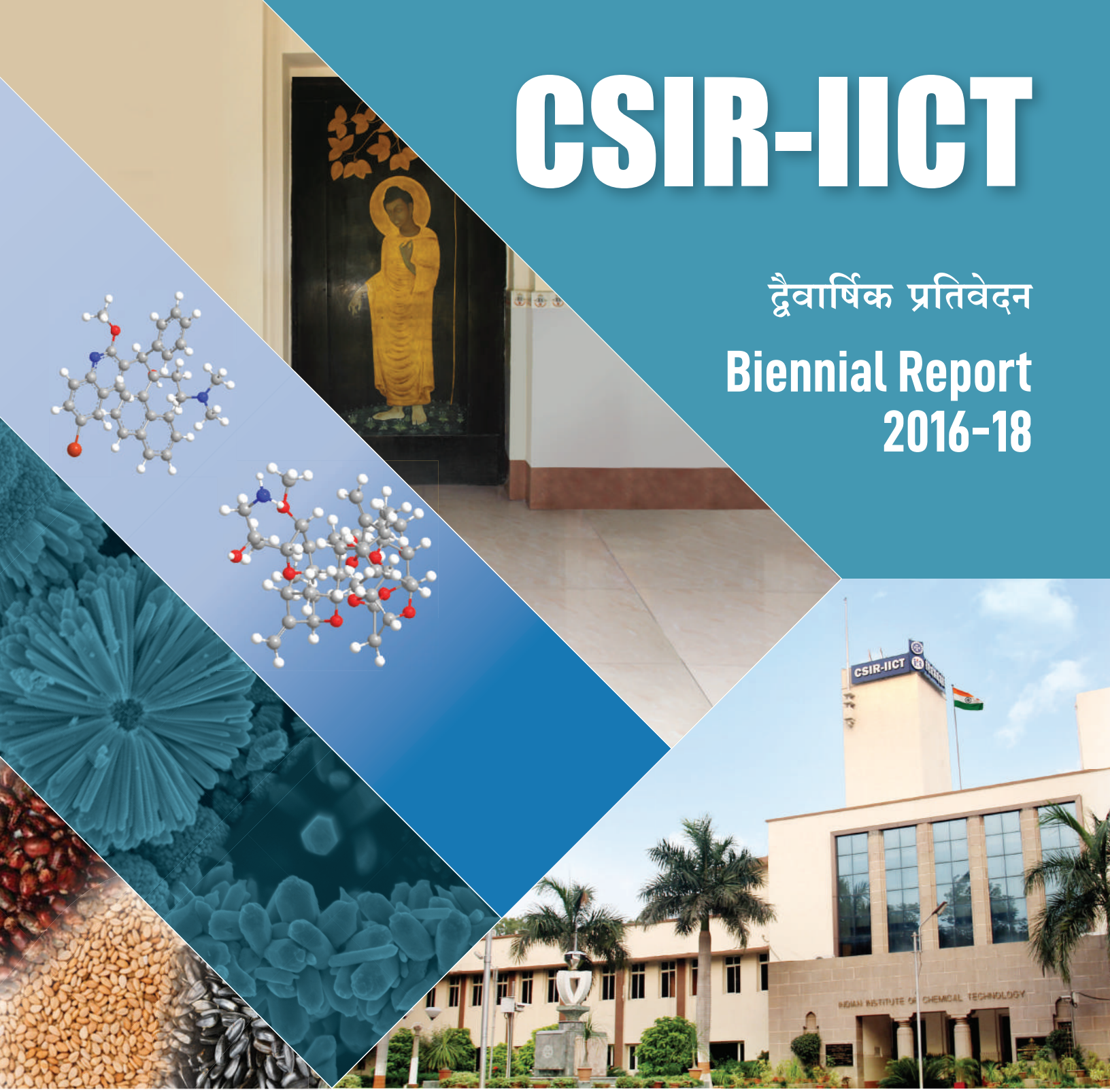
CSIR-IICT

द्वैवार्षिक प्रतिवेदन

Biennial Report 2016-18



सीएसआईआर–भारतीय रासायनिक प्रौद्योगिकी संस्थान

CSIR-Indian Institute of Chemical Technology

(Council of Scientific & Industrial Research)

Hyderabad - 500007

www.iictindia.org

PLATINUM JUBILEE 1944-2018

CSIR - IICT

Touching Lives

VISION

To Serve society by creating an outstanding knowledge base in chemistry and chemical technology.

MISSION

CSIR-IICT will strive towards knowledge intensive translational research in chemistry to meet the country's expectations with novel technologies.

THE ORGANIZATION

CSIR-Indian Institute of Chemical Technology (IICT), Hyderabad, established in 1944, is a constituent laboratory of Council of Scientific and Industrial Research (CSIR), New Delhi. With its expertise in chemistry and chemical technology, it provides solutions to challenges faced by Industry, Government Departments and Entrepreneurs through basic and applied research and process development. It is internationally recognized for its contributions to chemistry research and is an ideal place for taking ideas to commercialization through state of the art research and development.

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PLATINUM JUBILEE

1944-2018

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CONTENTS

प्रस्तावना

द्विवार्षिक वर्ष 2016-18 की अवधि के दौरान सीएसआईआर-आईआईसीटी के अनुसंधान और विकास उत्पादन एवं संबंधित उपलब्धियों के विवरण की रिपोर्ट प्रस्तुत करते हुए मुझे खुशी हो रही है। संस्थान में कर्मचारियों और छात्रों की समर्पित बौद्धिक गतिविधियों, प्रशासनिक कर्मियों का समर्थन, विभिन्न वित्तपोषित एजेंसियों से वित्तीय सहायता के फलस्वरूप उच्च गुणवत्ता वाला कार्य हो पा रहा है।

आरंभ से ही, संस्थान विज्ञान और प्रौद्योगिकी के अनुसंधान और विकास गतिविधियों के साथ ही साथ औद्योगिक और सामाजिक लाभ के लिए अपने शोध निष्कर्षों के उपयोग पर संतुलित महत्व दिया है। आवर्ती खर्चों के लिए समर्थन, और वैज्ञानिक तथा औद्योगिक अनुसंधान परिषद (CSIR), भारत द्वारा वार्षिक अनुसंधान खर्चों के पर्याप्त अंश के लिए भी सहायता प्रदान की जाती है। विज्ञान और प्रौद्योगिकी विभाग (DST), जैव प्रौद्योगिकी विभाग (DBT), रक्षा अनुसंधान और विकास संगठन (DRDO), एमओईएस (MoES), डीएई (DAE), आईसीएमआर (ICMR) सहित रासायनिक और दवा उद्योगों तथा विभिन्न एजेंसियों द्वारा वित्त पोषित बड़ी संख्या में अनुसंधान परियोजनाओं पर भी संस्थान के वैज्ञानिक कार्य कर रहे हैं। संस्थान ने राष्ट्रव्यापी कई शैक्षणिक संस्थानों और विश्वविद्यालयों के साथ समझौता ज्ञापन के लिए सहमति दी है। मैं उन सभी पूर्व निदेशकों के नेतृत्व का स्मरण करता हूँ, जो लगभग साढ़े सात दशकों से अनुसंधान कार्य के शीर्ष पर थे, और मैं संस्थान के अनुसंधान परिषद तथा प्रबंधन परिषद के अध्यक्ष एवं सदस्यों के मूल्यवान मार्गदर्शन के लिए अपना व्यक्तिगत आभार व्यक्त करता हूं।

(डॉ.एस.चन्द्रशेखर)
निदेशक

FOREWORD

I am pleased to present the CSIR-IICT Biennial Report detailing the Research & Development output and related achievements during the period 2016-18. The high quality work presented here resulted from the dedicated intellectual activities of the staff and students, support of administrative personnel, financial support from various funding agencies.

Since its beginning, the Institute has laid balanced emphasis on R & D activities in science and technology, as well as on the application of its research findings for the industrial and social benefit. The support for recurring expenses, and also for a substantial fraction of the annual research expenses are provided by the Council of Scientific and Industrial Research (CSIR), India. The scientists of the Institute also undertake a large number of research projects funded by chemical and pharmaceutical industries and also various agencies, including the Department of Science and Technology (DST), the Department of Biotechnology (DBT), the Defence Research and Development Organization (DRDO), MoES, DAE, ICMR. The Institute has facilitated MoU agreements with several academic institutions and universities nationwide. I recall the leadership of all the former Directors who were at helm of the affairs for almost seven and half decades, and I place on record my personal gratitude to the Chairman and the Members of the Research Council and Management Council of the Institute for their valuable guidance.

(Dr. S. Chandrasekhar)
Director

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Solid State and Structural Chemistry Unit,
Indian Institute of Science
Bengaluru

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CSIR-IICT, Hyderabad

Member-Secretary

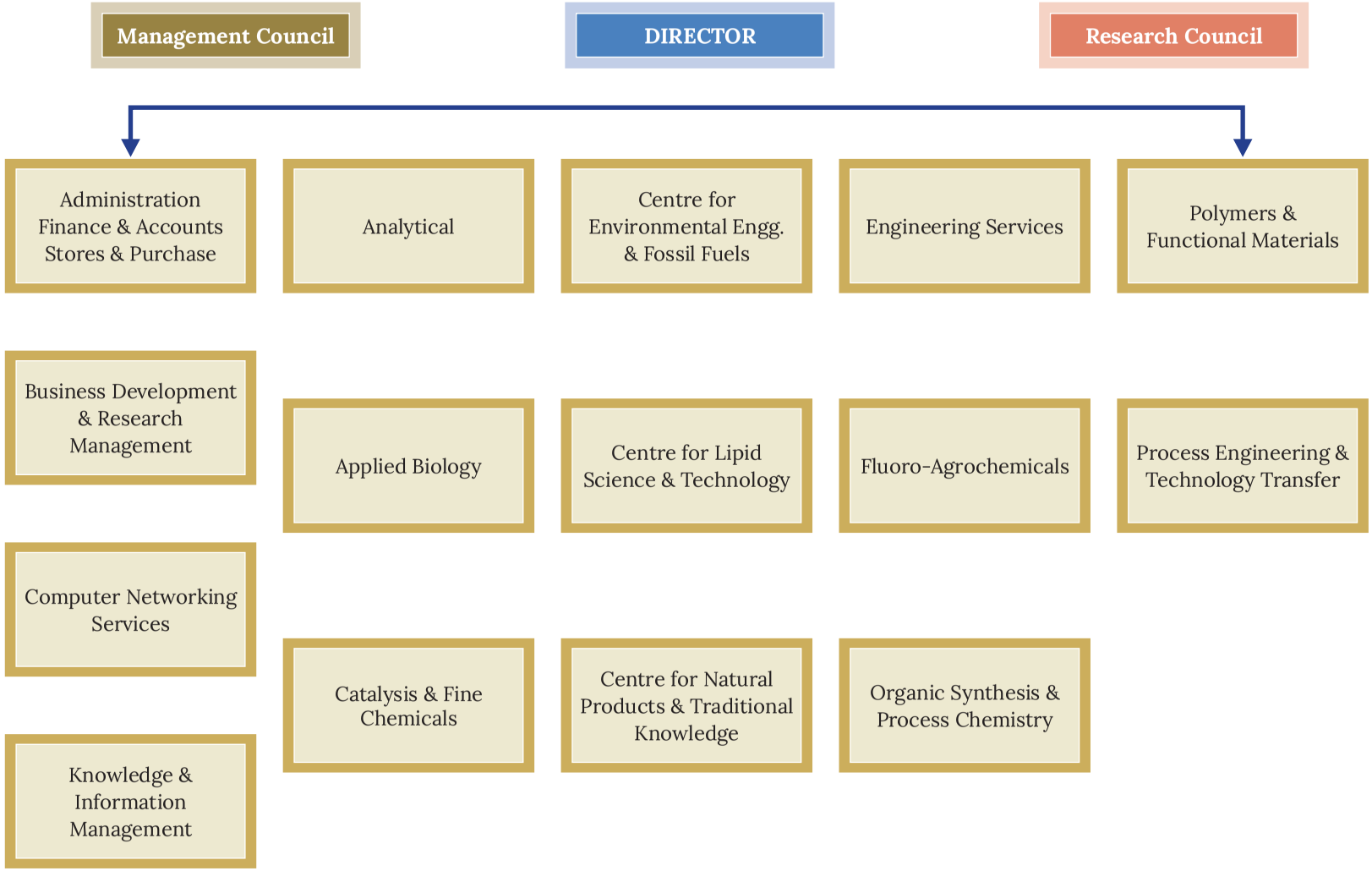
COA/AO, CSIR-IICT


Research Council in progress


62nd Research Council Meeting of CSIR-IICT Open Forum

CSIR-IICT

ORGANISATIONAL STRUCTURE

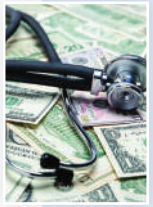


CSIR-IICT
RESEARCH FOCUS

Adequate Clean Energy

- Solar & Energy Materials
- Direct Coal Liquefaction
- Coal Gasification
- Carbon sequestration
- Biomass to energy
- Photobiological processes

Affordable Health Care



- Therapeutics
- Diagnostics
- Vaccines
- Designer Molecules
- Screening
- Delivery Systems

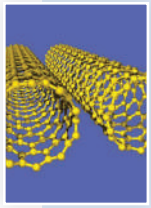
Environment

- Sustainable technologies
- Biohydrogen
- Waste utilization
- Biodigestors

Sustainable Chemistry

- Specialty Chemicals
- Fluorine Chemicals
- Membrane separations
- Biocatalysts
- Process Safety
- Process Intensification

Advanced Materials

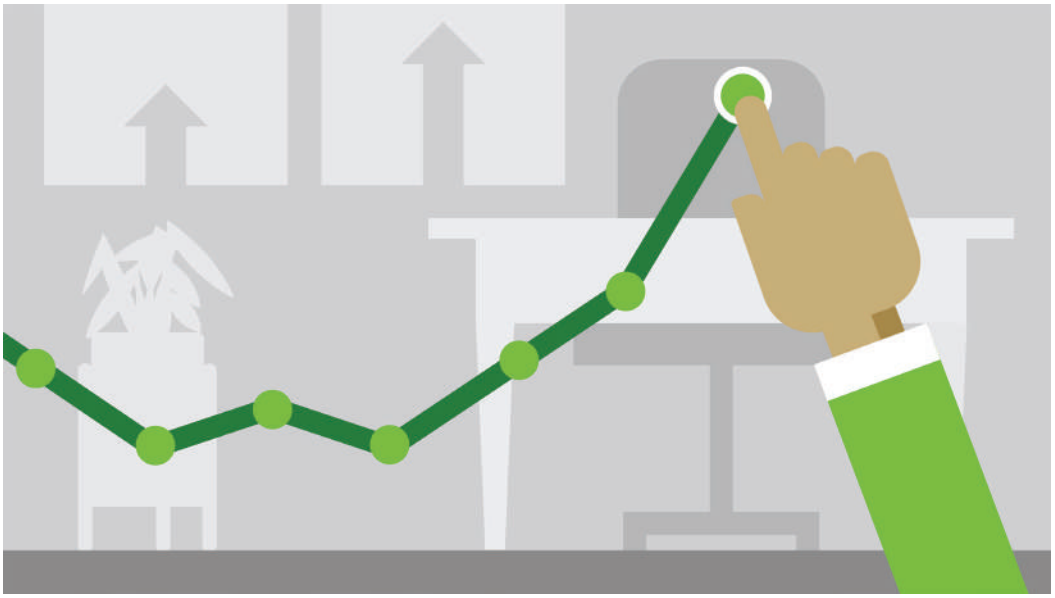


- Micro/nano materials for smart and intelligent coatings
- Stimuli responsive materials
- Graphene materials
- Photo functional materials

Agriculture, Food & Nutrition

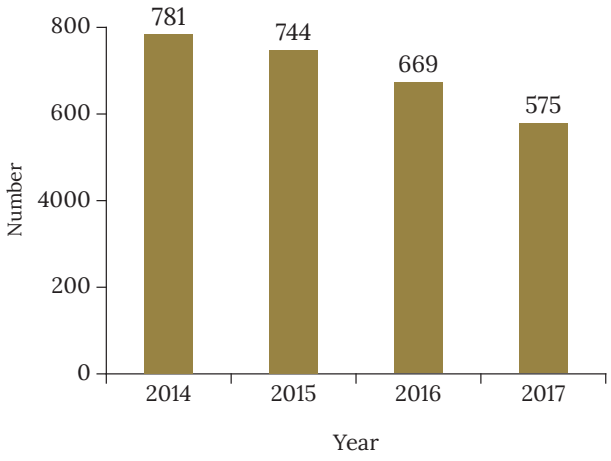
- Processes for edible non-edible oils
- Natural & synthetic Agrochemicals
- Plant volatiles
- Pheromone application

R&D OUTPUTS

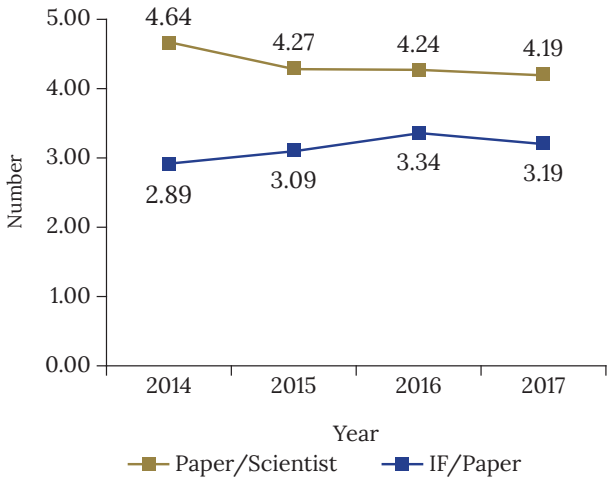


R&D OUTPUTS

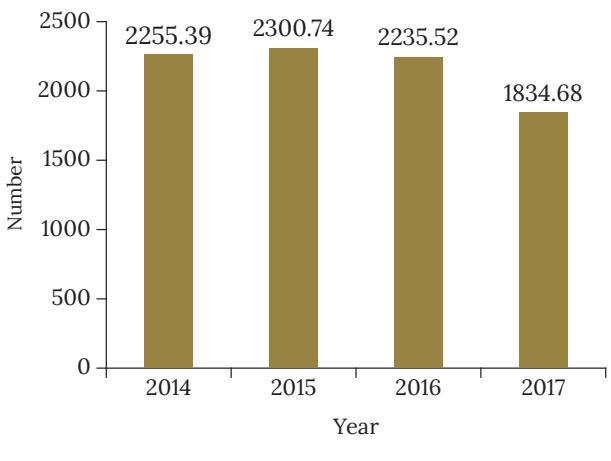
Research Publications



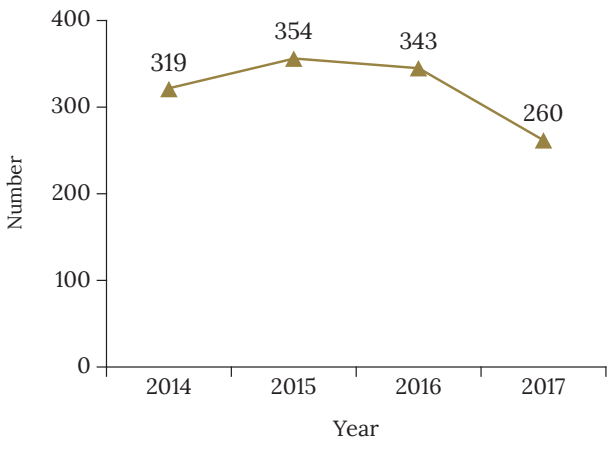
Paper/Scientist & IF/Paper



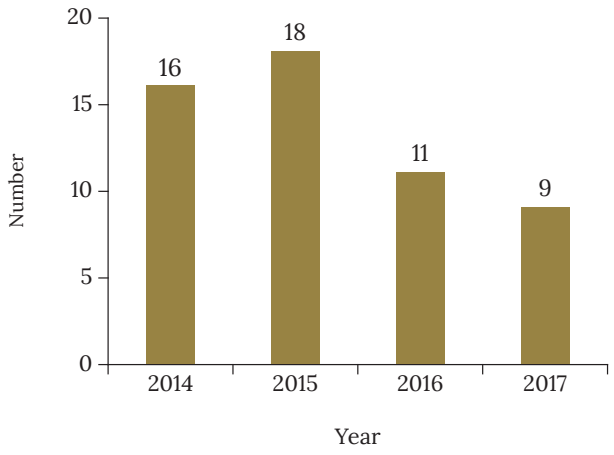
Research Papers Total IF



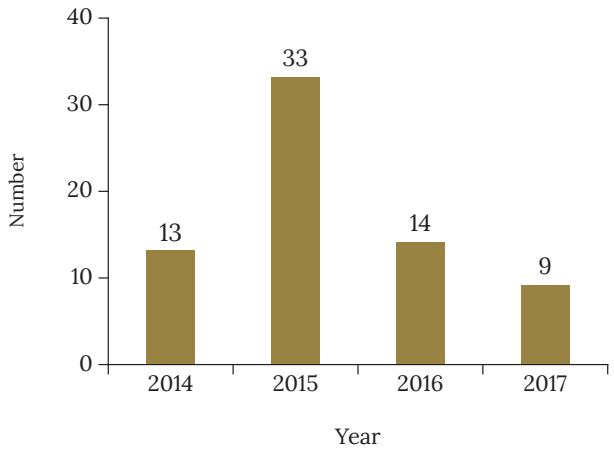
Publications with IF> 3



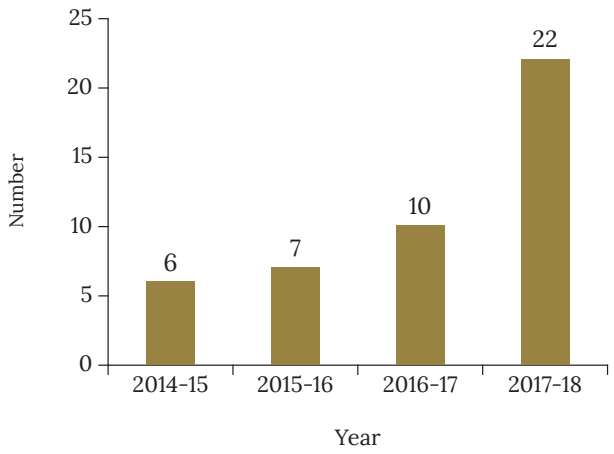
Patents Filed (India)



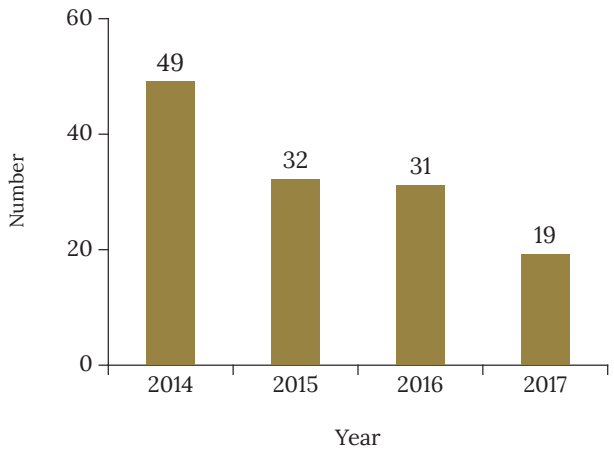
Patents Filed (Overseas)



Patents Granted (India)

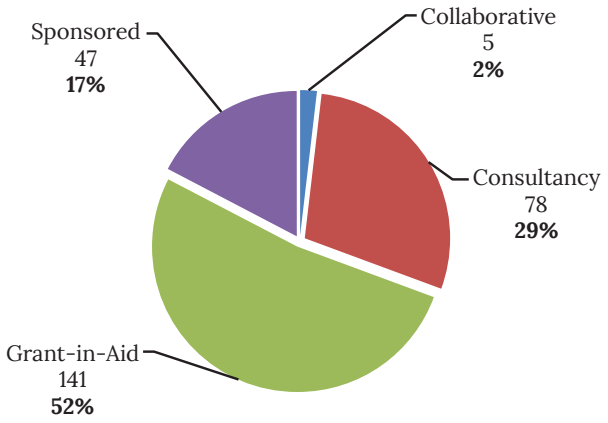


Patents Granted (Overseas)

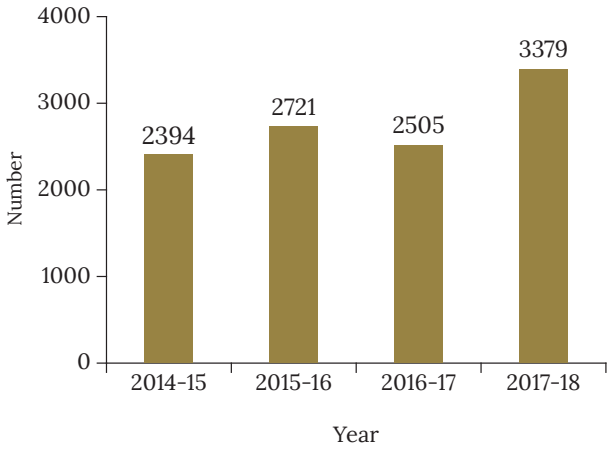


R&D OUTPUTS

Projects Undertaken (2016-18)



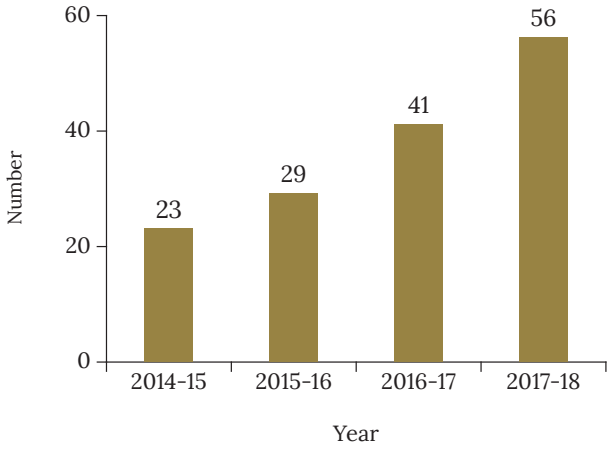
External Cash Flow



Human Resource Base

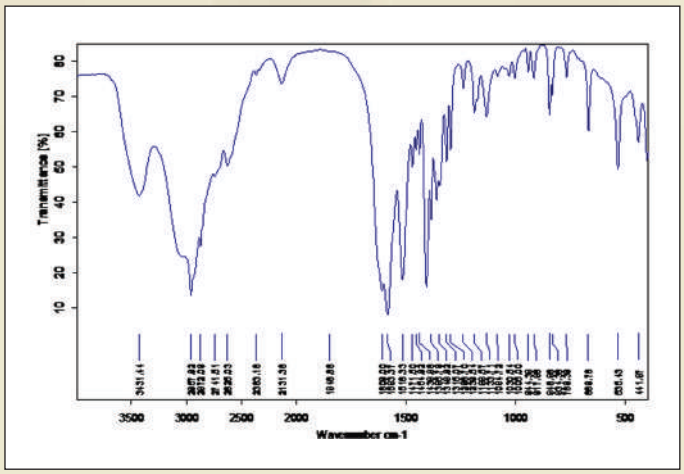
	2016-17	2017-18
TOTAL STAFF	**591**	**551**
***Total S & T Staff**		
• Scientist (Group-IV)	166	149
• Technical (Group-III)	114	111
• Technical (Group-II & I)	157	141
***Total Administrative & Non-Technical**	**154**	**150**
***Research Scholars/Assts.**		
• IF/RA/WOS/Others	29	29
• SRF/JRF's	40	16
• P I / P A's	04	22

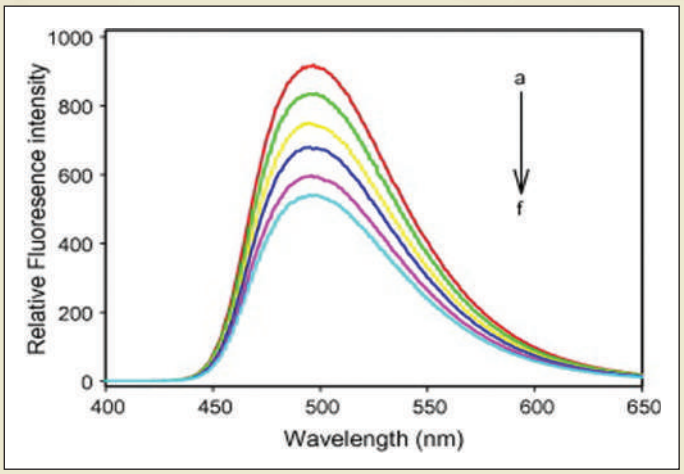
PhDs Awarded

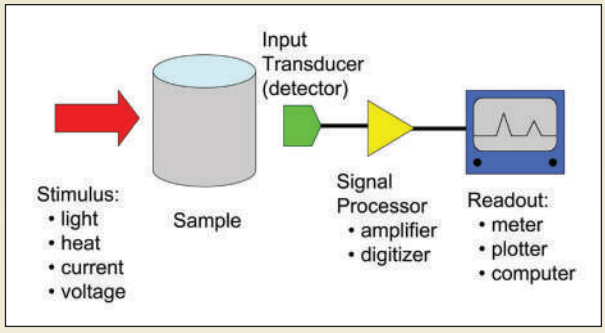


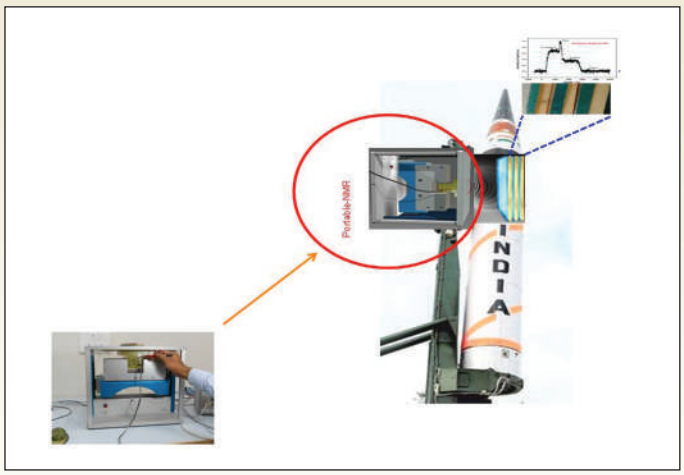
R&D PERFORMANCE

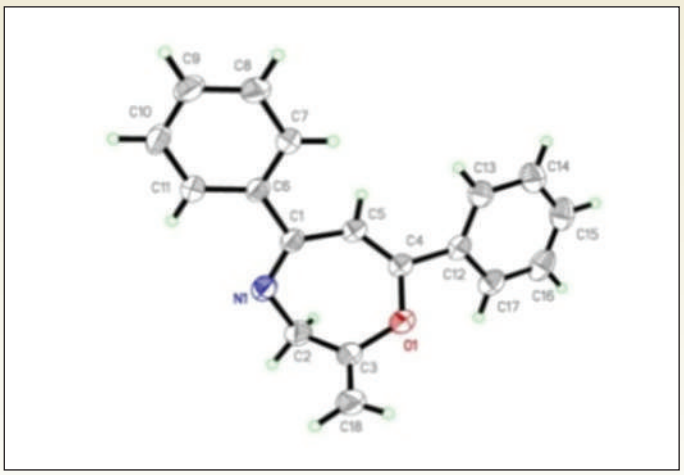
ANALYTICAL


Transmittance [%]
Wavenumber cm-1


Relative Fluoresence intensity
Wavelength (nm)
a
f


Input
Transducer
(detector)
Stimulus:
• light
• heat
• current
• voltage
Sample
Signal
Processor
• amplifier
• digitizer
Readout:
• meter
• plotter
• computer


Portable NMR
INDIA



Analytical department of CSIR-IICT is a multifaceted division with sophisticated analytical instruments for chemical analysis. The department is equipped with latest Nuclear Magnetic Resonance (NMR) spectrometers, Mass Spectrometers (MS), X-Ray, HPLCs, ICP-OES, GPC, CHNS analyzer, and HPTLC. The department has expertise to provide analytical solutions in the areas of pharmaceutical, environmental, forensic, biological and food interest in both qualitative and quantitative analysis. The department is serving many institutional R&D projects in different areas of chemical and biological research, providing analytical services to Industry and Academia and holding regulatory compliances such as ISO 9001 certification, ISO/IEC 17025 accreditation.

The Objectives of the department are:

- To provide knowledge based quick analytical solutions to the intended applications of various Industries
- Provide regulatory compliant analytical services to Industry and Academia
- To develop and validate analytical methods for the intended purposes and carryout advanced research in analytical chemistry to develop greener analytical methods
- Providing skill development training to postgraduate students and staff of industry and academia

The staff of the department has expertise to carry diverse research projects in the area of analytical chemistry and has capability to provide quick analytical solutions to the industrial applications. The scientists at analytical department have been engaged in basic and applied research and instrumental in developing various tools/techniques to solve many analytical problems. They are instrumental in developing various approaches in the identification, characterization and quantification of analytes of interests. Their efforts have yielded more than 500 research publications in reputed journals of international excellence.

Their contributions are well recognized and honored with awards and fellowships by several scientific academies like RSC, APAS, TAS, ISMAS etc. Several scientists are also acting as editorial board members in various international journals like PLOSONE, Rapid Communications in Mass Spectrometry, Journal of Mass Spectrometry etc. The department has awarded more than 60 PhDs till date and presently about 20 students are pursuing their PhD work. The department also catering the needs of various institutions by supporting their students for dissertation work and providing hands on experience on various analytical tools to make them fit for Industry and Academia set up.

RESEARCH GROUPS

The analytical department encompasses majorly five research groups. The facilities available at each group along with team members and the core competencies of the group are given under each group.

i) Nuclear Magnetic Resonance

ii) Mass Spectrometry

iii) X-Ray

iv) Hyphenated Analytical Separations

v) Thermal analysis

vi) Photochemistry & Photophysics

vii) Other Facilities

i) The NMR laboratory continues to focus on the following areas

- Basic research
- Applied research
- S & T services to internal as well as external

BASIC RESEARCH

Real-time homonuclear broadband decoupled pure shift COSY

The development and applications of real-time homonuclear broadband decoupled pure shift version of in-phase zeroquantum filtered COSY (PS-IPZF-COSY) and clean in-phase COSY PS-CLIPCOSY) pulse schemes is described. In contrast to the conventional COSY schemes, these pure shift versions provide enhanced spectral resolution and simplify the chemical shift correlation analysis of scalar coupled spins in complex organic molecules (**Figure 1**), which are exemplified for erythromycin A, estradiol, and a mixture of estradiol and testosterone.

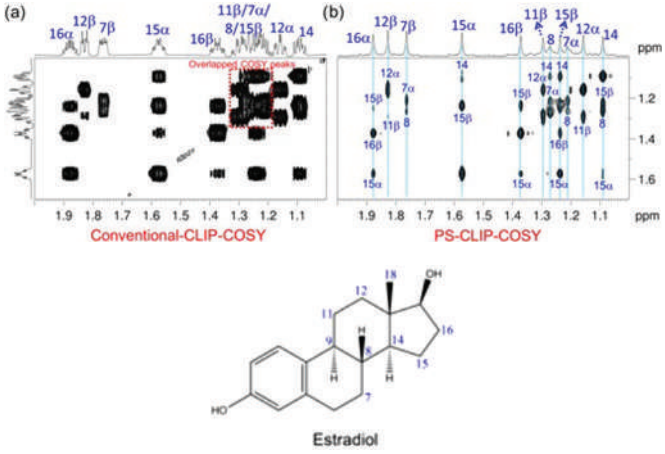
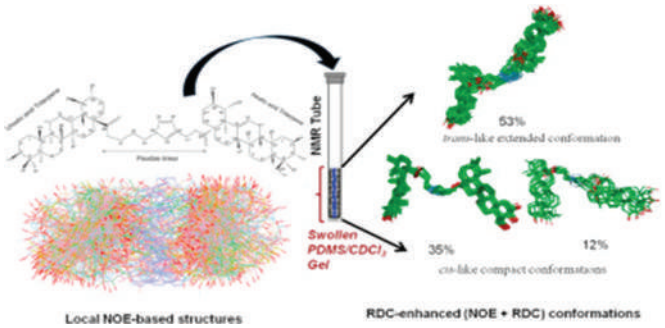


Figure 1: Comparison of expanded (a) CLIP-COSY and (b) PS-CLIP-COSY spectra recorded for estradiol (30 mM in DMSO-D6 solvent) at 800-MHz field strength. The results clearly highlight that the spectral complexity is greatly reduced and a significant enhancement in the resolution has been achieved for the PSCLIP- COSY. PS-CLIP-COSY = pure shift clean in-phase correlation spectroscopy

Conformation of flexibly linked triterpene dimers by using RDC-enhanced NMR spectroscopy

Dimers of flexibly linked pentacyclic triterpene ursolic acid (UA) and its related frameworks such as asiatic acid (AA) and oleanolic acid (OA) have recently attracted significant attention due to their enhanced anti-cancer and anti-HCV activity compared to their respective monomers. Determination of conformation/ inter-monomer orientation of these molecules is very important to understand their structure-activity relationship and to develop new scaffolds, which, however, is difficult through conventional NOE based solution-state NMR spectroscopy, due to lack of long-range NOEs. Here, we report a precise determination of conformation of two 1,2,3-triazole-linked triterpene dimer molecules, UA-AA and UA-OA, by employing one-bond C_H residual dipolar couplings (RDCs) as additional long-range orientational restraints, measured in anisotropic PDMS/CDCl3 solvent medium (**Figure 2**).



Selective measurement of $^1H–^1H$ scalar couplings from crowded chemical shift regions: Combined pure shift and spin-echo modulation approach

J_{HH} scalar couplings carry rich structural information and their measurements are fundamental in the ^1H NMR based elucidation of small and medium molecules, which, however, are hampered in the presence of large *J*-coupling network. Further, enhanced spectral resolution is often essential for precise determination of a specific set of $^1H–^1H$ *J*-couplings among the complex *J*-multiplets. In the light of the recent advancements in homodecoupling pure shift strategies, here, we report absorption mode, band-selective refocused pure shift spin-echo method, which helps in determining $^1H–^1H$ *J*-couplings from crowded spectral regions. The importance of the present band-selective refocused pure shift spin-echo experiment is exemplified for 2 steroid molecules, estradiol (**Figure 3**) and testosterone

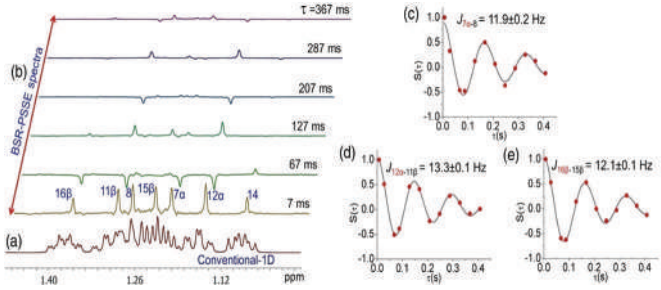


Figure 3: Comparison of the conventional-1D (a) and the BSR-PSSE (b) spectra recorded at different values of τ for estradiol sample dissolved in DMSO-d_6. The respective pure shift selective spin-echo modulations of spins $H_{7\alpha}$, $H_{12\alpha}$, and $H_{16\beta}$ fitted to the theoretical Expression 1 has resulted in scalar coupling values: $H_{7\alpha}–H_8$ (c), $H_{12\alpha}–H_{11\beta}$ (d), and $H_{16\beta}–H_{15\beta}$ (e)

APPLIED RESEARCH

Study of Diastereotopic left and right handed helical structures in peptides containing Amino Pyran Carboxylic acid and C- linked Carbo-β- amino acid

The present work described the study of a set of diastereomeric β-peptides from (R,R)- and (S,S)-APyC by alternating use of (R)-β-Caa and (S)-β-Caa respectively in a 1:1 ratio. The conformational analysis on these peptides revealed the presence of left and right handed 12/10-helices (Fig. 4), as was observed for the enantiomeric peptides. Thus, the study on the

formation of enantiomeric helical patterns from the diastereomeric peptides amply infers that the APyC monomers have profound influence on the outcome of helix screw sense. The **figure 5** below displayed the CD spectra of the diastereomeric peptides with enantiomeric handedness. Such an observation can be well adopted for the synthesis of diastereomeric peptides with enantiomeric handedness, from diverse diasteromeric amino acids and enantiomeric APyCs, to enrich the domain of foldamers.

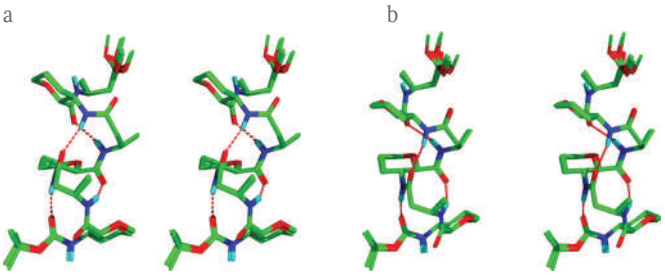


Figure 4: Stereoview of a superimposition of the 20 lowest energy structures for peptide (A) (R,R)-APyc and R-β-Caa showed a Left handed 12/10-helix (B) (S,S)-APyC and S-β-Caa showed a Right Handed 12/10-helix (The red dotted lines indicate hydrogen bonding between amide protons and carbonyl carbons)

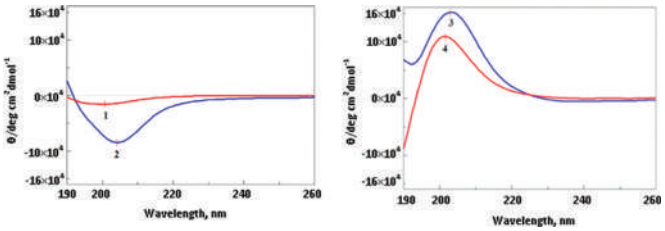


Figure 5: CD profiles of peptides made from A) (R,R)-APyc and R-β-Caa, B) (S,S)-APyC and S-β-Caa

Solvent-directed switch of a left-handed 10/12-helix into a right-handed 12/10-helix in mixed β-peptides

The present study describes the conformational analysis of a new series of peptides composed of β-hGly in 1:1 alternation with (S)- or (R)-β-Caa bearing a D-lyxo furanoside side chain. The peptides with an (S)-β-Caa(l) monomer at the N-terminus reveal the presence of a right-handed 10/12-helix, as supported by a theoretical study. Very interesting results are observed for the peptides with a β-hGly residue at the N-terminus in alternation with (S)-β-Caa(l) constituents. The NMR studies show the presence of a left-handed 10/12-helix (**Figure 6A**) in the solvent $CDCl_3$, However, the appearance of a maximum at 202 nm in the CD spectrum of this peptide in solvent CD_3OH indicates the opposite handedness in this solvent. Indeed, the NMR studies in the more polar solvent CD_3OH suggest the presence of a right-handed 12/10-helix (**Figure 6B**). This is an unprecedented 'switch' between two helical structures with different hydrogen bonding pattern and different handedness, which is reported in 12/10-helices for the first time. Moreover, the structural features of both helix types were observed in the polar aprotic solvent acetonitrile. The unusual solvent effect can well be understood by looking at the approximately energetic equivalence of both helices according to quantum chemical calculations. To the best of our knowledge, no other examples with such remarkable effects of an excessive change of helix type and handedness by a mere solvent change were found until now.

The peptides composed of (R)-β-Caa(l) constituents in alternation with β-hGly revealed results, that are in agreement with data of former investigations on the corresponding peptides with (R)-β-Caa(x) residues bearing a D-xylo furanoside side chain. The data of this study demonstrate several possibilities to influence helix type and handedness, as for instance by a different configuration of the amino acid constituents and the variation of their side chains and even by the nature of the solvent. The study shows the wide variety of possibilities to realize special types of secondary structures. Thus, experimental and theoretical methods may efficiently contribute to a rational peptide and protein design in a concerted action.

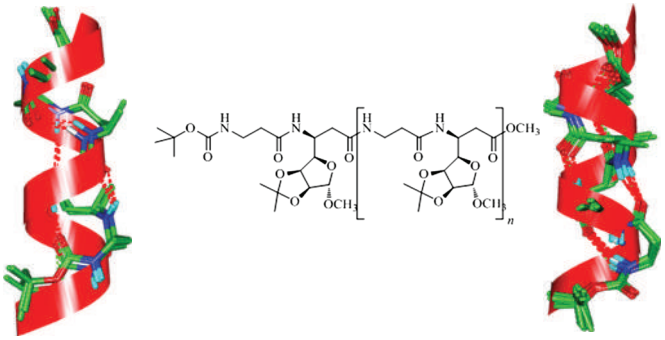


Figure 6: A) A left handed 10/12-mixed helix B) Chemical structure C) A right handed 12/10-mixed helix of a β-hGly in 1:1 alternation of β-Caa with D-lyxo furanoside side chain.

S & T SERVICES

Analytical Services to in-house projects of IICT

NMR Centre of CSIR-IICT is the largest NMR facility in the country with 9 high-field NMR spectrometers

ranging from 300 to 700 MHz capable of doing multi-dimensional NMR, covering both solution and solid-state experiments. The 600 MHz and 700MHz NMR spectrometers are equipped with sophisticated cryoprobe that enhance sensitivity and will enable to characterize samples of sub-millimolar concentrations. Centre for NMR & SC provides services to various departments in IICT for both in liquid as well as solid state NMR. Two new Bruker AVANCE III HD 400 MHz NMR spectrometers were added to meet the requirements of the institute.

Value added services for pharmaceutical industries

By virtue of its technical and scientific expertise, the NMR centre has become a natural choice for many pharmaceutical industries and academic institutes in the country, to seek high quality analytical services and NMR centre extensively provides these services. Several complex molecules, APIs are routinely characterized at our centre, which is USFDA inspected.

The following are some representative drugs and APIs for which NMR based analytical methods have been established at our centre and are routinely characterized.

1. Eribulin
2. Sevelamer HCl/Sevelamer Carbonate
3. Axitinib
4. Sacubitril-Valsartan
5. Lapatinib
6. Heparin, Enoxaparin
7. Bortezomib/Velcade
8. Prasugrel
9. Ivabradine
10. Evarolimus
11. Glatiramer Acetate
12. Sucralfate
13. Ticagrelor
14. Dapgliflozin

The NMR centre takes up projects with synergistic approach for value addition to basic and industrial Research. Further the centre contributes for the product developments with absolute confidentiality and the services are economically priced.

ii) Mass Spectrometry

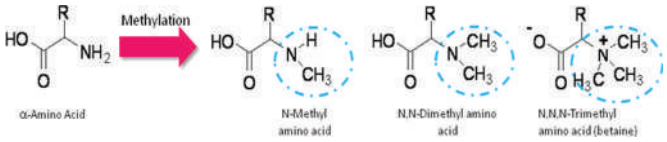
Mass spectrometry is a powerful and versatile analytical technique for the analysis of organic and biomolecules, mainly for determination of their molecular weight and structural characterization. Because of its high sensitivity, selectivity and speed, mass spectrometry finds application in several diverse fields, such as, chemistry, physics medicinal chemistry, biochemistry, pharmaceutical science, biological sciences, geology, cosmo chemistry, nuclear science, material science, archeology, petroleum industry, forensic science, and environmental science. Mass spectrometry has become an integral part of proteomics, metabolomics, lipidomics and the drug development process. Mass spectral analysis of products and various intermediates generated during process development helps in process control very effectively.

The Mass Spectrometry group has a dedicated facility (ISO/IEC 17025 accredited) for off-site analysis of chemicals related to chemical weapons convention (CWC). The laboratory obtained prestigious designation status from Organization for Prohibition of Chemical Weapons (OPCW), The Netherlands) in 2008. The laboratory has been participating in the international official OPCW proficiency tests every year. This laboratory is contributing to the mission of OPCW and NACWC, New Delhi in achieving the common goal for a world free of chemical weapons.

Characterization of N-methyl Amino Acids by ESI-MS/MS for metabolomic studies

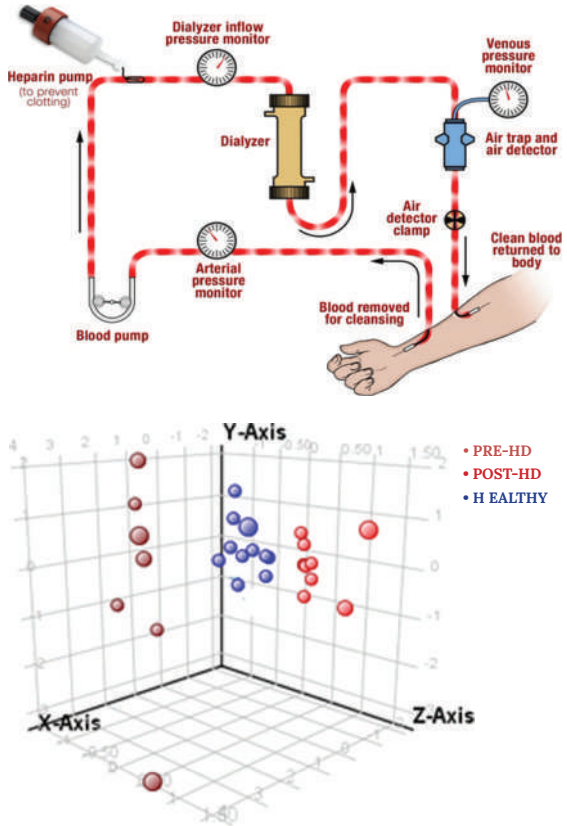
Methylation was an important component in numerous cellular processes including embryonic development, genomic imprinting, X-Chromosome inactivation, and preservation of chromosome stability. In human body methylation process was involved in critical functions such as thinking, repairing DNA, turning on and off genes, fighting infection. Methylated compounds are known to be involved in most of the bodily functions, and some of them serve as biomarkers. Further, methylated amino acids are biomarkers for several metabolic disorders. Theoretically, all α-amino acids can be methylated and it is possible to encounter them different sample sources. Thus, it is essential to generate mass spectral data and to develop mass spectrometry methods for the

identification of all possible methylated amino acids for future metabolomic studies. In these lines, we already reported synthesis of trimethyl and dimethyl amino acids and their characterization by ESI-MS/MS. Recently, we reported characterization of N-methyl and N,N-dimethyl amino acids by GC-MS after ECF derivatization. In this study aimed to characterize N-methyl amino acids by ESI-MS/MS conditions. The MS/MS spectra of all the studied N-methyl amino acids showed structure indicative product ions that made easy identification of isomeric N-methyl amino acids.



Assessment of Plasma Metabolites in CKD Patients on Maintenance Hemodialysis

Chronic kidney disease (CKD), also known as chronic renal disease is a slow progressive loss of kidney function over a period of several years. The CKD patients may not become apparent until the kidney function is significantly impaired. At this point the individual either has to have a kidney transplant or dialysis. Presently, commonly used uremic toxins that are easily estimated in all the available laboratories are two small molecules, urea and creatinine. The metabolomics technologies have been used in abroad to detect other uremic toxins in blood samples of CKD patients, however, research in these lines is not explored in India. After ingestion of food, amino acids especially aromatic amino acids suffer extensive metabolism with sulfate group converts into aromatic sulfonic acids (Indoxyl Sulfate, P-Cresol Sulfate, Phenyl Sulfate, Guaiacol Sulfate, Ethyl phenyl Sulfate, and Catechol Sulfate). These sulfates exist at higher concentration in the kidney disease, mostly hemodialysis patients, and the identification of these metabolites is an emerging area. In this study, we have focused on the screening of uremic toxins in blood samples of CKD, who are on hemodialysis. The samples are collected from Gandhi Hospital and analyzed at CSIR-IICT using direct ESI-MS, LC-MS/MS techniques. A number of uremic toxins were detected, and a few targeted uremic toxins were quantified. Thus, we developed a LC-ESI-MS/MS for quantitative screening of targeted uremic toxins in about 100 CKD patients' plasma samples before and after dialysis. The statistical data showed that all analyzed uremic toxins were highly significant in Pre- and Post- hemodialysis patients when compared with the healthy subjects.



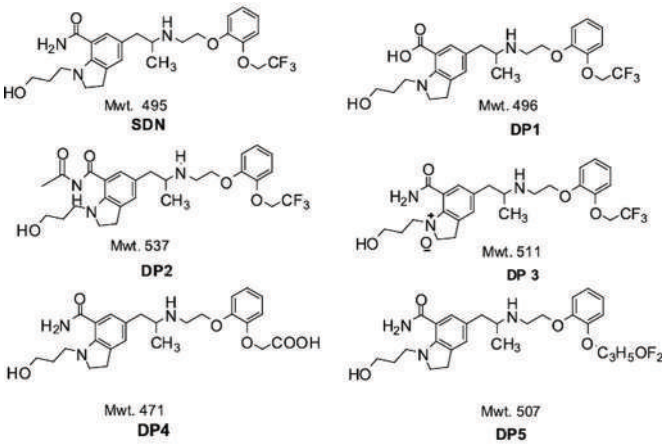
Phytochemical Profiling of Andrographis glandulosa

Despite the availability of synthetic or semi-synthetic drugs, continued efforts are required to identify naturally occurring safe anticancer compounds that are free from side effects. Plants contributed more than 50% of anticancer molecules that are being used in the treatment. The genus Andrographis belonging to the family Acanthaceae includes various species of medicinal importance and most of them are endemic to India. Andrographis glandulosa Nees found in and around forests of the Cuddapah and Nellore districts of Andhra Pradesh, India, is one of the species that remains unraveled for medicinal importance and chemical constituents. The present study for the first time unravels the chemical profiling and medicinal importance of an unexplored species, Andrographis glandulosa. LC-MS analysis of A. glandulosa methanolic extract disclosed it as a rich source of flavonoids, with 8 minor peaks and 2 major peaks (m/z 285.0749 and 283.0595). NMR and ESI-MS/MS analyses confirmed the major peaks as (R)

2',5-dihydroxy-7-methoxyflavanone and 2',5-dihydroxy-7-methoxyflavone. (*Planta Med. Int. Open*, **2017**, 4, e24)

Stress degradation products of silodosin studied by LC/MS

Silodosin (SDN) is being used for the treatment of benign prostatic hyperplasia. It acts as a α1- adrenoceptor antagonist with high uroselectivity. Forced degradation studies of a drug candidate is an important part of drug discovery and drug development, and are widely used to predict drug stability problems and identify degradation products or potential impurities. When a drug degrades, it may result in the loss of drug activity and degradation products may elicit possible adverse reactions. Thus, understanding the formation of degradation products is very important for defining product manufacturing conditions and choosing suitable packaging and storage conditions. No study so far has reported on the systematic forced degradation behavior of SDN under stress conditions prescribed by the International Conference on Harmonization (ICH) and World Health Organization (WHO). The present study is focused to conduct forced degradation of SDN under hydrolysis, oxidative stress, photolysis and thermal conditions, resolve the formed degradation products on an ultra-performance liquid chromatography (UPLC) column, characterize them by LC/MS studies, and postulate the degradation pathway of the drug based on the stress degradation behavior. SDN was found to be labile under hydrolytic and oxidative conditions. A total of five degradation products (DP1 to DP5) were identified. The structures of the degradation products were elucidated by using high-resolution mass spectral data. The most rational mechanisms for the formation of the degradation products under different stress conditions have been established.



Studies on variations of chemical composition of fruits due to artificial ripening

Artificial ripening of fruits is one of the major concerns around the world. Fruits are one of the majorly consumed food commodities around the world due to several benefits. Fruits are generally harvested after they ripen fully on trees. However, transportation of such fruits is often difficult owing to the damage that occurs to the fruits. Hence, the fruits are harvested in the pre-ripen stage and are ripened with ethylene gas in ripening chambers. The construction and maintenance of ripening chambers is expensive hence the farmers and traders they adapt various simpler techniques such as dipping the fruits in ethereal solution, placing calcium carbide and ethylene gas releasing pouches in between the fruits. This kind of procedures accelerates the ripening process and the required colour of fruits is obtained quickly. During this process, the actual enzymatic reactions are accelerated and there may be changes in the chemical composition. Hence, it is necessary to identify the changes that occur in the fruits due to artificial ripening. The studies were carried out on Mango, Banana and Sapota fruits ripened with different artificial ripeners. The studies were focused on the changes of amino acids composition, which represents the changes in proteins of the fruits, phenolic components which represent the various metabolic processes, sugars which represent the conversion of pectins, and volatile components which represent the changes in odour of the fruits. Studies were also conducted for identification various markers of artificial ripeners in fruits.

Quantitative estimation of acidic degradation products of chemical warfare agents by in-situ butylation

The hydrolysis products are chemical warfare agents are very polar in nature and often associate easily with inorganic metals. Hence, it is difficult to extract the samples in normal extraction processes. After extraction of the samples, they need to be derivatized using various derivatization protocols. The derivatization reagents are either explosive or corrosive in nature and hence safer means of derivatization methods are necessary. An in-situ butylation method for the derivatization of alkyl phosphonic acids was developed and applied for the analysis of complex environmental samples prepared in

the scenario of challenging inspection. The method was useful for quantitative measurement of phosphonic acid till 1 µg/L concentrations.

Quantitative estimation of organic diacids from food products

The organic diacids are common food additives to maintain the acidity balance of the foods. Excess of these acids in the foods is harmful as they affect the digestive system. A simple method based on derivatization with ethylchloroformate and analysis by gas chromatography – mass spectrometry system was developed for quantitative estimation of various organic diacids in the food stuffs up to concentration 10 parts per billion levels with high degree of precision and accuracy.

iii) Centre for X-Ray Crystallography

The centre for X-ray crystallography exists to support the activities of the chemical crystallography both within the institute and for various external pharmaceutical industries. Elucidation of crystal structures for several synthesized and natural product molecules, catalysts and pharmaceuticals was the prime activity and played a significant role in the proper analytical characterization. The crystallographic expertise was utilized for resolving structural ambiguities in terms of geometrical positions and stereo-centers, tautomerism, chirality, ring cyclization, and etc. Importantly, the formation of several unknown compounds from totally unexpected chemical reactions identified by crystallographic group paved way for the identification of lead molecules in the drug discovery programs. Since its inception, the crystallographic centre has constantly contributed towards the progress of several institutes R & D programs. The research productivity at CSIR-IICT was increasingly underpinned by crystallographic methods.

Single crystal X-ray diffraction is an important and powerful technique used by various pharmaceutical companies in the discovery process of new medicines. New drug discoveries secure financial health of pharmaceutical companies and are paramount to the management of diseases and benefit the human health and wellness. In the synthesis of new compounds for drug efficacy studies, structural complexities limit the chemical characterization of the synthetic products such ambiguities can be resolved by crystal structure determination. Similarly, X-ray powder diffraction is extensively used in the drug discovery, design, development and formulation processes to obtain critical knowledge about pharmaceutical products. Many parameters required by the FDA, legal patent issues and drug performance are only accessible by employing XRD. With the introduction of systems specifically developed with the pharmaceutical industry in mind, XRD is now both cost-effective and easy-to-use. Phase analysis and polymorph identification are common analytical needs within both pharmaceutical development and production.

Powder and single crystal analyses carried out during 2016-18

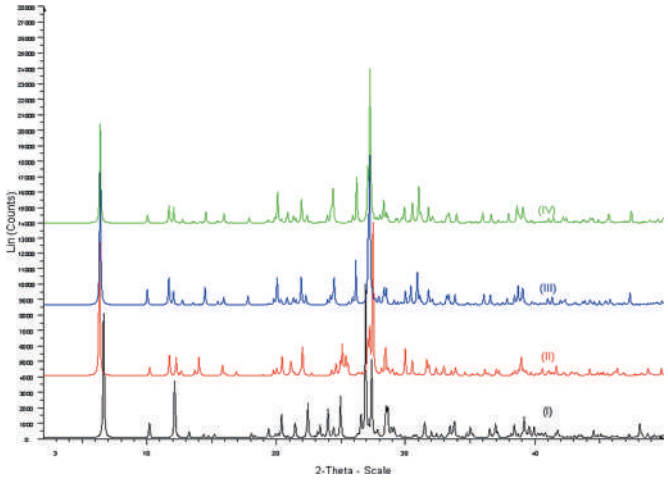
A total number of 7255 powder samples were analyzed and 695 crystal structures have been elucidated during the above said period. Externally funded industrial projects for Sai Life sciences, Hyderabad, Mylan Laboratories, Hyderabad, Dr.Reddy's Laboratories, Hyderabad, M/s. Alembic Pharmaceutical Ltd, Baroda, MSN, Hyderabad, Laurus, Hyderabad, Sreeni Labs, Hyderabad, Jubilant, Noida were successfully completed.

R & D ACTIVITIES

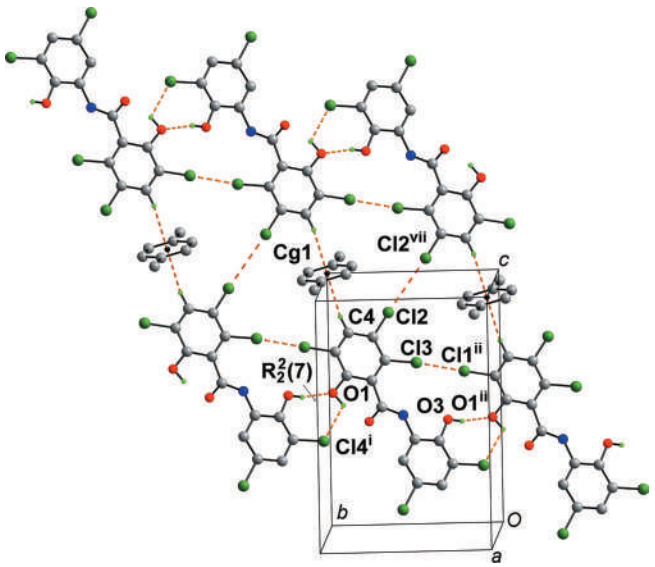
Chemical crystallography using single-crystal diffraction techniques has expanded beyond solely determining the structure of a molecule - increasingly, the interaction of molecules with each other in the solid state has become the focus of chemical crystallographic research. The systematic study of the way molecules pack in the solid has direct application in the pharmaceutical industry, in the study of polymorphism and further application in materials science for the design of new materials. The centre's R & D activities are focussed on crystal engineering aspects to design new solid forms, new drug formulation with improved the drug performance. The centre is also currently working on modern crystallization methods in making crystals of those compounds which are very difficult/ impossible to crystallize. The starting point of these studies is the preparation of suitable crystals of complexes with potential ligands which are achieved by using different strategies, and their evaluation for property enhancements.

Role of halogen–halogen contacts in the crystal structures of three new solvates of the drug oxyclozanide

Halogen–halogen contacts are electrostatic in nature and exhibit directionality similar to hydrogen bonds. Oxyclozanide [systematic name: 2,3,5-trichloro-N-(3,5-dichloro-2-hydroxyphenyl)-6-hydroxybenzamide] is a drug used for the treatment of fascioliasis in domestic animals. The molecule carries five chlorine substituents and represents an ideal candidate for the study of halogen bonds in the crystal. (*Acta Crystallogr. C*, **2017**, 73, 1056)



Overlay of the simulated powder X-ray diffraction pattern of solvates (I)–(IV), genarated from single-crystal data using Mercury (Version 3.8; Macrae et al., 2008).



A partial packing diagram showing one-dimensional hydrogen-bonded chains and Cl2...Cl2 contacts. The xylene solvent is encapsulated in the tetrameric cavity and is also linked by two equivalent C—H…Pi interactions.

Three new crystalline solvates of oxyclozanide, namely, oxyclozanide benzene hemisolvate, $C_{13}H_6Cl_5NO_3.0.5C_6H_6$, (I), oxyclozanide xylene hemisolvate, $C_{13}H_6Cl_5NO_3.0.5C_8H_{10}$, (II), and oxyclozanide toluene hemisolvate, $C_{13}H_6Cl_5NO_3.0.5C_7H_8$, (III), were structurally characterized. In this context, the crystal structure of oxyclozanide chlorobenzene hemisolvate, $C_{13}H_6Cl_5NO_3.0.5C_6H_5Cl$, (IV), was re-determined based on intensity data collected at 100 K. In all four solvates, the cocrystallized solvent molecules are located on crystallographic inversion centres. Solvates (I)–(IV) exhibit similar one-dimensional hydrogen-bonded chains generated by O—H---O, O—H---Cl and Cl---Cl interactions. The extension of these one-dimensional chains into two-dimensional layers is promoted by Cl---Cl and C—H--- π contacts. Solvates (III) and (IV) are isostructural and differ from (I) and (II) with respect to subtle details concerning the intermolecular contacts.

Crystal structure studies and antimicrobial activities of transition metal complexes of pyridine-2,6-dicarboxylic acid and imidazole containing water clusters

Two new copper(II) and chromium(III) complexes of tridentate 2,6-pyridine dicarboxylic acid (H2pydc) with imidazole (im), (Him)[Cu(Hpydc)(pydc)]·H2pydc·5H2O (**1**) and (Him)[Cr(pydc)2]·H2pydc·5H2O (**2**), have been prepared and characterized by elemental analysis, TGA measurements, FT-IR and UV-vis spectroscopy, powder and single crystal X-ray crystallography. Crystal structure analyses reveal that both copper(II) and chromium(III) ions are in a distorted octahedral environment. The optimized geometrical parameters were calculated using methods based on the density functional theory (DFT). These calculations agree closely with the X-ray structure. The antimicrobial activities of the ligand and the complexes were evaluated *in vitro* and compared with drugs in use. The results show that the complexes had stronger antibacterial activity than the corresponding ligand and the effectiveness was confirmed against *B. subtilis* (gram positive) and *K. pneumoniae* (gram negative) for **1**, and *E.coli* and *K. pneumoniae* (gram negative) for **2** by the well diffusion method. (*J. Coord. Chem.,* **2016**, 1602)

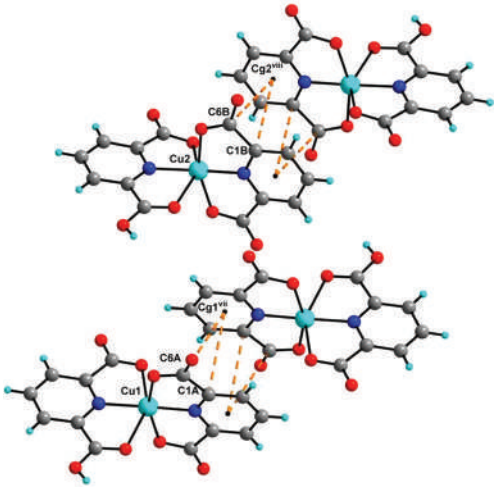
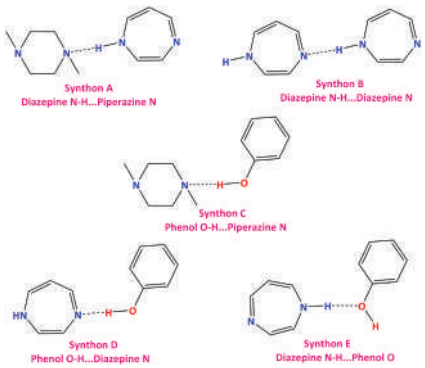


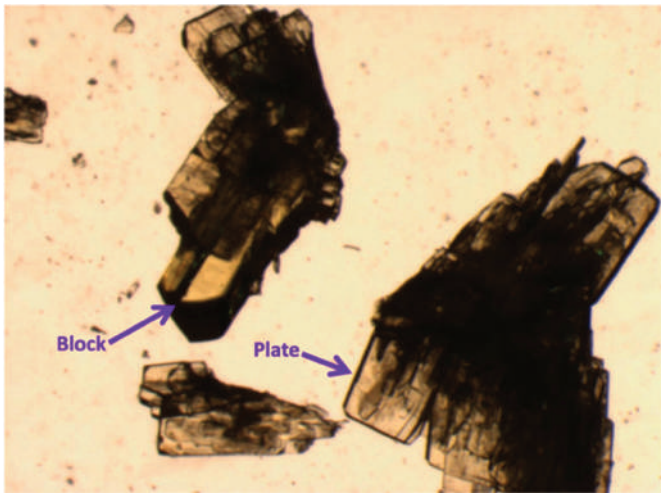
Figure representing the intermolecular offset π-stacking interactions (dashed lines) (the centroid of the pyridine ring Cg1stacks above the mid-point of the C1A-C6A

Designing a new cocrystal of olanzapine drug and observation of concomitant polymorphism in a ternary cocrystal system

Designing a co-crystal of olanzapine is an antipsychotic drug which shows donor-acceptor disparity in its polymorphic crystal structures. A strong hydrogen bonding acceptor, piperazine nitrogen, is left unutilized. We reasoned that including hydroquinone as a coformer with two hydroxyl donor groups could overcome the donor-acceptor disparity and facilitate the stronger phenol···piperazine and phenol···diazepine supramolecular synthons between the drug and coformer. Our co-crystallization attempts were successful in toluene solvent. Two distinct crystal morphologies were observed concomitantly and identified as two polymorphic forms of the drug cocrystal (block, form I & plate, form II). (*Cryst. Engg. Comm.*, **2017**, 19, 355)



Hydrogen bonding motifs observed in olanzapine polymorphs (synthons A), olanzapine dichloromethane solvate (synthon B), and the expected hydrogen bond motifs with hydroquinone (synthons C, D and E).



Concomitant appearance of block (form I) and plate (form II) crystal morphologies of olanzapine-hydroquinone-toluene system.

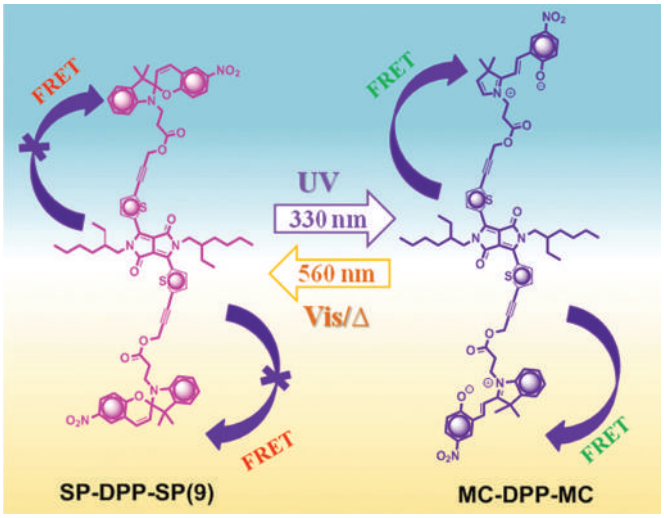
iv) Photophysics &Photochemistry

Fluorescence Switch Molecules

Diketopyrrolopyrrole - Spiropyran Dyad for Fluorescent Switch Application

We report the synthesis and characterization of a new fluorescent dyad **SP-DPP-SP(9)** via efficient palladium-catalyzed Sonogashira coupling of prop-2-yn-1-yl 3-(3',3'dimethyl-6-nitrospiro[chromene-2,2'-indolin]-1'-yl)propanoatespiropyran, **SP,** a well known photochromic accepter, with 3,6-bis(5-bromothiophen-2-yl)-2,5-bis((R)-2-ethylhexyl)-2,5-dihydropyrrolo[3,4-c]pyrrole-1,4-dione, **DPP,** a highly fluorescent donor. Under visible light exposure the **SP** unit is in a closed hydrophobic form, whereas under UV irradiation it converts to a polar, hydrophilic open form named Merocyanine (**MC**), which is responsible for functioning of photo-switch application. After absorption of UV light the spiropyran unit of the dyad under goes the rupture of the spiro C-O bond leading to the formation of **MC**. The absorption band of **MC** fairly overlaps to the fluorescence of **DPP** unit resulting quenching of fluorescence via fluorescence resonance energy transfer from exited **DPP** unit to ground state **MC**. In contrary, the fluorescence of **DPP** is fully regained upon transformation of **MC** to **SP** by exposure to visible light or thermal stimuli. Hence, the fluorescence intensity of dyad is regulated by reversible conversion among the two states of the photochromic spiropyran units and the fluorescence resonance energy transfer (**FRET**) between the **MC** form of **SP** and the **DPP** unit. Conversely, these scrutiny of the

experiment express that the design of dyad is viable as efficient fluorescent switch molecule in many probable commercial applications, such as, logic gates and photonic and optical communications. (*J. Fluorescence*, **2016**, 26, 1939)



v) Chromatography Separations

Projects in progress

- **National facility for scientific validation of traditional knowledge through modern approaches**

The project recommended for funding under Drugs and Pharmaceuticals Research Programme of DST, New Delhi. (Co-PI), 2018-2021.

- **Understanding the link between xenobiotic exposure and the onset/progression of type 2 diabetes using Drosophila as a model**

The project recommended for funding from Department of Health Research, MH&FW, GOI. (Principal Investigator@IICT), 2018-2021.

Projects completed

- **Identification and management of sewage effluent discharges to keep our rivers healthy: Comparative investigations in India and South Australia**

Selected for funding under Australia-India Strategic Research Fund (AISRF) (DST-DIISRTE Research Project), (PI @IICT), 2015-2018.

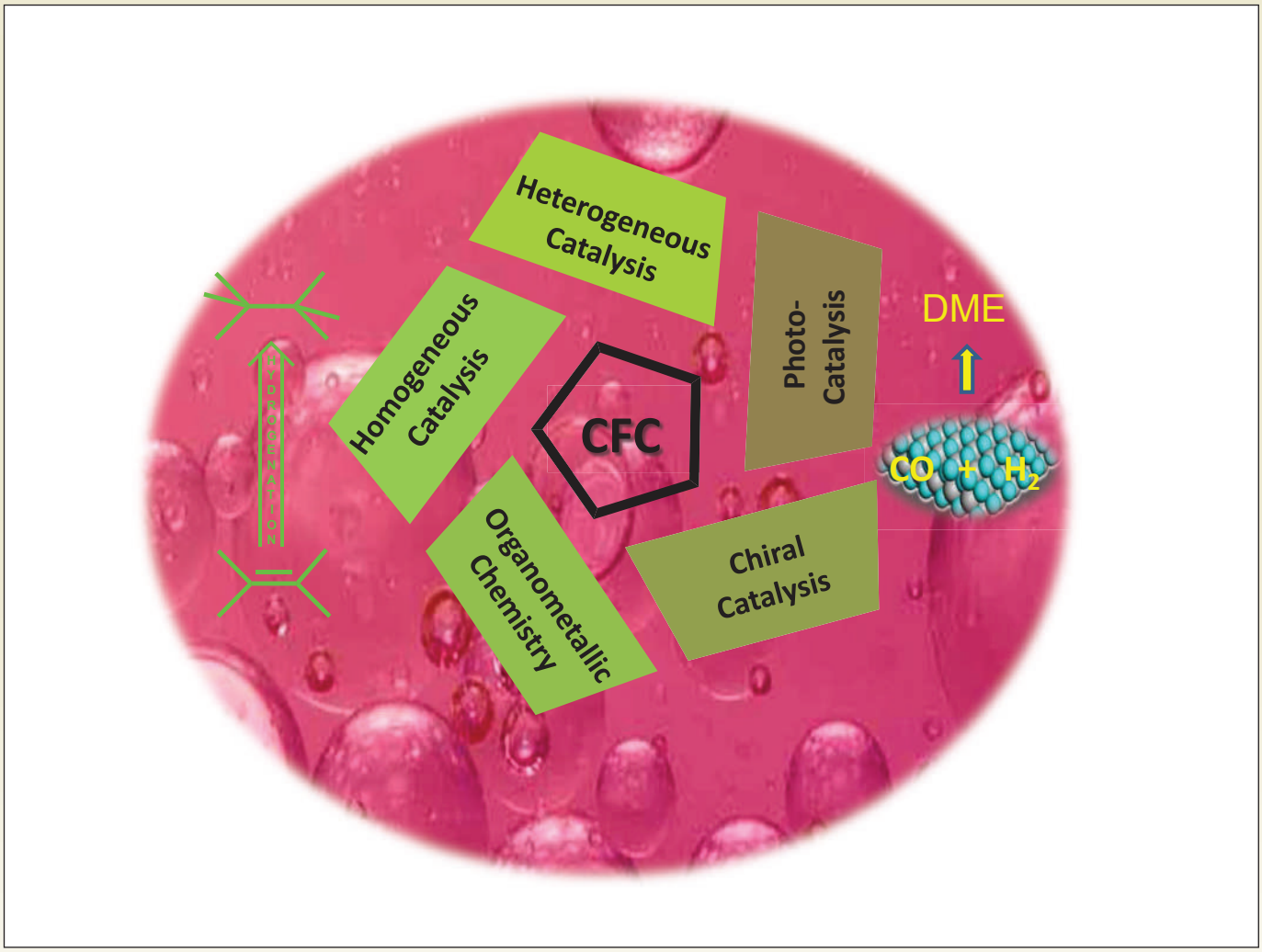
- **Evaluation of nanoparticle toxicity using mass spectrometry based comparative metabolomics in model organisms**

GAP-270 (funded by DST, New Delhi), **(**PI), 2013-16.

- **Integrated NextGen Approaches in Health, Disease and Environmental Toxicity (INDEPTH)**

CSIR-Network Programme **(**Work Package Leader**)**, 2012-17.

CATALYSIS & FINE CHEMICALS

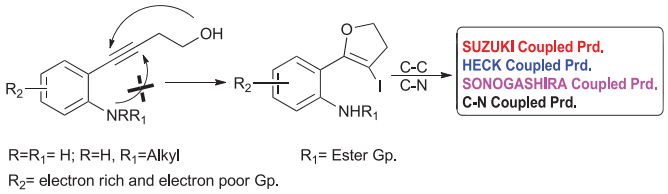


BASIC RESEARCH

Homogeneous Catalysis

Electronically Modified Amine Substituted Alkynols for Regio-selective Synthesis of Dihydrofuran Derivatives

An efficient and simple approach has been developed for the regio-selective synthesis of iodo-substituted dihydrofurans from amine substituted alkynols. The resulting iodo-substituted dihydrofurans have been further diversified by C-C couplings and C-N coupling reactions to afford a diverse range of substituted dihydrofuran derivatives. (*Org. Biomol. Chem.,* **2016,** 14, 288)

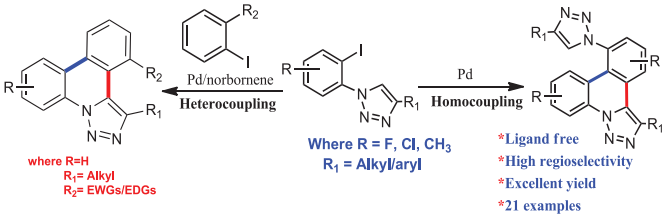


A Green Multi-Component Reaction for Synthesis of Trisubstituted Pyrroles in Ionic Liquid [bmim]BF4

2,4,5-Trisubstituted pyrrole derivatives were efficiently synthesized by one-pot condensation of 1,3-diones, α-bromoacetophenones, and ammonium acetate in ionic liquid [bmim]BF_4. The new synthetic method offers multisubstituted pyrroles with the advantages of mild reaction conditions, operational simplicity, higher yield, and environmental friendliness, (*Research on Chem. Intermed.,* **2016,** 47, 6873)

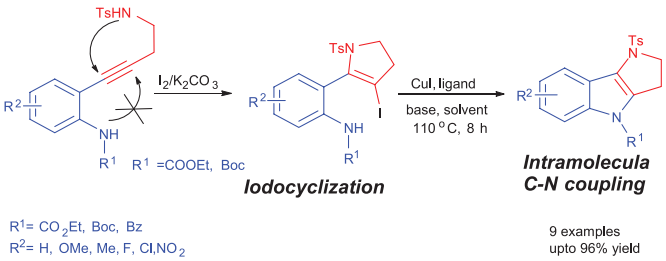
Palladium catalyzed domino reaction of 1, 4-disubstituted 1,2,3-triazoles via double C-H functionalization: one-pot synthesis of triazolo[1,5-f]phenanthridines

A palladium catalyzed domino coupling reaction of 1,4-disubstituted triazoles *via* homocondensation with a second molecule is presented. The domino couplings involve the formation of biaryl and bi(hetero)aryl bonds through a five membered carbopalladacycle intermediate. The approach provides a simple, straight forward and facile route to access triazolo[1,5-*f*]phenanthridines in high yields. Furthermore, the developed protocol was extended to heterocondensation in the presence of norbornene. (*RSC Adv.,* **2016**, 6, 43638)



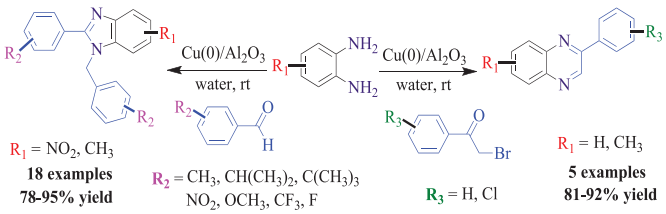
A New Synthetic Approach to Pyrrolo[3,2-b] indoles via Regioselective Formation of Pyrrole and Intramolecular C-N coupling

A new synthetic approach for the synthesis of pyrrolo[3,2-*b*]indoles has been developed in two steps. First step involves electrophilic iodocyclization of protected 2-alkynylanilines to regioselective formation of pyrroles followed by copper catalyzed intramolecular C-N coupling. (*Tetrahedron Lett.,* **2016,** 57, 4803)



Nano Copper(0)-Stabilized on Alumina: Efficient and Recyclable Heterogeneous Catalyst for Chemoselective Synthesis of 1,2-Disubstituted Benzimidazoles and Quinoxalines in Aqueous Medium

The present communication elicits the use of copper nanoparticles on aluminium oxide derived from Cu–Al hydrotalcite as a heterogeneous catalyst in the green and operationally simple approach for the synthesis of selective 1,2-disubstituted benzimidazoles and quinoxaline. Wide ranges of substituted *o*-phenylenediamines and aldehydes or α-bromo ketones were used to achieve the desired products using water as the reaction medium. The recoverability and reusability of the catalyst are the significant features in this eco-friendly green protocol. (*Catal. Lett.,* **2017**, 147, 2724)

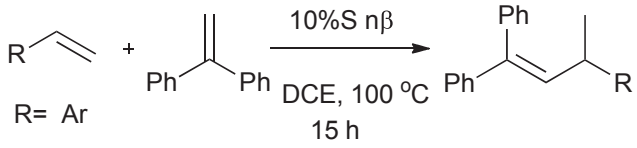


Iron-catalyzed C_{sp3}-C_{sp3} bond formation *via* dehydrative cross coupling reaction: facile access to new hybrid dihydroquinazolines having quinoline, isoquinoline, quinoxaline and azoles

An operationally simple, efficient and straight forward approach was developed for the synthesis of new hybrid nitrogen heterocycles bearing dihydroquinazoline with quinoline, isoquinoline, quinoxaline and azole *via* iron-catalyzed dehydrative cross coupling reaction between heterocyclic aminol and 2-methyl azaarenes. Furthermore, this protocol applied to couple simple methyl ketones to achieve C4-alkylated-dihydroquinazolines with broad substrate scope (*Tetrahedron Lett.,* **2017**, 58, 1501)

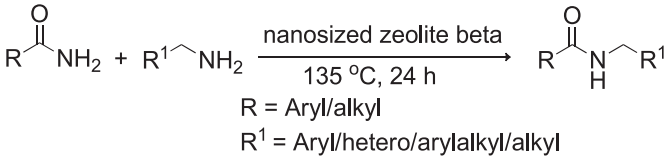
Chemo- and regioselective head-to-tail heterodimerization of vinylarenes with 1,1-diphenylethene over heterogeneous catalyst (Snβ zeolite)

We have developed a convenient Snβ zeolite catalyzed protocol for the highly chemo- and regioselective head-to-tail heterodimerization of vinylarenes with 1,1-diphenylethene under mild conditions. The scope and limitations of this process are demonstrated with various vinylarenes and 1,1-diphenylethene. Notable advantages offered by this strategy are use of non-hazardous and reusable catalyst, higher yields of the desired products, simple work-up procedure, which make this catalytic system an attractive and useful alternative to the existing method. (*RSC Adv.*, **2016**, 6, 1296)



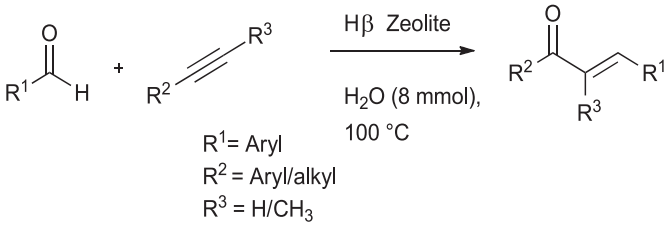
Transamidation of carboxamides with amines over nanosized zeolite beta under solvent-free conditions

A highly efficient approach to transamidation of carboxamides with amines over nanosized zeolite beta under solvent-free conditions has been successfully demonstrated. Transamidation of a variety of amides with amines produced the respective N-alkyl amides in moderate to excellent yields. (*Catal. Comm.*, **2016**, 81, 29)



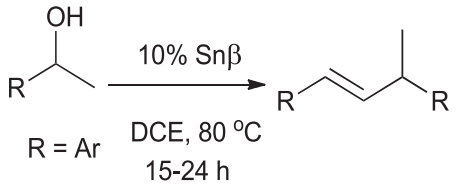
Synthesis of α,β-unsaturated ketones from alkynes and aldehydes over Hβ zeolite under solvent-free conditions

A facile Hβ zeolite-catalyzed strategy has been successfully developed for the synthesis of α,β-unsaturated ketones from alkynes and aldehydes under solvent-free conditions. The reaction proceeds *via* tandem hydration/condensation of alkynes with aldehydes to afford a range of α,β-unsaturated carbonyls in good to excellent yields. (*RSC Adv.*, **2016**, 6, 58137)



One-pot synthesis of 1,3-diaryl but-1-enes from 1-arylethanols over Snβ zeolite

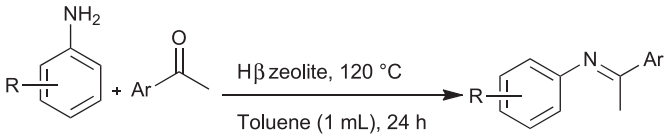
An environmentally benign catalytic protocol has been successfully developed for the one-pot synthesis of 1,3-diaryl but-1-enes from 1-arylethanols via dehydration of 1-arylethanols followed by head-to-tail dimerization of vinylarenes over heterogeneous catalyst (Snβ zeolite). The scope of the reaction was explored for various 1-arylethanols and afforded the corresponding dimers in good to excellent yields with high regio- and stereoselectivity. (*Catal. Comm.*, **2017**, 90, 95)



Hβ Catalyzed Condensation Reaction Between Aromatic Ketones and Anilines: To Access Ketimines (Imines)

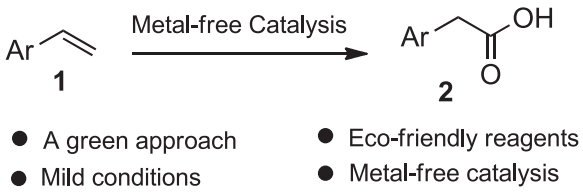
A simple approach for the formation of imines by condensation of ketones and anilines over heterogeneous catalyst (Hβ zeolite) has been successfully developed.

The present catalytic system scope was explored for various aromatic ketones and anilines. (*Catal. Lett.,* **2017**, 147(12), 2982)



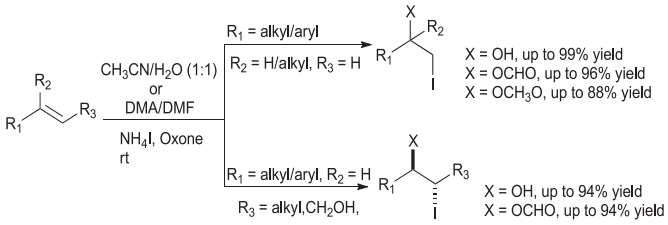
Metal-free, catalytic regioselective oxidative conversion of vinylarenes: A mild approach to phenylacetic acid derivatives

A new synthetic approach towards the synthesis of phenylacetic acids from aromatic alkenes has been developed for the first time under mild conditions by employing non-toxic reagents such as molecular iodine and oxone. This metal-free catalytic regioselective oxygenation of vinylarenes proceeds via tandem iodofunctionalization/de-iodination induced rearrangement. (*RSC Adv.,* **2016**, 6, 6719)



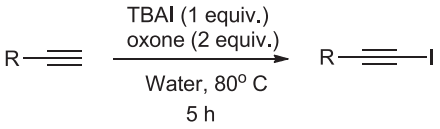
Regio- and stereoselective co-iodination of olefins using NH_4I and oxone®

A simple, efficient and environmentally benign protocol for the synthesis of vicinal iodohydrins and iodoesters from olefins using NH_4I and oxone® in CH_3CN:H_2O (1:1) and DMF/DMA, respectively, without employing a catalyst at room temperature is described. Regio- and stereo selective iodohydroxylation and iodoesterification of various olefins with anti fashion, following Markonikov's rule was achieved and the corresponding products were obtained in good to excellent yields. In addition, 1,2-disubstituted olefins afforded excellent diastereoselectivity. (*Synth. Comm.*, **2016**, 46 (13), 1133)



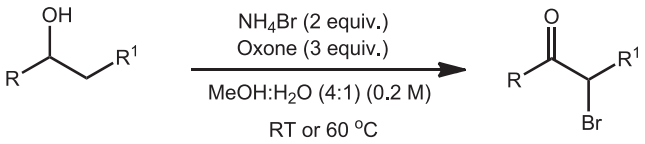
A Quaternary ammonium salt promoted regioselective iodination of terminal alkynes: A convenient access to 1-iodoalkynes in Aqueous Media

A new protocol for the synthesis of 1-iodoalkynes from terminal alkynes under metal-free conditions in aqueous media *via* quaternary ammonium iodide and oxone mediated oxidative iodination has been developed. Simple reaction conditions, low cost and commercial availability of reagents and the use of readily available, non-toxic and universal solvent i.e., water as a reaction media makes this approach as an eco-friendly and economically viable. (*ChemistrySelect*, **2017**, *2*, 748)



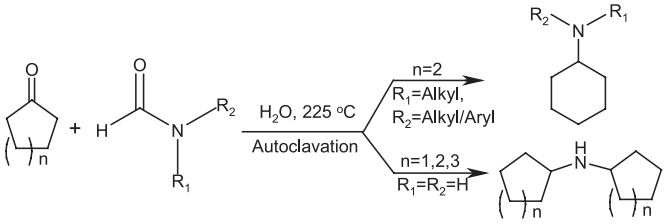
A new and versatile one-pot strategy to synthesize alpha-bromoketones from secondary alcohols using ammonium bromide and oxone

A new, efficient and green protocol for one-pot synthesis of α-bromoketones from secondary alcohols using cheap, air stable and non-toxic reagents such as NH_4Br and oxone has been developed. The scope and limitations of this protocol were investigated with various secondary alcohols such as 1-aryl-1-alkanols (containing halo, electron withdrawing and electronic donating groups on aromatic ring), aromatic ring fused and aliphatic (cyclic and acylic) alcohols. This reaction proceeds *via* two consecutive steps such as oxidation of secondary alcohol and oxidative bromination of *in situ* generated ketone. (*New J. Chem.,* **2017**, 41, 3710)



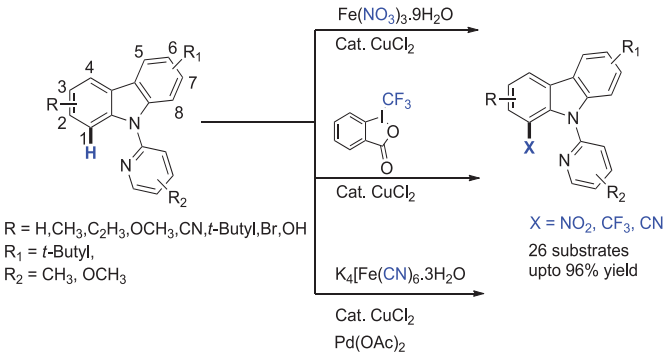
Catalyst-free synthesis of amines from cyclic ketones and formamides in superheated water

A novel and environmentally benign protocol for the synthesis of amines from cyclic ketones and formamides is developed. The reaction proceeds under catalyst-free and superheated water conditions and yields range from low to excellent. (*Synth. Comm.,* **2016**, 46(6), 516)



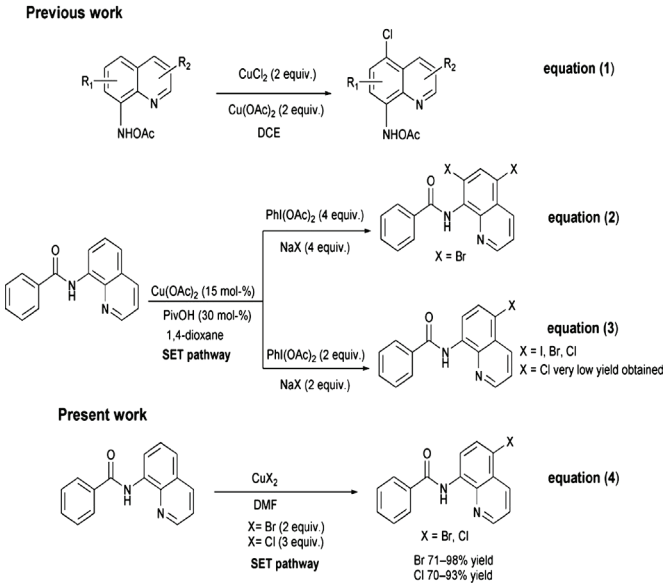
Highly Site-Selective and Direct Ortho-C-H Nitration, Trifluoromethylation and Cyanation at the C1-Position of Carbazole Frameworks

In summary, for the first time we have demonstrated that 9-(pyridine-2-yl)-9H-carbazoles readily undergo site-selective C1-H mono nitration, trifluoromethylation under copper catalyzed reaction conditions that are geometrically difficult to access. This protocol makes use of readily available $Fe(NO_3)_3.9H_2O$, Togni reagent-II as functional group source and shows good tolerance toward several substituted 9-(pyridine-2-yl)-9H-carbazoles giving the corresponding products in good to excellent yields. We have also demonstrated that when 5 mol% of $Pd(OAc)_2$ is used as catalyst in the presence of $CuCl_2$ also promotes important site-selective C1-H cyanation reaction of substrates containing 9-(pyridine-2-yl)-9H-carbazole core when $[K_4Fe(CN)_6].3H_2O$ is used as cyano source. Overall, our synthesis protocol tolerates as many as 26 substrate combinations and shows good yields toward numerous 9-(pyridine-2-yl)-9H-carbazoles giving the corresponding C1-functionalized products in good to excellent yields. The outstanding site-selectivity of our protocol was reflected by the fact that lack of formation of undesired C3 and C6 positions functionalized carbazole products that arise from unusually higher nucleophilic character of those sites wherein electrophilic substitutions are highly preferred. (*Asian J. Org. Chem.* **2017**, 6, 59)



Copper-Mediated Remote Highly Site-Selective C–H Bond Bromination and Chlorination of Quinolines at the C5 Position that is Geometrically Difficult to Access

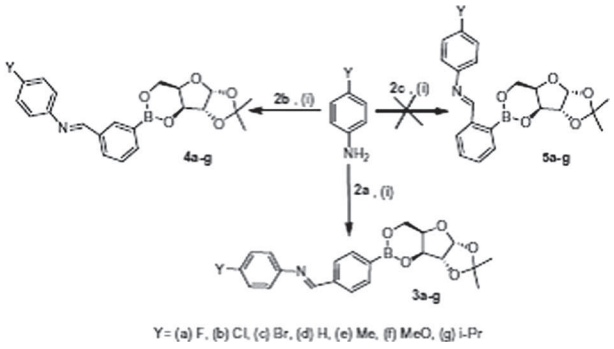
A concise, simple, and efficient method for remote C–H bond halogenation (Br and Cl) of 8-aminoquinoline scaffolds at the geometrically difficult-to-access C5 position was explored with diverse substrate combinations in DMF. This protocol made use of inexpensive $CuBr_2$ and $CuCl_2$ as mediators and showed good to excellent yields for as many as 24 substrate combinations. The outstanding site selectivity of the reaction was reflected by the lack of formation of the undesired C7-halogenated byproduct originating from the high nucleophilic reactivity of the 8-aminoquinoline scaffold at the C7 position,even if excess amounts of the CuX_2 salts were used. In summary, we developed a simple, concise, and efficient method for the remote C–H bond halogenation (Br and Cl) of 8-aminoquinolines at the geometrically difficult-to-access C5 position by by using 24 different substrate combinations. The outstanding site selectivity of the reaction was reflected by the lack of formation of the undesired C7-halogenated byproduct originating from the high nucleophilic reactivity of the 8-aminoquinoline scaffold at the C7 position, even if excess amounts of the CuX2 salts were used. *(Eur. J. Org. Chem.,* **2017**, 438)



Bioorganometallic Chemistry

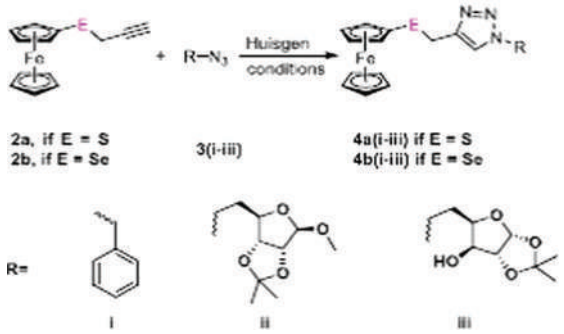
Synthesis, characterization and antimicrobial activity of novel Schiff base tethered boronate esters of 1,2-O-isopropylidene-α-D-xylofuranose

A series of twenty one Schiff bases based on boronate ester of 1,2-O-isopropylidene-a-D-xylofuranose scaffold were designed and synthesized by condensation of formyl or amino phenyl boronate esters with substituted anilines or 2-hydroxybenzaldehydes, respectively. *(Bioorg. Med. Chem. Lett.,* **2016**, 26, 3447)



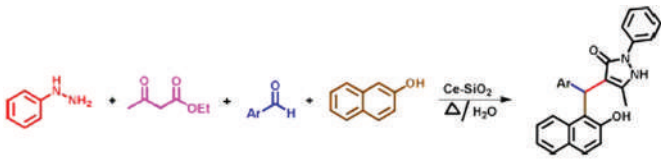
Ferrocenyl chalcogeno (sugar) triazole conjugates: Synthesis, characterization and anticancer properties

This work describes the synthesis, characterization and anticancer properties of a series of chalcogeno (S/Se) triazole bridged ferrocene-carbohydrate conjugates. (*J. Organomet. Chem.,* **2016**, 813, 125)



Ce/SiO_2 composite as an efficient catalyst for the multicomponentone-pot synthesis of substituted pyrazolones in aqueous media andtheir antimicrobial activities

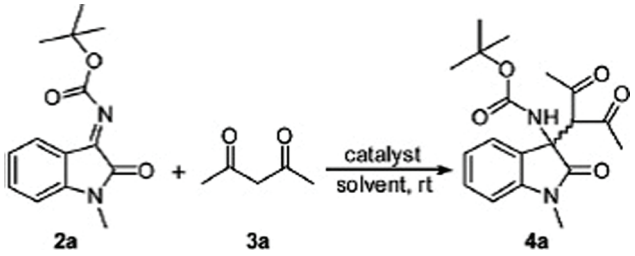
We describe here the preparation and characterization of a Ce/SiO_2 catalyst and its application in aneco-friendly and convenient synthesis of pyrazolone derivatives via one-pot multicomponent reactionof 2-naphthol, aldehydes, phenylhydrazine and ethyl acetoacetate under aqueous media. (*J. Mol. Catal. A: Chem.,* **2016**, 411, 325)



Scheme 1. General synthesis of 1H-3-pyrazolones.

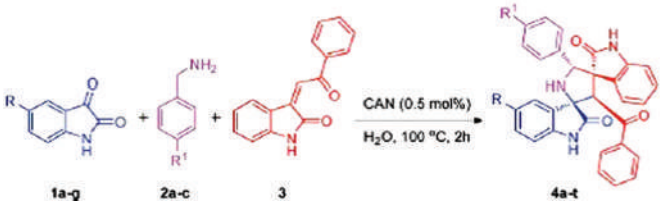
Asymmetric Mannich reaction: highly enantioselective synthesis of 3-amino-oxindoles via chiral squaramide based H-bond donor catalysis

We describe here a simple and facile asymmetric Mannich reaction catalyzed by chiral Cinchona alkaloid based squaramide containing H-bond donor catalysts, wherein, the reaction of 1,3-diketones with isatin (N-Boc) ketimines led to the formation of 3-aminooxindole derivatives. (*RSC Adv.*, **2016**, 6, 84242)



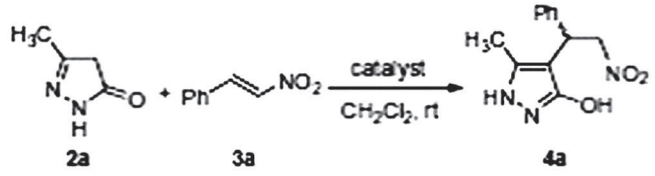
Highly efficient regio and diastereoselective synthesis of functionalized bis-spirooxindoles and their antibacterial properties

A simple, efficient, regioselective and diastereoselective method has been developed for the synthesis of diversely functionalized spirooxindole-pyrrolidines using 0.5 mol% of ceric ammonium nitrate in aqueous medium. (*RSC Adv.*, **2016**, 6, 26546)

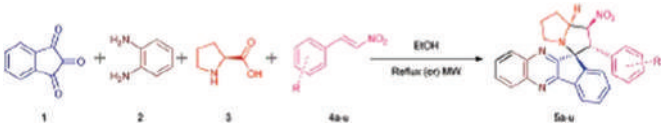


Chiral squaramide catalyzed synthesis of C4 substituted chiral pyrazol-3-ol derivatives via a facile asymmetric Michael addition of 3-methyl-2-pyrazolin-5-one to β-nitrostyrenes

Asymmetric Michael addition of 3-methyl-2-pyrazolin-5-one to b-nitrostyrenes, catalyzed by a series of chiral squaramide bifunctional catalysts derived from cinchona alkaloids, yielded chiral pyrazol-3-ol derivatives. (*Tetrahedron Lett.,* **2016**, 57, 1227)



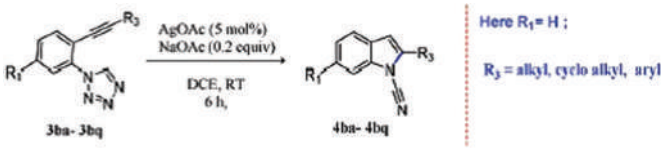
An expedient microwave assisted regio- and stereoselective synthesis of spiroquinoxaline pyrrolizine derivatives and their AChE inhibitory activity. *(New J. Chem.,* **2017**, 41, 873)



An efficient four-component cascade protocol is reported to afford spiro indeno[1,2-b]quinoxaline-11,30-pyrrolizines via the condensation of ninhydrin, phenylenediamine, proline, and nitrostyrene derivatives under microwave irradiation and classical conditions.

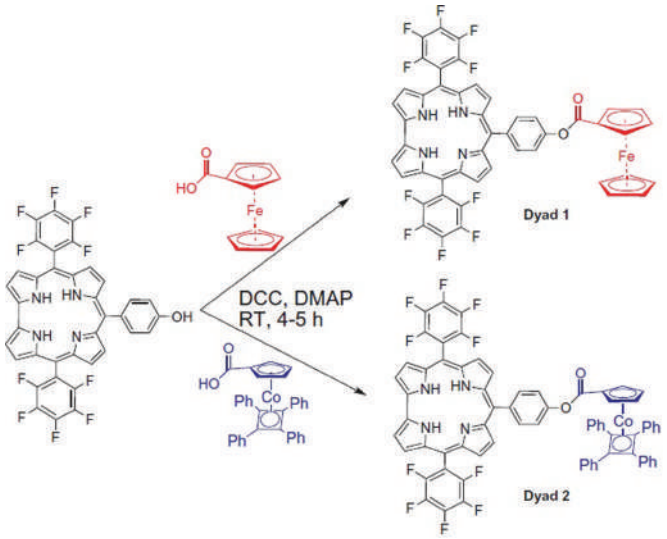
Silver(I) catalyzed intramolecular cyclization of N-(2-(alk-1-yn-1-yl))-1H-tetrazoles leading to the formation of N-cyano-2-substituted indoles under ambient conditions

A facile silver(I) catalyzed intramolecular cyclization reaction of alkynyl tetrazoles to form N-cyano-2-substituted indoles has been investigated. This unique cyclization involves the formation of a C–N bond during the intramolecular cyclization of N-(2-(alk-1-yn-1-yl))-1H-tetrazoles in the presence of silver(I) acetate. Good to excellent yields were obtained using low catalyst loadings, ~5 mol%, under mild conditions. (*Org. Chem. Front.*, **2017**, 4, 1574)



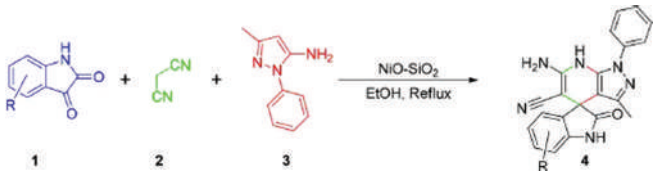
Synthesis, characterization and photophysical properties of ferrocenyl and mixed sandwich cobaltocenyl ester linked *meso*-triaryl corrole dyads

We report here the design and synthesis of corrole-metallocene dyads consisting of a metallocene (either ferrocene (Dyad 1) or mixed sandwich η^5-[C_5H_4(COOH)] Co(η^4-C_4Ph_4) (Dyad 2)) connected *via* an ester linkage at *meso* phenyl position. *(J. Porphy. Phthalocyan.,* **2017**, 21, 646)



Spirooxindole-fused pyrazolo pyridine derivatives: NiO–SiO_2 catalyzed one-pot synthesis and antimicrobial activities

One-pot synthesis of 13 spirooxindole-fused pyrazolo pyridine derivatives using NiO–SiO_2 catalyst via three-component reaction of isatin, 5-amino-3-methylpyrazole, and malononitrile is reported. This multicomponent one-pot protocol also features shorter reaction time, good yield, and simple work-up using a recoverable and reusable solid acid heterogeneous catalyst. (*Synth. Comm.*, **2017**, 48, 255)

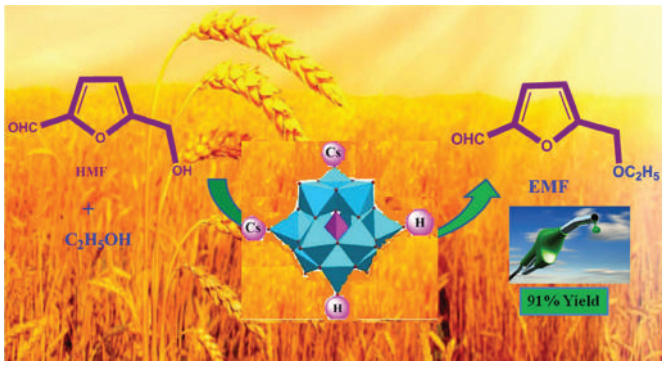


Heterogeneous Catalysis

Development of catalytic systems for conversion renewable resources:

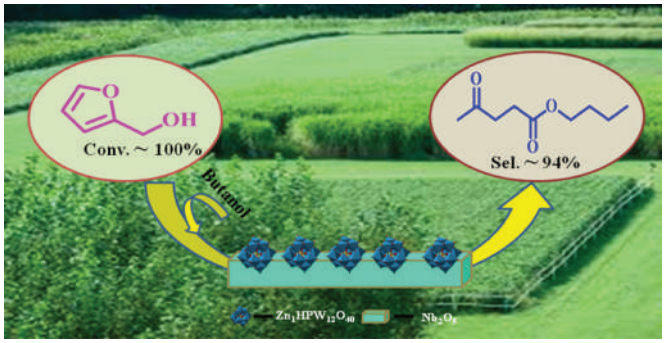
Conversion of biomass to chemicals/fuels:

Cesium-exchanged silicotungstic acid catalysts with retention of Keggin ion were developed for the conversion of 5-hydroxy methyl furfural to ethoxy methyl furfural, a fuel additive. The catalyst with two Cs ions exchanged with STA (Cs_2STA) showed highest activity. This catalyst showed about 91% yield of EMF at 120 °C with in 2.5 h. Different reaction parameters were studied and optimum conditions were established. (*Appl. Catal. A: Gen.*, **2016**, 520,105)



Furfuryl alcohol to butyl levulinate

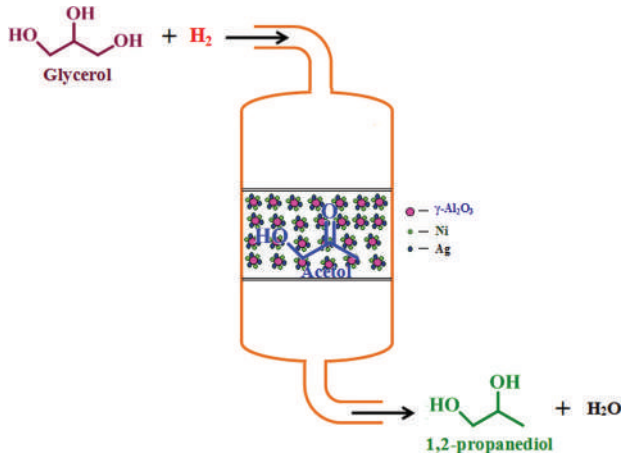
Niobia supported zinc exchanged tungstophosphoric acid catalysts were prepared with intact Keggin ion structure. Zn_1TPA/Nb_2O_5 was an efficient catalyst for the preparation of BL from FAL with n-butanol. The activity of the catalysts depended on the amount of zinc exchanged with TPA which directs the overall acidity of the catalyst. Exchange of protons of TPA with Zn^{2+} resulted in generation of Lewis acidic sites. The yield of BL also depends on the reaction temperature, reaction time and amount of catalyst. The catalyst is easy to recover and reusable without any loss in activity. (*Mol. Catal.*, **2017**, 427, 80)



Conversion of bio-glycerol to 1,2-propane diol

Alumina supported bi-metallic Ni-Ag catalysts were designed for continuous glycerol hydrogenolysis into 1,2-propanediol at atmospheric pressure. The catalyst with 10%Ni-5%Ag showed reasonable glycerol conversion of 80% with 58% selectivity to 1,2-propanediol. The high activity of the catalyst is due to the presence of highly dispersed metallic Ni and Ag species on γ-Al_2O_3 and also acidity of the catalyst The presence of Ag facilitates the reduction of NiO at relatively low temperature. The optimum conditions for the reaction were established. (*Catal. Lett.*, **2017**, 147, 1441)

Copper based Cu-ZrO_2-MgO catalysts were studied for selective hydrogenolysis of glycerol. The catalyst with 20%Cu-10%ZrO_2-MgO showed 62% glycerol conversion with 97% selectivity for 1,2-propanediol. A detailed kinetics was also evaluated. (*Catal. Lett.*, **2016**, 146, 1487)



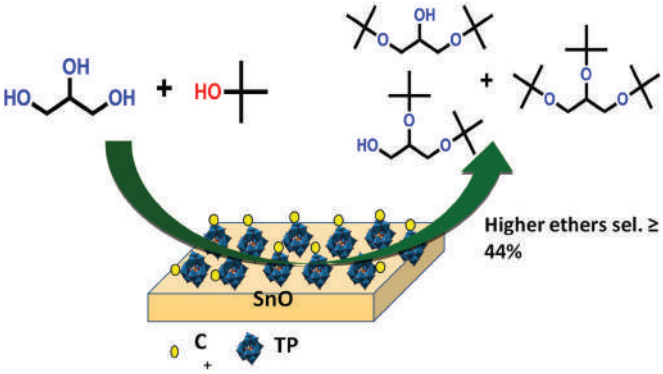
Glycerol to glycerol carbonate

Tungsten oxide supported on titania catalysts were prepared for the synthesis of glycerol carbonate from glycerol and urea. The interaction between tungsten oxide and titania influences the activity of the catalysts. The content of WO_3 on support and calcination temperature influences the activity of the catalyst. Highly dispersed amorphous WO_3 species are more active for the synthesis of glycerol carbonate. The catalyst is reusable with consistent activity without any pretreatment. (*Catal. Lett.*, **2016**, 46, 692)

Glycerol to fuel additives

Cesium salts of TPA supported on SnO_2 catalysts were prepared with retention of Keggin ion structure.

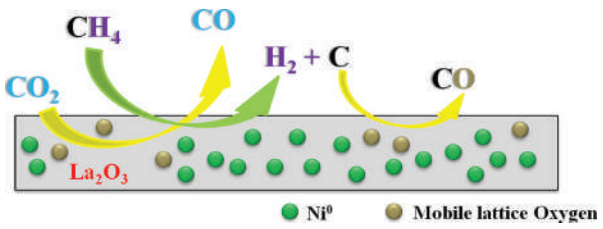
The characterization results suggest the presence of strong acidic sites, where acid strength depends on the exchangeable protons on TPA with Cs^+ ions and TPA loading on SnO_2. The etherification activity was related to the acidity of the catalyst. The Cs-containing catalysts possess stronger acidic sites compared to the catalyst without Cs. The 20% $CsTPA/SnO_2$ catalyst exhibited 90% glycerol conversion with 44% selectivity for higher ethers. The glycerol etherification activity and selectivity not only depended on the nature of the catalyst but also on some reaction parameters such as temperature, time and mole ratio of glycerol to tert-butanol. The catalyst exhibited reusability with constant activity. (*J. Mol. Catal. A: Chem*, **2016**, 413, 7)



Utilization of CO_2

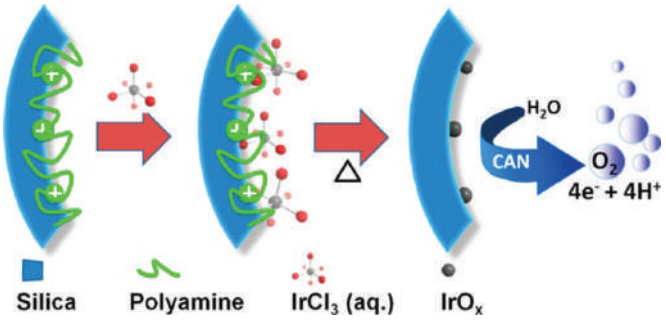
Oxidative dehydrogenation (ODH) of ethane with CO_2 was evaluated at atmospheric pressure over CaO–NiO/Al_2O_3 catalysts and in the temperature range of 600–700 °C. The addition of CaO in NiO/Al_2O_3 reversed the course of reaction leading to high selectivity to ethane. CaO addition increased the basicity and the coke resistance. The activity of these catalysts was compared to identify the best method of catalyst preparation.

Continuous syngas production by CO_2 reforming of methane was achieved over $LaNi_xAl_{1-x}O_3$ perovskite catalyst. La-Ni-Al tri metallic perovskite formation gives higher CH_4 and CO_2 conversions than the La-Ni bimetallic perovskite in the catalysts. Strong interaction between the metallic Ni and the defined structure prevents sintering of metal particles. The high dispersion of Ni enhances the activity. The incorporation of third metal into the bimetallic perovskite lattice increases the lattice defects thereby producing the mobile oxygen, which help decrease coke accumulation on the surface of the catalysts. (*J. Chem. Sci.*, **2017**, 129(11), 1787; *Catal. Lett.*, **2017**, 147, 82)



Water Oxidation Catalyst via Heterogenization of Iridium Oxides on Silica: A Polyamine-Mediated Route to Achieve Activity and Stability

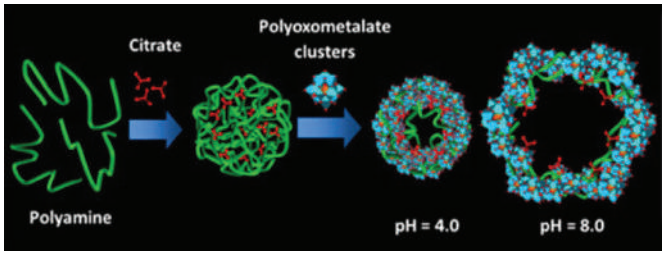
A polyamine-mediated assembly process to heterogenize iridium species on mesoporous silica spheres has been demonstrated. While the functionalization of the silica surface with polyamine facilitates interaction with the negatively charged iridium precursor, the presence of polyamine further enables control on the dispersion and crystallization of the generated nano-sized iridium oxides during the thermal treatment at 573 K. As a consequence, the catalyst exhibits enhanced activity with higher TON in water oxidation along with desirable stability to allow it to be recycled while keeping the activity intact. (*ACS Catal.,* **2016**, 6, 5699)



Microcapsule Structure with a Tunable Textured Surface via the Assembly of Polyoxomolybdate Clusters: A Bioinspired Strategy and Enhanced Activities in Alkene Oxidation

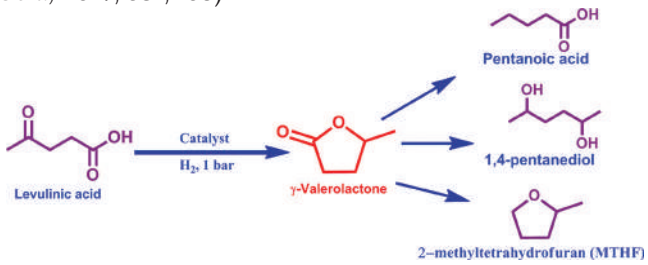
A bioinspired strategy to assemble Keggin-type phosphomolybdic acid (PMA) clusters is shown to result in microcapsule (MC) structures under very mild conditions. Besides the structural stability, the assembly process allows an interesting transition from a smooth to a wrinkled surface for the MCs alongside a change in the Keggin to its lacunary form depending on the pH of the medium. Moreover, the presence of isolated PMA

units in the hybrid structure enables them to be active in catalyzing the aerobic oxidation of alkenes with better selectivity and reusability. **(***ACS Appl. Mater. Interfaces,* **2017**, 9, 3161**)**



Biomass-derived levulinic acid conversion to fuel additives using supported Ni and Ru catalysts

Efficient and sustainable strategies are developed for the biomass derivable levulinic acid to fuel blending agents as γ-valerolactone and valeric acid over the supported Ni and Ru based catalysts at an atmospheric pressure. *(Appl. Catal. B: Environ.,* **2016**, 180, 113; *RSC Adv.,* **2016**, 6, 9872; *Appl. Catal. A: Gen.*, **2017**, 531, 169; *Appl. Catal. A: Gen.,* **2017**, 531, 169)



Possible levulinic acid conversion strategies

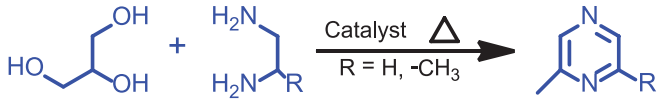
Catalytic CH_4 decomposition to produce CO_x free hydrogen over Ni-based catalysts

Different supported Ni and/or Ni-Cu based catalysts were developed for production of COx free hydrogen with a special attention on the long-term stability of the catalysts and production of high quality carbon nano fibers/nanotubes over a decade. (*Appl. Catal. A Gen.,* **2016**, 519, 85; *RSC Adv.,* **2016**, 6, 34600; *Int. J. Hydrogen Ener.,* **2016**, 61, 19855; *Energy Fuels*, **2017**, 31, 6374)

$CH_4 \rightarrow 2H_2$+ Carbon (CNT/CNF); $\Delta H° = 75.6$ kJ mol^{-1}

Synthesis of alkylpyrazines using bio-glycerol using Cu-Cr/Zn-Cr catalysts

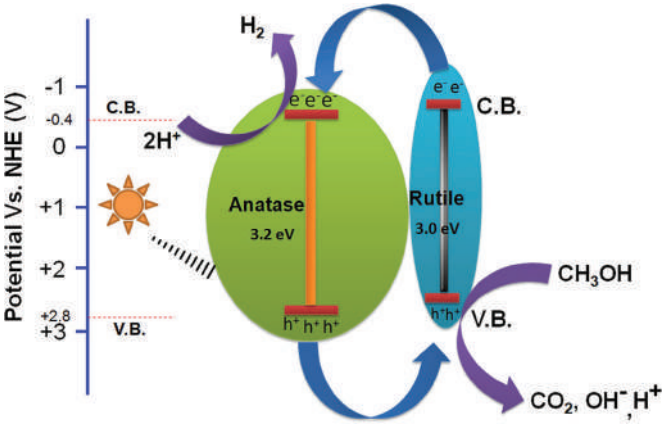
The effective utilization of bio-glycerol to alkylpyrazines has been demonstrating over the meta-chromite catalysts along with a focus on monitoring the active sites by in-situ DRIFT spectroscopic and adsorption data. (*Catal. Commun.,* **2016**, 74, 91; *Kinetics Catal.,* **2016,** 57(5), 602; *Appl. Catal. B: Environ.,* **2016**, 193, 58; *Current Catal.,* **2017,** 6, 135; *Catal. Sci. Technol.,* **2017**, 7, 3399; *New J. Chem.,* **2017**, 41, 9875; *Ind. Eng. Chem. Res.,* **2017**, 56, 11664)



Synthesis of alkylpyrazines using bio-glycerol and amines

Photocatalytic water splitting to produce hydrogen using doped titania-based materials

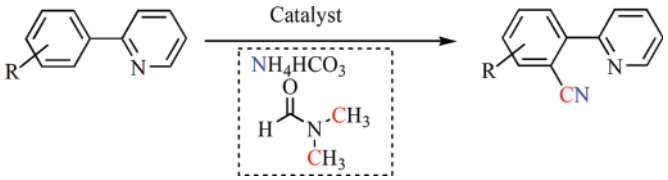
As a part of TAPSUN project, the research was also focussed on the band gap engineering of different TiO_2 materials for the photocatalytic H_2O splitting using natural sun light and developed some efficient materials that are active in sun light. *(Appl. Catal. A: Gen.* **2016**, 515, 91; *Appl. Catal. B: Environ.,* **2016**, 199, 282)



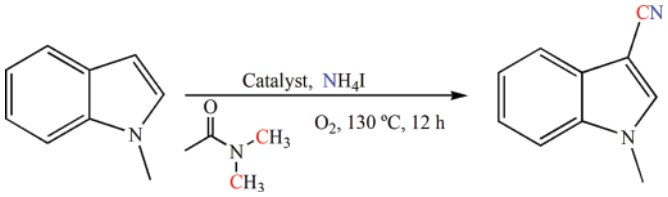
Hydrogen production and electron transfer in mixed phase of TiO_2

Catalyst development for industrially important organic reactions

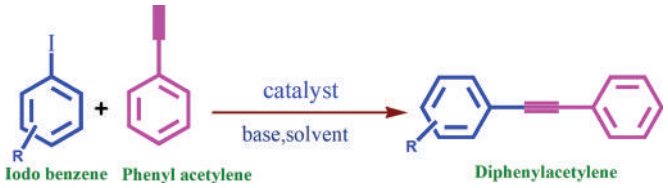
Research has also been focussed on the development of robust and active heterogeneous catalyst for industrially important organic transformations under mild reaction conditions and non-toxic solvents. A few of them are given below. (*Catal. Sci. Technol.,* **2016**, 6, 8055; *Energy Fuels*, **2017**, 31(6), 6320; *J. Phys. Chem. C.,* **2017**, 121(40), 22191)



Synthesis of aryl nitrile over the supported Cu catalysts



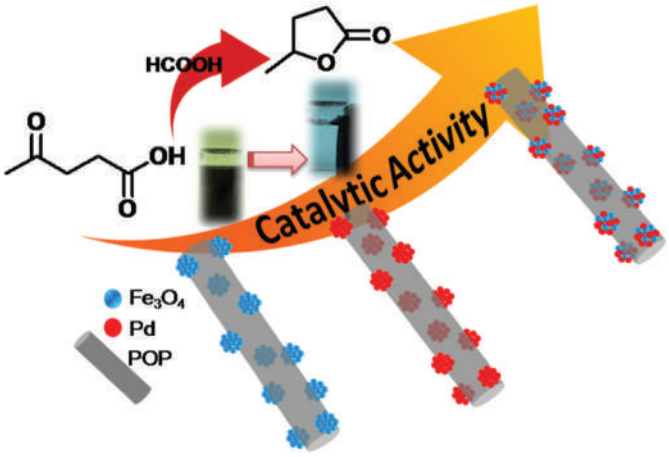
Cyanation of N-methylindole



Cross Coupling Reaction of Iodobenzene and Phenyl Acetylene

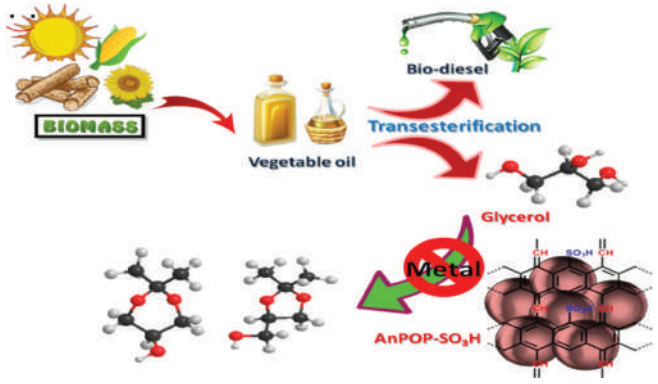
Magnetic Nanohybrid Decorated Porous Organic Polymer: Synergistic Catalyst for High Performance Levulinic Acid Hydrogenation

Herein we have developed a highly active, robust, and selective porous organic polymer (PPTPA-1, POP) encapsulated magnetically retrievable Pd-Fe_3O_4 nanohybrid catalyst in a one-step solvothermal route and investigated its catalytic performance in levulinic acid (LA) hydrogenation, a key platform molecule in many biorefinery schemes, to γ-valerolactone (GVL), employing formic acid as sustainable H_2 source. *(ACS Sust. Chem. Eng.*, **2017**, 5, 1033)



Constructing Sulfonic Acid Functionalized Anthracene Derived Conjugated Porous Organic Polymer for Efficient Metal-Free Catalytic Acetalization of Bio-Glycerol

Sulfonic acid (-SO_3H) functionalized anthracene derived conjugated porous organic polymer (AnPOP-SO_3H) have been constructed through Friedel-Crafts alkylation of anthracene by using formaldehyde dimethyl acetal as a cross-linker and anhydrous $FeCl_3$ as a promoter followed by sulfonation of aromatic rings using chlorosulfonic acid under controlled reaction conditions. This newly designed AnPOP-SO_3H metal-free organocatalyst exhibited an excellent catalytic activity in the acetalization of Bio-Glycerol with acetone, furfural, and benzaldehyde under solvent free and ambient temperature conditions to furnish 2,2-dimethyl-1,3-dioxalane-4- methanol (solketal) derivatives, with quantitative conversion and good selectivities. (*ChemstrySelect*, **2017**, 2, 4705)

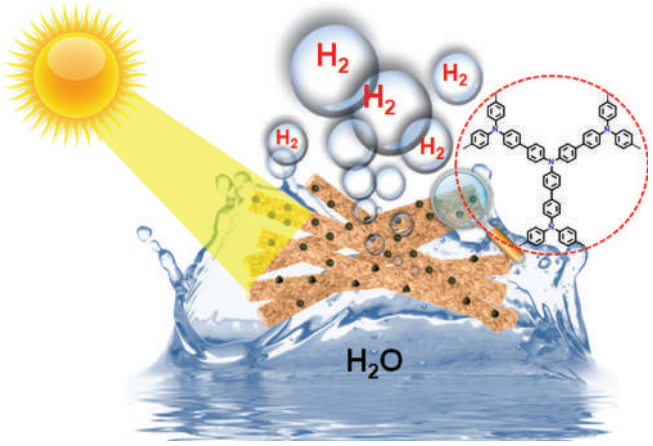


Palladium Nanoparticles Encaged in a Nitrogen-Rich Porous Organic Polymer: Constructing a Promising Robust Nanoarchitecture for Catalytic Biofuel Upgrading

Robust nanoarchitectures based on surfactant-free ultrafine Pd nanoparticles (NPs) (2.7–8.2:0.5 nm) have been developed by using the incipient wetness impregnation method with subsequent reduction of Pd(II) species encaged in the 1,3,5-triazinefunctionalized nitrogen-rich porous organic polymer (POP) by employing $NaBH_4$, HCHO, and H_2 reduction routes. The resulting Pd-POP based materials exhibit highly efficient catalytic performance with superior stability in promoting biomass refining (hydrodeoxygenation of vanillin, a typical compound of lignin-derived bio-oil). (*ChemCatChem*, **2017**, 9, 2550)

The Design of a New Cobalt Sulfide Nanoparticle Implanted Porous Organic Polymer Nanohybrid as a Smart and Durable Water-Splitting Photoelectrocatalyst

In this study, the design and sequential synthesis of a novel cobalt sulfide nanoparticles grafted Porous Organic Polymer nanohybrid (CoS_x@POP) is reported and used as an active and durable water-splitting photoelectrocatalyst in the hydrogen evolution reaction (HER). CoS_x@POP has been evaluated as a superior photoelectrocatalyst in HER, achieving a current density of 6.43 $mAcm^{-2}$ at 0 V versus the reversible hydrogen electrode (RHE) in a 0.5 m Na_2SO_4 electrolyte which outperforms its Co_3O_4@POP analogue. It was found that the nanohybrid CoS_x@POP catalyst exhibited a substantially enhanced catalytic performance of 1.07 mmolmin@1cm^{-2}, which is considered to be ca. 10 and 1.94 times higher than that of pristine POP and CoS_x, respectively. (*Chem. Eur. J.*, **2017**, 23, 14827)



Electro Catalysis

We undertakes the studies of new materials; process and device engineering based on metal–semiconductor composites, inorganic-organic hybrid materials and plasmonic metal nanoparticles in solar energy conversion and advanced oxidation process for environmental remediation application. In parallel, currently we are working on functional materials for coal to methane, CO_2 capture and formic production. The current research activity includes development of new stable 2D semiconductors, oxynitrides for photocatalytic hydrogen production from water and the understanding of photophysics to acquire efficient solar-to-chemical energy conversion at device level. In parallel, currently we are working on functional materials for coal to methane, CO_2 capture and formic production.

Recently, we have developed new $KNb(Zr)O_3$ perovskite materials and showed their enhanced photocatalytic hydrogen evolution activities (Fig.1)

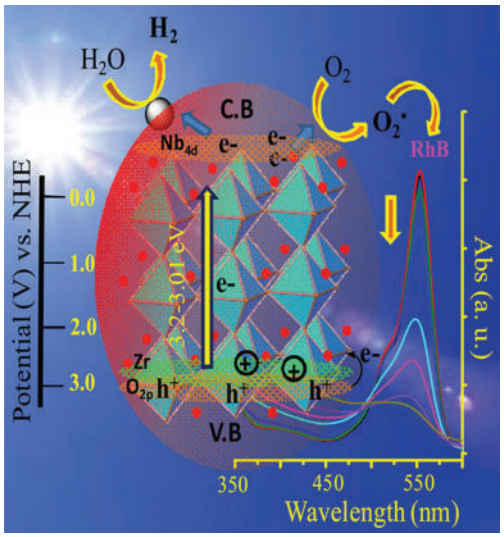


Fig.1: $KNb(Zr)O_3$ Perovskite for Enhanced Photoactivity

We realized very interesting changes in photophysical property and photocatalytic effect because of substitutional aliovalent metal ion doping in the host structure as depicted in the Fig. 2. *(Phys. Chem. C*, **2017**, 121, 2597).

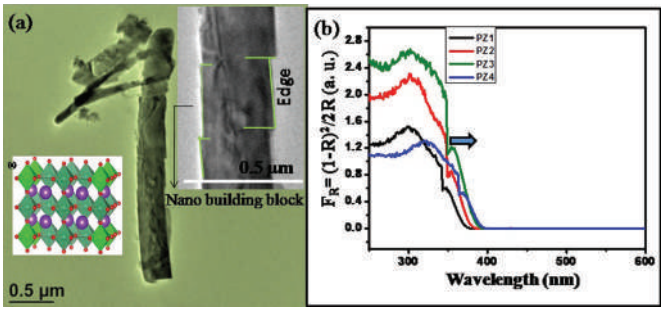


Fig.2: (a) TEM image and (b) absorption spectra of $KNb(Zr)O_3$

APPLIED RESEARCH

Industry Sponsored Project

Process Development for esterification of para-tert-Butyl benzoic Acid (PTBBA) to para-tert-butyl- methyl benzoate

In a series of two processes, alkylation of toluene to PTBT and oxidation of PTBT to para-tert-butyl benzoic acid, subsequent process development for esterification of PTBBA to para-tert-butyl methyl benzoate has been developed by CSIR-IICT. The esterification of PTBBA is achieved by the reaction of PTBBA with methanol in presence of methane sulphonic acid as a recyclable catalyst. In this process, both methanol and catalyst were recovered and reused in next batch of esterification and the overall yield and purity of product was 95% and <99% respectively. After transferring the technologies for PTBT and PTBBA, esterification of PTBBA has been studied at bench scale and later pilot scale and BDR. Based on the basic design report, the client has given its consent to commercialize the product (production at 5TPD. *Work carried out with Chem. Engineering Team)*

Process development for acylation of anisole to 4-MAP

Friedel-Crafts acylation is one of the most import ant methods for synthesizing aromatic ketones. Lewis acids or other catalysts are used in order to allow the reaction of anisole to proceed at a convenient rate. The use of such a conventional catalyst leads to a number of problems such as the loss of the catalyst, corrosion, pollution and waste and it is evident that only in the case of using a large amount of the catalyst under heating and for a longer reaction period can afford 4-methoxyacetophenone in a good yield. CSIR- IICT has developed the continuous mode process for acylation of anisole using heterogeneous catalyst and acetic anhydride under mild conditions. The preliminary work (process optimization, isolation of product, analysis of products & by-products and recovery of solvents and un-reacted materials) has been completed. (*Work carried out with Chem. Engineering Team)*

Process development for Paraectamol using acetic acid

Acetaminophen or paracetamol is widely used analgesic and antipyretic. It is widely used OTC drug in numerous countries and in different pharmaceutical formulations, alone or in combination with other active pharmaceutical ingredients. Drugs containing acetaminophen are used in the treatment and/or relief of minor aches and pains and are also included in formulations for cold and flu remedies due to its antipyretic effect.

The procedure for the preparation of acetaminophen is by catalytic reduction and hydroxylation of nitrobenzene to acetaminophen and by catalytic hydrogenation followed by acylation of para-nitrophenol to acetaminophen. The different acylating agents used in acylation of para aminophenol are acetyl chloride, acetic anhydride and acetic acid.

CSIR-IICT has made an agreement with the client for the process know how of paracetamol preparation using acetic acid as acylation reagent and subsequent scale up study for the commercial plant of 10000TPA.

The present process for acylation of para-aminophenol (PAP) is carried out using acetic acid under mild reaction conditions with high conversion and selectivity of paracetamol. The process is competitive to existing process which uses acetic anhydride and water is only by-product.

GOI has declared acetic anhydride as '*Controlled Substance* ' since its use in illicit manufacture of heroin and methaqualone. The process involves replacement of acetic anhydride with acetic acid which offers several advantages such as water as by-product, green process, inexpensive KSM. (*Work carried out with Chem. Engineering Team)*

Process Development for Avobenzone

Avobenzone is a primary agent in commercial sunscreens due to its effectiveness in absorbing a wide range of ultraviolet (UV) rays, specifically the type that is known to cause SUNBURN.

CSIR-IICT has already developed the technologies for the production of PMAP and PTBMB, raw materials for the Avobenzone. The process involves base mediated condensation of p-methoxy-acetophenone and p-tert-butyl methyl benzoate to yield avobenzone in moderate yield.

At present there is no commercial production of avobenzone in India. China is major supplier for the raw materials and Avobenzone product. The demonstration of the avobenzone process at one lit. scale capacity has given to the client.

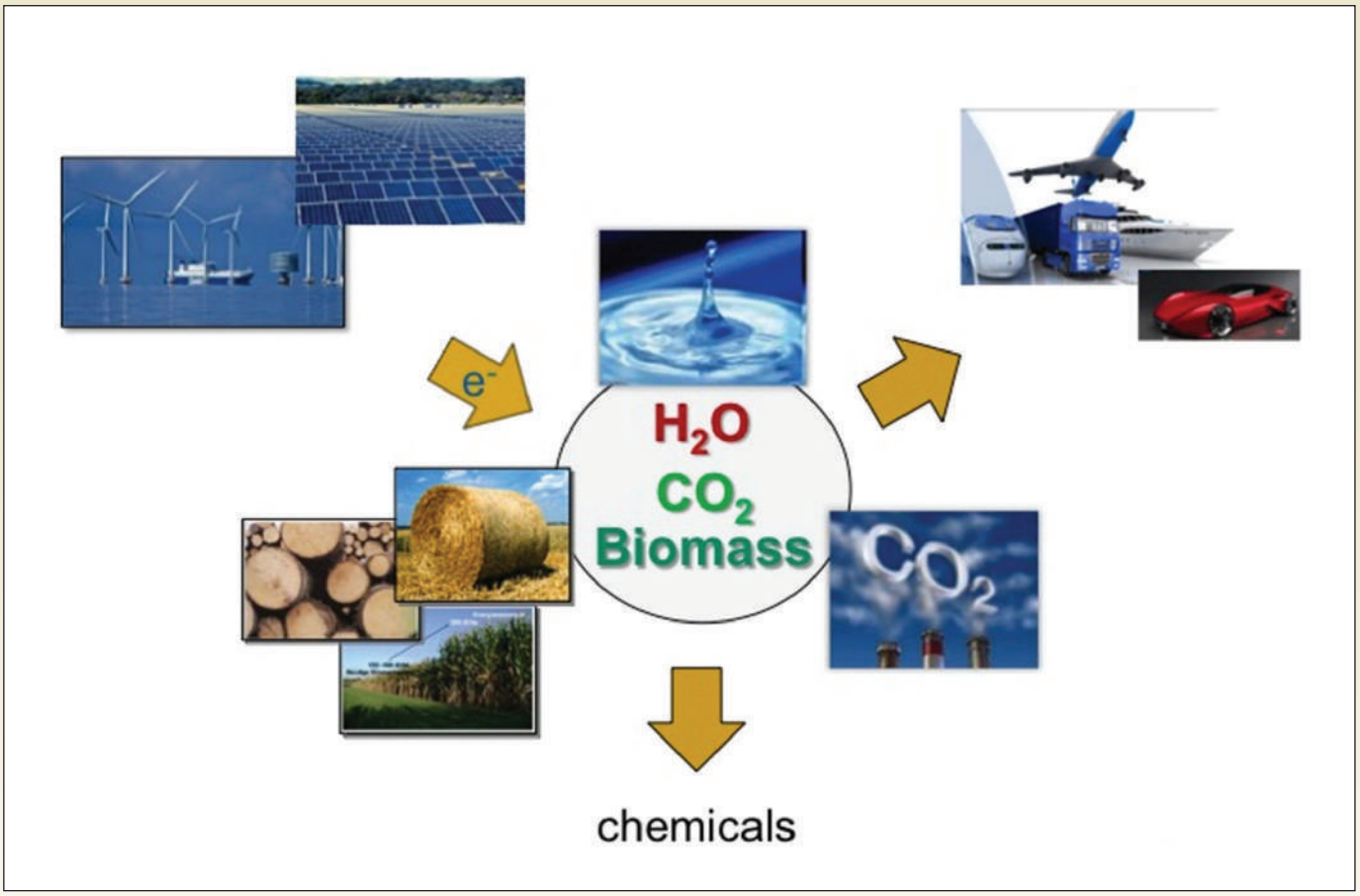
Selective catalytic hydroxylation of benzene with molecular oxygen

Selective hydroxylation of benzene to phenol is a challenge reaction in petrochemical industry as phenol has wide range of applications. Conventional phenol sysnthesis from Cumene oxidation (Hock Process) is a multi step process with high acetone production as a co-product, conversions are kept low at every step to keep the selectivity high. These issues are the driving force for the search of new catalytic process which will produce phenol directly from benzene in one step. We took this project to develop active catalysts for the selective synthesis of phenol from benzene.

Development of vapour phase catalytic process for the synthesis of iminostilbene from iminodibenzyl

Development of catalyst for synthesis of iminostilbene from iminodibenzyl byusing vapour phase fixed bed reactor is important process in pharma industry. There was no commercial catalyst for this reaction and we have been working on this project to develop an indigenous catalyst. We identified an active catalyst for this reaction and the standardization of reaction parameters are established.

CENTRE FOR ENVIRONMENTAL ENGINEERING & FOSSIL FUELS



Acidogenesis - Valorization of Renewable Fuels and Chemicals from Waste

Biohydrogen and Biohythane: In the realm of fossils depletion, the demand for chemicals and fuels is pushing the world towards higher sustainability. Biohydrogen (H_2) and biohythane (H_2+CH_4) hold an important place in renewable biofuel spectrum. The biological production of H_2 through acidogenic (dark) fermentation and biohythane through integrated anaerobic process is gaining perceptible interest that has an added advantage of the co-production of volatile fatty acids/ short chain carboxylic acids (VFAs/SCCAs). Pre-treated biocatalyst and higher carbon load showed marked enhancement in H_2 production, while untreated inoculum favored biohythane production. Pre-aeration helped in the improvement of H_2 production. To overcome the inhibitory concentrations of undissociated acids and the resultant pH drop during H_2 production, the role of inorganic sodium salts of hydroxide (OH^-), bicarbonate (HCO_3^-) and phosphate (PO_4^{3-}) as buffering agents was evaluated. It was observed that, H_2 production was highest in the HCO_3^- buffered system followed by OH^- and PO_4^{3-}. In addition, since microbial community play a key role in H_2 production the effect of selectively enriched biocatalyst and shifts in microbial communities during long term H_2 production process was studied. Pyrosequence distinguished the inter-species diversity of *Alphaproteobacterial* members and also showed increase in *Betaproteobacterial*, *Firmicute* sequences and decrease in *Epsilon proteobacterial* and other sequences in pretreated sample.

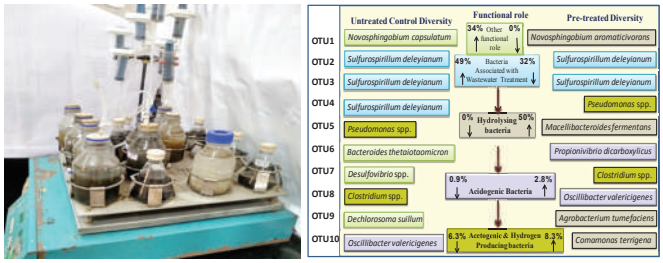


Fig 1: Acidogenic experiments for biohydrogen production and schematic representation of the functional roles of the ten foremost operational taxonomic units identified from un-treated control and pre-treated microbial consortia towards H_2 production

Short Chain Fatty Acids: Acidogenic fermentation facilitates the formation of simple compounds from the hydrolysis of organic compounds present in the waste by hydrolytic microorganisms and by the action of acidogenic bacteria leading to the formation of mixture of VFAs/SCCAs (VFA; C2: acetic, C3: propionic and C4: butyric), H_2 and CO_2. Biologically, these VFA can be converted to alcohols, methane (CH_4), bioplastics, microalgal lipids, bioelectricity, etc. VFA are renewable platform chemicals which are building blocks for polymers, acidulants, preservatives, flavor compound, and precursors for the synthesis of pharmaceuticals, etc. At present, commercial production of VFA is mostly accomplished by chemical routes through catalytic processing of petroleum-based precursors. VFA production was studied using waste activated sludge (WAS), defatted algal biomass (DAB) and food/vegetable wastes as primary feed stock. Several studies were performed towards the increase in VFA productivity. The application of pre-aeration strategy (AS) and head space pressure due to H_2, influenced the concentration and composition of fatty acids when renewable feed stock was used. Highest fraction of acetic, butyric and propionic acids was achieved with good degree of acidification (DOA). Selective enrichment of the biocatalyst, enhanced VFA production compared to untreated parent biocatalysts. In the microbial community analysis it was observed that acidogenic firmicutes (spore formers) and fatty acid producing bacteroides were enriched along with saccharolytic and proteolytic bacteria (*Bacillus cellulosilyticus* (alkalophile), *Soehngeniasaccharolytica*, etc.). The VFAs produced in the aforementioned mentioned process can be further used a substrate for synthesis of biopolymers (polyhydroxyalkanotes) in a closed loop approach.

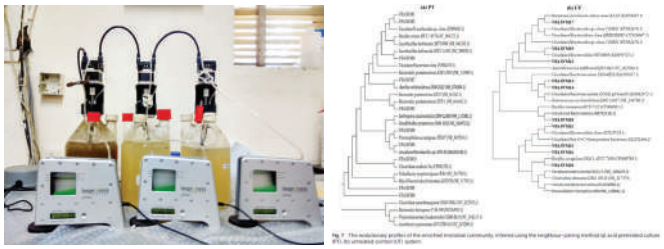


Fig 2: Acidogenic experiments for VFAs production with gas flow and schematic representation of the functional roles of the ten foremost operational taxonomic units identified from un-treated control and pre-treated microbial consortia towards VFA production

Polyhydroxyalkanoates (PHA): Polyhydroxyalkanoates (PHA) is a family of naturally-occurring biopolyesters synthesized by diverse microorganisms and has attracted significant research and commercial interests due to its biodegradability, diversity in chemical structure, biocompatibility and its feasibility to produce from renewable carbon resources. Although pure culture fermentation process offers high PHA content, the PHA produced is more expensive than conventional plastics

due to its high production cost, which includes substrate cost (50-60%), culture procurement, development, sterilization and maintenance. An attractive alternative to pure cultures and elevated substrate cost is the use of mixed cultures with acidogenic effluents (VFA), which eliminates the need of maintaining sterile conditions, thus lowering the energy and operating costs. PHA production was evaluated by varying the reactor microenvironment (aerobic and microaerophilic) and operating pH (6, 7 and 8) using aerobic consortia acquired from a full scale activated sludge. Maximum PHA production was observed in microaerophilic operation, compared to aerobic operation. Neutral pH showed better PHA synthesis than basic and acidic redox microenvironments. Biopolymer composition showed the presence of co-polymer, poly-(3-hydroxybutyrate-co-3-hydroxyvalerate). FISH showed the presence of phylum Proteobacteria, Acidobacteria and Firmicutes. These findings depict an economically and environmentally attractive method for optimizing mixed culture PHA production using acidogenic effluents and provide impetus for further process integrations.

Methanogenesis - Generation of Biogas and Biomanure

Dry Anaerobic Co-Digestion of Food Waste and Cattle Manure: Impact of Total Solids, Substrate Ratio and Thermal Pre-Treatment on Methane Yield and Quality of Biomanure: The objective of the present study is to assess the impact of TS concentration, substrate mixing ratio (co digestion) and thermal pretreatment on biogas production, methane yield, VS reduction (%) and quality of biomanure through dry anaerobic digestion (DAD) of food waste (FW) and cattle manure (CM). Results divulged that the optimum methane yield and biomanure of 0.18 and 0.21m3 CH4/(kg VS reduced) and 3.15 and 2.8 kg/kg waste was obtained from FW at TS of 25% and 30% at an HRT of 41 and 31 days respectively whereas it was 0.32 and 0.43m3 CH4/(kg VS reduced) and 2.2 and 1.15 kg/kg waste from pretreated FW at an HRT of 16 and 20 days correspondingly. Improvement of methane from 62 to 81% was obtained due to thermal pretreatment. The highest nutrient recovery in terms of N, P, K was found to be 5.14, 2.6 and 3.2 respectively.

Relative Evaluation of Micronutrients (Mn) and its Respective Nanoparticles (Nps) as Additives for the Enhanced Methane Generation: Effect of micro nutrients (MN) ($NiCl_2$, Fe_2O_3, $CoCl_2$, $(NH_4)_6Mo_7O_{24}$)) was compared with nanoparticles (NPs) of respective MN with cattle manure (CM) slurry in single and bi-phasic anaerobic digestion (AD) at a hydraulic residence time (HRT) of 20 days at a mesophilic temperature of 37 ± 2 ^oC for the generation of biogas with enhanced methane (70 - 80 %). Experiments were also carried out with CM slurry as control. During single phase AD, highest biogas production of 0.16 L/(g VS reduced) and 0.14 L/(g VS reduced) was obtained from Fe_3O_4 NPs and $CoCl_2$ MN respectively whereas in bi-phasic AD 0.3 L/(g VS reduced) and 0.2 L/(g VS reduced) was obtained from NiO NPs and $NiCl_2$ MN correspondingly. The results elucidated that $NiCl_2$ (either as MN or NPs) yielded highest biogas in comparison with either control or other MN and NPs.

Microbial Electrochemical Technology

Microbial Fuel Cells (MFC): Microbial fuel cell (MFC) is a bio-catalyzed electrochemical system which can directly convert chemical energy from an organic substrate to electrical energy through the artificially introduced electrodes (anode and cathode). The presence of electrode assembly induces the development of potential in the system that acts as a net driving force for bioelectrogenic activity. In order to enhance the power output, various strategies have been proposed in MFC. A prototype bio-catalyzed electrogenic system integrated with a biological treatment process (SBR-BET) in a multiphasic approach was evaluated to study specific function of anoxic condition on the electrogenic activity with focus on influence of DO and inter-electrode distance. Spatiometabolic function influenced by the electrode distance and DO showed diverse and specific bacterial enrichment. The DO levels in aqueous phase also influence the microbial diversity/profile. The major fraction of microbial community was from phylum proteobacteria (Alpha proteobacteria, Betaproteobacteria, Deltaproteobacteria and Gamma proteobacteria) followed by firmicutes belonging to the genera *Pseudomonas*, *Enterobacter*, *Bacilli* was observed with suspended biomass samples. Effect of various pretreatment methods was employed for selective enrichment of electrogenic bacteria from mixed culture. Iodopropane and heat-shock pretreatments showed enrichment of the exoelectrogenic bacteria from the mixed microbial community belonging to genera *Xanthomonas*, *Pseudomonas* and *Prevotella* while suppressing the growth of non-exoelectrons. Increased power output and coulombic efficiency was observed

in iodopropane and heat-shock MFC compared to untreated MFC. Pretreatment showed marked shifts in microbial community structure toward electrogenesis instead of fermentation. These results signify the role of iodopropane and heat pretreatments on enrichment of electrogenic bacteria for fuel cell application which helps to deliver higher and stable power outputs.

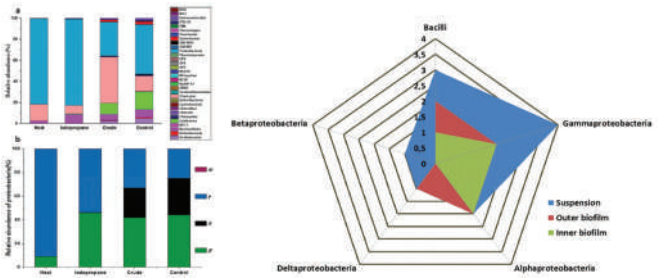


Fig. 3. (a) Relative abundance of phyla of proteobacteria in heat-shock, iodopropane, crude and control samples (b) Radar chart representing distribution of taxonomical classes of biocatalyst in samples.

A strategy to mimic nature and integrate anoxygenic and oxygenic photosynthesis was studied in two chambered MFC with major scope to provide self-sustainability. The synergetic interaction between oxygenic photosynthesis (microalgae; cathode) and anoxygenic photosynthesis (photosynthetic bacteria; anode) in hybrid biophotovoltaic cell facilitated multiple benefits viz., bioelectricity generation, biofuel production, CO_2 sequestration and wastewater treatment along with *in situ* generation of oxygen as terminal electron acceptor that facilitate the oxygen reduction reactions.

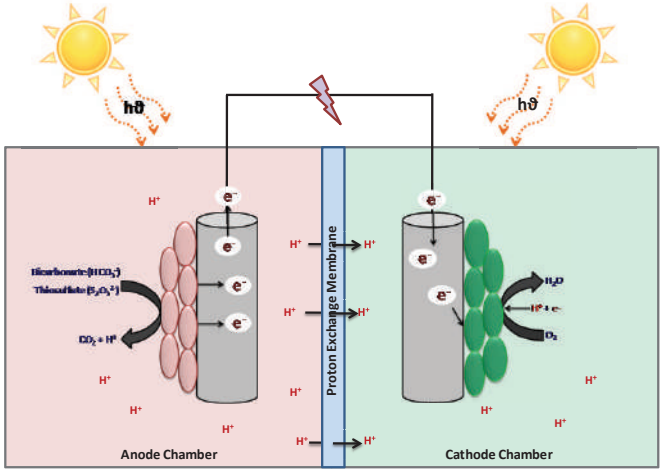


Fig. 4: Schematic representation of the hybrid Biophotovoltaic MFC cell

CO_2 to Chemicals using Bioelectrochemical System (BES): BES catalyzes CO_2 conversion to multi-carbon organic chemicals. Microbial community/biocatalyst promotes biochemical reactions under potential by utilizing CO_2 by homoacetogenic bacteria. Enriching acetogens and suppressing methanogenic bacteria for bioelectrochemical reduction of CO_2 towards synthesis of multi-carbon organic acids was evaluated towards maximizing acetic acid production. A polarized voltage of -0.8 V (vs Ag/AgCl (S)) was chronoamperometrically employed on working electrode (biocathode) of BES. Among the mixture of carboxylic acids synthesized, acetic acid concentration was high followed by butyric and propionic acids. Initially, CD was observed to be -250 mA/m^2 which successively progressed to a maximum of -720 mA/m^2. To elucidate the shifts/changes in bacterial community phylogenetic analysis was employed. Selectively enriching homoacetogenic bacteria was efficient in the development of a microbial community dominantly comprising of members belonging to Clostridiaecea. Study unraveled the potential of BES in not only synthesizing the multi-carbon organic chemicals but also minimizing the gaseous waste.

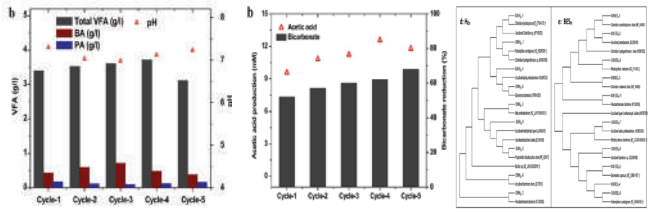


Fig. 5: Total VFA and acetic acid production from CO_2 reduction in BES and microbial community structure during operation

Bio-electrochemical Treatment (BET): Cathodic reduction reactions are significant in terms of bioelectrogenic activity as well as treatment. Influence of cathode material on electron accepting conditions during the treatment of recalcitrant pharmaceutical wastewater (PWW) was comparatively evaluated at different organic loads (3, 6, 9 and 15 g/l) in three BETs with different electrode materials viz., BET-SS (graphite (anode); stainless steel (SS; cathode)) and BET-G (graphite (anode/cathode)) in comparison to conventional anaerobic treatment (AnT) which lacks the electrode assembly. With the increase in organic loading rate and time of operation, increment in COD removal was observed in all the systems. Successive increment in COD removal efficiency was noticed at 6 g/l and 9 g/l. Efficient electron accepting conditions and high cathode potential in BET-G showed graphite as promising cathode material over SS for the treatment of PWW. The study provided insights into the interactions between anode and cathode electrode materials in BET reactors for treatment and energy generation. Opting

biocompatible electrode materials and their placement in a reactor can be considered as one of the essential elements in designing and operating BET reactors for the treatment of complex pharmaceutical wastewaters. The functional activity of anaerobic bacteria in the presence of an electrode as solid electron acceptor was evaluated in terms of azo dye based wastewater treatment with increasing dye concentrations (100, 200, 300 and 500 mg dye/l). BET documented positive influence on increasing dye concentration till 300 mg dye/l, which was reduced marginally thereafter. Presence of electrode assembly aided in development of bio-potential and contributed for enhanced dye degradation with simultaneous bioelectricity generation. The performance of BET at 500 mg/l was relatively low in comparison to operation at 300 mg/l. Hence, in order to enhance the dye degradation, TDS at varied concentration (1.25 g/l and 2.5 g/l) was supplemented to BET reactors and studied with two different dyes (acid and base dye). Acid dye degradation was relatively higher than base dye, and increased concentration of TDS aided in higher performance due to increased conductivity of anolyte. Multi-electrode bioelectrochemical treatment system (ME-BET; membrane less) consisting of six electrode assemblies (E1–E6) was designed and studied for the treatment of complex chemical-based wastewater with high salt concentration. The performance was compared with single electrode assembly BET reactor (SE-BET). Increased TDS and COD removal was observed in ME-BET (32%; 56%) compared to SE-BET (15%; 23%) as a result of *in situ* bio-potential from multi-electrodes through the oxidation of organic substrate in the wastewater. The study infers that designing of compact reactors with multiple electrodes in a single system enhances the anodic reactions and enable effective treatment of complex wastewaters with simultaneous power production.

Microbial Desalination Cell (MDC): The function of Microbial Electrochemical Systems (MES) was studied for simultaneous wastewater treatment, desalination and resource recovery. Two MDCs with abiotic cathode (MES-A) and algal biocathode (MES-B) were investigated with synthetic feed and saline water as proxy of typical real-field wastewater. Comparative anodic and cathodic efficiencies revealed a distinct disparity in both the MDCs when operated in open circuit (OC) and closed circuit (CC). The maximum open circuit voltage (OCV) read in MES-A and MES-B was about 700 mV and 600 mV respectively. Salinity and organic carbon removal efficiencies were noticed to be high during CC operation as 72% and 55% in MES-A and 60% and 63% in MES-B. These discrete observations evidenced the influence of microbial electrochemical induced ion-migration over cathodic reduction reactions (CRR). The study demonstrated notable difference in salinity removal and treatment efficiency observed with external circuit operation. Biofilm assisted electrochemical gradient was the driving force for ions migration. Cathodic product recovery at low salt concentration makes sense for future application in secondary wastewater treatment or as pre-treatment prior to reverse osmosis. A three-chambered microbial desalination cell (MDC) was specifically designed for salts removal from synthetic ground water and evaluated in different circuitry modes (open and closed) to assess the desalination efficiency, bioelectricity generation, resource recovery, substrate utilization and bioelectrokinetics. The closed circuit operation has showed efficient desalination efficiency (51.5%) and substrate utilization (70%). Owing to the effective electron transfer kinetics, closed circuit mode of operation showed effective desalination of the synthetic ground water with simultaneous power production (0.35 W/m^2). The design showed efficient inter-electrode communication by reducing the distance of separation and also maintained an appropriate surface area to volume ratio. MDC can function as sustainable and alternative solution for ground and surface water treatment with power productivity and resource recovery.

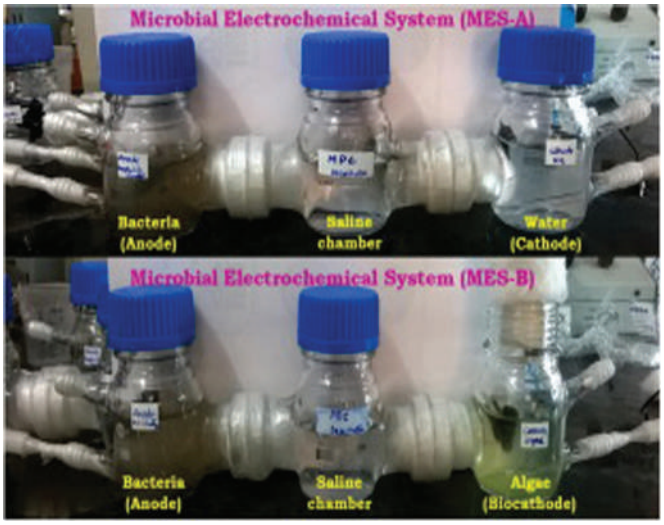


Fig. 6: Lab scale set-up of three chambered microbial desalination cell

Accelerated Anaerobic Composting of Water Hyacinth for the Production of Nutrient Rich Soil Conditioner:

*Eichhornia crassipes*solms commonly known as water hyacinth is a free-floating perennial hydrophyte belonging to the family Pontederiaceae. The leaves are broad, thick, glossy, and ovate and float above the water surface. They have long, spongy and bulbous stalks. The feathery, freely hanging roots are purple-black. It is one of the most productive plants on the earth and is considered the world's worst aquatic weed (Grodowitz, 1998). It tolerates annual temperatures ranging from 21°C to 27 °C and its pH tolerance is estimated at 5.0 to 7.5. The 'beautiful blue devil' water hyacinth, grows rapidly as a dense green mat over stagnant water bodies such as lakes, streams, ponds, waterways, ditches and backwaters and is recognized by its lavender flowers and shinning bright leaves. The plant is now considered as a serious threat to biodiversity. The environmental hazards associated with these plants degrade the water quality that leads to drastic changes in the plant and animal community, light and oxygen diffusion is severely curtailed by reduced water movement etc. (Gopal, 1987). To check its vigorous growth, control measures are required. One such method is its use as composting material as huge quantity of water hyacinth is available.

Fig. 7a: Steps of anaerobic composting of water hyacinth for production of nutrient rich soil

The technology has been successfully demonstrated at lab scale and it has been licensed to M/s KHAR Energy Optimizers, Hyderabad to setup a full scale facility. CSIR-IICT, M/s KHAR EO and GHMC jointly initiated a project for the removal of 12,000 tons of water hyacinth filled in Kapra lake, Hyderabad and its conversion to organic fertilizer. The same is being sold in the market as soil conditioner.

Fig. 7b: Anaerobic composting of water hyacinth at Kapra Lake

Purification of NDH-2 Protein and Elucidating its Role in Extracellular Electron Transport

In microbial electrochemical systems, transport of electrons from bacteria to an electrode is the key to its functioning. However, the role of several electron transport proteins, especially the membrane bound dehydrogenases which link cellular metabolism to extracellular electron transfer pathway is yet to be identified. This study focused on improvement of electrogenic performance of bioelectrochemical systems through genetic engineering of NADH dehydrogenase II (NDH-2) into *E.coli* cells. NDH-2 is a non-proton pumping

NADH dehydrogenase located in the inner membrane of several bacteria including, *Bacillus subtilis, Escherichia coli,* etc. Unlike NADH dehydrogenase I, NDH-2 is not impeded by a high protonmotive force thus helping in increase of metabolic flux and carbon utilization. NADH dehydrogenase II (*ndh2*) gene was heterologously expressed from *Bacillus subtilis* into *Escherichia coli* BL21 (DE3) to enhance electron flux and understand its role in bioelectrogenic activity. *E. coli* expressing NDH-2 has shown increased electron flux through EET which is evident from the 3 fold increase in current (1.9 µA) production when compared to parent strain (0.4 µA). Furthermore, expression of NDH-2 also resulted in increased biofilm formation which can be corroborated well with the decrease in charge transfer resistance for electron transfer from bacteria to electrode. NDH-2 expression has resulted in high catabolic activity of cell resulting in high NAD^+/NADH ratio indicating increased NADH oxidation. It was also found that NDH-2 strain can reduce metal oxides (Iron citrate) at a higher rate than parent strain suggesting increased electron flux thorough electron transport chain due to NADH dehydrogenase II activity. Purified Ndh2 was found to be ~42 kDa and has FAD as cofactor. This work demonstrates that the primary dehydrogenases like NADH dehydrogenases can be reengineered to increase the electron flux in EET pathways which can further enhance the microbial fuel cells performance.

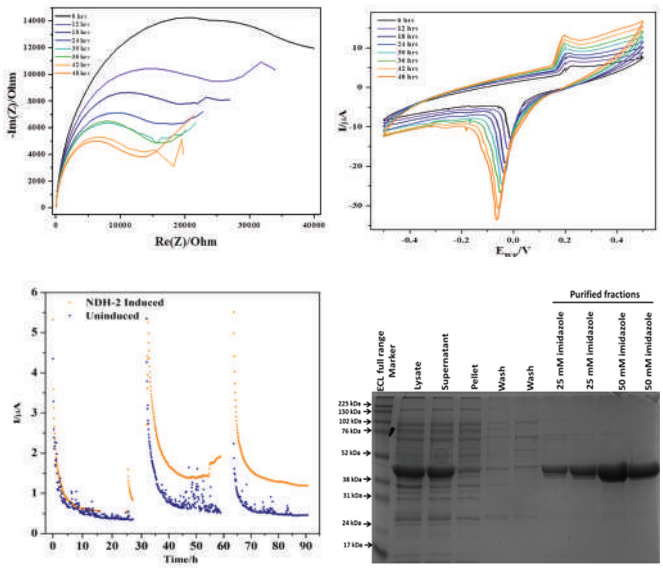


Fig. 8: Enhancement in bioelectrogenic activity for expression of NDH-2 protein can be seen in terms of (A) Electrochemical Impedance Spectroscopy [EIS] (B) Cyclic Voltammetry (C) Chronoamperometry (D) Purified fraction of NDH-2.

Gas purification - Biofilters

Gas phase Bio-Filter for the Removal of Triethylamine (TEA) from Air: Studies were carried out on packed bio-filter (PBF) of 2 L capacity for the removal of triethylamine (TEA) at inlet concentration in the range of 250–280 ppmV. Five different bacterial species viz; Aeromonas sp., Alcaligenes sp., Arthrobacter sp., Klebsiella sp., and Pseudomonas sp., were identified in PBF. It was observed that diethyl amine, ethylamine and nitrate were formed as metabolites during the degradation pathway.

Design and Development of Operating Strategies for the Abatement of Inorganic and Organic Gaseous Pollutants through Bio filters: Bio-degradation of ammonia (NH_3), hydrogen sulphide (H_2S), Triethylamine (TEA/$(CH_3CH_2)_3N$) and Ethanethiol (Ethylmercaptan/ CH_3CH_2SH) in biofilter with reference to the design, operation, optimization and microbial diversity was studied. Removal efficiency (RE) of 90-99 % was obtained in the laboratory scale biofilter which was loaded with nitrifying and anaerobic ammonia oxidizing (anammox) bacteria at an empty bed residence time (EBRT) of 20 s when the inlet ammonia (NH_3) concentration was about 250 parts per million by volume (ppmV). In another laboratory scale biofilter that was loaded with sulphur oxidizing bacteria (SOB), resulted in obtaining 98-100 % RE, at an EBRT of 50 s when the inlet hydrogen sulphide (H_2S) concentration at about 220 ppmV.

Laboratory scale studies were also carried out for the detoxification of air contaminated with triethylamine (inlet concentration of 250 to 280 ppmV) and CH_3CH_2SH (inlet concentration of 10 to 300 ppmV). It was learnt that both $(CH_3CH_2)_3N$ and CH_3CH_2SH could be detoxified to the level of 90-99 % (RE) with an EBRT of 20 s and 240 s respectively. Microbial species *viz*; *Aeromonas sps, Alcaligenessps, Arthrobacter sps, Klebsiella sp.* and *Pseudomonas sp.* were found to be responsible for bio-degradation of $(CH_3CH_2)_3N$. In the biofilter treating CH_3CH_2SH, microbial diversity analysis revealed that bedding material was enriched with bacterial species viz; *Enterobacter aerogenes, Thiobacillus denitrificans, Thiobacillus aquaesulis, Thiobacillus Q strain.*

Subsequent to this, studies were carried out on pilot scale biofilter for the simultaneous removal of H_2S and NH_3 from air. In this study, RE of 90-99 % was obtained when NH_3 and H_2S inlet concentrations were in the range of 200 to 210 ppmV with an EBRT of 55 s. Microbial diversity revealed that *Proteobacteria, Firmicutes* and *Acinetobacteria* were responsible for biodegradation

of NH_3 and H_2S in the polluted gaseous mixture and the metabolites formed were nitrite, nitrate, sulphate and sulfide which are innocuous products. A full scale biofilter for the purification of air emitted from the drum yard section (M/s SAA tannery) that is contaminated with NH_3 and H_2S was installed based on the pilot scale studies. RE of 99 % was obtained when NH_3 and H_2S inlet concentrations were 15 to 70 ppmV with an EBRT of 55 s.

Ammonia Odour Removal by Gas Phase Biofilter through Nitrification and Anammox Processes: Biofilter study was carried out on 1.2 L gas phase filter for the removal of ammonia at inlet concentration around 250 ppmV. Removal efficiency (RE) of biofilter remained in the range of 90–99% during the stable period of operation (80 days) at empty bed residence time (EBRT) of 20 s whereas RE of biofilter dropped to 65% when the EBRT was 10s. Metabolites were observed as ammoniacal nitrogen, hydrazine, nitrite and nitrate were formed during the degradation pathway in biofilter bedding material of a mixture of agricultural residue. It was inoculated with mixed microbial cultures of nitrifying and anammox bacteria were isolated from the active sludge of ETP of different industries.

Algal Research

Microalgae cultivation is attracting global interest due to its ability to produce diverse photosynthetic products including lipids, carbohydrates, protein and pigments. Mining of bio-based products from microalgae can create more sustainable economies. *Chlorella sp.* was isolated from lake receiving inflow of domestic wastewater rich in nutrient and organic loads. The *Chlorella* species partial ITS gene sequences was submitted to GenBank NCBI database (accession number KY350162). Microalgae cultivation by mixotrophic and heterotrophic modes were studied for enhancing the biomass and lipid productivities. Specific changes in fatty acid profile were observed with respect to trophic condition. Maximum biomass and relatively higher lipid content and higher carbohydrate content was observed with mixotrophic operation while heterotrophic mode showed higher protein and lipid contents. Fermented(acid rich) effluents (spent/diary wastewater) were employed for growth phase of mixotrophic mode cultivation. Mixotrophic cultivation documented higher biomass productivity. Higher total lipids was observed in mixotrophic mode of nutrition while higher neutral lipid was observed in heterotrophic mode of cultivation during stress phase. Enhancing microalgae biomass productivity through different abiotic and environmental factors optimization is crucial. Design of experimental (DOE) methodology using Taguchi orthogonal array (OA) was studied to evaluate the specific influence of eight important factors (light, pH, temperature, carbon concentration, nitrates, phosphates, magnesium ion concentration and carbon source) on the biomass production using three levels of factor (2^1 $X3^7$) variation with experimental matrix [L_{18}-18 experimental trails]. Substantial influence on biomass productivity was observed with carbon concentration followed by nitrates and light. Experimental condition (Light, pH-8.5, Temperature 25°C, Carbon concentration 10 g/l, nitrates 1.5 g/l, phosphates 0 g/l, magnesium 150 mg/l, glucose) showed maximum biomass growth (5.26 g/l) and good substrate degradation (63%, COD removal efficiency) contributing to carbohydrate production (257 mg/g biomass) which was further converted to lipids (20% Total lipid and 10% Neutral lipids). The effect of selected stress factors (pH, temperature, salinity, and carbon supplementation) on microalgal lipids and carbohydrate production during heterotrophic mode of operation was studied using design of experimental (DOE) methodology (Taguchi approach) with variation at four levels ($2^1 \times 4^4$). All the selected factors showed marked influence on the lipid production, whereas temperature and carbon concentration showed major influence on the carbohydrate synthesis. Interesting, relatively higher total lipid production (55% of DCW) was obtained from experimental condition (pH: 6; salinity: 1 g/l; temperature: 20°C; carbon concentration: 30 g/l). Relatively good neutral lipid fraction (13.6%) was observed with experimental condition (pH: 6; salinity: 5 g/l; temperature: 30°C; carbon concentration: 1 g/l). Good carbohydrate synthesis (262 mg/g biomass) was observed with experiment condition (pH: 4; salinity: 2 g/l; temperature: 30°C; carbon concentration: 15 g/l). Higher number of saturated fatty acids (C12:0 to C24:0) with biodiesel properties was specifically observed in both the above cases. Lab scale Flat Panel Photobioreactors (50 L X 4; 200 liters and Raceway Ponds (3000 L X 2 no) were constructed in CSIR-IICT for higher scale evaluation.

Fig. 9: Flat Panel and Raceway pond (3000 liters) systems for algal cultivation designed and developed at CSIR-IICT

Advanced Wastewater Treatment

Anaerobic systems for chemical/pharmaceutical effluent treatment, customized design for effluent/ sewage treatment plants, self-mixed anaerobic digester (SMAD), specialized consortia for enhanced treatment efficiency of chemical effluents, chemical disinfection treatment unit for liquid biomedical waste for decentralized application, *in situ* treatment of sewage in flow-through systems, compact and modular sewage treatment systems for decentralized applications, etc. are some of the key projects/technologies pursued. Integrated models for increasing the process efficiency for pharmaceutical and dye based wastewater treatment were evaluated. These waste management strategies for remediation and value addition are being designed in a coherent way to improve the process efficiency.

Designed Synthetic Consortium with embedded Wastewater Treatment Potential: Augmenting withexternal microorganisms with high degradation capability to biological unit operation can enhance the process efficiency significantly. In this study four different strains viz., P. otitidis, B. firmus, B. subtilis, and B. circulans were isolated, identified and further selected for the wastewater treatment. This was undertaken to explore the wastewater treatment potential of isolated strains and design of synthetic consortia based on carbon and nutrient removal. A comprehensive evaluation of both isolates and designed consortia with respect to substrate degradation efficiency, nutrients removal potential, enzymatic analysis, and bioelectrochemical behavior depicted the relative suitability of Microbiome to the complex wastewater system. The exploitation of such consortia can overcome the inefficiencies pre-existing with the biological wastewater treatment plants by acting as prospective candidates for bio-augmenting the native microflora. This study depicted the development of efficient consortia using lab isolated strains to improve the performance of wastewater treatment. Presence of interspecies bacterial strains and their synergetic relationship enhanced the wastewater treatment efficiency.

Energy-Positive Nitrogen Removal of Pharmaceutical Wastewater by Coupling Heterotrophic Nitrification and Electrotrophicdenitrification: The study cohesively assessed the aerobic nitrification treatment (ANT) and bioelectrochemical denitrification treatment (DNT) of real-field pharmaceutical wastewater. The ANT resulted in the removal of 73% ammonium and 78.5% organic carbon content. Subsequently, the outlet of ANT reactor was fed to DNT reactor and the relative influence of external circuitry was investigated. The DNT reactor operated with closed circuit mode (CCM) resulted in ~83% of nitrates and % ~61% of organic content removal even at low C/N ratio of 2.18 along with removal of other pollutant concentrations *viz.*, phosphates, sulfates and total dissolved salts. In this study, a sequential integration of both ANT and DNT processes exhibited high potential for self-sustained energy-positive nutrient removal.

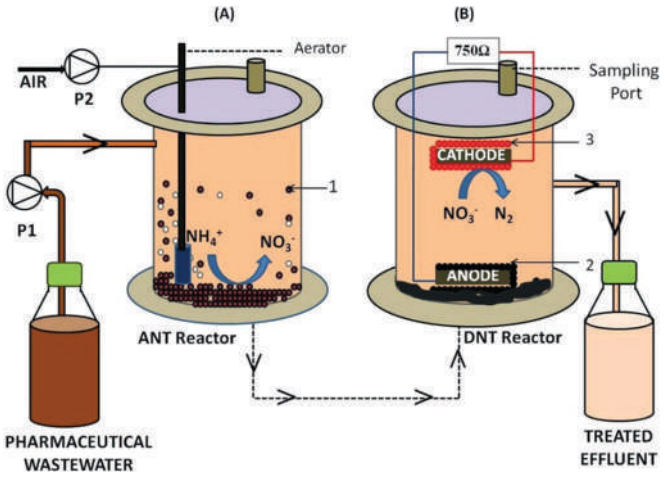


Fig. 10: Schematic view of (A) ANT (aerobic nitrification treatment) reactor and (B) DNT (denitrification treatment) reactor

Multi-Pollutant Treatment with Function of Dissolved Oxygen on Process Control: Biological processes are considered to be advantageous and sustainable in comparison to the physicochemical methods due to the cost effectiveness and eco-friendly nature for the treatment of microcrystalline cellulosic wastewater. The treatment efficiency of wastewater and its constituents in the biological process gets influenced by the presence of dissolved oxygen (DO) based on its role as terminal electron acceptor (TEA). The influence of DO on the biological wastewater treatment was evaluated using three different modes of periodic discontinuous batch systems (PDBR; sequential batch) operated with diverse microenvironments (aerobic, anoxic and anaerobic). The function of DO levels as TEA on the substrate degradation (COD removal) was quite evident with the varied PDBR operations. The higher COD removal was observed in PDBR-aerobic system [92%; 2.63 kg COD/ m3-day])] compared to PDBR-anoxic [71%; 2.12 kg COD/m3-day] and PDBR-anaerobic [63%; 1.81 kg COD/ m3-day] systems. The study signified that the redox microenvironments provided as TEA play a crucial role in the treatment.

Coupling of Aerobic/Anoxic and Bioelectrogenic Processes for Treatment of Pharmaceutical Wastewater: A sequential treatment strategy designed by integrating sequencing batch (anoxic/aerobic operation) reactor (SBR) with bio-electrochemical treatment (BET) was studied to enhance the remediation of real field pharmaceutical wastewater (PW). The study was executed in two steps in SBR with PW under anoxic and aerobic microenvironments. The performance of SBR and BET was comparatively assessed in terms of treatment and bio-electrochemical parameters. The self-induced bio-potential developed in BET system due to electrode assembly enabled higher organic and inorganic removal than SBR. The study concluded that the induction of bioelectrochemical potential aided in increased breakdown of complexity of wastewater in comparison to SBR. It provided a strategy of combining SBR as pretreatment step to BET process achieving the dual benefits of enhanced treatment efficiency and bioelectricity production.

Bio-Electrogenic Process for Bioelectricity Production and Cathodic Nutrient Recovery from Azo Dye Wastewater: This study attempted to understand the process of treating textile effluent using microbial electrochemical treatment (MET) processes in integration with periodic discontinuous batch reactor (PDBR). In this, the waste (effluent) obtained from one process was sequentially utilized for other to devour carbon present and recover nutrients for commercial purposes/farming aiming the process towards zero liquid discharge in the frame work of biorefinery. The results suggest that the use of MET can considerably degrade toxic pollutants and provides nitrate rich solution (biofertilizer). Utilization of recovered nutrients directly to farms without any energy intensive methods is reported in this communication. This study will help to comprehend few challenges and design effective integration strategy for complete mineralization of high strength wastewater and recovery of nitrates utilizing zero input energy methods and mixed culture as consortia. The experimental data illustrated the effective integration of PDBR and MET processes with regard to wastewater bioremediation, bioelectricity generation and recovery of nutrients. The integration of two different processes for azo dye treatment paves a way towards sustainability by addressing product recovery and bioremediation.

Integrated Ecotechnology Approach towards Treatment of Complex Wastewater with Simultaneous Bioenergy Production: Sequential integration of three stage diverse biological processes was studied by exploiting the individual process advantage towards enhanced treatment of microcrystalline cellulosic wastewater. A successful attempt to integrate sequence batch reactor (SBR) with bioelectrochemical treatment (BET) and finally with microalgae treatment was evaluated. Ecotechnology strategy used for this research provides options of maximizing extraction of various resources from the wastewater along with achieving enhanced treatment of wastewater. The advantage of sequentially integrating and maintaining a lineage between the three processes was exploited for enhanced treatment efficiency of wastewater used and product outcome in a biorefinery and circular format. The study resulted in providing a strategy of combining SBR as pretreatment step to BET process and finally polishing with microalgae cultivation achieving the benefits of enhanced wastewater treatment along with value addition.The integrated ecotechnology strategy exploited the advantages of the individual bioprocesses to overcome the individual limitations towards enhanced reduction of carbon footprints along with obtaining valuable products.

Ecological Engineered (Tri-Trophic) Treatment System: An ecologically engineered system was designed to have tri-trophic conditions embedded with electrode assembly for treatment of textile dye wastewater in *in-situ* and *in-vivo* conditions. EES was designed to mimic the functional role of natural aquatic ecosystems and evaluated their response to bio-electrogenic activity by cascadically interlinking three tanks with functionally diverse biota viz., floating macrophytes (Tank 1), submerged plants (Tank 2) and filter feeders (fish and snails) (Tank 3). Electrogenic microenvironment was created by placing the electrodes in plant rhizosphere. Anaerobic/anoxic microenvironments facilitate the reduction of the azo dye compound, and break down the dye molecules and aerobic microenvironment that direct the oxidation of carbon compounds and nitrification. Free-floating plants and filter feeders is intended to remove TSS and color effectively. The placement of electrodes and plant root zone enables higher redox reactions towards dye/substrate degradation, which in turn is influenced by co-substrate utilization. ETWS treatment process not only decolorizes the azo dye but also removes its toxic and mutagenic components.

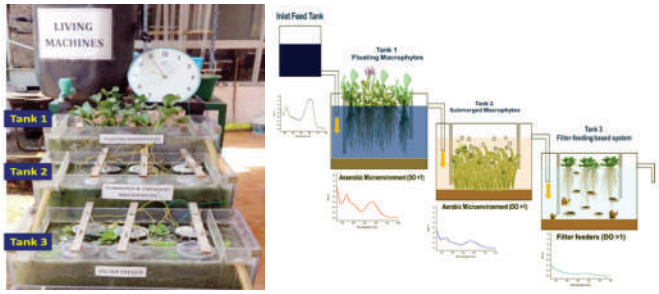


Fig.11: Lab Scale Ecological Engineering System with Schematic representation of EES components designed by CSIR-IICT

Microalgae Treatment of Pharmaceutical Wastewater: Microalgae are capable to grow in nutrient-rich wastewaters thus contributing to reducing the carbon and nutrients by heterotrophic/mixotrophic nutritional mode coupled with the production of biomass. Microalgae based treatment was designed and studied to polish biologically treated pharmaceutical wastewater under mixotrophic mode of operation. Good COD and nitrates removal of wastewater along with the maximum utilization of phosphates and sulphates was observed. Presence of saturated and unsaturated fatty acids with varying ratios indicates favorable profile towards biodiesel production. The biomass growth and fatty acid profile support the feasibility of integrating microalgae cultivation with advanced biological treatment process. The integration process offers multiple benefits to both bioenergy and environment sector.

Liquid Waste Treatment – Landfill Leachate

Biological Process for the Simultaneous Removal of Ammoniacal Nitrogen and COD from Industrial Wastewaters

Pilot scale process for simultaneous removal of ammoniacal nitrogen and COD from industrial wastewaters was developed which could be demonstrated for industrial applications Commercial industries could utilize this technology for the safe disposal of wastewaters into the sewers as per the standard disposal limits of state PCB which is 50 ppm for ammoniacal nitrogen. Society is greatly benefitted as the water bodies are safe guarded from pollution and eutrophication.

Evaluation of Single and Two Stage Anaerobic Digestion of Landfill Leachate: Effect of pH and Initial Organic Loading Rate on Volatile Fatty Acid and Biogas Production

Landfill leachate, a type of high strength organic liquid could be potentially reclaimed for bioenergy and value-added products generation. This paper aims to evaluate the impact of parameters such as pH and varying initial organic loading (IOL) in terms of COD on VFA production, methane yield and COD removal efficiencies during single and two stage anaerobic digestion (AD). Another objective is to assess the type of fermentation based on pH variance with respect to IOL. It was observed that dominant fraction of VFA at acidic pH 5.5 was acetic acid due to mixed acid type fermentation whereas at weak acidic and alkaline pH of 5.5 -6 and 10-11, it was butyric acid at an IOL of 48 g/L. The trend was as IOL increased, VFA production increased with a decline in pH due to rapid acidification during acidogenesis whereas methane yield decreased during single and two stage AD (methanogenesis).

Biohydrogen Production from Waste- Pilot Scale Operation

Acidogenesis is a versatile bioprocess that has the potential to play an important role for the transformation of waste into primary fermented biobased products which includes biohydrogen (H_2) and fatty acids. Biohydrogen pilot plant (10 m^3) reactor was designed, installed and operated at CSIR-IICT in 2017 with the financial support from MNRE (Fig 11). The design is unique and has process flexibility to convert diverse types of bio-degradable waste/wastewater to biohydrogen. The main acidogenic bioreactor (AB: 10 m^3) is connected with multiple units viz inoculum tank (ICT: 0.2 m^3: SS316L), biohydrogen holding tank (BHT: 0.2 m^3: SS316L), buffer tank (BT: 2 m^3: SS316L), water storage tank (WST: 2 m^3) and acid/base tanks (a/b: 0.05 m^3). Non-flammable pumps were fixed at different positions for product mixing (recirculation capacity: 5 m^3/h), inoculum mixing (magnetic bottom agitator) and transfer of inoculum to main bioreactor (screw pump) and for water supply (1HP) to AB, BT, ICT and WST. For online monitoring and controlling of the bioprocess, different probes like pH, temperature and level indicators, and gas flow meters were fixed in the appropriate units. AB was packed with high surface area (~750 m^2/m) polymer material as support for the growth of hydrogen producing acidogenic biocatalyst upto 50% of volume. Three flanged heaters were incorporated in IT to apply pretreatment to the mixed microbial culture towards selective enrichment of biohydrogen producing microbes at specific temperature before transferring in the AB. A gas flow meter with a gas measuring range of

100-850 lit/min is connected between AB and BHT. All the units were interconnected with SS316L pipelines and also facilitated with appropriate valves and connectors to collect the samples and regulate the flow during the bioprocess. An ignition in the automated flaring unit on the top of the roof finally flares out the gas when pressurized beyond 4bar in BHT. The bioreactor was operated with selectively enriched microbial culture with food waste and distillery wastewater. Food waste at 50 g COD/L organic load showed 54,000 L of H_2/day with 46% conversion efficiency. Biohydrogen is a green fuel with a high energy content (122 kJ/g). Along with biohydrogen, waste remediation is an added advantage with this technology.

Fig. 12: A 10 m^3 pilot plant for the production of biohydrogen from waste installed and operated at CSIR-IICT

Waste Biorefinery Platform-Pilot Plant Facility

CSIR-IICT has recently designed and constructed an innovative pilot scale waste biorefinery facility (Fig. 2). To the make the acidogenesis process sustainable and more economic it was integrated with waste biorefinery facility to harness a spectrum of biobased products from fatty acids rich acidogenic effluent. This biorefinery facility can sustainably convert acidogenic effluent to multiple biobased products with simultaneous wastewater treatment by advanced living machines. The first bioprocess in the integrated biorefinery is methanogenesis where acidogenic effluent (a mixture of C2, C3, and C4) will be converted to biomethane by methanogens. The resulting effluent from methane bioreactor is diverted to photosynthesis unit for the cultivation of algal biomass followed by bioelectrochemical treatment (BET; Bio-electrogenesis). The photosynthesis unit and microbial electrochemical unit efficiently reduce the carbon load in the wastewater, which is finally passed through an advanced ecological engineered system (EES). EES was designed to mimic the natural cleansing functions of wetlands to bring about wastewater treatment. EES system consisted of three tanks containing diverse biota viz., aquatic macrophytes, submerged plants, emergent plants and filter feeders connected in series. The waste biorefinery unit finally reduces down the COD of the water in the range of 20-40 mg COD/L. The treated water is again re-circulated to water storage tank to be used for biohydrogen production. This advanced waste biorefinery is a potential solution to address, energy and clean water in a sustainable way preserving the environment and ecosystems. Biorefinery offers a sustainable green option to utilize waste through decarbonization pathways to produce marketable biobased products analogous to the petro-based refinery and therefore supports bioeconomy in a circular loop approach.

Fig. 13: Waste Biorefinery: Integration of multiple bioprocesses (anaerobic digestion, algal cultivation, anoxic system, bioelectrogenic system, Ecologically Engineered system) with biohydrogen production for multi-product recovery

Biogas Plants - High Rate Biomethanation of Organic Solid Waste For the Generation of Biogas and Biomanure

Operational Strategy of High Rate Anaerobic Digester with Mixed Organic Wastes: Effect of Co-Digestion on Biogas Yield at Full Scale: This research work is aimed at providing an economically feasible solution

for the farmers to exploit the mixed organic wastes (MOW) as resources for the generation of biogas based electrical power and utilize the same for irrigation purpose to reduce the dependence on electricity board. A full scale biomethanation plant has been installed based on anaerobic gas lift reactor (AGR) technology to analyze, understand the operational parameters of anaerobic digestion and assess the performance of a high rate biomethanation plant by co digesting the MOW such as such as poultry litter (PL), cattle manure (CM) and napier grass (NG) at ambient temperature. The biomethanation plant was incorporated with inline pre and post processing unit assembly. The plant was fed with 1000 kg of MOW per day having 250kg of total solids, about 178 - 200 kg of volatile solids and operated continuously for 52 weeks under ambient temperature. Electrical power generated (84.5 - 104 kWh/day) from biogas (65 to 80 m3/day) containing methane (40 to 48 m3/day) was used for operating the water pumps for agricultural purpose and the digestate (115 - 130 kg/day) was exploited as organic manure for growing crops in the same field. Napier grass was grown in the same land and other feed stocks were procured from the nearby area at the cost of $10 to $15 per ton. Around 6 acres of land was being cultivated using the biogas based power generated from the MOW that was being used for growing vegetables and maize.

Biogas Plant Installation for the Treatment of One Ton Mixed Organic Waste Per Day: As an initiative, M/s Ahuja Engineering Services Pvt. Ltd, (AES), Hyderabad has installed its first plant based on AGR Technology at PeddaShivanoor, Chegunta Mandal near Hyderabad for the generation of biogas based power and bio-manure from mixed organic waste (poultry litter, cattle manure, vegetable waste). The plant was operated for a period of 3 years i.e. January 2013 to December 2015, and demonstrates the complete process. 80 m^3 of biogas and 200 kg of biomanure per day are produced from one ton of mixed organic waste. 89 kWh of electricity is generated from the biogas produced. The biogas based power is used for the operation of agricultural pumps. The digestate is being applied to the surrounding fields as bio-manure. Biogas based power plants would ensure a cleaner environment and provide long-term financial benefits to farm owners by offsetting their power requirements. Safe & timely waste disposal and saving energy costs will improve the profitability of the complete poultry industry.

Output from the Plant: POULTRY LITTER TO POWER

- Safe and secured treatment
- Generation of 100 m^3 biogas per 1.5 ton of poultry litter
- Biogas can be used for brooding to replace the LPG
- Biogas can be used for generating power in farm
- Digested slurry could be used for fish ponds
- Digested solid & liquid slurry can be used as organic fertilizer
- Conversion of biogas to electricity to power the farms
- Power in take from electricity board can be reduced
- Power generation from diesel (costlier option) can be avoided
- Saving grid and diesel electricity

Reference Biogas Plants Based on AGR Technology for the Treatment of Food Waste Food Waste (Cooked and Uncooked) as Feedstock

Currently, food waste across our cities and towns is rapidly increasing along with human population. Cooked and uncooked food waste collected from households, restaurants, institutional canteens etc. constitutes the food waste and it is known as organic fraction of MSW (OFMSW). Instead of land filling, OFMSW could be purposefully utilized for the generation of renewable energy (biogas) in order to save the land as well as conserve conventional energy. Besides this, fruit and vegetable wastes are produced in large quantities in markets, which is a source of nuisance in municipal landfills because of their high biodegradability. In India, most of the MSW related issues would be settled if the OFMSW could be used purposefully in a semi-decentralized manner. Food waste (cooked and uncooked) due to its nature of high biodegradability and high moisture content (75-90%) is considered to be a good substrate for recovery of bio-energy through anaerobic digestion process. CSIR-IICT and AES are collectively exploring the opportunities associated with food waste-to-energy in large kitchens, hotels, hostels, canteens, and temples etc where at least three to four LPG cylinders per day are used for cooking. Distributive biogas plants set-up near these kitchens can act as the primary energy source for production of LPG equivalent fuel. Waste disposal at source is also an important result of this process.

Beneficiary and Waste Generation Source: The Akshaya Patra Foundation (TAPF) is an NGO operates under the aegis of ISKON serves mid-day meals to children in school. There are approximately 40 large-scale kitchens set up by Akshaya Patra Foundation across the country. At each kitchen approximately meal for one lakh children is prepared every day and distributed to the schools in and around 50 square kilometer. Previously TAPF is facing the problem of disposing solid and liquid waste generated at their kitchens. The food waste generated at these kitchens is highly biodegradable and results in putrefication rapidly. This could damage the quality of food prepared in the kitchen. As a solution to the waste disposal problem, CSIR-IICT and M/s AESPL has installed its second biogas plant at Torangallu, Bellary, Karnataka based on IICT's AGR Technology. Upon successful commissioning of the plant and the intangible benefits accrued by the beneficiary, TAPF has given consent to install similar biogas plants at other kitchens of TAPF.

Biogas Plant at TAPF Torangallu, Bellary, (Karnataka): M/s AESPL Hyderabad has installed biogas plant at TAPF at Bellary, Karnataka for the generation of biogas and bio-manure from food waste generated at that kitchen. The plant is based on "AGR TECHNOLOGY" and the aim is to serve as a sustainable technology to provide a scientific waste disposal system to the kitchens as well as utilize the clean fuel (biogas) produced as a cooking fuel to replace LPG consumption. The plants run like a closed-loop system where the kitchen's waste is converted into biogas and fertilizer on day-to-day basis. Approximately 1000 kg of food waste (400 kg cooked food waste, 600 kg uncooked food waste) and 2000 L of organic wastewater (rice water/Ganji) is used for the generation of 130 to 140 m^3 of biogas per day to replace 55 to 60 kg of LPG at each plant. The plant is operational since June 2015.

Fig. 15: Biomethanation Process Flow

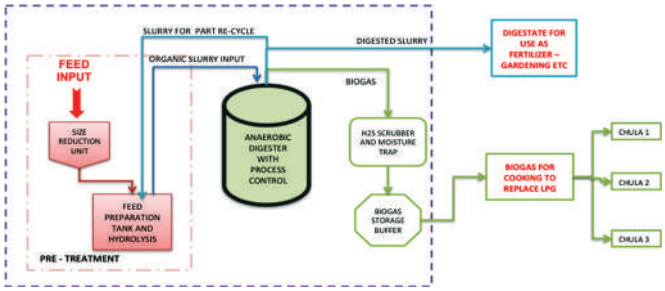


Fig. 16: Full scale biogas plant for the treatment of food waste based on AGR at Bellary

Biogas Plants at TAPF Hubli (Karnataka): The third biogas plant based on AGR Technology has been installed and commissioned by AESPL under the supervision of CSIR-IICT. Approximately 1000 kg of food waste (400 kg cooked food waste, 600 kg uncooked food waste) and 2000 L of organic wastewater (rice water/Ganji) is used for the generation of 130 to 140 m^3 of biogas per day to replace 55 to 60 kg of LPG at each plant. The plant is operational since June 2016.

Biogas Plants at TAPF Ahmadabad, Surat and Bhavnagar (Gujarat): Fourth, Fifth and sixth similar biogas plants based on AGR Technology have been installed and commissioned at the kitchens of TAPF at Ahmadabad, Surat and Bhavnagar (Gujarat) by AESPL under the technical guidance of CSIR-IICT. Few more installations based on the AGR technology have been executed and the list of installations is given in Table.1.

Fig. 17: Full scale biogas plant for the treatment of food waste based on AGR at Hubli, Ahmadabad, Surat and Bhavnagar

Output from Full Scale Biogas Plants installed at the kitchen's of TAPF

- One ton of food waste produces about 120 - 140 m^3 of biogas, which could replace around 55 - 60 kg of LPG on a daily basis.
- Waste generated in kitchen is being sent back to kitchen but in the form of renewable energy employing AGR technology.
- Bio-manure is used as a soil conditioner in the fields/ landscape area.
- Decentralized treatment of food waste
- Generation of clean fuel in the form of biogas
- Saving waste disposal cost
- Replacement of LPG with biogas for cooking
- Reduction of GHG emissions to atmosphere

Biogas Plant at M/s HIMSWL, Jawahar Nagar MSW Dump Yard, Hyderabad: M/s Ahuja Engineering, Services Pvt.ltd, Secunderabad as an executing organization, CSIR-IICT, Hyderabad as Technology partner and M/s HIMSWL, Hyderabad as beneficiary jointly undertook a project entitled "**High Rate Biomethanation of Organic Waste for Generation of Power for Off-Grid Applications**" sponsored by Indo-US Science and Technology Forum, PACESetter Fund. The formal award ceremony of the project was held on 27th of May 2016 at N.Delhi. The ambassador of USA to India Mr.Richard R. Verma and Secretary, MNRE, Dr. Upendra Tripathy awarded the project to IICT consortium. The aim of this project is Generation of Biogas Based Power From 5 – 6 TPD of Organic Fraction of MSW using the "Anaerobic Gas Lift Reactor (AGR) Technology" developed by CSIR-IICT. The project is ongoing and the biogas plant for the treatment of 5 – 6 TPD of OFMSW for the generation of power is installed and commissioned at M/s HIMSWL, Jawahar Nagar site, Hyderabad.

Output from the Biogas Plant

- Biogas based power (300 kWh/day)
- Biogas for cooking applications (35 – 40 m^3/day which is equivalent to 14.2 kg LPG/day)
- Biomanure (750 – 800 kg/day)

Fig. 18: Pilot plants established at various locations in India

5 TPD biomethanation plant based on AGR at Jawahar Nagar, Hyderabad

250 kg/day biomethanation plant at CSIR-IICT

Biogas plant (250 kg/day) installed at CSIR-IICT, Hyderabad

Biogas plant for the treatment of 3,000 – 5,000 kg/day of organic fraction of MSW, installed at Jawahar Nagar, MSW Processing Site, Hyderabad

Biogas plant at odhisha for the treatment of 250 kg/day of food waste

Biogas plant at CapGemini, Hyderabad for the treatment of 250 kg/day of food waste

Biogas plant at Kurnool Vegetable Market Yard, Kurnool for the treatment of 500 kg/day of market and vegetable waste

Table.1: List of Biogas Plants based on AGR Technology Installed at Various Places in India

S. No	Place of Installation	Capacity of the plant	Type of substrate	Biogas generation (m^3/day)	Biogas utilization	Biomanure generation (kg/day)	Foot print area required (m^2)	Status of the plant
1.	Bellary (Karnataka)	1000 kg/ day	Food waste	110 - 140	LPG replacement	100 - 150	55	Working successfully
2.	Hubli (Karnataka)	1000 kg/ day	Food waste	110 - 140	LPG replacement	100 - 150	55	Working successfully
3.	Ahmadabad (Gujarat)	1000 kg/ day	Food waste	110 - 140	LPG replacement	100 - 150	55	Working successfully
4.	Surat (Gujarat)	1000 kg/ day	Food waste	110 - 140	LPG replacement	100 - 150	55	Working successfully
5.	Bhavnagar (Gujarat)	500 kg/ day	Food waste	55 - 70	LPG replacement	50 - 70	32	Working successfully
6.	CSIR-IICT, Hyderabad	250 kg/ day	Food waste	25 - 40	LPG replacement	20 - 30	18	Working successfully
7.	Vrindavan (UP)	1000 kg/ day	Food waste	110 - 140	LPG replacement	100 - 150	55	Working successfully
8.	Rourkela (Odisha)	500 kg/ day	Food waste	55 - 70	LPG replacement	50 - 70	32	Working successfully
9.	Jawahar Nagar (Hyderabad)	3,000 – 5,000 kg/ day	Organic fraction of MSW	150 - 250	Electricity generation	300 - 50	550	Working successfully
10.	Dr. B. R Ambedkar vegetable market yard, Bowenpally, Hyderabad	10,000 kg/day	Vegetable and market waste	NA	NA	NA	NA	Under construction
11.	Vegetable market yard (Kurnool)	500 kg/ day	Vegetable and market waste	55 - 70	LPG replacement	50 - 70	32	Working successfully
12.	Capgemini (Hyderabad)	300 kg/ day	Food waste	NA	NA	NA	NA	Working successfully

Gas purification

Biofilter for Odour Control

- Developed BIOFILTER technology which is being licensed to all the users so that industry could benefit from this technology. This would fetch good amount of revenue and foreign exchange to CSIR-IICT and India as well.
- The scope of the Biofilter technology is being widened with compounds such as mercaptans, try ethyl amine etc.
- Occupational health greatly improves due to the implementation of this technology as workers are presently suffering from odour related health issues.
- In the 12th Plan network project, pilot scale BIOFILTER Technology was developed for the treatment of gaseous emissions having amines, mercaptans, H_2S, NH_3 etc.,. which is applicable for chemical and allied sectors. We have transferred this technology to M/s Ramky Enviro Engineers Limited (REEL) for the deodorization of off gases from compost plant at Jawahar Nagar, Hyderabad. We are also negotiating with various industries for the transfer BIOFILTER Technology.
- A 28 m3 biofilter design is given to M/s Kondapally Enviro Tech Private Limited, Vijayawada for the installation same at Common Effluent Treatment Plant (CETP) for the abatement of odour causing off gases emanating from ETP.

- A 17m3 biofilter is being fabricated for its installation at M/s Fleming Laboratories for the abatement of odour causing off gases emanating from bulk drug unit.

Influence of Inlet Concentration of Ethanethiol on Empty Bed Residence Time in Gas Phase Biofilter: Ethanethiol is a toxic organic pollutant with a low odour threshold and its density is more than air that makes it more vulnerable for causing health related issues. In the present work, biological degradation of ethanethiol using mixed microorganisms in gas phase biofilter was studied. Microbial consortia isolated from activated sludge plant of petroleum refinery was enriched and immobilized on biofilter bedding material. Biological waste gas treatment represents a new treatment alternative. CLRI, Chennai and IICT, Hyderabad developed a novel bio-filter process for removal of odor causing compounds in Tanneries under zero emission research initiative (ZERI) with the financial assistance of CSIR, Government of India. A full-scale modular (Three modules of 4.5 m^3 each) bio-filter was installed in SAA Tannery, Erode, Tamil Nadu for the removal of NH_3 and H_2S from drum yard section of the tannery.

Full scale Bio-filter for odour removal in Tannery

Impact on Industry

- Industry is very much eager to adopt this technology to solve odour problem
- Bio-filter for the removal of odour causing gases in a tannery was indigenously developed and patented and full-scale plant designed. Full-scale plant was erected at M/s Abdul Aziz Tannery, Eroad, TN and is working satisfactorily since August 2012.
- Commercialization of Bio-filter Technology for the removal of odour from CETP off gases is being erected at M/s Kondapally Envirotech Private Limited, Vijayawada.
- Commercialization of Bio-filter Technology for the removal of odour and VOC from chemical and allied sectors and a 17 m3 biofilter is under installation at M/s Flemings Laboratory.
- A consultancy project is being carried out for M/s Ramky Enviro Engineers Limited (REEL), Hyderabad for the deodorization of off gases from compost yard at Jawahar Nagar, Hyderabad with the knowledge generated from the biofilter project.
- A biofilter of 17 m3 is under commissioning at M/s Flemings laboratories private limited, Hyderabad for the purification of odorous gases.

Deodourization of Off Gases Emanating from Compost Yard at M/s HIMSWL: A new bacterial strain named as AGR/IICT/4 was isolated from a gas phase biofilter treating triethylamine (TEA) and it was used for understanding the removal pattern of TEA in designed synthetic and industrial wastewater. The strain was identified as *Pseudomonas aeruginosa* based on biochemical and 16S rRNA gene sequence analysis. Parameters affecting biodegradation of TEA were selected based on conventional approach as well as statistical analysis (full factorial design and central composite design model). It was observed that initial TEA concentration, temperature and pH are the key controlling factors and *Pseudomonas aeruginosa,* could completely degrade 300 mg/L of TEA to ammonia in 60 hr at a pH of 7.5 and temperature of 31°C. The strain could also effectively degrade diethyl amine, ethylamine and amine to ammonia as final product, which were identified as intermediates in aqueous medium. Maximum mono oxygenase activity of 315.29 U/mg was observed under optimized conditions. Currently, waste from the Hyderabad city is dumped at the 330-acre Jawaharnagar dump yard and treated by Ramky, a private firm. Though, a treatment plant is running, complaints about a foul smell emanating from the site haven't ceased. Citizens complain of the stench reaching a radius of 7 to 8 kms around Jawaharnagar. Ramky-HIMSWM approached CSIR-IICT to conduct experiments to control odour control (Fig. 27). In this regard supplied 10 lit of microbial culture, every week for 6 months. The experiments were conducted at site and measuring the deodorization potential of microbial culture. Experiments were shows good results in respective of odour abatement.

Biogas Plants

Establishment of 3 - 5 Tons/Day, Biogas Plant based on CSIR-IICT AGR Technology at Hyderabad Integrated MSW Limited (Hyderabad): Indo-US Science and Technology Forum (IUSTF) under Indo-US PACESetter Fund Awarded a project entitled "High rate biomethanation of organic waste for generation of power for off-grid applications" to the consortium comprising CSIR-Indian Institute of Chemical Technology (CSIR-IICT), Hyderabad, KL University - Vaddeswaram (Vijayawada,AP) and M/s Ahuja Engineering Services Pvt. Ltd, Secunderabad, with a total grant of Rs.192 lakhs. The aim of the project is to scale up "Anaerobic Gas-lift Reactor (AGR) Technology" developed by CSIR-IICT and establish a 3 - 5 tons/day (TPD) Bio-digester Plant for the generation of biogas & power from organic waste. The PACESetter fund was awarded to the Consortium after screening about 140 proposals. In the formal Award ceremony held on May 27, 2016 at New Delhi, the ambassador of USA to India and Dr. Upendra Tripathy Secretary, MNRE, awarded the project to the CSIR-IICT consortium.

A Bhumi Puja Ceremony was held on January 26, 2017 to launch the erection & commission of the plant. This program is taken up as a part of Prime Minister Swatch Bharat Program. The biogas plant has been commissioned in June 2018 and is in successful operation.

Installation of 10Ton/day of Organic Fraction of MSW and 2.5 m^3/day of Leachate for the Generation of Biogas and Biomanure based on CSIR-IICT AGR Technology at Dr. B. R Ambedkar Vegetable Market, Bowenpally (Hyderabad): Department of biotechnology (DBT) has awarded a project entitled "High rate biomethanation of organic fraction of MSW for the generation of biogas and biomanure for decentralized applications. CSIR-IICT as the technology provider is executing the project in association with greater Hyderabad municipal corporation (GHMC) for the installation of 10 ton/day of organic fraction of MSW and 2.5 m3/day of landfill

leachate for the concomitant treatment and generation of biogas and biomanure. This biomethanation plant serves as the demonstration plant to various stakeholders so that the same can be replicated at various municipalities and waste generation sources. This enables in the reduction of the transportation and waste handling costs by the municipalities. Apart from this there are numerous tangible and intangible benefits associated with the installation of this biogas plant. The plant is under installation and prior to that, the site at Bowenpally vegetable market yard and the raw material assessment was done.

Global Change and Climate Programmes: ISRO under Geosphere and biosphere Programme (GBP) sponsored a project on AT-CTM (atmospheric trace gases chemistry, transport and modelling) to CSIR-IICT. CSIR-IICT in collaboration with TIFR has set up an environmental observatory at TIFR-BF to monitor the levels of ozone and its precursor trace gases like NO_x, CO and SO_2 in the atmosphere. The observatory is also equipped with pyranometer to measure the total solar radiation and to study the role of photochemical oxidation of these trace gases in the formation of ozone.

CENTRE FOR LIPID SCIENCE & TECHNOLOGY

Centre for Lipid Science and Technology is recognized nationally and internationally in the area of lipid research with major thrust to vegetable oils and their allied products. The vision and goals of the lipids group mainly pertain to newer processing methodologies for vegetable oils, nutraceuticals, specialty oleochemicals, biolubricants and biodiesel. During 11th Five Year Plan Period, CSIR-IICT established "Centre for Lipid Research" with CSIR special financial grant consisting of with three specialized facilities for Vegetable Oils, Biodiesel and Lubricants, and one Process Equipment Pilot Plant on par with the International Standards. The centre is carrying out high quality research in several thrust areas which are relevant and contemporary to the needs of the Indian vegetable oil industry. During this period, Food Safety and Standards Authority of India (FSSAI) has recognized the Centre for Lipid Research as National Referral Food Testing Laboratory in the area of oils and fats. The Centre for Lipid Research organizes business meets, international and national conferences, refresher courses for the benefit of the vegetable oil and allied industry at regular intervals.

Dr. S. Chandrasekhar, Director, CSIR-IICT with participants and Faculty (2017)

Centre for Lipid Science and Technology organizes Refresher Course on "Processing and Analytical Methodologies of Oils & Fats" every year. The uniqueness of the course is that it is designed for the representatives of industries, R & D institutions and academia with both theoretical discussions and practical demonstrations and 34 and 21 participants attended this refresher course during March 22-24, 2017 and March 19-21, 2018 respectively. This course is divided into lectures on processing and analysis and demonstrations of different spectral and chromatographic analytical techniques and chemical analysis related to oils and fats. This help the participants from industry as well as R & D institutions to have a better understanding on the subject and to maintain high quality standards of the products available in the market. CSIR-IICT is conducting this course for more than ten years and till now trained around 325 participants primarily from Oil & Fats industry and National Food Laboratories. This refresher course has become very popular and created significant impact on this particular industry.

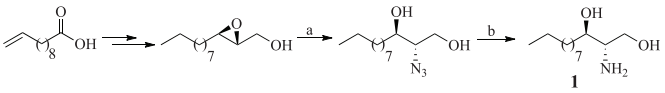
Participants with Course Faculties, Dr S Y Mhasker, Dr RBN Prasad and Dr K Ravikumar (2018)

Dr S Y Mhasker, the Chief Technology Officer of Marico Limited, Mumbai was the Chief Guest of the inaugural function in 2018 and in his inaugural address he thanked CSIR-IICT for organizing such course. He also explained the importance of such courses and in the present scenario of Food safety and Standards how the industries should align themselves with the latest developments. The majority of the participants were from leading oils and fats processing industries and R & D institutions and this helped them to have a better understanding on the subject and to maintain high quality standards of the products available in the market.

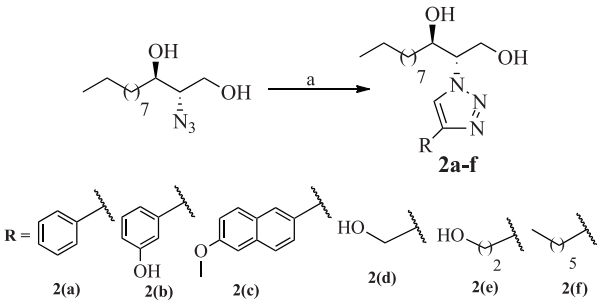
BASIC RESEARCH

Design and Synthesis of Short-chain Sphinganine and its 1,2,3-Triazole Analogs as Potential Antimicrobial and Anti-biofilm Agents

A conceptual synthetic approach of short-chain sphinganine **1** and a small library of 1,2,3-triazole analogs of C_{12}-sphinganine **2a-f** has been accomplished from commercially available and inexpensive 10-undecenoic acid as a starting material. Miyashita's C-2 selective *endo* mode azidolysis and Huisgen click reaction was employed for the synthesis of the designed analogs.



Reagents: (a) NaN_3, $(CH_3O)_3B$, DMF, 50 °C, 3 h, then $NaIO_4$ treatment, CH_3CN, rt, 30 min, 79% (over two steps); (b) H_2, 10% Pd/C, CH_3OH, rt, 4 h, 86%.

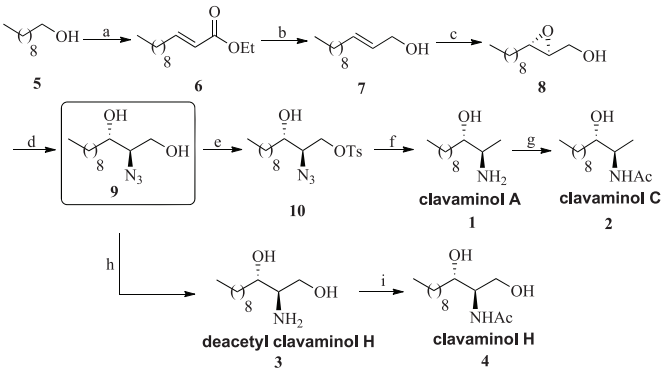


Reagents: (a) HC≡CR, *t*-BuOH:H_2O (1:1), $CuSO_4.5H_2O$, Na-ascorbate, RT, 8 h, 81-92%

Synthesis of Short-chain Sphinganine and its 1,2,3-Triazole Analogs

Based on biological evaluation studies of all the synthesized compounds, it was observed that the sphinganine derived hydroxy phenyl substituted triazole compound **2b** exhibited promising antimicrobial and antifungal activities. Furthermore, the compound **2b** displayed specific biofilm inhibition activity against *Staphylococcus aureus* MTCC 96 and *Micrococcus luteus* MTCC 2470. Based on its mode of action, the compound **2b** showed increased levels of reactive oxygen species (ROS) accumulation in *Candida albicans* MTCC 227. (*Eur. J. Med. Chem.,* **2016**, 118, 98)

Total Synthesis and *in vitro* Bioevaluation of Clavaminols A, C, H & Deacetyl clavaminol H as Potential Chemotherapeutic and Antibiofilm Agents



Reagents and conditions: (a) (i) PCC, CH_2Cl_2, 0 °C to rt, 1 h, (ii) Ph_3P=$CHCO_2Et$, dry THF, rt, 12 h, 89% (over two steps); (b) DIBAL-H, dry CH_2Cl_2, -78 °C to rt, 1 h, 93%; (c) 4Å molecular sieves, *L*-(+)-DIPT, $Ti(O^iPr)_4$, TBHP, dry CH_2Cl_2, -25 °C, 24 h, 91%; (d) (i) NaN_3, $(CH_3O)_3B$, dry DMF, 50 °C, 3 h, (ii) $NaIO_4$ impregnated over silica gel, CH_2Cl_2, 0 °C to rt, 1 h, 78.2% (over two steps); (e) *p*-TsCl, Et_3N, DMAP, dry CH_2Cl_2, 0 °C to rt, 4h, 79%; (f) $LiAlH_4$, dry THF, 0 °C to reflux, 6 h, 73%; (g) Ac_2O, dry THF, rt to reflux, 6 h, 83%; (h) H_2, 10% Pd-C, CH_3OH, rt, 5 h, 91%; (i) Ac_2O, dry THF, rt to reflux, 6 h, 85%

Total Synthesis of Clavaminols A, C, H & Deacetyl Clavaminol H

A highly concise and expedient total synthesis of bioactive clavaminols (**1-4**) has been executed using commercially available achiral compound decanol. The synthetic strategy relied on *trans*-Wittig olefination, Sharpless asymmetric epoxidation, regioselective azidolysis and *in situ* detosylation followed by reduction as key reactions with good overall yield. Based on biological evaluation studies of all the synthesized compounds, it was observed that the clavaminol A (**1**) exhibited good cytotoxicity against DU145 and SKOV3 cell lines with IC_{50} value of 10.8 and 12.5 µM, respectively. Clavaminol A (**1**) and deacetyl clavaminol H (**3**) displayed selective promising inhibition towards Gram-positive pathogenic bacterial strains and showed good antifungal activity against the tested *Candida* strains. In addition, compounds **1** and **3** have demonstrated significant bactericidal activity. Compound **3** was found to be equipotent to the standard drug Miconazole displaying MFC value of 15.6 µg/mL against *Candida albicans* MTCC 854, *C. albicans* MTCC 1637, *C. albicans* MTCC 3958 and *C. glabrata* MTCC 3019. Compounds **1** and **3** were also able to inhibit the biofilm formation of *Micrococcus luteus* MTCC 2470 and *Staphylococcus aureus* MLS16 MTCC 2940. Clavaminol A (**1**) increased the levels of reactive oxygen species (ROS) accumulation in *Micrococcus luteus* MTCC 2470. (*Eur. J. Med. Chem.,* **2016**, 120, 86)

Self- Assembly of Isomannide-based Monoesters of C18-Fatty Acids and their Cellular uptake Studies

The self - assembling behavior of oleic, elaidic and stearic acidisomannide glycolipids is revealed. The self - assembling behaviour of isomannide based glycolipids which differ only in their hydrophobic core. The self - assemblies of elaidic acid and oleic acid IMLs resulted in the formation of microspheres which were used in cellular uptake studies using MDA-MB-231 cells. The results suggest that, the self - assembled structures show an increase in the uptake of model hydrophilic

drug called fluorescein. Amongst these oleic and elaidic acid-based isomannide lipids self - assembled to form microspheres which were efficiently taken up by cancer cell lines enabling their usage for drug delivery applications. (*RSC Adv.,* **2016,** 6, 72074)

Synthesis and *In Vitro* Antioxidant and Antimicrobial Studies of Novel Structured Phosphatidylcholines with Phenolic Acids

Novel phenoylated phosphatidylcholines were synthesized from 1,2-dipalmitoyl phosphatidylcholine/ egg 1,2-diacyl phosphatidylcholine and phenolic acids such as ferulic, sinapic, vanillic and syringic acids. The structures of phenoylated phosphatidylcholines were confirmed by spectral analysis. 2-acyl-1-lyso phosphatidylcholine was synthesized from phosphatidylcholine via regioselective enzymatic hydrolysis and was reacted with hydroxyl protected phenolic acids to produce corresponding phenoylated phosphatidylcholines in 48–56% yields. Deprotection of protected phenoylated phosphatidylcholines resulted in phenoylated phosphatidylcholines in 87–94% yields. The prepared compounds were evaluated for their preliminary in vitro antimicrobial and antioxidant activities. Among the active derivatives, compound 1-(4-hydroxy-3,5-dimethoxy) cinnamoyl-2-acyl-sn-glycero-3-phosphocholine exhibited excellent antioxidant activity with EC_{50} value of 16.43 µg/mL. Compounds 1-(4-hydroxy-3-methoxy) cinnamoyl-2-acyl-sn-glycero-3-phosphocholine and 1-(4-hydroxy-3,5-dimethoxy) cinnamoyl-2-palmitoyl-snglycero-3-phosphocholine exhibited good antioxidant activity with EC_{50} values of 36.05 and 33.35 µg/ mL respectively. Compound 1-(4-hydroxy-3-methoxy) cinnamoyl-2-palmitoyl-sn-glycero-3- phosphocholine exhibited good antibacterial activity against *Klebsiella planticola* with MIC of 15.6 µg/ mL and compound 1-(4-hydroxy-3-methoxy) benzoyl-2-acyl-sn-glycero-3-phosphocholine exhibited good antifungal activity against *Candida albicans* with MIC of 15.6 µg/mL. (*Food Chem.,* **2017**, 221, 664)

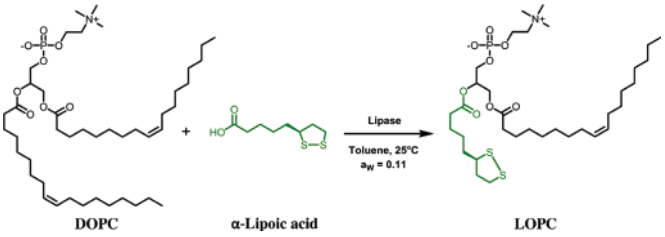
Synthesis and Evaluation of Anti-Oxidant and Cytotoxic Activities of Novel 10-Undecenoic Acid Methyl Ester-based Lipoconjugates of Phenolic Acids

The synthesis of five novel methyl 10-undecenoate-based lipoconjugates of phenolic acids from undecenoic acid was carried out. Undecenoic acid was methylated to methyl 10-undecenoate which was subjected to a thiol–ene reaction with cysteamine hydrochloride. Further amidation of the amine was carried out with different phenolic acids such as caffeic, ferulic, sinapic, coumaric and cinnamic acid. All synthesized compounds were fully characterized and their structures were confirmed by spectral data. The antioxidant activity of the synthesized lipoconjugates of phenolic acids was studied by the 2,2-diphenyl-1-picrylhydrazyl (DPPH) radical scavenging assay and also by the inhibition of linoleic acid oxidation in micellar medium by differential scanning calorimetry (DSC). The prepared compounds were also screened for their cytotoxic activity against five cell lines. It was observed that the lipoconjugates of caffeic acid, sinapic acid, ferulic acid, and coumaric acid displayed anticancer and anti-oxidant properties. The anticancer properties of these derivatives have been assessed by their IC50 inhibitory values in the proliferation of MDA-MB231, SKOV3, MCF7, DU 145 and HepG2 cancer cell lines. (*Beilstein J. Org. Chem.,* **2017**, 13, 26)

An Anti-Oxidant, α-Lipoic Acid Conjugated Oleoyl-*Sn*-Phosphatidylcholine as a Helper Lipid in Cationic Liposomal Formulations

Trans-esterification or acidolysis of dioleoylphosphatidylcholine (DOPC) with lipoic acid was carried out by enzymatic method. Substrate solution (DOPC and lipoic acid) in toluene and immobilized enzyme (Lipozyme RM IM) were separately adjusted to defined water activity of 0.11 by gas phase equilibration using saturated salt solution of Lithium Chloride in closed vials at room temperature for at least 24 h. In a typical reaction, trans-esterification was initiated by the addition of 75 mg of immobilized lipase to 1 ml of the substrate solution containing DOPC (7.86 mg, 0.01mmoles) and lipoic acid (62 mg, 0.3 mmoles) in toluene with 0.5% of cysteine. The reactions were performed in open vials secured in closed containers containing the saturated salt solution to maintain the desired water activity. This novel anti-oxidant lipid, α-lipoyl, oleyl-sn-phosphatidylcholine (LOPC) was used as a helper lipid in combination with a cationic amphiphile, Di-Stearyl Dihydroxy Ethyl Ammonium Chloride (DSDEAC) and 1,2-dioleoyl-sn-glycero-3-phosphocholine (DOPC) at varying concentrations of LOPC. DNA binding properties of the liposomal formulations (DS, DS LA1, DS LA2 and DS

LA3) revealed that increasing the percentage of single aliphatic chain lipid LOPC, did not affect the DNA binding properties. But, transfection profiles of these liposomal formulations in 3 different cell lines (HeLa, HEK 293 and MCF7) showed difference in their efficacies. Results showed that optimal percentage of LOPC i.e. 25% in DSDEAC and DOPC at 1:1 molar ratio (DS LA1) enhanced transfection as compared to DSDEAC:DOPC alone. The endosomal escape studies with NBD labelled lysotracker and Rhodamine labelled liposomal formulations revealed that DS LA1 and DS LA2 facilitated the release of genetic cargo with a better efficiency than their counter parts. Reactive Oxygen Species (ROS), a key modulator of necroptosis were lowered with the treatment of DS LA1 than other liposomal formulations. In this work, we present a novel liposomal formulation using DSDEAC and DOPC at 1:1 molar ratio doped with 25–50% (mole ratio) LOPC as an efficient delivery system for enhanced transfection with quenching of ROS levels compared to formulations without LOPC. (*Colloids Surf. B: Biointerf.,* **2017**, 152, 133)



Enzymatic Synthesis of 1-lipoyl,2- oleyl-*sn*-phosphatidylcholine (LOPC)

Synthesis and Cytotoxic Evaluation of Fatty Acid Based- Amino Alcohols

Synthesis of β-amino alcohols from a medium chain fatty acid, 10-undecenoicacid and evaluation of their cytotoxicity are reported. Nucleophilic ring opening reactions of epoxy undecanoates of varying ester chain lengths (C1-C8) with aniline in equimolar ratio (1:1) was carried out using Bronsted acidic ionic liquid, 1-methylimidazolium tetrafluoroborate, thus playing a dual role of solvent as well as a reaction medium. The cytotoxic properties of the amino alcohols of 10-undecenoic acid were evaluated. It was observed that the compound 4f showed promising cytotoxicity against HeLa, compound 4a showed good activity against A549 cell line, while compounds 4a, 4cshowed good activity against MDA-MB-231 cell line. All other compounds showed moderate activity against all the other tested cell lines. *(I.J.A.B.R.,* **2016***, 6*(3), 348)

Synthesis of Dihydrosterculic Acid-based Monoglucosyl Diacylglycerol and Its Analogues and their Biological Evaluation

Lactobacillus plantarum glycolipid (GL1) molecule in β-configuration and its fatty acid analogues were synthesized using trichloroacetimidate methodology. The β-configuration of the GL1 molecule was unambiguously assigned by NMR studies using 2D-ROESY (NOE) and J-coupling analysis. Dihydrosterculic acid was synthesized using Furukawa's reagent and the selective esterification of dihydrosterculic acid at C-3 position of glycerol was achieved with EDC-HCl at 0°C. *In vitro* cytotoxicity of the GL1 molecule and its fatty acid analogues was evaluated against DU145, A549, SKOV3 and MCF7 cell lines. Among all the synthesized molecules, the GL1 molecule (oleic-cyclopropane-based) and lauroyl analogue showed moderate activity, while the oleic acid analogue showed promising activity against all the tested cell lines with IC50 values of 20.1, 18.2, 19.1 and 17.6 mM, respectively. In addition, all tested compounds showed poor cytotoxicity against normal HUVEC cells. The MCF7 cells when treated with compound 7b showed lower bromodeoxyuridine incorporation levels as compared to untreated cells, suggesting that the oleoyl derivative was highly effective and inhibited the cell proliferation. In addition, the compounds showed significant increase in caspases 3 and 9 levels by inducing apoptosis in MCF 7 cells. (*Eur. J. Med. Chem.,* **2016**, 109, 134)

Effects of Natural Antioxidants Extracted from Cameroonian Ginger Roots on the Oxidative Stability of Refined Palm Olein

The objective of this study was to evaluate the effect of ginger roots methanolic extract on the stability of palm olein during accelerated storage. After analysis of the extract by the measurement of its total phenolic content by colorimetry and detection of some of its phenolic antioxidants by HPLC-DAD (high performance liquid chromatography-diode array detector) and ESI-MS (Electrospray ionization-mass spectrometer), preliminary antioxidants tests have been conducted. After these tests, the extract has been added in refined palm olein at concentration 200–1800 ppm for investigating its effect on it oxidative stability. Butylated hydroxytoluene (BHT) at it legal concentration of 200 ppm served as positive control, while palm olein without additive served as negative control. Induction

time, chemical indexes (peroxide, p-Anisidine, total oxidation, thiobarbituric acid and iodine values) and changes in linoleic acid profile (analyzed by gas chromatography coupled to a flame ionization detector) of oil samples were evaluated. Results of these investigations showed ginger roots methanolic extract to be rich in phenolic antioxidants. Ferulic acid and 6-gingerol were the antioxidants detected. The extract was also efficient in reducing palm olein oxidation on Rancimat and Schaal oven test of 30 days at 70 °C. Ginger roots extract might be a viable source of natural antioxidants for stabilization of palm olein. (*Eur. Food Res. Tech. Bull.,* **2017**, 8, 154)

Total Synthesis of (-)-Sachalinol A and Evaluation of its Cytotoxicity

(-)-Sachalinol A, a group of monoterpenoids, oxygenated derivatives of rosinidol, was synthesized employing a simple, eight step procedures. The compound demonstrated excellent cytotoxicity against MDA-MB-231 derived from human breast adenocarcinoma cells (ATCC No. HTB-26) and HeLa derived from human cervical cancer cells (ATCC No. CCL-2). Good activity against A549 derived from human alveolar adenocarcinoma epithelial cells (ATCC No. CCL-185) and Neuro2a derived from mouse neuroblastoma cells (ATCC No. CCL-131). While, moderate activity was observed against MCF-7 derived from human breast adenocarcinoma cells (ATCC No. HTB-22). (*Ind. J. Chem. B*, **2017**, 56B, 695)

Effect of Salinity Stress on Growth, Lipid Productivity, Fatty Acids Composition and Biodiesel Properties in *Acutodesmus Obliquus* and *Chlorella Vulgaris*

Two microalgae strains including *Chlorella vulgaris* and *Acutodesmus obliquus* were grown on BG11 medium with a different concentration of salinity ranging from 0.06 to 0.4 M NaCl. The dry biomass and lipid content of microalgae were improved as the concentration of NaCl increased from 0.06 to 0.1 M. Highest dry weight (0.92 and 0.68 gL^{-1}) and lipid content (49 and 43 %) of *Chlorella vulgaris* and *Acutodesmus obliquus* respectively, were obtained in BG11 amended with 0.06 & 0.4 M NaCl. The Fatty acid composition of the investigated microalgal strains was also improved by increased NaCl concentration. At 0.4 M NaCl, Palmitic acid (37%), Oleic acid (15.5 %) and Linoleic acid (20%) were the dominant fatty acids in *Chlorella vulgaris* while Palmitic acid (54%) and Stearic acid (26.6 %) were major fatty acids found in *Acutodesmus obliquus.* Fatty acids profiling of *Chlorella vulgaris* and *Acutodesmus obliquus* significantly varied with salinity concentration. Therefore, the study showed that salt stress is an effective stress that could increase not only the lipid content but also improved the fatty acid composition which could make *Chlorella vulgaris* and *Acutodesmus obliquus* potential strains for biodiesel production. (*Environ. Sci. Pollut. Res. Int.,* **2017**, 24(15), 13437)

Karanja Oil Polyol and Rigid Polyurethane Biofoams thereof for Thermal Insulation

Rigid polyurethane biofoams were prepared from karanja polyol derived by ring opening reaction of epoxidized karanja oil. The polyol which had a hydroxyl value of 186 mg KOH/g was thoroughly characterised and the structure confirmed by spectral techniques. The foam formulations were developed to achieve shrinkage free foams with closed cell structure. The resulting foams were characterised for their mechanical properties like density, compression strength and flexural strength. The densities and mechanical properties such as compression and flexural strength varied with the amount of MDI added for a fixed amount of polyol and other additives as a result of side reactions leading to allophanate and urea linkages. SEM results indicated that the cells are spherical and samples are isotropic. However, the cell size distribution varied with MDI content. The thermal conductivity was found to be in the 0.036-0.042 (W/m.K) range which is well suited for insulation purpose. (*J. Renew. Mat.,* **2017,** 5, 124)

Effects of Boiling and Roasting on Proximate Composition, Lipid Oxidation, Fatty Acid Profile and Mineral Content of Two Sesame Varieties Commercialized and Consumed in Far-North Region of Cameroon

The aim of this study was to determine the effect of boiling and roasting on the proximate, lipid oxidation, fatty acid profile and mineral content of two sesame seeds varieties. The proximate composition was significantly affected ($P < 0.05$) during treatments. The minerals of seeds roasting at 120°C for 10 min were significantly decreased. The free fatty acids content of sesame oil after processing was significantly increased ($P < 0.05$). Iodine and peroxide value were also affected

by processing. Totox and p-Anisidine values were significantly increased during processing. The fatty acids composition a little modified during processing, and roasting at 180°C for 10 min mostly affected the polyunsaturated fatty acids for all sesame varieties. C16:0, C18:0, C18:1 and C18:2 were quantitatively the most important fatty acids in sesame oil. Boiling appeared to be the best processing method for cooking the two sesame varieties concerning oxidative stability and fatty acid profile. (*Food Chem.*, **2016**, 221, 1308)

Synthesis of Novel Fatty Substituted 4-methyl-2HChromen-2-one via Cross Metathesis: Potential Antioxidants and Chemotherapeutic Agents

A series of novel fatty substituted 4-methyl-2H-chromen-2-one (coumarins) were synthesized by employing cross metathesis, a key step in the synthesis. The antioxidant activities of the title compounds were compared with the commercial antioxidants, namely butylated hydroxy toluene (BHT) and α- tocopherol, glycosidic and other substituted 4-methyl-2H-chromen-2-ones. Among the different 4-methyl2H-chromen-2-ones, the glycosidic substituted 4-methyl-2H-chromen-2-ones was excellent, while those with aliphatic fatty acid chain and hydroxyl substitutents were good. Among the substituted 4-methyl-2Hchromen-2-ones, glycosidic, hydroxyl and cyano containing 4-methyl-2H-chromen-2-ones exhibited good, while fatty substituted exhibited moderate anticancer activities against the four different cancer cell lines tested, namely DU145 (Prostate carcinoma cancer cell), HepG2 (Hepato cellular carcinoma cancer cell), SKOV3 (Ovarian cancer cell) and MDA-MB 231 (Human breast cancer cell). The study reveals that these substituted coumarins can be potential candidates in a number of food and pharmaceutical formulations. (*J. Oleo Sci.*, **2016**, 65(12), 1023)

Synthesis, Antimicrobial, Biofilm Inhibition And Antioxidant Activities of Some Novel Undecenoic Acid-based Substituted Benzaldehyde Oxime Ester Derivatives

A series of novel oxime ester conjugates comprising various substituted benzaldehyde oximes and undecenoic acid were synthesized and evaluated for antimicrobial and antioxidant activities. Among all the synthesized compounds, 3, 5-dichloro-2-hydroxyphenyl oxime ester exhibited promising antimicrobial activity against Gram-positive, Gram-negative bacteria and fungal strain and this also exhibited promising antifungal, minimum bactericidal concentration and biofilm inhibition activities. Among all the prepared compounds 4-fluoro oxime ester showed good antioxidant activity. Further studies on similar derivatives having 3, 5-dichloro-2-hydroxyphenyl oxime moiety may yield efficient antimicrobial agents. (*Indo Amer. J. Pharma. Res.,* **2016**, 6 (3), 4759)

Synthesis and Biological Evaluation of Some New N-Fatty Acyl Derivatives of 4,5-Dimethoxy Tryptamine

A series of novel N-fatty acyl derivatives of 4,5-dimethoxy tryptamine were synthesized and screened for *in vitro* anticancer, antioxidant and antimicrobial activities. The results revealed that short chain saturated (butyric) and long chain unsaturated (oleic) derivatives exhibited the highest anticancer activities. It was also observed that dimethoxy tryptamine derivative of undecenoic acid exhibited promising antibacterial and antioxidant activities. The antioxidant results also suggested that undecenoic and stearic acid derivatives exhibited significant lipid peroxidation inhibition as compared to BHT. (*Ind. J. Chem.*, **2017**, 56B, 531)

The Impact of Sugar and Fatty Acid on the Bioactivity of *N*-Fatty Acyl-*L*-Tyrosine Aglycone

A series of fatty acids-based (short, medium and long unsaturated chains) glycosylated *N*-fatty acyl-*L*-tyrosines and *N*-lipoyl-*L*-tyrosine methyl esters were synthesized and evaluated for their cytotoxic and antimicrobial activities. The aglycone moiety was synthesized using different chemical reagents. The glycosylation of aglycone moiety with different carbohydrates was performed using the Lewis acid, $BF_3.Et_2O$. All the synthesized compounds were tested against a panel of four cancer cell lines. The glycosylated *N*-fatty acyl-*L*-tyrosines showed moderate activity against all the cell lines and the IC_{50} values were in the range of 15.6–45.6 µM. However, the oleic acid analogues exhibited IC_{50} values of 15.6, 17.6 µM, respectively, against MDA-MB-231 cell line. Glycosylated *N*-lipoyl-*L*-tyrosine methyl esters showed promising activity against all the tested cell lines and the IC_{50} values ranged between 9.4–13.8 µM. The compound exhibited significant cytotoxicity and

IC_{50} values were 10.5, 9.4, 10.9 and 12.1 µM against A549, PC3, MDA-MB-231 and HepG2 cell lines, respectively. Moreover, the nonglycosylated *N*-fatty acyl-*L*-tyrosine and methyl *N*-fatty acyl-*L*-tyrosinate derivatives showed excellent and moderate antimicrobial activity against some of the tested bacterial strains. (*J. Chem. Sci.,* **2017**, 129, 663)

Synthesis and Biological Evaluation of 5-Fatty-Acylamido-1, 3, 4-Thiadiazole-2-Thioglycosides

The synthesis of 1, 3, 4-thiadiazole-based thioglycosides were accomplished in good yields with employing a convergent synthetic route. The starting material 5-amino-1, 3, 4-thiadiazole-2-thiol and followed by a series of 5-fatty-acylamido-1, 3, 4-thiadiazole-2-thiols were synthesized with different fatty acid chlorides. The glycosylation of compounds was achieved with trichloroacetimidate methodology. Antimicrobial and cytotoxicity activities of title compounds were evaluated. Among the entire compounds lauric acid and myristic acid derivatives showed good and moderate antimicrobial activity. In case of cytotoxicity results of compounds, the acetate protected short chain (C6:0, C8:0, C10:0) compounds and the free hydroxyl long chain saturated (C16:0, C18:0) and unsaturated (C18:1, C22:1) compounds exhibited good activity against different cancer cell lines. Further, the free hydroxyl compounds did not show any toxicity towards normal CHOK1 cell line whereas acylated compounds exhibited toxicity. (*Bioorg. Med. Chem. Lett.*, **2017**, 27, 3370)

APPLIED RESEARCH

Development of Sustainable Processes for Edible Oils with Health Benefits from Traditional and New Resources (*PEOPLE HOPE, CSIR Networking Project of 12th Five Year Plan*)

CSIR-IICT was the nodal laboratory and CSIR-NIIST, CSIR-NEIST, CSIR-IIP, CSIR-CFTRI, CSIR-NCL were the participating labs for this 12th Five Year Plan networking project. The project consists of six packages namely, Screening of unexploited tree-borne oilseeds of forest origin for edible and non-edible applications; Screening of microbial strains for the production of PUFA-enriched oils and development of processes for extraction, characterization and refining of microbial lipids; Genetic modification of microbes and plant cells for the production of PUFA-rich oils; National survey to assess the modernization needs of vegetable oil and vanaspati industry and preparation of a modernization package for the enhancement of efficiency of the industry; Development of sustainable and greener technologies like mechano-chemical processing and supercritical carbon dioxide extraction for vegetable oil extraction and value addition, and Nutritional biochemistry of lipids and their derivatives. The major achievements of the project in each work package is given below.

WP-1: CSIR-IICT along with NEIST, NCL and IIP, screened 204 tree-borne oil seeds for their oil content & FAME composition. Networking with various state forest departments and related organizations was carried out and links were established with some organizations for information and collection of tree-borne seeds. Survey of the Indian forest area for seed information was done with the help of IMRB International, Chennai, a consultancy company. During the screening of tree-borne seeds, main thrust was given to the oil content and fatty acid composition. Based on the data generated on oil content and fatty acid composition, about 6 species from CSIR-IICT (*Mesua ferrea, Calophyllum inophyllum, Swietenia mahagoni, Ailanthus excelsa, Melia dubia, Butea parviflora)* and about 10 species from CSIR-NEIST [*Cinnamomum impressinervium* (NST 20, 48% oil), *Litsea cubeba* (NST 24, 45% oil), *Garcinia morella* (NST 28, 38% oil), *Chrysophyllum roxhburghii* (NST 37, 35% oil), *Chisocheton paniculatus* (NST 39, 40% oil), *Litsea coriacea* (NST 42, 34.5% oil), *Dysoxylum procerum* (NST 48, 50.3% oil), *Cinnamomum obtusifolium* (NST 75, 38% oil), *Garcinia xanthochymus* (NST 32), *Magnolia champaca* (NST 80, 41.4% oil, 38.3% oil) containing 34-50% oil were shortlisted for further studies. About 20 seeds were collected and screened by CSIR-IIP and identified two potential seeds (*Prunus and Crambe*) for oleochemicals applications like bio lubricants, esters etc. CSIR-NCL supplied about 50 seeds for oil content and fatty acid composition analysis. Based on the data, 4 seeds namely *Garcinia talboti, Terminalia paniculata, Macaranga peltata and Knema attenuata* were identified by IICT for detailed study. Two potential varieties were identified by CSIR-IICT (*Swetinia mahagoni* and *Butea parviflora*) which are available in good quantities have been taken up for large scale extraction and refining studies. The refined oils will be evaluated for toxicity studies.

WP2: CSIR-NIIST along with CFTRI collected about 200 soil samples were from Western Ghat regions of Kerala, Karnataka and Tamil Nadu and 150-160 microbial strains were isolated. About 50-60 oleaginous fungal cultures were qualitatively isolated. Among them, 15 fungal strains were identified for the *production* of *PUFA* oil *with specific reference to GLA*. One potent fungal strain, *Cunninghamella elegans* CFR-C07 was found to be a good producer of GLA and was deposited and published in NCBI (GenBankANo. KF916583 sp). The CFR-C07 was shortlisted for scale up studies at NIIST. The lab scale fermentation optimization for the improved production of GLA from *Cunninghamella elegans* CFR-C07 under submerged and solid-state fermentation have been carried out.

WP-3: CSIR-NCL profiled 30 microbial cultures for fatty acids and 14 new fungi producing PUFAs were identified. Among these, 3 promising species namely *Cunningamella echinulata* producing high amount of γ- linolenic acid (GLA) -23.4%, *Rhizopus oligosporous* producing high amount of oleic acid (39%) and *Penicillium notatum* producing high amount of linoleic acid (42%) were identified. In addition, two new diatom isolates producing EPA and DHA were identified. Growth and media conditions were optimized for *Beauveriafelina*, which produced up to 58% linoleic acid. The fatty acid biosynthesis pathway was characterized from the selected microbes and the desaturase & elongase genes involved at each stage have been determined. The microbial Δ5 elongase and Δ6 desaturase genes were identified. The Δ5 elongase gene has been cloned and partial Δ6 desaturase gene has been cloned. The full-length gene is being cloned. Standardized *Agrobacterium* mediated transformation protocols for linseed. Cloning of microbial Δ5 elongase and Δ6 desaturase genes is in progress

WP-4: India is importing more than 60% of the domestic requirement of vegetable oils. Hence, the need of the hour is to have serious introspection in this sector in order to make India self sufficient in vegetable oils. Though, there are technological interventions worldwide in this sector for newer eco-friendly processes, India did not gear up in this direction due to lack of scientific auditing of the existing units. In this context, a national survey was proposed as the part of this project to assess the present status of oilseed expelling units and vegetable oil refineries to identify the major problems encountered by these industries with respect to raw material quality, processing parameters, energy conservation, water consumption, effluent handling, product quality, by-product utilization and testing facilities. CSIR-IICT Initially conducted Pilot Survey in two industries of each type: expelling and vegetable oil processing industry. Based on the pilot survey data analysis, questionnaires were prepared after thorough deliberations with professional bodies like OTAI, SEA etc. Survey was carried out in 12 expelling units and 11 vegetable oil refining industries and four major areas namely processing, quality control, instrumentation and effluent treatment were identified for modernization. The selection procedure of raw materials, processing methodologies followed by the industries, the equipments and facilities available with the industries, the quality of the man power present in the industry and the analytical facilities available with the industries were critically evaluated. The poor maintenance of the plant and machineries and loss in productivity and product qualities were also critically examined. As per the deliverables promised in this project, a modernization package particularly for the quality assurance cell of the vegetable oil refining industries was submitted for funding to FSSAI. In case, FSSAI does not fund, the same proposal will be submitted to some other agency.

WP-5: CSIR-IICT carried out Supercritical carbondioxide extraction of rice bran, linseeds, soybeans and safflower and the conditions were optimized by varying the parameters like pressure, temperature and extraction time. The yield of oils was found to be 16, 30.7, 12.4 and 28.1% respectively. Oil yield and physico-chemical properties such as FFA, 'P' content, I.V, P.V, S.V etc. for both solvent extracted and supercritical carbondioxide extracted oils was generated. The supercritical extracted oils contained less amount of phosphorous content compared to solvent extracted oils and were of light color. Enzymatic pretreatment of mustard seeds, groundnuts and soybeans was carried out using cellulase, viscozyme and alprolase. Enzymatic pretreated conditions such as enzyme dosage, temp, buffer pH, time, oil/buffer ratio optimized. It was found that the oil content was enhanced for the enzyme treated mustard seeds using viscozyme compared to traditional solvent extraction. The other treated oils did not show much improvement upon enzymatic pretreatment when compared to mustard oil. Feasibility studies were conducted on Mechano chemical processing (MCP) with prototype horizontal extrusion type expeller using mustard, groundnut and karanja seeds in 500 g/batch

and an efficiency of about 20% residual oil was achieved over multiple reprocessing.

WP-6: CSIR-IICT made efforts to establish network among regulatory authorities, industry & consumers for the development of quality and healthy products in the area of vegetable oils. Food Safety and Standards Authority of India (FSSAI) has recognized Centre for Lipid Research of IICT as the National Referral Laboratory for carrying out testing of food samples and other functions related to oils & fats under Regulation 2.2.1 of FSS (Laboratory and Sample Analysis) Regulation, 2011. Three types of indigenous edible oil blends were designed with WHO and AHA-suggested fatty acid profiles using rice bran, sunflower, soybean, palmolein and sesame oils. Synthetic oryzanol was prepared (50 g scale) for the fortification in vegetable oils. An appropriate design was made to evaluate the antihypercholesteremic effect of cooking oils fortified with oryzanol, employing 60 male Syrian Hamsters divided into control and different treated groups fed with palm and soybean oils either alone or fortified with oryzanol and comparing the results with those of rice bran oils. Taken help from NCLAS, NIN, Hyderabad for the preparation of rodent diet based on AIN 93 recommendations with 5% oil and 1% cholesterol in the diet. Special cages were fabricated in order to accommodate this powder diet for hamsters. Complete characterization of the synthetic oryzanol required for the fortification purpose was completed. Sunflower and palm oils were fortified with Synthetic Oryzanol (0.38 & 1.25%) in 500 and 800 g scale and were evaluated for their Hypocholesteremic activity in Syrian Male Hamsters in comparison with native oils and physically and chemically refined rice bran oils containing 0.38 & 1.25% γ-oryzanol respectively using the animals models for 3 months. Initial one month study resulted significant reduction in cholesterol and also improved lipid profiles compared to native oils. However, the results obtained after one month study were found to be disturbed. Hence, the animal model was modified by increasing the oil content (5 to 10%) and decreasing the cholesterol content (from 1% to 0.5%) in the diet. Initial studies with the fortified sunflower and palm oils with 1.45% synthetic oryzanol in comparison with native oils and physically refined rice bran oil containing 1.45% γ-oryzanol for Hypocholesteremic activity in Syrian Hamsters as per modified model and one month study is encouraging.

Swietenia mahagoni Seed Oil: A New Source for Biodiesel Production

Swietenia mahagoni seed oil contains common unsaturated fatty acids such as oleic (25.5%), linoleic (32.6%), linolenic (12.2%) and saturated fatty acids, namely, palmitic (13.0%) and stearic (14.1%) as major fatty acids with 58.1% oil content. In the present study, the oil with 1.39% free fatty acids was converted into biodiesel employing conventional acid-catalyzed esterification followed by base-catalyzed trans-esterification reaction. The resultant biodiesel was evaluated for physico-chemical properties namely iodine value (104.6), free fatty acids (0.05%), phosphorous content (0 ppm), flash point (165.0 °C), cloud point (7 °C), pour point (9 °C), viscosity at 40 °C (4.13 cSt), oxidative stability at 110 °C (3.7 h), density (0.880 g/cm^3 at 15 °C), and trace metals (Group I metals, 0.5 ppm). The physico-chemical properties were found to be within the range of ASTM and almost falling in the range of EN biodiesel specifications. (*Indus. Crops Prod.,* **2016**, 90, 28)

Isolation and Physico-Chemical-Characterization of *Butea Parviflora* Seed Oil

The seeds of *Butea parviflora* were investigated for oil extraction and the oil was studied for complete physico-chemical properties. The fatty acid profile of the seed oil showed oleic acid (18:1) at 27.5%, linoleic acid (18:2) at 26.4%, palmitic acid (16:0) at 16.1% and behenic acid (22:0) at 14.1% as the major fatty acids. The physico-chemical characteristics of the seed oil were studied for parameters such as free fatty acids (0.71%), iodine value (76.2 g/100g), peroxide value (5.95 ppm), saponification value (177.32 mg KOH/g), unsaponifiable matter (0.82%), phosphorous content (197 ppm), triglyceride analysis, tocols, specific gravity and refractive index following standard procedures. (*Gras. Y Aceite,* **2016**, 67(3), e151)

Physico-chemical Characterization and Biodiesel Preparation from *Ailanthus excelsa* Seed Oil

Seed oils from forest trees are considered as renewable sources for many industrial and edible applications and research is now focused on the exploitation of these tree-borne oil seeds for various applications. In this study, *Ailanthus excelsa* seed oil is identified as minor seed oil from forest origin for biodiesel production. The seed oil was initially characterized for various physico-chemical properties following standard protocols. The

extracted oil was further refined and transesterified to produce biodiesel. The prepared biodiesel was evaluated for fuel properties such as the iodine value, free fatty acids, phosphorous content, flash point, cloud point, pour point, viscosity, oxidative stability, density and trace metals. The properties were compared with international specifications and it was found that the oxidative stability of the prepared biodiesel was better compared to most of the biodiesels reported. (*Energy Sour., Part A: Rec. Utiliz. Environ. Effects*, **2017**, 39 (8), 811)

Comparison of Oil Content and Fatty Acid Compositions of Some Lesser Known Oilseeds from Andhra Pradesh Forest Region

The oil content and fatty acid composition of eight lesser known tree borne oil seeds namely, *Albizia odoratissima*, *Albizia lebbeck*, *Pterocarpus marsupium*, *Ailanthus excelsa*, *Casia siama, Dalbergia sissoo*, *Oroxylum indicum, Melia dubia* are reported for the first time from Andhra Pradesh (AP) forest region and the data are compared with previous results. Except for *M. dubia* (i.e., 43.5 %) and *O. indicum* (i.e., 22.2%) all the species exhibited oil content of less than 20%. Linoleic acid was the major fatty acid in six seed oils and oleic acid was the major fatty acid in two seed oils. Palmitic and stearic acids were the common fatty acids present in all the seed oils. Caprylic, capric, myristic acids were present in minor quantities. (*J. Lipid Sci. Tech.*, **2017**, 49, 5)

A Comparative Study of Solvent and Supercritical CO_2 Extraction of *Simarouba gluaca* Seed Oil

In the present study, optimization of conditions for supercritical carbon dioxide (CO_2) extraction of oil from *simarouba gluaca* seeds was carried out at varying conditions of pressure (300-500 bar), temperature (50-70 °C) and CO_2 flow rate (10-30 g/min). The optimized condition for maximum oil yield was obtained at 500 bar pressure, 70 °C temperature and at 30 g/min flow rate of CO_2. The extracted oil was analysed thoroughly for physico-chemical properties and compared with those of conventional solvent extracted oil. An interesting observation is significant reduction in phosphorus content of oil (8.4 ppm) extracted using supercritical CO_2 compared to the phosphorous content of solvent extracted oil (97 ppm). Moreover, the content of total tocopherol in supercritically extracted oil (135.6 mg/g) was found to be higher than solvent extracted (111 mg/g). Rest of the physico-chemical properties of two differently extracted oils matched well with each other. Results indicated possible benefits of supercritical CO_2 extraction over solvent extraction of *Simarouba gluaca* seed oil. (*Gras. Y Aceites,* **2017**, 68, 205)

BIOLUBRICANTS

Synthetic Aviation Lubricants

India is totally dependent on developed countries for its aviation lubricant requirements. Hence, it is necessary to develop the necessary aviation lubricants which are of immense strategic importance in the defence-preparedness of our country necessitating self-reliance in this field. Moreover, Indian aviation sector is growing at a very rapid pace with many small and big players entering the market and an indigenous technology is required for the production of aviation lubricants for both defence and civil aviation sectors. Hence, CSIR-IICT formed a consortium with 5 other organizations namely, IOC R&D, CSIR-NAL, HAL, GTRE, CEMILAC, and developed two synthetic aviation lubricants (SVS-11 and SVS-21) suitable for Garrett and Orpheus aero engines with funding from Centre for High Technology (CHT), Ministry of Petroleum & Natural Gas, New Delhi. DRDO, CSIR and HAL also supported this endeavour. The developed lubricants have passed all the mandatory tests and obtained provisional certificates for Airworthiness Approval from CEMILAC, which are essential for in-flight tests and further for commercial exploitation. In addition, SVS-11 lubricant passed the Ryder Test at US NAVAIR. With the successful completion of the Phase-I project; CSIR-IICT has initiated Phase-II activity in April 2016 with the funding of CHT (Ministry of Petroleum, Govt. of India, Rs 132 lakhs) in collaboration with HPCL, Indian Air Force (3BRD, Chandigarh), CEMILAC & DGAQA. During this period CSIR-IICT demonstrated the process for SVS-21 & SVS-11 base oils production to HPCL & CEMILAC representatives. CSIR-IICT prepared 250 Kg each of SVS 21 and SVS 11 to the collaborating institute HPCL, Mumbai for formulation and initial testing. HPCL, Mumbai evaluated the SVS 21 base oil for its physico-chemical and lubricant properties & then formulated. 3BRD, Chandigarh supplied the rubber seals used in TV-2 aero engine to HPCL. HPCL conducted elastomer compatibility & triobology studies for the SVS-21 lubricant in comparision with commercial OX-38 in presence of all the collaborating institutes namely, CSIR-IICT, CEMILAC, DGAQA & 3BRD representatives.

The Elastomer testing of TV-2 engine rubber seals with SVS-21 Lubricant was found to be on par with that of OX-38 & some of the triabology properties of SVS-21 were found to be superior to OX-38. Mean time, IAF has informed that the TV-2 aero engine is going to be phased out shortly and hence, it was decided to not to conduct inflight tests with SVS-21 lubricant. However, IAF agreed to conduct only short time (50 hr) engine test in TV-2 aero engine with SVS-21 in comparison with commercial OX-38 and is going to be initiated shortly. Further work on the formulation of SVS-11 base oil & its elastomer compatibility with TV-3 aero engine rubber seals & triobology studies are in progress. After that, IAF, 3BRD will conduct engine (TV-3 aero engine) tests & inflight tests to SVS-11 lubricant in comparison with commercial OX-27 lubricant.

Synthesis, Characterization, and Evaluation of Castor Oil-Based Acylated Derivatives as Potential Lubricant Base Stocks

Synthesis, characterization, and evaluation of a series of novel acylated derivatives of castor oil as biolubricant base stocks are reported. The acylated derivatives of castor oil, castor oil fatty acid methyl and 2-ethylhexyl esters were synthesized using different anhydrides (C1–C6) in about 90–95% yield. All the products were structurally characterized using NMR and IR spectral data. The acylated products were evaluated for their physicochemical and lubricant properties. Although these products belong to group V, based on viscosity index (130–156), acylated derivatives of castor fatty acid alkyl esters belong to group III, the category of base fluids as per API classification. The acylated products exhibited excellent pour point (–21 to –39 °C) and flash point (174–280 °C). The hexanoylated and butanoylated esters of castor oil exhibited excellent flash points of 280 and 272 °C, respectively. The air release value was found to be excellent in the range of 0.38–0.99 min, and NOACK volatilities in the range of 3.25–3.92%. The other lubrication properties such as load carrying capacity, and emulsion stability were found to be good. Therefore, these derivatives will have utility in hydraulic and metal working fluids and other industrial fluids with their wide range of properties. *(Ind. Eng. Chem. Res.,* **2016***,* 55, 9109)

Synthesis and Characterization of Novel 10-Undecenoic Acid based Acyloxy Ether Derivatives

Synthesis of novel 10-undecenoic acid based acyloxy ether derivatives was done in a two step reaction. Methyl epoxy undecanoate on oxirane ring opening by alkoxy anions from two different alcohols namely, methanol and n-butanol in presence of K 10 clay as a green reusable heterogeneous catalyst yielded a mixture of regioisomeric forms of hydroxyl ether undecanoates. These products on acylation of hydroxyl group with two different anhydrides gave acyloxy ether derivatives in good yields (90-92%). The synthesized products were characterized using different spectroscopic techniques like FTIR, ^{1}H NMR and ^{13}C NMR, GC, GC-MS and ESI-MS. These products could prove useful as biodegradable cold flow improvers for diesel and biodiesel fuels and potentially as lubricants. *(J. Lipid Sci. Tech.,* **2016***,* 48(3), 69)

Synthesis and Characterization of Ricinoleic Acid- based Cyclic Carbonates

Cyclic carbonates were synthesised from castor oil fatty acid, ricinoleic acid by intra molecular rearrangement of epoxy carbonate esters with Lewis acid. The first step was di/mono esterification of ricinoleic acid with 1,4-butane diol, and next step was carbonate interchange reaction between diester/monoester of ricinoleic acid and dimethyl carbonate followed by epoxidation using performic acid method to get epoxy linear carbonates. These products on treatment with Lewis acid formed di/mono cyclic carbonates by intramolecular rearrangement. Synthesized compounds were characterized by ^{1}H NMR, ^{13}C NMR, ESI-MS and FT-IR. In the present study, we report synthesis of novel cyclic carbonates from ricinoleic acid using a new approach. These carbonates are potential precursors for the synthesis of isocyanate-free linear polyurethanes, the most promising substitutes for conventional polyurethanes used in paints, coatings and/or as biomaterials. *(J. Lipid Sci. Tech.,* **2017**, 49(2), 44)

Synthesis of 10-undecenoic acid based C22-dimer acid esters and their evaluation as potential lubricant basestocks

A new class of C22-dimer acid esters was synthesized from 10-undecenoic acid by montmorillonite K10 clay

catalyzed polymerization to dimer acid followed by their esterification using straight and branched chain alcohols (C1 to C10). All the newly synthesized products were characterized by IR, ^{1}H NMR, ^{13}C NMR, ESI–MS and HPLC, and evaluated for their physicochemical and lubricant properties such as density, specific gravity, viscosity, pour point, flash point, thermal and oxidation stability, weld load, wear and copper corrosion. Structural features like chain length and branching of alcohols influence the physicochemical and lubricants properties of the C22-dimer acid esters. It was observed that the esters synthesized using branched chain alcohols showed lower pour point and higher oxidation stability than their counterparts synthesized using straight chain alcohols. Overall, the physicochemical and lubricants properties of all the synthesized C22-dimer acid esters indicate that they can be potential base oils for hydraulic, metal working fluids and low-temperature lubricant applications. (*Indus. Crops Prod.,* **2017**, 103, 141)

Polyol Esters and Epoxy Derivative as Lubricant Basestocks from *Calophyllum inophyllum* Oil

Different types of lubricant base stocks were prepared based on Calophyllum fatty acids with different polyols having 5-6 carbon atoms and a total of 2-3 hydroxyl groups and with C_6 iso alcohol. Calophyllum oil was epoxidised using formic acid and hydrogen peroxide in the presence of acid catalyst at 60°°C. All the products were characterized for their physicochemical properties and evaluated for their lubricant properties like viscosity, viscosity index, pour point, flash point, copper corrosion test, oxidation stability and thermal stability etc. The products exhibited excellent pour point (–12 to –18 °C) and flash point (164–300 °C), good oxidation stability with onset temperature above 150°C and high thermal stability with degradation temperature above 200 °C. These products can be potential lubricant basestocks for industrial applications.

Development of High Performance Lubricant Basestocks from Non-edible Oils *(GENLUBE, CSIR Networking Project of 12th Five year plan)*

Tribological performance of ten acylated derivatives was evaluated using four ball tester. Their antiwear performance and coefficient of friction were studied. The wear scar diameter varied from 0.8 to 1.0 mm and coefficient of friction varied from 0.0886 to 0.1294. Four jatropha oil-based acyloxy products were found suitable for hydraulic fluids. All the properties excepting pour point and lubricity properties were superior to mineral oil basestocks. Hence, pour point of these products was improved using a commercial pour point depressant. Propionoylated jatropha fatty acid isopropyl esters had pour point -4 °C and it was improved to -10 °C and other products such as hexanoylated, acetylated and butanoylated esters pour point was improved from -5, -6 and -8 to -10, -11 and -11 °C respectively. The extreme pressure properties were also improved using a commercial additive. All the four products have load carrying capacity of 140 kg and they were improved to 300 kg. These formulations can be potential substitutes for mineral oil based hydraulic fluids.

SURFACTANTS

Sulfosuccination of Methyl Ricinoleate and Methyl-12-Hydroxy Stearate derived from Renewable Castor Oil and Evaluation of their Surface Properties

Sulfosuccination of castor oil derived methyl ricinoleate and methyl 12-hydroxy stearate have been carried out in the present work. Synthesis involves malenization of secondary alcohol of methyl ricinoleate/ methyl 12-hydroxy stearate followed by sulfonation of maleic monoester to generate double headed dianionic surfactant with carboxylate and sulfosuccinate functionalities in the head group region. Various reaction conditions were optimized for maximum production of these two sulfosuccinates. Both compounds were evaluated for surface and detergency properties. The surface tension study indicated that the critical micelle concentration of sulfosuccinated methyl ricinoleate and methyl 12-hydroxy stearate is 0.26 and 0.11 mM respectively. Detergency property of these two surfactants indicated their excellencies in wetting time, emulsification and Ca-tolerance. However, these two surfactants exhibited very poor foam height and foam stability. (*J. Surf. Det.*, **2016**, 19, 447)

Stimuli Responsive Self Assembly of 3-(Octyloxy)-3-oxopropyl Acrylate-Co-Acrylic Acid Polymer in Aqueous Solution

A novel copolymer based on 3-(alkyloxy)-3-oxopropyl acrylate and acrylic acid was synthesized and

characterized. Surface tension and fluorescence probe techniques (using N-phenyl-1-napthylamine as probe) were employed to evaluate the surface property of the amphiphilic copolymer. The studied copolymer was found to reduce the surface tension of water to 40-46 mN m^{-1} depending on pH of the medium. The critical aggregation concentration (CAC) of the copolymer determined by surface tension method is found to be 0.28 mg/ml at pH 4, 1.13 mg/ml at pH 8 and 1.44 mg/ml at pH 10, pretty close to those obtained by steady state fluorescence probe technique (0.21, 1.13 and 1.48 mg/ml respectively at pH 4, 8 and 10). The pH-induced structure formation of the copolymer was also studied using various techniques such as steady state fluorescence using pyrene and 1,6-diphenyl-1,3,5-hexatriene (DPH) as probe, dynamic light scattering (DLS) and transmission electron microscopy (TEM). The protonation of pendant carboxylate moiety at acidic pH makes the aggregate compact and rigid. Conversely, fully ionized carboxylate moiety of the copolymer under alkaline condition resulted larger aggregate. (*J. Surf. Det.,* **2016**, 19, 619)

Synthesis and Evaluation of Surface and Biological Properties of some Lactic Acid-based Anionic Surfactants

In the present study, 11 lactic acid-based anionic surfactants were synthesized and evaluated for their surface and biological activities. The synthesis involved the esterification of lactic acid with a range of fatty alcohols differing in chain length as well as in branching and unsaturation. The resultant ester was sulfonated by treatment with chlorosulfonic acid followed by salt formation with aqueous NaOH solution. The surface properties of all the synthesized surfactants were determined using surface tensiometry. Synthesized surfactants showed low critical micelle concentration (CMC) values and a decreasing trend with an increase in the alkyl chain length. Alkyl branching also led to a mild change in CMC values when compared with linear counterparts having the same number of carbon atoms, though such decreases or increases were observed to be dependent on the position and number of the branching. Some of the synthesized surfactants exhibited good antimicrobial and anti-cancer activities against the tested microbial strains and cell lines. (*J. Surf. Det.,* **2016**, 19, 343)

Synthesis, Surface Properties of Undecanoic Acid & Vinylguaiacol-based Anionic Surfactants

The surface properties of biobased anionic surfactant synthesized from vinylguaiacol and 11-bromo undecanoic acid was reported. To further improve its hydrophilicity and bioavailability, amino acid head group incorporation was carried out. The performance properties such as foaming, wetting, emulsification value and calcium tolerance were evaluated. The studied surfactants possess excellent emulsion stability and moderate calcium tolerance as compared to commercially available surfactant sodium lauryl sulfate. The micelle formation and the thermodynamics involved at the air–water interface were estimated from surface tension measurements. These surfactants showed a higher tendency towards adsorption at the air–water interface than micellization. Dynamic light scattering and steady state fluorescence anisotropy study were carried out to shed light on the bulk micellization properties of the synthesized surfactant. Along with spherical micelles of 5 nm size, larger aggregates (35–84 nm) were observed with higher anisotropy values. FESEM images further confirmed the larger spherical micelles formed by these surfactants. The surfactants formed chiral aggregates above the critical micelle concentration as indicated by circular dichroism spectra. These surfactants may be suitable candidates as additives for detergents to improve their calcium tolerance properties especially in the case of hard water. Furthermore, a low foaming ability along with high emulsion stability may find these surfactants to be better replacement of the conventional surfactant used as emulsifiers in many industrial applications. (*J. Surf. Det.,* **2016**, 19(6), 1133; *Tenside Surf. Det.*, **2017**, 54(1), 18)

GLYCEROL-BASED CARBON CATALYSTS

Novel Heterogeneous SO_3Na-Carbon Transesterification Catalyst for the Production of Biodiesel

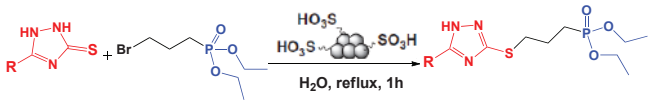
Glycerol, a major biodiesel by-product, was valorised into a novel and highly stable heterogeneous carbon-based solid base catalyst with transesterification activity. The SO_3H-carbon catalyst developed previously by us from glycerol was modified into base catalyst by treating with aqueous alkali under controlled

conditions. The reported solid base catalyst is first of its kind having polycyclic aromatic carbon sheets attached with $-SO_3Na$, -COONa and –ONa functionalities. The catalyst was characterized for its structural properties using XRD, FTIR, ^{13}C-MAS NMR, XPS, EDAX, SEM, TEM, TG/DTA, ICP-OES and Raman spectral techniques. The SO_3Na- catalyst was employed for the transesterification of sunflower oil to fatty acid methyl esters (biodiesel) in high yields (99%) at atmospheric pressure. The strong basic sites of the catalyst contributed to its remarkable performance and the activity was intact even after 8 cycles of reuse without any leaching, indicating its high structural stability. Thus, the reported SO_3Na-carbon catalyst possessed the potential of green and economic biodiesel production from oils & fats apart from clean glycerol as by-product.

Preparation of Heterogeneous Carbon-based Catalysts

An Efficient Nonconventional Glycerol-Based Solid Acid Catalyzed Synthesis and Biological Evaluation of Phosphonate Conjugates of 1,2,4-Triazole Thiones

A series of new diethyl (3-((5-aryl-1*H*-1,2,4-triazol-3-yl) thio)propyl)phosphonates (**7a–u**) has been synthesized in excellent yields by coupling 5-aryl-1*H*-1,2,4-triazol-3-thiones with diethyl (3-bromopropyl)phosphonate employing SO_3H-carbon catalyst derived from glycerol. The present investigation is concerned with the objective of discovering triazole derivatives as novel and potent anti-cancer, anti-bacterial and anti-fungal agents. Structures of the synthesized compounds were characterized by IR, NMR, and HRMS spectroscopic data. These triazole derivatives were screened for their in vitro cytotoxicity using the standard MTT (3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide) assay against a panel of five different human cancer cell lines (HeLa: Cervix, A549: Lung, A375: Skin, MDA-MB-231: Breast, and T98G: Brain). The anti-microbial activities of the synthesized compounds were investigated against four bacterial strains *Bacillus subtilis*, *Staphylococcus aureus*, *Escherichia coli*, *Pseudomonas aeruginosa*, and three fungal strains *Aspergillus niger*, *Aspergillus terreus*, *Aspergillus fumigatus. (Lett. in Drug Design Discov.,* **2016**, 13, 968)



Synthesis of diethyl (3-((5-aryl-1*H*-1,2,4-triazol-3-yl)thio)propyl)phosphonates

FOOD & NUTRITION

Generation of Data on Pesticide Residues and Metal Contaminants in Edible Vegetable Oils of Different Regions *(Sponsored by FSSAI, Govt. of India)*

Some countries have established maximum residue limits (MRLs) for each pesticide residue in different edible oils (crude and refined). The European Union standards, the Food and Agriculture Organization of the United Nations (FAO) and the World Health Organization (WHO) have defined MRLs in edible oils for various pesticide residues in the range of 0.002–2 mg/kg. However, MRL values for several pesticides that are currently being used in cultivation of vegetable oilseed crops in India have not yet been formulated. As of now FSSAI has notified allowed ranges for specific pesticide residue contaminants for only few oils like cottonseed oil, rapeseed oil and soybean oil. And further, there is no consolidated information available on heavy metal contamination of edible oils and fats at different parts of the country. Similarly FSSAI also notified allowed ranges for some selected heavy metal contaminants in edible oils and fats, hydrogenated, partially hydrogenated, interesterified vegetable oils and fats such as vanaspati, table margarine, bakery and industrial margarine, bakery shortening, fat spread and partially hydrogenated soybean oil. Therefore, the need of the hour is to conduct a study on contamination of pesticide residues, metal contaminants such as Cu, Sn, Zn, Cd, Cr, Fe, Ni, Pb, Hg, and As in edible oils and fats to address the safety aspects of consumers in India. Hence, the present proposal aims to screen ten selected oils namely soybean, sunflower, safflower, groundnut, rice bran, mustard, sesame, cottonseed, coconut, and palm for the presence of pesticides approved by CIBRC and also recommended by other appropriate Agriculture Research Institutes. Similarly these oils will also be screened for some selected metal contaminants such as Cu, Sn, Zn, Cd, Cr, Fe, Ni, Pb, Hg, and As. In this context, CSIR-IICT collected 131 edible oil samples of Sunflower, Groundnut, Soybean, Coconut, Cottonseed, Ricebran, Palm, Mustard, Rapeseed, Sesame, Palm Kernel, Vanaspati and Olive oils (crude and refined)

from different regions of India for the generation of data on pesticide residues & metal contaminants. Analytical methods and extraction protocols for the analysis of 52 pesticides by GC-MS/MS and LC-MS were standardized and also validated the methodology. The study showed that, the crude oils contain multiple pesticide residues namely, chloropyriphos, triazophos, triazophos, lamda-cyhalothrin, captan, dimethoate, endosulfan (I & II), tebuconazole and cypermethrin in high quantities, whereas most of the refined oils contain no pesticides. Even though, some of the refined oils showed the presence of some pesticides, they were found to be in much below than the MRL levels. None of the oils contains- trifluralin, chlorothalanil and dichlorvos pesticides. Soya bean oil was found contain the most common pesticide captan. Calibration studies for different metals were carried out on ICP-OES using the standard ASTM methods. The edible oil samples (131 no.) were also analyzed for some selected metal contaminants such as Cu, Sn, Zn, Cd, Cr, Fe, Ni, Pb, Hg, and As. In all the edible oils, heavy elements (As, Hg, Pb, Cd) were observed in very micro quantities. Especially, in refined edible oils negligible values were observed. Iron is the most common metal contaminant observed in majority of oils which may be due to the process reactors and storage tankers.

Assessment of the Quality of Vegetable oils while Frying and Formulation of Safety Guidelines for Fried Oils for Repeated Frying *(Sponsored by FSSAI, Govt. of India)*

Frying study was carried out by taking representative oils namely palmolein (saturated fatty acid-rich), groundnut and rice bran oils (mono unsaturated fatty acid-rich) sunflower (poly unsaturated fatty acid-rich), mustard (long chain fatty acid-rich) and coconut oils (Medium chain saturated fatty acid-rich) as each oil is unique in its nature and due to this reason the degradation characteristics may vary depending upon the fatty acid composition and the level of natural antioxidants present in the oils. Frying was carried out at 180-185°C for 20 cycles. Sample at each cycle was collected and studied for acid value, peroxide value, fatty acid composition and total polar material (TPM). Based on the analytical parameters, palm and rice bran oils with saturation and presence of native anti-oxidants were found to be more stable compared to soybean and sunflower oils with polyunsaturation.

Development of Novel Methodologies for the Identification and Quantification of Oils in Blended, Interesterified and Adulterated Oils based on TAG Structure, Fatty Acid Composition and Minor Constituents *(Sponsored by FSSAI, Govt. of India)*

Along with the nutritional and sensory need for consumption of oil vis-a-vis health risk associated with high intake, there are several man-made risk factors associated with consumption of edible oil. One such risk is adulteration of oil at different stages of food chain. Adulteration is done mainly for economic reason, by mixing cheap oil or used oil with good oil. In some cases, adulteration may happen with some unsafe oils like crude oils or produced with inefficient refining methods. Consumption of such oils adversely affects the health of people. Hence the proposed study aimed at generating data base of some commonly consumed edible oils in India to ascertain the presence or absence of a particular oil in blends as well as in adulterated oil. The proposed project is focused on generating data base on triacylglycerol (TAG) molecular species of all edible oils. Oil has characteristic TAG structure based on types and number of fatty acids present in it. The positioning of fatty acid over the glycerol backbone is very specific, with EFAs and PUFAs are mostly occupying 2-position of glycerol. Triolein in olive oil, triricinolein in castor oil, trilinolein in safflower, sunflower and soybean are some of the very specific symmetrical TAG molecular species. Cocoa butter is rich in SUS type TAG molecular species (like, POP, POS and SOS). In this proposed project, profiling of TAG molecular species of some of the commonly consumed edible oils was carried out. Developed method was validated by adopting some of the well-practiced adulteration (like Rice bran oil in Mustard oil; Cottonseed oil in sunflower or soybean oil; Palm oil in rice bran, groundnut or any other oil; High oleic sunflower oil in olive oil; Palm kernel oil/ palm oil in coconut oil) of edible oils at different ratios of blending.

Application of Low Calorie Hypocholesterolemic Structured Lipid as Potential Bakery Fat

The hypocholesterolemic effects of two low calorie structured lipids (SL1 and SL2) containing essential fatty acids, prepared by lipase catalyzed interesterification of ethyl behenate respectively with sunflower and

soybean oils were studied in rats and rabbits. The feeding experiment conducted on rats as well as rabbits, fed on normal and atherogenic diet containing 10% of SL1 and SL2 (experimental) and sunflower oil (control) indicated no adverse effects on growth and food intake. The structured lipids however beneficially lowers serum and liver lipids, particularly cholesterol, LDL cholesterol, triglycerides and also maintains the essential fatty acid status in serum and liver. The lipid deposition observed in the arteries of rabbits given atherogenic diets was significantly reduced when structured lipids were included in the diet. These observations coincided with reduced levels of serum cholesterol particularly LDL cholesterol observed in experimental groups. Therefore prepared structured lipids, designed to have low calorific value also beneficially lower serum lipids and lipid deposition in animals given atherogenic diets. (*Int. Food Res. J.*, **2016**, 23, 854)

Comparative Evaluation of Lysolecithin from Rice Bran Oil *vis-à-vis* Lipotropic Agents in Broiler Chicken Diet

The possibility of using lysolecithin from rice bran oil (LL) as a lipotropic agent was explored in the diet of broiler chickens. The LL was evaluated at 0.1 and 0.5% levels in diet vis-à-vis choline chloride, betaine or a commercial LL (0.1% of any) in broiler chickens (270) from 0 to 35 d of age. The diets were *isonitrogenous* and *isocaloric*. Body weight at 35 d was significantly higher in the group fed betaine, while LL showed no effect on growth, feed consumption, serum cholesterol concentration, slaughter variables and liver protein, and fat contents in comparison to control. The serum concentration of triglycerides at 35 d of age, however, decreased significantly with betaine, commercial LL and rice bran oil LL at both the levels. It is concluded that rice bran oil LL at dietary levels upto 0.5% showed no adverse effect on performance and reduced serum triglycerides content in broiler chickens, while betaine improved body weight. (*Ind. J. Animal Sci.,* **2017**, 87 (2), 241)

Effects of Dietary Inclusion of Lysolecithin from Rice Bran Oil on Performance, Serum Biochemical Profile, Organ Weights, Immune Response and Nutrient Digestibility in Broiler Chicken

Lysolecithin was included in diet at graded levels (0, 0.05, 0.1, 0.2, 0.4, 0.8, 1.6 and 3.2 % in diet) and fed to a total of 640 broiler chickens from 0 to 35 d of age. The diets were *isonitrogenous* and *isocaloric*. Body weight was higher in the group fed the highest level (3.2 %) of LL. Feed intake was significantly ($p<0.01$) lower in the groups fed 1.6 and 3.2 % LL in comparison to control, whereas feed conversion efficiency was significantly ($p<0.01$) improved at the highest level of LL (3.2 %). Serum concentration of protein, total cholesterol and triglycerides as well as slaughter parameters, organ weights, fat deposition in liver and muscle, and SRBC response were not affected. The fat digestibility was significantly ($p<0.05$) improved at the higher levels (1.6 and 3.2 %) of LL in diet. It is concluded that rice bran oil LL could be safely used in broiler chicken diet and at dietary levels of > 1.6 % the LL improved the body weight, feed conversion efficiency and fat digestibility in broiler chickens. (*Ind. J. Animal Res.*, **2017**, 51, 700)

Enzymatic Synthesis of Structured Lipid-based on Silkworm Oil and Palm Olein

Synthesis and characterization of structured lipid (SL) containing α-linolenic acid (ALA) was carried out employing palm olein (POo) and silkworm oils (SWO) by enzymatic interesterification method. POo was chosen as one of the substrate because it does not contain ALA and is oxidatively more stable compared to other vegetable oils. The study was aimed to obtain an ALA content of about 10% in the structured lipid which was achieved with the blend of POo and SWO in the ratio of 80:20 (wt/wt). The reactions were catalysed by a sn-1, 3-regiospecific lipase, Lipozyme RM IM. The effect of reaction time, temperature were studied and were found to be at 4 hr and 65°C-70°C respectively at a lipase concentration 4% (w/w) of substrates. Physico-chemical characteristics of both the substrate oils were determined and compared with those of initial physical blends and the prepared SL. The oxidative stability of SL was also studied and the induction time was found to be at 13.2 hr which was higher with respect to SWO. The SL prepared using refined POo, SWO has potential applications in nutraceutical, food and industrial applications. (*J. Oil Palm Res.*, **2017**, 29 (1), 81)

VALUE ADDITION TO VEGETABLE OILS & THEIR PROCESSING BY-PRODUCTS

Studies on mosquitocidal and larvicidal formulations based on extracts from *Madhuca longifolia, Pongamia glabra & Ocimum tenuiflorum* L. *(sponsored by TRIFED, Govt. of India)*

The karanja seed collected from the market for executing the project contain 25.7-27.1% of oil (dry basis) and 1.1-1.2% of karanjin. Karanja seeds were taken up for extraction of oil using both solvent extraction as well as expelling route to get the corresponding deoiled cake. Both solvent extracted and expelled cake was extracted using isopropanol (IPA) as eluting polar solvent to get karanjin-rich extract. However, the IPA-soluble extract obtained from expelled cake contains more karanjin (16.1%) than the IPA-soluble extract obtained from solvent extracted cake (11.1%). The karanjin-rich crude IPA-soluble polar extract showed excellent mosquito larvicidal activities against *Aedes aegypti* and *Culex quinquefasciatus* strains. LC_{50} and LC_{99} values of polar extract obtained in expelled route on the early fourth instar larvae after 24 h exposure were found to be 84.77 and 183.67 ppm against *Culex quinquefasciatus* and 69.02 and 188.21 ppm against *Aedes aegypti*. The ovicidal activity of the crude polar extract was also evaluated against eggs of two larval strains, *Aedes aeygpti* and *culex quinifacitus a*fter 48 hrs of exposure. EC_{50} and EC_{99} ovicidal values of polar extract obtained in expelled route were found to be 18.81 and 55.77 ppm against eggs of *Aedes aegypti* and 45.66 and 108.04 ppm against *Culex quinquefasciatus*. However, the knock down results during the evaluation of adulticidal activity of the extract is not good. This may be due to lack of mist formation and/or non-volatile nature of the active ingredient, i.e. karanjin. It was planned to use three alternate modes for checking adulticidal acitivity. The test was conducted using three types of formulations namely spray formulation, liquid vaporiser and aerosol. Even in these three modes of applications, adulticidal activity was found to be very poor. Hence this karanjin-rich crude polar extract can be used as mosquito ovicidal and larvicidal formulated product.

Process for the Preparation of Purified Gamma linolenic Acid (GLA, 98%) from Borage Oil *(Sponsored by M/s Fermish Clinical Technologies, New Delhi)*

CSIR-IICT developed an economically efficient process for the preparation of a high grade, pure form of Gamma-Linolenic-Acid (GLA, ≥98% pure)from borage oil. The process was demonstrated to M/s Fermish Clinical Technologies, at 2 Kg/ a batch scale of Borage oil in 3 consecutive batches to obtain 3x100 g of 97-98% GLA.

Characterization & Quantification of lipids in Hepatitis-B surface Antigen (HBsAg) Samples *(Sponsored by M/s Shantha Biotech, Hyderabad)*

Recombinant Hepatitis B surface antigen protein, a vaccine component is being manufactured at Shantha Biotechnics Ltd, Hyderabad. This protein is lipoprotein and the process of manufacturing involves a series of purification steps (altogether 9 steps). At every process step there is removal of contaminants which includes lipids and the extent of removal varies at different stages. The objective of the project is to quantify total lipid as well as its characterization during the 9 purification steps carried out at M/s Shantha Biotech. Total lipid content, total phospholipid content, composition of different classes of phospholipid and their quantities were determined for a number of sample submitted by the sponsoring agency at 7 different purification stages.

Process Know-how for the Upgradation and Bleaching of Crude Rice Bran Wax

Rice bran wax is a by-product of rice bran oil refinery and being sold at a low price of Rs 15-20/kg. Process for the upgradation and bleaching was developed from crude rice bran wax at 2 kg/batch. Refined rice bran wax has several applications as polishing agent in boot polishes, candles, fruit coating etc. This technology was transferred to the following 3 industries during 2016-18.

1. M/s Marico India Ltd., Mumbai

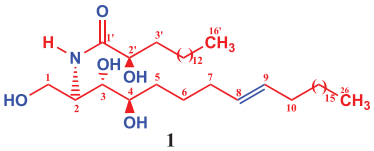
2. M/s Kanchan Oil Mills Ltd., Kolkata

3. M/s Sheel Chand Agroils Pvt Ltd., Uttarakhand

CENTRE FOR NATURAL PRODUCTS & TRADITIONAL KNOWLEDGE

Self Gelating Isoracemosol A, New Racemosaceramide A, and Racemosol E from *Barringtonia Racemosa*

Phytochemical investigation of the $CHCl_3$ extract of the fruits of *Barringtoniaracemosa* resulted in the isolation of two new metabolites along with isoracemosol A and betulinic acid as known metabolites. The new compounds were characterized as phytosphingosine-typeceramide [(2*S*,3*S*,4*R*)-2-[(2*R*)-2-hydroxyhexadecanoylamino]-hexacos-8(*E*)-ene-1,3,4-triol, **1**] and racemosolE[21β-acetoxy-22α-(2-methylbutyroxy)-olean-12-ene-3β,16α,28-triol, **2**] on the basis of extensive spectroscopic data analysis and chemical modifications. In addition, the self gelating property of isoracemosol A (3) was investigated for the first time, which leads to the unexpected agglomerated porous like morphology. (*Nat. Prod. Res.*, **2017**, 31, 63)



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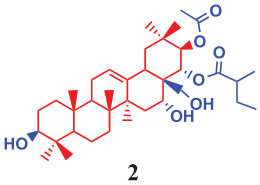
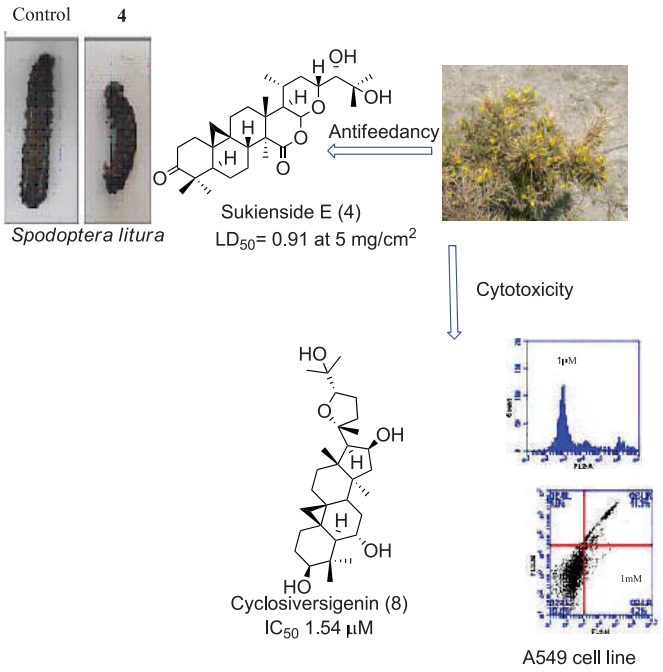


2

New Cycloartane type-Triterpenoids from the arial parts of *Caragana sukiensis*and their biological activities

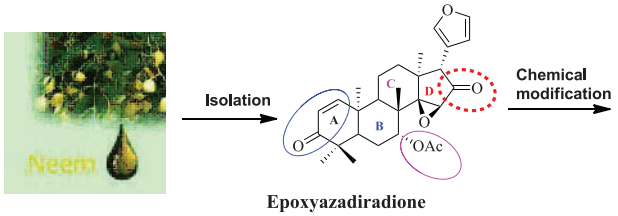
A comprehensive re-investigation of aerialparts of *Caragana sukiensis* resulted in the isolation of twelve compounds (**1-12**) including three new cycloartane type triterpenoids (**3-5**) respectively. Chemical structures of the isolated compounds were established by analysis of their IR, HRMSESI, 1D and 2D NMR spectroscopic data. In addition, these compounds were evaluated for their cytotoxic activity against cancer lines (HeLa, A549, MCF-7, DU-145) and Human embryonic kidney cell line (HEK-293). The results indicated that compound **8** showed potent cytotoxic activity against A549 with IC_{50} value of 1.54 µM which is comparable to standard drug, doxorubicin. Further, flow cytometric analysis showed that compound **8** arrested the cell cycle in the Go/G1 phase leading to apoptotic cell death. (*Eur. J. Med. Chem.,* **2017,** 136, 74)

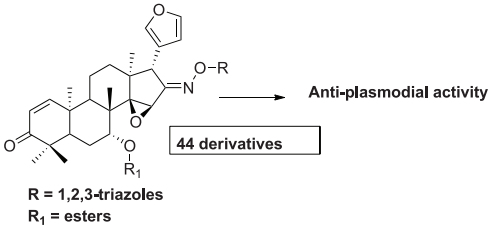
In addition, Hoechst 33258 staining, Annexin V-FITC assay and measurement of mitochondrial membrane potential also suggested that **8** induced cell death by apoptosis. All the isolates were also screened for their antifeedant and insecticidal activity against tobacco caterpillar (*Spodopteralitura*), using no-choice leaf disk method. Among screened compounds **1**, **3**, **4** and **6** showed potent antifeedancy with ED_{50} values of 0.59, 1.19, 0.67, and 1.68 µg/cm^2.



Synthesis and Evaluation of Anti-plasmodia and Cytotoxic activities of Epoxyazadiradione derivatives

Epoxyazadiradione (**1**), a major compound derived from Neem oil, showed modest anti-plasmodial activity against CQ-resistant and CQ-sensitive strains of the most virulent human malaria parasite *P. falciparum*. A series of analogues were synthesised by modification of the key structural moieties of this high yield natural product. Out of the library of all compounds tested, compounds **3c** and **3g** have showed modest anti-plasmodial activity against CQ-sensitive (IC_{50} 2.8±0.29 µM and 1.5±0.01 µM) and CQ-resistant strains (IC_{50} 1.3 ±1.08 µM and 1.2± 0.14), while compounds **3k**, **3l** and **3m** showed modest activity against CQ-sensitive strain of *P. falciparum*with IC_{50} values of 2.3±0.4 µM, 2.9±0.1 µM and 1.7±0.06 µM, respectively.

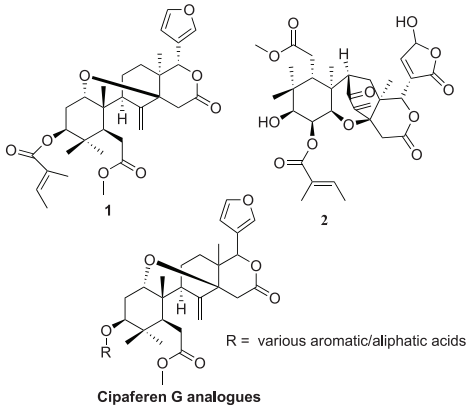




Additionally, cytotoxic properties of these derivatives against SIHA, PANC 1, MDA-MB-231, and IMR-3 cancer cell lines were also studied and the results indicated that low cytotoxic potentials of all the derivatives which indicating the high selectivity index of the compounds. (*Eur. J. Med. Chem.,* **2017,** 134, 242)

New Seco-Limonoids from *Cipadessabaccifera*: Isolation, Structure determination, Synthesis and Their Antiproliferative Activities

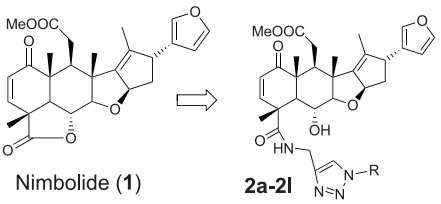
A comprehensive reinvestigation of chemical constituents from $CHCl_3$-soluble extract of *Cipadessabaccifera* led to the isolation of two new limonoids **1**, **2** together with six known compounds **3-8**. Their structures were established on the basis of extensive analysis of spectroscopic (IR, MS, 2D NMR) data. Further, a series of cipaferen G (**3**) derivatives were efficiently synthesized utilizing Yamaguchi esterification (2, 4, 6-trichlorobenzoyl chloride, Et_3N, THF, DMAP, toluene) at the C-3 position of the limonoids core, which is being reported for the first time.



The anti-proliferative activity of the isolates and the synthetic analogues were studied against HeLa, PANC 1, HepG2, SKNSH, *MDA-MB-231* and IMR32 cancer cells using the sulphorodamine B assay. Among the tested compounds, **13d** and **13h** manifested potent activity against IMR32, HepG2 cell lines with GI_{50} 0.013 and 0.01µM, respectively. (*Fitoterapia,* **2017,** 117, 34)

"Click" Reaction based Synthesis of Nimbolide derivatives and Study of their Insect Antifeedant Activity against *Spodopteralitura* Larvae

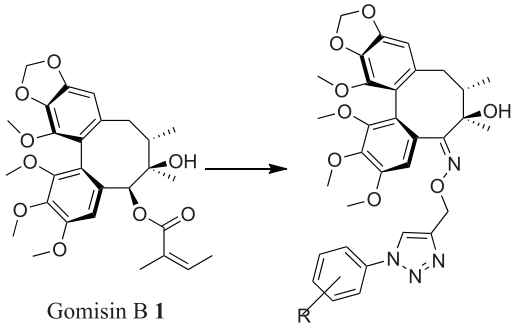
A series of Nimbolide-triazole conjugates were synthesized through copper(I)- catalyzed azide–alkyne "click" chemistry approach and these derivatives (**2-4**, **2a-2l**) were characterized using modern spectroscopic techniques. Antifeedant activities of these derivatives were studied on Tobacco Caterpillar, *Spodopteralitura* (F.)using no-choice leaf disk bioassay. Interestingly, the synthesized derivatives were more effective in reducing feedancy by insect species when compared to the parent nimbolide. Among the tested compounds, **2a**, **2c**, and **2d** showed potent antifeedancy with ED_{50} values of **0.49, 0.95** and **0.97** mg/cm^2 against *S. litura.* Several of the analogs were also toxic or caused developmental abnormalities following leaf disc assay. (*Fitoterapia,* **2017,** 123, 1)



Novel Gomisin B Analogues as Potential cytotoxicAgents: Design, Synthesis, Biological evaluation and Docking Studies

As part of pharmacological-phytochemical integrated studies on medicinal flora, Gomisin B (**1**) was isolated as major phytochemical lead from *schisandra grandiflora*, a plant traditionally used in different Asian systems of medicine. A series of 1,2,3-triazoles derivatives were synthesizedat the C-7' position of the gomisin B core through diastereoselective Michael addition followed by regioselective Huisgen 1,3-dipolar cycloaddition reactions. All these triazolyl derivatives (**5a-5q**) were well characterized using modern spectroscopic techniques and evaluated for their anti-cancer activity against a

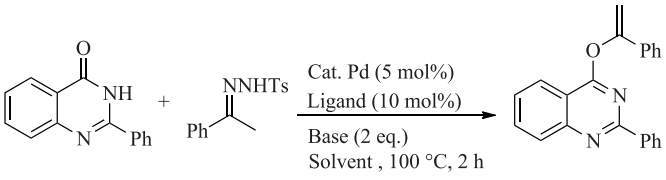
panel of five human cancerous cell-lines. Among them, compound **5b** exhibited the best cytotoxicity against SIHA cell (IC_{50} 0.24 mM) which was more than the standard drug doxorubicin, while the other derivatives were exhibited moderate to low activities in tested cell lines. The cell cycle analysis indicated that compound **5b** stalled HeLacells at G2/M phase. **5b** promoted tubulin polymerization and this was supported by the docking studies, wherein **5b** showed significant binding affinity at the colchicine binding pocket of tubulin. Overall, we identified a novel small molecule that demonstrated anticancer activity by promoting *in vitro* tubulin assembly. (*Eur. J. Med. Chem.,* **2017,** 139, 441)



Gomisin B **1** **5a-5q**

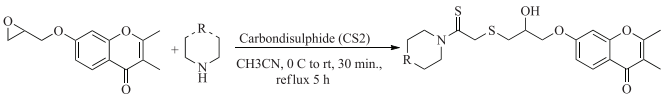
Palladium(II)-catalyzed direct O-alkenylation of 2- arylquinazolinones with N-tosylhydrazones: an efficient route to O-alkenylquinazolines

An efficient Pd(ii)-catalyzed direct O-alkenylation of 2-arylquinazolinones with simple ketone-derived N-tosylhydrazones is reported. In this reaction, O-alkenylquinazolines were obtained in good yields, with excellent functional group tolerance. Pd-carbene migratory insertion is proposed as the key step in the reaction mechanism. (*Chem. Commun.,* **2017,** 53, 1672)



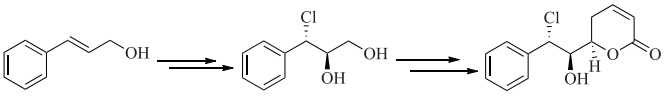
Synthesis of new chromeno-carbamodithioate derivatives and preliminary evaluation of their antioxidant activity and molecular docking studies

New chromeno carbamodithioates (7a-i), have been synthesized from 2, 3-dimethyl-7-(oxiran-2-ylmethoxy)-4H-chromen-4-one (5), carbondisulphide and commercially available acyclic and cyclic secondary amines in acetonitrile with good to excellent yields. The free radical scavenging activity of novel chromone-carbamodithioate analogues was quantitatively estimated by spectrophotometric method. Whereas, molecular docking studies were performed with the active site of cyclooxygenase-2 to identify hydrogen bonding, hydrophobic and ionic interactions between protein and ligands. The compounds 7g and 7h demonstrated potent antioxidant activity with IC_{50} of 1.405±0.019mM and 1.382±0.35mM respectively compared to Ascorbic acid. (*Bioorg. Med. Chem. Lett.,* **2017,** 27(5), 1256)



First Stereoselective synthesis of (6*R*, 7*R*, 8*S*)-8-chlorogoniodiol

A stereoselective synthesis of (6*R*,7*R*,8*S*)-8-chlorogoniodiol has been achieved in a linear sequence of 12 steps and 19.8% overall yield from cinnamyl alcohol. The key steps include Sharpless asymmetric epoxidation, regioselective ring opening of epoxide, indium-mediated Barbier allylation, and Still–Gennari olefination. (*Synthesis,* **2017,** 49, 2483)



Method validation and simultaneous determination of two bio-active marker compounds in *Pongamiapinnata*:seed and karanj oil by UPLC-MS

Seed of *Pongamiapinnata*(Linn.) Merr known as "Karanj" widely used in traditionalsystem of medicine. Oil from karanj seeds contain flavonoids which possess diverse pharmacological properties. The seed oil was subjected to karanj oil-liquid extraction with methanol to isolate karanjin and pongamol which are active principle of karanj. The oil mainly used for skin diseases such as psoriasis, eczema and vitiligo etc. A validated reversedphase ultra-performance liquid chromatography method with photodiode array detector was successfully developed for the first-time report to simultaneously determine two active compounds karanjin and pongamol in karanj seed extract and its oil. Separation carried

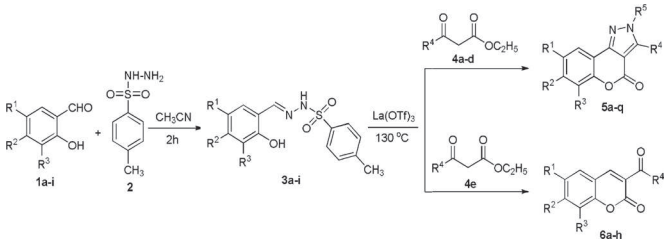
through a BEH C18 column by gradient elution using 0.1% formic acid in water (v/v):methanol: acetonitrile at 0.2 mL/min. Significant linear correlations were found between component concentrations and specific chromatographic peak areas. The % R.S.D. values found by the method indicating precision, range and recovery to be good. Thus, the proposed validated method can be applied as a reference standard for quality control analysis commercial samples of karanj oil. (*World J. Pharmaceut. Res.,* **2017**, 6, 846)

HPTLC method development and quantification of curcumin content indifferent extracts rhizome of *Curcuma longa* L.

Turmeric is very long known for its potent medicinal values in Indian traditional systems of medicine. *Curcuma longa* L. commonly known as turmeric (Haldi) is a well-known plant which is used as a drug in traditional medicine such as Ayurvedic and Unani system of medicine. Curcumin is main active component present in the rhizomes of *C. longa*. The contents of curcuminoids in turmeric rhizomes vary often with varieties, locations, sources, andcultivation conditions, while there are significant variations in composition of turmeric rhizomes with varieties and geographical locations. The present study reported a simple,sensitive and fast HPTLC method for quantification of curcumin in solvent extracts of rhizomes of *C. longa* L. The separation was performed on TLC aluminum plates precoated with silica gel G F254. Good separation was achieved in the mobile phase of chloroform: methanol: formic acid (9.6:0.4:0.1, v/v) at R*f* = 0.70 ± 0.05 for curcumin. The method was validated successfully having good resolution of peaks along with precision, accuracy and repeatability. Curcumin capsules (>95% curcumin) have not been emerged as a drug so far but had been taken in food or dietary supplement. In traditional medicine, it is well recommended to use 2 to 3 grams turmeric powder in our daily diet. Therefore, the objective of the study to extract turmeric and assess curcumin content and other constituents by HPTLC with a suggestion to use the whole extract derived from the equivalent 2 to 3 grams of the turmeric powder. Present study is to determine high content of curcumin 95-98% and recommended for many diseases. The HPTLC method can be used for quantification of Curcumin in extracts of rhizomes of *C. longa* L. (*Annals of phytomed.,* **2017,** 6, 74)

Neoteric Synthesis and Biological Activities of Chromenopyrazolones, Tosylchromenopy razolones,Benzoylcoumarins.

Chromenopyrazolones, tosylchromeno pyrazolones and benzoylcoumarins were prepared by the reaction of salicylaldehyde tosylhydrazones with 3-oxobutanoates. The title compoundswere screened for their in vitro



anti-microbial, DPPH, ABTS.+ free radical scavenging, a-glucosidase inhibitory and anti-inflammatory activities. The bioactivity profile studies revealed that the trifluoromethyl chromenopyrazolones were effective for anti-microbial activity. Trifluoromethyl chromenopyrazolones5h, 5j, 5l, tosyl chromenopyrazolones 5m-q and benzoylcoumarin 6g are the promising a-glucosidase inhibitors. The methyl chromenopyrazolones 5b-d, trifluoromethyl Chromenopyrazolones 5h-l, tosylchromeno pyrazolone 5m and methoxy benzoyl coumarin 6h denoted promising anti-inflammatory activity. (*ChemistrySelect,* **2017**, 2, 10628)

Diabesity: The unacknowledged Indian Knowledge

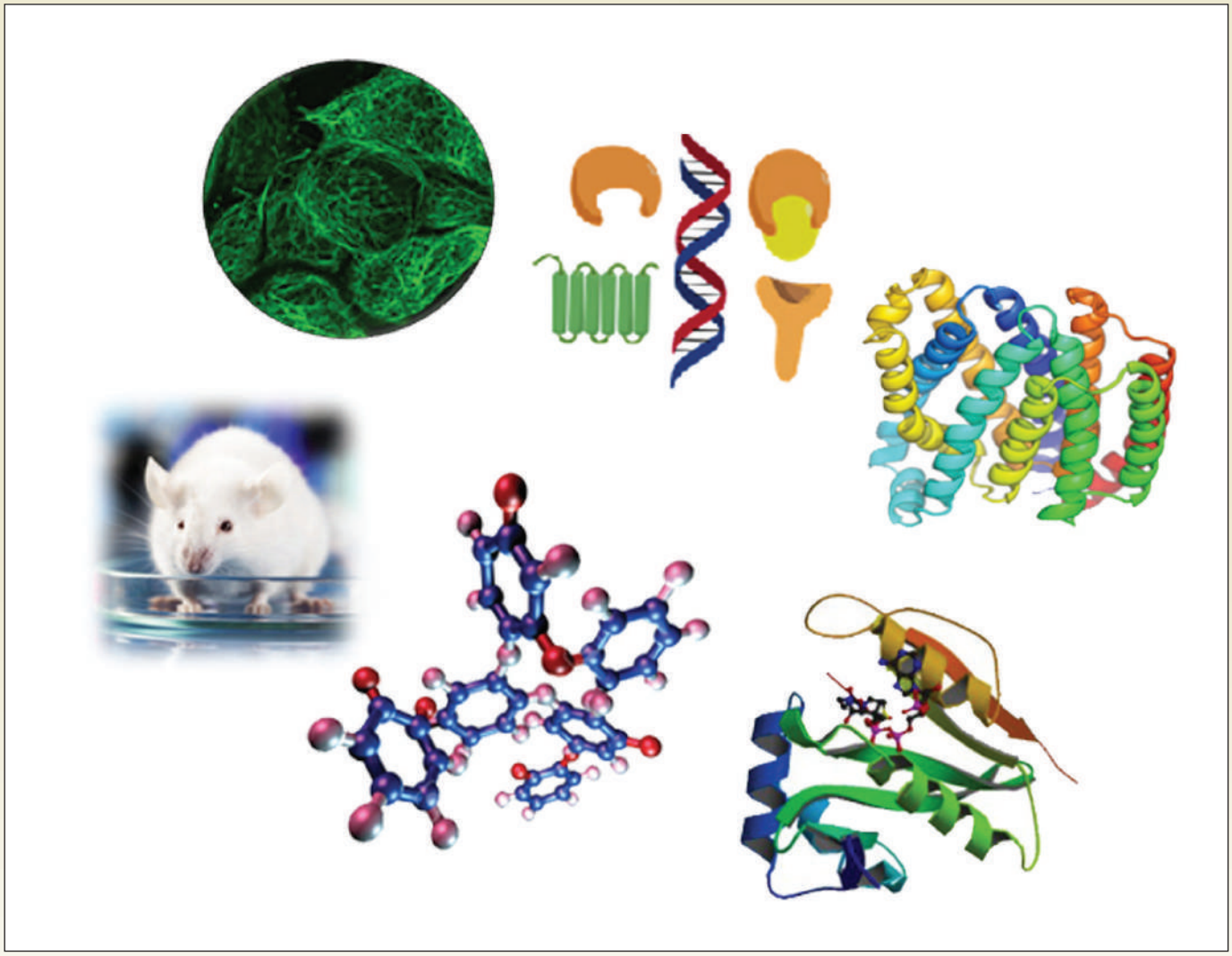
The monograph entitled Total dietary regulation in the treatment of diabetes published on October 15, 1919 from The Rockefeller Institute of Medical Research, New York finds that "The earliest mention of the sweetness of diabetic urine is contained in the Ayur Veda of Sustruta, dating from sixth century. The disease bore the distinctive name of Madhumeha or honey-urine. Thus the most prominent clinical feature, and one of the most widely supported modern hypotheses concerning etiology, received their first mention in India. But Hindu medicine failed to advance beyond this beginning, and exerted no influence on progress elsewhere". (Ch.1, p5) In a nutshell, the present monograph provides the informations which were unacknowledged at that time. **(***TAS popular science series,* **1st edition 2017,** Telangana Academy of Sciences)

Re: Patient commentary: the current model has failed. Failing Current Drug Discovery Models

Reading a patient's commentary is really eye opening and also moving when we read patients' anguish as a human being and not as a professional. In the course of drug discovery and development of therapeutics for not only cancer but also other diseases, we should also think about the root cause of disease. Public education and awareness about the origin of disease and their relationship to our current lifestyle should be the prime objective.

So far as the process of drug discovery is concerned, it involves money and after development industries will focus only on money. This business depends on money and only money. Here profit and loss matters a lot. Humanity is certainly involved but it is secondary. We have reached the moon, mars and other planets before reaching into the human heart. Cultivation of human sensitivity is required not only in professional organizations but also in public. Having achieved this goal, we may solve the majority of sufferings ourselves and reduce the burden on organizations involved in drug discovery process. Before we blame others, we should look at whether we took care of ourselves. Poor animals have become target for drug discovery. Business houses have emerged. In that business, laboratory animals are living lavish life. Humans are still suffering from poverty and hunger. *(Brit. Med. J.,* **2017**, 359, j4568)

CHEMICAL BIOLOGY



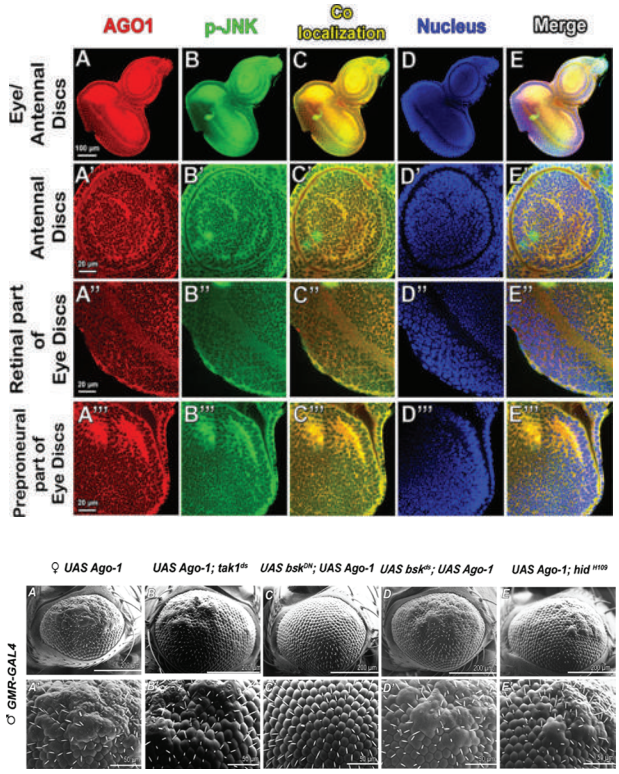
Research at Applied Biology Division at CSIR-IICT is dedicated to provide solutions for the health care issues. Majority of the research programs under this banner are inter-disciplinary in nature. Some of the strengths of this division are in the area of

- Cancer, cardiovascular and Neurobiology
- Stem cells and regenerative medicine
- Antitubercular agents
- Structural biology and Biotechnology
- Drug delivery and Nano-medicine

Cancer Research

- The limitations of the current prostate cancer (PCa) screening tests demands new biomarkers for early diagnosis of PCa. ESIMS/MS and GC-MS was performed for identification of significantly altered lipids in cancer patient's serum compared to controls. Lipidomic data from cancer patinet's serum (n = 18) compared to normal (n = 18) with no history of PCa followed by stringent validation criteria revealed that the altered lipids PC (39:6) and FA (22:3) offer a new set of biomarkers in addition to the existing diagnostic tests that could significantly improve sensitivity and specificity in PCa diagnosis. (*PLOS One,* **2016,** 0150253)
- Our previous study showed that Tumor protein D52 (TPD52), a proto-oncogene overexpression could increase migration and proliferation of LNCaP cells contributing to the development of prostate cancer. However, mechanism of TPD52 in prostate cancer initiation and progression remains elusive. Mechanistically, we found that TPD52 confers transactivation of nuclear factor-κB, thereby enhancing its target gene expression in LNCaP cells. Furthermore, TPD52 directly interacts with nuclear factor-κB p65 (RelA) and promotes accumulation of phosphorylated nuclear factor-κB (p65) S536 that is directly linked with nuclear factor-κB transactivation. Interestingly, in TPD52 overexpressing LNCaP cells, nuclear factor-κB inhibition prevented the autocrine/paracrine activation of STAT3. Collectively, these results reveal mechanism by which TPD52 is associated with prostate cancer progression and highlight the approach for therapeutic targeting of TPD52 in prostate cancer. (*Tumor Biol.,* **2017**, 1) Furthermore, in IMR-32 neuroblastoma (NB) cells retinoic acid (RA) stimulates an increase in expression of TPD52. Here, we demonstrate that TPD52 is essential for RA to promote differentiation of NB cells. TPD52 protects cells from apoptosis and arrest cell proliferation by varying expression of p27Kip1, activation of Akt and ERK1/2 thus promoting cell differentiation. Our data reveal that TPD52 act through activation of JAK/STAT signaling pathway to undertake NB cells differentiation induced by RA. (*J. Cellul. Biochem.*, **2017**, 9999, 1)
- The B-lymphoma Moloney murine leukemia virus insertion region-1 protein (BMI1) acts as an oncogene in various cancers, including breast cancer. Recent evidence suggests that BMI1 is rapidly recruited to sites of DNA double strand breaks where it facilitates histone H2A ubiquitination and DNA double strand break repair by homologous recombination. Our research showed that miR-15a and miR-16 expression is decreased during the initial period after DNA damage where it would otherwise down-regulate BMI1, impairing DNA repair. This suggested that miR-15a and miR-16 mediate the down-regulation of BMI1, which impedes DNA repair while elevated levels can sensitize breast cancer cells to doxorubicin leading to apoptotic cell death. This data identified a new target for manipulating DNA damage response that could impact the development of improved therapeutics for breast cancer. (*Sci. Rep.,* **2017**, 7(1), 4263)
- pH-sensitive drug carriers that are sensitive to the acidic (pH = ~6.5) microenvironments of tumor tissues have been primarily used as effective drug/gene/siRNA/microRNA carriers for releasing their payloads to tumor cells/tissues. We have developed a nanocarrier system from kojic acid backbone-based cationic amphiphile containing endosomal pH-sensitive imidazole ring. This pH-sensitive liposomal nanocarrier effectively delivers anti-cancer drug (Paclitaxel; PTX) and siRNA (Bcl-2), and significantly inhibits cell proliferation and reduces tumor growth. Tumor inhibition response attributes to the synergistic effect of PTX potency and MDR reversing ability of Bcl-2 siRNA in the tumor supporting that kojic acid based liposomal pH-sensitive nanocarrier as efficient vehicle for systemic co-delivery of drugs and siRNA. (*Sci. Rep.*, **2016**, 6, 35223)
- Role of Ago-1 in regulating apoptosis during Drosophila development. Over expression of Ago-1 resulted in reduced number of ommatidia in the eye and produced smaller size brain in adult and larval Drosophila. Study showed that Ago-1 stimulates phosphorylation of JNK through transforming growth factor-β activated

kinase 1- hemipterous (Tak1-hep) axis of JNK pathway and in-turn regulates pro-apoptotic genes hid, grim & reaper and induces activation of Drosophila caspases (cysteinyl aspartate proteinases);DRONC (Death regulator Nedd2-like caspase), ICE (alternatively Drice, Death related ICE-like caspase) and DCP1 (Death caspase-1) by inhibiting apoptotic inhibitor protein DIAP1. Ago-1 also inhibits miR-14 expression to trigger apoptosis. Our findings propose that Ago-1 acts as a key regulator in controlling cell death, tumor regression and stress response in metazoan providing a constructive bridge between RNAi machinery and cell death. (*PLOS One*, **2017**, 13(1), e0190548)



- Glioma amplified sequence 41(GAS41) is a potent transcription factor that play a crucial role in cell proliferation and survival. In glioblastoma, the expression of GAS41 at both transcriptional and post transcriptional level needs to be tightly maintained in response to cellular signals. We identified GAS41 as a novel target for endogenous miR-203 and demonstrate an inverse correlation of miR-203 expression with GAS41 in glioma cell lines (HNGC2 and U87). Over expression of miR-203 negatively regulates GAS41 expression in U87 and HNGC2 cell lines. Moreover, miR-203 restrained miR-10b action by suppressing GAS41. GAS41 is essential for repressing p53 in tumor suppressor pathway during cell proliferation. Conversely reconstitution of miR-203 expression induced apoptosis and inhibited migratory property of glioma cells. Taken together, we show that miR-203 is a key negative regulator of GAS41 and acts as tumor suppressor microRNA in glioma. (*PLOS One*, **2016**, 11(7), 0159092)

- Protacs are heterobifunctional molecules which bind two molecular targets in cancer cells. The first target is usually an oncogene and the second target is an E3 ubiquitin ligase (either Cereblon (CRBN) or von Hippel-Lindau (VHL) proteins in cells. The binding of a Protac molecule to two proteins is facilitated by their respective small molecule inhibitors (oncogene) or ligands (VHL or CRBN). A linker of various chain lengths is employed to hitch the two moieties on either side.After the cells are treated with Protacs, the inhibitor of the oncogene binds the target and the E3 ligase binds the E3 proteins (Cereblon or VHL). This binding leads to the recruitment of the oncoprotein to the E3 ligase complex, subsequently the ubiquitin chain bound to E2 protein (ubiquitin-loaded ubiquitin conjugating enzyme) is transferred to the oncoprotein. Thus, Protacs effectively degrade the target protein by a proximity-based ubiquitination. Hence, we aim to design, synthesize and evaluate chimeric molecules that will bind mIDH1 and recruit a cellular E3 ligase, leading to the degradation of mIDH1 protein. Glioblastomas (GBMs), acute myeloid leukaemias (AML) and chondrosarcomas harbour mutations in isocitrate dehydrogenase-1 (IDH1). Currently, the small molecule inhibitors of mutant IDH1 (mIDH1i) are in either Phase 1 or II clinical trials. However, all the inhibitors under clinical trials study inhibit only mIDH1 enzymatic activity, but also do not eliminate the protein. To achieve our goals, we designed the mIDH1-Protacs to harbour a linker (s) that is covalently linked to the chemical moieties on either side via chemical synthesis. Established small molecule inhibitor of mIDH1 will be hitched to the linker on one side and the ligands that bind E3 ubiquitin ligase, Cereblon or Von-Hippel Lindau (VHL) proteins, on the other. Further, to discern the specificity of the Protacs, CRISPR/Cas9 technology will be used to generate mIDH1 or E3 ligase specific knockouts. Finally, co-crystals of mIDH1 with an E3 ligase in the presence of Protacs will be performed to acquire structure-based information. Overall, the project deals with elucidating new paradigm in drug discovery.

- The recurrence of breast cancer in patients is a persistent challenge to the medical fraternity. Breast tumor contains a small population of cells with high tumor initiating and metastatic potential, known as cancer stem cells (CSCs), which are resistant to existing chemotherapeutics. CSCs contribute to the aggressiveness of triple negative breast cancers (TNBCs), thereby necessitating the identification of molecular targets on breast CSCs. TNBC cell line MDAMB-231, in comparison with MCF-7, demonstrated a higher expression of epidermal growth factor receptor (EGFR). Thus, the naturally occurring flavanone, chrysin, with limited potential as a chemotherapeutic agent, was structurally modified by designing an analog with EGFR binding affinity using a molecular docking approach and subsequently synthesised. Chrysin analog CHM-09 and known EGFR inhibitors demonstrated a comparable anti-proliferative, anti-migratory activity along with the induction of apoptosis and cell cycle arrest in MDA-MB-231. Furthermore, sorted CD24-/CD44+-breast CSCs and CD24+-breast cancer cells from MDA-MB-231 demonstrated a markedly high expression of EGFR in the former than in the latter. CHM-09 and EGFR inhibitors could perturb EGF-induced EGFR signalling of breast CSC proliferation, migration, mammosphere formation and mesenchymal tri-lineage differentiation. CHM-09 or EGFR inhibitors not only led to inactivation of EGFR downstream signalling pathways such as Akt, extracellular signal regulated kinase and signal transducer and activator of transcription 3, but also induction of mesenchymal–epithelial transition as confirmed by decreased N-cadherin and increased E-cadherin expression. Finally, combinatorial treatment of EGFR inhibitors and doxorubicin led to significant increase in breast CSCs responsiveness to a chemotherapeutic drug. The results of the present study suggest that EGFR is a therapeutic target in breast CSCs and that abrogation of EGFR signalling along with chemotherapeutic drugs is an effective approach against breast cancer. (*FEBS J.*, **2017**, 284, 1830)
- Glucocorticoid receptor (GR) synthetic ligand, dexamethasone (DEX) is known to antagonize side effects of chemotherapy but its sustained use induces steroid resistivity. We showed that upon a simple cationic lipid (C10) modification of DEX, the resultant compound DX10 inhibited STAT3 activation through lowering the production of IL-6. Hence, use of STAT3 synthetic inhibitor, WP1066, which is also in clinical trials, in combination with DX10 exhibited synergistic anticancer effect through significant inhibition of STAT3 activation. This resulted in enhanced melanoma tumor reduction. Together, the study repurposes the the role of GR in the context of p-STAT3 inhibition-mediated cancer treatment and advocates a novel combination strategy for treatment of STAT3 implicated cancers. (*Mol. Cell Biochem.*, **2017**, 436(1-2), 119)

Cardiovascular Research

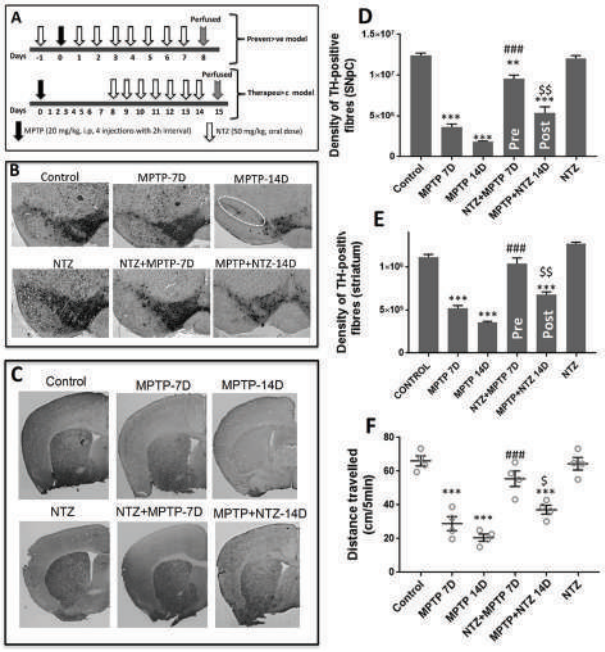
- Resveratrol attenuates monocyte-to-macrophage differentiation and associated inflammation via modulation of intracellular GSH homeostasis: Relevance in atherosclerosis. Monocyte-to-macrophage differentiation promotes an inflammatory environment within the arterial vessel wall that causes a mal-adaptive immune response, which contributes to the progression of atheromatous plaque formation. In the current study, we show that resveratrol, a well-known antioxidant, dose-dependently attenuated phorbol myristate acetate (PMA)-induced monocyte-to-macrophage differentiation, as measured by cell adhesion, increase in cell size, and scavenger receptor expression in THP-1 monocytes. Also, resveratrol significantly inhibited PMA-induced pro-inflammatory cytokine/chemokine and matrix metalloprotease (MMP-9) production. This inhibitory effect of resveratrol on monocyte differentiation results from its ability to restore intracellular glutathione (GSH) status, as resveratrol in the presence of buthionine sulfoximine (BSO) failed to affect monocyte differentiation. Furthermore, PMA-induced monocyte differentiation and inflammation was greatly inhibited when cells were co-treated with N-Acetyl-l-cysteine (NAC), a GSH precursor, while the presence of BSO aggravated these processes. These results also show that resveratrol mediated up-regulation of GSH is due to AMP-activated protein kinase (AMPK)-α activation, as compound C (AMPK inhibitor) treatment drastically depleted intracellular GSH and exacerbated PMA-induced monocyte differentiation and pro-inflammatory cytokine production. More importantly, chronic administration of resveratrol efficiently prevented monocyte infiltration and markedly diminished angiotensin (Ang)-II-induced atheromatous plaque formation in apolipoprotein-E knockout (ApoE(-/-))

mice. We conclude that, intracellular GSH status plays a critical role in regulating monocyte-to-macrophage differentiation and inflammation and resveratrol, by restoring GSH levels, inhibits these processes. Taken together, these results suggest that resveratrol can attenuate atherosclerosis, at least, in part, by inhibiting monocyte differentiation and pro-inflammatory cytokines production (*Free Radic. Biol. Med.,* **2016,** 96, 392)

- Cardiac hypertrophy leading to heart failure is one of the major causes of morbidity and mortality in the world. It is characterized by a chronic physiological increase in cardiac muscle mass resulting from systolic or diastolic wall stress, occurs normally during development, and other conditions. However, prolonged persistence and prevalence of this process leads to congestive heart failure, arrhythmia, and sudden death. Oxidative stress and mitochondrial dysfunction has been identified as one of the key contributing factors in the progression and development of cardiac Hypertrophy. Prohibitin (PHB) is rapidly emerging as a critical target molecule for cardiovascular signaling. Prohibitin (PHB) is overtly conserved evolutionarily and ubiquitously expressed protein with pleiotropic functions in diverse cellular compartments. However, regulation and function of these proteins in different cells, tissues and in various diseases is different as evidenced by expression of these proteins which is found to be reduced in heart diseases, kidney diseases, lung disease, Crohn's disease and ulcerative colitis but this protein is highly expressed in diverse cancers. The mechanism by which this protein acts at the molecular level in different subcellular localizations or in different cells or tissues in different conditions (diseases or normal) has remained poorly understood.

  In our previous studies in cardiac hypertrophy in SD rats, using proteomics approach we have identified prohibitin as a plausible marker having significant implications and potential in the disease biology. Further findings from our study on prohibitin and its overexpression and knockdown in cardiac hypertrophy identified that it plays a key role in regulation of oxidative stress and mitochondrial dysfunction in cardiomyocytes. We found that the protective defensive role of prohibitin (PHB) against ISO-induced hypertrophic response in rat H9c2 cells is via attenuation of oxidative stress-dependent signaling pathways. The intracellular levels of mitochondrial membrane potential along with cellular ROS levels and mitochondrial superoxide generation were determined. In order to understand the regulation of Akt/Gsk-3β signaling pathway, we carried out immmunoblotting for key proteins of the pathway such as PTEN, PI3K, phosphorylated, and unphosphorylated forms of Akt, Gsk-3β, and immunofluorescence experiments of p-Gsk-3β. Enforced expression of PHB in ISO-treated H9c2 cells suppressed cellular ROS production with mitochondrial superoxide generation and enhanced the mitochondrial membrane potential resulting in suppression of oxidative stress which likely offered potent cellular protection, led to the availability of more healthy cells, and also, significant constitutive activation of Gsk-3β via inactivation of Akt was observed. Knockdown of PHB expression using PHB siRNA in control H9c2 cells reversed these effects. Overall, our results demonstrate that PHB confers cytoprotection against oxidative stress in ISO-induced hypertrophy and this process is associated with modulation of Akt/Gsk-3β signaling mechanisms as evident from our PHB overexpression and knockdown experiments. and could be useful to predict the therapeutic response to established and novel therapies for the prophylaxis of cardiac hypertrophy and subsequent heart failure in cardiac patients. (*Mol. Cell Biochem.,* **2017**, 425, 155; *Curr. Drug Targets*, **2017**, 18, 1836)

Neurobiology Research



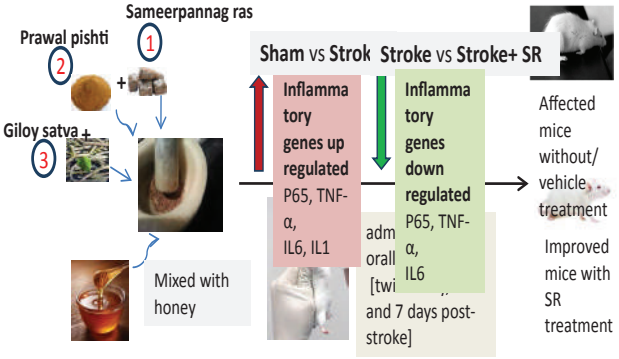
- The anti-helminth drug, nitazoxanide, confers protection against MPTP-induced experimental Parkinsonism in mice due to its unintended mitochondrial uncoupling effects.

  Mitochondria plays a primary role in the pathophysiology of Parkinson's disease (PD) and small molecules that counteract the initial stages of disease may offer therapeutic benefit. In this regard, we have examined whether the off-target effects of the FDA approved anti-helminth drug, nitazoxanide (NTZ) on mitochondrial respiration could possess any therapeutic potential for PD. Results indicate that MPP+ induced loss in oxygen consumption rate (OCR) and ATP production by mitochondria were ameliorated by NTZ in real-time by virtue of its mild-uncoupling effect. Pretreatment of cells with NTZ mitigated MPP+ induced loss in mitochondrial OCR and ROS. Similarly, addition of NTZ to cells pre-treated with MPP+ could reverse block in mitochondrial OCR and ROS induced by MPP+ in real-time. The observed effects of NTZ were found to be transient and reversible as removal of NTZ from incubation medium restored the mitochondrial respiration to that of controls. Apoptosis induced by MPP+ was ameliorated by NTZ in a dose-dependent manner. In vivo results demonstrated that oral administration of NTZ (50 mg/kg) in an acute MPTP mouse model of PD conferred significant protection against the loss of TH positive neurons of Substantia nigra. Based on the above observations we believe that repurposing of NTZ for PD may offer therapeutic benefit. (*J. Biol. Chem.*, **2017**, 292(38), 15731)

- Neuropsychiatric and neurologic disorders

  The neurobiology and the neuropsychiatric group has developed several cost effective zebra fish and mouse models to perform in vivo screening of new compounds as well as to understand the disease mechanism.

  Neuropsychiatric and neurologic disorders in combination, contribute a major chunk of the total global disease burden. According to World Health Organization (WHO) report, one in four people in the world suffers with some kind of mental disorders at some point in their life. Currently no proper curative measures available for these diseases due to poor understanding. In order to achieve a proper understanding of the disease mechanism, a cost-effective vivo model is needed for screening new drug molecules. Here we have developed a cost effective neuro disease vertebrate zebra fish model for better understanding of the disease mechanism and in identifying new drugs. (*Sci. Rep.*, **2017**, 7(1), 1492)



- Several studies were undertaken to understand the molecular basis of the gender difference that underlies stress response using a number of mouse models of stress-induced depression and related psychiatric disorders (*Neuroscience*, **2017**, 356, 89; *Biochem. Biophy. Res. Commun.*, **2017**, 486(4), 1122). Overall studies showed that different strategy should be employed in developing therapeutics and also in the dose of the existing medications to treat reward and cognitive disorders in females of different age groups. (*Behavioural Brain Res.*, **2017**, 318, 36)

- Studies using a newly developed mouse model of cerebral ischemia mimicking common human mild stroke condition (*Biochimica et Biophysica Acta*, **2017**, 1863, 152) revealed the novel role of epigenetic regulatory mechanisms in mediating the stroke-induced striatal damage, eventually was used to validate one of the ayurvedic formulations as potential stroke therapeutic. (*J. Ethanopharmacol.*, **2017**, 197(2), 147)

Stem Cells and Regenerative Medicine

Engraftment of transplanted stem cells is often limited by cytokine and noncytokine proinflammatory mediators at the injury site.We examined the role of Cyclooxygenase-2 (Cox-2)-induced cytokine-mediated inflammation on engraftment of transplanted bone marrow stem cells (BMSCs) at the wound site. BMSCs isolated from male C57/BL6J mice were transplanted onto excisional splinting wounds in syngenic females in presence or absence of celecoxib, Cox-2 specific inhibitor (50 mg/kg, body weight [b wt]), to evaluate engraftment and wound closure. Inflammatory cell infiltration and temporal expression of inflammatory cytokines at the wound bed were determined using

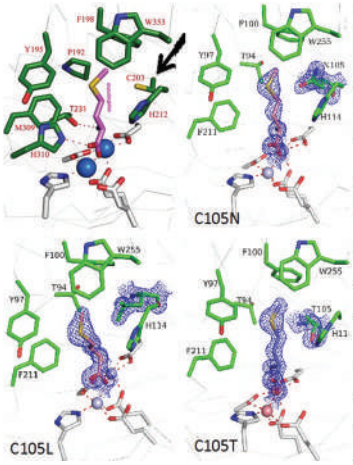
immunohistochemical and quantitative real-time polymerase chain reaction (qPCR) analysis, respectively. Mechanistic studies were performed on a murine macrophage cell line (J774.2) to evaluate the effect of interleukin (IL)-17A. Celecoxib administration led to a significantly high percent of wound closure, cellular proliferation, collagen deposition, BMSCs engraftment and re-epithelialization at the wound site. Interestingly, recruitment of CD4+T cells and F4/80+ macrophages as well as BMSC transplantation induced upregulation of Cox-2 and IL-17A gene expression levels were reverted by celecoxib administration. Exogenous supplementation of recombinant interleukin (rIL)-17 to J774.2 cells significantly increased proliferation and gene expression of cytokines -IL-1β, IL-6, IL-8, IL-18 and tumor necrosis factor (TNF)-α via nuclear translocation of nuclear factor kappa B (NFκB)p65/50 subunit. Conditioned media of rIL-17 treated J774.2 cells when supplemented to BMSCs depicted a dose-dependent increase in the number of apoptotic cells and proapoptotic protein expression that was perturbed by celecoxib or IL-17 neutralizing antibody. Finally, celecoxib led to a dose-dependent increase in BMSC differentiation into keratinocyte-like cells in vitro. Celecoxib protects transplanted BMSCs from Cox-2/IL-17–induced inflammation and increases their engraftment, differentiation into keratinocytes and re-epithelialization thereby potentiating wound tissue repair. (*Cytotherapy,* **2017**, 19, 756)

Antitubercular Agents

With the proposition of "affordable and accessible healthcare for all" to primarily deal with neglected tropical diseases of our country, including Tuberculosis, Malaria and Leshmaniasis, we have performed high throughput screening of small molecule libraries and validation in appropriate models at CSIR-IICT to facilitate discovery of novel anti microbial agents against Mycobacterium. Different CSIR laboratories, other national laboratories, universities and colleges across India used this platform across at CSIR-IICT. The main outcome of this facility including new chemical entities was identified as new anti-tubercular agents that are in the pipeline for further lead progression.

Structural Biology

Role of Active Site non-Cognate Residue in the Substrate Specificity of Type 1 Methionine Aminopeptidases



PDB ID	Type 1 MetAP	C-105
1C21	*Escherichia coli*	97%(C), 2%(N), 1%(L)
1QXY	*Staphylococcus aureus*	99% (C), 1%(N, F, T)
4JUQ	*Pseudomonas aeruginosa*	94%(C), 5%(N), 1%(L)
3TB5	*Enterococcus faecalis*	93%(C), 6%(N), 1%(T)
4KM3	*Streptococcus pneumoniae*	93%(C), 5%(N), 1%(L), 1%(T)
3MX6	Rickettsia prowazekii	99%(C), 1%(L)
1YI3	*Mycobacterium tuberculosis*	100%(C)
2B3L	*Homo sapiens*	100%(C)

Leucine assubstrate

Enzyme	Km (μM)	Kcat (min^{-1})	Kcat/Km ($M^{-1}min^{-1}$)
C105N	709.8±61	18.95	0.0267
C105T	635.9±63	22.81	0.0358
*Vco*MetAP1a	613.4±43.8	19.22	0.0314

Methionine aminopeptidase (MetAP) is an essential enzyme in all living cells. MetAP removes initiator methionine from 60-70% of the newly synthesized proteins in every living cell (ref). Given their importance in pathophysiology, large numbers of studies have been dedicated to understand their biochemical and structural aspects. MetAPs are broadly divided into two classes, Type 1 and Type 2. Type 1 enzymes have been studied for their antimicrobial while Type 2, specifically from humans for its antiangiogenic properties. One of the uniqueness of this class of enzymes is their strict substrate specificity towards methionine in the amino-terminus of a peptide. Others and we have demonstrated that a highly conserved cysteine (C70 in *E. coli* MetAP1a and C105 in *M. tuberculosis* MetAP1c) in the bottom of the S1 pocket provides the molecular support for specificity. Mutation of this residue to any other amino acid results either in the partial or complete loss of activity, or relaxed substrate specificity. X-ray crystal structure of C105S mutant of *Mycobacterium tuberculosis* Type 1c MetAP (*Mt*MetAP1c) suggested that the S1 pocket gets enlarged due to the conformational change of new serine there by accommodating the leucine as substrat. Use of biochemical, structural and quantum mechanical studies provided the evidence that there exists a C-H...S hydrogen bond between the substrate methionine and S1 pocket cysteine residue of *Mt*MetAP1. Such unique interaction is not possible between the enzyme cysteine and any other amino acid as substrate. This explains why MetAPs demonstrate specificity towards methionine alone.

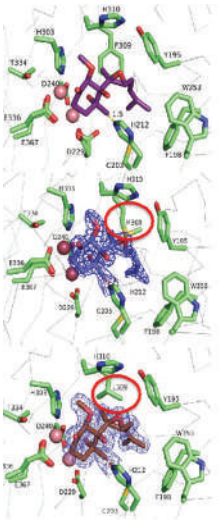
Bioinformatic analysis carried out in one of our previous studies suggested that a cysteine is conserved about 96% of the Type 1 MetAPs at the analogous position of C105 of *Mt*MetAP1c (ref). The other 4% is replaced by asparagine,

threonine, leucine and valine in the decreasing order of frequency. Till date none of the Type 1 MetAPs that have a non-cysteine residue at the homologous position of C105 of *Mt*MetAP1c have been reported. It is not clear if the MetAPs that have non-cysteine residues display relaxed specificity as observed in C105 mutants of *Mt*MetAP1c or have preserved the original specificity for methionine.

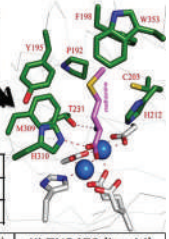
In the current study, we report the biochemical studies of two MetAPs that have an asparagine in the place of cysteine of *Mt*MetAP1c in the bottom of the active site. In addition we have carried out biochemical and structural studies of various mutants of *Mt*MetAP1c in complex with the amino acid methionine. We have carried out comparative bioinformatics to support the conclusions from biochemical and structural data. For the first time we show MetAP's in rare circumstances, also cleave other substrates like leucine.

Structure of the angiogenesis inhibitor ovalicin bound to three mutants of human Type 1 methionine aminopeptidase, a noncognate target

Methionine aminopeptidases (MetAPs) remove the initiator methionine during protein biosynthesis. They exist in two isoforms, MetAP1 and MetAP2. The anti-angiogenic compound fumagillin binds tightly to the Type 2 MetAPs but only weakly to Type 1. High-affinity complexes of fumagillin and its relative ovalicin with Type 2 human MetAP have been reported. Here we describe the crystallographic structure of the low-affinity complex between ovalicin and several mutants of F309 in Type 1 human MetAP at atomic resolution. For both Type 1 and Type 2 human MetAPs the inhibitor makes a covalent adduct with a corresponding histidine. At the same time there are significant differences in the alignment of the inhibitors within the respective active sites. It has been argued that the lower affinity of ovalicin and fumagillin for the Type 1 MetAPs is due to the smaller size of their active sites relative to the Type 2 enzymes. Comparison with the uncomplexed structure of human Type 1 MetAP indicates that there is some truth to this. Several active site residues have to move "outward" by 0.5 A° or so to accommodate the inhibitor. Other residues move "inward." There are, however, other factors that come into play. In particular, the side chain of His310 rotates by 134° into a different position where (together with Glu128 and Tyr195) it coordinates a metal ion not seen at this site in the native enzyme. In the mutant structures, large phenylalnine when replaced by leucine or flexible methionine, the affinity is increased in the range of low micromoles to nanomoles.



Ovalicin, a natural product is a selective inhibitor of Type 2 MetAP (nM). Type 1 is inhibited at mM.



	Ki-ovalicin (in μM)
*Ef*MetAP1a	1.49±0.1
*Sp*MetAP1a'	1.49±0.1

	Ki-ovalicin (in μM)	Ki-TNP470 (in μM)
*Ef*MetAP1a	1.49±0.1	3.45±0.25
*Sp*MetAP1a'	1.49±0.1	2.01±0.15
*Hs*MetAP1b	-ND-	-ND-
*Mt*MetAP1c	-ND-	-ND-
F309M	0.09±0.01	0.46±0.04
F309L	0.175±0.022	4.57±0.34
F309I	7.66±0.9	7.17±0.73
F309Y	-ND-	-ND-
T334A	51.62±6.07	35.17±3.91
H212A	-ND-	-ND-

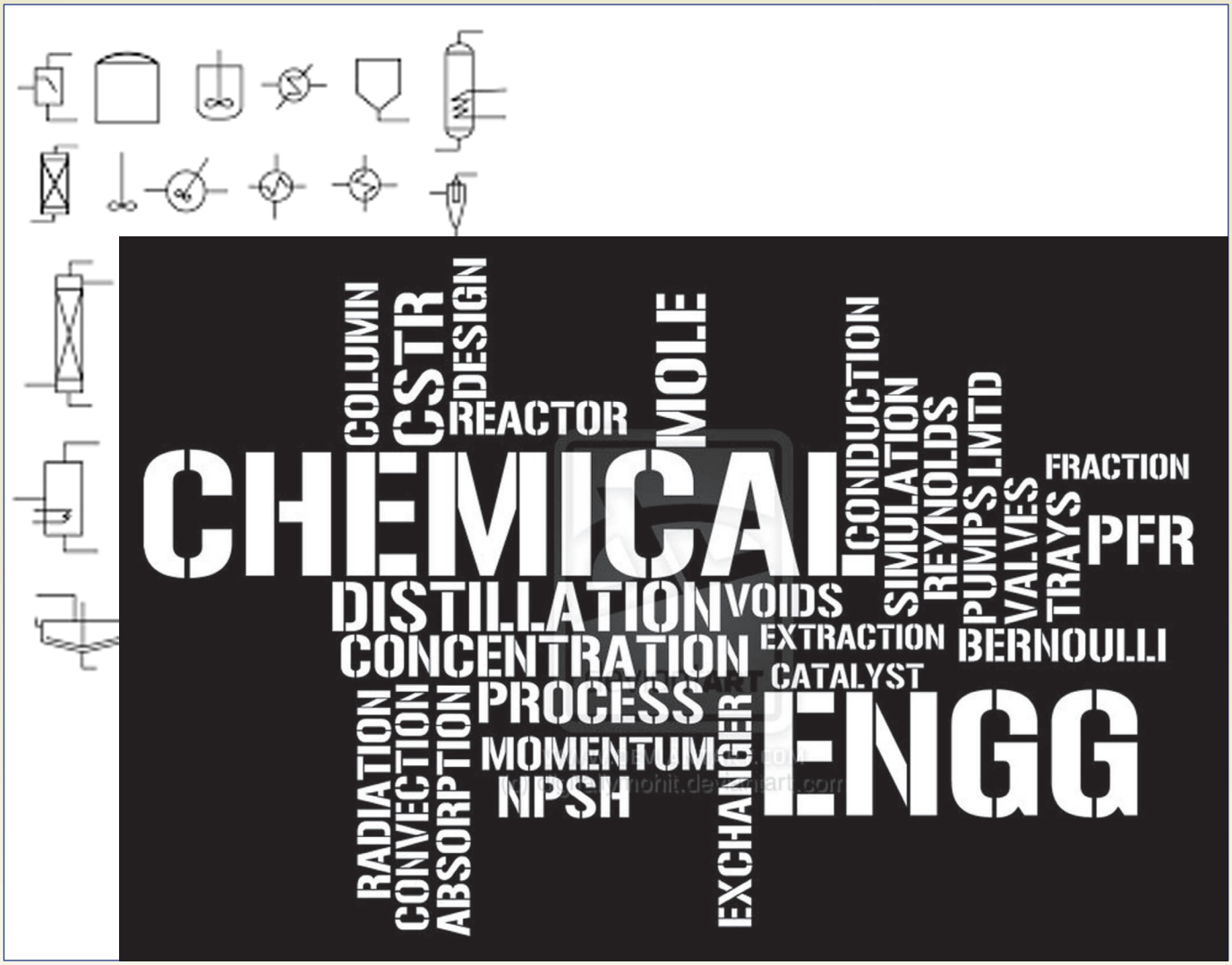
To be published

Drug Delivery and Nanomedicine Research

- N-end rule pathway, an ubiquitin dependent proteolytic system, counteracts cell death by degrading many antisurvival protein fragments like BCLxL, BRCA1, RIPK1, etc. RIPK1 also induces necroptosis. Strategy is to metabolically stabilise RIPK1 to induce enhanced anticancer effect. Earlier we designed and developed RFC11, the synthetic, hetero-bivalent N-end rule pathway inhibitor. Utilizing the over expression of biotin receptor in cancer cells, we showed that coadministration of RFC11 and anticancer drug shikonin (also an elevator of RIPK1 levels) solubilized in a stable biotin receptor-targeted liposome exhibited significant synergistic antitumor effect in both subcutaneous and orthotopic mouse colon tumor model through induction of necroptosis with distinctive upregulation of RIPK1. (*Mol. Ther. Oncolytics*, **2016**, 3, 16020)
- We showed that glucocorticoid receptor (GR), which is ubiquitously expressed in all cells, can be selectively targeted to elicit EMT reversal of aggressive cancers. Using this phenomenon, we liposomally co-delivered lipophilic drugs and anti-Hsp90 gene towards establishing the strategy to induce drug-sensitivity, EMT-reversal, and reduced malignancy in aggressive tumors of pancreas and skin. (*Mol. Pharm.,* **2016**, 13(7), 2507)

- We explored the potential of glucocorticoid receptor (GR)-targeted nano-gold formulation as antitumor drug sensitizing agent. Toward this, we modified GR-ligand dexamethasone (Dex) to carry sulphide (namely DSH) which was further utilized to tag on gold nanoparticles (GNP). The GNP surface, hydrophobically modified with DSH), then efficiently adsorbed hydrophobic anticancer drug withaferin. The resultant material showed maximum efficiency in melanoma tumor reduction with concomitant induction of EMT reversal. (*Nanomedicine(London),* **2016**, 11(19), 2529)
- The process of angiogenesis, involving generation of new blood vessels from the existing ones, is vital for the supply of oxygen and nutrients to various tissues of body system. Angiogenesis is directly associated with several physiological and pathological processes. It is well-established that impairment in angiogenesis process results in various fatal conditions. Recently, our group demonstrated the therapeutic angiogenesis of several metal oxide/hydroxide nanoparticles, observed by various in vitro and in vivo angiogenesis assays, for the treatment of ischemic diseases (limb, brain, heart), wound healing etc. In one study we have demonstrated the pro-angiogenic properties (in vitro and in vivo) of terbium hydroxide nanorods (THNRs) along with the detailed molecular mechanisms. The in vivo wound healing and nonimmunogenicity of the THNRs have been validated in the mouse models (*ACS Biomater. Sci. Eng.,* **2017**, 3 (12), 3635). This study will aid in the development of alternative treatment strategies for wound healing along with cardiovascular and ischemic diseases, where angiogenesis is the chief target. We also reported the investigation of role of nitric oxide driven angiogenesis by zinc oxide nanoflowers (*J. Mater. Chem.B,* **2017**, 5(18), 3391). In other studies, we have shown the pro-angiogenic properties of functionalize nanoceria and doped-titanium oxide nanomaterials (*J. Mater. Chem.B,* **2017**, 5, 9371; *Sci. Total Environ.,* **2017**, 599 & 1263). We have also demonstrated the enhanced vascularization and endothelial cell proliferation using electrospun ploycaprolactone (PCL) embedded pro-angiogenic europium hydroxide nanorods. (*J. Mater. Chem. B,* **2017**, 5, 4660)
- Our department is also pursuing various nanomedicine projects for cancer theranostics. Designed recombinant proteins comprising functional domains offer selective targeting of cancer cells for the efficient delivery of therapeutic agents. Using a combinatorial approach, we designed and fabricated a drug delivery system by combining gold nanoparticles (AuNPs) with an engineered bi-functional recombinant fusion protein TRAF(C) (TR), loaded with an anticancer drug, namely doxorubicin (DX), and erbB2-siRNA (si), to mediate target specific delivery into SK-OV-3, a model human ovarian cancer cell line over expressing HER2 receptors (i.e. human epidermal growth factor receptor-2). Intraperitoneal administration of our drug delivery systems (DDS) at 2.5 mg kg–1 of DX and 0.25 mg kg–1 of erbB2 siRNA into SK-OV-3 xenograft nude mice, revealed target specific uptake and consequent gene silencing resulting in significant tumor suppression (*J. Mater. Chem. B*, **2017**, 5, 7082). We have also successfully delivered the doxorubicin to cancer cells using biologically synthesized gold nanoparticles (*J. Ind. Chem. Soc.*, **2017**, 94, 1335). In collaboration with IIT-Guwahati, we have demonstrated the cancer theranostics applications of nanoparticles (*Chem. Sci.*, **2017**, 8, 7566; *ACS Appl. Mat. Interf.*, **2016**, 8, 32220; *Biosens. Bioelectron.*, **2017**, 89, 636). We have also demonstrated the curcumin-loaded silica-based mesoporous materials: Synthesis, characterization and cytotoxic properties against cancer cells. (*Mater. Sci. Eng. C*, **2016**, 63, 393)

CHEMICAL ENGINEERING



BASIC RESEARCH

Separation of water from lactic acid solution by membrane distillation

Microporous hydrophobic ZSM-5 loaded polyvinyl chloride (PVC) mixed matrix membrane was prepared by phase inversion technique for dehydration of lactic acid solution. 0.9 g of ZSM-5 zeolite was initially introduced into 81.1 ml *N*-Methyl-2-pyrrolidone (NMP) solvent with stirring for a period of 15-20 min followed by ultrasonication for 2 h at 30 ° C for uniform dispersion of zeolite particles. After that, 18 g of PVC polymer was added to the solution with stirring at ambient temperature for 6 h to obtain a homogenous polymer solution. The solution was cast over a non-woven polyester fabric support and kept in water bath to result a porous membrane.

Reactive extraction of tartaric acid by membrane contactors

Microporous hydrophobic polyvinylidene fluoride (PVDF) blend membrane was prepared using phase inversion technique for reactive extraction of tartaric acid from synthetic mixture. 4.8 g of glycerol was added to 83.2 ml of *N,N*-dimethylformamide solvent and the solution was stirred until complete dissolution of the additive in the solvent was ensured. After that, 8 g of PU polymer was added gradually followed by addition of 4 g of PVDF polymer. The solution was stirred for a period of 5-6 h and left undisturbed to remove air bubbles. The bubble free solution was cast over a non-woven polyester fabric support and kept in water bath to result a porous membrane.

Extraction of levulinic acid from industrial effluent by membrane contactors

Developed microporous PVC membrane for reactive extraction of levulinic acid from industrial effluent. 19% (w/v) PVC polymer solution was prepared by dissolving 4.75 g of PVC polymer in 20.25 ml of NMP solvent. The bubble free solution was cast over a non-woven polyester fabric support and kept in water bath to result a porous membrane.

Development of polyimide membranes for gaseous separations

Two isobaric gas permeation systems were constructed (Swagelok parts) which are connected to steel gas permeation cells (film membrane holder) and newly purchased gas cylinders/pressure regulators. Materials were selected after literature survey and purchased. Dense membrane films (non-porous <0.4nm) were fabricated by solution-casting/complete evaporation of solvent method. Permeability, diffusivity of pure gases, selectivity and extent of separation of mixed gases, by the membranes were experimentally determined.

Dense membrane films of four pure polymers were fabricated and studied to observe their intrinsic gas separation ability. These were polyethersulfone, polysulfone, Torlon® polyamide-imide and pebax(poly-ether block amide). Dense mixed matrix membrane films of Torlon with Zif8 nanoparticles were fabricated and tested and they showed enhanced gas separation compared to pure polymers.

Oil and Water Separation:

- The most important pollutants in the wastewaters that are conventional pollutants such as oil and grease, suspended solids. Among these pollutants oil is one of the most complicated pollutants to remove oil from water. Traditional ultrafiltration technology has been provided for relatively clean water that was once suitable for sewer discharge and also for reuse.
- The UF membrane having molecular weight cut-off (MWCO) 10 KDa showed around the flux 188 L/m^2.h, 86 % recovery and 5 KDa showed flux 180 L/m^2.h, 50 % recovery.

Preparation of sulfonated Polyether ether ketone membrane for use in microbial fuel cell

Sulfonation of PEEK polymer

15 g of the polymer was dissolved in 300 ml of concentrated (95–98%) sulfuric acid and vigorously stirred at 55 °C for 5 to 10 h. The reaction was terminated by immersing the flask containing the reaction mixture into a large excess of ice-cold water. The polymer thus formed was precipitated out in cold water and washed repeatedly to remove the excess of traces of acid until the pH gets neutral. The polymer was dried under vacuum at 80 °C for 8 –10 h. The final product thus obtained was called as SPEEK. The sulphonated PEEK was approximately weighed about 15gms out of which 5gms was dissolved in 15 ml of N-methyl pyrrolidine, stirring was continued at 50°C for 24h and then casted on a Petridish and dried

at 100^{0}c in the oven for 24h, while ensuring no bubble formation occurred.

SPEEK Membrane Synthesis

- SPEEK was prepared by taking PEEK (6 g) and adding into vigorously stirred 100 ml concentrated sulfuric acid (95–98 wt.%). The reaction was carried out at 50 °C. The sulfonation reaction was terminated by precipitating the resulting acid polymer solution into ice-cold water under mechanical agitation. The polymer precipitate was filtered, washed several times with deionized water until pH was neutral. Then, the polymer was dried at room temperature for several days, and then dried in a vacuum oven at 100 °C for 24 h.
- SPEEK polymer was dissolved in DMSO to make a 10 wt% SPEEK casting solution, which was then cast onto a flat glass. The cast membranes were dried at 60 °C for 6 h to remove the solvents, and annealed at 120 °C for 4 h. After cooling to room temperature, the resultant membranes were peeled from the glass in deionized water. Finally, the membrane was pretreated by boiling for over 1 h in 0.5 M H_2SO_4 and subsequently rinsed with deionized water several times. The thus-pretreated SPEEK membranes were kept in deionized water before testing. The thickness of the dried SPEEK membranes was about 80–120 µm.

APPLIED RESEARCH, HAVING SIGNIFICANT INDUSTRIAL / ECONOMIC / ENVIRONMENTAL / SOCIETAL / STRATEGIC IMPACT

Membrane contactors

Influence of Operating Parameters on Recovery of Tartaric Acid

Fig. 1 (a) shows the influence of tartaric acid concentration in aqueous solution on membrane extraction efficiency for an initial TOA concentration of 20% (v/v in 1-octanol). An increase in tartaric acid content from 0.2 mol/L to 1.07 mol/L in the aqueous phase resulted in reduction in extraction efficiency from 5.81% to 3.48%. Additionally, the influence of TOA concentration on extraction efficiency of tartaric acid for initial acid concentration of 100mol/m^3 was investigated. It was found that the % extraction efficiency increased linearly from 5.4 to 12% over a TOA concentration range of 10% to 30% v/v in 1-octanol (Fig. 1 (b)).

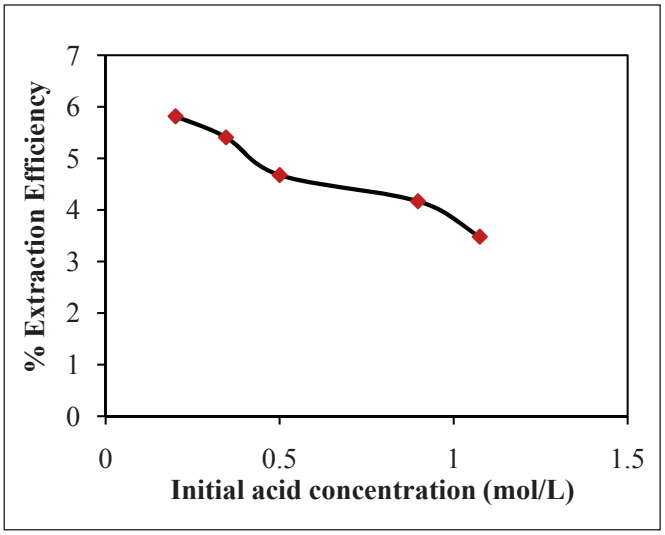


Fig1(a) Influence of Tartaric Acid Concentration on % Extraction Efficiency for Initial TOA Concentration of 20% (v/v) in 1-Octanol

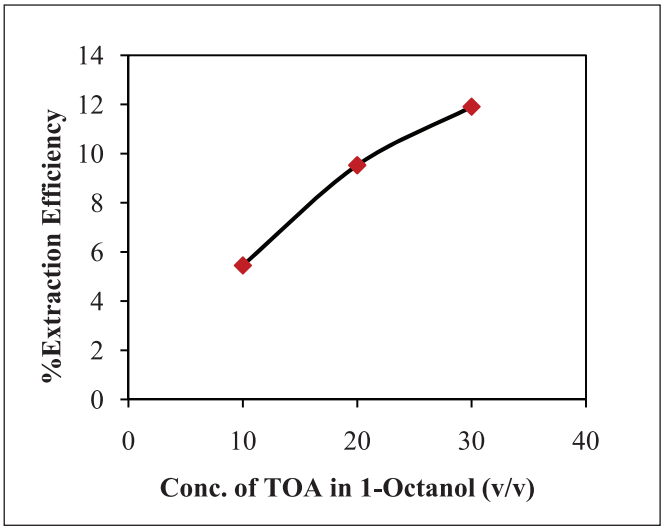


Fig2(b) Effect of TOA Concentration on % Extraction Efficiency for Initial Tartaric Acid Concentration of 100 mol/m3

Influence of Additives on Extraction of Levulinic Acid

Influence of additives such as $LiCl_2$, $ZnCl_2$, polyethylene glycol (PEG) 6000 and glycerol on extraction efficiency of levulinic acid from industrial wastewater was investigated. Four different polymer dopes containing 20 wt% PVC was prepared using NMP as solvent with additive in each dope constituting 20% of polymer weight. Fig. 2 shows membrane performance with respect to different additives for initial levulinic acid content of 575 mol/m^3 and TOA concentration of 10% (v/v in 1-octanol), respectively. The membrane

prepared with glycerol as additive exhibited higher extraction efficiency of 21.74% as compared to other formulations containing $LiCl_2$, $ZnCl_2$ or PEG as additive. This observation is attributed due to higher pore size formed in PVC membrane upon replacement of glycerol molecules with water in the precipitation bath.

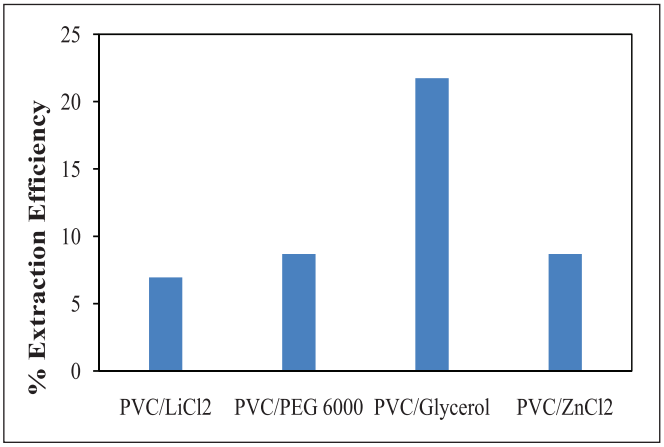


Fig 2: Influence of Additive Loading on Extraction Efficiency of Levulinic Acid for Initial Acid Concentration of 575 mol/m^3 and TOA Concentration of 10% (V/V)

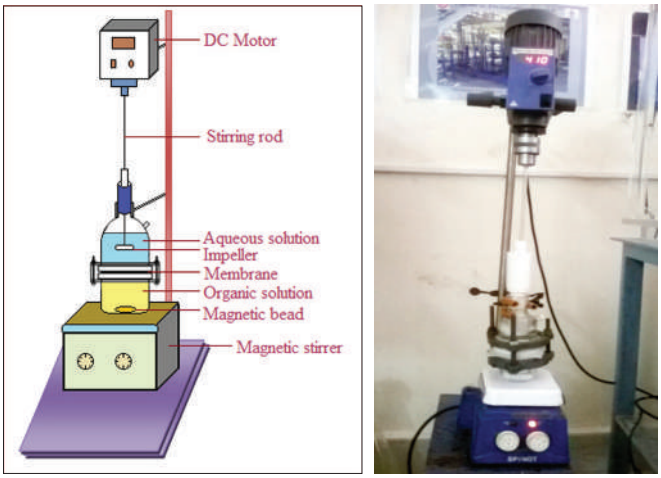


Fig 3 (a) Schematic Representation of Liquid-Liquid Membrane Contactor System and (b) Laboratory Set-Up of Membrane Contactor System

Membrane Distillation

Effect of Feed Lactic Acid Concentration on Total Flux

Fig. 4 (a) shows variation of total flux as a function of feed lactic acid (LA) concentration at constant downstream pressure of 5 mmHg and feed temperature of 303 K. An increase in lactic acid concentration in feed solution from 74% to 90% (v/v) resulted in enhancement of total flux from 0.17 to 0.61 kg/m^{2}h with presence of trace quantities of lactic acid in permeate. Strong hydrogen bonding of lactic acid with water molecule could cause its losses across the selective hydrophobic barrier. Concentration of lactic acid in permeate sample was determined by standard calibration plot of refractive index versus known compositions of lactic acid/water mixtures (Fig. 4 (b)).

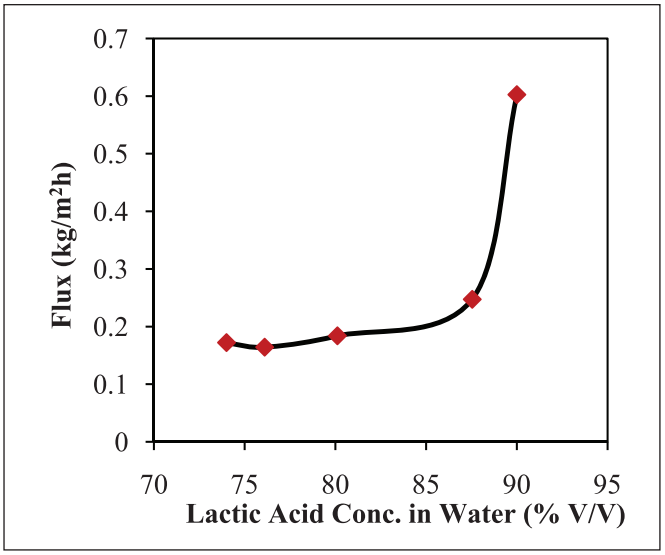


Fig 4(a): Effect of Feed Lactic Acid Concentration on Total Flux at Constant Downstream Pressure of 5 mmHg and Feed Temperature of 303 K

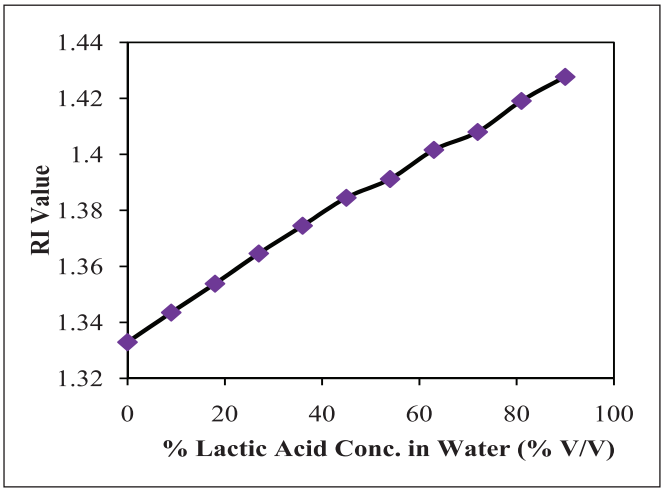


Figure 4(b): Refractive Index Calibration Curve for Lactic acid/Water System

Table 1 provides data recorded for dehydration of lactic acid concentration varying from 74% to 90% in the feed for which its content in permeate was quite low (1.28 to 0.36 %), implying highly selective nature of the membranes. The small losses of the acid could be attributed to coupling effect on account of the strong hydrogen bonding of LA with water.

Table 1: Data on Dehydration of Lactic Acid through PVC Membrane

Feed lactic acid concentration (v/v)	Feed RI value	Permeate RI value	%Lactic acid in permeate
74	1.4102	1.3344	1.28
74	1.4097	1.3342	1.28
76.1	1.4131	1.3342	1.09
80.11	1.4179	1.3337	0.7
87.54	1.4253	1.3335	0.506
90	1.4277	1.3333	0.36

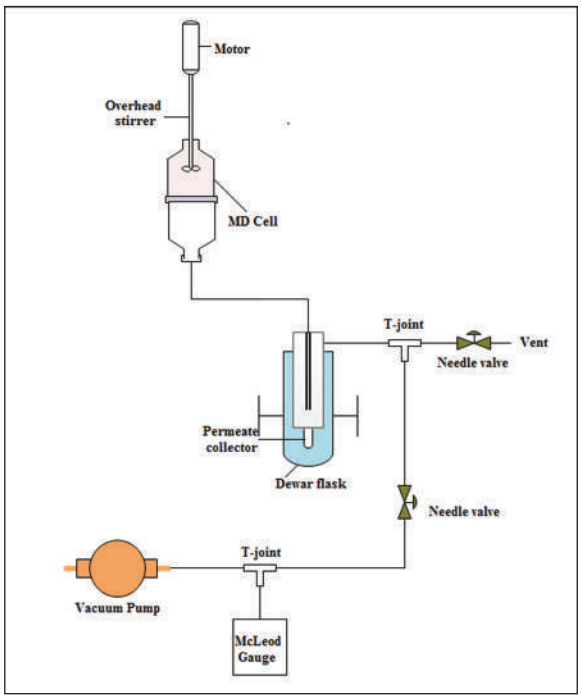


Fig 5 Schematic of Membrane Distillation System

Membrane Bioreactor

Performance of Submerged and Side Stream MBR for treatment of Domestic and Industrial Wastewater

This study focuses on the possibility of integrating membrane techniques with biological methods for treatment of domestic and industrial wastewater. However, several doubts and debates arose mitigating the technical feasibility and economic viability of these technologies on a large scale in real-world applications. Analysis of MBR treated effluents revealed a sharp reduction in various parameters like COD, TDS, turbidity, conductivity by using a mixed microbial consortium of bacterial strain in both submerged and side-stream MBR.

Experimental results for Submerged Membrane Bioreactor (SMBR)

- An indigenously developed spiral wound Hydrophilized Ultrafiltration (HF-UF) membrane of 10 kDa molecular weight cut off (MWCO) was immersed into a membrane bioreactor (SMBR) of novel design. A mixed microbial consortium was isolated from curd for treatment of kitchen wastewater, especially to reduce COD levels, by maintaining aerobic conditions maintained within the submerged MBR. The initial domestic feed wastewater sample values are 450 mg/L TSS, 1382 ppm TDS, 71 FAU turbidity, 23800 (mg/L) COD and 1.40 mS/cm. The MBR process was able to remove the impurities substantially in the final permeate to as low as 150 mg/L TSS, 1000 ppm TDS, 6 FAU turbidity, 120 (mg/L) COD and 1.40 mS/cm Conductivity respectively.

Experimental results for Side-stream Membrane Bioreactor (SSMBR)

- The low cost Hydrophilized Ultrafiltration (HF-UF) membrane of 10 KDa molecular weight cut off (MWCO) was used for the treatment of industrial wastewater. The membrane was placed under side-stream in to membrane bioreactor (SSMBR). A mixed microbial consortium was isolated from same effluent for treatment of dairy industrial wastewater, especially to reduce high content of COD levels, by maintaining aerobic conditions within the side-stream MBR. Initial values of industrial wastewater was recorded as 1492 ppm TDS, 96 FAU turbidity, 2.74 mS/cm 2 conductivity and 10,400 mg/L COD, the analysis post biological treatment revealed corresponding reduction in parameter values to 119 ppm, 16 FAU, 2.50 mS/cm and 800 mg/L respectively.

Gas Separation

Torlon based novel membranes exhibited good gas separation for three applications. Separation of carbon dioxide from nitrogen to enable power-plant off-gas capture and reduce CO_2 emissions was achieved. Separation of helium from nitrogen to lower cost of separation process was achieved. Separation of carbon dioxide from methane to increase purity of biogas was achieved. Polyethersulfone based face masks were also prepared to prevent inhalation of air pollution. Material characterization studies included DMTA, DSC, TGA, FTIR, SEM, FE-SEM, EDS, XRD and UTM.

Alkaline Water Production Devices

- A batch mode AIW unit of 20 L capacity is constructed using a flat-sheet ion exchange membrane of 50 cm^2 area that produces 20 L of 9.5 pH water in 15 h. The smaller table top AIW unit could process 200 mL of neutral pH water to pH 9.5 in just 15 min, by utilizing a membrane of molecular weight cut off (MWCO) 5 kDa and area of just 40 cm^2. The continuous electrolyser of 2.35 L/h capacity was designed using a hollow fiber membrane module of effective membrane area 0.045 m^2 and MWCO 30 kDa.
- Ultrafiltration membranes based on polyethersulfone (PES) and polysulfone (PSf) were synthesised and used for AIW generation. The performance of the electrolyser was evaluated in terms of feed TDS, flux, electrode durability, operating time, membrane stability and power consumption for the production of alkaline reduced water. In case of continuous AIW unit, stainless steel (SS) electrodes were found to be suitable, while in case of batch electrolyser, titanium anode is used to avoid corrosion problems. A pH of 10 could be attained at flux of 3.33 L/h in continuous mode using hollow fiber module while batch mode electrolyser exhibited 2.22 L/h and 2 L/h with PES and PSf membranes respectively.
- The developed electrolysers were found to be effective in producing AIW of9.5 pH by considering drinking water from nanofiltration(NF)/reverse osmosis(RO) as feed and utilising power from 36 V DC adapters wherein the average current was 0.4 A. The capital cost of 20 L batch AIW unit, hollow fiber based continuous unit and 200 mL table top unit worked out to be only Rs. 1025/-, Rs. 2500/-and Rs. 410/- respectively, which are several notches lower than commercial AIW units

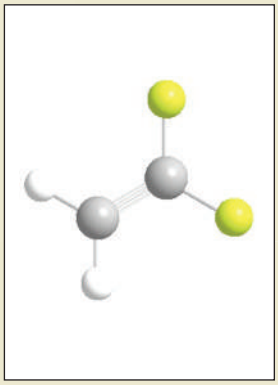
Preparation of A novel microbial fuel cell incorporated with polyvinylchloride / 4A zeolite composite membrane for kitchen wastewater reclamation and power generation

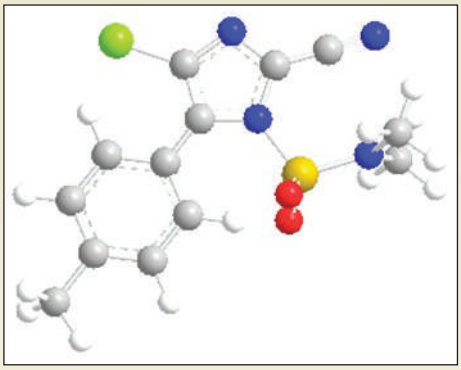
Synthesis of a alternative membrane to Nafion 117 that is based on hydrophlic zeolite 4A incoporated in hydrophobic polyvinylchloride (PVC) matrix for treatment of kitchen wastewater by microbial fuel cell (MFC). The indigenous membrane was prepared by solution casting-solvent evaporation technique and characterized by FTIR, XRD, TGA and SEM analysis. Sorption behavior, proton conductivity, ion exchange capacity (IEC) and MFC performance were thoroughly investigated. A molecular dynamics (MD) simulation was performed to determine oxygen diffusion coefficient through the membrane, which was found to be desirably low. Higher proton conductivity values were observed at increasing zeolite concentrations in PVC membrane until an optimum power density of 294 mW m-2 could be achieved at 15% loading. Corresponding performance of PVC and Nafion 117 membranes were observed to be only 94 mW m-2 and 193 mW m-2, respectively. Furthermore, the PVC/4A membrane exhibited substantial removal of chemical oxygen demand up to an extent 89%. The mixed matrix membrane exhibits vast potential for MFC application as demonstrated by its performance comparison with state of the art Nafion 117 membrane.

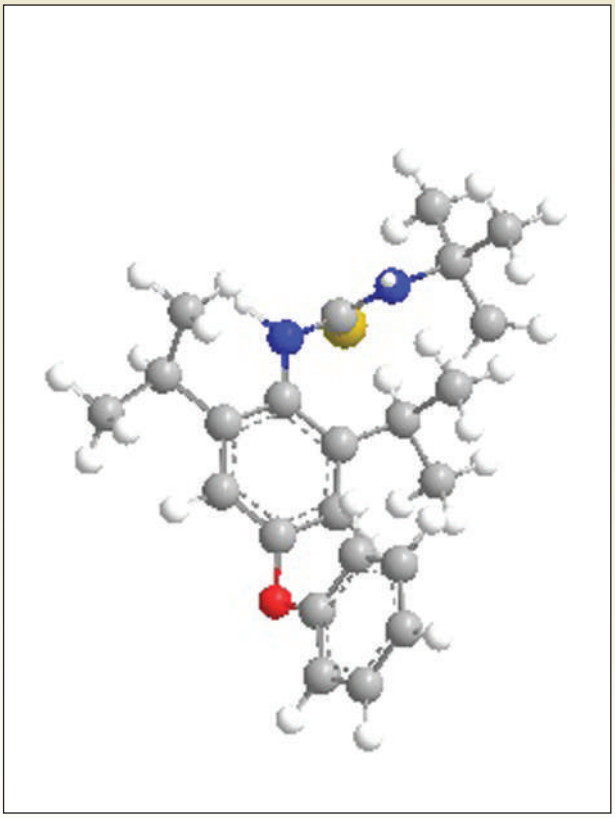
S & T SERVICES RENDERED INCLUDING MAJOR FACILITY / EQUIPMENT INSTALLED

- Laboratory scale forward osmosis and membrane distillation systems were installed at Membrane separations laboratory for processing aqueous systems.
- Design of Highly Efficient and In-expensive Membrane Equipment as Import Substitutes for Demineralized Water Production
- Installed pilot scale electro deionization unit for production of ultra pure water that could be integrated with the cascaded RO demineralization unit
- Two RO based water purification systems of 1000 L/h capacity deployed in line with automatic rinsing –filling -capping machine for production of packaged drinking water to be marketed by HPCL
- Nanofiltration based water purification unit of 1000 L/h capacity installed at Gandhi Hospital to serve the patients and hospital staff

FLUORO-AGROCHEMICALS





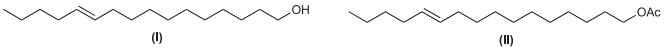


BASIC RESEARCH

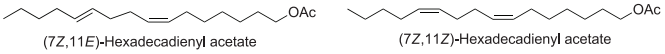
Scientists in Semiochemicals Lab (Fluoro & Agrochemicals Department) are active in Pheromone Application Technology (**PAT**). Here in the past two years activities of this particular group have been presented.

The following molecules were synthesized by the group and formulated as lures for use in the pheromone traps.

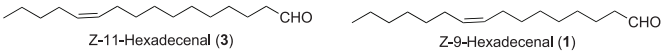
1. Brinjal Shoot and Fruit Borer (BSFB)



2. Pink Bollworm insect pheromones (PBW)

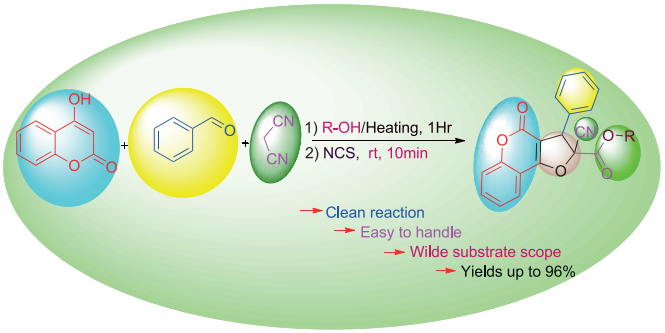


3. Yellow Stem Borer of Rice (*Scirpophaga incertulas*)



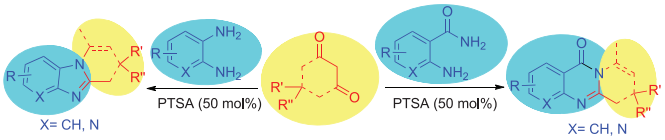
A simple, one pot synthesis of furo[3,2-*c*] chromenes and evaluation of antimicrobial activity

Synthesis of a number of 2-cyano-4-oxo-3-phenyl-3,4-dihydro-2H-furo[3,2-c]chromene-2-carboxylate compounds has been accomplished by a simple, multicomponent one pot reaction. The furo[3,2-*c*] chromenes antimicrobial activity was evaluated *in vitro* against different Gram-positive and Gram-negative bacterial strains. The outcome of the screening study showed that compound one compound exhibited promising activity against *Micrococcus luteus* MTCC 2470 and *Klebsiella planticola* MTCC 530. Another compound exhibited excellent activity against *Bacillus subtilis* MTCC 121, *Micrococcus luteus* MTCC 2470, *Klebsiella planticola* MTCC 530, *Escherichia coli* MTCC 739 and displayed a moderate activity against *Staphylococcus aureus* MTCC 96 and *Candida albicans* MTCC 3017 when compared with Ciprofloxacin (standard control). *(Bioorg. Med. Chem. Lett.,* **2016**, 26, 4899)



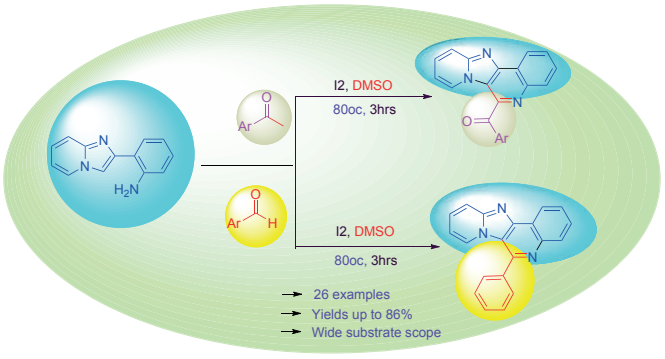
A simple one pot synthesis of novel tricyclic quinazolinones

Synthesis of a series of tricyclic quinazolinones has been accomplished starting from anthranilamide and 1,3-cyclic dione promoted by $TsOH.H_2O$. The protocol presented herein is based on retro-Dieckmann type reaction, leading to incorporation of dione as an acyclic unit into the product. Simple reaction conditions, broad scope, excellent yields are the advantages of this protocol. Further, this methodology is extended to the synthesis of pyridopyrimidinones and benzimidazopyridines. *(Tetrahedron Lett.,* **2017**, 58, 1071)



Synthesis of pyrido fused imidazo[4,5-*c*] quinolines by I_2-DMSO promoted oxidative cross coupling and intramolecular cyclization

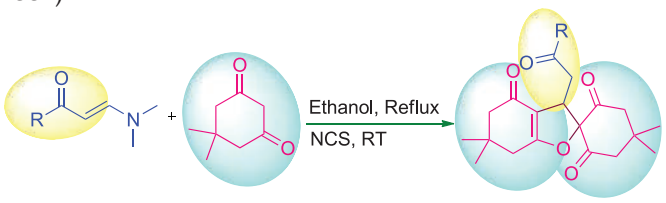
Synthesis of a series of novel pyrido fused imidazo[4,5-*c*] quinolines was accomplished by a simple, efficient, I_2-DMSO promoted sequential oxidative cross coupling followed by intramolecular cyclization of pyridoimidazole arylamines and carbonyl compounds in a one pot reaction. Simple reaction conditions, no metal catalyst, no additives, no ligand, selective product formation and high yields are the advantages of this method. *(Synthesis,* **2017**, 49, 1603)



A simple approach to access tricyclic spiro dihydrofurans in a one pot reaction

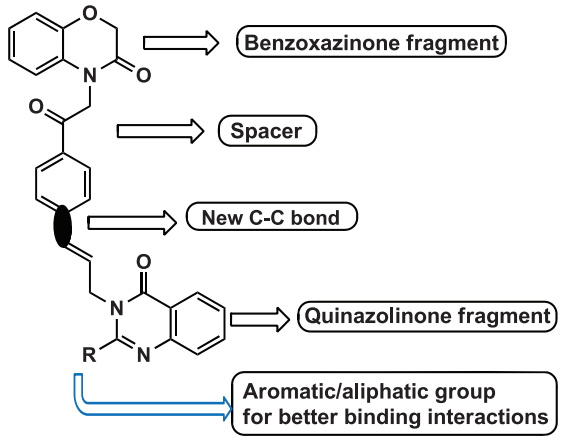
A simple and efficient one pot protocol is accomplished to access tricyclic spiro dihydrofurans by the reaction of β-enamino ketones and dimedone in ethanol followed

by sequential addition of N-chlorosuccinimide (NCS) at ambient temperature for the first time. The selectivity in desired product formation in good yields is the advantage of this protocol. (*Synth. Commun.,* **2017**, 47(14), 1332)



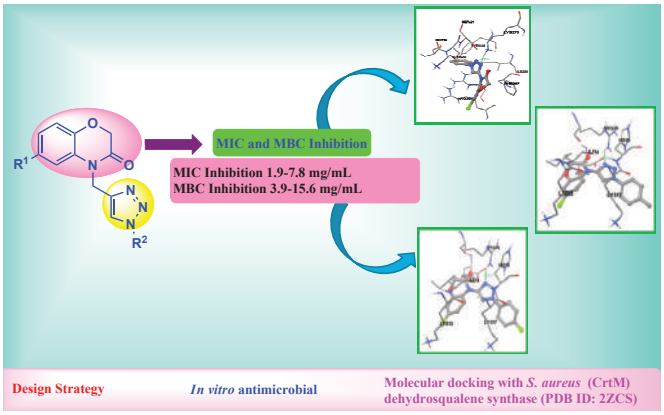
Potential anti-proliferative agents from 1,4-benzoxazinone-quinazolin-4(*H*)-one templates

A novel synthetic protocol has been developed for the synthesis of 1,4-benzoxazinone-acetylphenylallyl quinazolin-4(3*H*)-one hybrids by employing Pd-catalyzed C-H arylation in presence of 5-10% phosphine ligand in good to excellent yields and evaluated for their anti-proliferative activity against three cancer cell lines such as A549 (lung), HeLa (cervical), MDA-MB-231 (breast). Few compounds exhibited promising anti-proliferative activity with GI_{50} values ranging from **0.37** to **2.73** μM respectively against A549, HeLa, and MDA-MB-231. This is the first report on the synthesis and *in vitro* anti-proliferative evaluation of 1,4-benzoxazinone-acetylphenylallyl quinazolin-4(3*H*)-one hybrids. *(Bioorg. Med. Chem. Lett.,* **2017**, 27, 5481)



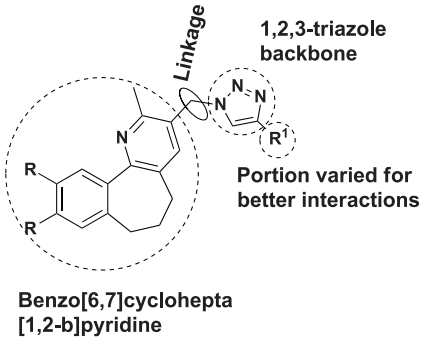
Potential antimicrobial agents from triazole functionalized 2*H*-benzo[*b*][1,4]oxazin-3(4*H*)-ones

A series of substituted triazole-functionalized 2*H*-benzo[*b*][1,4]oxazin-3(4*H*)-ones were synthesized and compounds were screened for their *in vitro* antimicrobial activity against Gram positive and Gram negative strains using Miconazole and Ciprofloxacin as standard drugs. (*Bioorg. Med. Chem. Lett.,* **2017**, 27, 5158)



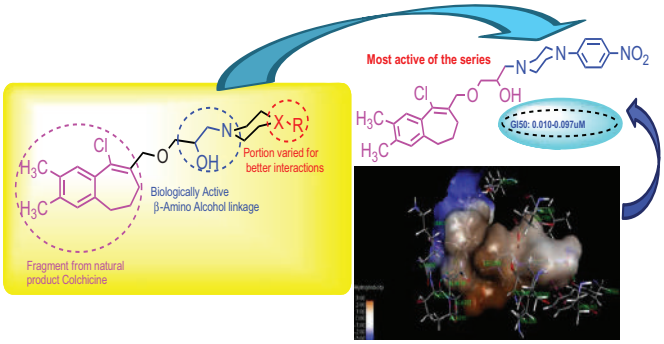
Design, Synthesis and *in vitro* anti-tuberculosis activity of *benzo[6,7] cyclohepta[1,2-b]pyridine-1,2,3-triazole* derivatives

A series of novel benzo[6,7]cyclohepta[1,2-*b*]pyridine-1,2,3-triazole hybrids have been designed and synthesized in excellent yields by Huisgen's [3+2] cyclo addition reaction of 3-(azidomethyl)-2-methyl-6,7-dihydro-5H-benzo[6,7]cyclohepta[1,2-*b*]pyridine with various alkynes in presence of copper sulphate and sodium ascorbate and the newly synthesized compounds were evaluated for their *in vitro* anti-mycobacterial activity against *Mycobacterium tuberculosis* H37Rv (ATCC27294). Among the compounds tested, the few compounds displayed most potent with MIC: 1.56 µg/mL. and has shown lower cytotoxicity. (*Bioorg. Med. Chem. Lett.,* **2017**, 27, 5119)



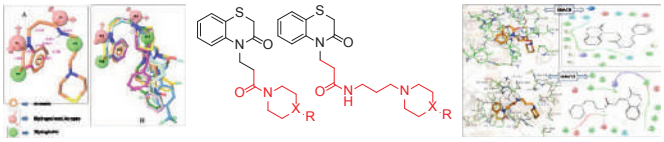
Novel piperazine linked β-aminoalcohols bearing a benzosuberone scaffolds as anti-proliferative agents

A series of novel 1-((9-chloro-2,3-dimethyl-6,7-dihydro-5*H*-benzo [7] annulen-8-yl)methoxy)-3-(4-phenylpiperzin-1-yl) propan-2-ols have been synthesized in excellent yields and evaluated for their *in vitro* anti-proliferative activity against four human cancer cell lines of HeLa, MDA-MB-231, A549 and MIAPACA with GI_{50} values ranging from 0.010 to 24.4μM. (*Bioorg. Med. Chem. Lett.,* **2017**, 27, 792)



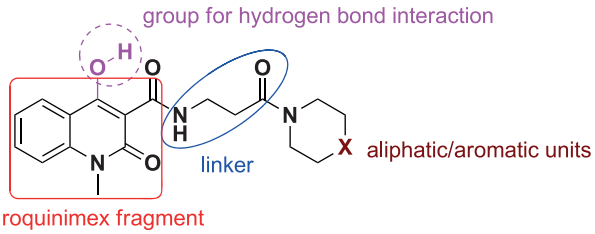
Novel benzothiazin-piperazine derivatives by peptide-coupling as potential anti-proliferative agents

Novel benzothiazin-piperazine derivatives has been synthesized by peptide-coupling and screened for their anti-proliferative activity against human cancer cell lines of HeLa, MIAPACA, MDA-MB-231 and IMR32. *(Bioorg. Med. Chem. Lett.,* **2017**, 27, 354)



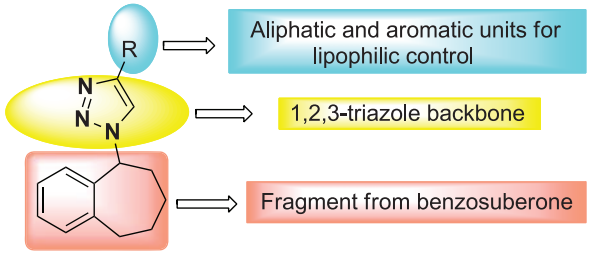
Synthesis, biological evaluation and molecular docking studies of novel 1,2-dihydro-4-hydroxy-2-oxoquinoline-3-carboxamide derivatives as potential anti-proliferative agents

A new series of 4-hydroxy-1-methyl-2-oxo-1,2-dihydroquinoline-3-carboxamide hybrids have been designed and synthesized using peptide coupling agents with substituted *N*-phenyl piperazines and piperidines with good to excellent yields. The synthesized compounds were evaluated for their *in vitro* anti-proliferative activity against PANC 1, HeLa and MDA-MB-231. The compounds exhibited considerable anti-proliferative activity with GI_{50} values ranging from **0.15** to **1.4** μM. The structure and anti-proliferative activity relationship was further supported by *in silico* molecular docking study of the active compounds against tubulin protein. *(Eur. J. Med. Chem.,* **2017**, 125, 400)



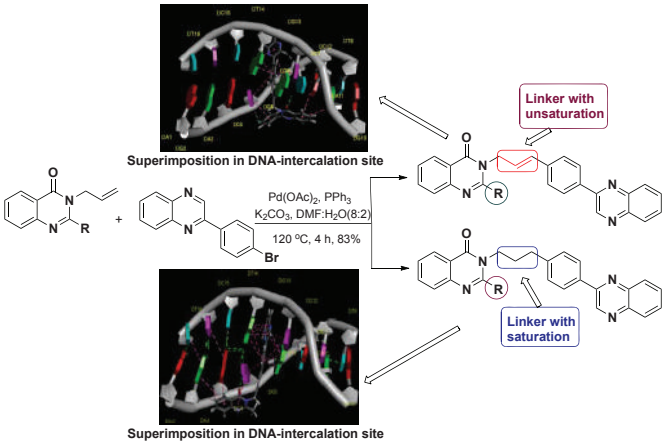
A convenient synthesis and screening of benzosuberone bearing 1,2,3-triazoles against *Mycobacterium tuberculosis*

A series of benzosuberone bearing 1,2,3-triazoles were rationally designed and alkyl/aryl groups appended on 1,2,3-triazole derivatives were synthesized using click chemistry and evaluated for their *in vitro* antimycobacterial activity against *Mycobacterium tuberculosis* H37Rv (ATCC27294). Few compounds (MIC: 3.125 µg/mL) and (MIC: 6.25 µg/mL) exhibited promising hits. This is the first report on the synthesis and *in vitro* antimycobacterial activity against *Mycobacterium tuberculosis* H37Rv of benzosuberone alkyl/aryl groups appended on 1,2,3-triazole derivatives. *(Bioorg. Med. Chem. Lett.,* **2016**, 26, 4292)



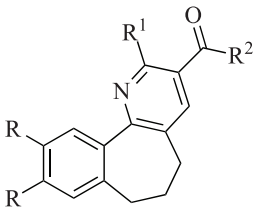
Quinazolinones-Phenylquinoxaline hybrids with unsaturation/saturation linkers as novel anti-proliferative agents

A new series of novel quinazolinones with allylphenyl quinoxaline hybrids were efficiently synthesized in good yields by the reaction of 3-allyl-2-methylquinazolin-4(3*H*)-one with bromophenyl)quinoxaline utilizing Pd catalyzed Heck-cross coupling and evaluated for anti-proliferative activity against four cancer cell lines and Docking results indicate a sign of good intercalation, suggesting that these compounds act as DNA intercalates. (*Bioorg. Med. Chem. Lett.,* **2016**, 26, 3014)



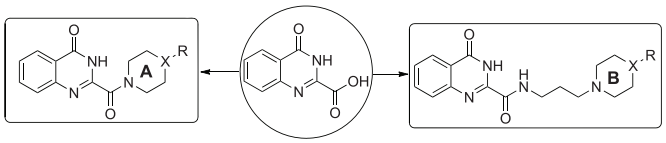
Three-component, one-pot synthesis of benzo[6,7]cyclohepta[1,2-*b*]pyridine derivatives under catalyst free conditions and evaluation of their anti-inflammatory activity

An efficient three-component protocol is described for the synthesis of benzo[6,7]cyclohepta[1,2-*b*]pyridine derivatives using β-chloroacroleins, 1,3-dicarbonyls and ammonium acetate under catalyst free conditions by using ethanol as reaction media. The mild reaction conditions, operational simplicity and high yields are the advantages of this protocol and the broad scope of this one-pot reaction makes this procedure promising for practical usages. All the final compounds were screened for anti-inflammatory activity. Among the compounds tested, few compounds exhibited significant inhibition of IL-1β and MCP-1secretion as a measure of anti-inflammatory activity. *(Bioorg. Med. Chem. Lett.,* **2016**, 26, 858)



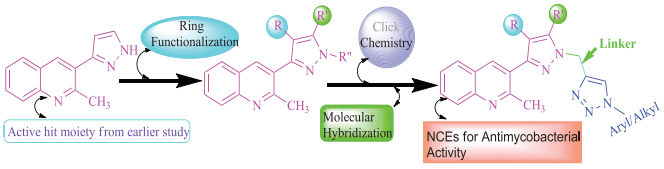
Synthesis and evaluation of anti-proliferative activity of novel quinazolin-4(*H*)-one derivatives

Two series of novel quinazolin-4(3*H*)-one derivatives have been synthesized and evaluated for their *in vitro* anti proliferative activity against human HeLa, MIAPACA, MDA-MB-231 and IMR-31 cancer cell lines. The synthesized compounds were characterized by spectral methods. Among them, few compounds exhibited potent *in vitro* anti proliferative activity with GI_{50} values 0.02, less than 0.01 μM against MIAPACA human cancer cell line. We have explored the probable binding mode and key active site interactions in HDAC8 and EHMT2 proteins. The docking results are complementary to the experimental results. *(Med. Chem. Res.,* **2016**, 25, 2070)



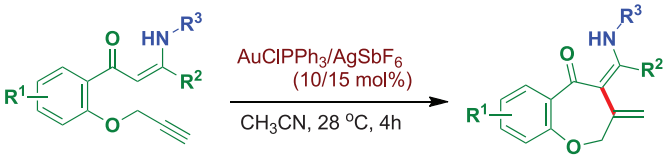
Ring Functionalization and Molecular Hybridization of Quinolinyl Pyrazole: Design, Synthesis and Antimycobacterial Activity

Synthesis of quinolinyl pyrazole analogues by ring functionalization as well as molecular hybridization strategy is adopted. Diverse functional groups were assembled around the privileged scaffold viz., 2-methyl-3-(1H-pyrazol-5-yl)quinoline. A series of quinolinyl pyrazole analogues with 1,4-disubstituted 1,2,3-triazole moiety, were synthesized employing Click reaction conditions. All 29 compounds synthesized compounds were evaluated for antitubercular activity against *Mycobacterium smegmatis* strain; wherein eight compounds were active and two promising. Compounds also exhibited the low cytotoxicity against A549 cell line. (*ChemistrySelect,* **2017**, 1, 1)



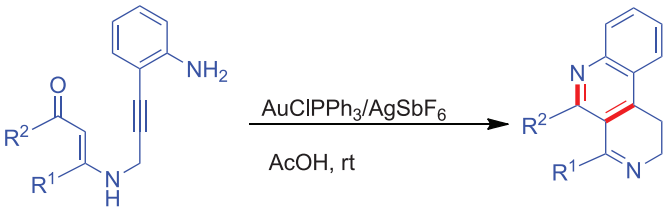
Gold-catalysed Synthesis of 3-Methylene-3,4-dihydrobenzo[b]oxepinones

An efficient gold-catalyzed synthesis of substituted 3-methylene-3, 4-dihydrobenzo**[***b***]** oxepinones have been achieved from *ortho-O*-propargyl substituted aryl enaminones**.** In this transformation new C-C bond formation was taken place regioselectively *via* **7-***exo-dig* cyclization. Benzooxepinone derivatives were obtained in good to excellent yields in one-pot at ambient temperature**. (***Org. Lett.,* **2017,** 19, 282)



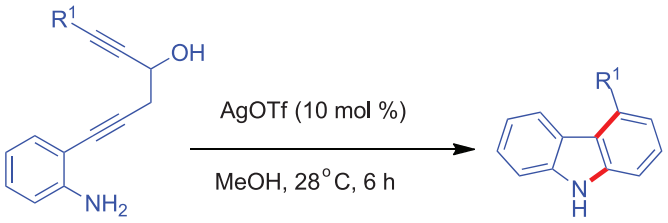
Synthesis of 1,2-Dihydro[c][2,7] naphthyridines

We have developed a novel and efficient gold catalyzed protocol for the construction of 1,2-dihydrobenzonaphthyridine derivatives from 2-aminophenyl prop-2-yn-1-yl enaminones. In this transformation a new C-C and C-N bond formation occured in one-pot fashion under mild reaction conditions *via* intramolecular *6-endo*-dig cyclization, condensation sequence. It is noteworthy that very good to excellent yields of 1,2-dihydrobenzonaphthyridine derivatives were achieved. (*Org. Biomol. Chem.*, **2017**, 15, 7813)



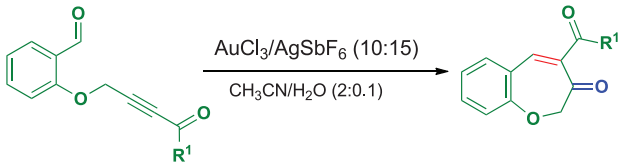
Synthesis of Substituted carbazoles *via* silver catalysis

We have developed an efficient synthetic protocol for generating carbazoles from **2-(6-substituted-3-hexanol-1,5-diynyl)anilines.** Significantly, in this transformation new C-C and C-N bonds were formed ***via* a sequence of hydroamination, cyclization, and dehydration.** Good to excellent yields of the carbazole derivatives were obtained in one-pot under mild conditions. This synthetic strategy provides a new, efficient and rapid method for the construction of carbazole derivatives in the presence of silver-catalyst. *(Asian J. Org. Chem.,* **2017**, 6, 1674)



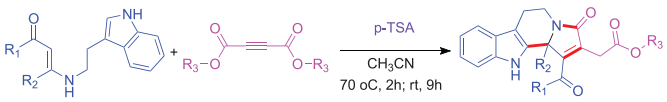
Synthesis of Benzooxepin-3-ones

An efficient gold-catalyzed intramolecular cyclization of *ortho-O*-propargyl-1-one substituted arylaldehydes has been achieved for the generation of substituted aroylbenzo[*b*]oxepin-3-one derivatives in moderate to good yields. This synthetic transformation proceeds *via* gold-catalysed oxidation of internal alkyne moiety followed by an intramolecular condensation leading to the seven-membered oxacycles. *(Org. Biomol. Chem.*, **2016**, 14, 3526)



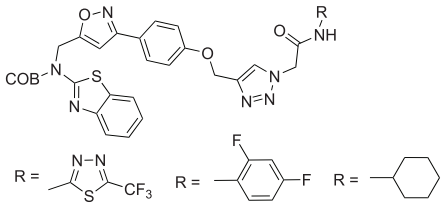
Synthesis of Tetracyclic Tetrahydro-β-Carbolines

An efficient *p*-toluenesulfonic acid promoted reaction of substituted β-enaminones and acetylenedicarboxylates has been achieved for the generation of tetracyclic tetrahydro-β-carboline derivatives. In this one-pot reaction two new C-C and one C-N bonds are formed sequentially to access moderate to good yields of tetracyclic tetrahydro-β-carboline derivatives having significant molecular complexity. *(Asian J. Org. Chem.,* **2016**, 5, 1378)



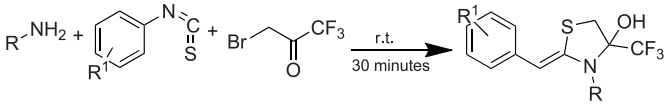
Novel Triazole linked 2-phenyl benzoxazole derivatives induce apoptosis by inhibiting miR-2, miR-13 and miR-14 function in Drosophila melanogaster

Novel Triazole linked 2-phenyl benzoxazole derivatives as a negative regulator of apoptosis inhibiting micro RNAs (*miR-2, miR-13 and miR-14*) in a well established in vivo model *Drosophila melanogaster* where the process of apoptosis is very similar to human apoptosis. (*Apoptosis,* **2017**, 22(6), 786)

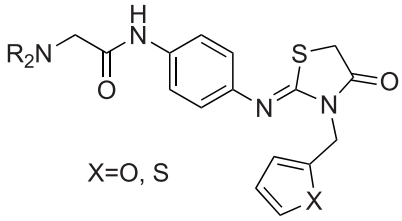


Fluorinated thiazolidinols cause cell death in A549 lung cancer cells via PI3K/AKT/mTOR and MAPK/ ERK signalling pathways

A series of 2-imino-4-(trifluoromethyl)thiazolidin-4-ol derivatives were synthesized from one pot, three component reactions of primary amine, aryl isothiocyanate and 3-bromo-trifluoromethyl acetone via *in situ* generation of both symmetrical and unsymmetrical thioureas. All the synthesized derivatives were screened for their in vitro anti-cancer activity against human cancer cell lines. The cell cycle showed that treatment of lung cancer cells with these compounds resulted in G0/G1 cell cycle arrest. Studies to understand the molecular mechanism of action of these compounds suggest that the compounds inhibit PI3K, pAkt and mTOR protein expression with concomitant up-regulation of tumour suppressor PTEN. These compounds contributed to LC-3 mediated cytoplasmic vacuolation leading to cell death in lung cancer cells. *(Med. Chem. Commun.*, **2016**, 7, 1197)



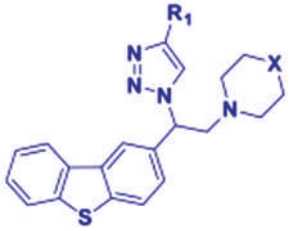
Synthesis and biological evaluation of novel 2-imino-4- thiazolidinone derivatives as potent anti-cancer agents



A new series of 2-imino-4-thiazolidinone derivatives has been synthesised and screened for their cytotoxicity against three cancer cell lines (B16F10, A549, PANC-1) and normal cell line (CHO). Among the compounds tested, compounds 3 compounds showed potent cytotoxicity against B16F10 cell line with IC_{50} between 3.4 and 7 µM. Interestingly these three compounds are non toxic to non cancerous CHO cells and induced apoptosis in B16F10 cells observed by DNA damage analysis through PI/Hoechst double staining method. (Bioorg. *Med. Chem. Lett.,* **2016,** 26, 5361)

Click-based synthesis and antitubercular evaluation of novel dibenzo[*b,d*]thiophene-1,2,3-triazoles with piperidine, piperazine, morpholine and thiomorpholine appendages

A series of novel piperidine, piperazine, morpholine and thiomorpholine appended dibenzo [*b,d*]thiophene-1,2,3-triazoles were designed and synthesized utilizing azide–alkyne click chemistry in the penultimate step. The required azide building blocks was synthesized from commercial dibenzo[*b,d*]thiophene in good yields following five step reaction sequence. Screening all thirty new compounds for invitro antimycobacterial activity against Mycobacterium *tuberculosis* H37Rv, resulted **three derivatives** as potent analogues with MIC 0.78 µg/mL, 0.78 µg/mL & 1.56 µg/mL respectively and has shown lower cytotoxicity. Interestingly, all six piperazine appended dibenzo[*b,d*]thiophene-1,2,3-triazoles exhibited *Mtb* inhibition activity with MIC 1.56–12.5 µg/mL. To some extent, the data observed here indicated *Mycobacterium tuberculosis* inhibition among the appendages is in the order, piperazine > thiomorpholine > morpholine. *(Bioorg. Med. Chem. Lett.*, **2016**, 26 (11), 2649)

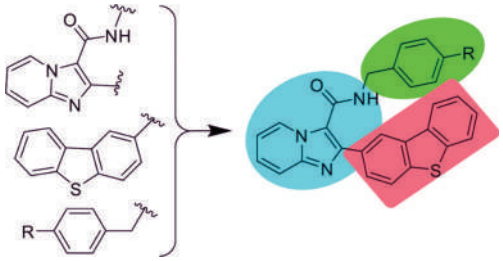


Synthesis and antitubercular evaluation of novel dibenzo[*b,d*] thiophene tethered imidazo[1,2-*a*]pyridine-3-carboxamides

A series of novel dibenzo[*b,d*]thiophene tethered imidazo[1,2-*a*]pyridine carboxamides were designed and synthesized. The required building block, 2-dibenzo[*b,d*] thiophenyl imidazo[1,2-*a*]pyridine carboxylic acid was synthesized from commercial dibenzo [*b,d*]thiophene in good yields following five-step reaction sequence. The desired carboxamides was prepared through coupling of acid with various benzyl amines. All the new analogues was characterized by their NMR and mass spectral analysis.

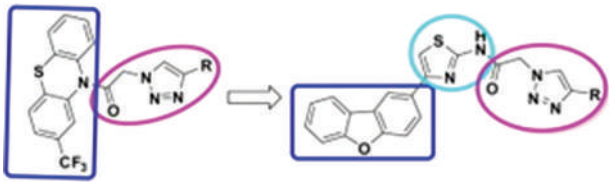
Among nineteen new compounds screened for invitro anti-mycobacterial activity against Mycobacterium *tuberculosis* H37Rv, three compounds were identified

as potent analogues with low cytotoxicity. The results reported here will help global efforts for identification of potential lead antimycobacterial agents. (*Bioorg. Med. Chem. Lett.*, **2016**, 26 (13), 3135)



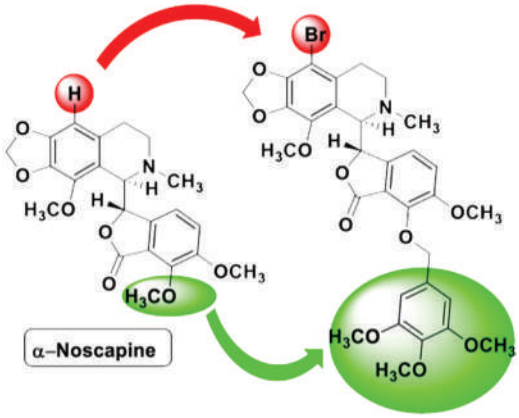
Click-based synthesis and antitubercular evaluation of dibenzofuran tethered thiazolyl-1,2,3-triazolyl acetamides

A series of novel dibenzofuran tethered thiazolyl-1,2,3-triazolyl acetamides, designed by assembling antitubercular pharmacophoric fragments, dibenzofuran, 2-aminothiazole and substituted triazoles in one molecular architecture, were evaluated against *Mycobacterium tuberculosis*. The new analogues accomplished in four step synthetic sequence utilizing click chemistry in the penultimate step, was fully characterized by their NMR and mass spectral data. Among the compounds screened for in vitro antimycobacterial activity against *Mycobacterium tuberculosis* H37Rv, three compounds was found to be most active (MIC: 1.56 µg/mL and 3.13 µg/mL) and exhibited lower cytotoxicity. Among these three, **one product** could be a candidate to consider as a drug like hit analogue for further development. *(Bioorg. Med. Chem. Lett.*, **2016**, 26(15), 3684)



Subtle Alterations in Microtubule Assembly Dynamics by Br-TMB-Noscapine Strongly Suppress Triple-Negative Breast Cancer Cell Viability without Mitotic Arrest

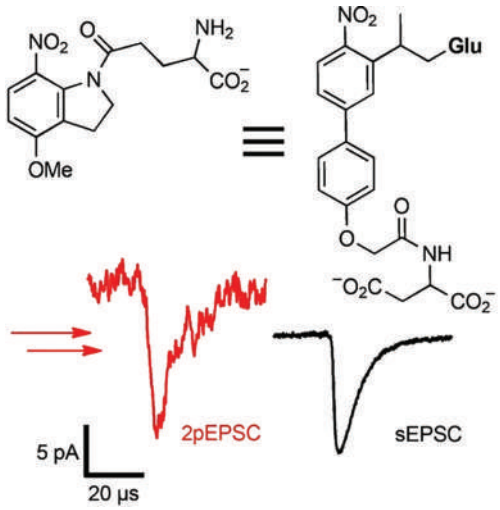
Triple-negative breast cancer (TNBC) is one of the most aggressive cancers in women with limited treatment options. We rationally designed a potent analogue of noscapine, Br-TMBNos, through a three-step reaction sequence starting from natural α-noscapine, fully characterized it by IR, ^{1}H & ^{13}C NMR and mass spectral analyses, examined its tubulin-targeted mechanism of action, and investigated its efficacy against TNBC using MDA-MB-231 cells. Far-UV CD spectra indicated disruption of helical stability in tubulin by Br-TMB-Nos. In addition, the noscapinoid altered the surface configuration of tubulin, promoted colchicine binding to tubulin, and slightly inhibited microtubule polymer mass. Among the cell lines tested (MDA-MB-231, HeLa, and PANC-1), it showed strongest inhibition of MDA-MB-231 cell viability (IC_{50}, 0.4 ± 0.05 µM), and strongly suppressed clonogenicity of this cell line. Despite targeting tubulin, Br-TMB-Nos did not induce mitotic arrest; instead, it prolonged S-phase. Thus, the structural alterations in the noscapinoid architecture changed its mechanism of action from G_2/M arrest to S-phase arrest. Interestingly, cellular microtubules and DNA appeared to be intact in the presence of the drug. Our findings suggest that Br-TMB-Nos may be investigated further as a tubulin-targeted, S-phase-specific, cytostatic, antibreast cancer agent, potentially devoid of severe side effects. *(Chemtryselect*, **2016**, 1(14), 4313)



Development of Anionically Decorated Caged Neurotransmitters: In Vitro Comparison of 7-Nitroindolinyl- and 2-(*p*-Phenyl-*o*-nitrophenyl)propyl-Based Photochemical Probes

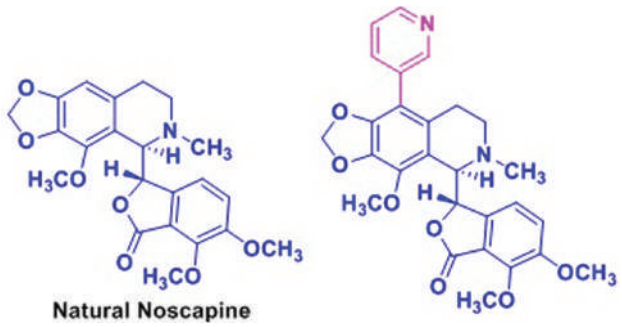
Neurotransmitter uncaging, especially that of glutamate, has been used to study synaptic function for over 30 years. One limitation of caged glutamate probes is the blockade of γ-aminobutyric acid (GABA)-A receptor function. This problem comes to the fore when the probes are applied at the high concentrations required for effective

two-photon photolysis. To mitigate such problems one could improve the photochemical properties of caging chromophores and/or remove receptor blockade. We show that addition of a dicarboxylate unit to the widely used 4-methoxy-7-nitroindolinyl-Glu (MNI-Glu) system reduced the off-target effects by about 50–70 %. When the same strategy was applied to an electron-rich 2-(*p*-Phenyl-*o*-nitrophenyl)propyl (PNPP) caging group, the pharmacological improvements were not as significant as in the MNI case. Finally, we used very extensive biological testing of the PNPP-caged Glu (more than 250 uncaging currents at single dendritic spines) to show that nitro-biphenyl caging chromophores have two-photon uncaging efficacies similar to that of MNI-Glu. *(ChemBioChem*, **2016**, 17(10), 953)



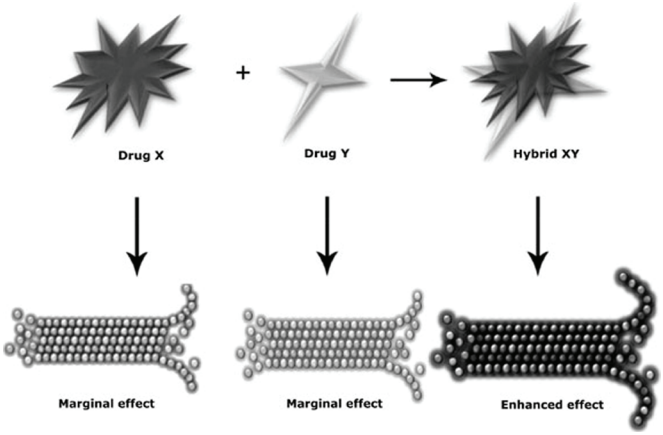
Elucidation of the Tubulin-targeted Mechanism of Action of 9-(3-pyridyl) Noscapine

We have recently reported the synthesis and antiproliferative potential of a series of biaryl type α-noscapine congeners. Among them, 9-(3-pyridyl) noscapine (9-PyNos, henceforth), which was synthesized by adding pyridine unit to the tetrahydroisoquinoline part of natural α-noscapine core, was found to be the most effective one to inhibit proliferation of a variety of cancer cell lines. However, details of its interactions with its cellular target, tubulin, remain poorly understood. In this report, we examined the nature of interactions of 9-PyNos with tubulin based on the methodologies of spectrofluorimetry, circular dichroism, and turbidimetry techniques. Far-UV circular dichroism spectra indicated perturbation of tubulin secondary structure in the presence of 9-PyNos, not amounting, however, to the perturbation induced by noscapine. The noscapinoid nevertheless altered the surface configuration of the protein considerably, as indicated by an anilinonaphthalene sulphonate binding assay, and promoted colchicine binding to tubulin, the latter indicating its adjacent binding site with colchicine. 9-PyNos however, did not alter microtubule assembly considerably. Investigating the possible reason behind this apparent lack of strong inhibition of microtubule assembly, we found that the binding interactions of tubulin with 9-PyNos do not involve modification of cysteine residues of tubulin. Taken together, our data suggest that the antiproliferative mechanism of action of 9-PyNos involves disruption of structural integrity of tubulin without strong inhibition of tubulin assembly. (*Curr. Top. Med. Chem.,* **2017**, 17(22), 2569)



Microtubule Targeting Agents as Cancer Chemotherapeutics: An Overview of Molecular Hybrids as Stabilizing and Destabilizing Agents

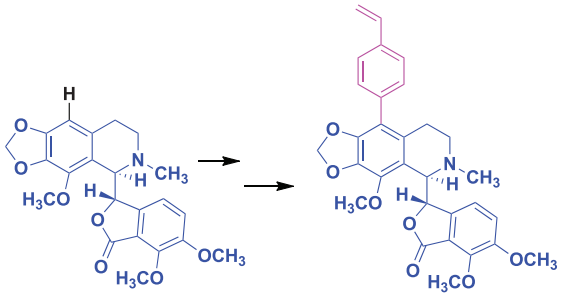
Microtubules form crucial dynamic structural cellular components of the cell and are composed of the alpha beta tubulin heterodimers. Microtubules are involved in a wide variety of functions in the cell such as attribution to cell shape, motility, intracellular trafficking and mitotic spindle formation. Owing to these reasons, tubulin and microtubules have gained significant interest as important targets for cancer therapy. A review of the existing microtubule targeting drugs specifies that these agents can be categorised into two of the major categories: Microtubule stabilizing agents such as paclitaxel, docetaxel, epothilones, and discodermolide which bind to the tubulin polymer and stabilize the microtubules, microtubule destabilizing agents such as vinca alkaloids, colchicine and combretastatins which bind to tubulin dimers and cause destabilization.



These agents ultimately alter the equilibrium between tubulin and microtubule resulting in disruption of mitotic spindle, thereby effecting a critical transition in the cell cycle, leading to cell death. Further, clinical studies of these agents are limited by toxicity effects and emergence of drug resistance. The hybrid drugs are a combination of two or more drugs wherein pharmacophores are incorporated into a single molecule to interact with multiple targets and enhance the cytotoxic action with minimal side effects. Such hybrid regimens can improve therapeutic efficacy and reduce drug toxicity. Therefore, studies on new hybrids with such biological properties form important part in chemistry. In this review, we present an overview of various recent hybrids of colchicines, combretastatin, phodophyllotoxin, etc generated by combination among themselves through linkers or with other pharmacophores and their properties like tubulin stabilization and tubulin destabilization. We also attempted to provide chemistry, toxicity, resistance, side effects of these molecular hybrids acting as microtubule targeting drugs. (*Curr. Top. Med. Chem.,* **2017,** 17(22), 2523)

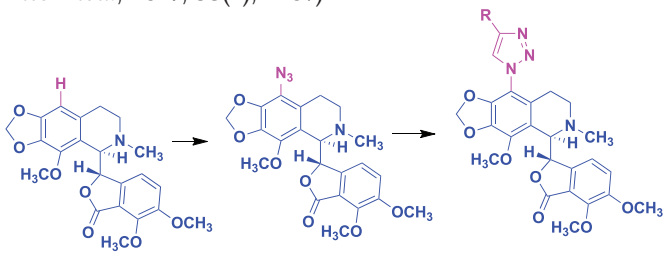
Induction of acetylation and bundling of cellular microtubules by 9-(4-vinylphenyl) noscapine elicits S-phase arrest in MDA-MB-231 cells

Noscapine is an alkaloid present in the latex of Papaver somniferum. It has been known for its anticancer efficacy and lack of severe toxicities to normal tissues. Structural alterations in noscapine core architecture have produced a number of potent analogues of noscapine. Here, we report an unusual activity of a novel noscapine analogue, 9-(4-vinylphenyl)noscapine (VinPhe-Nos) on cancer cells. As we reported earlier, VinPhe-Nos inhibited MDA-MB-231 cell proliferation with an IC_{50} of 6 μM. The present study elucidated a possible antiproliferative mechanism of action of VinPhe-Nos. The noscapinoid significantly inhibited clonogenic propagation of MDA-MB-231 cells. However, unlike the majority of tubulin-binding agents, it did not induce mitotic arrest; instead, it prolonged S-phase. Although prolonged presence of the drug show some disruption of cellular microtubule architecture, it did not affect microtubule recovery after cold-induced depolymerization. VinPhe-Nos, nevertheless, induced acetylation and bundling of microtubules. Our data suggest that rational modification of parent compound can alter its mechanism of action on cell cycle and that VinPhe-Nos can be investigated further as a less-toxic, S-phase-preferred, cytostatic anticancer agent. (*Biomed. Pharmacother.,* **2017**, 86, 74)



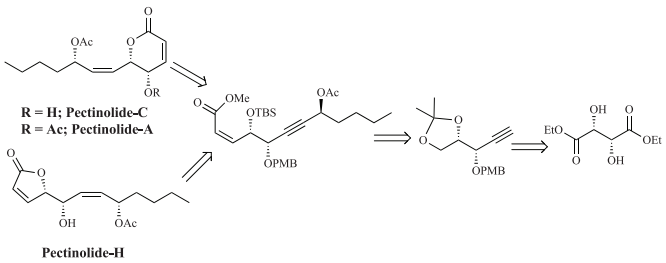
Synthesis and click reaction of tubulin polymerization inhibitor 9-azido-α-noscapine

An efficient protocol for the synthesis of tubulin polymerization inhibitor, 9-azido-α-noscapine from 9-amino-α-noscapine is developed using mild reaction conditions (*t*-butyl nitrite/trimethylsilyl azide in acetonitrile at room temperature). Operational simplicity, high product yield without formation of any side products are the advantages of this protocol. Further copper catalysed click reactions of 9-azido-α-noscapine with alkynes resulted 9-triazolyl nicotinoids resulted in excellent yields. (*Res. Chem. Intermed.*, **2017**, 33(4), 2457)



Stereoselective Total Synthesis of Pectinolides A, C and H:

Pectinolides A-C and H were isolated from the Mexican medicinal plant *Hyptis pectinata*, belonging to the Lamiaceae family, which is used in the treatment of fever, antiseptics for skin and eye infections, gastric disturbances, muscular pain, rhinopharyngitis and lung congestion. Pectinolide A displayed antimicrobial activity against *Staphylococcus aureus* and *Bacillus subtilis* in the concentration range of 6.25-12.5 μg/mL. Pectinolides B and C were active with an MIC of 12.5-25 μg/mL against *Bacillus subtilis* and a value of 100 μg/mL against *Staphylococcus aureus* and exhibited significant cytotoxic activity (ED_{50} <4 μg/ml) against a variety of tumor cell lines. Pectinolide H also displayed a significant antimicrobial activity against two multidrug resistant strains of *Staphylococcus Aureus*, XU-212, which is highly resistant to tetracycline and SA 1199 B, which is resistant to certain fluoroquinolones.



The potential biological activity of Pectinolides A, C and H attracted us to carry out their stereoselective total synthesis. Our synthetic strategy follows mainly $LiAlH_4$ reduction of *p*-methoxy benzylideneacetal, *Ohira-Bestmann* homologation reaction, coupling of a terminal alkyne with pentanal, *Corey-Bakshi-Shibata* (*CBS*) reduction and *cis*-olefination using the *Still-Gennari* reagent followed by cyclization. (*Helv. Chim. Acta,* **2016,** 99, 247)

APPLIED RESEARCH (INDUSTRY SPONSORED)

New Chemical Entities for Agrochemical Activity (*Insecticides (India) Limited*)

Industry sponsored programme focuses on development of small molecules of synthetic origin that can are screened as plausible crop protection agents. Industry specified frameworks were synthesized. Scientific inputs involve development of reactions and/or protocols capable of building biologically active small-molecules by integrating Multi component reaction protocols, green reaction protocols and Diversity oriented synthesis. A total of 315 compounds (50 mg each) were submitted to the client for evaluation as agrochemicals. Active compound frameworks were remodeled and diverse ring functionalization attempted.

Fulcrum Reference Molecules (*Sai Life sciences*)

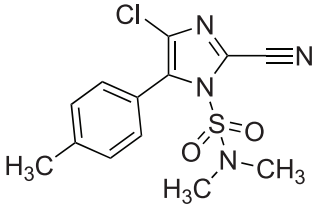
Accomplishing a time bound target synthesis for Fulcrum reference compounds. Four scientists were assigned six targets each. Each molecule involves multistep synthesis. Targets were successfully synthesized and compound given to the clients in 30-300mg quantities.

International Collaboration

A series of newchemical entities based on MCC950 were made as part of DBT-Indo-Australia collaboration project titled "Novel immunomodulatory agents for type II diabetes through targeting the NLRP3 inflammasome signaling cascade".

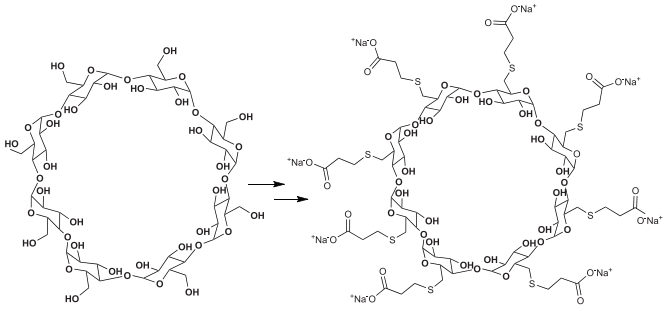
Process Development

Process development of fungicide, Cyazofamid (*Sponsored project*)



Cyazofamid is a foliar contact and protective fungicide. The mode of action is by inhibiting the complex-III Cytochrome bc1 at a site in mitochondria of Oomycetes Fungi. It is used in particularly on potatoes and tomatoes against Phytophthora infesting. It also controls mildew in vegetable crops and grapes. In view of its broad use CSIR-IICT started working on development of efficient process for the preparation of cyazofamid through sponsorship from agro industries.

Process improvement for Fluconazole and Sugammadex (*Sponsored project)*

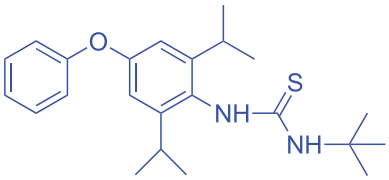


Sugammadex is synthesized from cyclodxtrin in two steps.

Improvement of yields in key steps in the process for the preparation of an antifungal drug. Fluconazole were also carried out in this project.

Diafenthiuron

Diafenthiuron is a broad spectrum insecticide having contact and stomach action with some ovicidal activity. It was introduced by Ciba Geigy corporation (Syngenta) in the year 1990. This product is mainly used to prevent and kill the pests and mites in cotton, fruit trees, vegetables, ornamental plants, soybeans and other crops. It also can be used to control the red spider on citrus tree and apple tree, the diamondback moth and other pests of cruciferous vegetables.

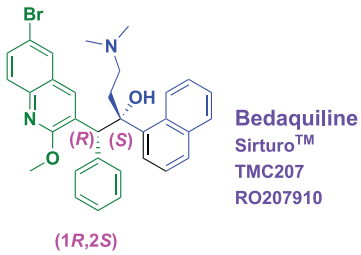


Country Demand evaluated based on imports data, from August 2015 to July 2016 is almost 152 tones @ Rs 2493/- kg product (accounting for 37.5 crores approximately) was imported from Switzerland. Realizing the importance of this insecticide, IICT has taken up the process development of this product and work carried out is as follows.

Initially, 2,6-diiisopropyl-4-phenoxyaniline moiety was prepared starting form *p*-nitrochlorobenzene and phenol followed by reduction and isopropylation. Thus obtained 2,6-diiisopropyl-4-phenoxyaniline was further reacted with CS_2 followed by t-butylamine leading to the desired product "Diafenthiuron". Scale-up studies from isopropylation stage onwards are in progress.

Process improvement of Bedaquiline

Bedaquiline is an oral drug, specifically used for the treatment of Multi-Drug Resistant Tuberculosis (MDR-TB). Bedaquiline was the first new drug approved for the treatment of TB in more than forty years (FDA Approval in December 2012). Bedaquiline affects the proton pump for ATP synthase of the *Mycobacterium tuberculosis*. It is on the World Health Organization's list of essential medicines

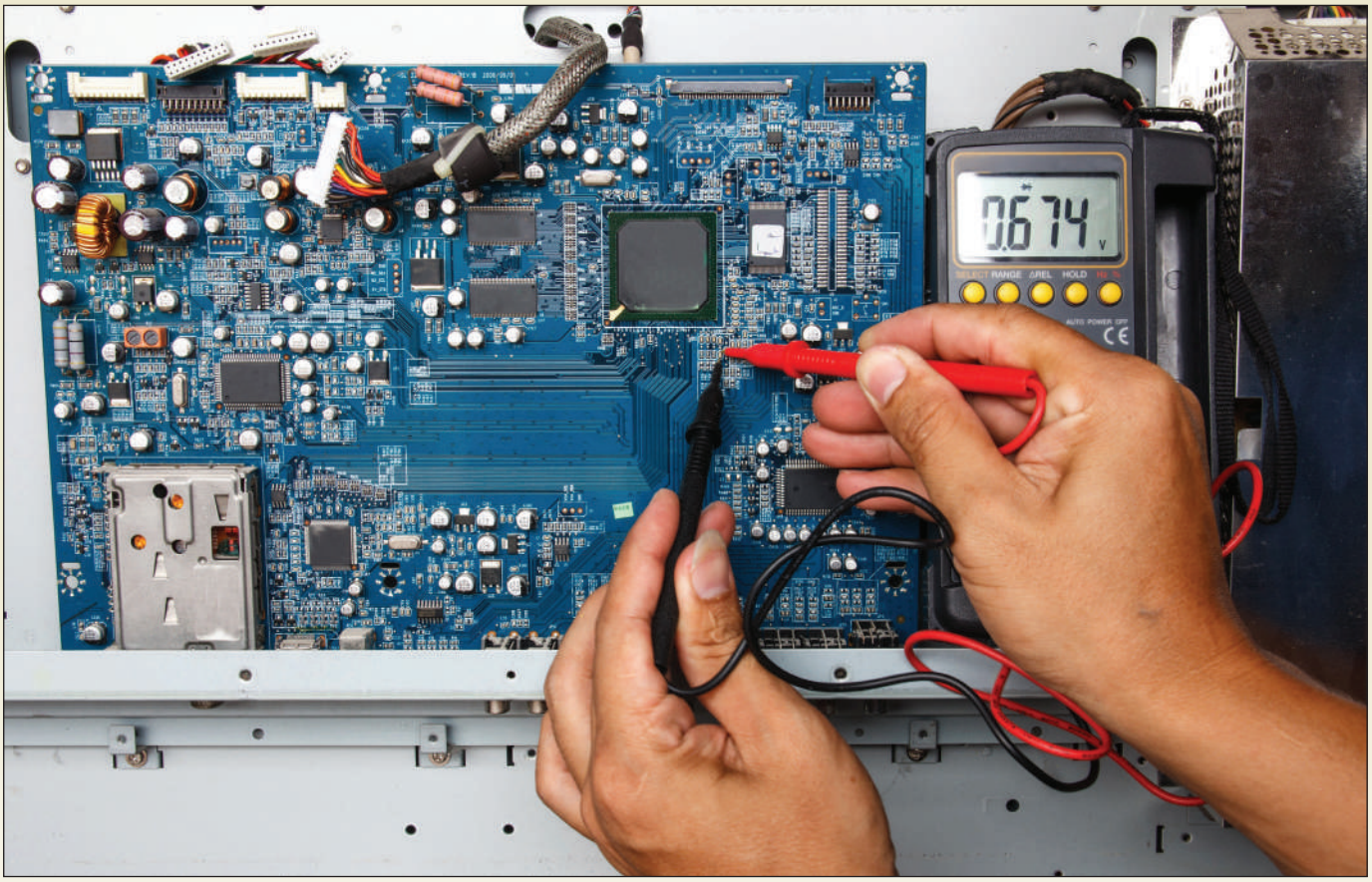


Process improvement of bedaquiline a drug molecule for tuberculosis was achieved. In this process, few steps yield improvement as well as undesired isomers were removed during the workup procedure.

Process improvement of Loxoprofen

Loxoprofen is a nonsteroidal anti-inflammatory drug. We are working on this molecule to reduce the reaction steps, non-infringing route of synthesis *via* cost effective synthetic procedures.

INSTRUMENTATION & REPP



Instrumentation, Reaction Engineering & Pilot Plants are catering the Institutes process development activities in the area of Instrumentation Engineering requirements for the existing and proposed R&D projects/activities & infrastructure of the Institute. State of the art pilot plant facilities are being established for scale up studies and for generation of engineering data for design of pilot or commercial plants.

In general the activities carried out by the department can be broadly classified as under:

- Process Development (R& D Projects)
- Establishment of Bench/Pilot scale facilities & Maintenance
- Design of Instrumentation & Process Automation systems
- Establishment of Instrumentation Facilities & Maintenance
- Human Resource Development

Process Development: (R&D Projects)

Instrumentation Engineering division & Reaction Engineering Pilot Plant are involved in the following R&D projects in various capacities in Instrumentation Design in Process measurement & Automation systems, providing Automation solutions, setting up of lab scale, pilot scale reactors for process development studies. Interfacing with multidisciplinary process development teams, in managing and providing Instrumentation solutions for the Institute to cater both in-house and Industrial projects.

The division provides basic & detailed engineering solutions in process plant automation using state of the art engineering software tools. Engineering services are offered in the form of i) Preparation of Process flow diagrams, ii) Process & Instrumentation diagrams, iii) Control philosophy, iv) Process automation design & v) Preparation of detailed engineering document for Instrumentation & process automation for pilot and commercial scale plants.

Following are the Major R&D Projects associated during this period:

- Hydrazine Hydrate Project (M/s GACL, Vadodara)
- Bio Ethanol -- Indo - US Project
- Commissioning of PTBT & PTBBA commercial plants at M/s Vinati Organics, Mumbai.
- Methyl Ester for M/s Vinati Organics, Mumbai
- PT Benzaldehyde Project for M/s Vinati Organics, Mumbai
- SAL project(Phase-II) – M/s HPCL

Establishment of Bench/Pilot scale facilities & Maintenance:

Established suitable Bench scale units for scale up of processes developed in-house and also for external industrial clients in the following projects:

- Biomass Multi feedstock Pretreatment process reactor facility at atmospheric conditions
- Biomass Pretreatment at high pressure and temperature reactor facility
- Biomass Hydrolysis/Saccharfication reactor
- Bioethanol Fermentation process reactor facility

Design of Instrumentation & Process Automation systems for the following projects:

Basic Engineering Package for 10,000 TPA capacity, Hydrazine Hydrate commercial plant for Gujarat Alkalies & Chemicals Limited.

Basic Design report for Methyl Ester & PMAP commercial plant for M/s Vinati Organics, Mumbai.

Establishment of Instrumentation Facilities & General Maintenance:

Process, Analytical, Utility Instruments & New Facilities installation, commissioning & Maintenance

Instrumentation division participates in Installation and commissioning of Instruments in various divisions, by closely interacting with user scientists to understand their needs and help further in maintaining these equipments for smooth and trouble free operation.

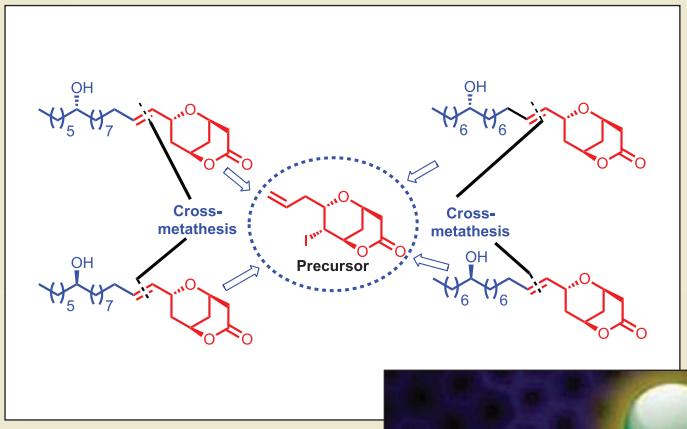
General Maintenance of lab instruments & equipment

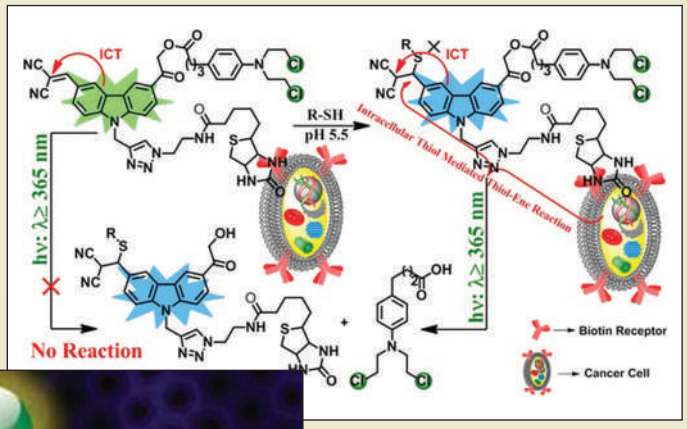
Our division renders services to all departments, receives work orders approximately around 800-1000 per annum for all types Instrumentation services which are being attended promptly and provided right & economical solutions for better performance.

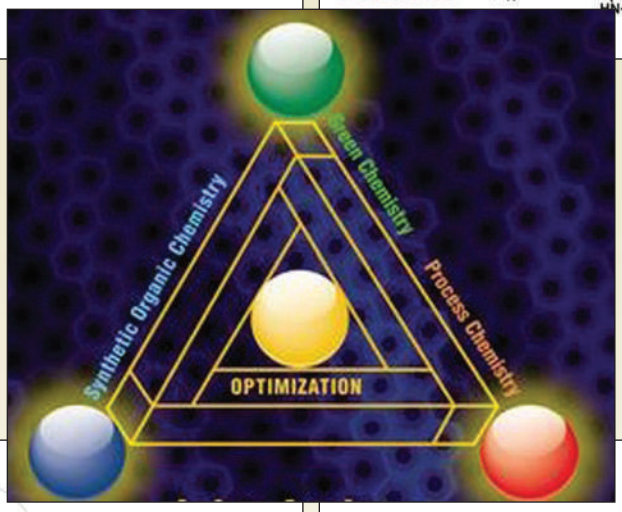
Human Resource Development Activity:

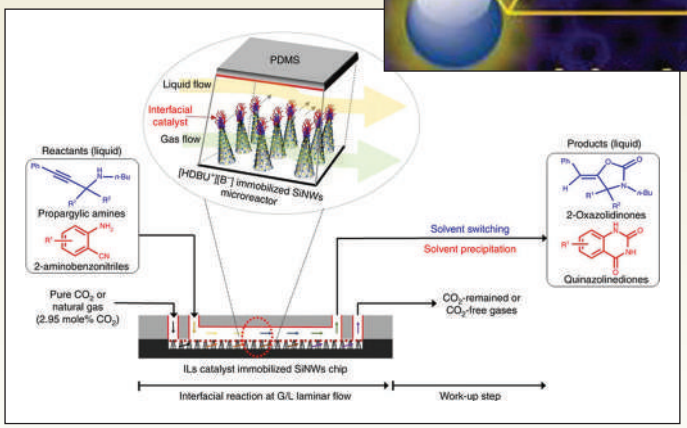
Short term and long term training for engineering students are taken up by our division for better understanding of Industrial Automation design and documentation. Several batches have undergone through this training and the trend is still continuing.

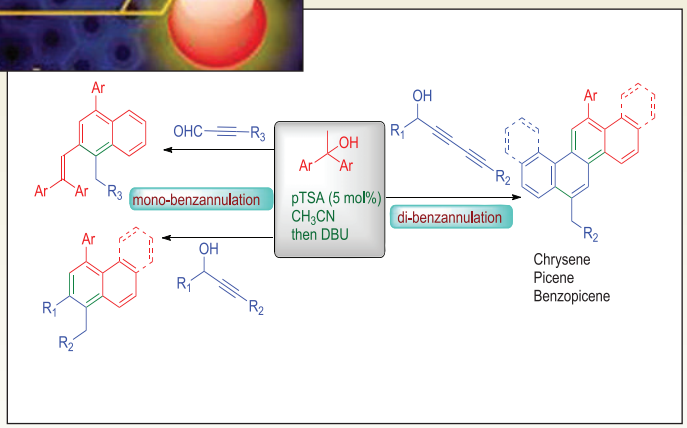
ORGANIC SYNTHESIS & PROCESS CHEMISTRY







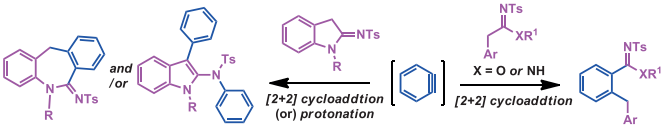




BASIC RESEARCH

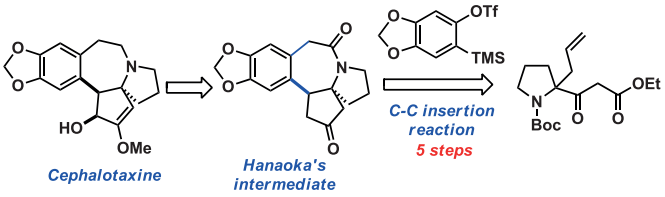
Insertion of *N*-Tosylacetimidates/ Acetimidamides onto Arynes via [2+2] Cycloaddition

A novel insertion reaction of *N*-tosylacetimidates and *N*-tosylacetimidamides onto arynes via a benzocyclobutene intermediate followed by ring cleavage is developed to afford *o*-benzylbenzoic acid derivatives in good yields. Interestingly, the use of cyclic 2-sulfonyliminoindolines provided two distinct products such as azepanimines via [2+2] cycloaddition and indolamines via protonation based on solvent medium. (*J. Org. Chem.*, **2016**, 81(6), 2451)



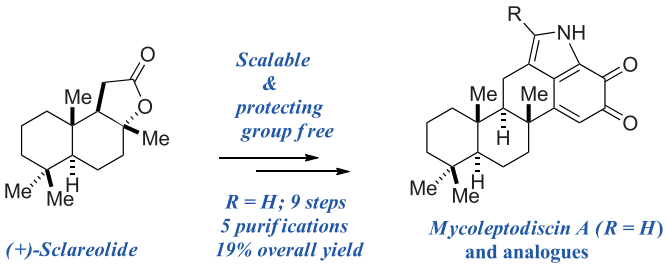
Formal Total Synthesis of (±)-Cephalotaxine and Congeners via Aryne Insertion Reaction

The formal total synthesis of pentacyclic core alkaloid, (±)-cephalotaxine is achieved in nine steps from known 2-allylpyrrolidine-2-carboxaldehyde using aryne insertion reaction as a key step in 10% overall yield. The developed novel strategy enabled easy access to cephalotaxine congeners. (*Org. Lett.*, **2016**, 18(11), 2044)



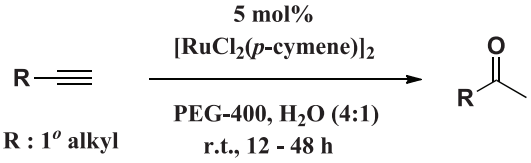
Expanding Diversity without Protecting Groups: (+)-Sclareolide to Indolosesquiterpene Alkaloid Mycoleptodiscin A and Analogues

Short and scalable synthesis of the complex pentacyclic indolosesquiterpene natural product mycoleptodiscin A has been achieved from commercially available diterpenoid (+)-sclareolide in 19% overall yield. This approach allows one to prepare various analogues of mycoleptodiscin using McMurry cyclization as a key reaction with just three chromatographic purifications. (*Org. Lett.*, **2016**, 18(11), 2684)



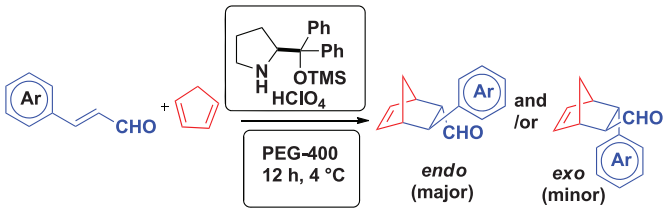
Ruthenium(II)-Catalyzed Hydration of Terminal Alkynes in PEG-400

A mild ruthenium(II)-catalyzed hydration of terminal alkynes in PEG-400 provides methyl ketones in high yield through Markovnikov addition of water. (*Synlett*, **2016**, 27(13), 1969)



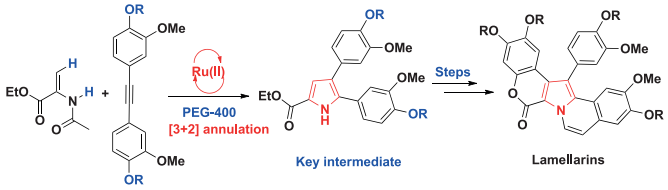
Caveat in the stereochemical outcome of the organocatalytic Diels–Alder reaction in PEG-400

The organocatalytic Diels-Alder reaction in non-conventional solvent (PEG-400) has yielded cycloaddition products with diastereoselectivities hitherto not reported in detail using classical reaction conditions. (*RSC Adv.*, **2016**, *6*, 76132)



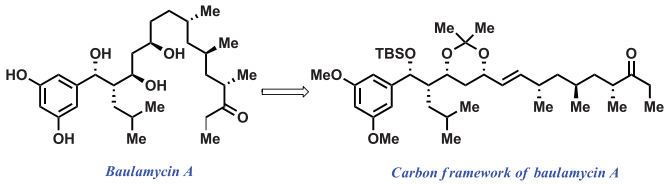
Total Synthesis of Lamellarin D Trimethyl Ether, Lamellarin D, and Lamellarin H

Total syntheses of three different lamellarins have been accomplished using a Ru(II)-catalyzed (3+2) annulation strategy to construct the central pyrrole ring. The striking features of this synthesis are the use of PEG-400 as a green solvent for the (3 + 2) annulation reaction and multiple catalytic reactions with excellent overall yield. The present route also enables the synthesis of various lamellarin analogues devoid of a B ring. (*J. Org. Chem.*, **2017**, 82(9), 4998)



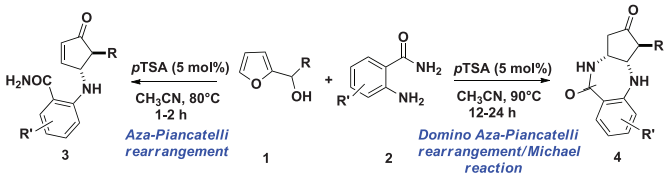
Synthesis of Complete Carbon Framework of Baulamycin A

The total carbon framework with all chiral carbons of proposed structure of baulamycin A is synthesized using Evans' aldol and Grubbs' cross-metathesis as key reactions. This strategy enables one to access all the isomers of this natural product. (*Tetrahedron Lett.*, **2017**, 58(28), 2784)



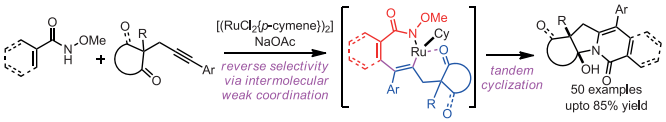
Brønsted Acid Catalysed Domino Aza-Piancatelli Rearrangement/ Michael Reaction: Construction of 1,4-Benzodiazepin-5-ones in One-Pot

A *para*-toluenesulfonic acid (*p*TSA) catalyzed domino aza-Piancatelli rearrangement/Michael reaction was developed for the construction of 1,4-benzodiazepin-5-ones in one pot. The method proceeds well in the presence of various furfurylcarbinols and *o*-aminobenzamides to give products that contain medicinally relevant chemical entities. (*Eur. J. Org. Chem.*, **2017**, 2017(37), 5671)



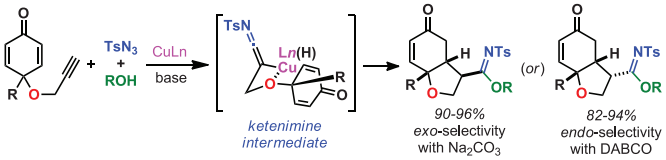
Carbonyl-Assisted Reverse Regioselective Cascade Annulation of 2-Acetylenic Ketones Triggered by Ru-Catalyzed C–H Activation

The first reverse regioselective intermolecular annulation of aryl substituted 2-acetylenic ketones with O-substituted N-hydroxybenzamides or acrylamides followed by tandem cyclization is reported via ruthenium-catalyzed C–H activation. Excellent reverse selectivity of alkyne insertion was induced by the weak coordination between carbonyl group and ruthenium complex. This highly efficient and practical reaction has broad range of substrate scope with excellent functional-group tolerance. The tandem reaction provides a wide range of polycyclic products having indozilidine structural motif, which found to be synthetically and pharmaceutically valuable potential. (*Chem. Sci.*, **2016**, 7, 4748)



Tunable Diastereoselective Desymmetrization of Cyclohexadienones Triggered by Copper-Catalyzed Three Component Coupling Reaction

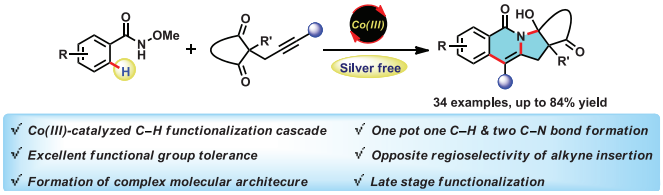
Catalytic tandem diastereoselective desymmetrization of cyclohexadienone-containing 1,6-enynes has been achieved through copper-catalyzed [3+2]-cycloaddition followed by ketenimine formation and subsequent intramolecular conjugate addition. The cascade reaction provides cis-hydrobenzofurans in good yields with excellent diastereoselectivity. The exo- or endo-selectivity of bicyclic scaffolds depends on the selection of the base in the reaction. In addition, N-tethered bicyclic products further transformed into tricyclic compounds via intramolecular Michael addition. *(J. Org. Chem.*, **2017**, 82(13), 6786)



Cp*Co(III)-Catalyzed C–H Functionalization Cascade of *N*-Methoxyamides with Alkynedione for the Synthesis of Indolizidines

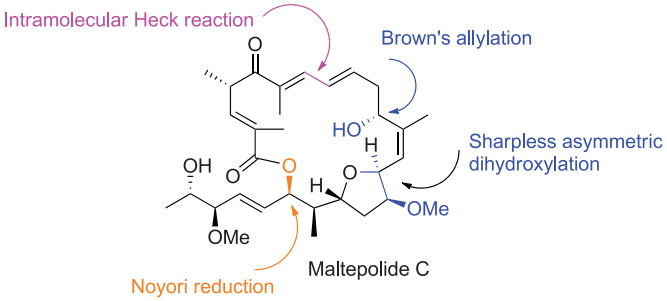
Cp*Co(III)-catalyzed C–H functionalization cascade of N-methoxyamides with alkynedione has been reported for the synthesis of indolizidine scaffolds under redox-neutral conditions. The reaction displays broad functional group tolerance along with excellent yield. The reaction proceeds with kinetically relevant C–H bond activation through carboxylate assistance with excellent diastereoselectivity and complete opposite

selectivity with respect to alkyne insertion. *(Org. Lett.,* **2017**, 19(8), 2186)



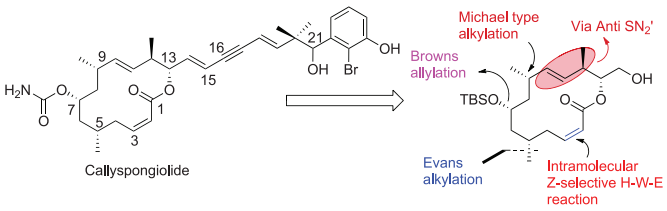
Total Synthesis of the proposed structure of Maltepolide C

Asymmetric total synthesis of the proposed structure of cytotoxic macrolide maltepolide C has been reported for the first time. An *E*-selective intramolecular Heck cyclization was used to construct the macrocycle. Other key reactions used in the synthesis are *cis* selective Wittig olefination, Sharpless asymmetric dihydroxylation followed by Williamson-type cyclo-etherification, Brown asymmetric allylation and Noyori reduction of an alkynone. Detailed NMR study confirms the structure and stereochemistry of the synthetic malepolde C unambiguously. However the deviation of the spectra of the synthetic maltepolide C from those of the natural maltepolide C indicates the error in the original structural assignment. (*Org. Lett.*, **2016**, 18(16), 4092)



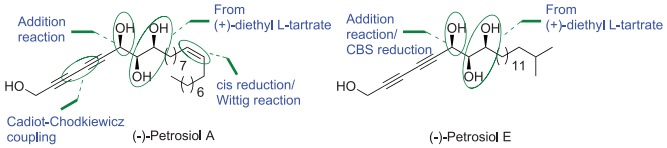
Synthetic studies of callyspongiolide: Synthesis of macrolactone core of the molecule

A concise synthesis of macrolactone core of a unique polyketide callyspongiolide was achieved. The C9 and C5 methyl centers in the macrocycle were installed via Evans asymmetric alkylation and diastereoselective Michael type alkylation reactions respectively. Browns asymmetric allylation reaction was used to fix the C7-hydroxy center whereas the C10-C11 *E*-configured olefin as well as the C12 methyl center were installed via allylic alkylation of an activated *Z*-allylic alcohol with organocopper reagent via S_N2' reaction. Finally the macrocycle with required *Z*-olefinic moiety was constructed through a *Z*-selective intramolecular H-W-E. (*Org. Biomol. Chem.*, **2016**, **14(28),** 6769)



A facile approach for the total synthesis of neurotrophic diyne tetraol petrosiol A and petrosiol E

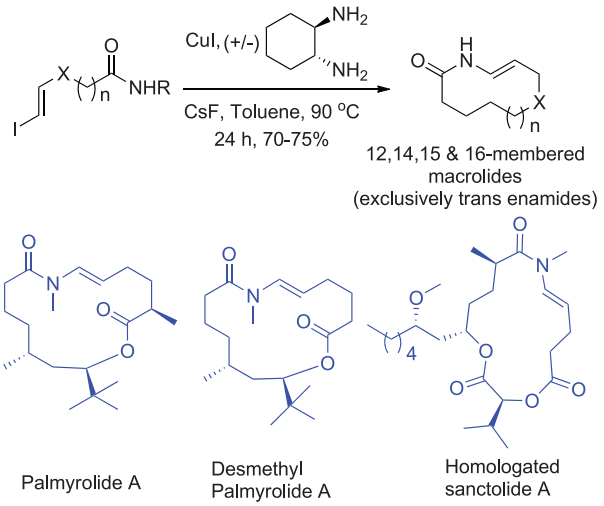
The first total synthesis of neurotrophic diacetylenic tetraol, petrosiol A and stereoselective total synthesis of petrosiol E was accomplished. The total synthesis involves Cadiot-Chodkiewicz coupling reaction as the key step for petrosiol A. The diastereorich chiral alcohol (third chiral center) was synthesized from CBS mediated stereoselective ketone reduction reaction for petrosiol E. Of the three chiral centers, the two chiral centers are originated from (+)-diethyl L-tartrate and the third chiral center was generated by an addition reaction of lithium trimethylsilylacetylide leading to two diastereomers which were used for the synthesis of both the natural products and their diastereomer C6-epi-petrosiol A and C6-epi-petrosiol E, respectively. (*Tetrahedron*, **2016**, 72(38), 5807)



Expedient synthesis of large-ring trans-enamide macrolides through CuI mediated intramolecular coupling of vinyl iodide with amide; Total synthesis of palmyrolide A

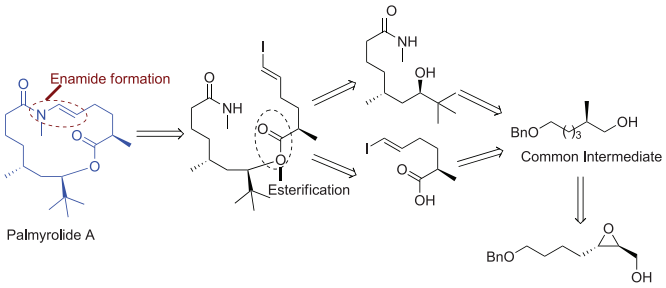
An efficient and improved procedure for copper catalyzed coupling of vinyl iodide with amide in an intramolecular fashion is described. The protocol utilizes combination of copper iodide, CsF and +/- 1,2-diaminocyclohexane as ligand. The vinyl iodide couples efficiently with amide to generate enamide macrolide without any alteration in the double bond geometry. The developed method was applied for the synthesis of several large ring enamide macrolides, total synthesis of natural product

palmyrolide A and homologated sanctolide A. (*Eur. J. Org. Chem.,* **2016**, 2016(14), 2509)



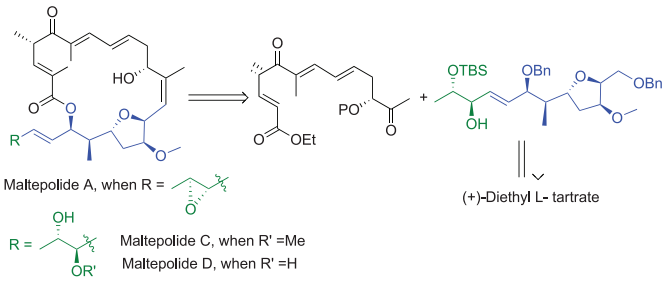
Stereoselective total synthesis of palmyrolide A via intramolecular trans *N*-methyl enamide formation

The stereoselective total synthesis of palmyrolide A was accomplished through macrocyclization reaction involving trans enamide formation by coupling of vinyl iodide with secondary amide in an intramolecular fashion. The two coupling partners, vinyl iodide and secondary amide were synthesized from the common intermediate alcohol. Yamaguchi esterification and CBS-reduction are the other key steps involved in the synthesis. (*Tetrahedron Lett.*, **2016**, 57(40), 4456)



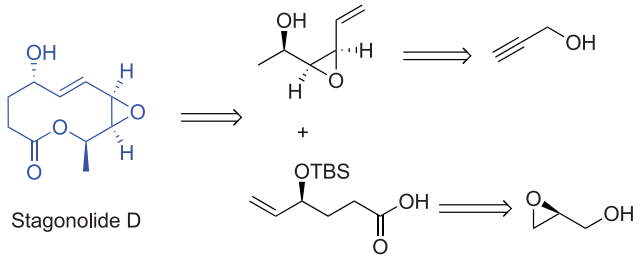
A facile approach for the synthesis of C13-C24 fragments of maltepolides A, C and D

A linear, chiron approach for the synthesis of C13–C24 fragments of cytostatic maltepolides A, C and D consisting of a tetrahydrofuran subunit and a chiral alkenyl/alkyl substituent is achieved from (+)-diethyl L-tartrate. The other chiral stereocenters were generated by employing key reactions such as Crimmins aldol, alkynylation and $CeCl_3 \cdot 7H_2O$ mediated Luche reduction reactions. (*Org. Biomol. Chem.,* **2016**, 14(40), 9629)



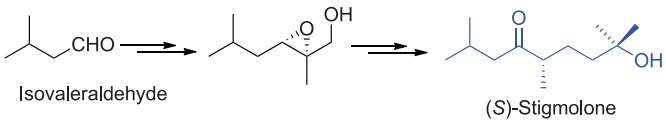
First stereoselective total synthesis and reconfirmation of absolute structure of nonenolide (-)-stagonolide D

The first stereoselective total synthesis of nonenolide (-)-stagonolide D has been accomplished. Midland Alpine borane reduction to install hydroxyl group at C4, Henbest epoxidation to introduce epoxide stereoselectively between C7 and C8, Yamaguchi esterification and Olefin metathesis reaction are the key steps involved in the total synthesis. *(Tetrahedron Lett.* **2016**, 58(6), 509)



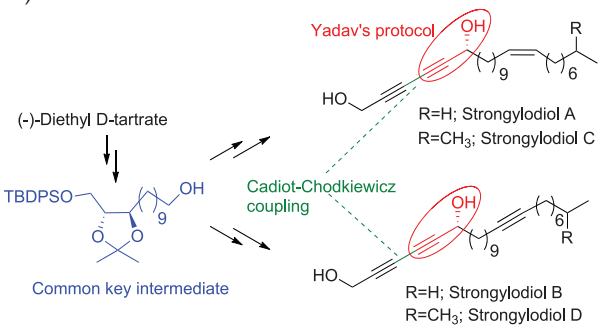
Stereoselective total synthesis of stigmolone: The fruiting body inducing pheromone

The total synthesis of (*S*)-stigmolone, a pheromone from the myxobacterium *Stigmatella aurantiaca* that induces the formation of fruiting bodies, is described. Sharpless asymmetric epoxidation followed by *tert*-butyldimethylsilyl trifluoromethanesulfonate/Hünig's base mediated intramolecular hydride ion transfer reactions were used to install the C-5 stereogenic center. Commercially available isovaleraldehyde is used as a starting material. *(Synthesis*, **2017**, 49(07), 1702)



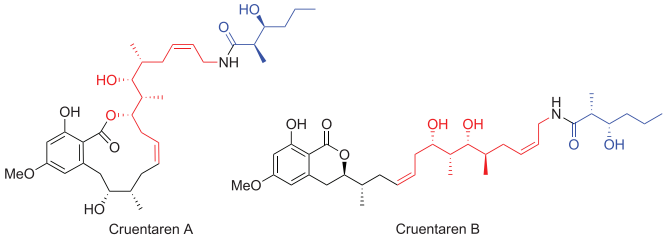
Stereoselective Total Syntheses of (R)-Strongylodiols A, B, C and D

A facile stereoselective approach for the total syntheses of (*R*)-strongylodiols A, B, C and D is described. A chiron approach has been followed wherein the stereochemistry at the chiral center is fixed and a methodology of base induced elimination of β-alkoxy chloride to get the chiral propargyl alcohol is employed. A key intermediate synthesized from commercially available (-)-diethyl D-tartrate has been utilized for the total syntheses of all the four titled compounds. (*ChemistrySelect,* **2017**, 2(14), 4106)



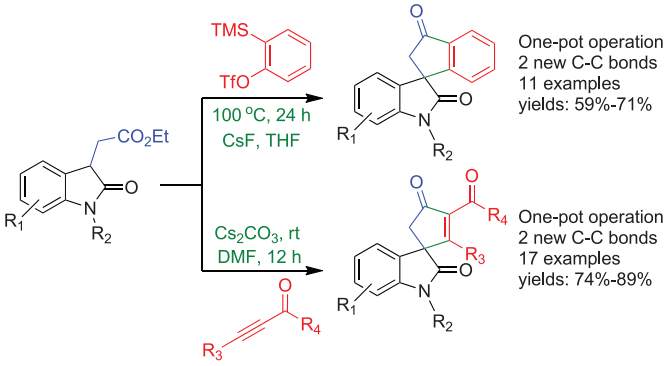
Studies towards the total synthesis of cruentaren A and B: Stereoselective synthesis of fragments C1-C11, C12-C22 and C23-C28

A convergent and stereoselective approach for the synthesis of C1-C11, C12-C22, and C23-C28 fragments of cytotoxic natural products cruentaren A and B are accomplished. Highlights of the strategy include a Sharpless epoxidation followed by a regioselective opening of epoxide to generate anti and syn-stereochemistry at C9-C10 and C15-C16, an Alder-Rickert reaction between a 1,5-dimethoxy-1,4-cyclohexadiene and dienophile to construct the aromatic ring, and a lithium-mediated aldol reaction to install the C17-C18 anti-stereochemistry. The synthesis of C1-C11 and C12-C22 fragments proceed with a longest linear sequence of 10 and 17 steps from commercially available 2-butyne-1,4-diol and cis-2-butene-1,4-diol respectively. (*Tetrahedron Lett.,* **2017**, 58(28), 2685)



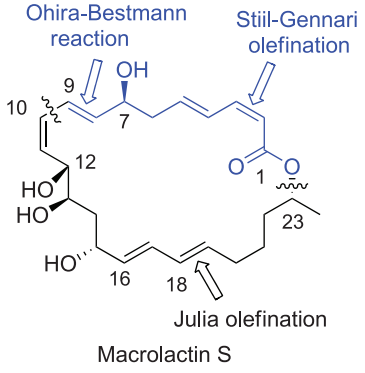
Spiroannulation of Oxindoles via Aryne and Alkyne Incorporation: Substituent-Diverted, Transition-Metal-Free, One-Pot Access to Spirooxindoles

A 'product control via substrate design' strategy has been conceptualized and implemented to harness the potential of aryne and activated alkyne insertions into oxindoles to readily and efficiently furnish pharmacophoric indano- and cyclopentannulated spirooxindole scaffolds in an operationally straightforward, one-pot, metal free protocol. (*Org. Lett.,* **2017**, 19(12), 3119)



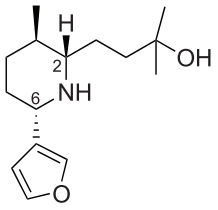
Studies on the total synthesis of antibiotic macrolactin S; A conventional approach for the synthesis

The C1–C9 and C10–C24 segments of the 24-membered polyene macrolide macrolactin S were synthesized by routes involving an epoxide-ring-opening reaction, an Ohira–Bestmann alkyne formation, a chelation-controlled nucleophilic addition reaction, and a Still–Gennari olefination as key steps. A chiron approach, starting from readily available glucose diacetonide, was used to synthesize a key intermediate, and a convergent approach was adopted for the synthesis of the key C10–C24 fragment. (*Synthesis,* **2017**, 50(03), 663)



Stereoselective total synthesis of (-)-Nupharamine

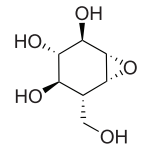
An efficient stereoselective synthesis of the nuphar alkaloid, (-)-nupharamine has been developed. The key features include the Lewis acid catalyzed reaction of an α-chloro sulfide with a silyl ketene acetal for C-C bond formation, creation of the stereocenter at C2 by a diastereoselective reaction of allyl indium with a sulfinimine and reductive amination for the introduction of the C6 stereocenter of the piperidine ring. (*Org. Biomol. Chem.,* **2016**, 14(1), 131)



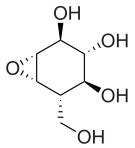
(-)-Nupharamine

Stereoselective formal synthesis of (+)-, (-)-cyclophellitol, (-)-conduritol B & (-)-conduramine B

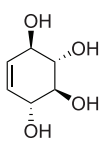
The formal total synthesis of both the enantiomers of cyclophellitol, conduritol-B and synthesis of conduramine-B derivative has been achieved from a common intermediate, obtained by regio- and stereoselective vicinal functionalization of a diene utilizing an intramolecular sulfinyl group as a nucleophile followed by stereoselective preparation of an allylic sulfide by reaction of vinylzinc bromide with an electrophilic α-chloro sulfide and lastly by ring-closing metathesis reaction as the key steps. The sulfoxide, sulfilimine and sulfur ylid prepared from this common intermediate have been transformed into derivatives of conduritol-B, conduramine-B and (–)-cyclophellitol respectively. The silyl sulfide was converted via sila-Pummerer rearrangement, hydrolysis and reduction in an one-pot operation to a hydroxymethyl group. [2,3]-Wittig-Still rearrangement was employed for the synthesis of (+)-cyclophellitol. (*J. Org. Chem.,* **2016**, 81(10), 4252)



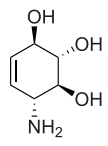
(+)-Cyclophellitol



(-)-Cyclophellitol



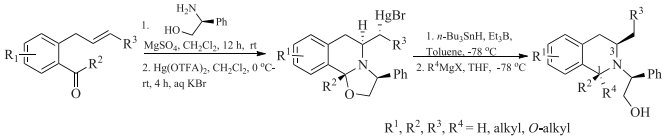
(-)-Conduritol B



(-)-Conduramine B

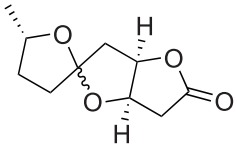
Oxazolidines as intermediates in the asymmetric synthesis of 3-substituted and 1,3-disubstituted tetrahydroisoquinolines

A diastereoselective mercury(II) promoted intramolecular cyclisation of an iminoalcohol/oxazolidine to prepare C-3 substituted tetrahydroisoquinoline, has been developed. The C-3 stereogenic center is subsequently exploited to create the C-1 stereocenter by coordination of the nucleophilic reagent to the oxygen atom of oxazolidine. Both *cis*- and *trans*-1,3-disubstituted tetrahydroisoquinolines can be readily prepared. Also using cationic rhodium complex intramolecular hydroamination was effected thus avoiding mercury(II) salts and demercuration. The reaction is general and works well using aliphatic and aromatic aldehydes. *(J. Org. Chem.,* **2016**, 81(15), 6201)



Synthesis of (-)-cephalosporolide E and (+)-cephalosporolide F utilizing the vinylogous Mukaiyama type reaction

The synthesis of cephalosporolide E and F is described utilizing diastereoselective reduction of a propargylic ketone using Noyori catalyst to create the C6 carbinol stereogenic center. A vinylogous silylketene acetal addition to an α-chloro sulfide is exploited for stereoselective carbon-carbon bond formation and introduction of the butenolide moiety. Oxidative radical cyclization is utilized for the creation of the [5,5] spiroketal moiety. (*RSC Adv.,* **2016**, 6(77), 72877)

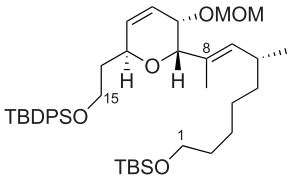


Cephalosporolide E & F

Convergent synthesis of the dihydropyran core of sorangicin A

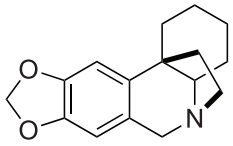
A convergent route to the C1-C15 subunit of sorangicin A has been developed. The key steps include carbon-carbon bond formation using an α-chloro sulfide, regioselective hydrozirconation of an internal alkyne for the preparation of a trisubstituted iodo alkene,

allene formation using Myers-Movassaghi protocol, stereoselective reduction of allylic and propargylic ketones using Noyori's catalyst and gold(I)-catalyzed cyclization of a β-hydroxy allene to construct the dihydropyran ring. (*J. Org. Chem.,* **2016**, 81(22), 10698)



Synthesis of Crinane

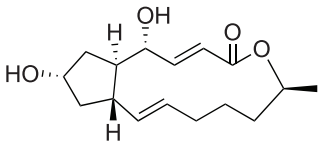
The synthesis of crinane is disclosed via intramolecular C-N bond formation by displacement of an allylic sulfoxonium salt. The allylic sulfide precursor was synthesized by a ring-closing metathesis reaction. The quaternary carbon stereocenter was created by alkylation of a benzylic cyanide. The allyl sulfide **14** was prepared by vinylmagnesium bromide addition to an α-chlorosulfide. (*Org. Biomol. Chem.,* **2016**, 14(43), 10222)



Crinane

Ru(II)-catalyzed enyne cyclization in the synthesis of brefeldin A

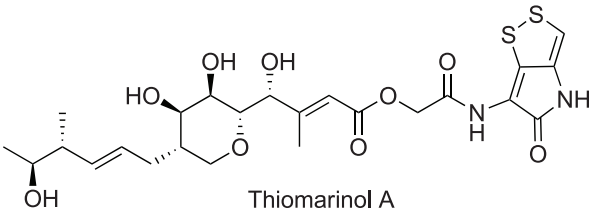
The approach to brefeldin A described herein hinges on Ru(II) catalyzed cycloisomerization of an enyne obtained by the reaction of an alkynylzinc reagent with a chloro sulfide. Other key steps include Mislow-Evans rearrangement, cross-metathesis, macrocyclization using Roush-Masamune protocol. (*J. Org. Chem.,* **2016**, 81(22), 10912)



Brefeldin A

Synthesis of an advanced intermediate enroute to thiomarinol

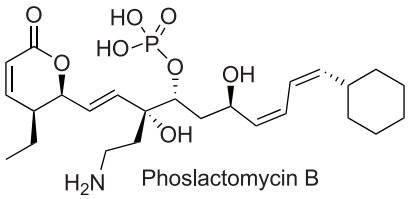
A stereoselective synthesis of the C1-C14 fragment of thiomarinols has been developed. The key steps include the stereoselective preparation of an allylic sulfide via a chloro sulfide by 1,2-asymmetric induction, ring-closing metathesis reaction, Kirmse-Doyle reaction for the preparation of a γ,δ-unsaturated ester, Nozaki-Hiyama-Kishi coupling and Julia-Kocienski olefination reaction. Substrate controlled asymmetric induction has been advantageously employed for the creation of stereogenic centers. Noyori transfer hydrogenation and asymmetric hydrogenation reactions have been utilized for the creation of carbinol stereocenters. (*Tetrahedron*, **2017**, 73(19), 2814)



Thiomarinol A

Stereoselective synthesis of phoslactomycin B

A convergent synthesis of the entire carbon framework of phoslactomycin B has been developed. The first route aimed at creating the C8 tetrasubstituted stereocenter by a regioselective intermolecular coupling between an internal alkyne and allyl silyl ether, adopting Trost's protocol followed by [2,3] sigmatropic rearrangement was not successful. In the second approach, a propargylic sulfide was rearranged to an unsaturated ketone which was further reacted with lithio acetonitrile to create the C8 stereocenter selectively. The C4 and C5 stereocenters were introduced by the non-Evans *syn*-aldol reaction using Crimmins' protocol. The C9 and C11 carbinol centers were created by asymmetric transfer hydrogenation. The (*Z*,Z)-diene moiety was introduced by a partial reduction of a diyne following Hansen's modification of Boland reduction reaction. (*Eur. J. Org. Chem.,* **2017**, 2017(20), 2981)

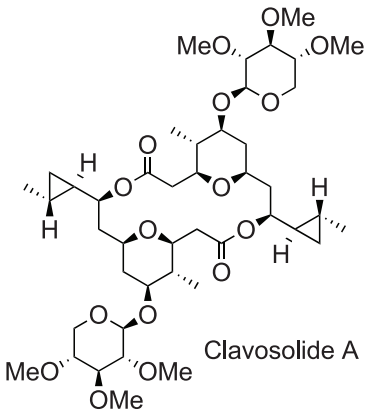


Phoslactomycin B

Synthesis of an advanced intermediate toward clavosolide A

A stereoselective route to an advanced intermediate toward the synthesis of clavosolide A has been developed. The key steps include Wadsworth-Emmons

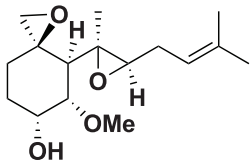
cyclopropanation, utilization of a sulfinyl moiety as an internal nucleophile to open a cycloprpane ring activated by Hg(II)- to create the C3-C5 stereogenic centers, C-C bond formation employing an α- chloro sulfide, asymmetric transfer hydrogenation, regioselective hydrosilylation and Tamao-Fleming oxidation. (*Tetrahedron Lett.*, **2017**, 58(25), 2465)



Clavosolide A

Formal synthesis of fumagillol

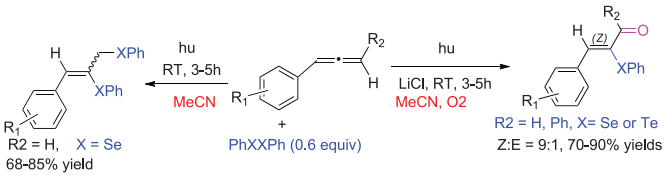
A formal synthesis of fumagillol, a congener of fumagillin that possesses varied biological activity, has been developed. Initial attempts at preparing an allylic sulfide via an α-chloro sulfide met with failure. The successful route involves a carbonyl-ene reaction, one-pot stannyl cupration, methylation of resulting alkenyl copper and further Stille-coupling of the alkenyl stannane as the key steps. (*Tetrahedron*, **2017**, 73(30), 4371)



Fumagillol

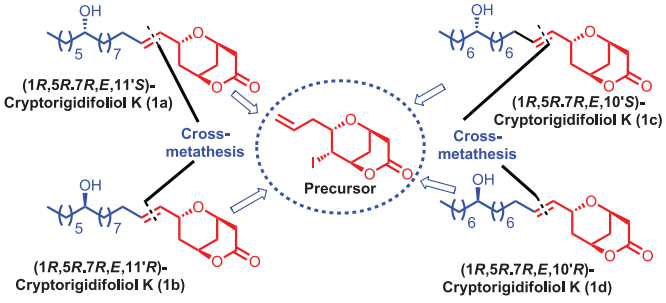
Visible-light-induced phenylchalcogenyl-oxygenation of allenes having aryl or electron withdrawing substituents with ambient air as a sole oxidant

We accomplished a new reaction that takes advantage of ambient air as a terminal oxidant for the chalcogenyl oxy-functionalization of aryl terminal allene and aryl alkenes. This reaction proceeds with high regio- and stereoselectivity and produce the respective products in single step at a high yield. This process is significant in that the O_2-promoted regio-selective sp^2 C-H oxidation process offers a carbon-heteroatom bond leading to the creation of formyl functional products having a substituent at α-phenyl Te- and Se heteroatom. Further, these newly introduced functional groups have a provision for the addition of pro-nucleophiles and the α-phenyl Te-/or Se heteroatoms are a source to generate a radicals. To the best of our knowledge, the single step syntheses of the α-heteroatom-functionalized α,β-unsaturated compounds and diselenation adducts from the same starting material promoted by visible-light photo-reaction are described here for the first time. (*Org. Biomol. Chem.*, **2016**, 14(48), 11415)



Total Synthesis of Four Isomers of the Proposed Structures of Cryptorigidifoliol K

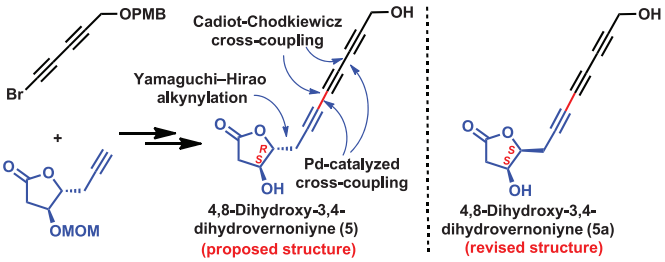
The first asymmetric convergent total synthesis of four isomers of proposed structures of cryptorigidifoliol K has been achieved from commercially available starting materials. The key steps in this synthesis involve tandem isomerization followed by C-O and C-C bond forming reaction for the construction of *trans*-2,6-disubstituted dihydropyran, iodolactonization, isomerization of terminal alkene and cross metathesis reaction. The large discrepancies of spectroscopic data (^{1}H and ^{13}C NMR) of synthetic cryptorigidifoliol K from the natural product suggest that the structure of the natural cryptorigidifoliol K requires revision. (*Org. Lett.*, **2017**, 19(24), 6506)



Total Synthesis and Stereochemical Revision of 4,8-Dihydroxy-3,4-dihydrovernoniyne

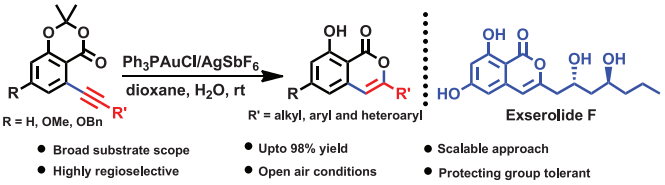
The first asymmetric total synthesis of two possible diastereomers (4S,5R)-4,8-dihydroxy-3,4-dihydro vernoniyne 5 and (4S,5S)-4,8-dihydroxy-3,4-dihydrovernoniyne 5a is accomplished. Salient features

of the synthesis involve Cadiot-Chodkiewicz coupling and Sonogashira cross-coupling of terminal acetylenes. Detailed comparison of the ^{1}H and ^{13}C NMR data and specific rotation with that of the natural product led to the revision of the absolute stereochemistry of the natural product as (4S,5S)-4,8-dihydroxy-3,4-dihydrovernoniyne 5. (*Org. Lett.,* **2017**, 19(16), 4167)



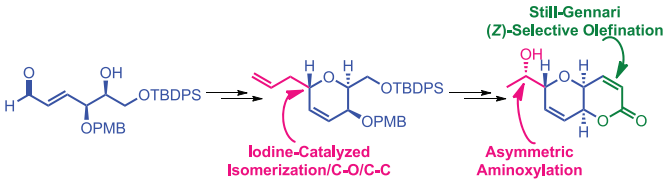
Gold(I)-Catalyzed Cyclization for the Synthesis of 8-Hydroxy-3- Substituted Isocoumarins: Total Synthesis of Exserolide F

A highly regioselective gold(I)-catalyzed 6-*endo-dig* cyclization of 2,2-dimethyl-5-(alkynyl)-4*H*-benzo-[*d*][1,3]-dioxin-4-ones for the synthesis of 8-hydroxy-3-substituted isocoumarins is described. Key features of the reaction include the broad substrate scope, is scalable and tolerant of protecting groups. The synthetic utility of this novel method is demonstrated by the first total synthesis of exserolide F, an isocoumarin containing polyol natural product. (*Org. Lett.,* **2017**, 19(8), 2074)



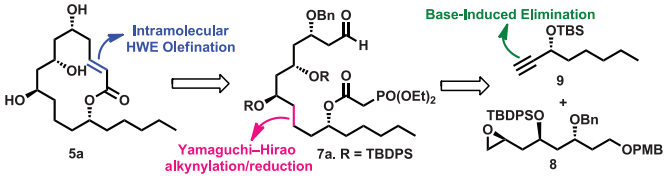
Asymmetric Total Synthesis of Putative Structure of Diplopyrone

The first asymmetric total synthesis of the putative structure of diplopyrone was achieved in 17 linear steps starting from *cis*-1,4-butene-diol. The synthetic route features iodine- catalyzed tandem isomerization followed by C-O and C-C bond formation reaction strategy developed by our own group to construct the *trans*-2,6-disubstituteddihydropyran ring, asymmetric α-aminoxylation reaction, and Still-Gennari (*Z*)-selective olefination reactions. Careful comparison of ^{1}H and ^{13}C NMR spectroscopic data as well as investigation of the UV and circular dichroism (CD) spectrum in trifluoroethanol for compound **2**, suggest that the the putative structure proposed for diplopyrone {6-[(1*S*)-1-hydroxyethyl]-2,4a(*S*),6(*R*), 8a(*S*)-tetrahydropyran[3,2-*b*]pyran-2-one} requires revision. (*J. Org. Chem.,* **2017**, 82(9), 4561)



Asymmetric Total Syntheses of Two Possible Diastereomers of Gliomasolide E and its Structural Elucidation

The first total syntheses of two possible diastereomers of gliomasolide E, a 14-membered macrolides isolated from the marine sponge Phakellia fusca Thiele, which was collected from the South China Sea, is reported. Highlights of the synthesis include macrolactonization through intramolecular Horner-Wadsworth-Emmons olefination, Yamaguchi-Hirao alkynylation, and base-induced elimination reactions for propargyl alcohol synthesis are the key reactions. Detailed comparison of their ^{1}H and ^{13}C NMR (1D and 2D NMR data) and specific rotation with those of the natural product revealed the absolute stereochemistry of gliomasolide E should be (2E,5R,7R,9R,13R). (*J. Org. Chem.,* **2017**, 82(2), 1053)

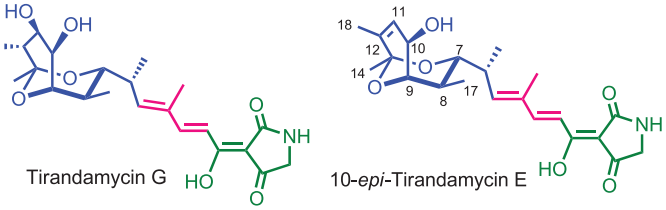


Genetic Validation of *Leishmania donovani* Lysyl-tRNA Synthetase Shows that It Is Indispensable for Parasite Growth and Infectivity

Leishmania donovani is a protozoan parasite that causes visceral leishmaniasis. Increasing resistance and severe side effects of existing drugs have led to the need to identify new chemotherapeutic targets. Aminoacyl-tRNA synthetases (aaRSs) are ubiquitous and are required for protein synthesis. aaRSare known drug targets for bacterial and fungal pathogens. Here, we have characterized and evaluated the essentiality of *L. donovani* lysyl-tRNA synthetase (*Ld*LysRS). (*mSphere,* **2017**, *2*, e00340-17)

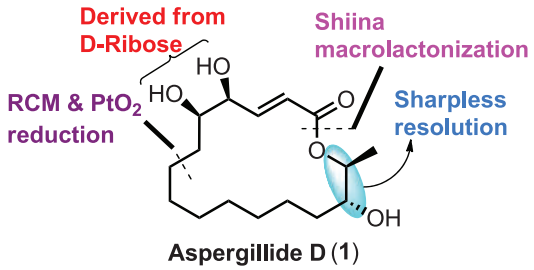
Stereoselective total synthesis of 10-*epi*-tirandamycin *E*

A stereoselective total synthesis of 10-*epi*-tirandamycin E is described, employing desymmetrization protocol, ring-closing metathesis (RCM), acid-catalyzed ketalization, substrate controlled dihydroxylation and Horner-Wadsworth-Emmons olefination as key reactions. (*Tetrahedron,* **2017**, 73(10), 1358)



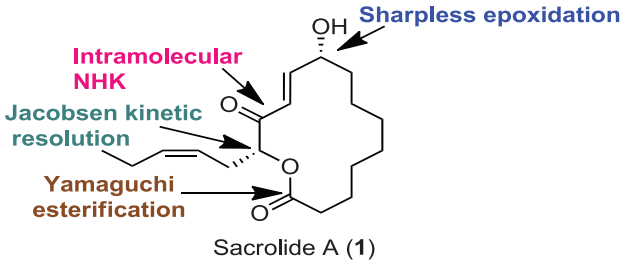
Total synthesis of the Proposed Structure of Aspergillide D

The first asymmetric total synthesis of the proposed structure of 16-membered macrolide aspergillide D is described. The chiral centers of the acid and alcohol subunits are derived from D-ribose and generated by Sharpless kinetic resolution, respectively. The other key reactions include Yamaguchi esterification, RCM reaction, Shiina macrolactonization to construct the fully functionalized macrocycle. (*Org. Biomol. Chem.*, **2017,** 15(8), 1863)



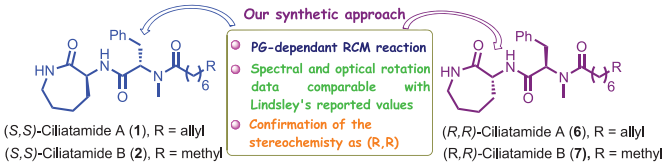
First Total Synthesis of Sacrolide A Following Nozaki-Hiyama-Kishi Macrocyclization Strategy

The first stereoselective total synthesis of oxylipin macrolide, (+)-sacrolide A was achieved in 13 steps with 12.1% overall yield. The key reactions are Jacobsen's hydrolytic kinetic resolution, Sharpless asymmetric epoxidation, Yamaguchi esterification and intramolecular Nozaki-Hiyama-Kishi (NHK) macrocyclization to construct the required 14-membered lactone. (*Asian J. Org. Chem.*, **2016**, 5(3), 340)



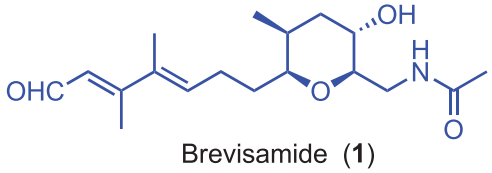
Ring-closing metathesis based total synthesis of ciliatamides A and B and their structural confirmation

Protecting group dependant ring-closing metathesis based approach to the total synthesis of the revised structures of ciliatamides A and B have been described and the present approach is more convenient to get the correct conclusion on absolute stereochemistry. Thus, on the basis of similar optical rotation values with Lindsley's reported data, we confirmed that the actual stereochemistry of both ciliatamides A and B is (*R,R*). (*Tetrahedron Lett.,* **2016**, 57(15), 1715)



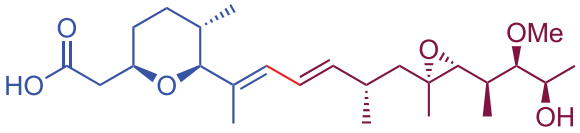
Formal Total Synthesis of Brevisamide Using Tandem Isomerization Followed by C-O and C-C Bond Formation Reaction

A highly stereoselective formal total synthesis of the brevisamide is described in a convergent and efficient manner utilizing our own methodology of tandem isomerization followed by C-O and C-C bond formation reaction for the construction of *trans*-2,6-disubstituted dihydropyran as the key step. In this synthesis iodolactonization, Crimmin's modified "non-Evans" *syn* aldol and Horner–Wadsworth–Emmons olefination were used as the key reactions. (*Eur. J. Org. Chem.*, **2016**, 2016(13), 2300)



Gold-Catalyzed Hosomi-Sakurai Type Reaction for the Total Synthesis of Herboxidiene

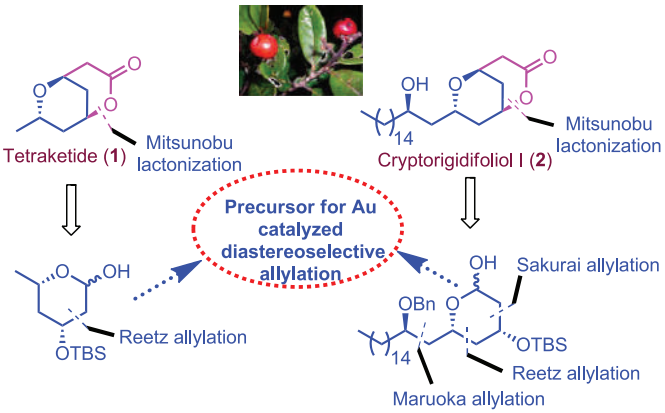
Total synthesis of herboxidiene/GEX1A/TAN-1609 has been accomplished in 22 longest linear sequence starting from 2-butyne-1,4-diol following our recently developed gold-catalyzed Hosomi-Sakurai type of reaction on lactols with allyltrimethyl silane and Stille cross coupling to assemble the advanced fragment. The synthesis of C10-C19 fragment was accomplished by means of Sharpless epoxidation and asymmetric alkylation reactions starting from (*R*)-methyl lactate. (*Org. Biomol. Chem.,* **2016**, 14(26), 6212)



Herboxidiene/GEX 1A

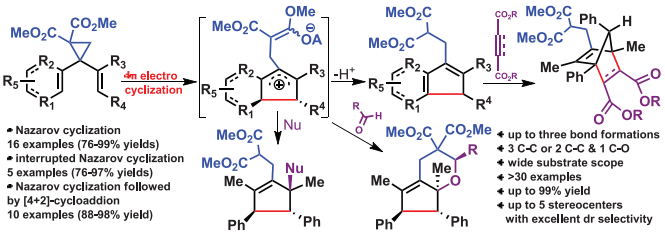
Total Synthesis of Tetraketide and Cryptorigidifoliol I via a Sequential Allylation Strategy

A unified and efficient synthetic route for both teraketide and cryptorigidifoliol I has been devised successfully from commercially available starting materials in 11 and 17 steps, with 16% and 11% overall yields, respectively. Highlights of the syntheses involved sequential Lewis acid-catalyzed highly regio- and diastereoselective allylations, and intramolecular Mitsunobu lactonization. (*J. Nat. Chem.,* **2016**, 79 (11), 2788)



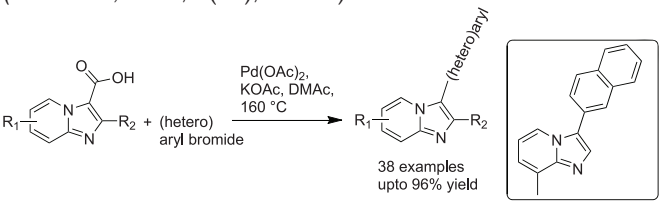
Nazarov Cyclization and Tandem [4+2]-Cycloaddition Reactions of Donor–Acceptor Cyclopropanes

We have developed aryl vinyl/divinyl donor–acceptor cyclopropanes (DACs) as novel Nazarov cyclization (NC) precursors and utilized in the synthesis of highly substituted indenes. The 1,3-zwitterion, generated from DACs embedded in the divinyl framework, acted as a pentadienyl cation, a requisite for Nazarov cyclization. A cyclic allyl cation in the course of electrocyclization reaction was trapped with external nucleophiles to provide substituted cyclopentene (interrupted NC products). Indeed, an allyl cation in this reaction is analogous to a 1,4-zwitterion that on reaction with dipolarophiles provided easy access to substituted pyrans with excellent yield and diastereoselectivity via electrocyclization followed by a formal [4+2] cycloaddition. (*Org. Lett.*, **2017**, 19(17), 4500)



Ligand-free Pd-catalysed decarboxylative arylation of imidazo[1,2-*a*]pyridine-3-carboxylic acids with aryl bromides

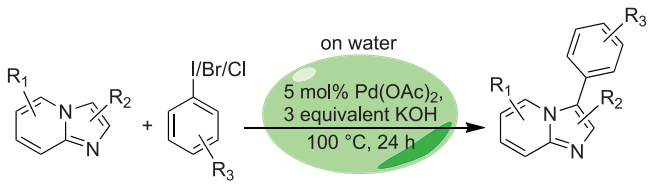
A facile ligand-free method for $Pd(OAc)_2$ catalysed decarboxylative arylation of imidazo[1,2-*a*]pyridine-3-carboxylic acids with hetero(aryl) bromides has been developed. This method is applicable to variety of (hetero) aryl bromides as coupling partner. Electron withdrawing and donating groups on imidazo[1,2-*a*]pyridine-3-carboxylic acids are well tolerated. It represent the first general protocol for ligand-free $Pd(OAc)_2$ catalysed decarboxylative arylation of imidazo[1,2-*a*]pyridine-3-carboxylic acids with (hetero)aryl bromides. Few of the compounds generated using this protocol showed antibacterial activity against *Staphylococcus aureus.* (*RSC Adv.,* **2016**, 6(69), 65095)



MIC = 25 μM against *S. aureus*

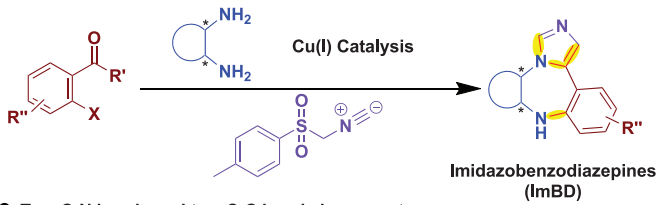
On water direct arylation of imidazo[1,2-*a*] pyridines with aryl halides

A simple, mild, and ecofriendly protocol for a palladium-catalysed direct arylation of imidazo[1,2-*a*]pyridines with aryl halides on water is reported. This protocol does not require any ligand and tolerate variety of functional groups on both the coupling partners. The simple base KOH is highly efficient in this transformation. *(Tetrahedron lett.,* **2017**, 58(29), 2818)



Tandem Copper-Catalyzed *N*-Arylation–Condensation and van Leusen Reaction: Synthesis of 1,4-Benzodiazepines and Imidazobenzodiazepines (ImBDs)

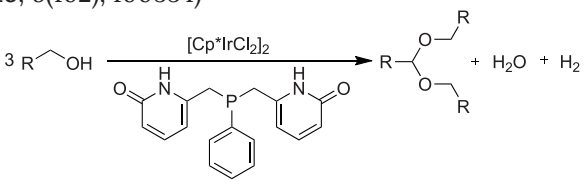
A straightforward tandem copper catalyzed *N*-arylation–condensation has been developed using chiral cyclic 1,2-diamines and *ortho*-halo aryl aldehydes or ketones. The corresponding chiral tricyclic 1,4-benzodiazepines were synthesized in high yields. Subsequently, the 1,4-diazepines have been converted to a new class of tetracyclic *N*-fused imidazobenzodiazepines (ImBDs) using van Leusen reaction. The one-pot sequential strategy has also been demonstrated for the synthesis of ImBDs. The synthetic utility of 1,4-benzodiazepines and ImBDs was described. (*Adv. Synth. Catal.,* **2016,** 358(8), 1309)



- Two C-N bonds and two C-C bonds in one pot
- One step synthesis of 1,4-benzodiazepines (18 examples)
- One pot synthesis of new class of ImBDs (14 examples)
- Gram scale

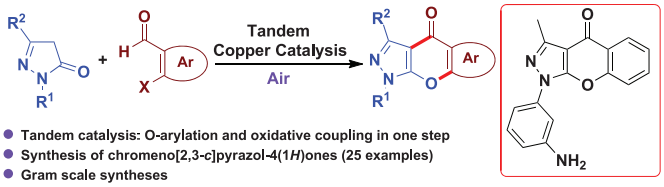
Acetals from Primary Alcohols with the Use of Tridentate Proton Responsive Phosphinepyridonate Iridium Catalysts

The association of the new phosphinepyridonate ligands along with an iridium metallic precursor resulted in the selective acetalization of various primary alcohols via a formal dehydrogenative coupling reaction. (*RSC Adv.* **2016**, 6(102), 100554)



Copper [Cu]-Catalyzed Tandem O-Arylation–Oxidative Cross Coupling: Synthesis of Chromone Fused Pyrazoles

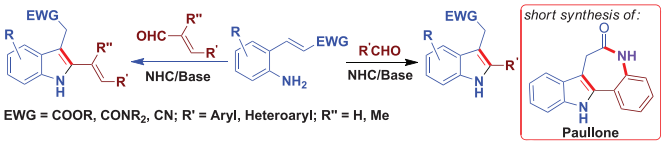
Intermolecular tandem copper-catalyzed O-arylation–oxidative acylation (cross dehydrogenative coupling-CDC) has been developed under air as an oxidant. The reaction between 2,4-dihydro-3*H*-pyrazol-3-ones and *ortho*-halo aryl carboxaldehydes furnished the corresponding chromone fused pyrazoles, in a straightforward manner. The synthetic utility of the presented tandem catalysis has been demonstrated with the synthesis of an A_2-subtype selective adenosine receptor antagonist in only two steps. (*J. Org. Chem.,* **2017**, 82(6), 2926)



- Tandem catalysis: O-arylation and oxidative coupling in one step
- Synthesis of chromeno[2,3-*c*]pyrazol-4(1*H*)ones (25 examples)
- Gram scale syntheses
- Synthesis of an A_2-subtype selective adenosine receptor antagonist

N-Heterocyclic Carbene (NHC) Catalyzed Atom Economical Construction of 2,3-Disubstituted Indoles

A novel organocatalytic approach, harnessing the unique reactivities of *N*-heterocyclic carbenes (NHCs), has been revealed for the construction of indoles. The NHC-catalysed atom economical synthesis of a wide range of 2-substituted indole-3-acetic acid derivatives is displayed. Strategic application of the developed method was demonstrated for a short synthesis of a cyclin-dependent kinase (CDK) inhibitor: paullone. (*Chem. Commun.,* **2017**, 53(23), 3338)

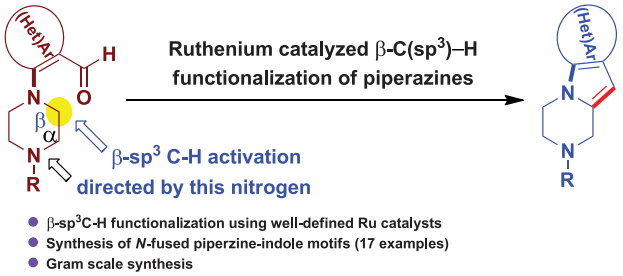


EWG = COOR, $CONR_2$, CN; R' = Aryl, Heteroaryl; R'' = H, Me

- N-Heterocyclic carbene (NHC) catalysed atom economical construction of indoles
- Synthesis of 2-substituted indole-3-acetic acid derivatives (37 examples)
- Gram Scale Synthesis
- Synthesis of Paullone in two steps

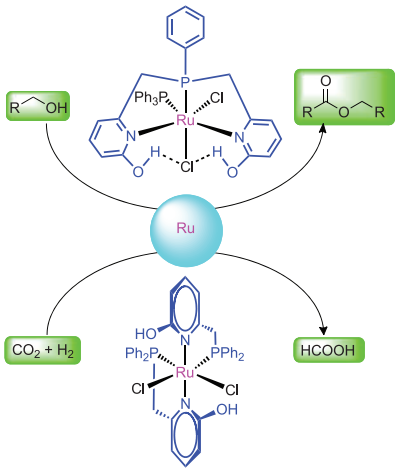
Ruthenium Catalyzed β-C(sp³)–H Functionalization on the 'Privileged' Piperazine Nucleus

β-C(sp³)–H functionalization on the 'privileged' piperazine nucleus has been disclosed using ruthenium catalysis. The ruthenium catalyzed synthesis of a variety of piperazine fused indoles from *ortho*-piperazinyl (hetero)aryl aldehydes is presented. This transformation takes place *via* the dehydrogenation of piperazine followed by an intramolecular nucleophilic addition of the transient enamine moiety onto the carbonyl group and aromatization cascade. (*Chem. Commun.*, **2017**, 53(75), 10448)



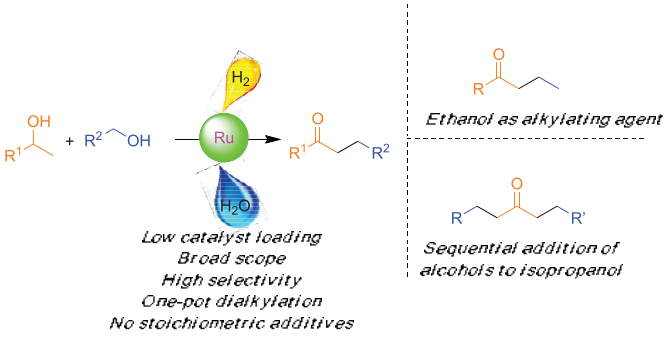
Phosphine-Pyridonate Ligands Containing Octahedral Ruthenium Complexes: Access to Esters and Formic Acid

The preparation of three well-defined ruthenium complexes arising from phosphine-pyridon-e/-ate ligands is described. Solvent dependent Lewis acidic species formation was observed with these complexes. Selective formation of acetals or esters from primary alcohols was observed in the presence of these catalysts. Preliminary evaluation of these complexes in the base free hydrogenation of carbon dioxide is also reported. (*Catal. Sci. Technol.*, **2017**, 7(16), 3492)



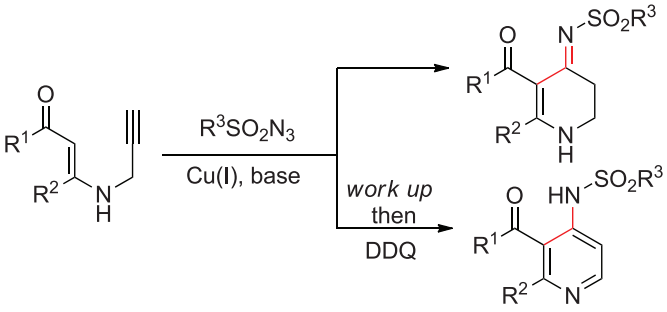
Ruthenium Phosphine–Pyridone Catalyzed Cross-Coupling of Alcohols to form α-Alkylated Ketones

An efficient and green route to access diverse functionalized ketones *via* dehydrogenative–dehydrative cross-coupling of primary and secondary alcohols is demonstrated. Selective and tunable formation of ketones or alcohols is catalyzed by a recently developed proton responsive ruthenium phosphine–pyridone complex. Light alcohols such as ethanol could be used as alkylating agents in this methodology. Moreover, selective tandem double alkylation of isopropanol is achieved by sequential addition of different alcohols. (*J. Org. Chem.*, **2017**, 82(19), 10727)



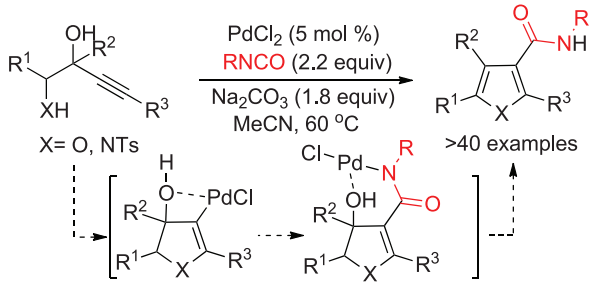
Cu-Catalyzed iminative hydroolefination of unactivated alkynes en route to 4-iminotetrahydropyridines and 4-aminopyridines

A general method for the construction of 4-imino tetrahydropyridine derivatives is reported from readily available β-enaminones and sulfonyl azides. It involves a tandem copper catalyzed ketenimine formation and its intramolecular hydrovinylation. The products are shown as ready precursors for highly valuable 4-sulfonamindopyridine derivatives via DDQ mediated oxidation. (*Chem. Commun.*, **2016**, 52(92), 13475)



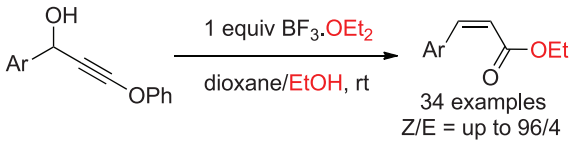
Synthesis of Substituted Furan/Pyrrole-3-Carboxamides Through a Tandem Nucleopalladation & Isocyanate Insertion

An access to furanyl- and pyrrolyl-3-carboxamides from readily available 3-alkyne-1,2-diols and 1-amino-3-alkyn-2-ols using isocyanate as amido surrogate is demonstrated. The approach constitutes a successful unprecedented combination of heteropalladation and isocyanate insertion, a new avenue for novel amide bond constructions. The mechanism likely involves a 6-membered oxa-amino-pallada cycle as the key intermediate. *(Org. Lett.,* **2016**, 18(17), 4332)



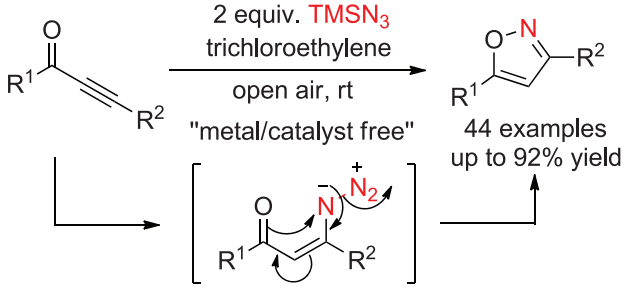
BF3.OEt2-Mediated Syn-Selective Meyer-Schuster Rearrangement of Phenoxy Propargyl Alcohols for Z-β-Aryl-α,β-Unsaturated Esters

Synthesis of Z-β-aryl-α,β-unsaturated esters from readily available 1-aryl-3-phenoxy propargyl alcohols is achieved via BF3-mediated syn-selective Meyer-Schuster rearrangement under ambient conditions. The reaction mechanism is postulated to involve an electrophilic borylation of allene intermediate as the key step to kinetically control the stereoselectivity. (*Org. Biomol. Chem.,* **2016**, 14(29), 7001)



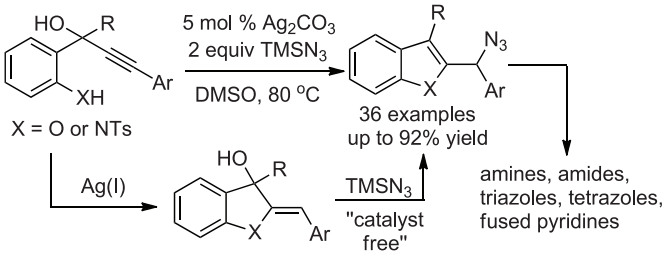
A Direct Access to Isoxazoles from Ynones using Trimethylsilyl Azide as Amino Surrogate under Metal/Catalyst free Conditions

A general method for isoxazoles from readily available ynones using trimethylsilyl azide as amino surrogate, likely via an unprecedented hydroazidation of alkyne and denitrogenative cyclization, is demonstrated. The method neither required any catalyst nor demanded the unusual conditions to afford the products with outstanding functional group compatibility. *(Chem. Commun.,* **2016**, 52(39), 6589)



Synthesis of benzofuranyl and indolyl methyl azides by tandem silver-catalyzed cyclization and azidation

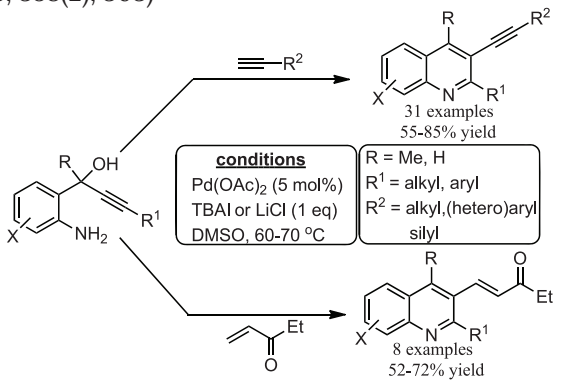
Ag(I)-catalyzed synthesis of 2-azidomethyl benzofurans/indoles from linear and readily available hydroxyl/amino-phenyl propargyl alcohols is described via a highly regioselective C–O and C–N bond formation. Control experiments reveal that the reaction involves the sequential Ag(I)-catalyzed 5-exo-dig cyclization and a catalyst free γ-allylic azidation. The synthetic utility of this method has been demonstrated by using the azidomethyl unit of the above synthesized heterocycles as the base for a variety of other functionalizations, such as triazole-, tetrazole-, amide-, amine-, and pyrido-derivatives. *(Org. Biomol. Chem.,* **2016**, 14(17), 4077)



Palladium(II)-Catalyzed Sequential Aminopalladation and Oxidative Coupling with Acetylenes/Enones: Synthesis of Newly Substituted Quinolines from 2-Aminophenyl Propargyl Alcohols

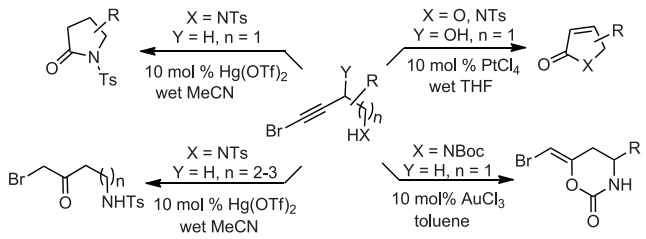
Palladium catalyzed conversion of 1-(2-aminophenyl)-propargyl alcohols to 3-alkynyl quinolines is realized via a cascade that involves aminopalladation, oxidative coupling with alkynes and dehydration. The method is shown to have a broad substrate scope with respect

to propargyl alcohols as well as alkynes. Vinyl ketones as coupling partners in the same reaction afforded 3-alkenyl quinolines with equal ease. *(Adv. Synth. Catal.,* **2016**, 358(2), 303)



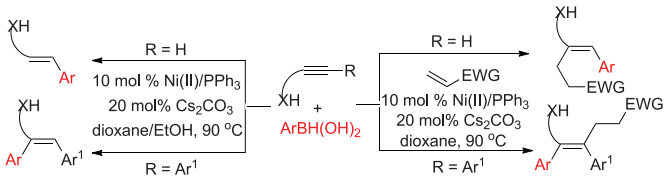
Hg/Pt-catalyzed conversion of bromo alkynamines/alkynols to saturated and unsaturated γ-butyrolactams/lactones via intramolecular electrophilic cyclization

A convenient and general Hg(II)/Pt(IV) catalyzed syntheses of γ-butyrolactams and α,β- unsaturated γ-butyrolactones/lactams are described via an intramolecular electrophilic cyclizations of bromoalkynes with tosylamino and hydroxyl tethers. The reaction features the use of wet solvents, the exclusion of any base and additive, mild conditions and practical yields. We also synthesised few chiral lactams through this pathway. Additionally, it is shown that NHTs group distanced farther from homopropargylic position assists for regioselective bromoalkyne hydration to yield useful α-bromoketones. Further, Boc protected bromo homo propargyl amines undergo 6-endo-dig cyclization through Boc oxygen to give bromomethylene substituted oxazinones. *(Org. Biomol. Chem.,* **2016**, 14(4), 1252)



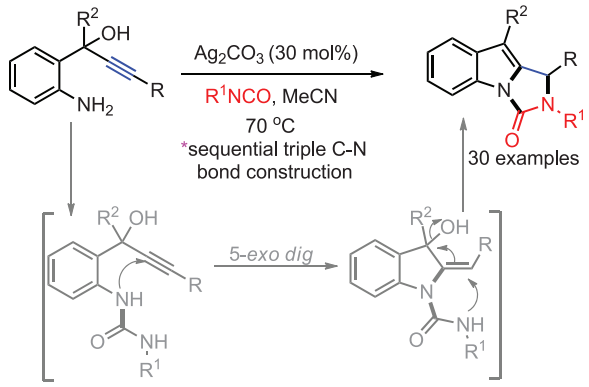
Ni-Catalyzed regio- and stereoselective addition of arylboronic acids to terminal alkynes with a directing group tether

Addition of arylboronic acids to directing group tethered acetylenes in a regio and stereoselective manner using an inexpensive catalytic system is achieved for the first time to access highly sought after allyl/homoallyl alcohol/amine units. The apparent inylnickel intermediate was successfully trapped by the Michael electrophiles to get defined tri- and tetra-substituted olefins. An interesting selectivity switch was observed with internal alkynes. (*Chem. Commun.,* **2017**, 53(27), 3894)



Ag-Catalyzed Intramolecular Sequential Vicinal Diamination of Alkynes with Isocyanates: Synthesis of Fused Indole-Cyclic Urea Derivatives

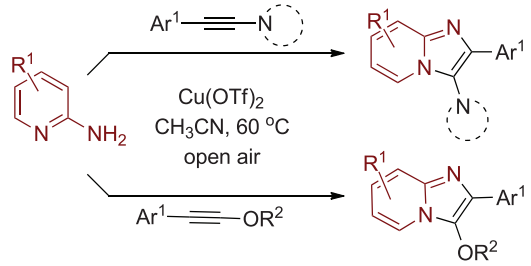
A formal intramolecular vicinal 1,2-diamination of alkynes is achieved for the synthesis of indole-cyclic urea fused derivatives through double cyclization process from readily available aminophenyl propargyl alcohols. This sequential triple C-N bond construction event was possible using isocyanate as urea precursor and Ag(I) catalyst as alkyne activating agent. Control experiments reveal that the cyclization followed by 1,3-allylic amino dehydroxylation is preceded by urea formation. (*J. Org. Chem.,* **2017**, 82(10), 5169)



Copper Promoted Regioselective Intermolecular Diamination of Ynamides: Synthesis of Imidazo[1,2-*a*]pyridines

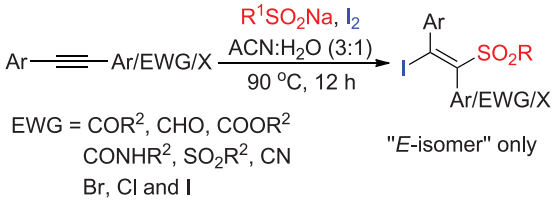
A facile access to 3-heterosubstituted (3-oxazolidinonyl/indolyl/phenoxy) imidazo[1,2-a]pyridines from readily available 2-aminopyridines and electron rich (internally activated) alkynes like ynamides/ynamines/ynol ethers is achieved via $Cu(OTf)_2$ mediated intermolecular

diamination under aerobic conditions. The reaction is highly regioselective owing to internal electron bias and thus led to a single regioisomer with heterosubstitution at C3. (*ACS Omega,* **2017**, 2(6), 2770)



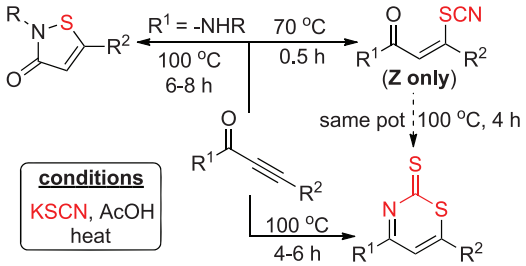
Metal-Free Iodosulfonylation of Internal Alkynes: Stereodefined Access to Tetrasubstituted Olefins

Stereoselective E-iodosulfonylation of internal alkynes for synthesizing highly defined tetrasubstituted olefins using sodium phenyl sulfinate and iodine is achieved. Most of the alkynes explored are non-symmetrical and the regioselection is in full control. Aryl alkynes with various with-drawing groups like keto, aldehyde, ester, amide, cyano, sulfone, bromo, chloro and iodo on the other end are identified as successful precursors to yield the highly functionalized olefins. Alkynes directly tethered with heteroatoms are also found as suitable substrates. (*Adv. Synth. Catal.* **2017**, 359(16), 2847)



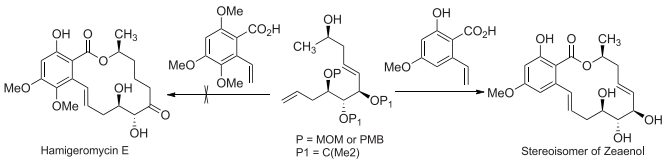
A stereoselective thiocyanate conjugate addition to electron deficient alkynes and concomitant cyclization to N,S-heterocycles

A regio- and stereoselective thiocyanate addition to ynones is achieved using KSCN in AcOH at 70 8C. The reaction is extendable to ynals, ynesulfones, ynoic acids and ynoates. Adducts from ynones were readily transformed into thiazine-2-thione derivatives under slightly modified reaction conditions. In contrast, thiocyanated adducts from ynamides underwent an in situ decyanative amido cyclization towards isothiazolones. None of these events needed any transition metal or catalyst, attaining a high synthetic value. (*Chem. Commun.,* **2017**, 53(80), 11060)



Carbohydrate Based Studies Towards the Synthesis of Hamigeromycin E: A Stereoselective Total Synthesis of an Isomer of Zeaenol

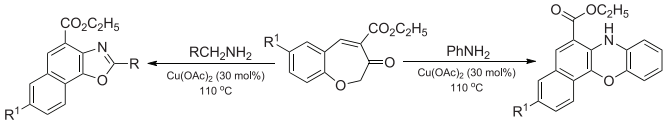
A stereoselective synthesis of 14-membered macrolide hamigeromycin E has been studied by employing *ortho*-lithiated formylation, *Barbier* allylation, *Julia-Kocienski* olefination, *Mitsunobu* esterification and ring-closing metathesis (RCM) reactions. The final RCM reaction did not provide the target molecule. This study has prompted us to synthesize a stereoisomer of zeaenol and accomplish the total synthesis with the above protocols. *(Helv. Chim. Acta*, **2016**, 99(6), 425)



Copper catalyzed C-H oxygenation of benzoxepine-4-carboxylates: A facile approach for the synthesis and photophysical properties of naphtho[2,1-*d*] oxazoles, benzo[*c*]phenoxazines

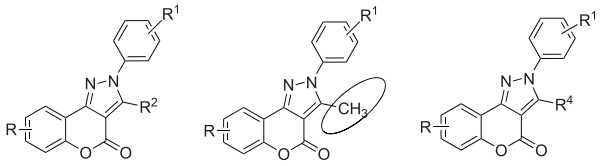
An efficient, solvent free, one-pot protocol has been developed for the preparation of naphtho[2,1-*d*]oxazoles and benzo[*c*]phenoxazines by the C-H oxygenation of benzoxepine-4-carboxylates with benzylamines and anilines in the presence of $Cu(OAc)_2$. The synthesis, UV-Vis absorption, fluorescence emission and electrochemical properties have been studied for these novel heterocyclic compounds for the first time. The benzo[*c*]phenoxazines displayed UV-Vis absoption in the range of 449-461 nm and fluorescence emission in the range of 562-627 nm. The nitro and dimethyl substituted benzo[*c*]phenoxazines and exhibited better fluorescence emission in the present series of compounds (627, 603 nm, Φf = 0.51, 0.37). Optical and electrochemical properties of these compounds suggest

that the compounds may act as electron transporting materials for OLED applications. *(Asian J. Org. Chem.*, **2016**, 5(6), 819)



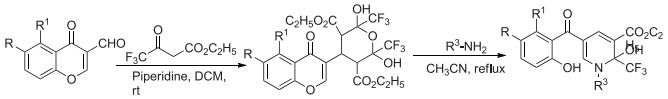
$La(OTf)_3$ catalyzed reaction of salicylaldehyde phenylhydrazones with β-ketoesters and activated alkynes: Facile approach for the preparation of chromenopyrazolones

A facile approach has been developed for the preparation of chromenopyrazolones by the reaction of salicylaldehyde phenylhydrazones with β-ketoesters and activated alkynes in the presence of $La(OTf)_3$ with good yields. However, the reaction of salicylaldehyde phenylhydrazones with ethyl 4-chloro-3-oxobutanoate underwent cyclization with reductive dechlorination and provided the methyl chromenopyrazolones instead of chloromethyl chromenopyrazolones. The present solvent free protocol provided the novel heterocyclic compounds. (*RSC Adv.*, **2016**, 6(110), 108654)



Convenient synthesis of 4*H*-chromenyltetrahydro-2*H*-pyrancarboxylates and cleavage of chromone and pyran rings leading to 5-(2-hydroxybenzoyl)-2-(trifluoromethyl)-1,2-dihydropyridine-3-carboxylates

4*H*-Chromenyl-tetrahydro-2*H*-pyrancarboxylates have been conveniently prepared by the reaction of 3-formylchromones and ethyl 4,4,4-trifluoro-3-oxobutanoate with good yields. Thus obtained 4*H*-chromenyl-tetrahydro-2*H*-pyrancarboxylates were reacted with amines to provide series of 5-(2-hydroxybenzoyl)-2-(trifluoromethyl)-1,2-dihydropyridine-3-carboxylates. The reaction proceeded *via* Michael addition (C-N bond formation) and followed by cleavage of chromone and pyran rings (C-O bond cleavage) in one-pot. (*Synth. Commun.*, **2016**, 46(24), 1963)



Biological evaluation of 3-hydroxybenzyl alcohol, an extrolite produced by *Aspergillus nidulans* strain KZR-132.

A bioactive extrolite was purified from *Aspergillus nidulans* strain KZR-132 whose chemical structure was elucidated as 3-hydroxylbenzyl alcohol (3-HBA) based on ^{1}H and ^{13}C NMR, FT-IR and mass spectroscopic analysis. The antimicrobial efficacy of 3-HBA was established against Gram-positive, Gram-negative bacteria and different *Candida* strains. It also showed promising anti-biofilm activity against various tested microbial strains. Reactive oxygen species induced by 3-HBA treatment on different *Candida* strains killed most of the cells and showed necrotic effect. It also exhibited dose-dependent antioxidant and anti-inflammatory activities. HBA exhibited broad-spectrum antimicrobial and anti-biofilm activities which are reported for the first time. (*J. Appl. Microbiol.*, **2017**, 122(6), 1518)

Statistical optimization of production conditions of β-glucosidase from *Bacillus stratosphericus* strain SG9

β-Glucosidases are industrially important finding application for use in producing different flavouring compounds such as terpenols, phenylethyl and benzyl alcohols, therapeutic importance in Gaucher's disease; biofuels, pharmaceutical and cosmetic industries. *Bacillus stratosphericus* strain SG9 was identified as a promising bacterial strain responsible for β-glucosidase production and the 16S rRNA gene sequence was deposited in Genbank (Accession number KY078548). Nutritional and environmental parameters were optimized to maximize β-glucosidase enzyme production using one factor at a time (OFAT) approach as well as Plackett–Burman design followed by Box–Behnken response surface methodology. Based on the Box–Behnken DOE statistical optimization, the maximum enzyme production increased by fivefold (from 660 to 3340 IU). (*Biotech*, **2017**, 7(3), 221)

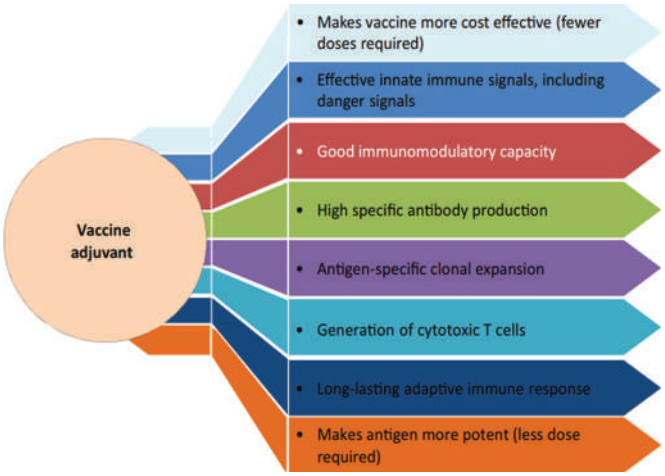
The use of databases, data mining and immunoinformatics in vaccinology: where are we?

Vaccinology has evolved from a sub-discipline focussed

on simplistic vaccine development based on antibody-mediated protection to a separate discipline involving epidemiology, host and pathogen biology, immunology, genomics, proteomics, structure biology, protein engineering, chemical biology, and delivery systems. Data mining in combination with bioinformatics has provided a scaffold linking all these disciplines to the design of vaccines and vaccine adjuvants. Areas covered: This review provides background knowledge on immunological aspects which have been exploited with informatics for the in silico analysis of immune responses and the design of vaccine antigens. Furthermore, the article presents various databases and bioinformatics tools, and discusses B and T cell epitope predictions, antigen design, adjuvant research and systems immunology, highlighting some important examples, and challenges for the future. Expert opinion: Informatics and data mining have not only reduced the time required for experimental immunology, but also contributed to the identification and design of novel vaccine candidates and the determination of biomarkers and pathways of vaccine response. However, more experimental data is required for benchmarking immunoinformatic tools. Nevertheless, developments in immunoinformatics and reverse vaccinology, which are nascent fields, are likely to hasten vaccine discovery, although the path to regulatory approval is likely to remain a necessary impediment. (*Expert Opin. Drug Discov.*, **2017**, 13 (2), 117)

An Overview of Novel Adjuvants Designed for Improving Vaccine Efficacy

Adjuvants incorporated in prophylactic and/or therapeutic vaccine formulations impact vaccine efficacy by enhancing, modulating, and/or prolonging the immune response. In addition, they reduce antigen concentration and the number of immunizations required for protective efficacy, therefore contributing to making vaccines more cost effective. Our better understanding of the molecular mechanisms of immune recognition and protection has led research efforts to develop new adjuvants that are currently at various stages of development or clinical evaluation. In this review, we focus mainly on several of these promising adjuvants, and summarize recent work conducted in various laboratories to develop novel lipid-containing adjuvants. (*Trends Pharmacol. Sci.,* **2017**, 38(9), 771)



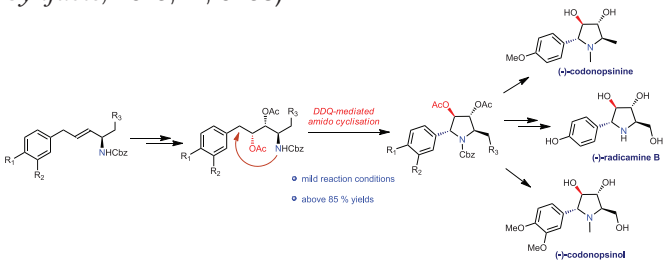
Optimization of recombinant vaccine antigen dose in mouse model by ELISA and immunophenotyping

Mass administration of vaccines against particular disease to produce protective immunity is the ultimate goal of developing recombinant vaccine antigens. Preclinical optimization and standardization of antigen dose is highly crucial for the clinical development of vaccines. In this present study, we have optimized the dose of HBsAg, Dengue and JEV recombinant antigens, through estimation of antibody titer by ELISA method (IgG, IgG1 and IgG2a) and Flow cytometric immunophenotyping of CD4+ and CD8+ surface markers in vivo in BALB/c mice and determined the minimum detectable antigen dose for immunization as well as antibody reactivity. (*Global Vaccines and Immunology*, **2017**, 2(1), 1)

DDQ-Promoted Benzylic/Allylic sp3 C–H Activation for the Stereoselective Intramolecular C–N Bond Formation: Applications to the Total Synthesis of (–)-Codonopsinine,(+)-5-epi-Codonopsinine,(+)-Radicamine B, and (–)-Codonopsinol

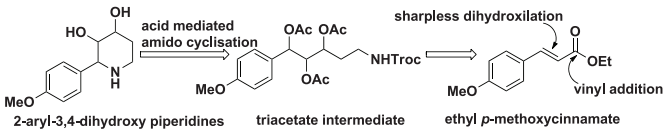
This is the first report on an intramolecular C–N bond formation of an amide-tethered benzylic/allylic system using DDQ under neutral conditions which has been successfully applied to the total synthesis of naturally occurring pyrolidine alkaloids. The key steps for the synthesis of corresponding precursors involve Julia–Kociensky olefination/cross-metathesis and dihydroxylation reactions, and this methodology is

also extended to the ω-unsaturated *N*-sulfanilamide to furnish piperidines. (*J. Org. Chem.,* **2016**, 81(4), 1367; *Synfacts,* **2016**, 12, 0458)



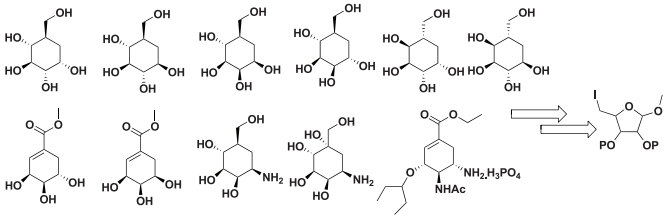
Influence of A1, 3 Strain on the Stereochemical Outcome of Acid-Mediated Amido Cyclization in the Synthesis of 2-(4-Methoxyphenyl)-3, 4-(dihydroxy) piperidines

The synthesis of 2-(4-methoxyphenyl)-3,4-(dihydroxy) piperidines was accomplished by using ethyl *p*-methoxycinnamate as the starting material and an acid-mediated amido cyclization reaction as the key step. This short and straightforward strategy avoids extra steps to create the chiral center and does not require a leaving group at the benzyliccarbon. This study also showed that the stereochemical outcome of the cyclization reaction is influenced more by allylic1,3-strain (A1,3 strain) than by the participation of a neighboring group. (*Eur. J. Org. Chem.,* **2016**, 2016(9), 1693)



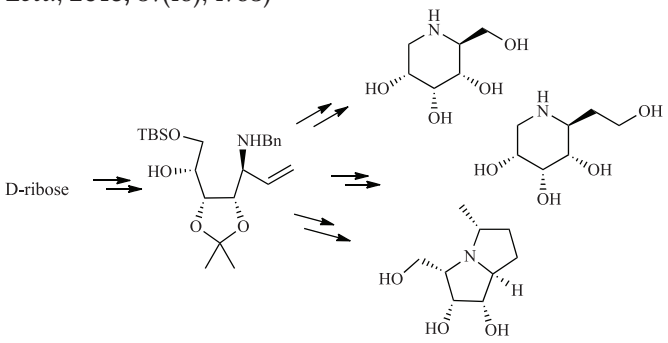
Synthesis of some carbahexopyranoses using Mn/CrCl 3 mediated domino reactions and ring closing metathesis

An efficient and common method for the synthesis of 5a-carba-α-d-mannopyranose **5**, 5a-carba-β-d-mannopyranose **6**, (+) methyl shikimate **9**, (+) methyl-5-*epi*-shikimate **10**, validamine analogue **15** and valiolamine analogue **16** from d-mannose, formal synthesis of Tamiflu **17** from d-ribose and also synthesis of 5a-carba-α-d-glucopyaranose **1**, 5a-carba-β-d-glucopyaranose **2**, 5a-carba-β-l-altropyranose **7** and 5a-carba-α-l-altropyranose **8** from d-xylose is described using Nozaki–Hiyama–Kishi (NHK) condition and ring closing metathesis (RCM). In this transformation 5-deoxy-5-halo-manno/ribo/xylo furanoside undergoes reductive elimination in the presence of $Mn/CrCl_3$to give corresponding olefin-aldehyde which was trapped by nucleophile under the same condition to afford diolefinic species which on metathesis reaction with appropriate Grubbs catalyst produced required carbocycles. (*Tetrahedron,* **2016**, 72 (15), 1838)



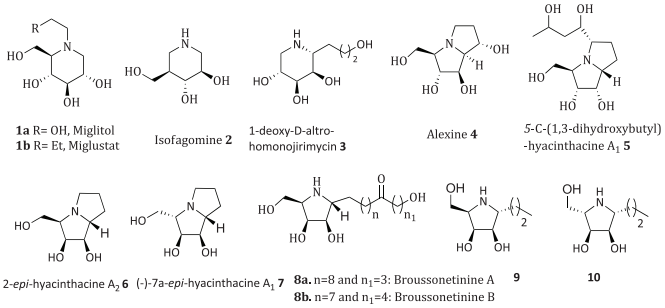
A common approach to the total synthesis of l-1-deoxyallonojirimycin, l-homo-1-deoxyazaallose and triacetyl derivative of 5-*epi* hyacinthacine A_5

A common strategy for the synthesis of polyhydroxylated piperidines l-1-deoxyallonojirimycin, l-homo-1-deoxyazaallose and triacetyl derivative of 5-*epi* hyacinthacine A_5 from the readily available d-ribose as a starting material has been described. (*Tetrahedron Lett.*, **2016,** 57(16), 1763)



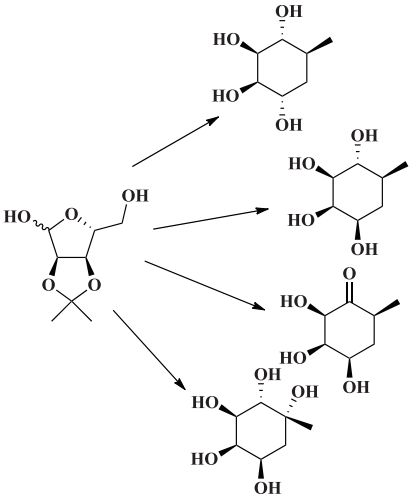
Stereoselective Approach for the Synthesis of 2-epi-Hyacinthacine A2, (–)-7a-epi-Hyacinthacine A1, 1-Deoxy-D-altro-homonojirimycin, and Some Pyrrolidine Iminosugars

A divergent approach has been developed for the synthesis of some important iminosugars by stereoselective allylation of the lyxosylamine derived from D-lyxose and intramolecular 5-exo-tet ring opening of the epoxide. The strategy described in this paper will be useful for the synthesis of some other biologically active iminosugars for the drug-discovery program. (*Synlett.,* **2016,** 27(16), 2391)



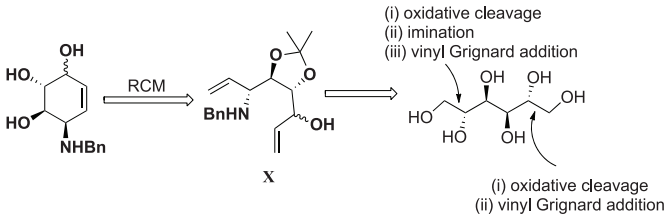
Concise stereo selective synthesis of Carba -α-D-rhamnose, Carba-β-D-rhamnose, and (-) Gabosine O

Stereoselective strategy was developed for the synthesis of Carba -α-D-rhamnose, Carba –β-D-rhamnose, (-) Gabosine O and polyoxygenated methyl cyclohexanoid **4** from D-ribose and also the glycosidase inhibitory activity of Carba -α-D-rhamnose, Carba –β-D-rhamnose have been studied. (*J. Carbohydr. Chem.,* **2016,** 35(3), 150)



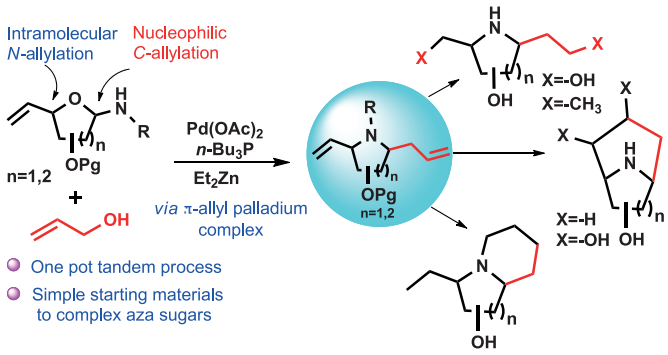
Stereoselective synthesis of *N*-benzyl conduramine F-1, *N*-benzyl *ent*-conduramine E-1, dihydroconduramine F-1 and *ent*-dihydroconduramine E-1

A short and stereoselective synthesis of conduramine F-1 and *ent*-conduramine E-1 derivatives have been achieved starting from D-mannitol using nucleophilic vinylation on imine. A concise sequence of vinylation at both ends of D-mannitol and followed by RCM allowed us to prepare target compound. (*Tetrahedron Lett.,* **2017,** 58(6), 559)



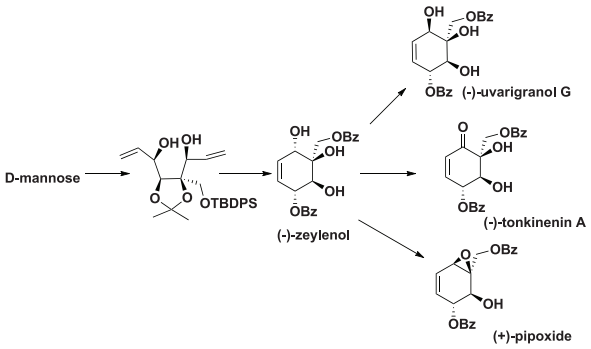
Palladium-Catalyzed Double Allylation of Sugar-Imines by Employing Tamaru-Kimura's Protocol: Access to Unnatural Iminosugars

Conversion of vinyl pyranosylamine and vinyl furanosylamines to 2,6- and 2,5-disubstituted pyrrolidine and piperidine iminosugars respectively in one pot has been developed, using Kimura and Tamaru's procedure, where a palladium salt in the presence of Et_2Zn was used for this domino reaction. In this procedure, double allylation, which involves nucleophilic allylation-heterocyclization, has taken place to give desired nitrogen heterocycles. This strategy was further elaborated to synthesize some unnatural deoxy-calystegines, hydroxylated pyrrolidines, piperidines and indolizidine analogues. (*Org. Lett.,* **2017**, 19(7), 1642)



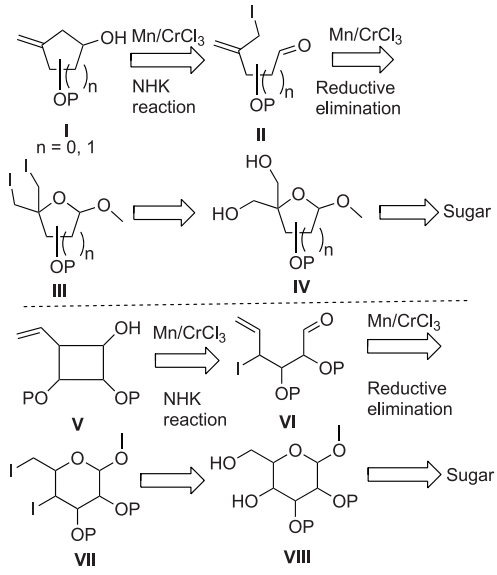
Stereoselective total synthesis of (–)-zeylenol, a key intermediate for the synthesis of (+)-pipoxide, (–)-uvarigranol G and (–)-tonkinenin A

Total synthesis of (–)-zeylenol, a key intermediate for the synthesis of (+)-pipoxide,(–)-uvarigranol G and (–)-tonkinenin A was achieved from commercially available starting material d-mannose. The key steps are mixed aldol condensation, Grignard reaction, ring closing metathesis and regioselective benzoylation. (*Tetrahedron Lett.,* **2017**, 58(11), 1075)



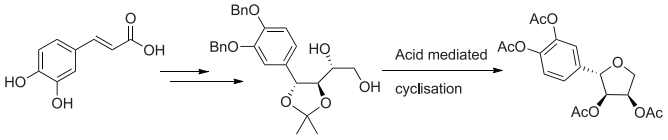
Carbohydrates to cyclitols using Mn/$CrCl_3$ mediated domino *Bernet-Vasella* reductive elimination and NHK Reaction

A novel, general and efficient approach for the conversion of carbohydrates to cyclitols was developed utilizing Mn/$CrCl_3$ mediated domino *Bernet-Vasella* reductive elimination of diiodo precursor of a sugar and NHK reaction to produce four, five and six membered cyclitols. And also, the specific reactivity of Mn/$CrCl_3$ over Zn on diiodo compounds was studied. (*ChemistrySelect,* **2017**, 2(36), 11949)



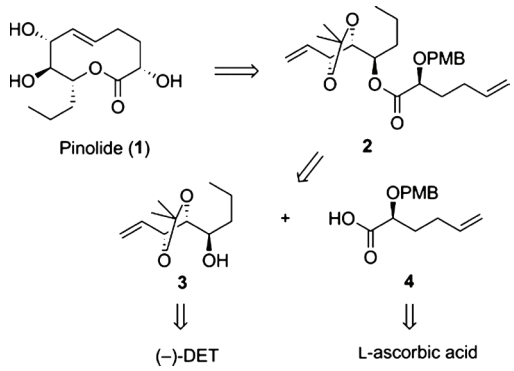
Stereoselective synthesis of peracetylated (-)-gloeosporiol *via* acid catalysed intramolecular etherification

A simple and an efficient strategy have been developed for the stereoselective synthesis of peracetylated (-)-gloeosporiol by acid catalysed cyclisation from the commercially available starting materials. (*Tetrahedron Lett.,* **2017**, 58(6), 563)



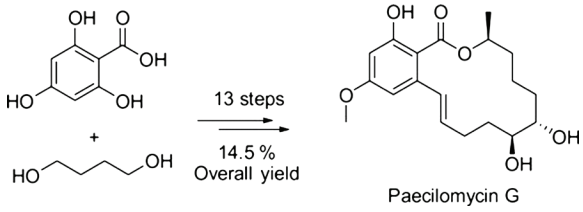
An Enantioselective Approach to Pinguisane Sesquiterpenes: Total Synthesis of (−)-Pinguisenol and (−)-Isonaviculol

A short and efficient enantioselective approach to pinguisane-type sesquiterpenes has been developed starting from a Hajos–Parrish-type ketone. This led to the first total syntheses of isonaviculol (10 steps, 6.6 % overall yield) and natural pinguisenol (9 steps, 12 % overall yield). The key reactions were regioselective thioketal protection, stereoselective cyclopropanation using Furukawa's protocol, diastereoselective hydrogenation of an olefin using a Thalesnano H-Cube Pro flow reactor, Li/liquid NH_3 mediated cyclopropane reduction, and a PCC-mediated 1,3-oxidative transposition sequence. (*Eur. J. Org. Chem.,* **2017**, 2017(19), 2824)



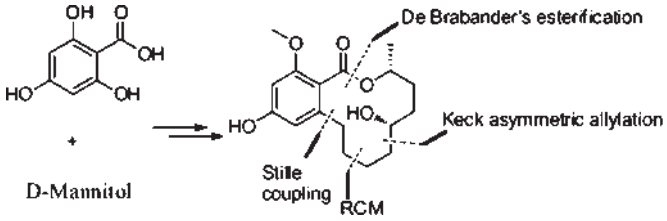
First stereoselective total synthesis of paecilomycin G

The stereoselective total synthesis of resorcylic acid lactone, paecilomycin G has been accomplished. The key steps involved are the Corey–Fuchs reaction, Sharpless asymmetric dihydroxylation, Jacobsen hydrolytic kinetic resolution, Stille coupling, Mitsunobu reaction, and Ring-closing metathesis (RCM) reaction as the key reactions in 13 longest linear steps with an overall yield of 14.5%. (*Tetrahedron Lett.,* **2016**, 57(25), 2800)



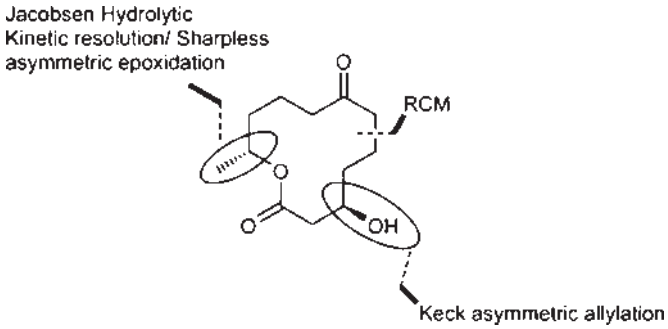
Stereoselective synthesis of (3R,6S)-6-hydroxylasiodiplodin

The first stereoselective synthesis of polyketide natural product (3*R*,6*S*)-6-hydroxylasiodiplodin has been described starting from commonly available starting materials D-mannitol and 2,4,6-trihydroxybenzoic acid. The key reactions involved are Keck asymmetric allylation, Stille coupling, De Brabander's esterification, and ring-closing metathesis (RCM) reaction. The total synthesis was achieved in 19.3% overall yield making the route significant. (*Tetrahedron Lett.,* **2016**, 57(15), 1653)



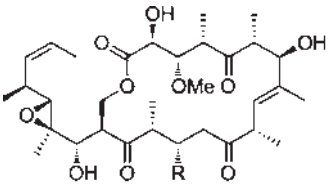
Stereoselective synthesis of dendrodolide-L

An efficient stereoselective total synthesis of 12-membered macrolide dendrodolide L has been achieved. The key reactions involved are Keck asymmetric allylation, Jacobsen's hydrolytic kinetic resolution, Sharpless asymmetric epoxidation, Mitsunobu reaction and ring-closing metathesis reaction as the key steps with an overall yield of 19.7% starting from enantiopure epoxide. (*Tetrahedran: Asymmetry*, **2016**, 27(6), 254)



Studies towards the total synthesis of (+)-13-deoxytedanolide: stereoselective synthesis of C1–C9 and C9–C17 fragments

A facile and stereoselective synthesis of C1–C9 and C9–C17 fragments of (+)-13-deoxytedanolide and studies towards the synthesis of (+)-13-deoxytedanolide was accomplished in 20 linear steps in a concise manner using Sharpless asymmetric dihydroxylation, Sharpless epoxidation and Crimmins' syn aldol and esterification under Yamaguchi conditions as key steps with an overall yield 4.2% and preparation of terminal olefin from primary alcohol utilising organo selenium reaction. (*Tetrahedron Lett.*, **2016**, 57(7), 728)

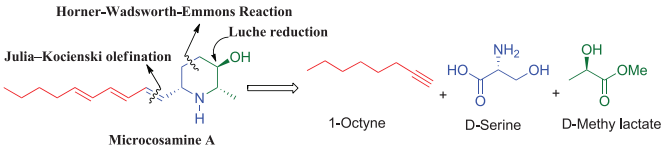


(+)-13-deoxytedanolide (1) R=H

(+)-tedanolide (2) R=OH

Total synthesis of a piperidine alkaloid, Microcosamine A

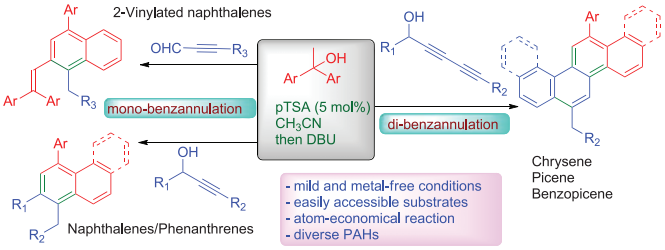
The first asymmetric total synthesis of a new natural piperidine alkaloid, microcosamine A, has been accomplished from *D*-Serine and *D*-methyl lactate as chiral pool starting materials. Key features of the strategy include the utility of Horner-Wadsworth-Emmons reaction, Luche reduction, intramolecular carbamate *N*-alkylation to form the piperidine framework and Julia-Kocienski olefination to install the triene side-chain. The approach is handy for the synthesis of other natural products and their analogues having different side chains. This work is a part of XII five-year programme project under ORIGIN (CSC-108) **(***Org. Biomol. Chem.*, **2016**, **14(1),** 251)



Atom- and Pot-Economical Consecutive Multi-Step Reaction Approach to Polycyclic Aromatic Hydrocarbons (PAHs)

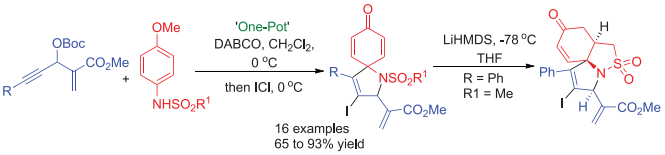
One-pot benzannulation reaction has been established for the synthesis of substituted polycyclic aromatic hydrocarbons (PAHs) from the direct coupling of propargylic aldehydes/alcohols with 1,1-diarylethanol through an atom-economical uninterrupted three/four-step reaction sequence under mild and metal-free reaction conditions. The strategy involves an acid-catalyzed dehydration and carbon-carbon bond formation followed by DBU-promoted cycloisomerization. Naphthalene and phenanthrene were obtained via mono-benzannulation and chrysene,

picene and benzopicene were obtained involving consecutive di-benzannulation reactions in good yields starting from easily accessible starting materials. This work is a part of XII five-year programme project under ORIGIN (CSC-108) (*Chem. Commun.*, **2017**, **53(11),** 1904)



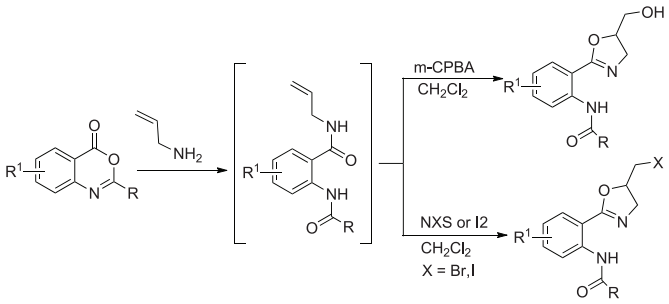
One-Pot Consecutive Sulfonamidation/ipso-Cyclization Strategy for the Construction of Azaspirocyclohexadienones

One-pot protocol for the synthesis of azaspirocyclohexadienones *via* sequential sulfonamidation/*ipso*-cyclization reactions using MBH carbonate and *N*-aryl sulfonamide are described for the first time. This tandem reaction represents a simple and efficient approach to azaspirocyclohexadienones involving sequential C-N, C-I and C-C bond formations. Usefulness of the spirocyclohexadienones has also been demonstrated to access tricyclic-fused sultam and other diversified derivatives. This work is a part of XII five-year programme project under ORIGIN (CSC-108) (*J. Org. Chem.*, **2017**, 82(13), 6932)



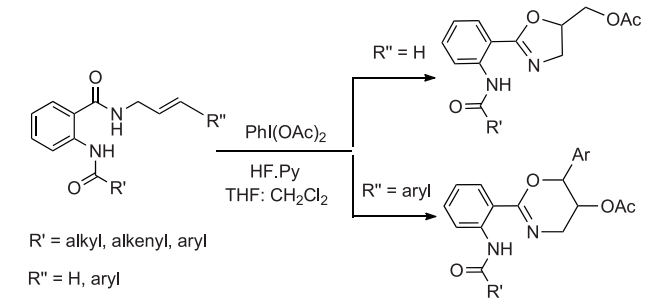
A metal-free tandem ring-opening/ ring-closing strategy for the heterocyclic conversion of benzoxazin-4-ones to oxazolines

A facile metal-free tandem ring-opening/ring-closing strategy was developed for the synthesis of oxazolines in good to excellent reaction yields under mild reaction conditions. This reaction essentially describes a novel tool for the heterocyclic conversion of benzoxazin-4-ones to 2,5-disubstituted oxazolines directly in one-pot. (*RSC Adv.*, **2016**, 6(8), 6058)



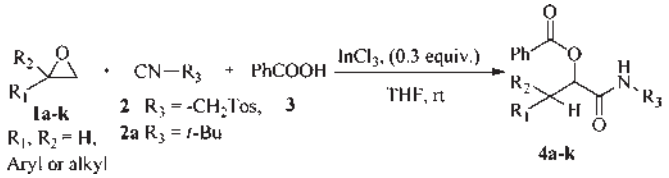
Intramolecular Oxyacetoxylation of *N*-Allylamides: Synthesis of oxazolines and oxazines by PhI(OAc)$_2$/Hydrogen fluoride–Pyridine System

The synthesis of oxazolines and oxazines from N-allylamides was accomplished via an unprecedented reaction set. This reaction involved an intramolecular cyclization of N-allylamides resulting from nucleophilic attack of the allylamine on the benzoxazin-4-one. Unlike the previous literature, the isolable N-allylamide could readily be subjected to exo and endo fashion ring-closure under conditions to afford the title compounds. (*Org. Biomol. Chem.*, **2016**, 14(42), 10074)



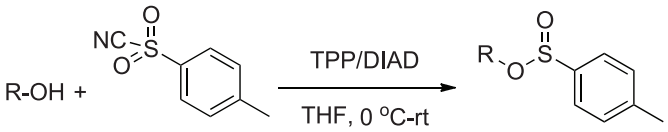
Facile access to α-acyloxyamides via epoxide rearrangement/three-component domino reaction catalyzed by indium(III) chloride

Highly regioselective rearrangement of epoxide to aldehyde/three component Passerini reaction catalyzed by indium(III) chloride is described. In the present protocol, epoxides served as wonderful substrates to furnish a library of α-acyloxyamides under mild reaction conditions in shorter reaction times and in good yields. (*Synth.Commun.*, **2016**, 46(15), 1275)



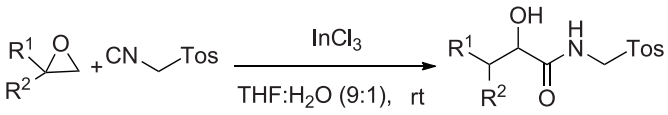
Sulfination of Alcohols with p-Toluenesulfonylmethyl Isocyanide under Metal-Free Conditions: A Mitsunobu Approach

A Mitsunobu approach for the synthesis of sulfinate esters by direct nucleophilic substitution of alcohols is described. The salient features of this strategy include neutral and metal-free conditions for the rapid synthesis of sulfinates in high yields. The present protocol using p-toluenesulfonylmethyl isocyanide (TosMIC) and the triphenylphosphine (TPP)/diisopropyl azodicarboxylate (DIAD) reagent system represents the general synthetic route to this important class of compounds. *(Adv. Synth. Catal.*, **2016**, 358(23), 3863)



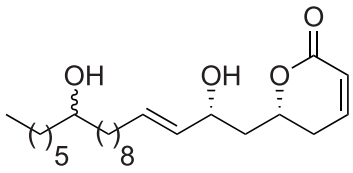
Indium(III) Chloride Promoted Highly Efficient Tandem Rearrangement–α-Addition Strategy towards the Synthesis of α-Hydroxyamides

A new tandem process is reported that provides access to α-hydroxyamides from epoxides for the first time. Herein, we explore InCl3-mediated tandem rearrangement of epoxides to aldehydes and α- addition of TosMIC to in situ derived aldehydes. An unprecedented C–C bond-forming reaction is disclosed that features mild conditions, high yields, and shorter reaction times. *(Synlett,* **2016,** 27(11), 1693)



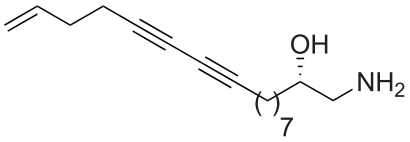
Total Synthesis of the Proposed Structures of the Novel Antimalarial Pyranone Cryptorigidifoliol E

The total syntheses of the proposed structures of the antimalarial lactone cryptorigidifoliol E are described. The synthetic sequence notably features a Bartlett–Smith halocyclization to give a chiral epoxide, followed by its regioselective ring-opening reaction, Still–Gennari olefination, Corey–Bakshi–Shibata (CBS) ynone reduction, and olefin cross-metathesis. (*Synthesis,* **2016,** 48(23), 4213)



Total synthesis of distaminolyne A

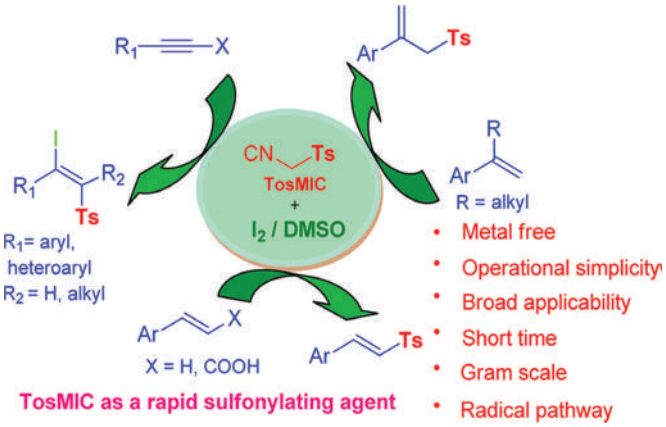
Herein we report the stereoselective total synthesis of first occurrence distaminolyne A via aminolytic kinetic resolution, Corey-Fuch's reaction for alkyne formation and Cardiot-Chodkiewicz cross coupling followed by Wittig olefination as the key steps. (*Tetrahedron Lett.*, **2017**, 58(13), 1273)



distaminolyne A

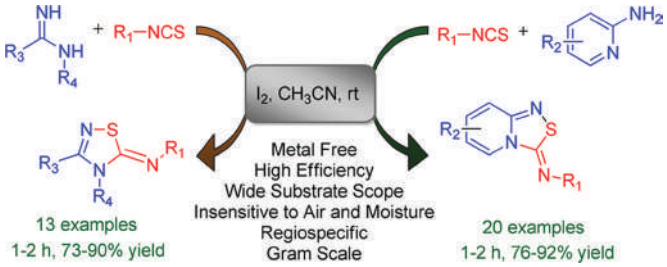
Iodine-Catalyzed Facile Approach to Sulfones Employing TosMIC as a Sulfonylating Agent

A novel iodine-catalyzed functionalization of a variety of olefins and alkynes and direct decarboxylative functionalization of cinnamic and propiolic acids with TosMIC to provide access to various vinyl, allyl, and β-iodo vinylsulfones is described. This simple, efficient, and environmentally benign approach employing inexpensive molecular iodine as a catalyst demonstrates a versatile protocol for the synthesis of highly valuable sulfones, rendering it attractive to both synthetic and medicinal chemistry. (*Org. Lett.*, **2017**, 19(10), 2580)



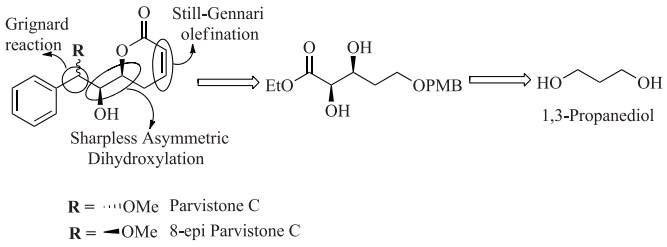
I_2-Catalyzed Oxidative N–S Bond Formation: Metal-Free Regiospecific Synthesis of N-Fused and 3,4-Disubstituted 5-Imino-1,2,4-thiadiazoles

A novel and expeditious approach for the synthesis of N-fused and 3,4-disubstituted 5-imino-1,2,4-thiadiazole derivatives has been achieved through the molecular iodine-catalyzed oxidative cyclization of 2 aminopyridine/amidine and isothiocyanate via N–S bond formation at ambient temperature. The present one-pot transition-metal-free protocol provides the facile and highly efficient regiospecific synthesis of various 1,2,4-thiadiazole derivatives in a scaled-up manner with good to excellent yields using inexpensive I2 as a catalyst. *(J. Org. Chem.*, **2017**, 82(10), 5310)



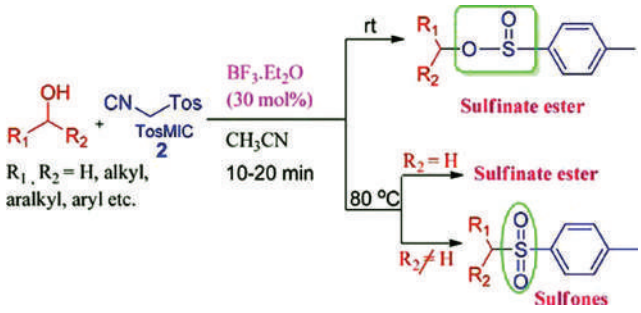
First total synthesis of parvistone C and its C8-epimer

Diastereoselective first total synthesis of parvistone C **1** and C8-epimer **1a** are described. The key features of our synthesis include Sharpless asymmetric dihydroxylation, stereoselective aryl Grignard reactions, Still–Gennari olefination, and intramolecular cyclization. (*Synth. Commun.*, **2017**, 47(20), 1879)



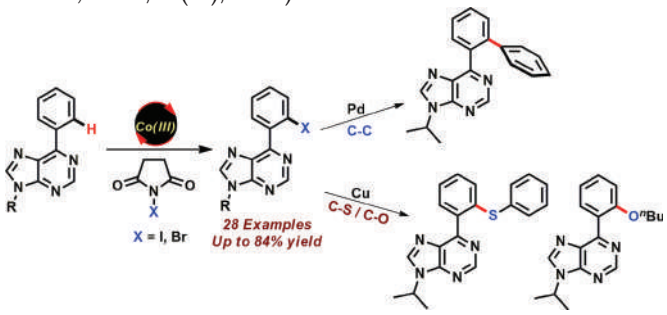
Substrate- and temperature-controlled divergence in reactions of alcohols with TosMIC catalyzed by $BF_3 \cdot Et_2O$: Facile access to sulfinates and sulfones

An efficient $BF_3 \cdot Et_2O$-catalyzed divergent synthesis of sulfinate esters and sulfones through C–O and C–S bond formation has been achieved from alcohols and *p* toluenesulfonylmethyl isocyanide (TosMIC).Various alcohols reacted smoothly with TosMIC under the present conditions at room temperature providing sulfinate esters exclusively. By tuning the reaction temperature, the alcohols that provide highly stabilized carbocation in the reaction medium afforded sulfones as sole products. This study was aimed at understanding the regioselectivity of ambidentate sulfinate ion and to elucidate the interpretation of sulfinate/sulfone scaffolds. (*Synth.Commun.*, **2017**, 47(13),1239)



Cobalt(III)-Catalyzed C–H Halogenation of 6-Arylpurines: Facile Entry into Arylated, Sulfenylated and Alkoxylated 6-Arylpurines

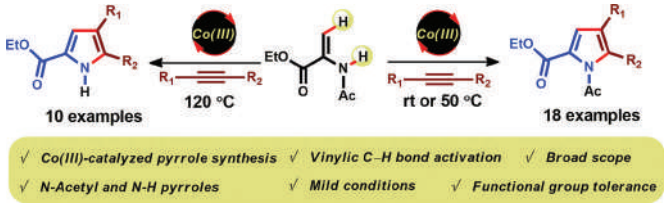
Cobalt-catalyzed C–H halogenation of biologically important 6-arylpurines has reported under mild conditions with good functional group tolerance. The regioselective halogenation of thiophenes as well as the synthetic applicability of the present protocol for the synthesis of arylated, sulfenylated and alkoxylated purine analogues was also demonstrated. (*Org. Biomol. Chem.*, **2016**, 14(12), 3275)



Cp*Co(III)-Catalyzed Vinylic C–H Bond Activation under Mild Conditions: Expedient Pyrrole Synthesis via (3+2) Annulation of Enamides and Alkynes

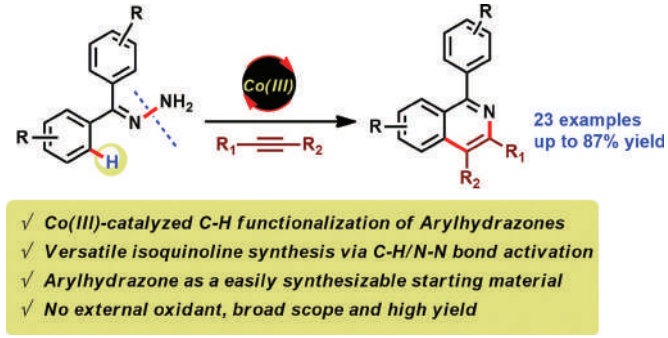
Cobalt(III)-catalyzed (3+2) oxidative annulation of enamides and alkynes for the synthesis of pyrroles has been developed under exceedingly mild conditions. The

reaction works well with various internal alkynes with broad scope and functional group tolerance. In most of the cases, the reaction proceeds at room temperature leading to *N*-acetyl pyrroles in excellent yields. The synthetically useful *N*-H pyrroles can also be obtained at elevated temperature. (*Org. Chem. Front.*, **2016**, 3(7), 836)



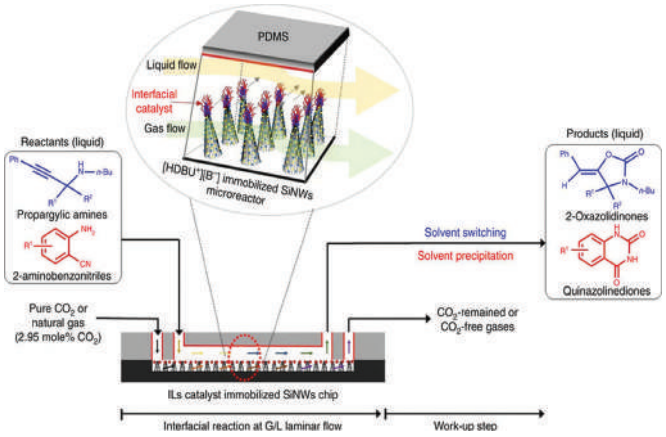
Cp*Co(III)-Catalyzed C–H/N–N Functionalization of Arylhydrazones for the Synthesis of Isoquinolines

Cationic Co(III)-catalyzed C–H/N–N bond functionalization of arylhydrazones with internal alkynes has been developed for the synthesis of isoquinoline derivatives. The arylhydrazones are easy to prepare and require inexpensive and commercially available hydrazine hydrate. The reaction works well with a variety of internal alkynes and arylhydrazones and offers broad scope, good functional group tolerance and high yields under redox-neutral conditions in presence of air. (*J. Org. Chem.*, **2016**, 81(22), 11409)



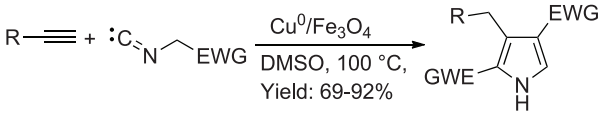
Integrated CO_2 capture-fixation chemistry via interfacial ionic liquid catalyst in laminar gas/liquid flow

Simultaneous capture of carbon dioxide (CO_2) and its utilization with subsequent work-up would significantly enhance the competitiveness of CO_2-based sustainable chemistry over petroleum-based chemistry. Here we report an interfacial catalytic reaction platform for an integrated autonomous process of simultaneously capturing/fixing CO_2in gas–liquid laminar flow with subsequently providing a work-up step. The continuous-flow microreactor has built-in silicon nanowires (SiNWs) with immobilized ionic liquid catalysts on tips of cone-shaped nanowire bundles. Because of the superamphiphobic SiNWs, a stable gas–liquid interface maintains between liquid flow of organoamines in upper part and gas flow of CO_2 in bottom part of channel. The intimate and direct contact of the binary reagents leads to enhanced mass transfer and facilitating reactions. The autonomous integrated platform produces and isolates 2-oxazolidinones and quinazolines-2,4(1*H*,3*H*)-diones with 81–97% yields under mild conditions. The platform would enable direct CO_2 utilization to produce high-valued specialty chemicals from flue gases without pre-separation and work-up steps. (*Nat. Commun.*, **2017**, 8, 14676)



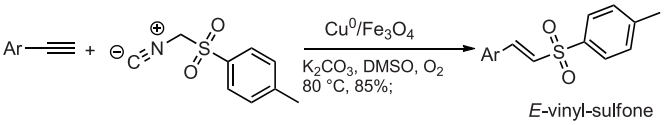
Cu^0/Fe_3O_4 Catalyzed Highly Regioselective Synthesis of 2,3,4-Trisubstituted Pyrroles From Unactivated Terminal Alkynes and Isocyanides

An efficient, one pot tandem nano Cu0/Fe_3O_4 catalyzed highly regioselective synthesis of 3-substituted pyrrole-2,4 dicarboxylates from unactivated terminal alkynes and isocyanides has been developed. This strategy exhibits an unprecedented double addition of isocyanides on unactivated terminal alkynes to obtain trisubstituted pyrroles in high yields. Furthermore, the catalyst was magnetically recovered and reused five times without any appreciable loss of activity. (*Chem. Commun.*, **2016**, 52(25), 4675)



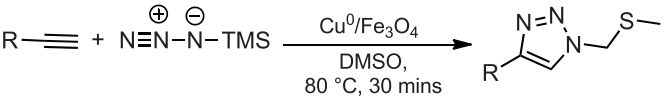
Magnetically Separable Nano Copper Catalyzed Unprecedented Stereoselective Synthesis of *E*-Vinyl Sulfones from Tosylmethyl isocyanide and alkynes: TosMIC as a Source of Sulfonyl group

An unprecedented efficient and mild catalytic route for stereoselective synthesis of *E*-vinyl sulfones from terminal alkynes and tosylmethyl isocyanide (TosMIC) in the presence of magnetically separable nano-copper (0) stabilized on Fe_3O_4. A variety of vinyl sulfones were obtained in moderate to good yields. In this newly developed protocol TosMIC acts as a sulfonyl source. *(Org. Chem. Front.,* **2016**, 3(7), 795)



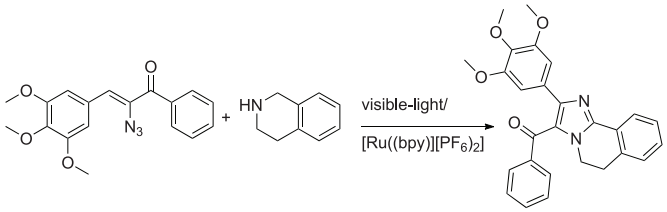
Magnetically Recoverable Cu^0/Fe_3O_4 Catalyzed One Pot Tandem Synthesis of Sulfur Containing Triazoles from Alkynes and Azide: DMSO acts as a alkylating agent

An efficient one-pot tandem nano Cu^0/Fe_3O_4-catalysed synthesis of sulfur-containing triazoles from alkynes and azide has been developed. In this newly developed method, the readily available TMS-azide and dimethyl sulfoxide act as nitrogen and sulfur sources, respectively. The catalyst was magnetically recovered and reused six times without any significant loss of activity. (*Eur. J. Org. Chem.*, **2016**, 2017(27), 4629)



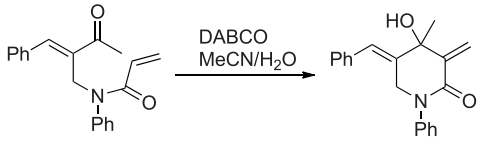
Visible Light Photoredox Mediated sp^3C-H Functionalization and Coupling of Secondary Amines with Vinyl Azides in Flow Microreactors

Structurally diverse imidazole derivatives were synthesized by a visible-light/[Ru(bpy)3][(PF6)2]-mediated coupling of vinyl azides and secondary amines in flow microreactors. This operationally simple and atom-economical protocol allows the formation of three new C-N bonds through the functionalization of sp3 C-H bonds adjacent to the secondary nitrogen atom. (*Chem. A Eur. J.,* **2016,** 22(2), 526)



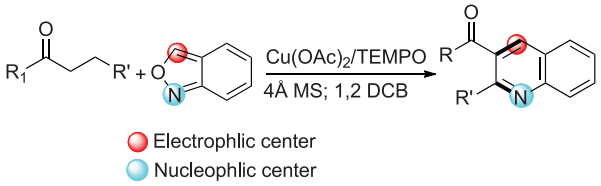
Double Morita–Baylis–Hillman (MBH) strategy; an intermolecular and a chemo selective intramolecular MBH reactions for 5/6 substituted, functionalized piperidine unit

A novel approach utilizing dual Moritae-Baylis-Hillman (MBH) reactions in form of intermolecular and a chemo selective intramolecular version, has been developed. With three electrophilic and a nucleophilic site in precursor, selective condition for intramolecular MBH reaction has been optimized. Role of water was found to be crucial. The dual strategy was applicable for synthesis of a variety of medicinally and synthetically important piperidine unit whose 5/6 atoms of ring were substituted, featuring a stereo defined trisubstituted olefin, a Michael acceptor (with a methylene moiety), trivalent nitrogen and a tertiary alcohol. (*Tetrahedron,* **2016**, 72(2), 312)



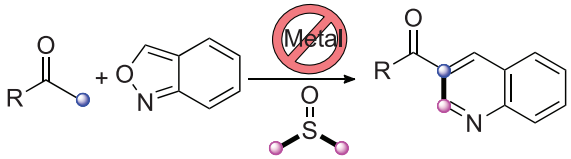
α,β-Functionalization of Saturated Ketones with Anthranils via Cu-Catalyzed Sequential Dehydrogenation/Aza-Michael Addition/ Annulation Cascade Reactions in One-Pot

An efficient method to access functionalized quinolines from the readily available saturated ketones and anthranils has been explored. This one-pot cascade reaction involves the in situ generation of α,β-unsaturated ketones by the copper catalysed dehydrogenation of saturated ketones followed by the aza-Michael addition of anthranils and subsequent annulations. (*Chem. Commun.,* **2017,** 53(38), 5302)



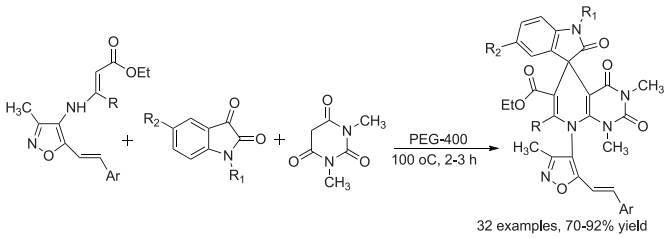
Transition Metal Free Quinoline Synthesis from Acetophenones and Anthranils via Sequential One Carbon Homologation/ Conjugate addition/Annulation Cascade

A transition-metal-free method for the construction of functionalized quinolines from readily available acetophenones and anthranils is reported. This one-pot reaction cascade involves in situ generation of α,β-unsaturated ketones from the acetophenone via one-carbon homologation by DMSO followed by the aza-Michael addition of anthranils and subsequent annulation. DMSO acted in this reaction not only as solvent but also as one carbon source, thus providing a highly atom-economical and environmentally benign approach for the synthesis of 3-substituted quinolines. (*Org. Lett.,* **2017**, 19(18), 4948)



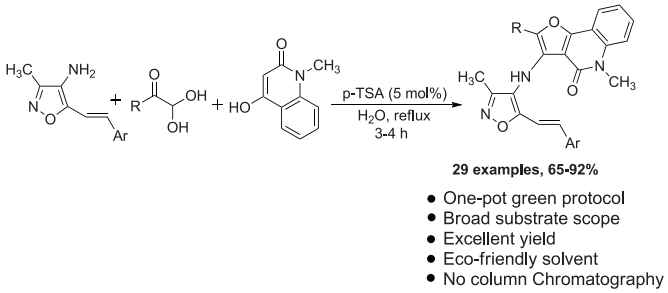
Polyethylene glycol (PEG-400) promoted as an efficient and recyclable reaction medium for the one-pot eco-friendly synthesis of functionalized isoxazole substituted spirooxindole derivatives

An efficient, inexpensive and environmentally friendly synthesis of novel isoxazole substituted spirooxindole-pyridopyrimidines/ indenopyridine/ chromenopyridine/ naphthayridine/ quinoline derivatives has been developed *via* one-pot three-component reaction of isoxazolyl enamino esters, isatins and 1,3-dimethylbarbituric acid/1,3-indandione/chromene-2,4-dione/quinoline-2,4-dione/ naphthalene-1,2,4-trione/dimedone using PEG-400 as a solvent as well as catalyst. Twenty six isoxazolyl enamino esters, seven 1,3-diketo compounds, and eleven substituted isatins were selected for the library validation. The superiority of this method is environmental safety, catalyst free, operational simplicity, metal free, diverse substrate scope, high yield, excellent functional group tolerance, less reaction time and PEG-400 can be recovered and reused. (*New J. Chem.,* **2017**, 41(23), 14062)



p-TSA-Catalyzed facile and efficient one-pot eco-friendly synthesis of novel isoxazolyl amino furo[3,2-*c*]quinolinone derivatives in aqueous medium

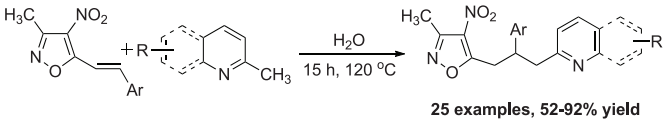
A green and operationally simple approach for the synthesis of novel isoxazolyl amino furo[3,2-c] quinolinone derivatives by a one-pot three-component reaction of 4-amino-3-methyl-5 styrylisoxazoles, aryl glyoxal monohydrates and 4-hydroxy-1-methyl-2-quinolinone using p-TSA as the catalyst in aqueous medium was developed. The protocol proves to be an efficient and an environmentally benign in terms of high yields, operational simplicity, clean reaction profile, compatibility with wide range of substrates, water as a solvent and easy purification. (*Tetrahedron Lett.,* **2017**, 58(40), 3859)



Water-mediated and promoted eco-friendly one-pot synthesis of azaarene substituted isoxazoles

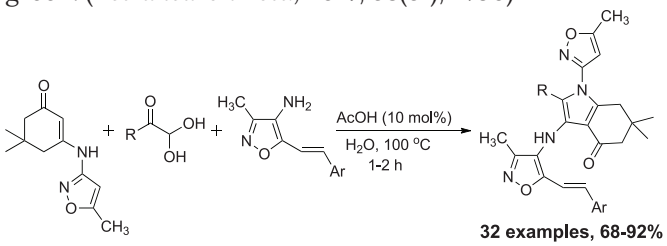
An efficient and green approach for the sp^3 C–H bond functionalization of 2-methyl azaarenes to 3-methyl-4-nitro-5-styrylisoxazoles in water has been described. Nitrostyrylisoxazoles were proven to be good C=C electrophilic acceptors for the construction of various azaarene-containing Michael addition products. This method provides an efficient and environmentally benign method for the one-pot synthesis of biologically important azaarene-substituted isoxazole derivatives in good yields. The important aspects of the present methodology are the use of non-toxic solvent, catalyst

free, the ease of purification and the large substrate scope. (*New J. Chem.,* **2017**, 41(12), 4783)



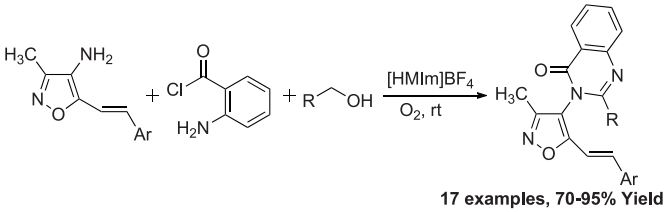
Water-acetic acid mediated an efficient and eco-friendly protocol for the one-pot synthesis of bis-isoxazolyl amino dihydro-1*H*-indol-4(5*H*)-ones under mild reaction conditions

A cost-effective and eco-friendly straightforward synthesis of new bis-isoxazolyl amino dihydro-1*H*-indol-4(5*H*)-ones is successfully achieved *via* one-pot three-component reaction of *N*-isoxazolyl enaminone, aryl glyoxal monohydrates and 4-amino-3-methyl-5-styrylisoxazoles by using water as a reaction medium and acetic acid (AcOH) as cheap and green promoter. The protocol proves to be an efficient and environmentally benign in terms of high yields, low reaction time, operational simplicity, metal-free and wide substrates scope. Most important of all, this reaction process is green. (*Tetrahedron Lett.,* **2017**, 58(51), 4790)



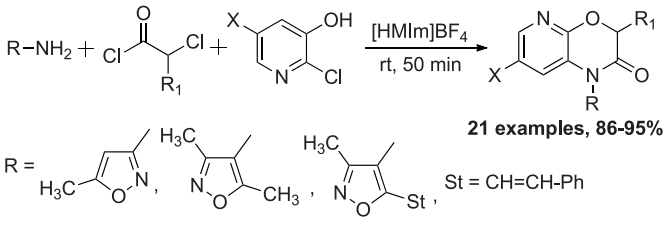
Ionic Liquid [HMIm]BF_4 Mediated and Promoted Eco-Friendly One-Pot Sequential Synthesis of New Isoxazolyl Quinazolin-4(3*H*)-ones

1-Methyl imidazolium tetraflouroborate ([HMIm]BF_4) has been discovered to be an effective eco-friendly solvent cum activator for a novel one-pot sequential coupling and oxidative cyclization of 4-amino-3-methyl-5-styrylisoxazoles, 2-aminobenzoyl chloride and benzyl alcohols to produce new isoxazolyl quinazolin-4(3*H*)-ones under ambient conditions. The protocol proves to be an efficient and an environmentally benign in terms of high yields, low reaction times, ease of recovery, and reusability of reaction medium. (*ChemistrySelect,* **2017**, 2(9), 2651)



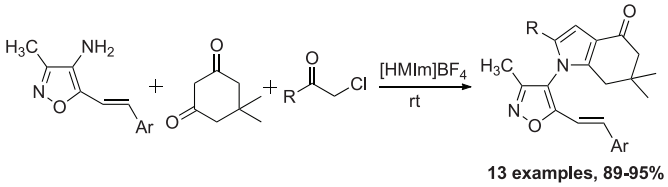
A fast and highly efficient one-pot synthesis of novel isoxazolyl pyrido[2,3-*b*][1,4]oxazin-2(3*H*)-ones *via* Smiles rearrangement using task-specific ionic liquid [HMIm]BF_4 as green solvent

A facile and convenient procedure for the synthesis of isoxazolyl pyrido[2,3-*b*][1,4]oxazin-2(3*H*)-ones *via* Smiles rearrangement from isoxazole amine, chloroacetyl chloride and 2-chloro-3-hydroxypyridine using [HMIm]BF_4 as task-specific ionic liquid has been described. The protocol proves to be an efficient and an environmentally benign in terms of high yields, eco-friendly solvent, ease of recovery, and reusability of reaction medium. (*Green Chem. Lett. Rev.*, **2017**, 10(1), 48)



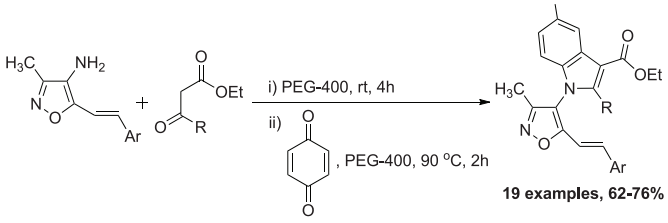
Ionic liquid mediated and promoted one-pot green synthesis of new isoxazolyl dihydro-1*H*-indol-4(5*H*)-one derivatives at ambient temperature

We report a mild, inexpensive, fast, highly efficient, and eco-friendly protocol for the synthesis of new isoxazolyl dihydro-1*H*-indol-4(5*H*)-ones by a catalyst free, one-pot three component reaction of 4-amino-3-methyl-5-styrylisoxazoles, dimedone and 2-chloroacetophenones under 1-methyl imidazolium tetraflouroborate ([HMIm]BF_4) as task-specific ionic liquid at room temperature. The important aspects of the present methodology are: use of green solvent, short reaction time, catalyst free, compatibility with wide range of substrates, ease of recovery, reusability of reaction medium and good yields. (*Cogent Chemistry*, **2017**, 3(1), 1318693)



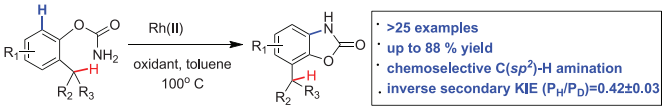
PEG-400 Mediated an Efficient Green Synthesis of Isoxazolyl Indole-3-carboxylic Acid Esters *via* Nentizescu Condensation Reaction and Their Anti-Inflammatory and Analgesic Activity

Polyethylene glycol-400 (PEG-400) has been discovered as an efficient and eco-friendly reaction medium for the synthesis of new isoxazolyl indole-3-carboxylic acid esters **11** from 4-amino-3-methyl-5-styrylisoxazoles **7**. Compounds **7** on treatment with β-keto ester **8** afforded the corresponding isoxazolylamino-2-butenoates **9** at ambient temperature in PEG-400. The Nentizescu condensation of compounds **9** with 1,4-benzoquinone **10** to give the title compounds isoxazolyl indole-3-craboxylic acid esters **11** under PEG-400. Structures of compounds **9** and **11** were established on the basis of IR, ^{1}H NMR, ^{13}C NMR and HRMS analysis. All the final compounds **11a-s** were evaluated for their anti-inflammatory and analgesic activities. Among the compounds tested, the compounds **11b**, **11g**, **11n**, **11o**, **11p and 11s** exhibited significant anti-inflammatory and potent analgesic activities as that of standard drugs. The advantages of this protocol are: operational simplicity, environmental safety, broad substrate scope, excellent functional group tolerance, and good yields. The PEG-400 can be recovered and reused. (*ChemistrySelect*, **2017**, 2(18), 5110)



Rhodium(II)-Catalyzed Undirected and Selective C(sp^2)-H Amination en Route to Benzoxazolones

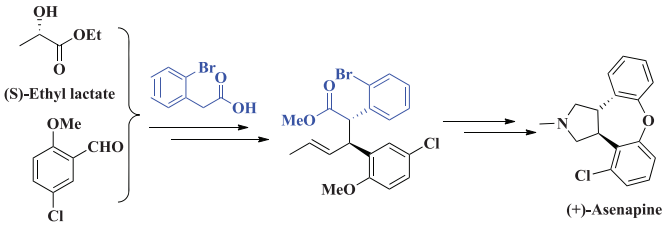
Rhodium (II) can effectively promote the activation and cyclization of arylcarbamate substrates to yield benzoxazolones via an intramolecular nitrene C—H insertion reaction. Investigation of the substrate scope show that the reaction undergoes selective aromatic C(sp^2)—H amination over more labile o-C(sp^3)—H bonds. Observation of inverse secondary KIE (P_H/P_D = 0.42±0.03) indicates involvement of aromatic electrophilic substitution mechanism for this aryl C—H amidation transformation. (*ACS Catalysis,* **2016**, 6(10), 6520)



APPLIED RESEARCH

The Ireland-Claisen rearrangement strategy towards the synthesis of the schizophrenia drug, (+)-asenapine

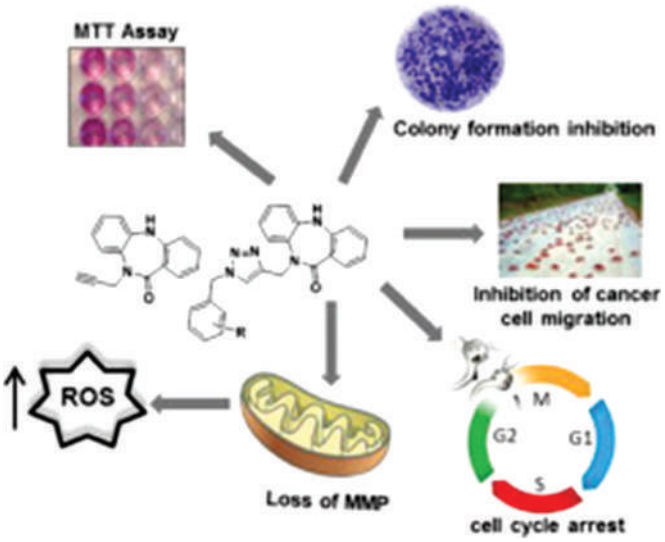
(±)-Asenapine, sold in the market as Saphris/Sycrest for the treatment of bipolar disorders, is synthesized in an optically pure form involving an Ireland–Claisen rearrangement as the key step. This approach allows access to all diastereomers. (*Org. Biomol. Chem.* **2016**, 14(4), 1332)



Synthesis and biological evaluation of 5,10-dihydro-11*H*-dibenzo[*b,e*] [1,4]diazepin-11-one structural derivatives as anti-cancer and apoptosis inducing agents

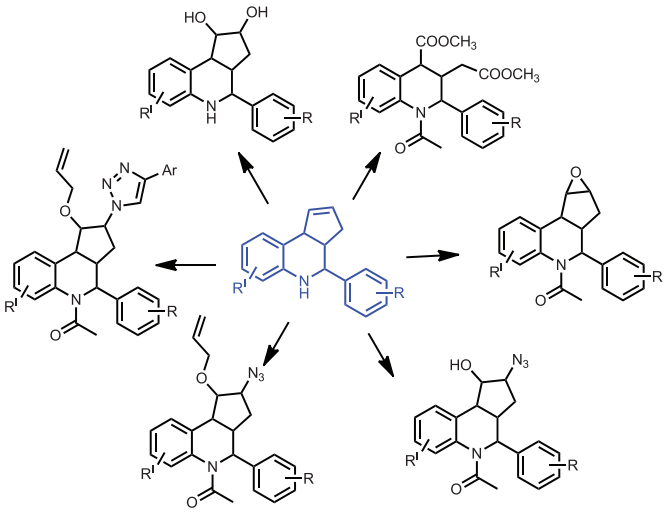
A series of thirteen 5H-dibenzo [*b,e*][1,4]diazepin-11(10*H*)-one structural derivatives has been synthesized and evaluated for anti-proliferative activity against five human cancer cell lines. Compound 9a exhibited potent tumour growth inhibition in all cell lines with IC_{50} values in the range of 0.71-7.29 µM. Experiments on lung (A549) and breast (MDAMB-231) cancer cell lines to investigate the mechanisms of growth inhibition and apoptosis inducing effects of 9a showed that it arrested both cancer cell lines in the G2/M phase of cell cycle in a dose dependent manner. Hoechst staining analysis revealed that 9a inhibited tumour cell proliferation through

apoptosis induction. Additionally, the mitochondrial membrane potential was affected and the levels of reactive oxygen species (ROS) were raised. The simple synthetic preparation and their biological properties make these dibenzodiazepinone-triazole scaffolds promising new entities for the development of cancer therapeutics. (*Eur. J. Med. Chem.* **2016**, 108, 674)



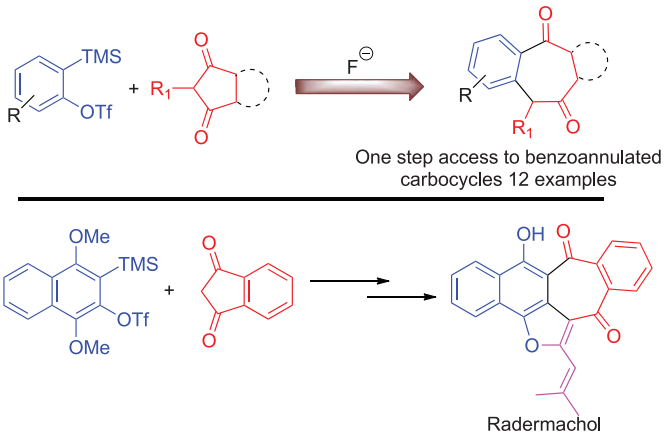
Expanding the tetrahydroquinoline pharmacophore

Tetrahydroquinoline is a privileged scaffold with a large number of biological applications. The tetrahydroquinoline pharmacophore has been expanded to yield 34 compounds. Biological screening of these compounds led to the identification of tetrahydroquinoline as neurotropic agents not reported earlier. (*Bioorg. Med. Chem. Lett.*, **2017**, 27(8), 1714)



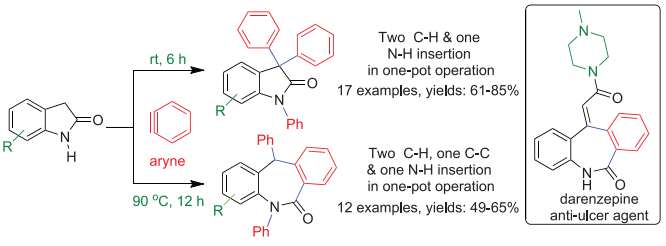
Versatile Route to Benzoannulated Medium-Ring Carbocycles via Aryne Insertion into Cyclic 1,3-Diketones: Application to a Synthesis of Radermachol

A general approach involving the insertion of *in situ* generated aryne into the C–C bond of cyclic 1,3-diketones for rapidly assembling functionalized benzo-fused medium ring carbocycles is delineated. The efficacy of the methodology has been demonstrated through a concise total synthesis of pentacyclic natural product radermachol. (*Org. Lett.*, **2016**, 18(12), 2832)



Multiple Aryne Insertions into Oxindoles: Synthesis of Bioactive 3,3-Diarylated Oxindoles and Dibenzo[b,e]azepin-6-ones

An aryne insertion cascade reaction on oxindoles has been observed and constitutes a convenient 'one pot' preparation of bioactive di- and tri-arylated oxindoles in good yields under mild conditions. A temperature controlled 'reaction switch' enables ready access to dibenzo[b,e]azepin-6-one derivatives employing the same reaction regime. This tactic has been extended to a short synthesis of potent anti-ulcer agent darenzepine. (*Org. Lett.*, **2016**, 18(23), 6184)

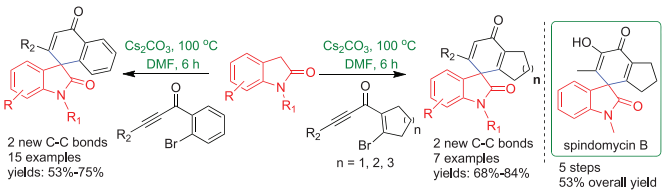


A 2-oxa-spiro[5.4]decane scaffold displays neurotrophic, neurogenic and anti-neurotrophic, neurogenic and anti-neuroinflammatory activities with high potential for development as a versatile CNS therapeutic

After our recent discovery of a new scaffold exhibiting significant neurotrophic and neurogenic activities, a structurally tweaked analogue, embodying a 2-oxa-spiro [5.4]decane framework, has been conceptualised and found to be more potent and versatile. It exhibits enhanced neurotrophic and neurogenic action in *in vitro*, *ex vivo* and *in vivo* models and also shows robust neuroprotection in mouse acute cerebral stroke model. The observed attributes are traceable to the predominant activation of the TrkB-PI3K-AKT-CREB pathway. In addition, it also exhibits remarkable anti-neuroinflammatory activity by concurrently down-regulating pro-inflammatory cytokines IL-1α and IL-6, thereby providing a unique molecule with a trinity of neuroactivities, i.e. neurotrophic, neurogenic and anti-inflammatory. The new chemical entity disclosed here has the potential to be advanced as a versatile therapeutic molecule to treat stroke, depression, and possibly other neuropsychiatric disorders associated with attenuated neurotrophic/ neurogenic activity, together with heightened neuroinflammation. (*Scientific Reports,* **2017**, Art no.149)

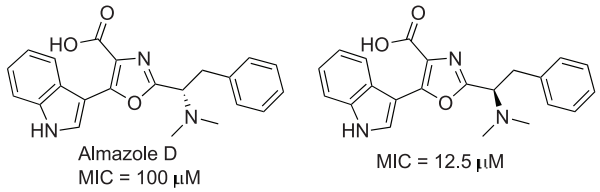
Stitching Oxindoles and Ynones in a Domino Process: Access to Spirooxindoles and Application to a Short Synthesis of Spindomycin B

A general, transition-metal-free, one-pot, domino Michael-SNAr or AdNE substitution protocol has been devised for the spiroannulation of oxindoles with ortho-bromoaryl ynones, β-bromoalkenyl ynones and β-bromoalkenyl enones in a convenient and efficient manner. As an application, a short synthesis of tetracyclic alkaloid spindomycin B has been accomplished. (*Org. Lett.,* **2017**, 19(22), 6152)



A facile synthesis and antituberculosis properties of almazole D and its enantiomer

An efficient route for the synthesis of almazole D has been developed using oxidative cyclization as a key step. This approach is successfully applied to the first synthesis of almazole D enantiomer. (*R*)-almazole D and synthesized intermediates showed potent inhibition of *Mycobacterium tuberculosis*. This hybrid 5-(3-indolyl) oxazole scaffold has drug like properties and is a good starting point for further exploration in antituberculosis drug discovery. (*ChemistrySelect,* **2017**, 2(3), 1250)



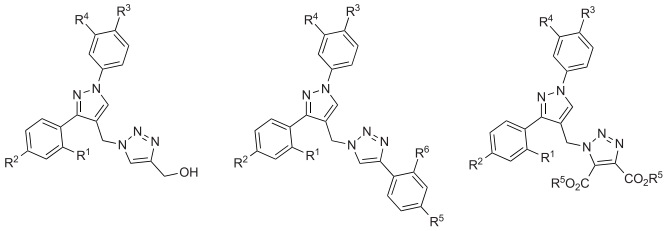
Minimum inhibitory concentration (MIC) against *M. tuberculosis* H37Rv

Chain-length-specific anti-Candida activity of cationic lipo-oxazoles: a new class of quaternary ammonium compounds

Candida species have become resistant to commonly used anti-fungal drugs like fluconazole and echinocandins. In our screen, a series of quaternary ammonium compounds (QACs) emerged as an alternative treatment choice for drug-resistant Candida infections. Medium alkyl chain cationic lipo-oxazoles comprising six to thirteen twin carbon chains and a quaternary ammonium unit were synthesized and evaluated for their in vitro anti-Candida and biofilm inhibition activity. SEM was performed to visualize membrane distortion.Results/Key findings. Heptyl and octyl chain analogues showed promising anti-fungal activity. Compound with octyl chain was active against both fluconazole-sensitive and resistant clinical isolates of Candida albicans as well as non-albicans Candida strains. It also inhibited the adhesion of C. albicans cells to a polystyrene surface and restricted biofilm formation. SEM further confirmed Candida cell membrane distortion. A novel class of QACs, called cationic lipo-oxazoles, was tested and found to exhibit anti-fungal activity against planktonic cells as well as biofilms of Candida. (*J. Med. Microbiol.*, **2017,** 66(12), 1706)

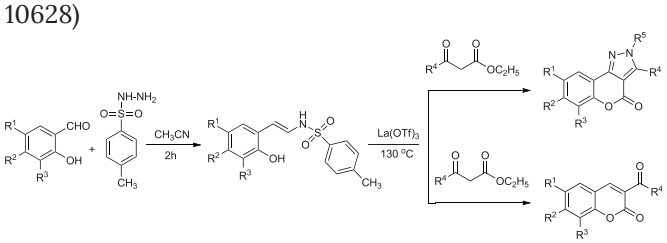
Synthesis, pharmacological activities and molecular docking studies of pyrazolyltriazoles as anti-bacterial and anti-inflammatory agents

A series of novel pyrazolyl alcohols, pyrazolyl azides, and pyrazolyltriazoles were prepared and evaluated for their bioactivity (anti-bacterial and anti-inflammatory) profile. The compound displayed the potent anti-bacterial activity against *Micrococcus luteus* (MIC 3.9 and MBC 7.81 µg/mL). *In vitro* anti- inflammatory activity data denoted that compound is effective among the tested compounds against IL-6 (IC_{50} 6.23 µM). Docking analysis of compounds and displayed high binding energies for the compounds and towards TNF-α dimer (2AZ5 protein) and IL-6 (1ALU protein). *In vivo* anti-inflammatory activity of compounds and with respect to LPS induced mice model indicated that compound showed significant reduction in TNF-α. (*Bioorg. Med. Chem.*, **2017**, 25(20), 5678)



Neoteric Synthesis and Biological Activities of Chromenopyrazolones, Tosylchromenopyrazolones, Benzoylcoumarins

Chromenopyrazolones, tosylchromenopyrazolones and benzoylcoumarins were prepared by the reaction of salicylaldehyde tosylhydrazones with 3-oxobutanoates. The title compounds were screened for their *in vitro* anti-microbial, DPPH, $ABTS^{\cdot+}$ free radical scavenging, α-glucosidase inhibitory and anti-inflammatory activities. The bioactivity profile studies revealed that the trifluoromethyl chromenopyrazolones were effective for anti-microbial activity. Trifluoromethyl chromenopyrazolones, tosyl chromenopyrazolones and benzoylcoumarin are the promising α-glucosidase inhibitors. The methyl chromenopyrazolones, trifluoromethyl chromenopyrazolones, tosylchromenopyrazolone and methoxy benzoylcoumarin denoted promising anti-inflammatory activity. (*ChemistrySelect*, **2017**, 2(32), 10628)



Anti-proliferative and antioxidant activities of 1-methoxy-3-methyl-8-hydroxy-anthraquinone, a hydroxyanthraquinoid extrolite produced by *Amycolatopsis thermoflava* strain SFMA-103

An actinobacterium isolated from sunflower rhizosphere soil sample was identified as *Amycolatopsis thermoflava* strain SFMA-103. The pigmented secondary metabolite was purified by silica gel column chromatography using methanol-chloroform solvent system. Structural elucidation studies based on 1D and 2D-NMR, FT-IR, and MS analyses confirmed the structure as 1-methoxy-3-methyl-8-hydroxy-anthraquinone. It showed significant *in vitro* anticancer activity against lung cancer and lymphoblastic leukemia cells with IC_{50} values of 10.3 and 16.98 µM, respectively. In addition, the anthraquinone showed good free radical scavenging activity by DPPH method with EC_{50} value of 18.2 µg/mL. It also showed other promising superoxide radical scavenging, nitric oxide radical scavenging and inhibition of lipid peroxidation activities. This is a first report of antiproliferative and antioxidant activities of 1-methoxy-3-methyl-8-hydroxy-anthraquinone isolated from *A. thermoflava* strain SFMA-103. (*Microbiol. Biotechnol. Lett.*, **2017**, 45(3), 200)

Phenazine-1-carboxamide, an extrolite produced by *Pseudomonas aeruginosa* strain CGK-KS-1 isolated from Ladakh, India and its evaluation against various *Xanthomonas* species.

Pseudomonas aeruginosa strain CGK-KS-1, produced a major bioactive metabolite which was purified and structurally elucidated as phenazine-1-carboxamide (PCN) based on ^{1}H and ^{13}C NMR, FT-IR, EI-HR-MS and 2D NMR spectroscopic techniques. PCN exhibited antimicrobial activity (MIC values: 1.9–3.9 µg/mL) against various bacterial pathogens and *Xanthomonas* species. PCN showed anti-biofilm property (IC_{50} values: 17.04 to 60.7 µM) against different test pathogens. *In silico* docking studies showed that PCN strongly interacted with various proteins of different *Xanthomonas* spp. with high binding energies. The extrolite from *P. aeruginosa* strain CGK-KS-1 showed promising bioactivities and could be a potential candidate for various biocontrol strategies. (*Microbiol. Biotechnol. Lett.*, **2017**, 45(3), 209)

Design, synthesis and biological evaluation of novel pyrazolochalcones as potential modulators of PI3K/Akt/mTOR pathway and inducers of apoptosis in breast cancer cells

Phosphatidyl-inositol-3-kinases (PI3Ks) are a family of lipid kinases involved in a number of cellular processes including cell growth, proliferation, nutrient uptake, differentiation, motility, survival, and intracellular trafficking. There is significant evidence that the PI3K/Akt/mTOR pathway is crucial for the survival of many human cancer cells and regulates cell metabolism as well as proliferation. Forty pyrazolochalcone conjugates were synthesized and explored for cytotoxic activity against a panel of sixty cancer cell lines. Among the series, 15 conjugates showed excellent growth inhibition (GI_{50} for MCF-7: 0.4-20 mM). Some promising candidates induced cell cycle arrest, mitochondrial membrane depolarization and apoptosis in MCF-7 cells at 2 mM concentration. Furthermore, the inhibition of PI3K/Akt/mTOR pathway-regulators such as PI3K, p-PI3K, p-AKT, and mTOR were observed; as well as upregulation of p-GSK3β and tumor-suppressor protein, PTEN. The study indicated that pyrazolochalcone conjugates could serve as potential leads in the development of tailored cancer therapeutics. (*Eur. J. Med. Chem.*, **2017**, 139, 305)

US-India Consortium for Development of Sustainable Advanced Lignocellulosic Biofuel Systems

Sorghum and pearl millet were evaluated as lignocellulosic feedstocks. Size reduction by mechanical commutation was adopting for conducting pretreatment experiments. After initial evaluation of different pretreatment methodologies and based on the generated data, the alkaline peroxide pretreatment process was evaluated at length for its effectiveness at both lab and bench scale. The developed pretreatment process was simple, with very low dosage of chemical input and high solid loading (20%), coupled with simple operating conditions, such as atmospheric pressure, normal temperature (40-50 °C) and a reaction time of 3-4 hours with recycling and reuse of 100% treated water. The developed pretreatment process was also evaluated for its suitability towards different lignocellulosic biomass materials (approx. 10-12 varieties - sorghum, pearl millet, maize, wheat and rice straw) at 3-5 Kg batch levels and data indicated that this process could be effectively used for multiple biomasses either individually or in combination. The pretreated biomass was further evaluated for its saccharification efficiency, wherein, it effectively underwent saccharification with commercial enzymes at 45-50 °C and pH 5.0-5.5. The conversions were found to be around 65-70% within 6-8 h or more than 80% within 18-24 h, with selected saccharification enzyme preparations. The hydrolysate containing sugars (glucose and xylose) was evaluated for bioethanol production using selected *Saccharomyces cerevisiae* strain. (*The overall developed process was demonstrated to the industrial partner, Hindustan Petroleum Corporation Limited, Bengaluru.)*

Synthesis of Triazole Derivatives of 9-Ethyl-9H-carbazole and Dibenzo[b,d]furan and Evaluation of Their Antimycobacterial and Immunomodulatory Activity

Disubstituted 1,2,3-triazole derivatives of 9-ethyl-9H-carbazole and dibenzo[b,d]furan were synthesized by the Huisgen's 1,3-dipolar cycloaddition reaction between azides and terminal alkynes. The synthesized derivatives 7d, 8a, 8b, 9e, and 10c exhibited good MIC values, especially against Mycobacterium smegmatis and these compounds were further evaluated for their immunomodulatory activity. Majority of the compounds exhibited no toxicity on splenocytes and macrophages and the compounds 8a and 8b are proved as induced proliferator. These compounds have shown decreased production of TNF-α from LPS stimulated RAW 264.7 cells and among all these compounds, 7d has shown significant inhibition of TNF-α production. Molecular docking studies into the active site of mycobacterial DprE1 enzyme helped to establish a structural basis for inhibition of Mycobacterium tuberculosis and understand the type of ligand-protein interactions governing the binding affinity. (*ChemistrySelect*, **2017**, 2(24), 7309)

Synthesis of a new class of glycolipids and the evaluation of their immunogenicity using murine splenocytes

A new class of glycolipids were generated by the incorporation of lipid entities at the C-6 position of D-glucose through oxidation of the primary hydroxyl group of tetrabenzylated D-glucose to form corresponding aldehyde, which in turn was subjected to Grignard reaction with C8 and C16 alkyl magnesium halides. The resulting lipidated secondary alcohol

was further subjected to esterification with long-chain carboxylic acids to afford novel glycolipids. All of the derivatives 4a–b, 6a–d, and 8a–b exhibited low cytotoxicity and induced strong T and B cell proliferation and IL-2, IL-4, and IFN-γ expression from stimulated splenocyte culture, signifying their potent immunostimulating activity. (*Carbohydr. Chem.,* **2016**, 35(6), 1)

Design and synthesis of ring C opened analogues of α-santonin as potential anticancer agents

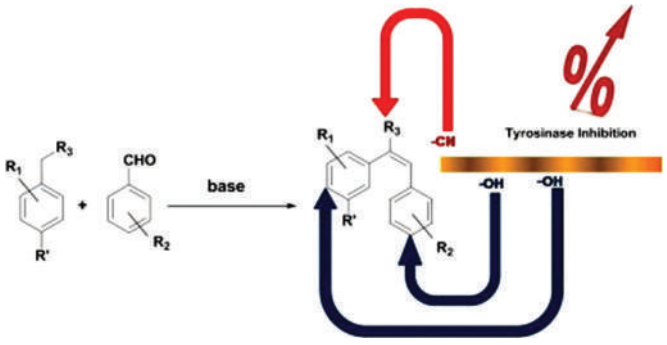
Here we describe ring opening reaction of a novel halo triene derivative viz., (3S, 5aS)-8-chloro-3a, 4, 5, 5a-tetrahydro-3, 5a, 9-trimethylnaphtho [1, 2-b] furan-2(3H)-one of α-santonin upon nucleophillic attack with alcohols. Halo-triene was synthesized from α-santonin upon reaction with vilsmeier reagent. The synthesized compounds from ring opening reaction were evaluated for anticancer activity against a panel of four human cancer cell lines (A-549, THP-1, HCT-15, and IMR-13). Most of the compounds exhibited promising anticancer activity against all cancer cells in vitro; however compound. 3d with benzyl substitution showed most potent anticancer activity with an IC50 value of 0.3, 0.51, 0.6 and 0.23 μM against A-549, THP-1, HCT-116 and IMR-13 cell lines respectively. (*Med. Chem. Res.*, **2016**, 25(9), 2030)

Synthesis and immunopotentiating activity of novel isoxazoline functionalized coumarins

A novel series (13) of isoxazoline functionalized coumarins was synthesized through 1,3-dipolar cyclization of nitrile oxides with Allylated coumarins. Synthesis of effective and target selective immunostimulators through conjugation of diversely substituted isoxazolines and 7-hydroxycoumarins is the focus of the present article. The proposed synthetic scheme was observed to be highly regiospecific yielding attempted conjugates in good yield (>90%). Kinetic resolution of the racemates was carried out by employing lipase B from Candida antarctica (CALB). The synthesized compounds were screened in vitro and in vivo for their biological activities viz. toxicity and impact on splenocyte proliferation (T- and B-cell proliferation), antibody production (HA titre), delayed-type hypersensitivity reaction (DTH), T-cell subtypes (CD4 and CD8), cytokine production (IL-2, IFN-γ, and IL-4) and NO (macrophage) production. Our results establish that isoxazoline functionalized coumarins exhibit excellent immune potentiating activity especially compounds 2, 4 and 8 whose activity is more than that of Levimasole as standard. The structure activity relations are explained in light of the structural/functional aspects of tested compounds. To the best of our knowledge the presented work is first of its kind and is presaged to prove very useful for the design and synthesis of bis-heterocycle based novel, therapeutically selective and effective immunopotentiators. (*Eur. J. Med. Chem.*, **2016**, 123, 90)

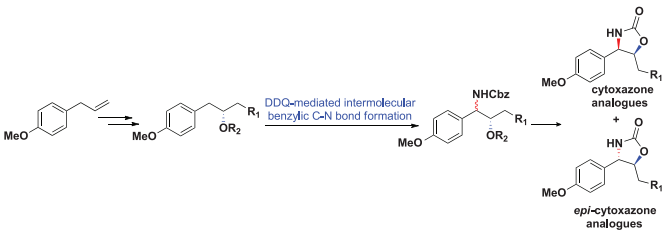
Synthesis and Tyrosinase Inhibition activity of trans-Stilbene Derivatives

Synthesis of a focussed library of trans-stilbene compounds through Wittig and other base catalysed condensation reactions is presented. The synthesized stilbenes were screened for their inhibitory potential against murine tyrosinase activity to explore the structure activity relationship (SAR). Presence of electron withdrawing group (-CN) at the double bond and hydroxyl group or halogen atom especially at para-position on the aromatic rings was found to significantly elevate the inhibitory activity. Among all the compounds screened, compounds 2, 6, 8, 10, 11, 15 and 21 were found to exhibit appreciable inhibitory activity. Compound 21 ((E)-2,3-bis(4-Hydroxyphenyl)acryonitrile) was found to be the most active with an IC50 value of 5.06μM which is less than half of the value 10.78μM observed for resveratrol (common standard used in murine tyrosinase activity studies) under similar conditions. The results obtained from the present study reveal structural/functional group sensitivity for the tyrosinase inhibitory activity of stilbenoid moieties and are expected to be very helpful for the design and synthesis of novel, selective and effective tyrosinase inhibitors. (*Bioorg. Chem.*, **2016**, 64, 97)



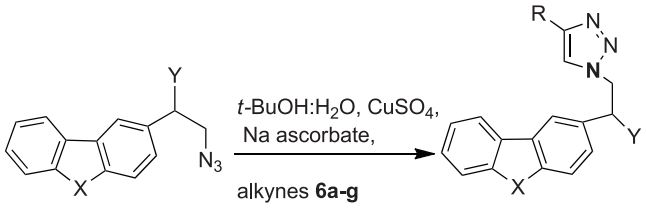
DDQ-Mediated Stereoselective Intermolecular Benzylic C–N Bond Formation: Synthesis of (-)-Cytoxazone, (-)-4-*epi*-Cytoxazone and their Analogues and Immunological Evaluation of their Cytokine Modulating Activity

A short and efficient strategy for the synthesis of (-)-cytoxazone, (-)-4-*epi*-cyoxazone and their analogues by using DDQ mediated diastereoselective intermolecular benzylic amination has been described. Immunological evaluation of their cytokine modulating activity revealed that the change of hydroxy methyl to methyl group increased the cellular immunity in *in-vitro* cultures. Changes in the stereochemistry of oxazolidine haven't influenced the biological activity. (*Tetrahedron,* **2017,** 73(11), 1473)



Synthesis of Triazole Derivatives of 9-Ethyl-9H-carbazole and Dibenzo [*b, d*] furan and Evaluation of Their Antimycobacterial and Immunomodulatory Activity

1,4-Disubstituted 1,2,3-triazole derivatives of 9-ethyl-9H-carbazole and dibenzo[b,d]furan were synthesized by the Huisgen's 1,3-dipolar cycloaddition reaction between azides and terminal alkynes. Molecular docking studies into the active site of mycobacterial DprE1 enzyme helped to establish a structural basis for inhibition of *Mycobacterium tuberculosis* and understand the type of ligand-protein interactions governing the binding affinity. (*ChemistrySelect,* **2017,** 2(24), 7309)

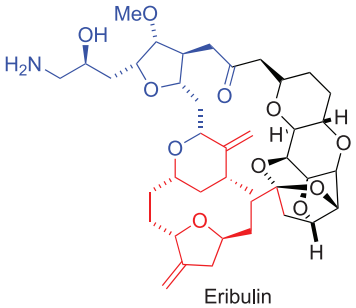


X=NEt, Y=Me
X=NEt, Y=Ph
X=O, Y=Me
X=O, Y=Ph

X=NEt, Y=Me, R= **6a-g**
X=NEt, Y=Ph, R= **6a-g**
X=O, Y=Me, R= **6a-g**
X=O, Y=Ph, R= **6a-g**

Process development for Eribulin

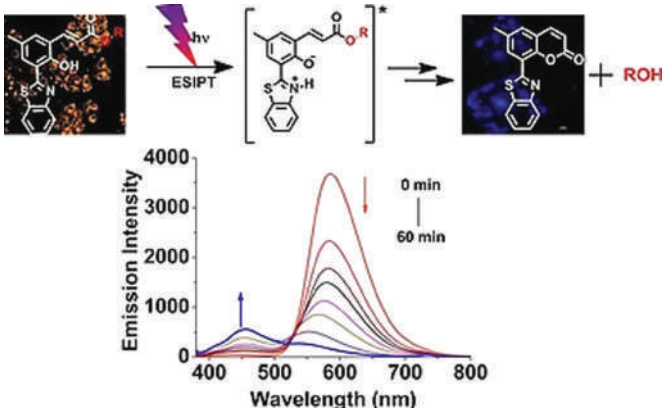
Eribulin is very important drug for the treatment of cancer and synthesis of this molecule in large scale is necessary to serve the market demand. Although, presently there is an approach for its synthesis, development of novel, economically viable non-infringing efficient synthetic processes are highly desirable. During this period this project has been taken up with the following objectives. Novel route has been developed for three key fragments required for the synthesis of Eribulin in less number of steps. The process will be optimized in 100g scale, which will be further developed for Kilogram scale. The total requirement for the country is less than five-kilograms. We have accomplished the synthesis of precursor for Eribulin and synthesis of final target molecule is in progress.



Eribulin

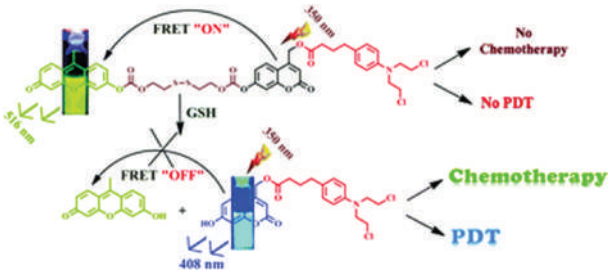
ESIPT-induced fluorescent *o*-hydroxycinnamate: a self-monitoring phototrigger for prompt image-guided uncaging of alcohols

We have developed a new fluorescent *o*-Hydroxycinnamate derived drug delivery system (DDS) which can serve as the self-monitoring phototrigger for prompt image-guided uncaging of drugs with alcohol functionality. (*Org. Biomol. Chem.*, **2017**, 15(40), 8544)



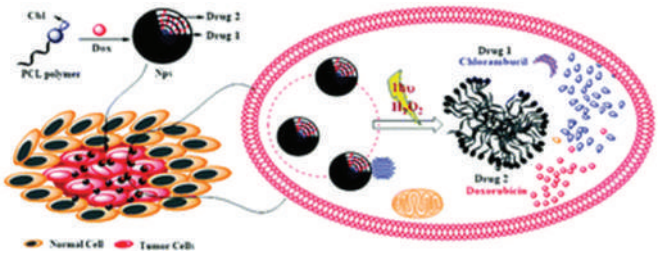
Redox-responsive xanthene–coumarin–chlorambucil-based FRET-guided theranostics for "activatable" combination therapy with real-time monitoring

A FRET donor–acceptor xanthene–coumarin conjugate has been designed for redox-regulated synergic treatment of photodynamic therapy and chemotherapy with real-time monitoring. The "locked" FRET pair was selectively "unlocked" by biological reducing thiols *via* rupture of a sacrificial disulfide linker. A distinct change in fluorescence color and selective cancer cell toxicity were observed *in vitro*. (*Chem. Commun.,* **2017**, 53(65), 9109)



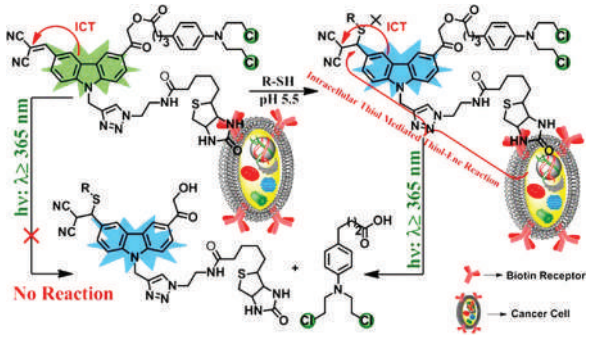
Coumarin polycaprolactone polymeric nanoparticles: light and tumor microenvironment activated cocktail drug delivery

Highly sensitive hypoxia (H_2O_2)-activated photoresponsive polymeric nanoparticles for cocktail delivery of anticancer drugs doxorubicin (Dox) and chlorambucil (Cbl) were developed. The photoresponsive polymer conjugate was constructed by ring-opening polymerization (ROP) of caprolactone (as the tail) with 7-hydroxycoumarin chlorambucil (as the head). During nanoprecipitation, the polycaprolactone chain wrapped around the hydrophobic core (coumarin chlorambucil) to form a "shell". Interestingly, the polycaprolactone-tagged coumarin-chlorambucil (PCL-CC) NPs provided sufficient space for co-encapsulation of another hydrophobic anticancer drug Dox with a loading efficiency of 13 wt%. The controlled release of Dox and Cbl from Dox–PCL-CC NPs was investigated under three different conditions: (i) in the presence of H_2O_2 (tumor microenvironment), (ii) photoirradiation using UV light of ≥365 nm for 60 min, and (iii) photoirradiation using UV light of ≥365 nm for 15 min in the presence of H_2O_2. Results showed that photoirradiation in the presence of H_2O_2 results in generation of reactive oxygen species (HOO–, OH–), which assist hydrolysis of the ester group in the polymeric backbone of Dox–PCL-CC NPs and UV irradiation leads to cleavage of the coumarin-chlorambucil ester linkage, leading to burst release of Dox and Cbl. The drug release profile from the NPs under three different conditions was monitored by different instrumental techniques, *e.g.* emission spectroscopy, MALDI-Tof mass spectrometry, DLS and HPLC analysis. *In vitro* biological studies revealed that the present system can efficiently deliver the cocktail anticancer drugs with full control over release into the tumor cells by means of H_2O_2 and light activation. (*J. Mater. Chem.* B, **2017**, 5(9), 1734)



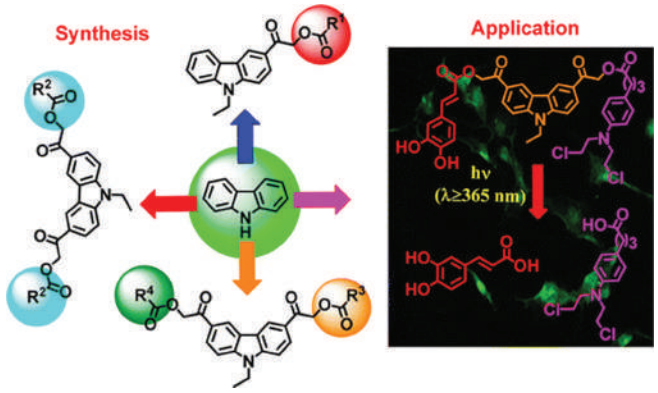
Three-Arm, Biotin-Tagged Carbazole–Dicyanovinyl–Chlorambucil Conjugate: Simultaneous Tumor Targeting, Sensing, and Photoresponsive Anticancer Drug Delivery

The design, synthesis, and in vitro biological studies of a biotin–carbazole–dicyanovinyl–chlorambucil conjugate (Bio-CBZ-DCV-CBL; **6**) are reported. This conjugate (**6**) is a multifunctional single-molecule appliance composed of a thiol-sensor DCV functionality, a CBZ-derived phototrigger as well as fluorescent reporter, and CBL as the anticancer drug, and Bio as the cancer-targeting ligand. In conjugate **6**, the DCV bond undergoes a thiol–ene click reaction at pH<7 with intracellular thiols, thereby shutting down internal charge transfer between the donor CBZ and acceptor DCV units, resulting in a change of the fluorescence color from green to blue, and thereby, sensing the tumor microenvironment. Subsequent photoirradiation results in release of the anticancer drug CBL in a controlled manner. (*Chem. Asian J.,* **2016**, 11(24), 3482)



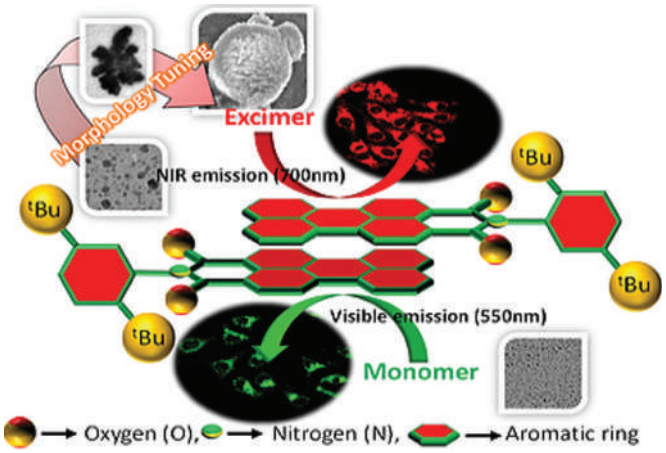
Photocaging of Single and Dual (Similar or Different) Carboxylic and Amino Acids by Acetyl Carbazole and its Application as Dual Drug Delivery in Cancer Therapy

A new fluorescent photoremovable protecting group (FPRPG) based on acetylcarbazole framework has been explored for the first time release of single and dual (similar or different) substrates from single chromophore. Mechanistic studies of the photorelease process revealed that photorelease of two (similar or different) substrates from acetyl carbazole proceeds via a stepwise pathway. Further, we constructed photoresponsive dual drug delivery system (DDS) to release two different anticancer drugs (caffeic acid and chlorambucil, 1 equiv each). In vitro study reveals that our DDS exhibit excellent properties like biocompatibility, cellular uptake, and photoregulated dual drug release. (*J. Org. Chem.*, **2016**, 81, 11168)



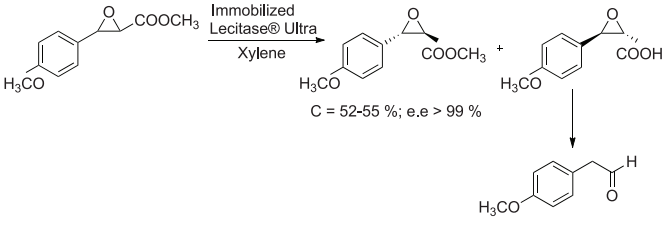
Morphology Tuning of Self-Assembled Perylene Monoimide from Nanoparticles to Colloidosomes with Enhanced Excimeric NIR Emission for Bioimaging

We have demonstrated an aggregation induced excimeric NIR emission in aqueous media from a suitably substituted perylene monoimide (PeIm) dye. Controlled entrapment of the dye into pluronic F127 micellar system to preserve its monomeric green emission in aqueous media was also established. The aggregation process of the PeIm dye to form organic nanoparticles (NPs) was evaluated experimentally by the means of transmission electron microscope. Tuning the morphology along with the formation of colloidosomes by the controlled self-aggregation of PeIm NPs in aqueous suspension was demonstrated successfully. Finally, both excimeric and monomeric emissive PeIm NPs as well as PeIm colloidosomes were employed for the bioimaging *in vitro*. (*ACS Appl. Mater. Inter.*, **2016**, 8(30, 2336)

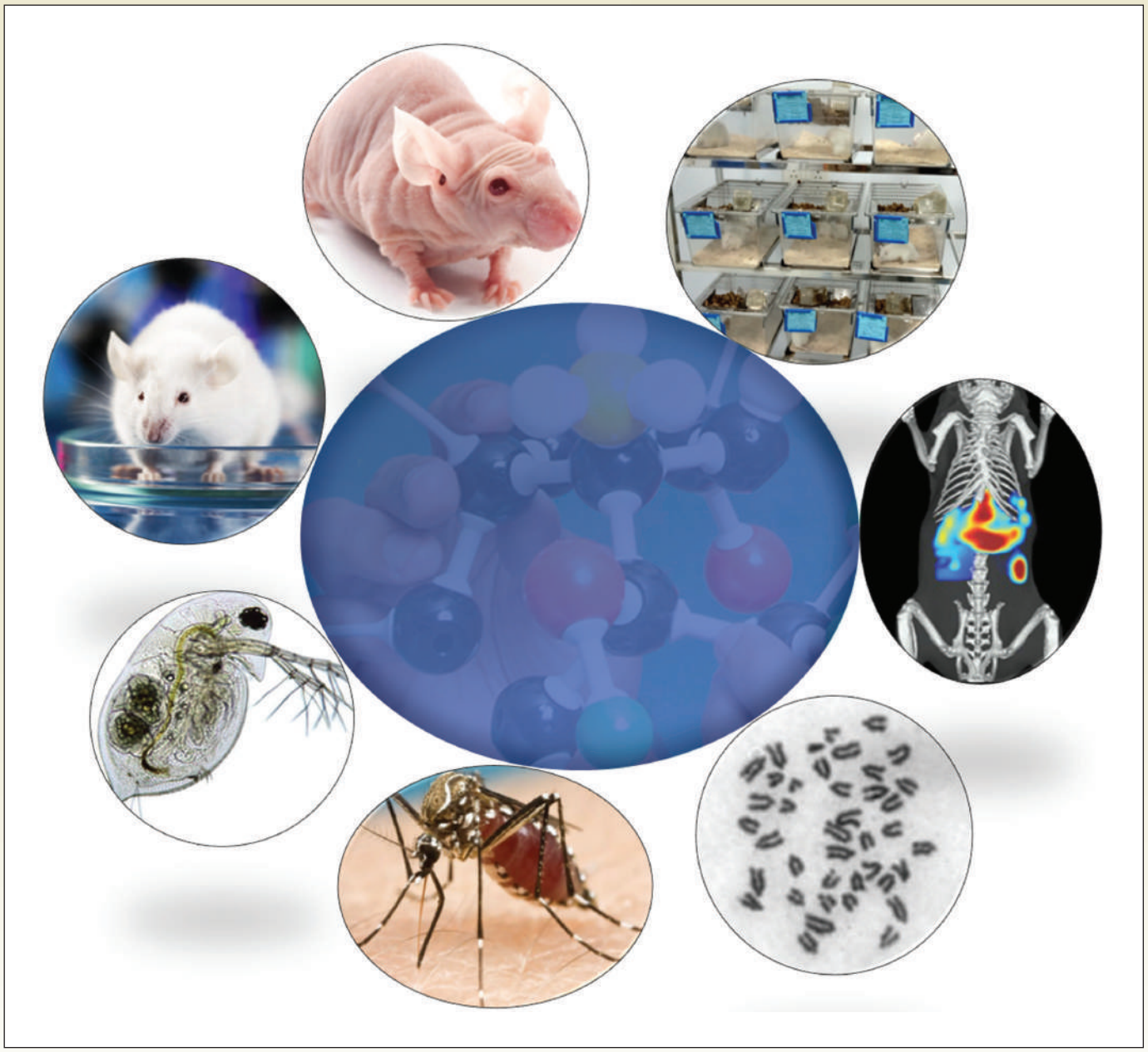


Immobilization of Lecitase® Ultra on recyclable polymer support: Application in resolution of *trans*-methyl (4-methoxyphenyl)glycidate in organic solvents

Immobilization of Lecitase® Ultra on recyclable polymer support was studied. Immobilization of the enzyme in PEI-Coated polymer matrix leads to a marginal improvement in the enzyme stability and enantioselectivity for the glycidate ester resolution. The resolution of methyl *trans*-(±)-3-(4-methoxyphenyl) glycidate in organic solvent (*e.e* > 99 %, conversion 50 %) was studied with additional advantage that the immobilized enzyme is not inhibited by the aldehyde (4-methoxy phenyl acetaldehyde) produced during hydrolysis. The immobilized enzyme is sufficiently hydrophobic to work efficiently in an organic phase and at the same time it is able to hold water, enough to carry out hydrolysis of the ester and it can be recyclable several times. *(Tetrahedron:Asymm.,* **2017,** 28(11)**,** 1612)



PHARMACOLOGY & TOXICOLOGY



Pharmacology and Toxicology Division of CSIR-IICT is actively involved in the various areas of research such as pharmacology, regulatory toxicology including genetic toxicology, entomology, mosquito borne diseases modeling, bioinformatics and microbiology.

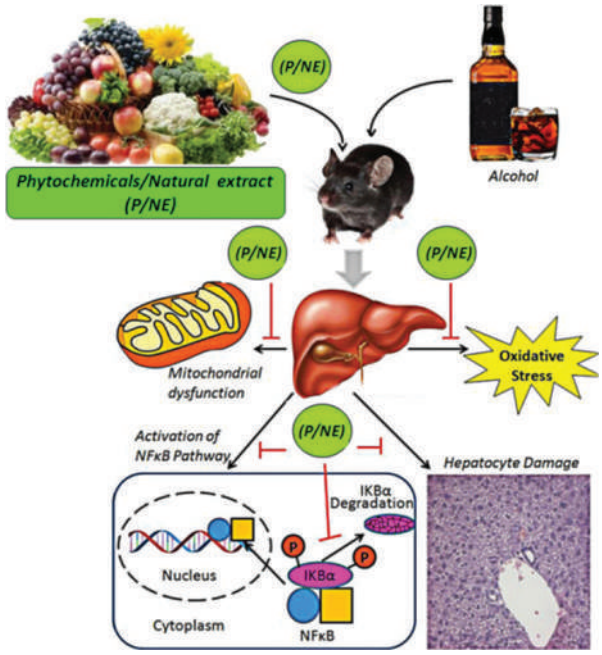
BASIC RESEARCH

Pharmacology & Drug delivery:

Pharmacology & Toxicology division focuses its research in the areas of in vitro and in vivo pharmacological evaluations, Novel Drug Delivery Systems (NDDS) and Regulatory Toxicology. The division has the expertise and is fully equipped instruments for conducting the toxicity studies on the NCEs in the drug development phase (Regulatory Toxicology). Current areas of research in the pharmacology is focused on evaluation of protective role of phytopharmaceuticals against drug induced toxicity on the vital organs such as heart, kidney and liver, various inflammatory conditions such as arthritis, inflammatory bowel disease (IBD), cancer, diabetes etc.

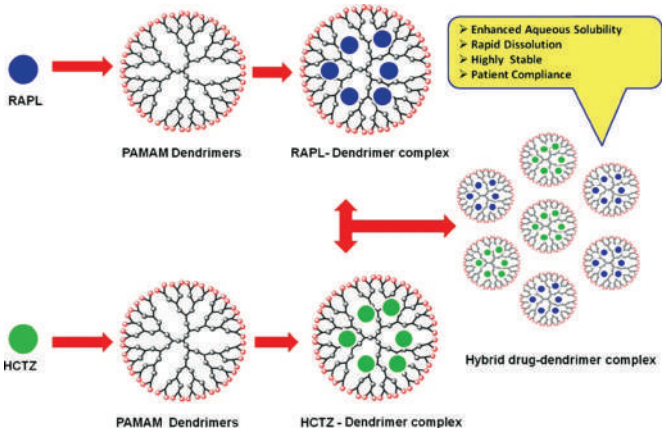
Phytochemicals/Natural Extracts against acute organ failure

Alcoholic liver disease (ALD) remains a major cause of morbidity and mortality worldwide accounting to approximately 5.9% of the deaths globally (World Health Organization). Modulation of oxidative stress and the inflammatory events represents an important strategy for protection against alcoholic liver injury. Our studies have demonstrated that phytochemicals (Fisetin, Polydatin, Capsaicin) and natural extracts (Phenolic-rich oats extract) are effective in preventing alcohol induced liver injury in mice models. IBD is a chronic condition involving inflammation of the GIT. Extracts of *Rosmarinus officinalis* L. extract (RE), were found to be an effective therapeutic food ingredient and dietary supplement for inflammatory bowel disease. Acute kidney injury (AKI) is another serious clinical syndrome that has to be addressed as complicates the course and worsens the outcome in a significant number of hospitalised patients. Our study reported that, Ferulic acid exhibits marked protective effects on AKI in mice and holds a strong potential to translate into the clinic. (*Phytomedicine*, **2017**, 27, 23; *J. Funct. Foods*, **2016**, 22, 588)



Functionalized Nano Carrier Systems for Drug Targeting

Targeting specific receptors or proteins over expressed on the abnormal cells is a major therapeutic strategy for various diseases. cRGDfK-conjugated nanoparticles [RCPN] for camptothecin and gemcetabine were synthesized with enhanced efficacy representing a new approach for improved delivery. Wheat germ agglutinin (WGA)-conjugated solid lipid nanoparticles increased the effectiveness of paclitaxel, by targeting lectin receptors. Poly (amidoamine) dendrimer-mediated hybrid formulations were synthesized for delivering combination therapy of ramipril and hydrochlorothiazide and tratuzumab. (*Mol. Pharmaceut.*, **2016,** 13(5), 1491; *Mol. Pharmaceut.*, **2016**, 13(11), 3903; *Eur. J. Pharm. Sci.*, **2017**, 96(1), 84)



Despite the development of novel therapeutics, poor drug transport, low bioavailability, poor stability, side effects, are the major problems associated. We developed various ligand coupled nanoparticle formulations, and evaluated their potential both *in vitro* and *in vivo*. Solid lipid nano-formulations for oral delivery of olmesartan medoxomil, increased its bioavailability 2.32 folds. EGCG loaded nanoparticles (EGCG-SLN), increased the stability of EGCG, and exhibited profound anticancer activities. TPNS nano-formulations increased the solubility and bio-availability of naringenin. HPβCD (hydroxyl propyl beta cyclodextrin) conjugated PLGA (poly-lactide-co-glycolic acid nanoparticles) nano particles of Fisetin, enhanced its activity and increased its bioavailability. (*Chem. Phys. Lipids*, **2016**, 198, 51; *Drug Deliv.,* **2017**, 24(1), 224)

Regulatory Toxicology including genotoxicity:

The division is actively involved in conducting acute, subchronic, chronic, and dermal toxicity studies in small rodent species employing OECD guidelines and schedule Y guidelines of Drugs & Cosmetics Act 1940. These studies are conducted for both public and private stake holders for the regulatory submissions. THe institute has state of the art animal house facility constructed based on GLP guidelines and the regulatory toxicology studies conducted in this facility.

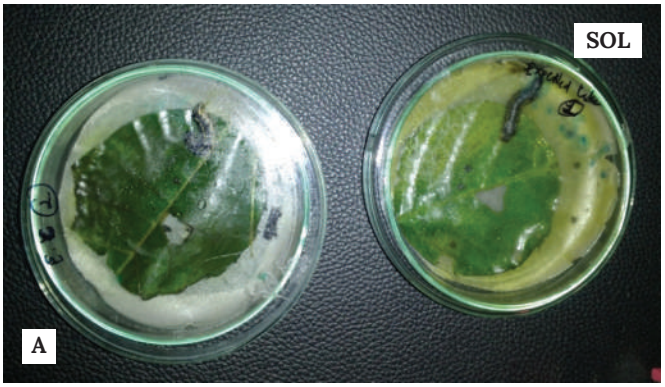
In addition the division is also involved in conducting *in vitro* and *in vivo* genotoxicity studies. Cytogenetic toxicity studies were carried out by analyzing the chromosomal aberration, mitotic index and micronucleus tests in somatic cell lines of bone marrow cells and spermatogonial, primary spermatocytes and sperm morphology assay from germ lines cells of Swiss mice.

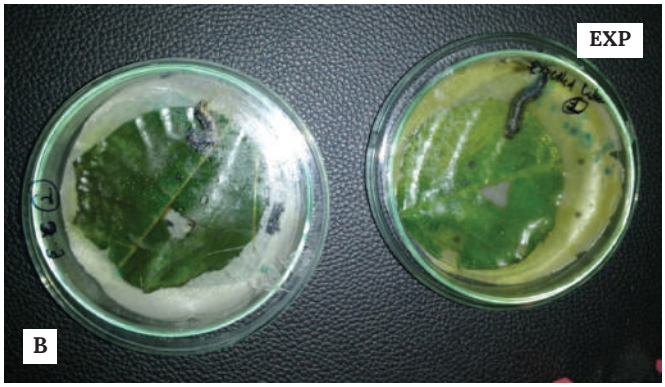
Studies on mosquitocidal and larvicidal formulations based on extracts from *Madhuca longifolia, Pongamia glabra & Ocimum tenuiflorum* L (*Funded by TRIFED, Govt. of India*)

Karanjin-rich crude extract, obtained both by solvent extraction and expelling route was taken up for evaluation. The extract from solvent extraction pathway (SOL) contained 11.11% of karanjin and the same from expelling pathway (EXP) contained 15.6% karanjin.

Mosquito larvicidal activity: Karanjin-rich crude extract, obtained both by solvent extraction and expelling route was taken up for evaluating its mosquito larvicidal activity against *Aedes aeygpti* larvae. The extract from solvent extraction pathway (SOL) contained 11.11% of karanjin and the same from expelling pathway (EXP) contained 15.6% karanjin. The larvicidal activity was performed according to the standard procedure recommended by World Health Organization (1981). Mosquito larvicidal activity of seed extract and expelled cake of Karanjia on 4th instar *A. aeygpti* after 24 hrs of exposure reveals that the karanjin-rich extract (EXP) obtained from expelled cake indicated better LC_{50} and LC_{90} values compared to the same obtained from solvent extracted cake (SOL). This result is in agreement with the content of karanjin as EXP contains 15.6% karanjin compared to 11.11% karanjin contain in SOL.

Antifeedant activity: Antifeedant activity studies, extracts from solvent extracted cake and expelled cake of karanja seed was assessed against lepidopteran agricultural pests, *S. litura*. Three different doses of both these karanjin-rich extracts were exposed *S. litura* to understand the repellent efficacy of the pest. The experiments were conducted using leaf-disc bioassay method. The leaf area consumed was measured after 24 hrs in both treated and control leaf discs using leaf area meter. In the distilled water and DMSO treated groups, larvae consumed 96.3% and 43.3% of leaf respectively. In the experimental groups, a dose dependent increase in the antifeedant index was observed. Hence from the above results, it can be concluded that extracts from both SOL and EXP possess antifeedant activity and can be used as a biocontrol against lepidopteron pests of agriculture crops.





Antifeedant activity of (A) extracts from solvent extracted cake (SOL) and (B) extracts from expelled cake (EXP)

Studies on mahua seed/flower extraction: (*Funded by TRIFED, Govt. of India*)

Madhuca longifolia flower samples were obtained from Bhadrachalm of Khammam district, Telangana. The flower samples were kept shade dried at room temperature (28±2 °C) till samples dried. The extracts from flower samples were used for various bioefficacy studies like Mosquito larvicidal activity and antimicrobial activity.

Larvicidal activity of *Madhuca longifolia* flower extracts against *Aedes albopictus* & *Culex quinquefasciatus* at 24 h post treatment. The results indicate that the percentage of mortality is higher in methanol extract in both *Culex* and *Aedes* species compared to ethyl acetate extract. Compared to *Culex* sp. larvae, larvae of *Aedes* sp. was found to be more tolerant to these extracts. The LC_{50} value at 24 h post treatment for *Culex quinquefasciatus* is 33.17 ppm and 44.60 ppm respectively for methanol and ethyl acetate extracts. In case of *Aedes albopictus*, LC_{50} value for methanol and ethyl acetate extracts is 209.20 and 236.40 ppm respectively.

Anti microbial activity: The extract with methanolic solvent has shown potential activity at different concentrations (4,6,8,10 mg/ml) against the *Escherichia coli* and *Staphylococcus epidermis* species and has no activity against the remaining four species i.e. *Bacillus subtilis*, *Staphylococcus aureaus*, *Psuedomonas aregunosia* and *Klebsilla pneumonea*. The ethyl acetate extract of mahua, on the other hand has shown potential activity at different concentrations (2, 4, 6, 8 and 10 mg/ml) against the *Bacillus subtilis* and *Psuedomonas aregunosia* species. No activity was observed against *Escherichia coli, Klebsilla pneumonia*, *Staphylococcus aureaus*, and *Staphylococcus epidermis.*

Nano-toxicology: The essence of toxicity testing is to check the toxicity and the effects it can produce. To check the effect of the test substances on laboratory animals and in understanding the possible hazards which can be extrapolated to man. Toxicology studies of various nanomaterials by oral acute and repeated dose studies were conducted to identify and generate data enabling us to understand their effects in Wistar rats.

Toxicological assessment of nano and micron-sized tungsten oxide after 28 days repeated oral administration to Wistar rats

Tungsten oxide (WO_3) nanoparticles (NPs) are being used in various applications. However, the health consequences of WO_3 NPs exposure have not been explored extensively. Hence, the goal of this study was to evaluate the toxicity of WO_3 NPs and their microparticles (MPs) after 28 days repeated oral administration in Wistar rats. The particles were characterised by transmission electron microscopy (TEM), dynamic light scattering (DLS), laser Doppler velocimetry (LDV), Brunner-Emmett-Teller (BET), X-ray diffraction (XRD), and inductively coupled plasma optical emission spectrometer (ICP-OES). Genotoxicity was determined using comet assay in blood and liver and micronucleus test in bone marrow. Biochemical parameters such as aspartate aminotransferase and alanine aminotransferase in serum and reduced glutathione content, catalase and lipid peroxidation in liver tissue were determined. Histopathological changes in tissues were documented. Biodistribution of tungsten (W) in rat's blood, urine, feces and tissues were analysed. The mean size of WO_3 NPs and MPs by TEM was 52±2.97 nm, and 5.73±7.58 µm and morphology were spherical in both the particles. DLS of NPs was 195.6 nm. XRD and BET data of WO_3 NPs and MPs showed a hexagonal and tetragonal crystal structure and surface area of 19.33 and 15.15 (m^2/g), respectively. The results revealed a significant increase in DNA damage and micronuclei, a difference in biochemical levels and histopathological alterations after exposure to 1000 mg/kg dose of WO_3 NPs. W biodistribution was detected in all the tissues in a dose and organ-dependent manner in both the particles. The highest amount of W was found in the liver and lowest in the brain of the treated rats. The tested NPs were found to have little toxicity hazard. (*Mutat. Res.,* **2017,** 819, 1)

Toxicological assessment of tungsten oxide nanoparticles in rats after acute oral exposure

Advances in and the rapid growth of the nanotechnology sector have escalated manufacture of nanoparticles (NPs), resulting in a significant increase in the probability of exposure of humans and wildlife to these materials. Many NPs have been found to exert genotoxicity. Therefore, genotoxicity studies are mandatory to assess the toxicity of NPs as a concern of succumbing to genetic diseases and cancers are universal. Tungsten oxide (WO3) NPs are being explored extensively in various fields. However, the toxicological data of WO3 NPs by oral route in mammals is limited. Hence, the goal of the current investigation was to evaluate the acute toxicity of WO3 NPs and microparticles (MPs) after single oral administration with 100, 500 and 1000 mg/kg bw doses in female Wistar rats. TEM, DLS and LDV techniques were used to characterise the particles. The genotoxicity studies were conducted using comet, micronucleus and chromosomal aberration assays. Alterations in biochemical indices and metal distribution in various organs were also evaluated. The mean size of WO3 NPs and MPs by TEM was 53.2±1.91 nm and 5.17±3.18 µm, respectively. The results revealed a significant increase in DNA damage, micronuclei and chromosomal aberrations after exposure to 1000 mg/kg dose of WO3 NPs. Significant alterations in aspartate transaminase, alanine transaminase, reduced glutathione, catalase and malondialdehyde levels in serum and liver were found only at the higher dose of WO3 NPs. Tungsten (W) biodistribution was observed in all the tissues in a dose, time and organ-dependent manner. In addition, the maximum concentration of W was found in the liver and the least in the brain was observed. The test substances were found to have a relatively low acute toxicity hazard. The data obtained gives preliminary information on the potential toxicity of WO3 NPs and MPs. (*Environ. Sci. Pollut. Res. Int.,* **2017**; 24(15), 13576)

Iodine catalyzed simple and efficient synthesis of antiproliferative 2-pyridones

A simple and efficient method for the selective synthesis of 2-pyrdones from 4H-pyrans using iodine as catalyst and ethanol as solvent was developed. The present method is equally effective for both aromatic and hetero aromatic ring containing 4H-pyrans. The compatibility with various functional groups, mild reaction conditions, high yields and application of inexpensive, readily and easily available iodine as catalyst and formation of 2-pyridones as major products are the advantages of the present procedure. In vitro antiproliferative activity of the final synthesized compounds was evaluated with four different human cancer cell lines (Lung adenocarcinoma-A549, Hepatocarcinoma-HepG2, Breast carcinoma- MCF-7 and Ovarian carcinoma-SKOV3) and normal human lung fibroblast cell line (MRC-5). Compounds 2b showed better inhibition against MCF-7, HepG2 and A549 cell lines (IC50 8.00 ± 0.11, 11.93 ± 0.01 and 15.85 ± 0.04 lM, respectively) as compared with doxorubicin and also 2e showed moderate inhibition against MCF-7, HepG2 (IC50 9.32 ± 0.21 and 20.22 ± 0.01 lM, respectively, cell lines, respectively) as compared with doxorubicin. As many clinically used antiproliferative agents induce apoptosis in cancer cells hence, the 2-pyridone analogues were also tested for their ability to induce apoptosis in MCF-7 cells using the caspases-3 and -9 assays. **(***Bioorg. Med. Chem. Lett.,* **2016,** 26(9), 2159)

Synthesis and evaluation of anticancer and antiobesity activity of 1-ethoxy carbonyl-3,5-bis (3'-indolyl methylene)-4-pyperidone analogs

A series of eleven novel bisindole derivatives were synthesized and screened for anticancer and antiobesity potentials in in vitro mode. The reaction of 1-ethoxy carbonyl 4-pyperidone 1a with indole-3-carboxaldehyde 1b in presence of catalytic amount of piperidine gave 2 which was N-alkylated with different benzyl halides in the presence of potassium carbonate to afford compounds 3a–3k in quantitative yields. Among the compounds tested for anticancer activity against different human cancer cell lines, 3f significantly inhibited HepG2 cell line (IC50 7.33 lM) when compared with standard doxorubicin (IC50 10.15 lM). Compounds 3e (IC50 2.75 lM), 3f (IC50 4.21 lM) and 3i (IC50 15.98 lM) showed better activity than the standard curcumin (IC50 23.54 lM) against A549 cell line. Also, among the synthesized compounds, 3g (IC50 14.89 lM), 3c (IC50 56.41 lM) and 3i (IC50 30.88 lM) have potentially inhibited enzyme lipase when compared to standard Orlistat (IC50 62.25 lM). In in silico docking assays, piperidones 3e, 3f, 3i, 3c and 3a showed higher binding affinity towards anti-cancer target of A549 (3e: 11.1, 3f: 10.3, 3c: 11.3, 3i: 11.2 kcal/mol), HepG2 (3f: 10.5 kcal/mol), HeLa (3d: 10.0 kcal/

mol) and SKOV3 (3f: 8.4 kcal/mol) cell lines better than standard drug doxorubicin. Docking to lipase protein for compounds 3i, 3g and 3c showed scores of 11.1, 10.7 and 10.5 kcal/mol when compared to that of standard drug Orlistatwith 6.9 kcal/mol. (*Bioorg. Med. Chem. Lett.,* **2016**, 26(6), 1633)

Assessment of genotoxicity in female agricultural workers exposed to pesticides.

This study was designed to determine the genotoxic effect of exposure to a mixture of pesticides in 106 female agricultural workers employed in cotton fields from India. Methods: Comet, micronucleus and chromosomal aberrations tests were carried out in peripheral blood lymphocytes. Micronucleus test was also performed in buccal epithelial cells. Levels of antioxidant enzymes, RBC acetyl cholinesterase and hematological parameters were analyzed in the blood samples of the study subjects. Results: The results indicated significant DNA damage, increased frequency of micronuclei and chromosomal aberrations in the exposed subjects ($p<0.05$). The levels of antioxidant enzymes were significantly lowered and the rate of lipid peroxidation was elevated in the exposed subjects. Conclusion: The outcome of the study revealed an increased risk of genotoxicity and health implications in female agricultural workers. **(***Biomarkers,* **2017**, 22(5), 446)

Genotoxicity study of nickel oxide nanoparticles in female Wistar rats after acute oral exposure

Nanoparticles (NPs) apart from their widespread advantages and increased utilisation, have aroused concerns over their safe use. Nickel (II) oxides (NiO) NPs are used as catalysts, biosensors and in many of the consumer products. The increasing use of NiO NPs necessitates an improved understanding of their potential impact on the environment and human health. In this study, we investigated the acute genotoxic effects of NiO NPs by oral route administration with three different doses (125, 250 and 500 mg/kg bw). Before the in vivo toxicological evaluation, characterization of particles by Transmission Electron Microscopy, X-ray diffraction, Dynamic Light Scattering (DLS) and Laser Doppler Velocimetry analysis was performed. Genotoxicity biomarkers such as comet, micronucleus and chromosomal aberrations (CAs) assays were utilised in this study. To document the uptake, retention and elimination of the NPs, biodistribution studies were also performed. The particle size obtained from Transmission Electron Microscopy analysis for NiO NPs was 15.62 ± 2.59 nm. The mean hydrodynamic diameter and PdI of NiO NPs in MilliQ water suspension obtained by DLS was 168.9 ± 17.13 nm and 0.375, respectively. Comet assay revealed significant ($P < 0.001$) DNA damage at 500 mg/kg bw dose in the PBL, liver and kidney cells of rats at the 24-h sampling time. The result of micronucleus and CAs tests was in agreement with the comet assay data. Biodistribution of NiO NPs revealed a maximum accumulation of Ni in the liver tissue at the 24-h sampling time. Our study showed significant DNA damage at the high dose level and the effect was more prominent at 24-h sampling time, providing preliminary evidence that the NiO NPs are capable of inducing genotoxicity when administered through the oral route. However, mechanistic investigations are needed before drawing any firm conclusion regarding the toxicology of NiO NPs. (*Mutagenesis,* **2017**, 32, 417)

Acute oral toxicity study of magnesium oxide nanoparticles and microparticles in female albino Wistar rats

Advancements in nanotechnology have led to the development of the nanomedicine, which involves nanodevices for diagnostic and therapeutic purposes. A key requirement for the successful use of the nanoparticles (NPs) in biomedical applications is their good dispensability, colloidal stability in biological media, internalization efficiency, and low toxicity. Therefore, toxicological profiling is necessary to understand the mechanism of NPs and microparticles (MPs). MgO NPs have attracted wide scientific interest due to ease of synthesis, chemical stability and unique properties. However, their toxic effects on humans should also be of concern with the increased applications of nano MgO. The present study was aimed to assess the toxicological potential of MgO NPs in comparison to their micron counterparts in female Wistar rats. Toxicity was evaluated using genotoxicity, histological, biochemical, antioxidant and biodistribution parameters post administration of MgO particles to rats through oral route. The results obtained from the investigation revealed that the acute exposure to the high doses of MgO NPs produced significant ($p < 0.01$) DNA damage and biochemical alterations. Antioxidant assays revealed prominent oxidative stress at the high dose level for both the particles. Toxicokinetic analysis showed significant

levels of Mg accumulation in the liver and kidney tissues apart from urine and feces. Further, mechanistic investigational reports are warranted to document safe exposure levels and health implications post exposure to high levels of NPs. (*Regulat. Toxicol. Pharmacol.,* **2017**, 90, 170)

Assessment of genotoxicity and biodistribution of nano- and micron-sized yttrium oxide in rats after acute oral treatment

The increasing use of yttrium oxide (Y_2O_3) nanoparticles (NPs) entails an improved understanding of their potential impact on the environmental and human health. In the present study, the acute oral toxicity of Y_2O_3 NPs and their microparticles (MPs) was carried out in female albino Wistar rats with 250, 500 and 1000 mg kg^{-1} body weight doses. Before the genotoxicity evaluation, characterization of the particles by transmission electron microscopy, dynamic light scattering and laser Doppler velocimetry was performed. The genotoxicity studies were conducted using micronucleus and comet assays. Results showed that Y_2O_3 NP-induced significant DNA damage at higher dose (1000 mg kg^{-1} body weight) in peripheral blood leukocytes and liver cells, micronucleus formation in bone marrow and peripheral blood cells. The findings from biochemical assays depicted significant alterations in aspartate transaminase, alanine transaminase, alkaline phosphatase, malondialdehyde, superoxide dismutase, reduced glutathione, catalase and lactate dehydrogenase levels in serum, liver and kidneys at the higher dose only. Furthermore, tissue biodistribution of both particles was analyzed by inductively coupled plasma optical emission spectrometry. Bioaccumulation of yttrium (Y) in all tissues was significant and dose-, time- and organ-dependent. Moreover, Y_2O_3 NP-treated rats exhibited higher tissue distribution along with greater clearance through urine whereas Y_2O_3MP-dosed animals depicted the maximum amount of Y in the feces. Hence, the results indicated that bioaccumulation of Y_2O_3 NPs via its Y ions may induce genotoxic effects. (*J. Appl. Toxicol.,* **2017,** 37, 1379)

APPLIED RESEARCH

Having Significant Industrial/ Economic/ Environmental/ Societal/ Strategic Impact

Influence of socioeconomic aspects on lymphatic filariasis: A case-control study in Andhra Pradesh

Lymphatic filariasis (LF) is a major public health problem in India. A longitudinal study was conducted to assess the impact of socioeconomic conditions on LF in Chittoor district of Andhra Pradesh, India. The microfilaria positive samples were taken as cases and matched with control group by sex and age (1:1) for case-control study. Multivariate analysis showed that the risk of filariasis was higher in groups of people with income < ₹1000 per month [OR = 2.752 (95%CI, 0.435-17.429)]; ₹1000-3000 per month [3.079 (0.923-0.275)]; people living in tiled house structure [1.641 (0.534-5.048)], with kutcha (uncemented) drainage system [19.427 (2.985- 126.410)], respondents who did not implemented mosquito avoidance measures [1.737 (0.563-5.358)]; and in people who were not aware about prevention and control of filariasis [1.042 (0.368-2.956)]. Similarly using principal component analysis a socioeconomic index was developed which showes that respondents with low (41.6%) and medium (33.8%) socioeconomic status are more prone to filariasis (p=0.036). The identified socioeconomic risk factors can be used as a guideline for improving the conditions for effective management of filariasis. (*J. Vector Borne Dis.,* **2016**, 53, 272)

Importance of climatic parameters on dengue transmission in India

For the past ten years, the number of dengue cases has gradually increased in India. Dengue is driven by complex interactions among host, vector and virus that are influenced by climatic factors. Here we have studied the Extrinsic incubation period (EIP) and its variability in different climatic zones of India. The EIP was calculated by using daily and monthly mean temperatures for the states of Punjab, Haryana, Gujarat, Rajasthan and Kerala. Among the studied states, a faster/low EIP in Kerala (8–15 days at 30.8 and 23.4 °C) and a generally slower/ high EIP in Punjab (5.6–96.5 days at 35 and 0 °C) were simulated with daily temperatures. EIPs were calculated for different seasons, and Kerala showed the lowest EIP during the monsoon period. In addition, a significant association between dengue cases and precipitation was also observed. The results suggest that temperature is important in virus development in different climatic regions and may be useful in understanding spatio-temporal variations in dengue risk. Climate-based

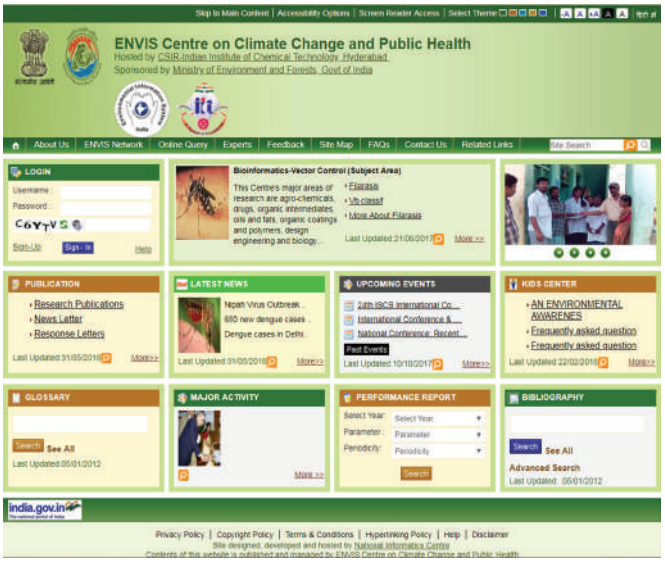
disease forecasting models in India should be refined and tailored for different climatic zones, instead of use of a standard model. (*Nature Emerg. Microb. Infect.*, **2017**, 6, e70)

Environmental Information System (ENVIS) Centre on 'Climate Change & Public Health'. (*Sponsored by the Ministry of Environment and Forests (MoEF) Govt. of India*)

Environmental information plays a vital role not only in formulating environmental management policies but also in the decision making process aiming at environmental protection and improvement of environment for sustaining good quality of life for the living beings. Ministry set up an Environmental Information System (ENVIS) in 1983 as a plan programme as a comprehensive network in environmental information collection, collation, storage, retrieval and dissemination to varying users, which include decision-makers, researchers, academicians, policy planners and research scientists, etc. ENVIS was conceived as a distributed information network with the subject-specific centers to carry out the mandates and to provide the relevant and timely information to all concerned. The ENVIS centre in CSIR-IICT is first of its kind to have a centre exclusively for information dissemination on *Climate Change and Public Health*. More details at: www.iictenvis.nic.in

Activities Pursued:

- Organizing awareness programs to school children's on Public Health and Hygiene
- Periodical upgradation of the information on latest disease outbreaks mosquito borne diseases
- Upload the information on impact of Climate change-vector borne diseases
- Publishing news letters on Climate change on public health and GIS applications on Public Health aspects
- Developed a web portal on encyclopaedia on vector borne disease transmitted by Flies, Fleas, Ticks and Lice. This portal consist of Epidemiology of disease, lifecycle and control and preventive measures was provided



ENVIS centre-home page

Toxicity evaluation of Ayurvedic herbo-metallic preparations

(Funded by Ministry of Ayurveda, Yoga & Naturopathy, Unani, Siddha & Homeopathy (AYUSH))

Traditional systems of medicines are being used since centuries for healthcare by people all over. They continue to be a valuable source of remedies to the people around the world to secure their health because such drugs are easily available, comparatively safe. People have faith in such remedies. Their industrial production is environment friendly, and is the best alternative to synthetic drugs. Ayurveda exclusively uses various processed metals and minerals (bhasmas) in therapeutics, which will remove the hazardous properties from these drugs. But a poorly prepared ayurvedic drug however used skillfully, may prove to be toxic to man. This project involves the oral acute and sub-chronic toxicity evaluation of four Ayurvedic herbo-metallic preparations (Arsho Kuthara Rasa, Chandramrit rasa, Ekangaveer rasa and Nityanand rasa) in albino Wistar rats. These Ayurvedic drugs are used to treat diseases like piles, anorexia, fever, caugh, paralysis, nervous disorders, elephantiasis, gout and tumors in man.

Toxicity evaluation of Ayurvedic herbo-metallic preparations

Objectives:

- To assess the genotoxic potential and the effect on the expression of ROS genes.
- To estimate hematological and biochemical alterations.
- To analyse the metals in HM drugs and their biodistribution in serum
- To perform the histopathological studies on the vital organs.

S&T Consultancy services rendered: The division has taken up consultancy project from industries mentioned bellow:

- Micellar Characterization study for Docetaxel Injection, - M/s Amneal Oncology Pvt Ltd, Ahmedabad, 2016.
- Acute toxicity evaluation of plant nutrient - M/s Nagarjuna Fertilizers and Chemicals Limited, Hyderabad, 2016.
- Evaluation of anti diabetic potential of herbal extracts in db/db mice – M/s Laadh Bio Pvt Ltd, Hyderabad, 2017.

Testing & evaluation services for industries (respect to particle size, zeta potential analysis & Differential Scanning Calorimetry):

1. Aurobindo Pharma, Hyderabad,
2. Alkem laboratories Ltd., Raigad;
3. Orbicular Pharmaceutical Technologies Pvt Ltd, Hyderabad
4. Therdose Pharma Pvt Ltd., Hyderabad,
5. Celon Laboratories Pvt Ltd., Hyderabad,
6. Rubicon Research, Mumbai
7. Sri Krishna Pharmaceuticals, Hyderabad.

Anti-termite test of industrial samples:

1. Antitermite study against termite species *Odontotermes obesus,* supplied by M/s.K Kalpana Industries,Silvassa.
2. Antitermite study against termite species *Odontotermes obesus,* supplied by M/s. ANCHOR Electricals Private Limited, Bhimpore, Nani Daman.
3. Antitermite study against termite species *Odontotermes obesus,* supplied by M/s Vindhya Telelinks Ltd, Rewa.
4. Antitermite study against termite species *Odontotermes obesus,* supplied by Sterlite Technologies Limited, Rakholi.
5. Antitermite study against termite species *Odontotermes obesus,* supplied by M/s.Birla Cable Ltd, Rewa.
6. Antitermite study against termite species *Odontotermes obesus,* supplied by M/s Universal Cables Limited, (Unit-Goa).
7. Antitermite study against termite species *Odontotermes obesus,* supplied by M/s. U M Cables Limited,Silvassa.
8. Antitermite study against termite species *Odontotermes obesus,* supplied by M/s. APAR Industries Ltd., Gujrath.
9. Antitermite study against termite species *Odontotermes obesus,* supplied by M/s.Narayani Polypipes,Kolkata.
10. Antitermite study against termite species *Odontotermes obesus,* supplied by Dura-Line India Pvt.Ltd.,Telangana.
11. Antitermite study against termite species *Odontotermes obesus,* supplied by M/s Universal Cables Limited, (Unit-Goa).
12. Antitermite study against termite species *Odontotermes obesus,* supplied by Sterlite Technologies Limited, Rakholi.
13. Antitermite study against termite species *Odontotermes obesus,* supplied by M/s. Shakun Polymers Limited,Gujrath.
14. Antitermite study against termite species *Odontotermes obesus,* supplied by M/s. Shakun Polymers Limited,Gujrath.
15. Antitermite study against termite species *Odontotermes obesus,* supplied by M/s.BSH Household Appliances Manufacturing Pvt. Ltd.,Tamilnadu.
16. Antitermite study against termite species *Odontotermes obesus,* supplied by M/s KEI Industries Ltd,Rajasthan.
17. Antitermite study against termite species *Odontotermes obesus,* supplied by M/s.Aksh OFC Ltd., Rajasthan.

18. Antitermite study against termite species *Odontotermes obesus,* supplied by M/s.Thermo Cable Ltd., Telangana.
19. Antitermite study against termite species *Odontotermes obesus,* supplied by M/s.Aksh OFC Ltd., Rajasthan.
20. Antitermite study against termite species *Odontotermes obesus,* supplied by M/s.Dura-Line India Pvt.Ltd.,Telangana.
21. Antitermite study against termite species *Odontotermes obesus,* supplied by M/s. ANCHOR Electricals Private Limited, Bhimpore, Nani Daman.
22. Antitermite study against termite species *Odontotermes obesus,* supplied by M/s.Servel India, New Delhi.
23. Antitermite study against termite species *Odontotermes obesus,* supplied by M/s Sterlite Technologies Limited, Rakholi.
24. Antitermite study against termite species *Odontotermes obesus,* supplied by M/s Sterlite Technologies Limited, Rakholi.
25. Antitermite study against termite species *Odontotermes obesus,* supplied by M/s Vindhya Telelinks Ltd, Rewa.
26. Antitermite study against termite species *Odontotermes obesus,* supplied by M/s.Birla Cable Ltd, Rewa.
27. Antitermite study against termite species *Odontotermes obesus,* supplied by M/s. ANCHOR Electricals Private Limited, Bhimpore, Nani Daman.
28. Antitermite study against termite species *Odontotermes obesus,* supplied by M/s.Dura-Line India Pvt.Ltd.,Telangana.
29. Antitermite study against termite species *Odontotermes obesus,* supplied by M/s. ANCHOR Electricals Private Limited, Bhimpore, Nani Daman.
30. Antitermite study against termite species *Odontotermes obesus,* supplied by M/s. U M Cables Limited,Silvassa.
31. Antitermite study against termite species *Odontotermes obesus,* supplied by Ms.Paramount Wires, Rajasthan.
32. Antitermite study against termite species *Odontotermes obesus,* supplied by M/s. ANCHOR Electricals Private Limited, Bhimpore, Nani Daman.
33. Antitermite study against termite species *Odontotermes obesus,* supplied by Himalaya communications Ltd., New Delhi.
34. Antitermite study against termite species *Odontotermes obesus,* supplied by M/s.HTL Ltd., Chennai.

Antirodent test of industrial samples:

1. Acute Oral toxicity study of Dantinanganagainst Albino Wistar rats, supplied by M/s.A.R Enterprises, Hyderabad.
2. Acute Oral toxicity study of fresh coat B#01 against Albino Wistar rats, supplied by M/s. IINRG- Indian Institute of Gums and Resins, Ranchi.
3. Acute Oral toxicity study of Triyz-Al-Amraaz against Albino Wistar rats, supplied by M/s. Triyaz-Al-Amraaz Pharmacy, Hyderabad.
4. Acute Oral toxicity study of Pigeon repellent additive against Albino Wistar rats, supplied by M/s. Lifeline Technologies Thane (west)-400604, Mumbai.
5. Acute Dermal toxicity study of Pigeon repellent additive against Albino Wistar rats, supplied by M/s. Lifeline Technologies Thane (west)-400604, Mumbai.
6. Antirodent study of 24F SM Composite OFC against a wild rodent species *Rattusrattus,*supplied by M/s. AkshOptifibre limited, Alwar-301019, Rajasthan.
7. Antirodent study of Rubber Sheet against a wild rodent species *Rattusrattus,* supplied by M/s.Taprath Elastomers LLP, Andheri (west), Mumbai- 4000853.
8. Antirodent study of Baby Carton Stripes against a wild rodent species *Rattusrattus,*supplied by M/s.V-Guard Industries Ltd, Uttarakhand- 244713.
9. Antirodent study of Mesh against a wild rodent species *Rattusrattus,* supplied by M/s.SparcoMultiplast Private Limited- Ahmedabad-15, Gujarat.
10. Antirodent study of Thermosetting Eva Sheath with LSLH properties doped with non-toxic anti-rodent master batch cable against a wild rodent species *Rattusrattus,* supplied by M/s.Thermocables limited, Hyderabad.

11. Antirodent study of40/32 MM, 78/63MM, 90/75 MM DWC HDPE pipes against a wild rodent species *Rattusrattus, Bandicotabengalensis, Tetra indica* supplied by M/s.Rex Polyextrusion Pvt.Ltd., Sangli, Maharastra.
12. Antirodent study of4 cable samples and 4 carton samples against a wild rodent species *Rattusrattus,*supplied by M/s. -V-Guard Industries, Wire & Cables Division, Coimbatore.
13. Antirodent study of DWC HDPE 150mm, 200mm pipes against a wild rodent species *Rattusrattus,*supplied by M/s.Rex Polyextrusion Pvt.Ltd., Sangli, Maharastra.
14. Antirodent study of Warning Mat samples against a wild rodent species *Rattusrattus,*supplied by M/s. SparcoMultiplast Private Limited- Ahmedabad-15, Gujarat.
15. Antirodent study of Anti-rodent warning Mat samples against a wild rodent species *Rattusrattus,*supplied by M/s.AkshOptifibre limited, Alwar-301019, Rajasthan.
16. Antirodent study of 2F Armoured OFC agaomstupir samples against a wild rodent species *Rattusrattus,* supplied by M/s.AkshOptifibre limited, New Delhi.
17. Antirodent study of DWC HDPE 75mm, 63mm pipes and BSNL sample HDPE ducts 75mm/63mm against a wild rodent species *Rattusrattus,*supplied by M/s. Rex Polyextrusion Pvt.Ltd., Sangli, Maharastra.
18. Antirodent study of 63/51 MM, 120/103MM DWC HDPE pipes against a wild rodent species *Rattusrattu s,Bandicotabengalensis, Tetra indica* supplied by M/s. Rex Polyextrusion Pvt.Ltd., Sangli, Maharastra.
19. Antirodent study of Halogen free flame retardant thermoplastic compound against a wild rodent species *Rattusrattus,*supplied by M/s.Shakun Polymers Ltd., Vadodara, Gujarat.
20. Antirodent study of 12F TPU UA cable against a wild rodent species *Rattusrattus,* supplied by M/s. Vindhya telelinks. Ltd., Rewa.
21. Antirodent study of 75/63 mm in all eight colors DWC HDPE ducts agains a wild rodent species *Rattu srattus,Bandicotabengalensis, Tetra indica*supplied by M/s. Rex Polyextrusion Pvt.Ltd., Sangli, Maharastra.
22. Antirodent study of Mesh against a wild rodent species *Rattusrattus,* supplied by M/s.SparcoMultiplast Private Limited, Ahmedabad, Gujarat.
23. Antirodent study of 2F multimode armoured optical fibre cable sample against a wild rodent species *Rattusrattus,*supplied by M/s.AkshOptifibre limited, Bhiwadi, Rajasthan.
24. Antirodent study of 75mm/63 mm, 110mm/95mm and 315mm/275mmin all eight colors DWC HDPE ducts agains a wild rodent species *Rattusrattus, Bandicotabengalensis, Tetra indica*supplied by M/s. Rex Polyextrusion Pvt.Ltd., Sangli, Maharastra.
25. Antirodent study of black purarmoured sample against a wild rodent species *Rattusrattus,* supplied by M/s.Rosenberger Electronic Co., India Pvt., Ltd., Verna, Goa.
26. Antirodent study of sample against a wild rodent species *Rattusrattus,*supplied by M/s.Apar Industries Ltd, Hyderabad.
27. Antirodent study of 75mm/63 mm, 50mm/38mm and 180mm/153 mm DWC HDPE pipes agains a wild rodent species *Rattusrattus,Bandicotabengalensis, Tetra indica*supplied by M/s. Rex Polyextrusion Pvt. Ltd., Sangli, Maharastra.
28. Antirodent study of black purarmoured sample against a wild rodent species *Rattusrattus,* supplied by M/s.Rosenberger Electronic Co., India Pvt., Ltd., Verna, Goa.
29. Antirodent study of 2F multimode armoured optical fibre cable sample against a wild rodent species *Rattusrattus,* supplied by M/s.AkshOptifibre limited, New Delhi.
30. Antirodent study of6 test pieces of warning Mat samples against a wild rodent species *Rattusrattus,* supplied by M/s.SparcoMultiplast Private Limited-Ahmedabad-15, Gujarat.
31. Antirodent study of black HDPE armoured outdoor sample against a wild rodent species *Rattusrattus,*supplied by M/s.Rosenberger Electronic Co., India Pvt., Ltd., Verna, Goa.
32. Antirodent study ofgreen colour wire sample against a wild rodent species *Rattusrattus,*supplied by M/s. Shilpicable technologies limited Alwar Rajasthan.
33. Antirodent study of DWC HDPE BSNL ducts 63mm/51mm, 90mm/76mm, 120mm/103mm of against a wild rodent species *Rattusrattus,* supplied by M/s.Rex Polyextrusion Pvt.Ltd., Uttarakhand.

34. Antirodent study of black purarmoured sample against a wild rodent species *Rattusrattus,* supplied by M/s.Rosenberger Electronic Co., India Pvt., Ltd., Verna, Goa.

35. Antirodent study of green colour wire sample against a wild rodent species *Rattusrattus,* supplied by M/s. Shilpicable technologies limited Alwar Rajasthan.

36. Antirodent study of A&B 75mm and 120mm DWC HDPE pipes against a wild rodent species *Rattusrattus,Bandicotabengalensis, Tetra indica*supplied by M/s. Rex Polyextrusion Pvt.Ltd., Sangli, Maharastra.

37. Antirodent study of Mat samples against a wild rodent species *Rattusrattus,*supplied by M/s. SparcoMultiplast Private Limited- Ahmedabad-15, Gujarat.

38. Antirodent study of Halogen free flame retardant thermoplastic compound against a wild rodent species *Rattusrattus,*supplied by M/s.Shakun Polymers. Ltd., Vadodara- 390021 Gujarat.

39. Antirodent study of HDPE Optical Fiber Cable sample against a wild rodent species *Rattusrattus,*supplied by M/s.TE Connectivity India Pvt.Ltd, Bangalore.

40. Antirodent study of Power Cord Sample against a wild rodent species *Rattusrattus,*supplied by M/s.Vi-SON Industries Estate, Kala-Amb, Himachal Pradesh.

41. Antirodent study of MM Armoured DX cable against a wild rodent species *Rattusrattus,*supplied by M/s. AmphenolOmniconnect India Pvt Ltd.

42. Antirodent study of PE warning mat/tapes against a wild rodent species *Rattusrattus,*supplied by M/s. Singhal Industries Pvt.Ltd.

43. Antirodent study of 175 mm, 90mm, 160mm DWC HDPE pipes against a wild rodent species *Rattusrattus,Bandicotabengalensis, Tetra indica*supplied by M/s. Rex Polyextrusion Pvt.Ltd., Sangli, Maharastra.

44. Antirodent study ofDWC HDPE (BSNL) Ducts in all eight coloursagainst a wild rodent species *Rattusrattus*supplied by M/s. Rex Polyextrusion Pvt. Ltd., Uttarakhand.

45. Antirodent study of 12F TPU UA cable against a wild rodent species *Rattusrattus,*supplied by M/s. Vindhya telelinks. Ltd., Rewa, M.P.

46. Antirodent study of 2F FTA sample against a wild rodent species *Rattusrattus,*supplied by M/s. Vindhya telelinks. Ltd.,Rewa, M.P.

47. Antirodent study of 7/63mm DWC HDPE ducts against a wild rodent species *Rattusrattus,Bandicotabengalensis, Tetra indica*supplied by M/s. Rex Polyextrusion Pvt.Ltd., Sangli, Maharastra.

48. Antirodent study of 48 Fibre Metal optical fibre cable with double HDPE sheath against a wild rodent species *Rattusrattus,*supplied by M/s. Vindhya telelinks. Ltd., Rewa, M.P.

49. Antirodent study of anti-rodent UV- protected HDPE grey outdoor cable against a wild rodent species *Rattusrattus,*supplied by M/s. Svarn Infratel Pvt. Ltd., Faridabad, Haryana.

50. Antirodent study of 24 metal free DS HDPE OFC for BSNL sample against a wild rodent species *Rattusrattus,*supplied by M/s. Finolex Cables Ltd., Verna, Goa.

51. Antirodent study of Disc Marker, 1401 Ball Marker, 1421 Ball Marker against a wild rodent species *Rattusrattus,*supplied by M/s. 3M India Ltd., MIDC.

52. Antirodent study of Anchor PVC Insulated RoHS REACH cable sample (black) against a wild rodent species *Rattusrattus,*supplied by M/s.Anchor Electricals Private Limited., Daman.

53. Antirodent study of three samples OD 315mm,OD 110 mm & OD 40mm ducts against a wild rodent species *Rattusrattus,Bandicotabengalensis, Tetra indica*supplied by M/s. Rex Polyextrusion Pvt.Ltd., Sangli, Maharastra.

54. Antirodent study of Polyamide 12 optical fibre cable sample (black) against a wild rodent species *Rattusrattus,*supplied by M/sEvonik India Pvt Limited., Andheri (E), Mumbai.

55. Antirodent study of advance cable 4 pair armoured GPS against a wild rodent species *Rattusrattus,*supplied by M/s Advance Cable Technologies (P) Limited., Bangalore.

56. Antirodent study ofoptical fibre cable against a wild rodent species *Rattusrattus,*supplied by M/sUM Cables Limited., Silvassa.

57. Antirodent study of three samples 160/135 mm pipes against a wild rodent species *Rattusrattus*supplied by M/s. Rex Polyextrusion Pvt.Ltd., Sangli, Maharastra.

58. Antirodent study of two PVC compound samples against a wild rodent species *Rattusrattus*supplied by M/s.KKalpana Industries (India).Ltd,D&NH.

59. Antirodent study of way chambers against a wild rodent species *Rattusrattus*supplied by M/s.Ashirvad Pipes Pvt. Ltd, Bangalore.

60. Antirodent study of optical fibre cable against a wild rodent species *Rattusrattus,*supplied by M/sSterilite Technologies Limited., D&NH.

61. Antirodent study of two Polyamide optical fibre cable samples against a wild rodent species *Rattusrattus,*supplied by M/sEvonik India Pvt Limited., Andheri (E), Mumbai.

62. Antirodent study ofsamples against a wild rodent species *Rattusrattus*supplied by M/s. Rex Polyextrusion Pvt.Ltd., Sangli, Maharastra.

63. Antirodent study of 63mm HDPC DWC pipesagainst a wild rodent species *Rattusrattus*supplied by M/s. Crescent India Polymers., Dharwad, Karnataka.

64. Antirodent study of120mm HDPC DWC pipes against a wild rodent species *Rattusrattus*supplied by M/s. Crescent India Polymers., Dharwad, Karnataka.

65. Antirodent study of DWC Duct pipeagainst a wild rodent species *Rattusrattus* supplied by M/s.CIPET, Hyderabad.

SOCIETAL ACTIVITIES

Information Education and Communication (IEC) cum distribution of Long Lasting Insecticide Nets (LLINs) in Arunachal Pradesh: LLINs were distributed and an awareness camp on malaria was conducted on **07.07.2017** in Hong village of Lower Subansiri district of Arunachal Pradesh in coordination with District Health Department, Ziro.

Shri. Er.Tage Taki, Hon'ble Parliamentary secretary Food & Civil Supplies Govt. of Arunachal Pradesh addressing the gathering on the occasion of IEC cum distribution of LLINs in Hong village of Lower Subansiri district of Arunachal Pradesh.

CSIR-IICT officials Dr.Srinivasa Rao and Dr.Madhusudhan Rao with Shri. Er. Tage Taki, Parliamentary secretary Food & Civil Supplies Govt. of Arunachal Pradesh, Kemo Lollen, Deputy Commissioner, Dr.Tage Kano DMO, Dr.Kuru Tama, DIPRO, ZPM members of Hong village during *IEC cum distribution of LLINs* in Hong village of Lower Subansiri district, Arunachal Pradesh.

Shri. Er.Tage Taki, Hon'ble Parliamentary secretary Food & Civil Supplies Govt. of Arunachal Pradesh distributing LLINs to the local populace of Hong village, Lower Subansiri district of Arunachal Pradesh

Serological testing for malaria and followed by distribution of LLINs for the local community in Hong village of Lower Subansiri district of Arunachal Pradesh

BACK TO SCHOOL: An ENVIS awareness program on "Public Health & Hygiene" @ Govt. High School JAMA-E-Osmania, OU, Hyderabad on 14-02-2018.

In connection ENVIS program a half a day programme on "*Public Health and Hygiene*" was conducted for the students of 8th 9th and 10th classes of Government High School, Jama E Osmania, Hyderabad on

14.02.2018 (*Wednesday*). The students were told about the engineering aspects to be followed to prevent stagnation of water so as to avoid the breeding of the mosquitoes in and around their dwellings. The students were also taught about the life cycle of the vectors and the parasites they transfer from unhealthy personnel to the healthy ones. It was also highlighted to them to avoid contact from mosquitoes and keep the doors and windows shut during the swarming period.

ENVIS awareness program @ Jama-E-Osmania Govt. High School

ENVIS coordinator Dr.M.Srinivasa Rao speaking on the occasion of Public Health & Hygiene

Teachers and students gathered on the occasion of *Public Health and Hygiene* workshop.

Student explained about mosquito borne diseases and its preventive measures during *Public Health and Hygiene* workshop.

RECOGNITIONS

The division is **recognized** as testing laboratory for Active Pharmaceutical Ingredients (APIs) and finished dosage forms by State Licensing Authority, **Drugs Control Administration, Govt of Telangana**.

XII FIVE YEAR PLAN PROJECTS:

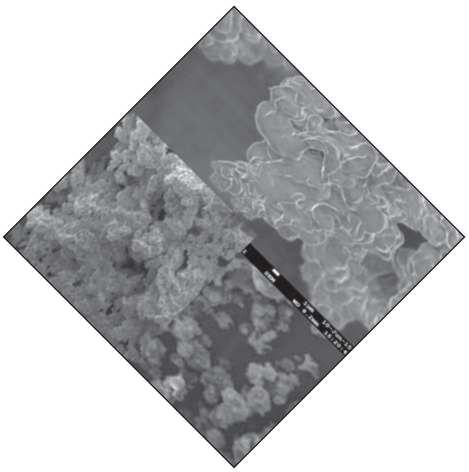
- Pharmacology Division is actively involved in the following XII FYP projects namely, SMiLE (Screening Molecules in Lead Exploration), ADD (Advanced Drug Delivery) and People HOPE (Development Sustainable Processes for Edible Oils with Health Benefits from Traditional and New Resources).
- Biology Division is actively involved in XII FYP project "Genomics and Informatics solution for Integrating Biology (GENESIS) for Advanced diseases forecasting system for mosquito borne diseases in India".

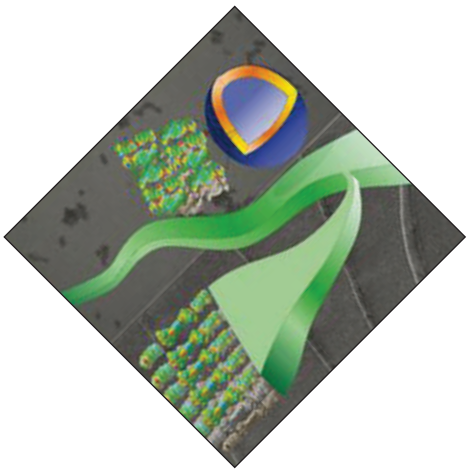
EXTRA MURAL RESEARCH:

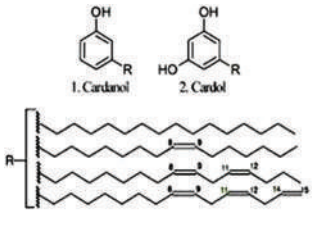
Grant in Aid Projects:

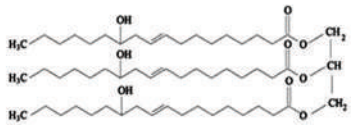
- Exploring selected natural plant sources of North East parts of India as potential therapeutic agents useful for the treatment of cancer – DBT
- Use of lipid nanoparticles for effective delivery of siRNA against chikungunya virus – DST Nanomission
- National facility for scientific validation of traditional knowledge through modern approaches - DST

POLYMERS & FUNCTIONAL MATERIALS









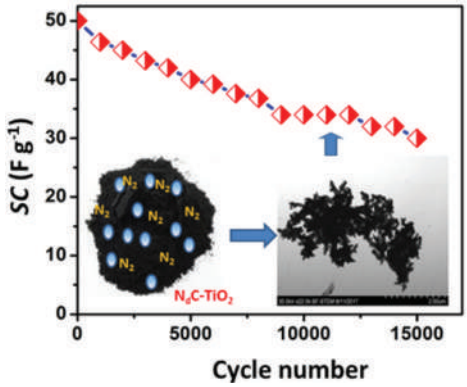
Castor polyol

BASIC RESEARCH

Energy

Polyaniline based Supercapacitor cell - 1.5 V (Symmetric Configuration)

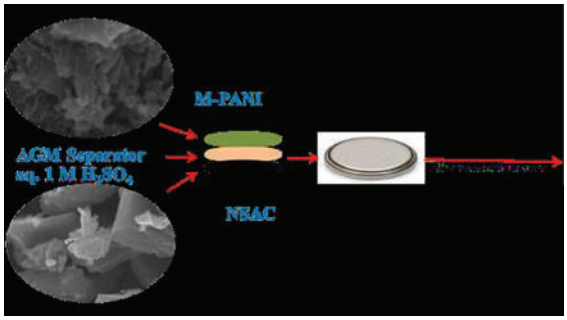
A carbon based material was designed in an aqueous electrolyte for high performance supercapacitor system by designing nitrogen doped carbon-titanium dioxide composite (N_dC-TiO_2). This was prepared by the oxidation of acidic aniline by peroxotitanium acid in addition to ammonium persulfate, followed by calcinating the sample under the nitrogen atmosphere, wherein, peroxotitanium acid is also a source material for TiO_2.

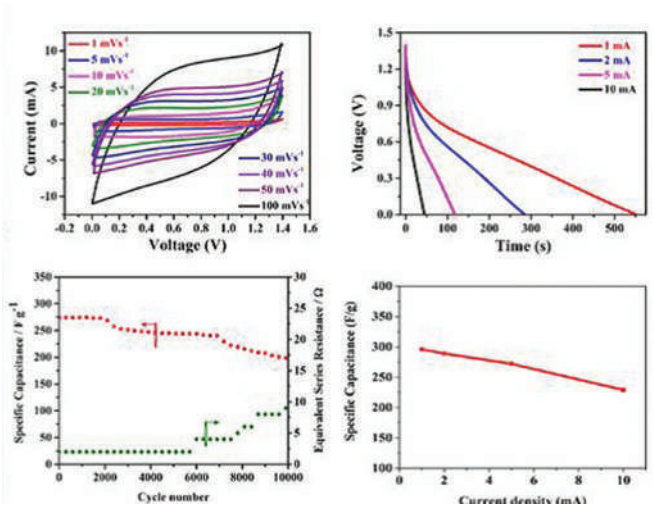


Specific capacitance Vs Charge-Discharge cycles

Polyaniline based Supercapacitor cell - 1.5 V (Asymmetric Configuration)

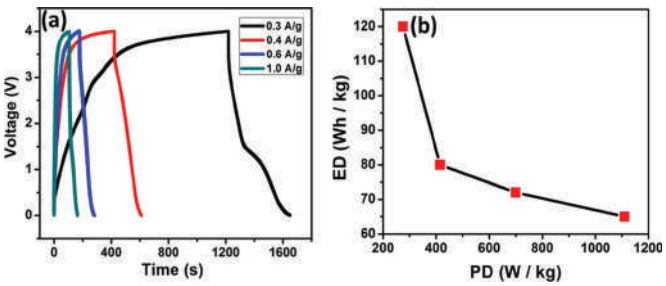
We report a high energy density asymmetric supercapacitor based on pseudocapacitance and electrochemical double layer (EDLC) electrodes, wherein, MnO_2 assisted polyaniline (MPANI) salt as a pseudocapacitative positive electrode and heteroatom (N, S) doped activated carbon (NSAC) as an EDLC negative electrode in aqueous H_2SO_4 electrolyte. Asymmetric supercapacitor cell was cycled up to the voltage of 1.4 V in spite of the use of aqueous electrolyte. Asymmetric supercapacitor exhibited excellent performance with a high specific capacitance of 296 F g^{-1} with energy density as high as 80 W hKg^{-1} at a power density of 500 W kg^{-1}. Furthermore, good cycling stability retaining over 72% of its initial capacitance at 10,000 charge-discharge cycles at a higher discharge current, 5 mA, was obtained. Practical device was demonstrated in the form of CR-2032 coin cell, highlighting the path for its Enormous potential in energy management.





Polyaniline based Novel 4 V supercapacitor system

An asymmetric supercapacitor system using commercially available molybdenum trioxide (MoO_3) as negative electrode and prepared composite of polyaniline hydrochloride salt with manganese dioxide and multi walled carbon nanotube (PANI-HCl•MnO_2•MWCNT) as positive electrodes in organic electrolyte was made and studied its electrochemical performance. This supercapacitor system showed high voltage up to 4 V, specific capacitance 54 F/g with energy density of 120 Wh kg^{-1} at a power density of 275 W kg^{-1}.



CD curves for the PANI-HCl•MnO_2•MWCNT//MoO_3aSC at various current densities from 0 to 4V, and (b) corresponding ED *vs.* PD plot

Polyaniline-Metal oxide – Supercapacitor Cell

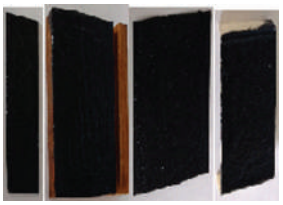
Polyaniline-nickel cobaltite composite was prepared with hydrothermally prepared manganese dioxide instead of ammonium persulfate. Asymmetric capacitor with nickel cobaltite composite exhibited excellent performance with a specific capacitance of 230 F g-1 with energy density of 45 Wh kg-1 at a power density of 790 W kg-1.

Electrochemical parameters of some of the supercapacitor cell

System	(V)	C_s (CD)at 0.35 A g^{-1} (F g^{-1})	E_d (Wh kg^{-1})	P_d (W kg^{-1})	Cycle life Retention (%)
C-TiO_2 // C-TiO_2	1.5	104	32	480	15000@0.2 Ag^{-1} 70%
PANI // rGO-TiO_2	1.6	270	95	17140	10000@1 Ag^{-1} 70%
PANI•TiO // MoS_2 [2]	2.8	84	92	2240	1000@ 1.6 Ag^{-1} 70%
PANI•MnO // MoO_3 [2]	4.0	84	96	2400	500 @ 0.6 Ag^{-1} 57%

Electrostatic Discharge Materials

Epoxy resin-polyaniline in the form of coating was developed for coating on various substrates such as concrete, wood, transparency sheet, paper, glass plate etc. for electrostatic discharge application.



A process for the preparation of low density polyethylene-polyaniline composite in the form of sheet was developed for electrostatic discharge application. Also, polyaniline-polyethylenevinylene acetate. Resistivities were observed in the range of ESD.

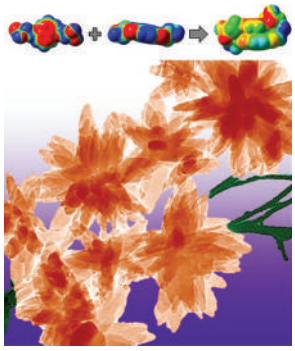
Polyethylene-Polyaniline sheet

Copper Chromite-Polyaniline Nanocomposite: An Advanced Electrode Material for High Performance Energy Storage

A novel copper chromite-polyaniline ($CuCr_2O_4$-PANI) nanocomposite electrode material for fabrication of high-performance energy storage is reported. The as synthesized nanocomposite with optimized ratio exhibits a specific capacity of 479.2 Cg^{-1} at 2 mVs^{-1} and high cycling stability with 93.9% capacity retention after 1000 charge-discharge cycles. Furthermore, it shows energy and power densities of 26.6 W h kg^{-1} and 3600 W kg^{-1}, respectively. (*Electrochimica Acta*, **2017**, 248, 486)

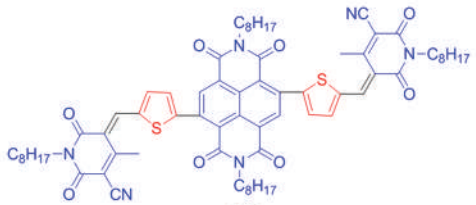
Novel naphthalene diimide derivatives for energy

A Charge Transfer (CT) complex self-assembled from an organic acceptor (NDI appended diamine (NDI-EA)) and donor (phosphonic acid-appended dialkoxynapthalene DAN1) in aqueous medium was developed. The aromatic core of the NDI and the structure of DAN1 were designed to optimize the dispersive interactions (π-π and van der Waals interactions) in the DAN1–NDI-EA construct, while the amino groups of NDI also interacted with the phosphonic acid of DAN1viaelectrostatic forces. (*Scientific Reports*, **2017**, 7, 16501)



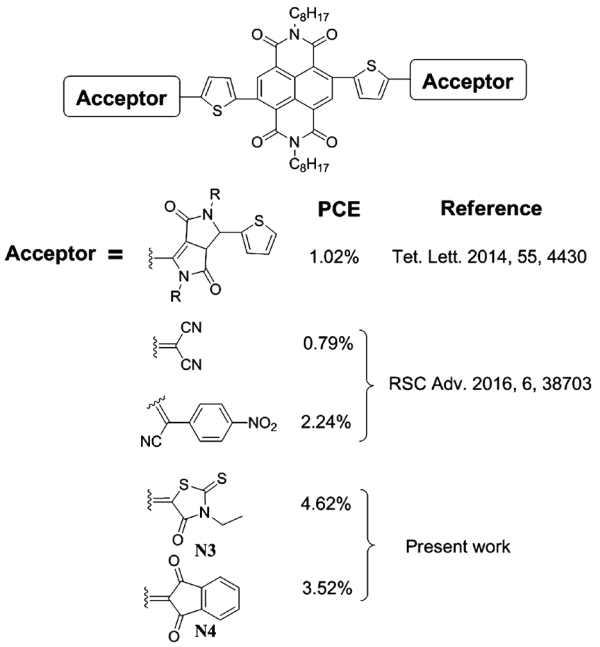
Schematic representation of CT complex flower formation

Naphthalene diimide (NDI) core-based non-fullerene acceptors, N5 and N6,comprising respectively of 2-methoxyethyl-2-cyanoacetate and cyanopyridone acceptor functionalities at the terminals were developed. The target chromophore bearing cyanopyridone acceptor units (N6) afforded a power conversion efficiency of 6.10% when paired with the conventional donor polymer poly(3-hexylthiophene), a result that is highest for the NDI core-based non-fullerene acceptors. (*Chem. Commun.*, **2017**, 53, **11157)**



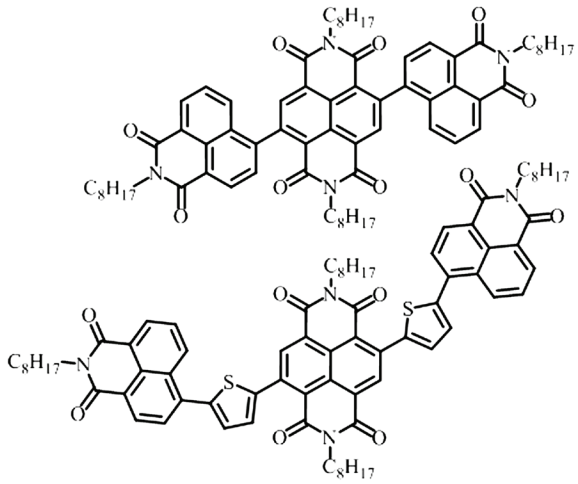
Structure of NDI derivatives

Through the conjunction of central naphthalene diimide and terminal rhodanine and 1,3-indanedione functionalities, two new non-fullerene electron acceptors, coded as N3 and N4, were designed, synthesized and characterized. Both of the materials exhibited good solubility, thermal stability, and displayed energy levels matching those of the conventional and routinely used donor polymer poly(3-hexyl thiophene) (P3HT). A high power conversion efficiency of 4.62% was obtained in simple, solution-processable bulk-heterojunction devices (P3HT: N3 1: 1) which is the best result for NDI core-based small molecular acceptors. (*Chem. Commun.*, **2017**, 53, 7080)



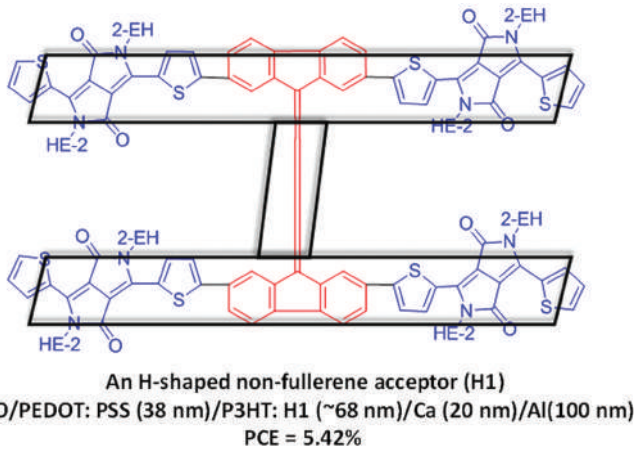
Chemical structures of the newly designed and synthesized NDI core-based acceptors N3 and N4

Through the conjunction of naphthalenediimide and benzoisoquinoline-dione functionalities (figure 17), two novel solution-processable non-fullerene electron acceptors were designed, synthesied and used as active components for organic photovoltaic devices. One of the acceptor materials afforded an unprecedented efficiency of >4% when used with the archetypal electron donor poly(3-hexylthiophene). (*Dyes and Pigments*, **2017**, 143, 1)



Structure of N1 and N2 used as an acceptor in BHJs

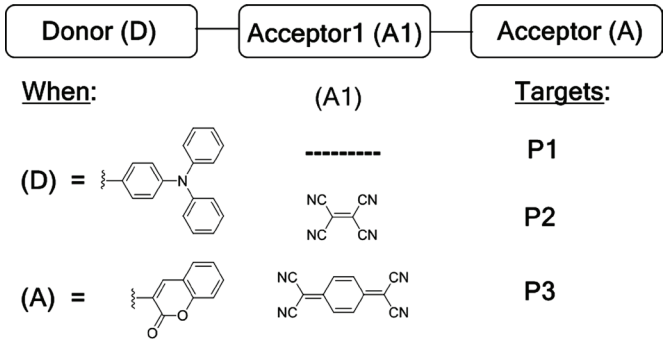
A bifluorenylidene-functionalized, H-shaped, small molecular non-fullerene electron acceptor, coded as **H1**, that used diketopyrrolopyrrole as terminal functionalities was designed, synthesized and characterized. **H1** displayed very high optical absorption coefficient, good solubility and thermal stability, promising optoelectronic properties and high electron mobility, and afforded an encouraging efficiency of 5.42% when paired with the archetypal electron donor poly(3-hexylthiophene). (*Mat. Chem. Front.*, **2017**, 1, 1600)



Structure of H-shaped non-fullerene acceptors

Donor–acceptor–acceptor-based non-fullerene acceptors

A D–A_1–A modular format in BHJ solar cells was developed. The new materials **P2** and **P3** were designed and synthesized based on the D–A_1–A format and their optoelectronic and photovoltaic properties were directly compared with a structural analogue **P1**, which was based on a simple D–A modular design. It was observed that **P2** and **P3** exhibited superior properties, such as light-harvesting, enhanced photocurrent density and overall device performance, when compared with **P1**. Overall, **P3** performed better than any of the three materials reported herein. It is notable to mention that not only are **P1**, **P2** and **P3** (figure 13) the first examples in the literature which comprise promising building blocks, such as TPA and terminal chromen-2-one, but the device parameters outlined herein are among the highest numbers reported in this class of materials. (*Dyes and Pigments*, **2017**, 146, 502)



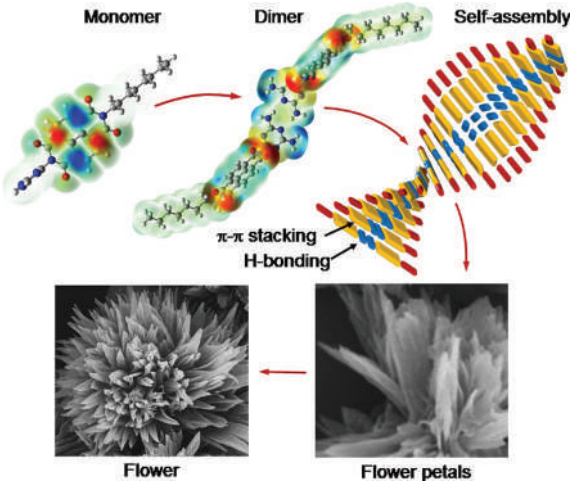
Non-fullerene electron acceptors **P1**, **P2** and **P3**

Structure of P1, P2 and P3

Functional materials

Naphthalenediimide (NDI) derivatives for sensing

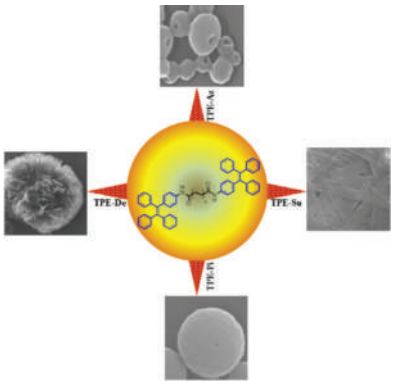
We report upon the formation of flower-like structures from a single precursor by self-assembly of a π-conjugated naphthalenediimide with melamine as the head group. The self-assembled flowers exhibit porous structures similar to natural flowers, and may find practical applications in the field of optoelectronic materials, mimicking enzyme catalysis and biosensors. (*ChemistrySelect*, **2017**, 2, 10118)



Schematic illustration of self-assembled microflower assembly formation of naphthalene diimide amphiphile and respective SEM images

Tetraphenylethylene based molecules with mechanochromic properties

Tetraphenylethylene (TPE) based dumbbell shaped molecules **TPE-Pi, TPE-Su**, **TPE-Az,** and **TPE-De** were synthesized bearing odd-even alkyl chains containing 7, 8, 9, and 10 carbons respectively. These molecules reveal typical Aggregation Induced Emission (AIE) behaviour. The mechanochromic properties of **TPE-Pi, TPE-Su,** and **TPE-Az** were also demonstrated by the process of grounding, fuming, and heating. (*Appl. Sci.,* **2017,** 7, 1119)

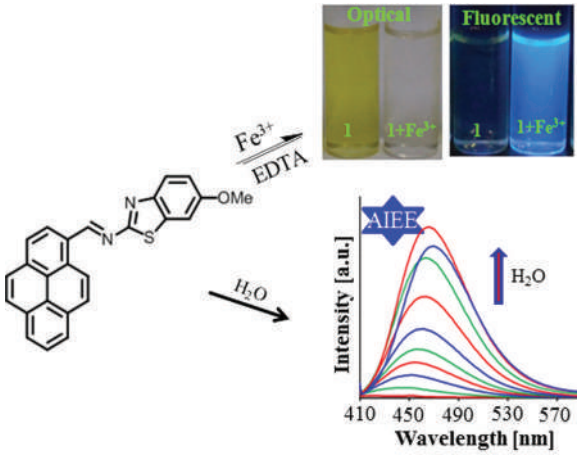


Structure of TPE derivatives and morphology

Chemosensor for detection of Fe3+ and Fe2+

A pyrene-based probe bearing benzothiazole ionophore (Py-BTZ) was synthesized as a “turn-on” fluorescent chemosensor for detection of Fe3+and Fe2+ ions in CH3CN:H2O (1:1, v/v) solvent mixes. The chemosensor showed optical as well as colorimetric changes towards Fe3+ and Fe2+ ions along with a remarkable enhancement in fluorescence emission. The detection limit of Py-BTZ

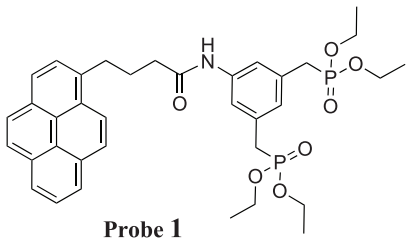
towards Fe3+ and Fe2+ ions was found to be 2.61 µM and 2.06 µM, respectively. Interestingly, Py-BTZ shows aggregation induced emission enhancement (AIEE) properties in polar solvents mixes such as CH3CN:H2O (1:1, v/v) (figure 8). (*Photochem. Photobiol. Sci.,* **2017**, 16, 1591)



Structure of pyrene sensor and optical properties

Pyrene phosphonate receptor

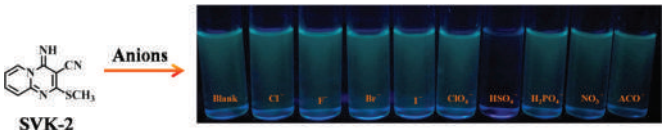
A new pyrene-phosphonate colorimetric receptor **1** has been designed and synthesized in one-step via amide bond formation between pyrene butyric acid chloride and phosphonate appended aniline (figure 11). The pyrene-phosphonate receptor **1** showed aggregation induced enhanced emission (AIEE) properties upon addition of water to acetonitrile (ACN) solution. Among the tested metal ions, the receptor **1** is capable of recognizing the Fe^{3+} ion selectively. The receptor **1:Fe^{3+}** complex showed a reversible UV-vis response in presence of EDTA. (*Molecule*, **2017**, *22*(9), 1417)



Phosphonate appended pyrene receptor 1

Fused pyridopyrimidine for HSO_4^- detection

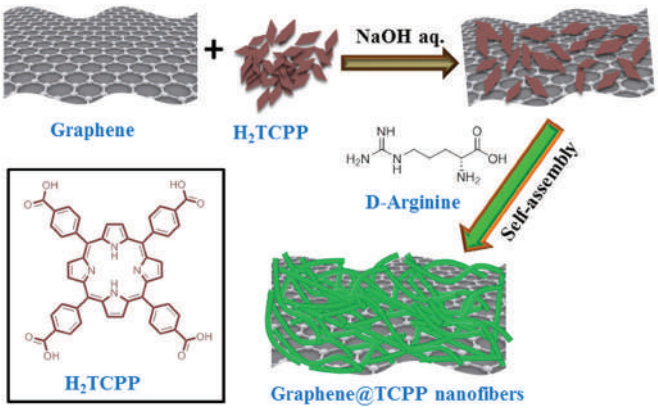
A new selective and sensitive HSO_4^- ion receptor probe based on fused pyridopyrimidine was developed. The detection of HSO_4^- over other anions such as Cl^-, F^-, Br^-, I^-, ClO_4^-, $H_2PO_4^-$, NO_3^-, and AcO^- was confirmed by fluorescent color changes, UV-vis and fluorescence spectroscopy. The HSO_4^- ion binding with the receptor was also investigated with a binding constant 1.09387 × 10^5 M^{-1}, which revealed that the receptor showed a remarkable binding ability towards the HSO_4^- ion. The limit of detection was calculated to be 6.0378 × 10^{-5} M in ACN:H_2O (1:3, *v:v*) solvent mixture. (*Chem. Biol. Interf.,* **2017**, 7, 209)



A novel selective and sensitive HSO_4^- anion receptor probe based on fused pyridopyrimidine (SVK-2) was developed and characterized

Porphyrin nanostructures for visible-light photocatalysis

A graphene@porphyrin nanofibre composite was successfully fabricated *via* arginine-mediated self-assembly of tetrakis(4-carboxyphenyl) porphyrin (TCPP) on graphene nanoplates (GNPs). The GNPs@TCPP nanofibers showed enhanced visible-light photocatalytic activity in comparison with free standing TCPP nanorods for the degradation of Rohdamine B (RhB) and methyl orange (MO). The possible photodegradation mechanism of these dyes by the GNPs@TCPP nano fiber photocatalyst was proposed (figure 15). (*Appl. Sci.*, **2017,** 7, 643)

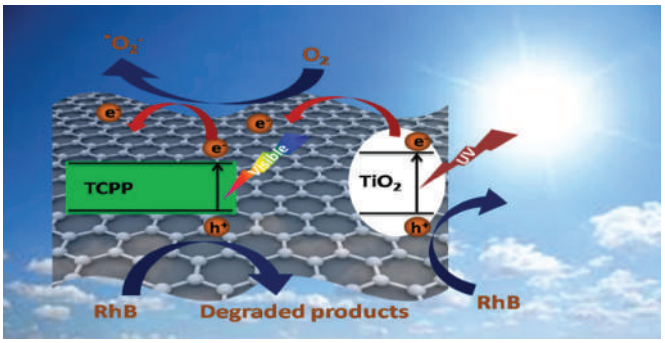


Schematic diagram of arginine-mediated self-assembly of porphyrin nanofibers on graphene surface

Nanostructure composites for pollutant degradation

The fabrication of a nanostructured graphene@TiO_2@TCPP composite was achieved *via* surfactant-assisted self-assembly. The applications of three components

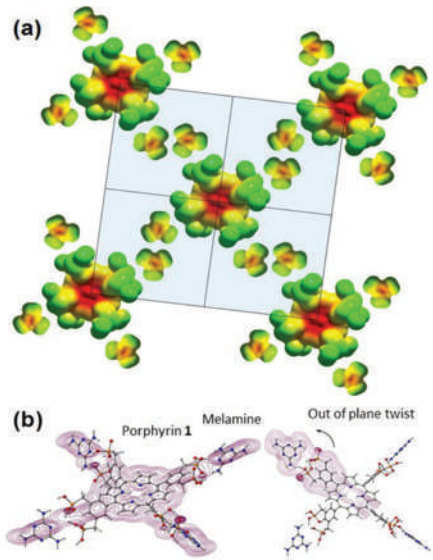
(graphene-TiO_2-TCPP) based nanostructure in photocatalytic pollutant degradation Rhodamine B is reported, where TiO_2 and TCPP are shown to be activated for UV and visible light repectively, resulting in a high performing composite. (*ChemistrySelect*, **2017**, 2, 3329)



Proposed mechanism of photocatalytic activity by graphene@TiO_2@TCPP composites

Supramolecular self-assembly of porphyrin

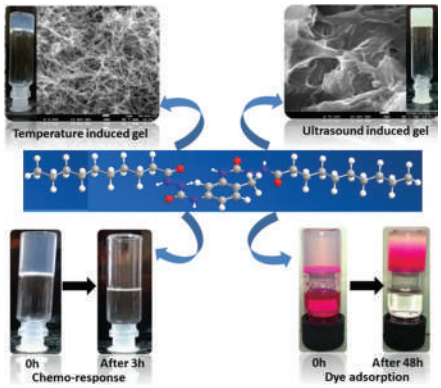
supramolecular self-assembly of porphyrin in the presence of melamine and spermine. The morphology of porphyrin in the presence of melamine and spermine was different, indicating that change in analytes could be used to control nanostructures. UV-vis and fluorescence spectroscopic methods were employed to investigate aggregation mode. The self-assembled nanostructure was confirmed by SEM imaging and XRD measurements. (*ChemistrySelect*, **2017**, 2, 1573)



Model of the melamine and piprhyrin 1 co-assembly in highly crystalline model, and in plane and out of plane electron density distribution in 1:4 porphyrin 1: melamine aggregation

Anion tuning and dye adsorbing properties thermal and ultrasound induced gels of Bis(acylsemicarbazides)

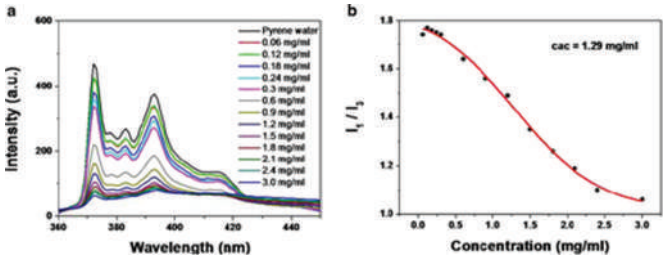
Aromatic bis(acyl-semicarbazides) carrying aromatic core and substituents of varying alkyl chain length was found to undergo gelation in selected organic solvents by thermal and Ultrasound treatment. The gels could be tuned in the presence of anions at different concentrations and addition of 5 equivalents of fluoride and acetate induced gel-sol transition. In addition, these organogels adsorbed dyes such as crystal violet and rhodamine-B from water every effectively which was confirmed by visual method and quantified by UV-vis spectrophotometry. (*Sens. Actuat. B: Chem.*, **2017**, 245, 711)



Environment

Surfactants for eco-friendly emulsion process

GPDPMA nanocomposite was modified amphiphilically to develop novel surfactants for eco-friendly emulsion process. The amphiphilic polymer-modified graphene displayed low CAC (critical aggregation concentration) value of 1.29 mg/ml as determined from the fluorescence study, similar to that of polymeric surfactants as shown in Figure.



(a) Fluorescence spectra of pyrene dispersed in aqueous solutions of S-GPDPMA at different concentrations (0.06 to 3.0 mg/mL) from top to bottom. (b) The corresponding relative fluorescence intensity (I1/I3) of pyrene against concentration of polymer-modified graphene surfactant and the CAC value. All measurements were carried out at 25 °C

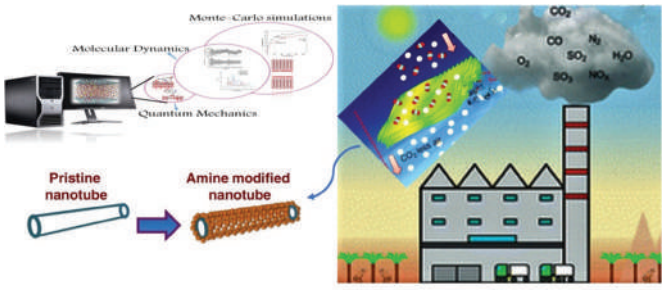
Monomers from cardanol

Cardanol derivatives and hydrogenated cardanol was utilized in the development of polymerizable monomers. The derivatives were subsequently polymerized using Controlled radical polymerization (CRP) techniques to facilitate the preparation of sequence controlled polymers like block, graft or comb polymers. Atom transfer radical polymerization (ATRP) is widely investigated for the synthesis of sequence controlled copolymers. In this work the copolymerization of styrene/methyl methacrylate with cardanyl acrylate / pentadecyl phenyl methacrylate via ATRP will be studied towards the development of novel pressure sensitive adhesives. Pure phenolic and cardanol modified phenolic resins were prepared and utilized as tackifier for nitrile latex (XNBRL) based adhesives. adhesive formulations were prepared by varying the amount of resin in XNBR latex along with other compounding ingredients and the bonding properties of these formulations were determined by lap shear test

The methacrylate derivative was sulphonated to yield reactive surfactant starting from cardanol and 3-pentadecyl phenol. The surfactant was evaluated in the semi-continuous emulsion copolymerization of acrylates and the effect of varying surfactant concentration (0.07 - 0.66 wt%) on the synthesis and polymer properties was studied. The copolymer prepared using reactive surfactant exhibits improved properties when compared to copolymer prepared using conventional surfactant. The tensile strength of the films increased from 6.6 MPa to 8.9 MPa, where the elongation at break decreased slightly from 260% to 235%. The incorporation of reactive surfactant further increased the hydrophobic characteristics of the films. The water contact angle of the film increased from 73°-92°. In summary, reactive surfactants improved the technical properties of the latex films.

Development of eco-friendly, cost-effective adsorbents for the selective capture of air-pollutants: computational screening and molecular engineering approaches

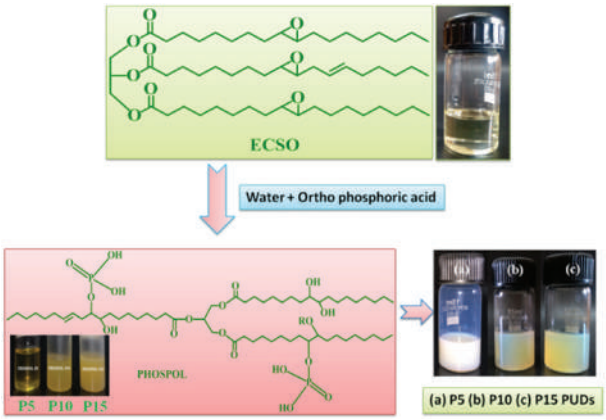
Novel adsorbents based on metal oxides for the CO_2 capture from industrial flue gases based on non-volatile amino acids and alkanol amines that are chemically grafted on TiO_2 surface were developed. The study explores the possibility of using *f*-TiO2 surface as a potential solid adsorbent to capture CO_2 at much reduced cost.



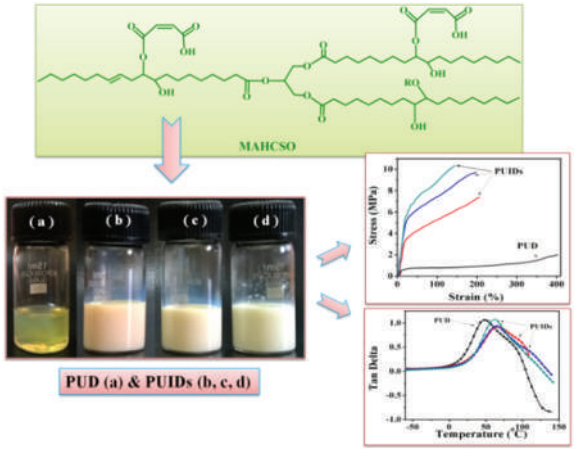
Computational Studies of Novel Solid Adsorbents for Selective Capture of CO_2 ,CH_4, NO_x and SO_x Gases

Water borne dispersions from vegetable oils for coating applications

Three different phosphorylated polyols (phospols), bearing both hydroxyl and ionizable phosphoryl groups (phospol-P5, P10, P15) having hydroxyl numbers 130, 160 and 180 mg KOH/g, were synthesized through the ring opening hydrolysis of epoxidised cottonseed oil (ECSO) in presence of *ortho* phosphoric acid and were used as internal emulsifiers in waterborne PUDs with isophorone diisocyanate and 3-aminopropyl triethoxysilane (APTES). All the three PU dispersions showed excellent storage stability (> 6 months) and the average particle size of PUDs ranged from 30 to 68 nm. The films of phospol-P5 based dispersion, exhibited the highest tensile strength, thermal stability, T_g value, contact angle and good anticorrosive property. (*ACS Sustain. Chem. Engg.*, **2017**, *5* (8), 6447)

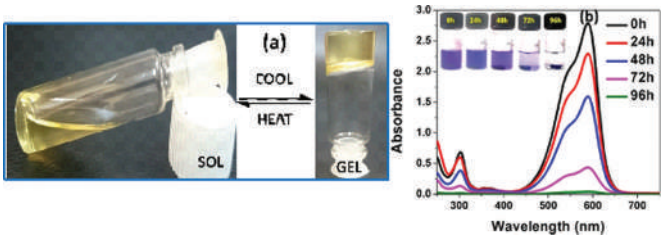


DMPA free, catalyst free, anionic waterborne polyurethane-imide (PUID) dispersions have been successfully synthesized by using maleated cottonseed oil polyol (MAHCSO) as an ionic soft segment, tolylene diisocyanate and dianhydrides as chain extenders. It was found that the tensile properties, thermal stability, water contact angle, and T_g values of PUIDs were remarkably high compared to conventional PUDs. (*Indust. Crops Prod.*, **2017**, 96, 132)



Stimuli responsive gels for selective adsorption of dyes from wastewater

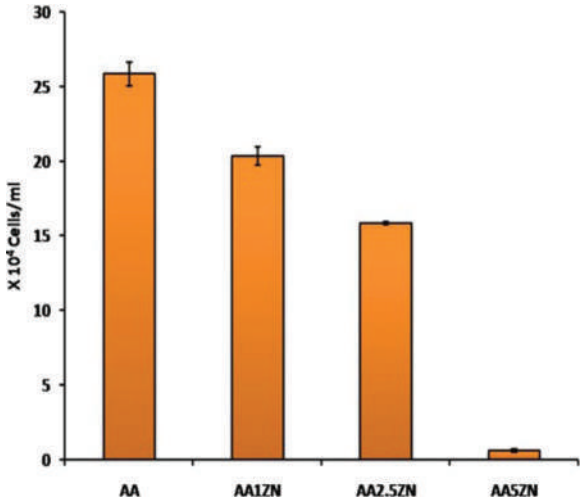
The polymers with a slightly different chemical backbone had capability of adsorbing crystal violet from their aqueous and desorbing in organic solvents like acetone and methanol in the xerogel state as well as native state. (*Polymer,* **2017**, 114, 199)



Health care

Cell Adhesion Resistant Polymers for Intraocular Lens Application

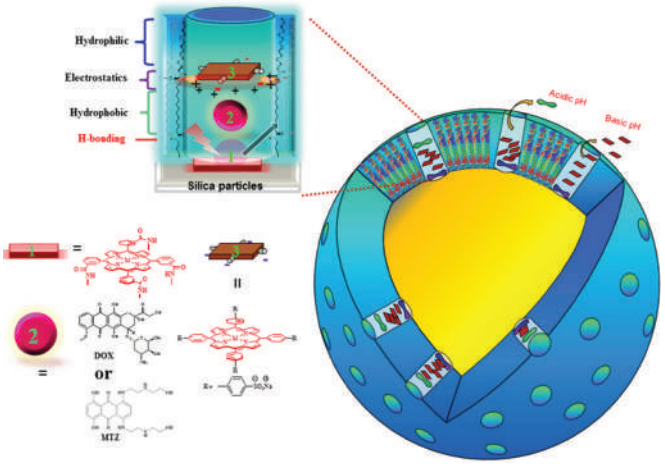
Patients afflicted with cataract suffer vision loss due to opacified intraocular lens (IOL) in eye. Most preferred treatment for this is replacing the diseased natural lens with artificial polymeric lens. Following surgery, many times, a secondary cataract (Posterior capsular opacification, PCO) occurs due to proliferation of remaining endothelial cells which attach to the lens and thus compromise vision. We found that addition of Zinc oxide nanoparticles (5 pph concentration) to a transparent polymer drastically reduces the number of fibroblast cells that are attached to it otherwise. These ZnO polymer nanocomposites have all other optical, physical, chemical, processing and handling properties required for manufacture and use of IOLs. (*Polymers for Adv. Tech.,* **2017**, 29(4), 1234; *J. Appl. Polymer Sci.*, **2017**, 134(8), 44496)



Number of cells attached to films. [AA: Film without ZnO, AA1ZN, AA2.5Zn and AA5Zn are nanocomposites of AA with 1, 2.5 and 5 pph ZnO]

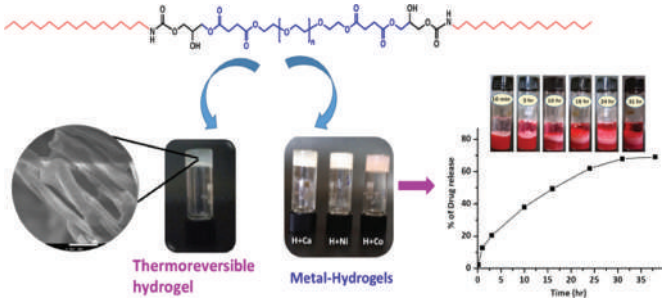
Magnetic silica nanoparticles for targeted delivery

Octowells on the magnetic silica nanoparticles for targeted delivery and reusable applications, and second is the encapsulation drug DOX or MTZ and their release by manipulating naturally occurring stimuli in vivo, that is, pH is reported for first time. Designer yoctowells, may act as tiny chemical reactors or alternatives in vivo drug-delivery systems by manipulating the interactions between drug molecules and the walls of yoctowell gaps and/or base porphyrin, and are thought to provide a useful supramolecular tool and could open new opportunities in the realm for targeted therapies. (*Open Access J. Sci.,* **2017**, 1, 00013)



Graphical illustration to demonstrate encapsulation of drug molecules 2 and capping porphyrin on the top to cover the wells and their step-by-step release by manipulation naturally occurring stimulus

Gels for controlled release of vitamins



A class of biscarbamates with hydrophilic PEG chains in the core and hydrophobic alkyl chains at the termini linked through hydroxyurethane moieties were found to aggregate in water into thermoreversible gels. The gel-sol transition took place upon repeated heating and cooling cycles. In addition, incorporation of metal ions increased the mechanical strength and thermal stability which was assisted by complex formation between the metal ions and gelator molecules. One of the metal ion responsive hydrogel was capable of entrapping vitamin B_{12} and the slow release of drug molecule was triggered in acidic medium.

APPLIED RESEARCH

Laboratory process for synthesis of Crospovidone

Crospovidone polymers are synthetic, insoluble, cross-linked homopolymers of N-vinyl-2-pyrrolidone (NVP). They find wide use in pharmaceutical industry, mainly for their swelling properties. Their use as pharmaceutical excipients depends mainly on their disintegration effect in tablets, their ability to hydrolyze insoluble drugs, to stabilize suspensions and to form complexes. Due to their non ionic nature, pyrrolidone chemistry and porous morphology, Crospovidones are the disintegrants of choice for rapid disintegration, enhanced rate of drug dissolution and robust tablets. These polymers combine multiple mechanisms to achieve disintegration at low levels of use. They also provide other advantages like swelling without gelling, increase tablet breaking force, reduce friability, enhance solubility of poorly soluble drugs etc. Apart from Pharmaceutical applications, Crospovidone finds utility in beverage industry also as a filtering aid. For example it is used in breweries to enhance clarity of beer during storage.

A laboratory scale process has been developed and optimized to synthesize Crospovidone that meets pharmacopeia specifications. The same process was demonstrated and transferred to a client.

Development of Carboxylated Butadiene-Nitrile Latex (CBNL)

Butadiene-nitrile latex polymers possess several unique and excellent properties like oil resistance, abrasion resistance and are elastomeric in nature. Carboxylated nitrile rubber lattices are used in a wide variety of industrial applications, such as in the manufacture of gloves, non-woven fabrics, masking tape, gaskets and an array of other products. The carboxyl modification of nitrile rubber (NBR) produces a material that has outstanding abrasion resistance.

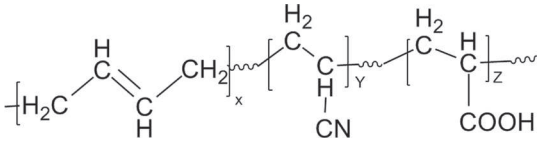


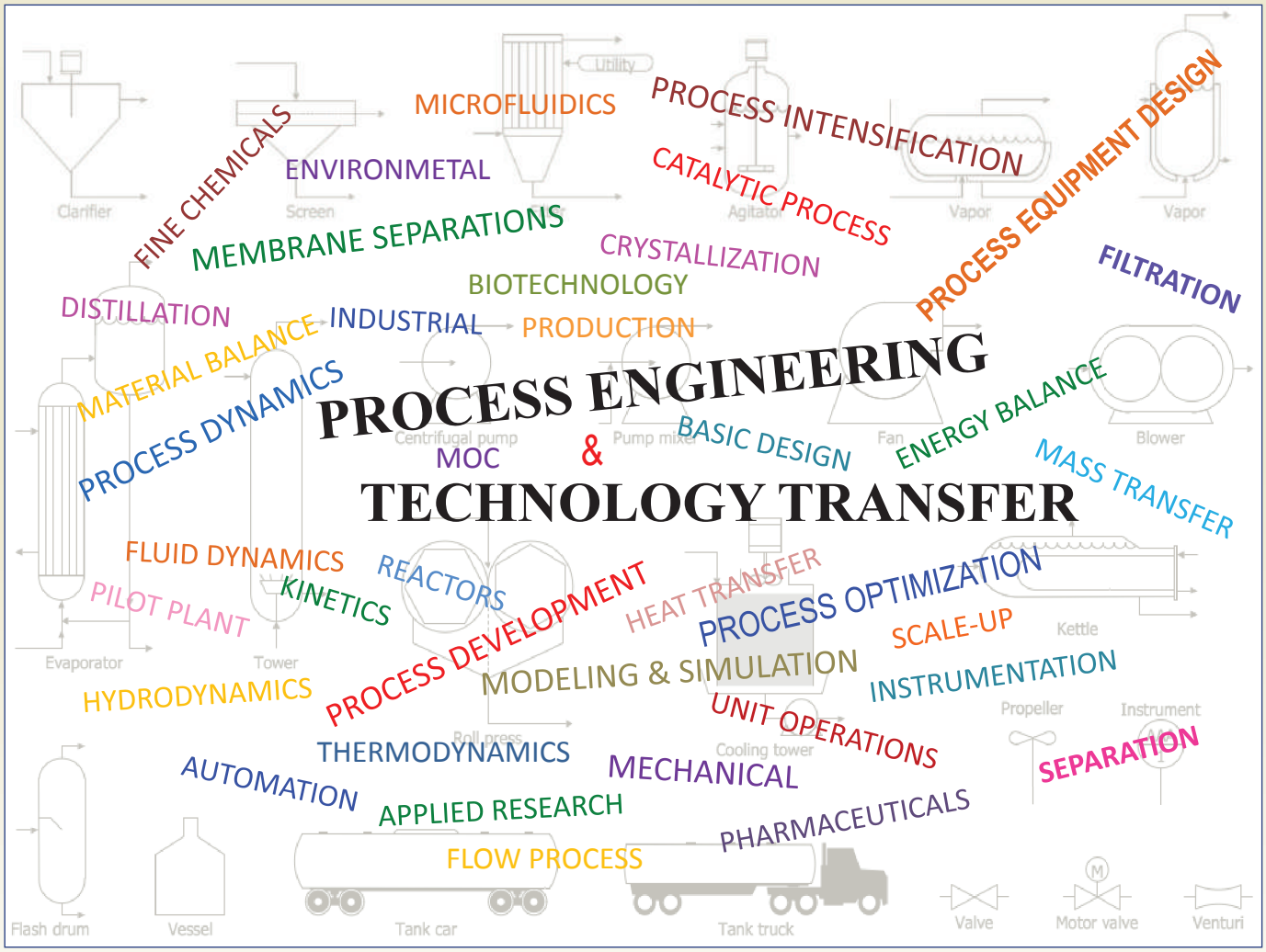
Figure 5

They contain pendent carboxyl groups at random sites along the main chain. The introduction of pendent carboxyl groups and the subsequent formation of ion rich aggregates at these sites profoundly affect vulcanizate properties. In a project sponsored by DRDO, the synthesis and compounding of CBNL on 500 g scale has been carried out.

Polyols from non edible vegetable oils for rigid PU foam applications

Biopolyols are now in demand because of growing environmental legislations, Technology knowhow for polyols from castor oil was demonstrated to industry as per the work proposed in the project titled "Technology for the development of polyols from renewable plant oils/agro based non edible oils" sponsored by Ministry of environment, forests and climate change on 500 g scale. The polyols with hydroxyl value ranging from 300 to 550 can be used for rigid PU foam development in the place of petro based polyol for a similar application.

PROCESS ENGINEERING & TECHNOLOGY TRANSFER

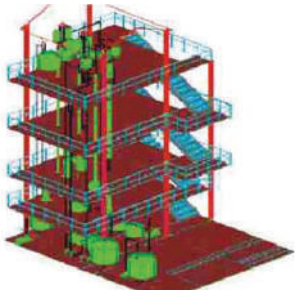


The Process Engineering and Technology Transfer (PETT) Department has a unique facility 'Mechanical Design and Engineering'; which forms the final link before the technology is transferred to the industry. The Group offers Mechanical Design and detailed engineering inputs for the establishment of Bench/ Pilot/Commercial scale process plants for the processes developed at CSIR-IICT and other CSIR Labs. Design and development of specialized equipment and test facilities is also one of the major activities of the Division. The expertise of the Division extends to other related areas like Project Engineering, Process Safety and Applied Research in Process Plant Engineering. A Computer Aided Engineering & Design (CAED) Centre was established to modernize the detailed engineering activities. A number of CAED software useful for speedy transfer of technology to chemical and bio-chemical process plants have been developed. Facilities exist at the CAED Centre for preparing 2D process plant engineering drawings, piping analysis and engineering, design appraisal utilizing finite element analysis, conversion of old drawings by large format scanning, 3D photorealistic modeling, Solid modeling, training, multimedia and engineering documentation.

Detailed Engineering of Pilot Plants

Design Appraisal

CAED Centre



3D Modeling of the plant

APPLIED RESEARCH

Vibration behavior of non-metallic bellows and pipes

The dynamic behavior of non-metallic bellows under different end and operating conditions is being studied. An experimental set-up has been established and work

is in progress to develop a theoretical model and to validate the model by collecting experimental data. Similarly, vibration behavior of fluid conveying pipes with different end conditions was studied for their natural frequencies and validated by experiment and simulation.

(Int. J. Mech. Engg. Automat., **2017**, 4(3),77; *Int. J. Mech. Engg. Automat.,* **2016**, 3(6),239; *Int. J. Mech. Engg. Automat.,* **2016**, 3(12),471; *J. Hydrocarbon Process.,* **2016**, 1; *Int. J. Mech. Engg. Automat.,* **2016**, 3(3), 96*; Int. J. Mech. Engg. Automat.,* **2016**, 3(8), 319)

Severe Plastic Deformation

Study on production of nanomaterial by the SPD methods is underway, which is a top-down approach-Experimental and theoretical (multi-scale modeling and simulation) studies are required to develop a SPD method. Study will include use of SPD method to process different materials and alloys.

ENGINEERING DESIGNS

Detailed Engineering for Hydrazine Hydrate Technology

IICT has developed a new process route for the production of Hydrazine Hydrate and has transferred the technology to Gujarat Alkalies and Chemicals Ltd, Gujarat. The scaled-up process at the pilot plant level was successfully commissioned and process demonstrated and product had met the international specifications. The design data for the commercial plant were collected from the process trials at the pilot scale, which was utilized for scale-up and commercial plant designs. This technology is further scaled up to the commercial level of 10000 TPA for which the Basic Engineering Design Package was submitted. The complete detailed engineering package was vetted by LTHE –Mumbai.

It is envisaged that the 10000TPA commercial plant for production of 80% hydrazine hydrate, will be commissioned by 2021.

The work involves:

- Detailed specifications of process equipment
- Detailed Drawings of specialized equipment
- Layout and elevation of the plant
- Piping specifications and piping engineering and detailing

Basic Engineering Package for: PTBMB; Benz aldehyde; Lily aldehyde; 4-MAP Paramethoxy acetophenone and Para methyl phenyl acetic acid Technologies

Processes for the manufacture of the above have been developed by IICT and the technology to manufacture these chemicals shall be transferred to Vinati Organics Ltd., Mumbai, in the form of a Basic Engineering Package.

The PTBT and PTBBA commercial plants were commissioned successfully in 2017-18. CSIR Technology Award for PTBT and PTBBA technologies was awarded to the Team.

Bioprocess

Pretreatment is the key process step in 2G ethanol technology mainly involves modification of biomass material and making accessible to enzymatic saccharification. The saccharification process is influenced by process steps- milling and pretreatment. Several pretreatment processes developed consume high energy. CSIR-IICT has developed simple and novel chemical treatment process which operates at 45-50 deg. C and atmospheric pressure. The pretreated biomass retains more than 98% cellulose and hemicelluloses; and removes 80% of lignin. The pretreated water can be recycled 5-6 times and lignin rich water is passed through membrane to recycle 80% back. The remaining 20% can be sent for lignin valorization. The pretreated biomass showed effective saccharification of cellulose and hemicelluloses with commercial enzyme and obtained more than 70% saccharification within 16-20hr which depends on the substrate enzyme ratio. The above data was generated using high biomass sorghum and rice straw in a makeshift pilot facility to process up to 50kg of biomass on a batch mode.

This group was associated in trial runs conducted in pilot plant for pretreatment of biomass by the chemical and steam explosion methods. The pretreated biomass has applications: in making of ethanol, as cattle fodder etc.

3D Plant modeling

The hydrazine Hydrate pilot plant, which was successfully commissioned, was modeled in 3D using Solid works software, as an experiment. The aim of this work was to determine the capabilities of the software in modeling process plants and piping and also get an

idea of the ease with which the modeling can be done. It also served to train the staff in the use of the software. Precise 3D models were created for various components like:

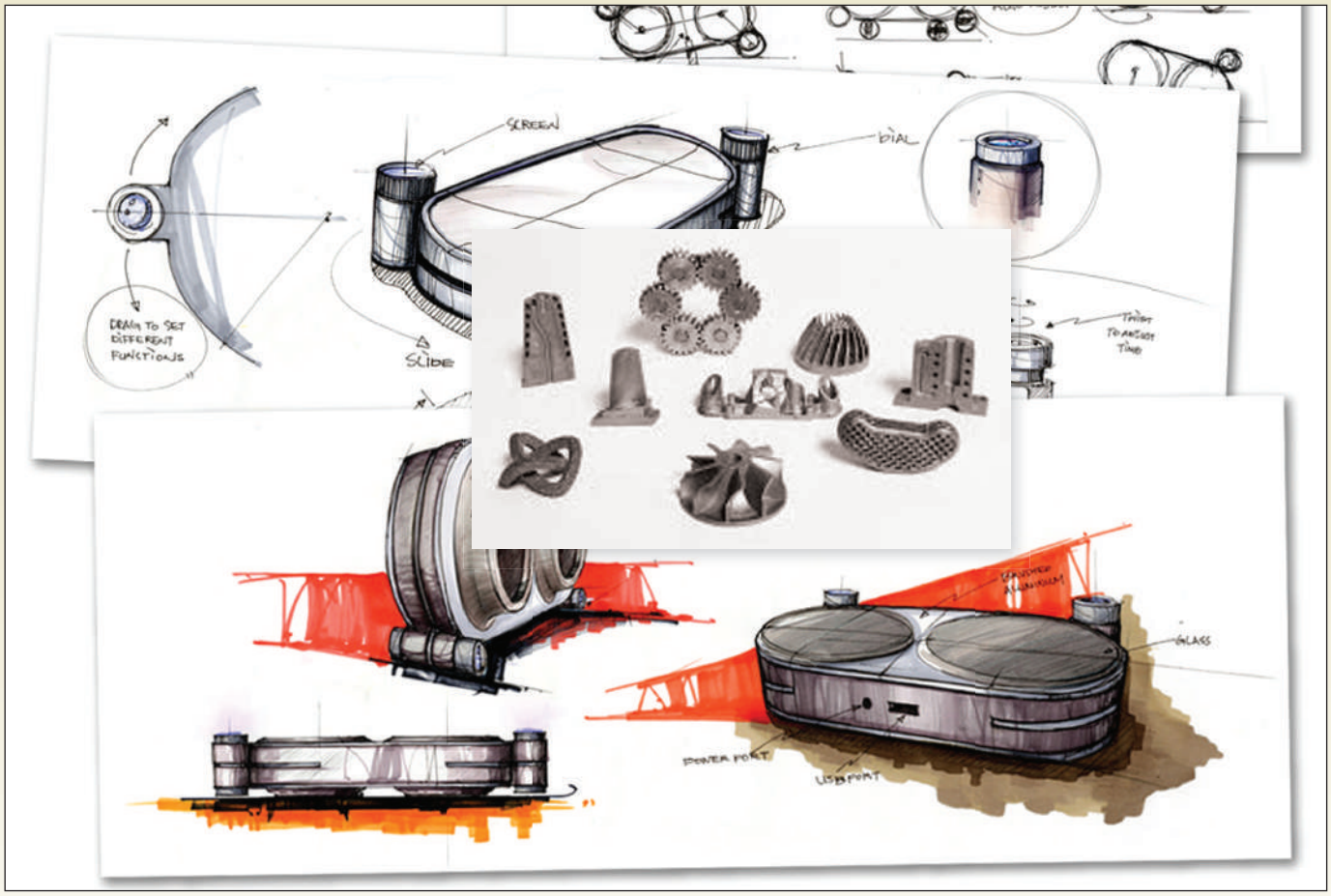
- All the structural members
- Fabricated process equipment
- Vendor equipment like pumps
- Piping and piping components Database were created for subsequent use
- The utility of software is a 3d view of plant is modeled to have clarity on equipment positioning and get good estimate of piping and piping components

CAD model of the HH pilot plant

New Equipment Installed

- AutoCAD 2015 - 2D & 3D Drafting / modeling software
- Up gradation of solid works premium software
- ABAQUS software for fluid flow and thermal problems

PROTOTYPE DEVELOPMENT & PROJECT ENGINEERING



The Prototype Development and Project Engineering (PDPE) division administers a big Central Workshop & a Pilot Plant Complex (PPC) at Moula-Ali to provide vital *prototype development* and *project engineering* support to R&D activities. Besides, the division pursued its own R&D activities in the areas of vegetable oil extraction & Gasification of Biomasses.

The PDPE Division was re-organized from its earlier composition that also included electrical, standby power generators, air-conditioning and carpentry on December, 26th, 2016. Further, on 21 February 2018, the PDPE Division, Chemical Engineering, Design & Engineering Division and Instrumentation Division were amalgamated into a new entity namely, Process Engineering & Technology Transfer (PETT) Division.

The Project Engineering Support Activities:

1. Catering to the general engineering support associated with R&D of the institute through the administration of Machine Shop, Fabrication Shop, Foundry and Black Smithy unit, Mechanical Maintenance Services, Boilers, Glass Blowing. In all about 450 work orders were executed.
2. Installation and commissioning of modern chemical laboratory lab fixtures. overseeing installation and commissioning of modern chemical laboratory lab fixtures namely the state of the art Fume Hoods and Work Benches complete with chemical storage and fireproof solvent storage units (meeting international standards such as ASHRAE 110(95) and EN 14175 (2003)) across various chemical laboratories continued in the reporting period. The reminder unfinished work part of about 10-15% of renovation works has been completed. The entire project installed quantities since the beginning of the project was accounted and handed over to the respective scientists and staff. Further, verification of all the invoices and preparation for consolidated invoice and submission of bills was facilitated and completed.
3. Planning, procurement and installation of Class 10000, HVAC facility for NEW Animal House. Provided basic designs inputs, scrutinizing the tenders, the recommendation of modifications in the area of air-conditioning and electrical component part of the project. The order is placed with M/s I-clean Pvt. Limited and the project is completed & commissioned.
4. Facilitated installation and commissioning of the pilot plant for production of Bio-Hydrogen from industrial/ domestic waste through dark fermentation Route in a 1000Ltrs reactor at PPC Moula Ali.
5. Installation and commissioning of over 50 air conditioners in various configurations (Split type, Verticool type, Cassette type) across the institute including maintenance services of ACR equipment air-conditioners, refrigerators, chillers, water coolers, HVAC systems for Animal House, cold rooms, central plants for Auditorium, New Lecture Hall and committee rooms, conference rooms.
6. Maintenance of wooden furniture of the Institute and development of storage units and stand-alone fume hoods.
7. Renovation IICT substation-2 and HT yard were completed. This will improve the electrical reliability of the connected areas and decrease the electrical breakdowns. This will leave an indelible positive impact on IICT R&D activities in the years to come.
8. Stricter monitoring of power factor close to unity improved energy savings and reduce breakdown of electrical equipment and other sophisticated instruments across the Institute. Improvements in electrical infrastructure across IICT ensured safety and reliable power supply with zero electrical accidents.
9. Conceptual design, verification of specifications, technical, administrative and financial planning, overseeing execution, troubleshooting and financial closure in respect of following electrical works as part of institute's electrical renovation, modernization and upgradation and maintenance.
   - Renovation of Lighting & Power circuits at Old Laboratory Buildings at IICT (Phase – I).
   - Electrical Renovation of BMA and X-Ray Divisions Ground floor.
   - Replacement of Power Control Centres at NPC building Ground & First floor.
   - Electrification of HRTEM and XPS instruments at Discovery building Ground floor- south wing.
   - Augmentation of Power supply cable & Power Control Centre at Chemical Engineering Pilot Plant (Biodiesel plant).
   - Electrification for Extension of Computer Division.

- Electrical renovation of Chemical Engineering Pilot plant.
- Electrical Renovation of BMA and X-Ray Division Extension.
- Electrical Renovation of block housing A.O. Office.
- Electrical Renovation of Biology Division Laboratory Ground floor.
- Renovation of Renovation of Toilets at various parts of ICT.
- Providing Power supply to the New Servers at Computer Division, IICT Hyderabad.
- Providing false ceiling Luminaries for Biomaterials Laboratory and Fluoro-Organics Division.
- Electrification of High Mast Flag near Main Gate.
- Electrical renovation of ground floor sitting room of the Engineering Services Division.
- Providing UPS power supply for newly installed Network switches & Wi-Fi Access points at various locations of CSIR IICT.
- SITC of LED Street Lights and other street light luminaries across various parts of IICT and staff quarters.
- Electrical renovation of various vehicle parking areas and staff quarters.
- Preventive and breakdown maintenance of electrical switchgear at one no. 33/11kV and 4nos of 11kV/415V substations IICT and PPC Moulali Complex, 6nos. DG Sets and one no. synchronization panel.

R&D and Prototype Development Activities:

Development of sustainable and greener technologies using mechano-chemical processing for vegetable oil extraction and value addition under PEOPLE HOPE project (CSC-0112) Investigations into the extraction of oil directly from the comminuted seed mass using lab scale high-speed centrifuge with or without extraction aids. Batch centrifuges with vessel capacities ranging from 5ml to 200ml were tried with speeds ranging from 7500rpm to 70000rpm with milling times ranging from 5mins to 5 hours for the extraction of oil directly from the comminuted seed mass.

- The maximum achievable yield was 25% residual oil in the oil cake.
- Various additives, both physical and chemical, were screened for improving the extraction efficiency during centrifugal separation of oil from the comminuted seed mass during the reporting period.
- Aqueous ammonia and lactic acid addition in the range of 10% to 15% showed decent improvement in the extraction yield to an extent of 10% to 15% residual oil in the oil cake.

Extraction of Oils using Lactic Acid Addition

- The lactic acid addition has been tried at 5%, 10% and 15%. The lactic was added to the comminuted seed mass and subjected to centrifugal separation at 12000RPM for 30 min duration as earlier studies. The oil recovery was found to be 85% to 90% which is closer to mechanical expelling efficiencies reported in the literature.
- Although lactic acid addition has shown decent extraction efficiency of about 10% residual in the cake the FFA of the cake shown very high value.

Extraction of Oils using Ammonia as an additive

- Trials with 10% aqueous ammonia in a 50gms per batch showed extraction efficiencies up to 8% residual oil in the cake.
- Aqueous ammonia assisted oil extraction was tried at 1kg per batch at 8% to 24% addition concentration on a weight basis in a basket centrifuge of 2.5 litres vessel capacity capable of running at 4500RPM. Experiments were conducted with two types of seeds namely comminuted ground nut and comminuted mustard. Addition of aqueous ammonia at 20% to 24% showed better extraction efficiencies of approx. 15% to 18% residual oil in the oil cake in a three-stage centrifugation of 30 min duration each at 4500RPM both in the cases of groundnut and mustard.
- Analysis for the presence of ammonia in the oil and oil cake was conducted using the N-H-C-S analyser. Oil samples did not show the presence of ammonia in the extracted oil. On the other hand, oil cake showed the presence of ammonia measured in the form of Nitrogen levels.
- In addition, FFA content of the aqueous ammonia assisted extracted oil was measured according to AOCS standards. FFA to an extent of about 0.15% on the weight basis was found to be present in the oil.

Other Extraction Routes tried

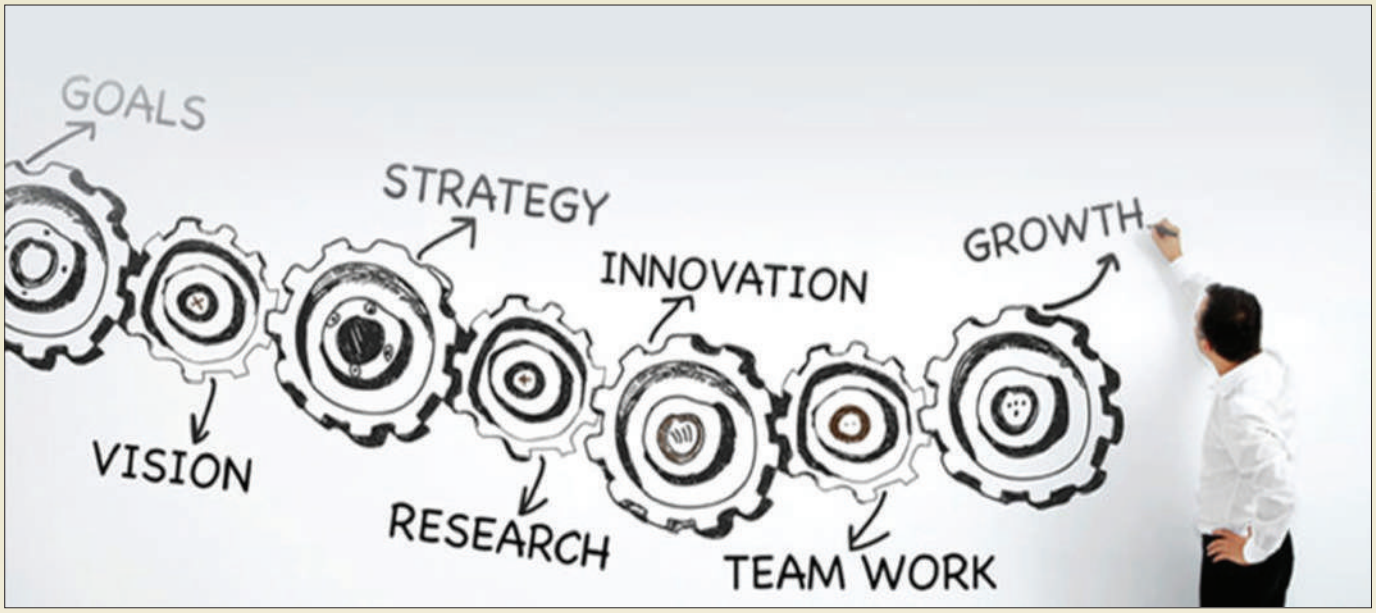
- **Aqueous extraction:** Comminution in an aqueous medium followed by centrifugal separation seems to show decent extraction efficiency (18% oil in the residual meal)
- **Solvent extraction of groundnut oil using D-Limonene, a green solvent, an agricultural by-product from the citrus industry:** An extraction efficiency of over 94% was achieved at seed powder to solvent ratio of 1:6 and centrifugation times of over 60 mins. Cost of the solvent is an issue.
- **Solvent extraction of groundnut oil by acid hydrolysis route using citric acid as a solvent:** Approximately 82% clear oil has been extracted from the seed. A gel was formed after centrifugation which contains sugars and proteins.

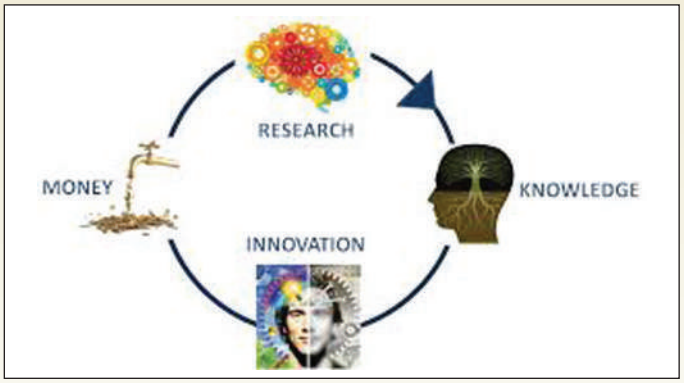
1. **Development of a prototype solar-powered window air-conditioner with automobile compressor**. A circuit was developed integrating MPPT (30-40Amps & 48V) and DC output from SMPS into a single module and connected to the power input to the 48V DC automobile compressor procured for the purpose. The entire air conditioner system was connected to 1.5kWp solar panels and test ran successfully.
2. **Engineering interventions to grassroot innovations as part of Corporate Social Responsibility of CSIR-IICT.** A MoU was signed with an NGO named Palle Srujana and activities have been taken up. In the first phase, the following Grass root innovations were supported in the reporting period.
   - Development of 5-speed tiller based on the 7-speed tiller
   - Improvements to the multiple brick making unit
   - Development of water pumping units resisting sand particle erosion and saltwater corrosion for the mastless windmill. The in-house fabricated units were installed at the project site West Gogulapally, Nellore District. It is undergoing service trials.
3. Coordinated **the Scientific Interventions Societal Problems (***as part of an initiative from CSIR Head Quarters***)** activity from a short listing of the potential problems to the approval, in-house financial sanction and overseeing execution.
   - Development of a cost-effective portable catalytic device for controlling microorganism in drinking water
   - Marker Compounds based Standardization of Herbal Drugs/Formulations
   - Establishing Drug Testing Facility
   - Promotion of Sustainable Agriculture using Pheromone Application Technology (PAT) for the control of Horticultural Insect Pests
4. **Repair and overhauling of Bio-Mass Gassification Unit**: Skid mounted bio-mass system comprising gasifier, feeder, pre-heater, pre-mixture, scrubber, GLS, peristaltic pump, Mass flow controller is reinstalled at PDPE Division to carry out R&D in the gasification of various bio-masses.

   Modifications were carried out in the system in the following sections.
   - The suction or feeding pipe of size 2" connecting to the hopper to Preheater was not properly aligned for the rice husk. The same is arranged for a new pipe of diameter 3" MS with a reducer angled at 55 Deg from the hopper through the drive to the preheater so as to feed the husk into the pre-heater without choking in the feed pipe.
   - The new pre-heater vessel was designed with 6" Dia. MS pipe to enable to test the heating patterns in the pre-heater with new feeding pipe. The grate for ash removal is designed with a coarse mesh.
   - The solid state relays (SSRs) in the control panel were replaced with new SSRs and the control panel was re-commissioned and tested all the controls were functioning properly including heating systems for the pre-mixture and the gasifier.
   - An online NUCON make Gas Chromatography unit was procured and commissioned with viz., Hydrogen, Nitrogen, Zero air cylinders and a gas station in between the gas cylinders and the GC unit.
   - The portable gas operated genset is run tested for power generation.
5. Rendering technical services to M/s BHEL R&D at Pilot Plant Complex, Moulali the Division generated revenue in the reporting period.

R&D SUPPORT

BUSINESS DEVELOPMENT & RESEARCH MANAGEMENT





Business Development and Research Management is a liaison & facilitation intensive, core department of CSIR-IICT that enables in realization of the roadmap laid by the organization. The department activity focuses on promoting the strengths & capability of the institute at all appropriate forums as part of business development and deals with management of projects funded by industry / strategic / CSIR and has been nodal for execution of various outreach programs.

The following encompass the major activities of the Department:

A) Business Development
B) Management of industry funded projects
C) Management of CSIR Funded Projects
D) Skill Development & Entrepreneurship Programs
E) International Collaborations
F) Outreach activities (Aspirational districts by NITI Aayog)

A) Business Development:

Based on the current R&D trends knowledge generated by interacting with industry and academicians from time to time the department passes on the information to concerned scientists for working on novel and need based problems. To harness this potential, the department creates seamless interaction platforms to identify areas of collaboration that match the business interests of the clients. In this connection, the department works closely with the research groups of CSIR-IICT by organizing Industry-Interaction meetings. This industry outreach program, aims to facilitate one-to-one interaction between industry personnel and scientists of the Institute that culminates into fruitful collaborations.

The core strengths of the institute are classified into five major streams of chemistry (pharma, industrial chemicals, agrochemicals, materials & environment) with support departments of analytical, biology and engineering. Prospective industries are mapped against these sectors for building businesses. Connects with major associations like IDMA, BDMA, PCB and PMFAI are made with B2B meetings to advertise and propagate the strengths and capabilities of the institute showcasing both scientific expertise and infrastructure that can cater to the requirements of the industry.

Industry meets/ Road shows are organized biannually with panel discussions by experts on topics pertaining to current R&D issues and probable solutions that CSIR-IICT can offer.

Visits to major exhibitions & events like ISC, iPhex, CPhi, ICC, FICCI etc, are made where posters & exhibits are displayed. Also appropriate lectures with clear objectives are delivered on such occasions to capture the interest of new clientele.

B) Management of Private Industry Funded Projects:

The department undertakes project management of technical, consultancy and sponsored research. The following are the multifarious activities executed:

- Facilitating interactions between CSIR-IICT management, scientists and industrial clients to finalise the scientific framework of collaboration
- Conducting negotiations with industries for identifying and finalizing new research collaborations.
- Arranging Non-Disclosure Agreements for exchange of information.
- Preparation of financial estimates and project to management and clients the financial aspects of collaboration
- Drafting, negotiating and finalizing agreements for sponsored, consultancy, and collaborative projects with scientific, technical, Intellectual Property Rights, financial, administrative aspects of collaboration in regular contact with clients and scientists.
- Obtaining necessary approvals from CSIR-IICT management, Management Council and CSIR HQ, wherever they are needed.
- Facilitating for realization of obligations spelled out by clients in the contracts
- Project Monitoring and Evaluation of all Industrial projects through periodical review meetings.
- Regular contact with clients and scientific teams to monitor the progress and activities of ongoing collaborations to facilitate for smooth and timely completion of the projects.
- Raising Invoice and processing the payments received from clients
- Coordinating GST payments with Accounts department
- Attending audit queries related to industry projects whenever necessary.

- Facilitating Vendor Registration Forms, Receipts and TDS forms with Clients.

Total no of projects undertaken with industries during the period of 2016-2017 is 82.

S.No	Title of the Project
1	Advisory consultancy in the field of organic synthesis, process development
2	Preparation of local oil spill disaster contingency plan
3	Micellar characterization study for Decetoxel injection
4	Providing consultancy in improvement in the process of production of Hi Strength Hypo
5	Estimation of Impurity in Voriconazole Drug using Ion Exchange Chromatography (IEC)
6	Consultancy in Analysis NMR samples
7	Consultancy in analyzing samples using microwave facility
8	Providing consultancy in PXRD analysis of pharmaceutical samples
9	Consultancy in NMR analysis
10	Analysis and data interpretation of Biodiesel samples
11	Consultancy on moisture cured PU coal tar black
12	Consultancy in NMR analysis
13	Consultancy on testing of epoxy and coal based paints on water pipe lines
14	Analysis and data interpretation of fatty oils for physicochemical characterization
15	Analysis of samples through LCMS, GCMS and EIMS
16	Utilization of existing facilities of Chemical Biology Division
17	Consultancy on analysis of NMR Samples
18	Providing consultancy in the field of Molecular Modeling
19	Evaluation of chemical disinfection unit plant
20	Analysis of samples to test for 100% solvent less food grade epoxy (6 samples)
21	Physico-Chemical and compositional studies of Soldier Fly Insect Oil
22	Testing of Dettol Antiseptic liquid & Harpic disinfectant
23	Cooperative Bioefficacy data generation of Prallethrin Neem and combined mosquito coil formulations
24	Comparative bio-efficacy data generation of Transfluthrin Neem liquid vaporizer
25	Classification of Triphenyl Phosphene
26	Consultancy on Anti-Rodent tests for DWC pipe samples
27	Consultancy on Anti-Rodent tests
28	Preparation and supply of microbial culture for deodorization
29	Testing of polymer coated samples
30	Consultancy on NMR analysis
31	Consultancy on NMR analysis
32	Fatty acid composition analysis of algal biomass samples (34 samples)
33	Consultancy on NMR analysis
34	Consultancy services in the area of vegetable oil, vanaspathi and allied products
35	Consultancy on NMR analysis
36	Consultancy on NMR analysis
37	Consultancy on anti rodent testing (4-samples)
38	Process optimisation of intermediates
39	Analysis and data interpretation of Biodiesel samples
40	Hazop study and risk analysis for soda recovery plant-II
41	Consultancy on NMR analysis
42	Providing consultancy in PXRD analysis of pharma samples.
43	Antirodent evaluation of samples
44	Providing consultancy in making of 2-octyl-cyanocrylate
45	Analysis of samples using Microwave facility.
46	High rate biomethanation of organic waste for generation of power for off-grid applications
47	Providing consultancy in upgardation of commercial plant design from 2000 TPA to 3000TPA for paratertiary butyl methyl benzoate (PTBMB)
48	Providing Oligonucleotide facilities
49	Analysis of samples using NMR analysis

S.No	Title of the Project
50	Analysis of samples using NMR analysis
51	Providing consultancy in the process development of Fexofenadine, Flucanazole and suggamoneddex
52	Processing and Analytical methodologies of oils and fats
53	Evaluation of antidiabetic potential of two herbal extracts in diabetic
54	Analysis of samples through Proton NMR, Mass spectrometer, HPLC
55	Characterization and refining of crude tobacco seed oil
56	Synthesis of New Chemical Entities (NCE's)
57	Biosyn gas derived dimethyl ether synthesis for LPG Blending.
58	Process knowhow for the upgradation and bleaching of crude rice bran wax.
59	Nanofiltration process for removal of chloride from TATA Steel effluent on bench scale with a feed capacity of 20L.
60	Process knowhow for Annona squamosa extracts and isolation
61	Labscale process for Anisole
62	Development of vapour phase catalytic process for the synthesis of iminostillene from umunodinezyl
63	Development of process knowhow for the upgradation and bleaching of crude rice bran wax
64	Development of process knowhow for the up gradation and bleaching of crude rice
65	Design and development of active layer materials for flexible solar cells
66	Cyclization of Arene by photochemical reaction
67	Synthesis of 5-Benzyloxy 4-hydroxy-6-(hydroxymethyl) pyridine 3-carboxylic acid
68	Process development of Cyazofamid (Fungicide)
69	Development of Crospovidone (Type A)
70	Development of process knowhow for APIs/ intermediates
71	Collaboration for research and development of processes for new molecules and API's
72	Water purification technology for fabrication of membrane based demineralised water plants of 25-50 2PH capacity plant
73	Development of an advanced Mg Ion battery
74	Licensing of Anaerobic gas lift reactor
75	Licensing of modular high rate Biodigester
76	Development of process knowhow for APIs/ reference compounds
77	Process development for the production of Paracetmol using Acetic acid and submission of BDR for commercial plant of 10000TPA capacity
78	Selective catalytic hydroxylation of benzene with molecular oxygen
79	Process development for the enrichment of GLA atleast 98% Boraglonl
80	Development of rechargeable Mg Ion battery chemistry for powering defence ground applications
81	Process Development and BDR for the commercial plant of Arobenzene
82	Licensing of Modular High rate biodigester

Total no of projects undertaken with industries during the period of 2017-2018 is 47.

S.No	Title of the Project
1	Anti rodent evaluation of rodent species
2	Providing advisory consultancy in the field of organic synthesis
3	Providing advisory consultancy in the area of heterogeneous catalysis
4	Providing technical report on the use of thermal resistant coating on chimney
5	Testing of thermal and corrosion resistant coating
6	Single crystal studies on Novel Polymorphic forms of API's
7	Providing consultancy on PXRD analysis of pharmaceuticals samples
8	Providing advisory consultancy in the area of double shooting in chemistry
9	Consultancy in the field of novel adjuvants including emulsions
10	Analysis of samples using LC-HRMS (50-samples)
11	Providing advisory consultancy in the field of Natural Product extraction and Isolation

S.No	Title of the Project
12	Providing consultancy services in the area of vegetable oil, Vanasapathi
13	Advisory consultancy in installing biofilters control odour
14	Advisory consultancy in the field of for castor poluols based rigid foams
15	Providing advisory consultrancy in making of 2-octyl-cyanoacrylate
16	Validation and estimation of impurity -E in voriconazole drug using Ion Exchange Chromatograph
17	Report on import of Bromofluoromethane
18	Consultancy on import of purchase of Carbon tetrachloride to use in bv acid chloride process
19	Consultancy on anti rodent testing
20	Providing NMR spectrometer services
21	Consultancy on import or purchase of HCFC-13a to use in manufacture of Halothane
22	Processing and analytical methodologies of oils and fats (18 participants)
23	Literature renew & opinion report on four catalogue chemicals
24	Design & fabrication of membrane based water purification plants of 300-2000 litres/hr capacity
25	Process development for preparation of Extra White Starch
26	Providing incubation space to carryout projects related to API's
27	Modelling and simulation of blending unit operation
28	Licensing of Modular high rate Biodigester
29	Licensing of Biodigester
30	Development of VK 2 glue
31	Synthesis and supply of (1R, 4R)-4-Hydroxycyclopent-2-en-1yl acetate
32	Process for preparation of CTFE Monomer
33	Providing incubation space
34	Providing incubation space
35	Providing incubation space
36	Preparation of core shell emulsion polymers with core containing acrylic acid and shell containing fluorinated monomers
37	Epoxy polyaniline coating for static control
38	Production of ultrapure water for Biomedical and Biochemical applications
39	Synthesis of Polychloro-trifluoroethylene (PCTFE) from Chlorotrifluoroethylene (CTFE)"
40	Development of process knowhow for total synthesis of Eribulin
41	Process improvement of Loxoprofen
42	Development of prices for perfurmery chemicals
43	Development of process knowhow for Na-TCP
44	Standardisation & Denitrosation reaction of low molecular weight heparins
45	Feasibility studies on enzymatic degumming process developed by CSIR-IICT
46	Demonstration of synthetic methodologies for pheromones
47	Transformation of water hyacinth to scalable nutrient rich organic fertilizer

C) Management of CSIR Funded Projects:

Project Management of CSIR funded projects:

The department plays a key role in handling major projects like Fast Track Translational projects, CSIR-800 projects, Mission Mode projects, Theme projects, In-House projects etc. Department maintains the complete database of all projects with fund sanction and receipts, expenditure, deployment of temporary manpower, R&D achievements etc., of the staff of the laboratory. Department conducts project Review meetings and project monitoring committee meetings (PMC) periodically for performance evaluation. Department gives wide publicity regarding information of various opportunities/ avenues available for R & D funding by CSIR-HQ. Scientific staff desirous of submitting new R & D project proposals for financial support in challenging areas, submit their proposals to the department, for their scrutiny and obtaining the approval of competent authority. Department handles CAG/Internal Audit and the liaison/Coordination of ongoing projects such as Mission mode, theme projects, Fast Track Translational Project, CSIR-800 project, etc., with CSIR-HQ.

The Overview of CSIR-Funded projects during the financial year 2016-17 and 2017-18:

Project Code	Project Type	Project Title
HCP009	Mission Mode	CSD-Catalysis for Sustainable Development
HCP0011	Mission Mode	INPROTICS-Pharma and Agro
RSP4027	CSIR-800	Polpularization of pheromone Technology (PAT): An upcoming versatile Agro Practice for pest Management
RSP4053	CSIR-800	Tassar Culture development in Warangal district & Improvement of Socio-Economic Conditions of Tribal Tasaar.
RSP4054	CSIR-800	Development of water purification plants
RSP4055	CSIR-800	Heating of cocoons with the biogas Generated from Sericulture (Left over mulberry leaves & Silkworm litter)
RSP4056	CSIR-800	Integrated Approaches for control of Malaria in various parts of India.
MLP0024	Fast Track Translational	Development of multipurpose thermal insulation coatings for different substrates
MLP0025	Fast Track Translational	Development of novel processes towards Eribulin, Nicotin, Bedaquiline.
MLP0026	Fast Track Translational	Discovery of Novel Anticancer Agent (HDAC Inhibitor)
MLP0027	Fast Track Translational	Polymeric Excipients for Pharmaceutical Applications

D) Skill Development & Entrepreneurship:

Skill programs:

The skill India programme at CSIR-IICT aims to create opportunities and scope for the development of talented Indian youth and enable them with better employment and entrepreneurship. As part of CSIR-Integrated Skill initiative, job oriented Skill Development Training Programmes are designed in Chemical Sciences, Analytical Sciences and Mechanical Engineering Services. Inauguration of Skill Development Training Programmes was held in CSIR-IICT Auditorium on 12th June 2017. Prof. Arun Tiwari, Author-Scientist inaugurated and launched the four courses.

CSIR-IICT conducted an "Advanced Pharma & Biotechnology" Programme in association with APSSDC (Andhra Pradesh State Skill Development Corporation) in three identified locations of Andhra Pradesh.

Following are the details on the Skill Development Training programmes being conducted by CSIR-IICT.

- Advanced Organic Chemistry Training (6 Weeks)
- Advanced Analytical Chemistry Training (6 Weeks)
- Advanced Cell & Molecular Biology (6 Weeks)
- Water Purification Systems (4 Weeks)
- Process Plant Drafting using AutoCAD (4 Weeks)
- Basic Chem-informatics (2 Weeks)

Entrepreneurial Programme with CSIR labs S&T Interventions:

A major change in the job market has been noticed in recent times with the advent of start-ups and increasing number of students choosing entrepreneurship over service.

CSIR-IICT has conceived a program entitled **"Be an Entrepreneur of Science and Technology - BEST"** in collaboration with NGO's, NRDC & CSIR HQ'rs for effective deployment of relevant CSIR technologies in rural areas of AP & Telangana states. The program involves an awareness campaign of the technologies at various Universities, followed by selection of the potential candidates and subjects them to grooming classes on the Technical and Business management aspects supported by NRDC for commercial feasibility assessment, followed by mentoring the candidates for start-up and incubation with financial assistance from Bankers.

Here is the link for registration for interested candidates:

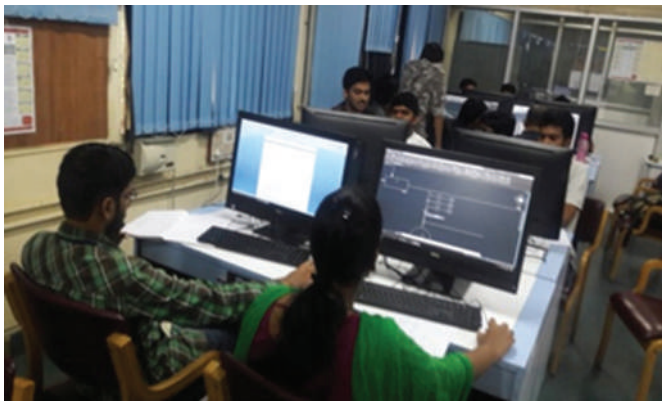
URL link: www.iictindia.org/best

Contact us: best.csir@iict.res.in

Skill Training Programme Inauguration by Prof. Arun Tiwari

Address by Dr. S. Chandrasekhar, Director, CSIR-IICT to Skill trainees

AutoCAD Course Trainees



AutoCAD Course Trainees

Analytical Course Trainees

Analytical Course Trainees

E) International Collaborations:

CSIR-IICT has international R&D collaboration programmes with Australia and France.

CSIR-IICT-RMIT Joint PhD Program

CSIR-IICT and RMIT (Royal Melbourne Institute of Technology) extended the Research Agreement up to 2020. The extension of this IICT-RMIT Research agreement was signed by the authorised signatories from both the Institutes and the signed documents were exchanged between both the Institutes on 23rd April, 2016. Dr. S. Chandrasekhar, Director, CSIR-IICT and Professor Peter Coloe, Pro Vice-Chancellor and Vice-President, RMIT University exchanged the agreement and Professor Suresh K Bhargava, Deputy Pro Vice Chancellor (Intl) and Director, CAMIC, RMIT University was also present on the occasion. A variation agreement to the existing MoU was made on 11.04.2017 to accommodate additional 7 candidates adding up to total 14 Ph.D students and one post doc.

Dr. S Chandrasekhar, Director, CSIR-IICT and Prof. Peter Coloe, Pro Vice-Chancellor and Vice-President, RMIT University exchanged the agreement. Prof. Suresh K Bhargava, Deputy Pro Vice-Chancellor (Int) was also present

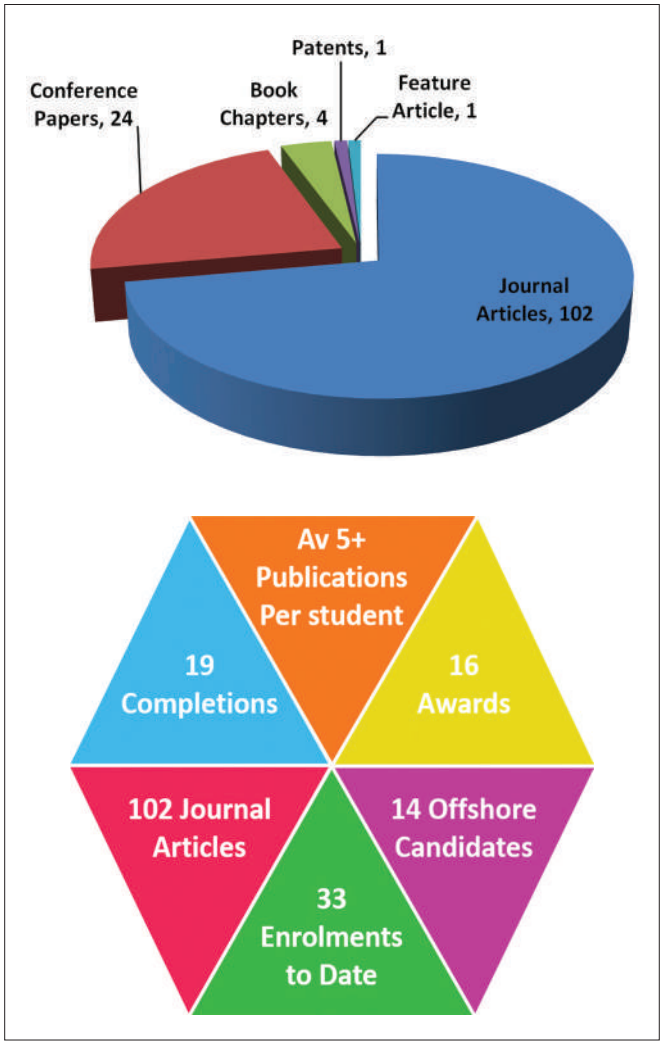
Exchange of Variation Agreement between Dr. S. Chandrasekhar, Director, CSIR-IICT and Prof. Suresh K Bhargava, Deputy Pro Vice Chancellor (Intl) on 11 April 2017

RMIT University and the Academy of Scientific and Innovative Research signed on to a joint badged PhD agreement during a formal ceremony in Melbourne on the 27th July 2017.

Under the joint PhD program the students will be enrolled at institutions, spending majority of their program at the AcSIR host institute and coming onshore to RMIT for up to 12 months at the later stages of their program.

RMIT students with RMIT University Supervisors Prof Ravi Shukla and Prof Gary Bryant during Review meeting at CSIR-IICT

Outcomes of RMIT Programs



RMIT-CSIR-IICT PhD Student Outcomes

Indo-French Joint Laboratory

CSIR-IICT signed an MoU with University of Rennes 1, France to renew the ongoing Indo-French research collaboration with a new title **"Natural Products and Synthesis towards Affordable Health"**. LIA NPSAH" was signed on 9th October 2017 in Rennes in collaboration with University of Rennes, France along with 3 other scientific reputed institutes in France for joint research and student exchange program given below.

- Centre National de la Recherche Scientifique
- The Ecole Nationale Supérieure de Chimie de Rennes
- The Institut National des Sciences Appliquées de Rennes

Signing of MoU in Rennes

Inauguration of Indo French Laboratory by Prof Joel Boustie, CNRS Research Director, University of Rennes with Dr S. Chandrasekhar, Director, CSIR-IICT; Dr D. Shailaja, Head, BDRM; Dr P. Srihari and Dr Raji Reddy

Inauguration event at Indo French Centre with scientists of CSIR-IICT

Outcome of Indo-French Programmes

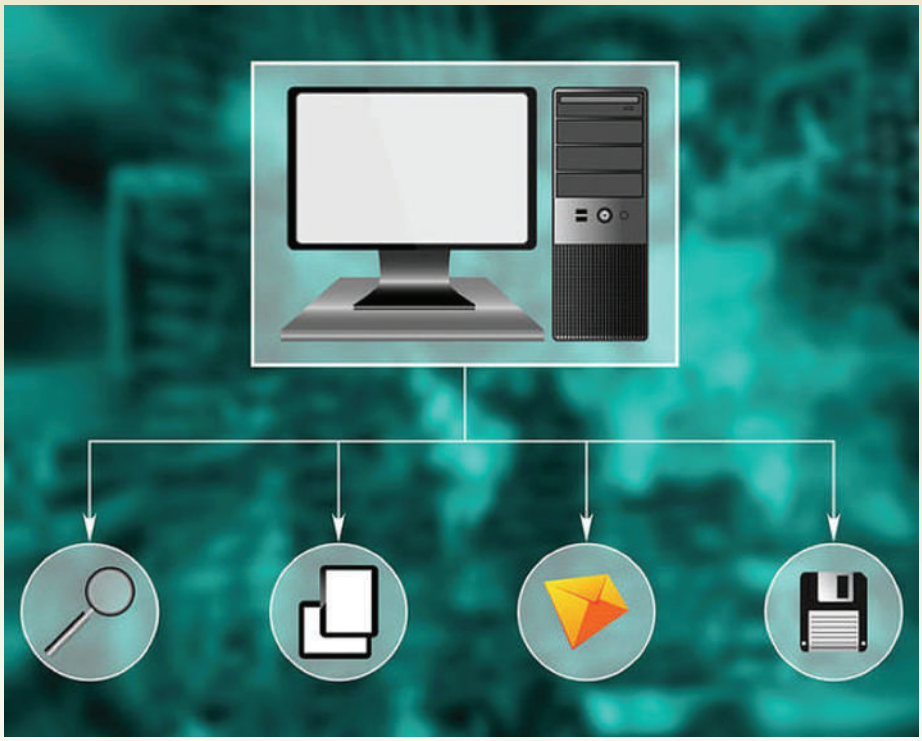
Total 62 Scientists (33 in France and 29 in India) are in the New Program from 2017-2021. Over 80 publications, published from Joint Lab research, 68 students participated to these research programmes [16 in Rennes, 28 in India]. Two Joint seminars and one CEFIPRA workshop have been organized together. Several important awards and special recognitions have been given to Joint Lab members.

In addition, CSIR-IICT is also having bilateral collaborations with Russia, UK, Poland, Sweden, France, and South Korea. These projects are sponsored by DST, DBT, and IFCPAR etc.

Additional Management activities handled are as follows:

- Processing of foreign deputations of permanent staff, students and temporary staff.
- Processing of bilateral exchange agreements & visits, sensitivity and security clearance of overseas project proposals (such as Indo-French Joint lab and RMIT etc.)
- arbitration cases, replies to parliament questions, audit paras, RTI queries etc.;
- Interaction with CSIR headquarters and other Govt. agencies related to R&D planning, overseas projects,
- Employment verification of temporary manpower,
- ISO Archives,
- Role mapping of employees and project mapping in ERP
- Monthly R&D Achievement Reports.
- Quarterly & Annual Research Utilization Data.
- R&D achievements information for CSIR Annual Report.

COMPUTER CENTRE



IICT COMPUTER CENTRE is one of the oldest computer centres in Andhra Pradesh existing since 1966. Computer Centre is the centralized resource facilitator for entire IICT Campus. The main aim of computer centre is to provide IT enabled facilities to ongoing R & D projects. Following activities/facilities provided by computer centre in 24/7 mode.

NATIONAL KNOWLEDGE NETWORK (NKN)

NKN is a state of art multi gigabit PAN-India network designed to ensure highest level of availability, quality of service, secure reliable and robust connectivity for extending network based services. NKN is designed and implemented by National Informatics Centre (NIC), Department of Information Technology, Govt. of India, 1 GB Network Bandwidth which interconnects the leading Scientific and Technical Institutions across India was commissioned at IICT.

CSIR-ICT 2016

Under the CSIR ICT-2016 Computer Centre modernized the **Data Centre** by establishing Campus Wide Network Backbone **10 GBPS** for connecting all 40 buildings/100 VLANs in single OFC enabling Biometric, Surveillance, Data, Video, and **Wi-Fi** services deploying 300 No Aruba Access Points in 20 Zones of IICT. The Campus wide 24x7 Wi-Fi services for smart devices was launched operation in 2017.

HIGH PERFORMANCE COMPUTING (HPC)

IICT computer centre team is capable of designing and establishing HPC environment. We have designed and established HPC for Molecular Modelling Group and Computational Chemistry Group in the IICT campus using Linux open source environment. Most of the resources, like operating system, software for certain applications like mail, squid proxy, MRTG, SARG etc., used in IICT Campus are open source based. As software is not procured from any OEM/company we save lot of money on license fees and renewals.

INFRASTRUCTURE FACILITIES

IICT commissioned below infrastructure to cater novel research facilities in 24x7 operation mode.

- 9 numbers of HP DL 380 G9 Servers with 128GB RAM, 12x600GB storage in Virtualisation each in to 4 Containers for Wi-FI/Wired Environment related Monitoring tools Air Wave/Clear Pass/IMC.
- 2 numbers of HP DL 375 G7 Servers with 48GB RAM, 6x300 GB storage RDBMS ORACLE/MSSQL/MySql.
- 5 numbers of IBM two way X6=5670 model servers with 48 GB RAM, 6x300 GB storage dual port HBA cords, redundant AC power supply connected to SAN Storage in HPC Cluster.
- 8 numbers of HP DL 360 G5 Servers with 16GB RAM, 2x128 GB storage OS Windows/Linux DC/ADC/DNS/DHCP/SUS/AV.
- 3 numbers of DELL PowerEdge R420/520 Servers with 48GB RAM, 1TB storage COMPAS/KIMS/BDRM.
- Fujitsu ETERNUS DX440make with 20TB usable storage, 8 GB 24 port Brocade Fiber Channel Switch, 2x LT 60 Tape library with 24 tape slots each and COMMVAULT backup software.
- 2 numbers UTM Cyberoam 1500iNG Security Appliances in High Availability Mode for WAN.
- 300 nos. **Aruba** 802.11 n/ac (Clear Pass, Airwave) 3x3 & 2x2 access points for **Wireless Network.**
- 10 Gigabit Ethernet capabilities of 100 VLANs across 4000 Desktops/Laptops/Smart devices.

CORE COMPETENCIES

- Security Management (UTM in High Availability, Servers, Clients)
- High Performance Computing
- Windows/Linux Server Administration

- Virtualization
- Database management: RDBMS: Oracle/MSSQL/ Postgre-SQL
- Syslog management for network devices
- ISPs: NIC/TATA
- Routing/Switching Fast Ethernet capabilities of 100 VLANs across 4000 devices
- Software development (ASP/.Net/PHP/Web technologies)
- Email/ Internet Proxy services
- Network Management System
- K7 Endpoint Security Management
- Operating System: Windows/Linux
- RDBMS: Oracle/MSSQL/Postgre-SQL
- System: LDAP/DHCP/DNS/WINS/Samba
- Network – Firewall/NFS/NIS/PPP dialin/SSL/SSH/ VPN
- Web Server: Apache/IIS

SOFTWARE DEVELOPMENT

The Computer Centre is undertaking applications of software development in the areas of scientific importance to institutional research programs. Additionally, it provides scientific inputs based on computer aided techniques to ongoing R&D Projects. The Centre also undertakes the application software development of various internal departments depending upon their requirement viz.

- Application for distribution of monies (Honorarium and Royalty)
- Application for the Visitor's Pass System at main gate of IICT.
- Application for the Medicine disbursement at IICT Dispensary
- Application for the Pathological Department for generating various pathological reports.
- Website development/Publicity of forth coming seminars
- Website development for Research Career/ Opportunities
- Internal website for the various maintenance modules/software installations/software patches/ general instructions etc. CCNET

Support Groups	Ongoing Software Projects
• Molbank IT support • Research Instruments IT support • NEERI Zonal lab IT support • MPDS: Molecular Modelling • Bio-Envis • Computational Chemistry • Biometric & Surveillance support • Software support for Admin Groups	• E-Notebook • Chem-Draw Professional • GIGW Compliant website • BEST • Analytical facilities Portal • Online Recruitment Portal • Continuous vulnerability assessment

SERVICE CENTRE

The Service centre extending Facility Management activities to institute in house users and they successfully executing several work orders (jobs) placed by internal users comprising following nature.

- Network Card Fixing/Configuration/Connectivity Testing
- Print/File services sharing across workgroup
- Display drivers downloading/fixing
- Virus patches downloading/applying to PC
- Operating System upgradation/fresh installation/ Hard Disk Error fixing
- Providing User/e-mail Id's to the users
- Creation/uploading personal folder (emails) on user desktops
- Browser installation and configuration of internet access with User-ID
- Providing HTTP, FTP, TELNET services to Power Users
- VC/Skype/Multimedia Services/display for seminars/ high level meetings etc
- All the client modules of Scientific Software implementation
- Application Software Installation and User training

Mostly they attend complete OS Installation on PCs with prime option of preserving user files backup in all the instances. The completed work orders an average of **150** per month in a calendar Year.

KNOWLEDGE & INFORMATION MANAGEMENT

Knowledge & Information Management (Library) is a combined facility for two National Laboratories, CSIR-IICT and CSIR-CCMB and has precious internationally acclaimed reference collections in frontier areas of chemical, engineering and life sciences. KIM plays a vital role in acquisition, organization, and dissemination of knowledge. It is consulted not only by the Institutional users but also by researchers in and around Hyderabad. It has an impressive collection both of print and electronic resources including books, journals, technical reports, standards, patents, theses and other material. It has adequate infrastructure to meet the information requirements of its users. The main thrust of the library continues to be the improvement of the quality services and facilities, achieving higher degree of user's satisfaction and modernization of its activities and operations.

Print holdings include books, dictionaries, handbooks, encyclopedias, reference book series and back volumes of journals. These total print collections are more than a lakh in number. Library subscribes to both National and International print journals and electronic journals. Apart from this CSIR- DST e-journal consortium known as National Knowledge Resource Consortium (NKRC) also provides/supports access to some E-journals and databases.

RESOURCES

IICT-CCMB library is one of the few signature libraries in the states of Telangana and Andhra Pradesh which has a complete collection of Chemical Abstracts from the year of its inception i.e. 1907 and now it is available online from January 2012. Library's computer infrastructure has been upgraded and user rooms were created to facilitate the usage of CD-Rom databases and browsing of E-Resources. Online databases and E-Journals are made available at user's desktops. The CD-Rom/ E databases include Chemical Abstracts, Indian and ASTM Digital Library, collection of Company's Annual Reports, CDs received through print subscriptions etc.

- **SciFinder:** It is a paid online database from American Chemical Society. SciFinder is a research discovery tool that allows the user to explore the CAS databases that contain literature from many scientific disciplines including biomedical sciences, chemistry, engineering, materials science, agricultural science etc. One can explore one single source for scientific information in journal and patent literature from around the world. Unlimited access has been provided in using this database to all the scientific staff of IICT.
- **Chemical Abstracts (Web Edition):** Chemical Abstracts includes a broad spectrum of technical and scientific information including Biochemistry, Physical, Inorganic and Analytical Chemistry, Applied Chemistry and Chemical Engineering, Macromolecular Chemistry and Organic Chemistry. References may be in the form of journals, patents, technical reports, dissertations, conference proceedings and books. From 1996-2011 it is available on CD's. From January 2012, CA is available online to the scientific staff of IICT.
- **Reaxys:** Reaxys is a web-based search and retrieval system for chemical compounds, bibliographic data and chemical reactions. It is built to support chemists in their daily work with focus and relevant information in chemistry by providers of Crossfire platform. Now crossfire has been migrated to Reaxys. Reaxys is an advanced platform over Crossfire.
- **Web of Science:** The Web of Science was provided through CSIR consortium provides seamless access of the most prestigious, high impact research journals in the world along with a unique search method, cited reference searching.
- **Patent Database:** Through NKRC the patent database is available to IICT researchers namely Derwent World Patents Index. It is searchable to give patent titles and abstracts using clear, descriptive, industry-specific terms. This is available at user's desktops.
- **Science Direct:** Some of the most referred Science Direct journals have been subscribed for the benefit of institutional users.

Besides E-Journals subscribed by the Library, access has also been provided to various open access journals and other information related to Chemistry and Chemical Sciences which are freely available on the Internet. Trial access of several databases and E-Journals has also been provided for the benefit of users as and when available. Apart from the available resources, information requirements of the users have been satisfied for procuring copies of the journal articles and books through Inter Library Loan requests from CSIR, DST and other libraries. By virtue of E-journal consortium of CSIR and as an add on to print journals of IICT, scientists can access many journals at their desktops.

LIBRARY HOME PAGE

Library Home page **http://libdoc** has been designed and maintained by this division, serves as a one point access to all the above mentioned E-Resources. Its features have been enhanced by adding more utilities from time to time.

DIGITAL REPOSITORY OF IICT (DRI)

DRI is a digital archive of the research output of IICT's scientists, has been designed and implemented. It is a mechanism for making research more widely available to academics and others. This knowledge base covers journal articles, technical reports, presentation/ lectures, preprints, Theses, images etc. One can browse the documents by author, division, subject and date. Both simple and advanced search facilities have been provided. Available publications from the year 1947onwards and bibliographic details of Ph.D thesis from the year 1945 onwards are available. 9797 full text articles and bibliographic details of 1165 thesis are included in DRI. The software that was chosen amongst the landscape of software platforms for building DRI is ***Dspace*** (Dspace 1.5) with Java, Apache Ant, Maven, PostgreSQL and Apache Tomcat on Linux OS. Soft ware has the facility to upload preprints by the scientists themselves in to DRI.

ACTIVITIES

The main activities of the division are as mentioned below:

- Scientometric analysis of IICT research publications

  Information on the bibliographical details along with the Impact factors of the research papers of IICT to the management and NISCAIR of CSIR in calculating the research output of the Institute and thus assisting the top management in evaluating quality and quantity of research.

- Archiving of IICT Publications

  It is essential to preserve IICT's research outputs and make it readily available for reference. Reprints of research papers of IICT scientists are collected/ downloaded from source publications, indexed and bound into volumes and displayed in the library.

- Replying Audit queries from time to time

SERVICES

Provides a range of Library and Information services like

- Circulation service
- Inter-Library Loan service
- Newspaper Clipping service
- Photocopying service
- Reference service
- Translation service for foreign language research articles

Services to Industry & Outside Agencies

KIM provides library utilization facilities to Industry and other Agencies on membership basis. Apart from Internal users, facilities have been extended to research scholars from any University registered for Ph.D and corporate sector through membership in the library.

HUMAN RESOURCE DEVELOPMENT

ACADEMY OF SCIENTIFIC AND INNOVATIVE RESEARCH

AcSIR | Academy of Scientific & Innovative Research

The Academy of Scientific & Innovative Research (AcSIR) has adopted the mandate to create and train young scientists to lead and the best of tomorrow's Science & Technology leaders through a combination of innovative and novel curricula and evaluation to face the challenges of inter-disciplinary and trans-disciplinary transformation of the biological, chemical and engineering sciences. AcSIR was established by an Act of Parliament, the Academy of Scientific Innovative Research Act, 2011 and now operating in 37 laboratories of CSIR are extending the services of their scientists, expertise and infrastructure to the Research Academy.

The courses of study by the candidates are organized on semester pattern and also its mandate to prepare Research proposals before comprehensive examination or evaluation, by selecting topics of high relevance and novelty, one in the area of candidate's research another in a contemporary area and with state-of -art review and methodologies.

The Academy at CSIR-IICT, Hyderabad offers Ph.D. programs in chemical, biological and engineering sciences and extending all infrastructure facilities, scientific manpower and other resources of this Institution to the candidates who are pursuing their doctoral work.

Till March 2018, **579 students were enrolled as Ph.D students** and the **143** scientists of CSIR-IICT, Hyderabad are extending their services as faculty members to the AcSIR Academy in the disciplines of Chemical, Biological and Engineering Sciences.

AcSIR FUNCTIONARIES

Dr. S. Chandrasekhar	Member, AcSIR Senate
Dr. Ramanuj Narayan	Associate Dean, Chemical Sciences (from October 2014)
Dr. Ch. Raji Reddy	AcSIR Coordinator, CSIR-IICT (from February 2016)

To streamline the activities of AcSIR at CSIR-IICT, Director had constituted the following committees.

ACADEMIC COUNCIL - ACSIR, CSIR-IICT

Dr. K. Ravi Kumar	Chairman
Dr. P. Radhakrishna	Director's Nominee
Dr. Pradosh P. Chakrabarti	Admissions
Dr. Ch. Raji Reddy	AcSIR
Dr. K. Rajender Reddy	Student Affairs
Dr. Sanjit Kanjilal	Student Welfare
Dr. Ramanuj Narayan	Alumni
Section Office (Recruitment and E& T)	Administration
Director Secretariat	Policy Matters and Approvals

COMMITTEES FOR CARRYING OUT ACSIR ACTIVITIES AT CSIR-IICT

Thesis Supervision Committee - AcSIR, CSIR-IICT

1	Dr. P. Radhakrishna	Chairman
2	Dr. M. Chandrashekaram	Co-Chairman
3	Dr. M. Sridhar Reddy (CS)	Member
4	Dr. P. Aruna (CS)	Member
5	Dr. G.V. Karunakar (CS)	Member
6	Dr. C. Sumana (ES)	Member
7	Dr. Shasi Vardhan Kalivendi (BS)	Member
8	Dr. Ramesh Ummanni (BS)	Member

AcSIR STUDENT INFORMATION (August 2016 to March 2018)

Number of Students Enrolled for PhD (Session wise)					
Discipline	**August 2016**	**January 2017**	**August 2017**	**January 2018**	**Total**
Chemical Sciences	43	40	36	20	**139**
Biological Sciences	23	05	08	04	**40**
Engineering Sciences	01	02	02	-	**05**
Total	**67**	**47**	**46**	**24**	**184**

COURSES OFFERED IN ALL DISCIPLINES (August 2016 to March 2018)

S. No	Course Offered	No. of Students Participated
1	CHE-IICT-1-2901: Research Methodology	77
2	CHE-IICT-1-2902: Analytical Tools and Instrumentation	85
3	CHE-IICT-2-2904: Advanced Polymer Chemistry	35
4	CHE-IICT-208: Advanced Photochemistry	66

S. No	Course Offered	No. of Students Participated
5	CHE-IICT-214: Advanced Materials Science	69
6	CHE-IICT-229: Natural products	42
7	CHE-IICT-231: Synthetic methods for organic chemists	56
8	CHE-IICT-3-2902/ CHE-IICT-3-2903 Total Synthesis/ Asymmetric Synthesis	99
9	CHE-IICT-323: Homogeneous Catalysis/ CHE-IICT-325: Catalysis for organic synthesis	104
10	CHE-IICT-2-2913: Medicinal Chemistry	68
11	CHE-IICT-2-2909: Green chemistry	84
12	CHE-IICT-2-2904: Advanced Polymer Chemistry	50
13	CHE-IICT-3-2921 Process Chemistry	35
14	Advanced Functional Materials	06
15	BIO-IICT-1-0001: Biostatistics	35
16	BIO-IICT-1-0002: Computation/ bioinformatics	36
17	BIO-IICT-1-0003: Basic Chemistry	79
18	BIO-IICT-1-0004:Research Methodology, Communication/ethics/ safety	35
19	BIO-IICT-2-2901: Biotechniques & Instrumentation	37
20	BIO-IICT-2-2902: Chemical Biology	48
21	BIO-IICT-2-2906: Proteomics and its application	37
22	BIO-IICT-3-2905: Disease Mechanisms	45
23	BIO-IICT-3-2907: Protein Science and Structural Based Drug Design and Development	45
24	ENG-IICT- 3-2901 Process Engineering	11
25	ENG-IICT-2910: Bioenergy And Bioproduct Engineering	13
26	ENG-IICT- 2-2906 Advanced Process Optimization	04
27	ENG-IICT- 2-2901 Numerical methods and Process Modeling	04

NO. OF STUDENTS COMPLETED DAC AND PRE-VIVA (August 2016 to March 2018)

DAC/CEB Meetings	PRE-VIVA
300	**106**

NUMBER OF STUDENTS SUBMITTED PH.D. THESIS (August 2016 to March 2018) AND AWARDED

Discipline	PhD Awarded
Chemical Sciences	80
Biological Sciences	16
Engineering Sciences	01
Total	**97**

Total number of Ph. Ds awarded From CSIR-IICT through AcSIR till March 2018: 152

AcSIR 400 LEVEL COURSE: SOCIETAL PROGRAM – SCIENCE TO SCHOOLS

As part of the above programme 20-Research Scholars along with AcSIR staff visited the Zilla Parishad High School, Anksapur village, Nizamabad district on December 21, 2017 to motivate the school children towards science and research as their future study. In this place, more than 300 students were gathered from 9-different schools. In the beginning, all the members did the plantation in school premises. Later, three scientists, Dr. Ramanuj Narayan, Dr. Ch. Raji Reddy and Dr. K. Rajender Reddy gave lectures to inspire the school students. All the research scholars demonstrated the various experiments showing how they carry out the research at CSIR-IICT and its importance for the society. School students were excited by listening to these demonstrations and interacted with the scientists. Overall this programme was successful to take the science to schools.

AWARDS AND HONOURS 2016-2017

Name of the Awardee (s)	Prize/Award/Honour
CSIR - IICT, Hyderabad **Team:** Dr. T. Prathap Kumar, Dr. B. Satyavathi, Dr. Pravin R Likhar, Dr. M. Lakshmi Kantam, Mr. M. Ramulu, Mr. S. Anand Kumar, Mr. K. Ravindranath, Mr. K.Vijay Murty	"Certificate of Merit" under the category of "Physical Sciences including Engineering" of the CSIR Technology Awards 2016.
CSIR - IICT, Hyderabad	1. Excellent implementation of Raj Bhasha Hindi for the year 2015. 2. CSIR-IICT Stall received Special Award by All India Industrial Exhibition (AIIE) at 77th AIIE, Nampally, Hyd.
Dr. S. Chandrasekhar	1. Kinnera-Sri Durmukhinama Ugadi Puraskaram-2016 (Science and Technology) by Government of Telangana. 2. Goyal Prize in Chemical Science by Kurukshetra University.
Dr. Arabinda Chaudhuri	Fellow of the Royal Society of Chemistry.
Mr. P. Chiranjeevi	First Prize for the Paper Presentation
Dr. Chittaranjan Patra	Dr. DS Bhakuni Award from Indian Chemical Society.
Dr. C. Ganesh Kumar	Fellow of Biotech Research Society India (BRSI)- 2016.
Dr. A. Gangagni Rao	1. Industrial Gold Medal Award-2015 by Biotech Research Society, India (BRSI) 2. Distinguished Scientist Award by Venus International Foundation
Dr. A. Krishnaiah	Member of the Expert Committee, Department of Chemicals and Petrochemicals, Govt. of India, New Delhi.
Ms. M. Madhumala	Young Scientist Award (TASYS-2015) in Chemical Sciences.
Mr. C. Nagendranatha Reddy	Best Poster Presentation
Namdev Vitthalrao Ghule	Best Oral Presentation Award
Mr. K. Narayanaswamy	Best Oral Presentation Award
Mr. Omprakash Sarkar	Junior Scientist Award
Dr. T. Pavan Kumar	Young Scientist Award (TASYS-2015) in Chemical Sciences.
Mr. V.S. Phani Babu	1. Best Poster Award 2. Best Student Oral Award
Dr. Prathama S. Mainkar	Organization of pharmaceutical producers of India (OPPI) Woman Scientist Award 2016
Rajnish Kumar	Indian Paint Association Award
G. Ramasatyaveni	1. Young Scientist Award in Biological Sciences 2. Best Poster Award
Mr. Reddi Kamesh	Best Paper Award
Mr. Sai Kishore Butti	1. Best Poster Presentation 2. Junior Scientist Award
Dr. Sarala Devi	Distinguished Scientist Award instituted by the Venus International Research Awards - VIRA 2016.
Mr. Siddhartha Moulik	IEI Young Engineers award 2016-17 in Chemical Engineering.

Name of the Awardee (s)	Prize/Award/Honour
Ms. M. Sowmya	Best Poster Award
Dr. S. Sridhar	CIPET National Award-2016
Mr. Sudip Mukherjee	1. Dr. K.V Rao Research Award-2016 2. Best Poster Award
Mrs. P. Swathi	Junior Scientist Award
Team: Dr. S. Sridhar, Dr. N.L. Gayatri, Mr. N. Shiva Prasad, Ms. B. Nagasandhya, Ms. Bukke Vani	Winner - 7th National Award for Technology Innovation in the category of 'Innovation of Polymer Processing Machinery & Equipments'.
Team: Dr. S. Sridhar, Mr. Siddhartha Moulik, Ms. Pavani Vadthya, Mr. N. Shiva Prasad, Ms. Madhumala	Runner - 7th National Award for Technology Innovation in the category of 'Innovation in Polymeric Material'.
Team: Dr. S. Sridhar, Harsha Nagar, Nazia Shaik, M. Madhumala, Y.V.L. Ravikumar	GYTI-Appreciation Award-2017 for 'Cutting Edge Innovation in Design of Highly Efficient and Inexpensive Membrane Equipment'
Dr. P. Usha Rani	Highly Cited Research for publishing in Journal of Asia Pacific Entomology
Mr. Vinayak Botla	Best Oral Presentation Prize
Mr. B. Vishnu Sravan	Best Poster Award
Dr. K. Yamuna Rani	Best Paper Award

Goyal Prize in Chemical Science (Dr. S. Chandrasekhar)


Industrial Gold Medal Award-2015 (Dr. A. Gangagni Rao)

Special Award by 77th AIIE, Nampally, Hyd (IICT Stall)

AWARDS AND HONOURS 2017-2018

Name of the Awardee (s)	Prize/Award/Honour
CSIR-IICT's Hydrazine Hydrate Project Team	FICCI Award for "Development of the Hydrazine Hydrate Process and Commercialization of the Technology".
Dr. S. Chandrasekhar	C. V. Raman Birth Centenary Award 2017-18
Mr. Ajay Anand	Best Oral Presentation award
Dr. P. Anand	Associate Fellow of the Telangana Academy of Sciences-2016
Dr. Debendra Kumar Mohapatra	NASI-Reliance Industrial Platinum Jubilee Award 2017
Dr. C. Ganesh Kumar	Fellow of the Telangana Academy of Sciences-2016
Dr. A. Gangagni Rao	1. SKOCH Order of Merit Award by SKOCH GROUP 2. I.C.I India Ltd Award for Excellence in Process or Product Development-2017 by IIChE.
Dr. John Mandal	Young Scientist Award-2016 by Telangana Academy of Sciences.
Dr. M. Madhumala	1. TAS-Young Scientist Award for the year 2015 in 'Engineering Sciences'. 2. Best Poster Presentation Award
Ms. K Naga Jyothi	IICHE Award: Acharya P C Ray Award
Dr. C. Nagendranatha Reddy	Best Ph.D Thesis Award 2017
Dr. B. Narsaiah	Fellow of the Telangana Academy of Sciences-2016
Ms. Neha R Dhoke	Zydus-Lipaglyn Third Prize for Oral Presentation
Dr. B.L.A. Prabhavathi Devi	Fellow of the Telangana Academy of Sciences-2016
Mr. S.M. Rajesh	1. Dr. K.V. Rao Research Award (2nd Prize) 2017-18 2. Best Oral Presentation Award
Dr. K.S. Rama Rao	Fellow of the Telangana Academy of Sciences-2016
Mr. B. Rama Rao	Third Award for Oral Presentation
Dr. S. Sridhar	1. CIPET National Award-2017 2. VIRA-2017 Distinguished Scientist in Chemical Engineering Award
Mr. N Susheel Kumar	First Award for Oral Presentation
Team: Dr. S. Sridhar, Mr. Siddhartha Moulik, Ms. Pavani Vadthya, Y.V.L. Ravi Kumar, B. Govardhan, S.S. Chandrasekhar	Nina Saxena Excellence in Technology Award–2017
Dr. Usha Virendra	Women in Education Award by Business School Affaire & Dewang Mehta National Education Awards in Collaboration with Institute of Public Enterprise

Name of the Awardee (s)	Prize/Award/Honour
Dr. S. Venkata Mohan	**1.** Environmental Engineering Design Award-2017 from NDRF of Institute of Engineers, India **2.** Fellow of the International Bioprocessing Association (FIBA) for 2015 **3.** The Most Cited Researcher in both Environmental Science and Engineering, Chemical Engineering categories, Shanghai Ranking's Global Ranking of Academic Subjects 2016 by Elsevier. **4.** SERB-IGCW 2017 Award for "Biohydrogen Technology"
Dr. K. Yamuna Rani	Women in Education Award by Business School Affaire & Dewang Mehta National Education Awards in Collaboration with Institute of Public Enterprise

FICCI Award to CSIR-IICT (Project Team)

SERB-IGCW 2017 Award (Dr. S. Venkata Mohan)

CIPET National Award - 2017 (Dr. S. Sridhar)

DISTINGUISHED LECTURES (2016-17)

- A V Rama Rao Technology Award Lecture on "Drugs and Diseases: An overview" by Dr. V K Subburaj, IAS, Secretary to Government of India, Department of Pharmaceuticals, Ministry of Chemicals and Fertilizers. **May 10, 2016**
- A Popular Science Lecture on "How to translate Research into Innovation" by Prof. Suresh Bhargava, Director of the CAMIC, RMIT University, Melbourne, Australia. **June 02, 2016**
- A Lecture on "Development of High-Performance Ionic Polymer Actuators" by Dr. Ravi Kumar, Research Professor, School of Material Science and Engineering, Ulsan National Institute of Science and Technology, South Korea. **July 2016**
- A Talk on "Metabolomic profiling reveals altered xenobiotic metabolism in bladder cancer: a mechanistic insight" by Dr P. Nagi Reddy, Asst. Professor, Bayor College of Medicine, Houston, USA. **July 2016**
- A Talk on "Engineered Hybrid-Porous Materials for Energy Storage Applications" by Dr. Satish K Nune, Senior Scientist, Pacific Northwest National Laboratory (PNNL), Washington, United States. **July 2016**
- A Lecture on "Development of Nanoparticulate Drug Delivery System for the Treatment of Diabetic Retinopathy" by Prof. D S Katti, Department of Biological Sciences & Bioengineering. IIT, Kanpur. **July 2016**
- A Lecture on "Integrated biochemical and imaging approach to decipher the molecular mechanisms of tropical diseases and tumorigenesis" by Dr. Anil Shukla, from NCI, NIH (F), USA. **July 2016**
- 73rd Foundation Day Lecture by Bharat Ratna Prof. C N R Rao. **August 05, 2016**
- A Talk on "Good Laboratory Practices (GLP) in Cell Culture lab: Cell Line Authentication and Cross-Contamination" by Dr. Jameel Ahamed Khan, Managing Director, Lifecode Technologies Pvt. Ltd., New Delhi. **August 2016**
- A Lecture on "Global Quality & Cost Effective Biosimilar Development" by Dr. A. Durgaprasad, Stelis Biopharma, Bangalore. **August 2016**
- A Talk on "Disease-responsive drug delivery: An emerging concept in biomedical sciences" by Dr. Praveen Vamula, Institute for Stem Cell Biology and Regenerative Medicine (inStem), National Centre for Biological Sciences (NCBS), Bangalore. **August 2016**
- A Lecture on "Catalytic Processes in Organic Synthesis: From Metal to Metal-Free" by Dr. Shikha Gandhi, Department of Chemistry, IISER, Bhopal. **September 2016**
- A Popular Lecture on "Molecules with Celebrity Status" by Dr S. Chandrasekhar, Director, CSIR-IICT, Hyderabad. **September 2016**
- A Talk on "Recycling Biopolymers to Value-Added Carbon Products and Green Plasticizers" by Prof. Minna Hakkarainen, KTH-Royal Institute of Technology, Sweden. **November 2016**
- A Lecture on 'Path of success: As learnt from Dr. APJ Abdul Kalam' by Prof. Arun Tiwari, Author & Scientist as part of the platinum jubilee celebrations. **November 2016**
- A Lecture on "Functionalized Nucleoside Toolbox for Studying Nucleic Acid Structure and Function" by Dr. Seergazhi G. Srivatsan, Associate Professor, IISER, Pune. **November 2016**
- A Lecture in Hindi on "Nano-significant technology of 21 century" by Dr. D. D. Ojha, Chief Scientist (retired), Ministry of water resources. **November 2016**
- A Special Lecture on "Chemical Technology" by Dr. S. Sridhar, CSIR-IICT, Hyderabad. **December 2016**
- A Talk on "Charge Separation in Photo catalysts for Artificial Photo synthesis" by Prof. Can Li, Director, Dalian National Laboratory for Clean Energy, China. **January 2017**
- A Mentor Lectures on "Path of Success" by Prof. Arun Tiwari, Author & Scientist. **January 2017**
- National Youth Day Lecture on "Swami Vivekananda and Science" by Shri. Jayant Sahasrabuddhe, National Organizing Secretary, Vigyan Bharati. **January 2017**
- CSIR Platinum Jubilee Celebrations Lecture by Prof. Kurt Wuthrich, Nobel laureate, The Scripps Research Institute, USA. **February 08, 2017**

- National Science Day Lecture on “Serendipity and Curiosity-driven Research” by Prof. Rene Gree, CNRS Director of Research (Em.), University of Rennes, France. **February 28, 2017**
- CSIR Platinum Jubilee Lecture on “The Art and Science of Organic Synthesis and Its Impact on Science and Society ” by Prof. K.C. Nicolaou, Harry C. and Olga K. Wiess, Professor of Chemistry, Department of Chemistry, Rice University, USA. **March 30, 2017**
- A Lecture on “Accelerating Discovery, Drug Development and Clinical Trials in Neuro-Oncology” by Dr. Santosh Kesari, Chair and Professor, Department of Translational Neurosciences and Neurotherapeutics, John Wayne Cancer Institute. **March 06, 2017**
- A Talk on “Discovering novel genes for environmental applications” by Dr. Gunjan Pandey from CSIRO, Australia. **March 2017**
- A Lecture on "Principles of Toxicology and Human Safety Evaluation" by Prof. Syed M GhiasUddin (Ghias), Toxicologist and Section Chief, Indiana Department of Environmental Management (IDEM), Indianapolis, USA. **March 2017**

CSIR Platinum Jubilee Celebrations Lecture by Nobel laureate Prof. Kurt Wuthrich

National Science Day Lecture by Prof. Rene Gree

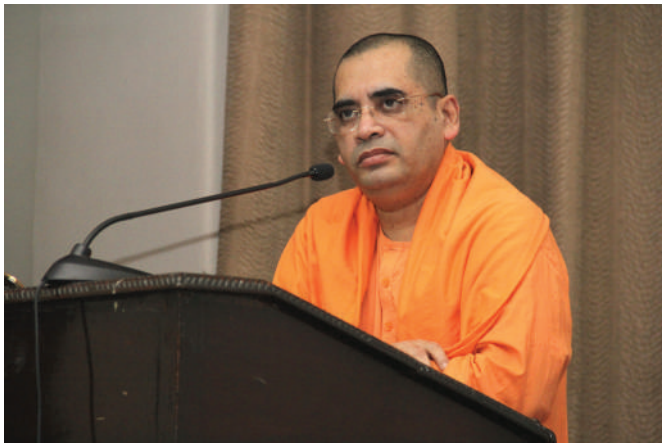
Lecture by Prof. Syed M GhiasUddin

CSIR Platinum Jubilee Lecture by Prof. K.C. Nicolaou

DISTINGUISHED LECTURES (2017-18)

- A Lecture on “Sustainable Water Management Under Climate Change Scenario” by Prof. K.V. Jaya Kumar, Professor of Civil Engineering and Dean (Planning & Development) NIT, Warangal. **April 2017**
- A Lecture on “Enantioselective Organocatalytic Reactions: Applications in Synthesis” by Dr. Nirmal K. Rana, Department of Chemistry, IIT Kanpur. **April 2017**
- A Lecture on Path of Success “Mentor Lecture No. 3: Self Confidence” by Prof. Arun Tiwari, Author & Scientist. **April 2017**
- A V Rama Rao Technology Day Award Lecture on “Use of Space Technology in India” by Sri. A. S. Kiran Kumar, Chairman, ISRO. **May 12, 2017**
- A Lecture on “Engineering Biomaterials and Antibacterials in the Era of Drug Resistance” by Dr. Jayanta Haldar, Associate Professor, Antimicrobial Research Laboratory, New Chemistry Unit, JNCASR, Jakkur, Bangalore. **May 2017**
- Inaugural Lecture in 21st National Symposium in Chemistry by Bharat Ratna Prof. C.N.R. Rao. **July 14, 2017**
- A Special Lecture on "An Inspiration" On the occasion of the 156th Birth Anniversary of Prof. Acharya P. C. Ray by Dr. Ramanuj Narayan, CSIR-IICT, Hyderabad. **August 02, 2017**
- CSIR-IICT’s Foundation Day Lecture on "Methanol Economy - Opportunities and Options for Energy Security " by Padma Bhushan Dr. Vijay Kumar Saraswat, Hon'ble member, NITI Aayog, Government of India, New Delhi. **August 05, 2017**
- Sixth Mentor Lecture on “Path of Success” by Prof. Arun Tiwari, Author & Scientist. **August 29, 2017**
- A Lecture on "Tolerable Upper Limits for vitamins and minerals - is indiscriminate use a safety issue?" by Dr. Sesikeran, Nutritional Pathologist and Former Director of National Institute of Nutrition. **September 2017**
- Prof. T. Navaneetha Rao Best Teacher Award Lecture on “Our Strategies to counter emergent drug resistant TB” by Prof. Nagaraja, President, JNCASR, Bangalore. **September 2017**
- Foundation Day Lecture on “India at 70: Next 30 Years” by Prof. Vijay P. Bhatkar, President VIBHA & Chancellor, Nalanda University. **September 27, 2017**
- A Lecture on “Antioxidant Tail to a DNA damage Responsive Ser/Thr Protein Kinase in a Radioresistant Bacterium" by Dr. H.S. Misra, Head-Molecular Biology Division & Professor, Homi Bhaba National Institute, BARC, Mumbai. **October 2017**
- A Talk on “How to write a Scientific Paper and Get Published” by Dr. Jan Willem Wijnen, Executive Publisher Chemistry of Elsevier. **October 04, 2017**
- Eighth Mentor Lecture on "Path of Success: "Self Control" by Prof. Arun Tiwari. **October 2017**
- Vigilance Awareness Week-2017 Lecture by Shri. V. Nagi Reddy Former State Election Commissioner, Telegana. **November 03, 2017**
- Ninth Mentor Lecture on "Path of Success: "The Habit of Doing More Than Paid For" by Prof. Arun Tiwari. **November 2017**
- An Inspiring Lecture by Prof. Hiroshi Amano, Nobel Laureate in connection with Platinum Jubilee Year Celebrations of CSIR-IICT. **January 4, 2018**
- A Lecture on " The First Stereoselective Total Synthesis of a Dimeric (Naphthoquinono)pyrano-γ-lactone: (+)-γ-Actinorhodin" by Prof. Reinhard Brüeckner, Albert-Ludwigs-Universität, Freiburg, Germany. **March 01, 2018**
- A Popular Lecture on "Scientific Temper and Spirituality" by Swami Bodhamayananda, Director, Vivekananda Institute of Human Excellence, Ramakrishna Math, Hyderabad. **March 05, 2018**

Inspiring Lecture by Nobel Laureate Prof. Hiroshi Amano



A Popular Lecture by Swami Bodhamayananda

Technology Day Lecture by Sri. A. S. Kiran Kumar

Mentor Lecture by Prof. Arun Tiwari

CONFERENCES/SEMINARS/ SYMPOSIA/WORKSHOPS ORGANISED BY CSIR-IICT 2016-17

- National Conference on "Advanced Cancer Therapeutics (ACT-2016)" organized by CSIR-IICT, Hyderabad. **April 4-5, 2016**
- Seminar on "Advances in Chemical Engineering" jointly organized by CSIR-IICT and IIChE, Hyderabad. **April 6, 2016**
- One day Symposium on "Science and Society" at CSIR-IICT organized by IGNA in association with CSIR-IICT and Gothe-Zentrum. **April 30, 2016**
- 3-Day National Scientific Seminar in Hindi 'Make in India - CSIR Contribution' organized by CSIR-IICT in association with CSIR-CCMB and CSIR-NGRI. **May 25 - 27, 2016**
- 17th National Workshop on "Challenges in Catalysis Science and Technology" (CCST-2016) CSIR-IICT Organized on behalf of Catalysis Society of India (CSI). **June 23–25, 2016**
- A workshop on implementation of official language on "Rules, Day-to-Day work and Correspondence using Hindi language" conducted by CSIR-IICT. **July 20, 2016**
- A two day INDO-US Workshop on "Vulnerability Assessment for Weaponizable Dual Purpose Chemicals" conducted jointly with CSIR-IICT, PNNL-USA and USDSCSP, USA at Resort Leonia, Hyderabad. **July 28-29, 2016.**
- A Tributary Symposium on "100 Years of Chemical Bonding by Gilbert N. Lewis" organized by CSIR-IICT, Hyderabad. **August 4-5, 2016**
- International Conference on "Nature Inspired Initiatives in Chemical Trends" (NIICT-2016) organized by CSIR-IICT, Hyderabad. **September 19-20, 2016**
- "21st International Conference on Organic Synthesis" at IIT Bombay, Mumbai, India. Organised by IIT Mumbai, CSIR-IICT, and IUPAC. **December 11-16, 2016**
- Indo-EU Workshop on 'Microbial Electrochemical Technologies for Sustainability: Fuels, Chemicals and Remediation(metSUS-2017)' organized by CSIR-IICT, Hyderabad. **February 28, 2017**

Workshop on implementation of official language

Participants of Indo-EU Workshop

- One day workshop on "Integrating CSIR and Chemical Industries for make in India" organized by CSIR-IICT, Hyderabad. **February 23, 2017**

Bharat Ratna Prof. C.N.R. Rao interacting School children at Tributary Symposium

Workshop on "Integrating CSIR and Chemical Industries for make in India"

CONFERENCES/SEMINARS/ SYMPOSIA/WORKSHOPS ORGANISED BY CSIR-IICT 2017-18

- GHMC has organized a One day Conference on "National Waste Management Summit (NSWM) – 2017". CSIR-IICT extended its affiliation in this event by displaying the technologies developed by CSIR-IICT for solid waste management. **June 24, 2017**
- 21st CRSI National Symposium in Chemistry and CRSI-ACS symposium in Chemistry organized by CSIR-IICT, Hyderabad along with CRSI. **July 14-16, 2017**
- CSIR-IICT Jointly with RSC (London)- India Deccan Local Section, CSIR-IICT Science India Portal and White Board, Hyderabad organized a SCIENCE FAIR on "Chemistry–It's applications" for School Children at CSIR-IICT, Hyderabad. **July 29, 2017**
- CSIR-IICT in collaboration with Royal Society of Chemistry (Deccan Section) organized a programme "Chem Careers India" for students at CSIR-IICT. **January 06, 2018**
- Two day Indo – US Bilateral symposium on Nanotechnology & Regulatory Science organized by CSIR-IICT, Hyderabad in association with IUSSTF, Food and Drug administration (FDA), USA and Government of Telangana. **February 21-22, 2018**

Prof.C.N.R.Rao at 21st CRSI National Symposium

A programme on "Chem Careers India" for students

Indo – US Bilateral symposium

TRAINING PROGRAMMES ORGANIZED BY CSIR-IICT 2016-18

- *Orientation cum Training programme* for science students of North Eastern India. **3-Months**
- Mechanical Design & Engineering Department of CSIR-IICT conducted a unique *certificate course* in Process Plant Drafting Using Autocad under the CSIR Integrated Skill Development Program. **May 29-June 23, 2017**
- *Skill development program* entitled "IICTAnalChemSkill Course on Advanced Analytical Chemistry Training" to postgraduate students with duration of 3 months. **July-September, 2017**
- *Training Program* on 'Content Enrichment for TGTs (Science) ' to 35 No.s of teachers from Navodaya Vidyalaya Samithi(NVS), Navodaya Leadership Institute, R.R Dist. **November 10, 2017**
- *Training programs* to the staff of A.P Prohibition and Excise laboratories on the program entitled "Advanced Analytical Techniques" for a duration of one month. **January 18- February 16, 2018**
- *Training programs* to the staff of A.P Prohibition and Excise laboratories on program entitled "Advanced Analytical Techniques" for a duration of one month. **February 21-March 23, 2018.**
- *An Orientation Program* for the Editorial Members of Science India Portal. **February 26, 2018**
- *Hands on training* on Analytical Instruments to different batches of Bachelor/Master students from A.P under "***Pratyancha***" program during **2017-2018**.


Training program to the staff of A.P Prohibition and Excise laboratories


CSIR Integrated Skill Development Program at IICT

OTHER EVENTS ORGANIZED BY CSIR-IICT 2016-18

- CSIR-IICT celebrated "World Earth Day Celebrations". **April 22, 2016**
- CSIR-IICT celebrated "International Yoga Day Celebrations'. **June 21, 2016**
- CSIR-IICT celebrated "73rd Foundation Day celebrations". **August 05, 2016**
- CSIR-IICT celebrated "Hindi Day" with a special lecture. **September 14, 2016**
- CSIR-IICT organized "Industry Meet" at Hotel Park Hyatt. **October 18, 2016**
- CSIR-IICT organized "GIGYASA" (Vibrant Student-Scientist Interactions) program. **October 25, 2016**
- CSIR-IICT organized a pre-IISF event, under the theme "Science for the Masses: A Public Outreach Program", as part of India International Science Festival (IISF -2016). **November 10, 2016**
- CSIR-IICT celebrated "World Environment Day Celebrations". **June 5, 2017**
- CSIR-IICT organized "JIGYASA - a scientist and KV student connect program". **July 03, 2017**
- CSIR-IICT organized "Open day" for science teachers on the occasion of 86th Birth Anniversary of Bharat Ratna late Dr. A. P. J. Abdul Kalam. **October 17, 2017**
- CSIR-IICT organized a program in Commemoration of Pandit. Deendayal Upadhyay to mark his Birth anniversary. **December 18, 2017**
- A program entitled "Be an entrepreneur of Science & Technology" (BEST) under 'CSIR Integrated Entrepreneurial Initiative' coordinated by CSIR-IICT in collaboration with NGO's & NRDC at Andhra University campus, Visakhapatnam. **January 25, 2018**
- Pratyancha - an initiative of CSIR-IICT in association with Andhra Pradesh State Skill Development Corporation (APSSDC) inaugurated at Rayalaseema University, Kurnool. **February 16, 2018**
- CSIR-IICT celebrated "World Women's Day Celebrations". **March 8, 2018**

World Women's Day speech by Dr.D.Shailaja

World Environment Day Programme

International Yoga Day

Pre - IISF- 2016 Event

Societal Impact Activities

- CSIR-IICT put up a Stall at the 77th All India Industrial Exhibition (AIIE), Nampally, Hyderabad. **January 2017**
- Dr. S. Sridhar & Dr. N. Lakshmi Gayatri (DST Woman Scientist) of CSIR-IICT have installed a membrane based water purification plant of 300 Lit/hr capacity for Madipally School in Khammam District. This venture is sponsored by Department of Science and Technology, New Delhi under a Woman Scientist scheme. **June 2017**
- Dr. S. Chandrasekhar, Director, CSIR-IICT Hyderabad led a team comprising of Dr. S. Sridhar, and Dr. Prathama S. Mainkar, exhibited CSIR technologies at the Royal Australian Chemical Institute's (RACI) Centenary Conference held at Melbourne. **August 2017**
- Poster Presentation on IICT contributions to Agrochemical sector for visiting Parliamentary delegation. **August 26, 2017**
- Put up Two Stalls- A Pheromone Application Technology and Agrochemicals Interventions by CSIR-IICT at CSIR 75th Platinum Jubilee Exhibition, Dr. Zaheer Memorial School, IICT Campus. **September 01-06, 2017**
- A Stall on pesticides and their usage at IIOR Rajendra Nagar campus. **September 10, 2017**
- CSIR Platinum Jubilee Celebrations live Programme with honorable Prime Minister of India Shree. Narendra Modi. **September 26, 2017**
- A Team led by Dr. S. Sridhar installed a Nanofiltration Pilot Plant of 30,000 Lit/day. It aims to provide free drinking water to inpatients of the 1400 bed government hospital, 3000 outpatients per day, their attendants, doctors, nurses and staff. The plant was inaugurated by Shri Laxma Reddy, the honorable health minister of Telangana State. **December 21, 2017**
- CSIR-IICT put up a Stall at the 78th All India Industrial Exhibition (AIIE), Nampally, Hyderabad. **January 2018**
- CSIR-IICT put up "Pheromone Application Technology Stall" for farmers and visitors at National Conference on BHUMI SUPOSHAN conducted by Ekalavya foundation and Akshaya krishi pariwar at CSIR-IICT. **March 24-25, 2018**

Pheromone Application Technology stall at CSIR-IICT

CSIR-IICT Stall at Exhibition (AIIE), Nampally, Hyderabad

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Dr. Vineet Aniya

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Sri. Lakshma Nayak V
Sri. Malavath Ratanlal
Sri. Nagendra Prasad T
Sri. Ramachandra D.V.N.S
Sri. Rama Linga Murthy T
Sri. Rasheed Khan N
Sri. Sai Krishna G
Sri. Siva Satish G
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Sri. Srinivasan T
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Sri. Uttam Kumar M
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Sri. Anjaiah N
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Sri. Farhath Hussain
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Sri. Kameshwar Rao K
Sri. Krishna Reddy T
Sri. Lingam D
Dr. Madhusudan Rao K
Sri. Mohd Tajuddin
Sri. Murthy J.V.S.N
Sri. Prasad K.S.S.Ch
Sri. Pulya Naik M
Sri. Rama Krishna K.V.S
Sri. Rama Krishna M
Sri. Ramesh P
Sri. Ramesh N
Sri. Ramesh Babu T
Sri. Ramulu K
Sri. Ramulu P
Sri. Ravi P.V
Dr. Rohini Kumar D.B
Sri. Sai Babu PV
Dr. Shailaja S
Sri. Sri Ram Murthy J
Sri. Sridhar B
Sri. Srinivas B
Mrs. Sumathi Reddy S
Mrs. Swapna V
Dr. Swarajya Lakshmi V.V
Ms. Swarna Latha Ch
Sri. Vardharajan S
Sri. Venkatanarayana K
Sri. Venkateshwara Rao M
Sri. Vivekananda T.G

Group II (3)

Sri. Aziz Pasha
Sri. Achal Singh
Sri. Bhupal S
Sri. Madan Kumar S/O Sambaiah
Sri. Meharban Singh S
Mrs. Mercy Joseph
Sri. Naqvi S.B.A
Sri. Narsing Rao N
Sri. Prasad P.L
Sri. Satyanarayana B
Mrs. Vijay Mary L

Group II (2)

Sri. Hari Krishna Reddy L
Sri. John Ramesh
Sri. Khaja Mansoor Ahmed
Sri. Mahender M
Sri. Mahender R
Sri. Munendra Kumar M
Sri. Mohd Rafiq Basha
Sri. Raja Shekar Rao G
Sri. Salaiah S
Sri. Soori Babu K
Sri. Subba Rao N
Sri. Sudarsana Rao B
Sri. Suresh Y

Group II (1)

Sri. Amaralingeswara Rao N
Sri. Ganji Ashok
Sri. Jarupula Shankar
Sri. Mohd Shabuddin
Sri. Murali Chikalametla
Sri. Naresh Kumar T
Sri. Sambhu Sankar Badtya
Sri. Sanjeev Kumar Pradhan
Sri. Venkatesh K

Group I (4)

Sri. Alimullah Khan

Ms. Asghari Banu
Sri. Ashok / Mankaiah G
Sri. Bal Narsimha A
Sri. Damodar G
Sri. Dasarath J
Sri. Eashwar Rao K.M
Sri. Fareed Ahmed S
Sri. Gajula Sai Ganesh
Sri. Ganeshwar C
Sri. George Anthony Das
Sri. Gopalakrishna D
Sri. Hussain / Afzal Sk
Sri. Jaikishan / Nagaiah D
Sri. James Paul D
Sri. Madan M
Sri. Mallesh / Gandaiah B
Sri. Mallesh / Ramaiah J
Sri. Mir Mumtaz Ali
Sri. Mishiah / Achaiah K
Sri. Mohd Ahemed/Akbar
Sri. Mohd Jaffar
Sri. Mohd Khaja Moinuddin
Sri. Mohd Maqbool
Sri. Mohd Moinuddin / Md Jaffar
Sri. Mohd Odud/Md. Younus
Sri. Narsing Rao D
Sri. Narsing Rao / Kumaraiah T
Sri. Narsing Rao / Ramulu N
Sri. Omprakash K
Sri. Rajveeraiah / Istari A
Sri. Ramamurty G
Sri. Ramesh K
Sri. Ramulu / Chandraih M
Sri. Ravinder / Ramaswamy C
Sri. Razak Ali / Sadiq Ali
Sri. Sathyanarayana K
Sri. Sd Moinuddin / Sd Asadullah
Sri. Shaik Muneer / Maqdoom
Ms. Shiva Parvathi D
Sri. Shivaramudu D
Sri. Sudershan / Bagayya L
Ms. Sujatha R
Sri. Suryaprakash L.B
Sri. Syed Abdul Khader
Sri. Venkatesh G / Swamy G
Sri. Yadagiri / Balaiah T
Sri. Yadagiri / Rajaiah N
Sri. Yadaiah / Pochaiah M
Sri. Yousuf / Ismail Khan Md
Sri. Zaheed Hussain M

Group I (3)
Sri. Bhikshapathi T
Smt. Durga Bai B
Sri. Ghulam Taher
Sri. Mushtaq Ahmed
Smt. Padma T
Sri. Ramulu P
Sri. Ramulu P
Sri. Satyanarayana Raju R
Sri. Venkatesh J

Controller of Stores & Purchase
Sri. Uma Sankar Das

Administrative Officer
Sri. Prasad D.J.N
Smt. Sailaja Maddaly

Finance & Accounts Officer
Mrs. Krishnaveni P.V
Smt. Manoja Prasad T

Stores & Purchase Officer
Dr. Srinivas Bandi
Sri. Vijay Kumar Mahto

Sr. Hindi Officer
Dr. Naseema S

Section Officer (F & A)
Dr. Sujatha D.S

Section Officer (G)
Sri. Venkateswarlu Gadde

Section Officer (S & P)
Sri. Ravi Rajalingam G

Security Officer
Sri. Ganesh K.R

Private Secretary
Sri. Mohan Rao V
Sri. Sailendra Rao P
Mrs. Sanjeeva Rani N
Mrs. Sujatha Y
Mrs. Sundari N.N.S.V.B.T
Smt. Vanisree M
Smt. Venkata Lakshmi K

Senior Steno (ACP)
Mrs. Madhavi Y
Mrs. Saroja M
Mrs. Seshalakshmi K
Mrs. Shashikala H.S

Sr. Hindi Translator
Sri. Satyanarayana N

Asst. Sec. Officer (F&A)
Mrs. Annapurna C
Sri. Muhammad Zafar Ahmad
Mrs. Kalaimathi R Anbarasu
Miss. Latha J
Sri. Sudhakar K
Sri. Shujath Hussain S

Asst. Sec. Officer (Gen)
Sri. Anand N
Mrs. Geetha C.S
Mrs. Husn Afroze S
Mrs. Koteshwari B
Mrs. Lakshmi G.V
Mrs. Prabhavathi S
Sri. Praveen Raju S
Sri. Rajesh Chelle
Sri. Ravi Kiran G
Mrs. Sai Bhavani S
Sri. Shanker P
Sri. Srikanth G
Sri. Veera Prakash
Sri. Vincent Thomas

Asst. Sec. Officer (S & P)

Sri. Ankit Parmanand Bagde
Mrs. Indira T.S
Sri. Krishnaiah S
Sri. Naga Raju M
Sri. Nataraju C
Sri. Ratan Raj P
Sri. Srinivas B.C

Senior Steno

Sri. Balaram M
Mrs. Harathi Jawahar P
Mrs. Jaishi Rani V
Mrs. Kavitha K.L
Mrs. Lakshmi Sunitha N
Sri. Murali Krishna Y
Sri. Naveen Kumar N.K
Sri. Revathi Kumar S
Sri. Sainadh G
Mrs. Saritha Kumari M
Mrs. Shamantha D
Sri. Yadu Krishna R.R

Sr. Sec. Assistant (Gen)

Mrs. Saraswathi J
Sri. Shiv Shankar A
Ms. Sunita Devi
Ms. Uma Maheshwari G
Sri. Venkateshwara Rao A
Sri. Yadagiri K

Sr. Sec. Assistant (S & P)

Sri. Ganesh V

Sr. Security Assistant

Sri. Sudersan P

Jr. Sec. Assistant (F&A)

Sri. Madhava Subrahmanya Kumar T
Sri. Rakesh Doure
Sri. Suneel Kumar T

Jr. Sec. Assistant (Gen)

Sri. Jayaprakash U
Sri. Panidhar K
Sri. Srinivas Karthik V
Sri. Yakaiah M

Jr. Sec. Assistant (S & P)

Sri. Madhusudhan D
Sri. Prasad G.L.S

Junior Steno

Miss. P. Akhila
Sri. Dumpati Saikumar
Smt. Gosula Divya Bharathi
Sri. Kethavathu Kumar
Sri. Praful Paswan
Miss. Tayyaba Unnisa

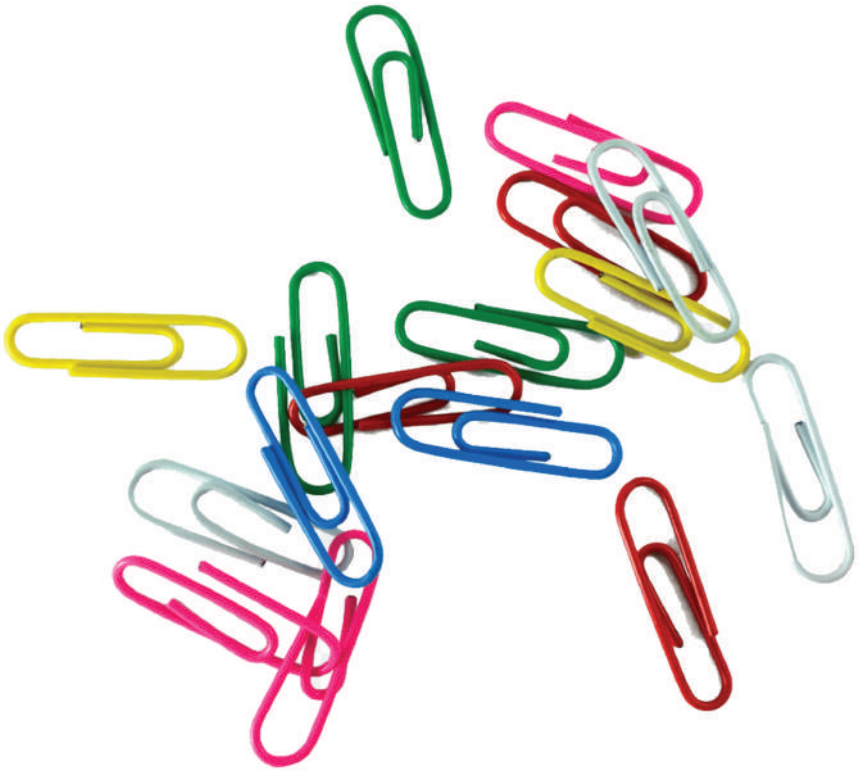
Staff Car Driver

Sri. Murali Krishna B
Sri. Nageswara Rao P
Sri. Sidda Ramulu B
Sri. Venkatesham P

Other Staff

Sri. Abdul Rehman
Sri. Babul A
Sri. Balaiah M
Sri. Chandra Mohan A
Sri. Chittaiah S
Sri. Dasarath M
Ms. Devamma M
Sri. Krishna E
Sri. Krishna C
Sri. Krishna N
Sri. Kumar G
Sri. Laxmaiah D
Mrs. Laxmamma M
Mrs. Laxmi J
Mrs. Laxmi T
Sri. Mahender B
Sri. Mallesh T
Sri. Mankiah D
Sri. Masood Ali
Sri. Meghanath D
Sri. Mohan Rao M
Sri. Mohd Khadir
Sri. Nagabhushanam P
Ms. Nagamani C
Sri. Narender V
Sri. Narsimha N
Sri. Narsing Rao C.K
Sri. Narsing Rao R
Smt. Padma M
Sri. Pandari
Sri. Parushaiah M
Smt. Prabhavathi Nair P
Sri. Rajasekhar K
Sri. Ramesh A
Sri. Ramulu
Mrs. Renuka P
Sri. Sajith P S
Sri. Sangeeta Rao P
Sri. Sathyanarayana A
Sri. Satyanarayana A
Sri. Satyanarayana B
Sri. Satyanarayana K
Sri. Shaik Ismail
Sri. Shaik Jahangir
Sri. Shankar R
Sri. Shankar D
Mrs. Shashikala A
Sri. Srinivas S
Mrs. Sumathi V
Ms. Sundari Kaur
Sri. Suryanarayana M
Sri. Swamy N
Smt. Swarnalatha M
Ms. Syeeda Sirajunnisa Begum
Sri. Vaman Rao K
Sri. Venkatesh L
Sri. Venkatesh M
Sri. Vishwanath C
Sri. Yadaiah M
Mrs. Yesupadamma K.C

ANNEXURE



NEW CONTRACTS SIGNED/ ASSIGNMENTS UNDERTAKEN 2016-17

OVERSEAS

Sponsored/Collaborative/Consultancy

Project Title	Party
Development of an advanced Mg Ion battery	M/s. AOS Technology Incorporation, USA

NATIONAL

Project Title	Party
Advisory consultancy in the field of organic synthesis, process development	M/s. Cipla Ltd., Mumbai
Analysis and data interpretation of Biodiesel samples	M/s. APSRTC, Vijayawada
Analysis and data interpretation of Biodiesel samples	M/s. TSRTC, Hyderabad
Analysis and data interpretation of fatty oils for physicochemical chracterisation	M/s. Food Safety and Standards Authority of India, Chennai
Analysis of samples through LCMS, GCMS and EIMS	M/s. Hygro Chemicals Pharmatek Pvt. Ltd., Hyderabad
Analysis of samples through Proton NMR, Mass spectrometer, HPLC	M/s. Accura Research Chemicals Pvt. Ltd., Hyderabad
Analysis of samples to test for 100% solvent less food grade epoxy (6 samples)	M/s. Vani Constructions, Visakhapatnam
Analysis of samples using Microwave facility.	M/s. Sri Lakshmi Bhargavi Pharma Pvt Ltd., Hyderabad
Analysis of samples using NMR analysis	M/s. Natco Pharma Ltd., Maharashtra
Analysis of samples using NMR analysis	M/s. Cipla Ltd., Maharashtra
Antirodent evaluation of samples	M/s. Shakun polymers Ltd., Gujarat
Biosyn gas derived dimethyl ether synthesis for LPG Blending.	M/s. HPCL, Bangalore
Characterization and refining of crude tobacco seed oil	M/s. ICAR-Central Tobacco Research Institute, Rajahmundry
Classification of Triphenyl Phosphene	M/s. Roopa Industries Limited., Hyderabad
Collaboration for research and development of processes for new molecules and API's	M/s. Accura Research Chemicals Ltd., Hyderabad
Comparative bio-efficacy data generation of Transfluthrin Neem liquid vaporizer	M/s. Plant Protection Consultant, New Delhi
Consultancy in Analysis NMR samples	M/s. Mylan Laboratories Ltd., Hyderabad
Consultancy in analyzing samples using microwave facility	M/s. Shree Lakshmi Bhargavi Pharma Pvt.Ltd., Medak
Consultancy on analysis of NMR Samples	M/s. Biocon Limited., Bangalore

Project Title	Party
Consultancy on anti rodent testing (4-samples)	M/s. BSNL, Pune
Consultancy on Anti-Rodent tests	M/s. Vindhya Telelinks Pvt.ltd., MP
Consultancy on Anti-Rodent tests for DWC pipe samples	M/s. Rex Polyextrusion Pvt. Ltd., Sangli
Consultancy on moisture cured PU coal tar black	M/s. Solvosol paints Pvt. Ltd., Hyderabad
Consultancy on NMR analysis	M/s. Indian Immunologicals
Consultancy on NMR analysis	M/s GE India Technology Centre Pvt. Ltd., Bangalore
Consultancy on NMR analysis	M/s. Dr. Reddy's Laboratories Ltd., Hyderabad
Consultancy on NMR analysis	M/s. Amneal Pharmaceuticals Pvt. Ltd., Ahmedabad
Consultancy on NMR analysis	M/s.Biocon Ltd., Bangalore
Consultancy on NMR analysis	M/s. Neuheit Pharma Technologies Pvt. Ltd., Hyderabad
Consultancy on testing of epoxy and coal ta based paints on water pipe lines	M/s. Solvosol paints Pvt. Ltd., Hyderabad
Consultancy services in the area of vegetable oil, vanaspathi and allied products	M/s Kaleesuwari Refinery Pvt Ltd., Chennai
Cooperative Bioefficacy data generation of Prallethrin Neem and combined mosquito coil formulations	M/s. Plant Protection Consultant, New Delhi
Cyclization of Arene by photochemical reaction	M/s. Sapala Organics Pvt. Ltd., Hyderabad
Design and development of active layer materials for flexible solar cells	M/s. Manipal Technologies Ltd., Manipal
Development of Crospovidone (Type A)	M/s. Lucas Technologies Ltd., New Delhi
Development of process knowhow for APIs/ intermediates	M/s. Sai Life Sciences Ltd., Hyderabad
Development of process knowhow for APIs/reference compounds	M/s. Sai Life Sciences Ltd., Hyderabad
Development of process knowhow for the up gradation and bleaching of crude rice	M/s. Sheel Chand Agrooils Pvt. Ltd., Uttarkhand
Development of process knowhow for the upgradation and bleaching of crude rice bran wax.	M/s. Marico Ltd., Solan
Development of rechargeable Mg Ion battery chemistry for powering defence ground applications	M/s. Research Centre of Imarat (RCI), Hyderabad
Development of vapour phase catalytic process for the synthesis of iminostillene from umunodinezyl	M/s. Divi's Laboratories Ltd., Vishakapatnam
Estimation of Impurity in Voriconazole Drug using Ion Exchange Chromatography (IEC)	M/s. Lee Pharma Ltd., Hyderabad
Evaluation of antidiabetic potential of two herbal extracts in diabetic	M/s. Laadh Biotech Ltd., Hyderabad
Evaluation of chemical disinfection unit plant	M/s. Cynosure Enterprises Ltd., Hyderabad

Project Title	Party
Fatty acid composition analysis of algal biomass samples (34 samples)	M/s. Defence Institute of Bioenergy Research (DIBER), Uttarkhand
Hazop study and risk analysis for soda recovery plant-II	M/s. ITC Limited., Secunderabad
High rate biomethanation of organic waste for generation of power for off-grid applications	M/s. Ahuja Engineering Services Pvt. Ltd., Secunderabad
Labscale process for Anisole	M/s. Vinati Organics Ltd., Mumbai
Licensing of Anaerobic gas lift reactor	M/s. Ahuja Engineering Services Pvt. Ltd., Secunderabad
Licensing of modular high rate Biodigester	M/s. Enbiopac, Kochi
Licensing of Modular High rate biodigester	M/s. The Enbiopac CO. Bengaluru
Micellar characterisation study for Decetoxel injection	M/s. Epsilon Pharmaceuticals., Ranga Reddy
Nanofiltration process for removal of chloride from TATA Steel effluent on bench scale with a feed capacity of 20L.	M/s. Tata Steel Ltd., Jamshedpur
Physico-Chemical and compositional studies of Soldier Fly Insect Oil	M/s. Green Carbon Fuels & Feeds Pvt. Ltd., Hyderabad
Preparation and supply of microbial culture for deodorization	M/s. Hyderabad Integrated MSW ltd., Hyderabad
Preparation of local oil spill disaster contingency plan	M/s. Visakhapatnam Port Trust, Visakhapatnam
Process Development and BDR for the commercial plant of Arobenzene	M/s. Vinati Organics Ltd., Mumbai
Process development for the enrichment of GLA atleast 98% Boraglonl	M/s. Fermish Chemical Technologies Pvt. Ltd., New Delhi
Process development for the production of Paracetmol using Acetic acid and submission of BDR for commercial plant of 10000TPA capacity	M/s. Bharat Chemicals, Mumbai
Process development of Cyazofamid (Fungicide)	M/s. Insecticides India Ltd., New Delhi
Process knowhow for Annona squamosa extracts and isolation	M/s. Dhana Crop Sciences Ltd., Hyderabad
Process knowhow for the upgradation and bleaching of crude rice bran wax.	M/s. Kanchan Oil Mills Ltd., Kolkata
Process optimisation of intermediates	M/s. Vamshi Labs Ltd., Solapur
Processing and Analytical methodologies of oils and fats	M/s. Clients from various Industries
Providing consultancy in the process development of Fexofenadine, Flucanazole and suggamoneddex	M/s. Virupaksha Organics Ltd., Hyderabad
Providing consultancy in upgardation of commercial plant design from 2000 TPA to 3000TPA for paratertiary butyl methyl benzoate (PTBMB)	M/s. Vinati Organics Ltd., Mumbai
Providing consultancy in improvement in the process of production of Hi Strength Hypo	M/s. Sree Rayalseema Hi Strength Hypo Ltd., Kurnool

Project Title	Party
Providing consultancy in making of 2-octyl-cyanocrylate	M/s. Stride organics Ltd., Hyderabad
Providing consultancy in PXRD analysis of pharma samples.	M/s. AET Laboratories Ltd., Hyderabad
Providing consultancy in the field of Molecular Modelling	M/s. Hetero Drugs ltd., Hyderabad
Providing Oligonucleotide facilities	M/s. BioArtis Life Sciences Pvt. Ltd., Hyderabad
Selective catalytic hydroxylation of benzene with molecular oxygen	M/s. Sabic Research & Technology Pvt. Ltd., Bengaluru
Synthesis of 5-Benzyloxy 4-hydroxy-6-(hydroxymethyl) pyridine 3-carboxylic acid	M/s. Vasudha Pharma Chem Ltd., Hyderabad
Synthesis of New Chemical Entities (NCE's)	M/s. India Insecticides Ltd., New Delhi
Testing of Dettol Antiseptic liquid & Harpic disinfectant	M/s. DD Reg Life Sciences Pvt. Ltd., Gurgoan
Testing of polymer coated samples	M/s. Amchem Products Ltd., Noida, U.P.
Utilization of existing facilities of Chemical Biology Division	M/s. Laadh Biotech Pvt. Ltd., Hyderabad
Water purification technology for fabrication of membrane based demineralised water plants of 25-50 2PH capacity plant	M/s. Plantris Ventures Pvt. Ltd., Delhi

Grant-in-Aid

Project Title	Sponsor
A knowledge based approach to drug repurposing for socially important and rare diseases	DST, New Delhi
Assessment of the quality of vegetable oils while frying and formulation of safety guidelines for fried oils for repeated frying	Food Safety and Standards Authority of India, New Delhi
Biochemical and molecular analysis of novel type of mutanase from paracoccus sp	DST, New Delhi
C V Raman International Fellowship for African Researchers	DST, New Delhi
Carbon-Alumina composites for defluoridiation of water	DST, New Delhi
Comparative studies of artificially ripened fruits ripened with various artificial ripeners for identification of changes in chemical composition and the residues of artificial ripeners	Food Safety and Standards Authority of India, New Delhi
Computational Studies of Intermolecular Interactions: Understanding the Mechanism of Fouling of Polymeric Membranes in Water Treatment using Molecular Dynamics simulations and DFT methodologies	SERB, New Delhi

Project Title	Sponsor
DBT/BINC-JRF	DBT/BINC, New Delhi
DBT-JRF	DBT-BCIL, New Delhi
Development of internally plasticized high impact graphene/clay-polyvinyl chloride nanocomposites	DST, New Delhi
Development of new heterogeneous catalytic methods for the synthesis of industrially important N-heterocycle compounds	DST, New Delhi
Development of noval methodologies for the identification and quantification of oils in blended, interesterified and adulterated oils based on triglyceride structure, fatty acid composition and minor constituents	Food Safety and Standards Authority of India, New Delhi
Development of novel cationic electrocyclization precursors and application in the synthesis of highly substituted cyclopentenes/indenes	SERB, New Delhi
Development of sustainable water treatment system based on microbial desalination process for salt removal	DST, New Delhi
Elucidating the role of DJ-1 mediated mitochondrial bioenergetics and chaperone activity in the pathophysiology of parkinsons disease	SERB, New Delhi
Energy efficient solar and DUV LEDs for next generation luminescent lighting and bio medical applications	SERB, New Delhi
Evaluation of nanoparticle toxicity using mass spectrometry based comparative metabolomics in model organism	SERB, New Delhi
Exploring selected natural plant sources of North East parts of India as potential therapeutic agents useful for the treatment of cancer	BCIL, New Delhi
Generation of data on pesticide residues and metal contaminants in edible vegetable oils of different regions	Food Safety and Standards Authority of India, New Delhi
ICMR Fellowship	ICMR,New Delhi
ICMR Fellowship-SRF	ICMR, New Delhi
INSPIRE Faculty Award	DST, New Delhi
INSPIRE Fellowship	DST, New Delhi
Mitochondria-targeted escultein as an anti-atherosclerotic agent: Mechanisms and its relevance in vascular aging	SERB, New Delhi
NASI Senior Scientist Platinum Jubilee Fellowship	The National Academy of Sciences, India, Allahabad

Project Title	Sponsor
National facility for Combinatorial Natural Products - Phase-II	DST, New Delhi
National Post-Doctoral Fellowship	SERB, New Delhi
Oxidative dehydrogenation of butane to butadiene using CO2 as a soft oxidant	DST, New Delhi
Regulatory pathways and role of zinc oxide (ZnO) nanoparticles in angiogenesis	DST, New Delhi
Strong NIR absorbing BODIPY incorporated Ru and Porphyrin dyes for design of efficient dye-sensitized solar cells (DSCs)	DST, New Delhi
Structural genomics of methionine aminopeptidase from pathogenic microbes: Interdisciplinary approach to identify specific inhibitors	SERB, New Delhi
Sustainable bioprocess for the production of high value succinic acid from municipal waste	DST, New Delhi
Unlocking therapeutic potential of glycoconjugates and isoprenoids of Indian mangrove flora	SERB, New Delhi
Valorization of waste to carboxylic acids by integrated acidogenic fermentation process using biorefinery approach	DBT, New Delhi

Projects Completed/Reports submitted to User Agencies

Project Title	Party
Process knowhow, scale-up studies on Pilot plant and design of Commercial Plant for Hydrazine Hydrate (HH)	M/s. GACL, Vadodara, Gujarat
Basic Engineering Report (BEP) on Hydrazine Hydrate	M/s. GACl, Vadodara, Gujarat
Improvement for the process of insecticidal coating composition	M/s. Meenakshi Agrochemicals Ltd., Hyderabad
Development of process knowhow for the upgradation and bleaching of crude rice bran wax	M/s. Sheel Chand Agrooils Pvt. Ltd., Uttarkhand
Characterization and quantification of lipids in Hepatitis B surface antigen samples	M/s. Shantha Biotecnics Ltd., Hyderabad
Evaluation report on the disinfection treatment unit developed by client for liquid chemical/biomedical waste pretreatment	M/s. Cynosure Enterprise Ltd., Hyderabad
Laboratory process for Lightly Cross-Linked Polyacrylic acid	M/s. Lucas Technologies, Hyderabad
Preparation of biopesticide from Annona Squamosa	M/s. Dhana Crop Science, Hyderabad

Processes / Technologies Demonstrated / Released / In Commercial Production

Project Title	Party
Process for producing 200 ml of Isrosene by catalytic hydrogenation of Linear Alkyl Benzene (LAB) affinate to reduce aromatic content 24% to less than 5 % by Volume	M/s. Andhra Sugars, Ltd., Tanuku
Demonstration of process of lily aldehyde from Para-tert butyl benzaldehyde involving the steps Aldol condensation and hydrogenation at 500 gm batch with recycle of catalyst	M/s. Vinati Organics Ltd., Mumbai
Demonstration of process knowhow for bio adhesive 2-Octylcyanocrylate	M/s. Stride Organics Pvt. Ltd., Hyderabad
Demonstration of Nanofiltration process for removal of chloride from TATA Steel effluent on bench scale with a feed capacity of 20L.	M/s. Tata Steel Ltd., Jamshedpur
Process knowhow for the upgradation and bleaching of crude rice bran wax	M/s. Kanchan Oil Industries Ltd., Kolkata
Process know-how for Anonna Squamosa Extraction & Isolation	M/s. Dhana Crop Sciences Ltd., Hyderabad
Process know-how for the preparation of defatted wax from crude rice bran wax	M/s. Marico Ltd., Solan H.P.
Demonstration of process knowhow for xylose and xylitol production from biomass	M/s. Lucas Technologies, Hyderabad
Demonstration of process of Benzaldehyde in 600 ml autoclave with recycle of catalyst	M/s. Vinati Organics Ltd., Mumbai
Demonstration of process knowhow for the upgradation and bleaching of crude rice bran wax	M/s. Sheel Chand Agrooils Pvt. Ltd., Uttarkhand
Demonstration of process for xylitol	M/s. Lucas Technologies Ltd., Hyderabad
Demonstration of process for xylose	M/s. Lucas Technologies Ltd., Hyderabad
Laboratory process for Lightly Cross-Linked Polyacrylic acid	M/s. Lucas Technologies Ltd., Hyderabad

Exchange of Agreements with M/S. AOST, USA & M/S. Laadh Biotech Ltd., Hyderabad

NEW CONTRACTS SIGNED/ ASSIGNMENTS UNDERTAKEN 2017-18

OVERSEAS

Sponsored/Collaborative/Consultancy

Project Title	Party
Modelling and simulation of blending unit operation	M/s. Daichii Sankyo Europe GmbH, Germany

NATIONAL

Project Title	Party
Advisory consultancy in installing biofilters control odour	M/s. Kondapally Enviorntech Pvt. Ltd., Vijayawada
Advisory consultancy in the field of for castor poluols based rigid foams	M/s. Sweetech Environ India Pvt. Ltd., Secunderabad
Analysis of samples using LC-HRMS (50-samples)	M/s. Sai Life Sciences., Hyderabad
Anti rodent evaluation of rodent species	M/s. V-Guard Industries Ltd., Coimbatore
Consultancy on anti rodent testing	M/s. Crescent India Polymers, Dharwad
Consultancy in the field of novel adjuvants including emulsions	M/s. Bharat Biotech Pvt. Ltd., Hyderabad
Consultancy on import of purchase of Carbon tetrachloride to use in bv acid chloride process	M/s. Bharat Rasayan Ltd., New Delhi
Consultancy on import or purchase of HCFC-13a to use in manufacture of Halothane	M/s. Piramal Pharma Solutions, Mumbai
Demonstration of synthetic methodologies for pheromones	M/s. Nova Agritech Pvt. Ltd., Hyderabad
Design & fabrication of membrane based water purification plants of 300-2000 litres/hr capacity	M/s. Kewaunce Scientific Co-op India Pvt. Ltd., Bangalore
Development of prices for perfurmery chemicals	M/s. M.K. Aromatics & Chemicals, Maharashtra
Development of process knowhow for Na-TCP	M/s. PMFAI, Mumbai
Development of process knowhow for total synthesis of Eribulin	M/s. Cipla Ltd., Mumbai
Development of VK 2 glue	M/s. 3BRD Airforce, Chandigarh
Epoxy polyaniline coating for static control	M/s. Monarch Industrial Products (I) Pvt. Ltd., Theni
Feasibility studies on enzymatic degumming process developed by CSIR-IICT	M/s. Danisco India Pvt. Ltd., Gurgoan
Licensing of Biodigester	M/s. BEIL Research and Consulting Pvt. Ltd., Gujarat
Licensing of Modular high rate Biodigester	M/s. Mamco Design Engg. Pvt. Ltd., Maharashtra

Project Title	Party
Literature renew & opinion report on four catalogue chemicals	M/s. Laxai Life Sciences Pvt. Ltd., Hyderabad
Preparation of core shell emulsion polymers with core containing acrylic acid and shell containing fluorinated monomers	M/s. Pidilite Industries Ltd., Mumbai
Process development for preparation of Extra White Starch	M/s. Lucas Technologies Ltd., Hyderabad
Process for preparation of CTFE Monomer	M/s. Gujarat Flurochemicals Ltd., Gujarat
Process improvement of Loxoprofen	M/s. Enal drugs Pvt. Ltd., Hyderabad
Processing and analytical methodologies of oils and fats (18 participants)	18 Different Industrial Participants
Production of ultrapure water for Biomedical and Biochemical applications	M/s. Althion Tech Information Innovation (P) Ltd., Hyderabad
Providing advisory consultancy in the area of double shooting in chemistry	M/s. Intonation Research Laboratories Pvt. Ltd., Hyderabad
Providing advisory consultancy in the area of heterogeneous catalysis	M/s. Sreeni Labs, Hyderabad
Providing advisory consultancy in the field of Natural Product extraction and Isolation	M/s. Sri Kartikeya Pharma., Hyderabad
Providing advisory consultancy in the field of organic synthesis	M/s. Cipla Ltd.
Providing advisory consultrancy in making of 2-octyl-cyanoacrylate	M/s. Stride Organics, Hyderabad
Providing consultancy on PXRD analysis of pharmaceuticals samples	M/s. AET Laboratories Ltd., Hyderabad
Providing consultancy services in the area of vegetable oil, Vanasapathi	M/s. Kalewswari Refinary Ltd., Mylapore
Providing incubation space	M/s. Meshram Life Sciences., Hyderabad
Providing incubation space	M/s. Aaltramed Health Care Services, Hyderabad
Providing incubation space	M/s. Virupaksha Life Pvt. Ltd., Hyderabad
Providing incubation space to carryout projects related to API's	M/s. Vamshi Pharma Pvt. Ltd., Hyderabad
Providing NMR spectrometer services	M/s. Dr. Reddy's Labs Ltd., Hyderabad
Providing technical report on the use of thermal resistant coating on chimney	M/s. M.P. Power Generation Company Ltd., Jabalpur
Report on import of Bromofluoromethane	M/s. Cipla Ltd., Mumbai
Single crystal studies on Novel Polymorphic forms of API's	M/s. Alembic Pharmaceuticals Ltd., Vadodara
Standardisation &Denitrosation reaction of low molecular weight heparins	M/s. Biological (E) Ltd., Hyderabad

Project Title	Party
Synthesis and supply of (1R, 4R)-4- Hydroxycyclopent-2-en-1yl acetate	M/s. Dev Synthesis, Hyderabad
Synthesis of Polychloro-trifluoroethylene (PCTFE) from Chlorotrifluoroethylene (CTFE)"	M/s. Gujarat Fluorochemicals Products (I) Pvt. Ltd., Gujarat
Testing of thermal and corrosion resistant coating	M/s. Kirloskar Corrocat Pvt. Ltd., Pune
Transformation of water hyacinth to scalable nutrient rich organic fertiliser	M/s. Khar Energy Optimusers, Hyderabad
Validation and estimation of impurity -E in voriconazole drug using Ion Exchange Chromatograph	M/s. Lee Pharma Ltd., Hyderabad

Grant-in-Aid

Project Title	Sponsor
An investigative study on the optoelectronic properties of group 16 pi-conjugated materials containing peripheral boron moieties	SERB, New Delhi
Assessment of plasma metabolites in patients on maintenance hemodialysis	TSCOST, Telangana
Asymmetric dearomatization of phenols and indoles and their application in the total synthesis of complex natural products	DST, New Delhi
Bioassay guided search for active constituent/s of A. mericata and their therapeutic effect on AMPK with reference to diabetes	DBT, New Delhi
Bioconversion of CO2 to platform chemicals through microbial catalyzed electrochemical approaches	DBT, New Delhi
Central Sector Scheme (2017-2018)	Food Safety and Standards Authority of India, New Delhi
Chemistry and biology of maltepolides A-F and their analogs	SERB, New Delhi
Co delivery of Erlotinib and Luteolin with chitosan-g-TGS nanocarriers-Potential modulators of EGFR mediated P13K/AKT/mTOR pathway for overcoming multidrug resistance	DST, New Delhi
DBT-JRF	DBT-BCIL, New Delhi
DBT-RA	IISc, Bangalore
Design of highly efficient and inexpensive membrane equipment as import substitutes for demineralized water production and haemodialysis	SRISTI-BIRAC, Ahmedabad
Design, synthesis and biological evaluate of imidazopyridines, imidazopyridine fused chromenes and diazepines: A green chemistryapproach	SERB, New Delhi
Development of choline hydroxide	Semi-Conductor Laboratory, Mohali

Project Title	Sponsor
Development of efficient and cost effective catalysts for C-H bond activation through simultaneous production of CO free hydrogen and carbon nanotubes from renewable H4: A value addition process	DST, New Delhi
Development of next generation BRAF protein kinase inhibitors: Rational design, green synthesis and biological evaluation on B-Raf inhibition and signaling in melanoma	SERB, New Delhi
Development of novel benzocycloheptenone templates by C-H bond activation relevance to application in medicinal chemistry	SERB, New Delhi
Development of novel enyne-assisted annulations towards the construction of fused polycyclic alkaloids	SERB, New Delhi
Development of novel heterocyclic compounds as inhibitors of influenza virus neuraminidase	DST, New Delhi
Development of pharmacopoeial monographs on single drugs of plant, mineral, metal and animal origin	PCIMH, Ghaziabad
Development of semi-automatic equipment for large area dye-sensitized solar module fabrication	DST, New Delhi
Elucidating factors affecting thermal stability of a protein: Computational studies on selected proteases of industrial significance	DBT, New Delhi
Environmental begin smart micro-total process machine developments for on demand safe chemical synthesis	SERB, New Delhi
Exploring the possibility of developing semiochemical based control strategy for the management of cossus cadambae the borer pest of tectona granidis through isolation & identification of its pheromone system	SERB/KFRI, New Delhi
Exploring the possibility using venom-derived peptides to mitigate stroke-induced brain damage by targeting acid sensing ion channel	ICMR, New Delhi.
High rate biomethanation of organic fraction of MSW for the generation of biogas based power and bio-manure	DBT, New Delhi
Identification of natural antioxidants and radioprotectors from extremely radioresistant and oxi	BRNS/DAE, Mumbai
INSPIRE Faculty Award	DST, New Delhi
INSPIRE Fellowship	DST, New Delhi
Integrated and sustainable sewage and organic solid waste treatment for decentralized applications	DST, New Delhi
Integrated control of dengue through predictive models in Telangana,India	DST, New Delhi

Project Title	Sponsor
Integrated eco-electrogenic system for efficient and sustainable treatment of textile wastewater	DBT, New Delhi
Laboratory scale investigation on chemical treatment of subsurface lignite deposits to enhance the conversion of lignite to methane	ONGC, Delhi
Methane to methanol transformation over metal encapsulated zeolites: A DFT study of mechanism	DST, New Delhi
Mitochondria-targeted escultein as an anti-atherosclerotic agent	BIRAC, New Delhi
National facility for scientific validation of traditional knowledge through modern approaches	DST, New Delhi
National Post-Doctoral Fellowship	SERB, New Delhi
New semiconductors based solution - Processed small molecule for optoelectronic devices	DST, New Delhi
Novel adjuvants for malaria vaccine development	DST/BBIL, New Delhi
Phytochemical investigation and anti-malaria activity evaluation of medicinal plants used by indigenous tribes of Andman and Nicobar Islands	SERB, New Delhi
Raja Ramanna Fellowship Scheme	DAE, Mumbai
Role of AMP-activated protein kinase in vascular aging	DBT, New Delhi
Role of GAS41 in miRNA Biogenesis	ICMR, New Delhi
Sequestration of carbon-dioxide for the synthesis of value added products using microbial catalyzed electrochemical system	SERB, New Delhi
Skill Development Programme on Advanced Pharma Biotechnology	APSSDC, Govt. of A.P.
Strategic biorefinery platform with integrated bioprocess in a self-sustained closed loop for multi-biobased product output	DST, New Delhi
Structure based target exploration for the discovery of new leads for antibiotics	ICMR, New Delhi
Sustainable wastewater treatment through bio-photoelectro catalysis and biofuel production	IMPRINT-MHRD, Govt. of India
Synthesis of new fluoro analogues of bedaquiline and study of their antimycobacterial activity	DST, New Delhi
Synthesis,characterization and evaluation of structured lipids for potential bioactive applications	SERB, New Delhi
Toxicity evaluation of ayurvedic herbo-metallic preparations	Ministry of AYUSH, New Delhi
Use of lipid nanoparticles for effective delivery of siRNA against chikungunya virus	DST, New Delhi

Projects Completed/Reports submitted to User Agencies

Project Title	Party
Sampling and analysis of proposed grades of seams of collieries/sidings	M/s. Office of Coal Controller, CCO, Kolkata
Development on process knowhow for Hydroxy Propyl Cellulose (HPC) at 100 gm batch	M/s. Lucas Technologies Pvt. Ltd., Hyderabad
Validation and estimation of Impurity-E in Voriconazole drug using Ion Exchange Chromatography	M/s. Lee Pharma Ltd., Hyderabad
Report on the use 3,3,3-trifluropropylene (1234zf) instead of Ethylene to make 343mdf instead of 250fb.	M/s. Chemours Company, USA

Processes / Technologies Demonstrated / Released / In Commercial Production

Project Title	Party
Improvement in the process of production of High Strength Hypo (HSH)	M/s. Sree Rayalseema Hi Strength Hypo Ltd., Kurnool
Demonstration of process development for preparation of extra white starch	M/s. Lucas Technologies Pvt. Ltd., Hyderabad
Demonstration of process development for Crospovidone (Type A)	M/s. Lucas Technologies Pvt. Ltd., Hyderabad
Demonstration of process development and Basic Design Report (BDR) for 3 TPD para-methoxy phenyl acetic acid	M/s. Vinati Organics Ltd., Mumbai
Demonstration of process knowhow for hydroxy propyl cellulose at 100gm batch	M/s. Lucas Technologies Pvt. Ltd., Hyderabad
Demonstration on process know how scale up studies on pilot plant and designs for commercial plant for hydrazine hydrate	M/s. GACL, Hyderabad
Preparation of Epoxy-Polyaniline coating for static control (ESD) flooring with resistance in the range of 10^3 to 10^9 ohm/sq	M/s. Monarch Industrial Products (I) Pvt. Ltd., T.N.
Process development of "Avobenzone" in 1 Lit. capacity jacketed reactor	M/s. Vinati Organics Ltd., Mumbai

Exchange of Agreements with M/S. Bharat Biotech Pvt. Ltd., Hyderabad & M/s. Althion Tech Information Innovation (P) Ltd., Hyderabad

PATENTS FILED IN INDIA & OVERSEAS

2016-17

2-Pyridone based derivatives useful as potential Phosphodiesterase 3A(PDE3A) inhibitors and a process for the preparation thereof **Application No. PCT/IN2016/050371 Dt: 28-10-16 (PCT)**

A New Porous Polymer Scaffold for On-site delivery of Stem Cells: Neo-vascularization Potentiates Tissue Regenaration while Protecting from Oxidative Stress by Enhanced Engraftment **Application No. 15/336187 Dt: 27-10-16 (US)**

A Process for the preparation of Nicotine **Application No. PCT/IN2017/050007 Dt: 06-01-17 (PCT)**

A process for the synthesis of silver nitroprusside nanoparticles and its Biomedical applications **Application No. 201611039557 Dt: 21-11-16 (India)**

An improved process for production of hydrazine hydrate **Application No. 201611033667 Dt: 03-10-16 (India)**

C5, C6 substituted and/or fused oxindoles as anti-cancer agents and process for preparation thereof **Application No. 201611037409 Dt: 02-11-16 (India)**

Development of solid base catalyst for the single step synthesis of glycidol from glycerol **Application No. 201611030495 Dt: 07-09-16 (India)**

Enzyme-Assisted Extraction of Stevio-Glycosides from the leaves of Stevia rebaudiana **Application No. 15/366120 Dt: 01-12-16 (US)**

Gold nanoparticles based new formulations for the delivery of drugs and nucleic acids for HER2+cancer therapy **Application No. 201611036499 Dt: 25-10-16 (India)**

Isothiocyanate Compouds as SMARI Stabilizers **Application No. 201611028762 Dt: 24-08-16 (India)**

Molecular engineered fullerene electron acceptors for optoelectronic applications **Application No. 201611034418 Dt: 07-10-16 (India)**

N-((3,4,5 - Trimethoxystyryl)aryl) cinnamamide derivatives as potential anticancer agents **Application No. 15/504985 Dt: 17-02-2017 (US); Application No. 15780946.8 Dt: 21-02-2017 (EP)**

One Pot Synthesis of High Performance N-Methylfulleropyrrolidine Derivatives for Organic Solar Cell Applications **Application No. 201611043425 Dt: 20-12-16 (India)**

Process for preparation of (2S,3S)-Taxifolin-6-C-Â¿-D-Glucopyranoside(ulmoside A) AND (2R,3R)-Taxifolin-6-C-Â¿-D-Glucopyranoside **Application No. 15/135983 Dt: 22-04-16 (US)**

Process for the preparation of novel propiolamides and pyrrolidine-2,5-diones and their use as potential pancreatic lipase inhibitors for the management of obesity **Application No. 201611041430 Dt: 05-12-16 (India)**

Process for the preparation of novel propiolamides and their use as potential pancreatic lipase inhibitors for the management of obesity **Application No. 201611041429 Dt: 05-12-16 (India)**

Progesterone-cationic lipid hybrid as anticancer agent and the process of synthesis thereof **Application No. 201611025818 Dt: 28-07-16 (India)**

Pyridone derivatives useful as potential insect antifeedant of the compounds against a major agricultural pest spodoptera litura and process for the preparation there of **Application No. PCT/IN2016/050451 Dt: 21-12-16 (WO)**

Simultaneous application of targeted chemotherapy and cancer immunotherapy to Inhibit and increase the survival of established pancreatic cancer in syngeneic mouse tumor model **Application No. 15/460701 Dt: 16-03-17(US)**

Synthesis and Biological Evaluation of (E)-4-(4-Acrylamidophenoxy)-N-Methylpicolinamide Conjugates as Potential Anticancer Agents **Application No. PCT/IN2017/050004 Dt: 04-01-17 (WO)**

Synthesis and Biological evaluation of (Z)-3,4,5 - Trimethoxystyryl - benzene sulfonamides as potential anti cancer agents **Application No. 2017-517275 Dt: 30-03-17 (Japan)**

Synthesis and Biological Evaluation of 4Â¿-Amidotriazole linked Podophyllotoxin derivatives as Potential Anticancer Agents **Application No. PCT/IN2017/050088 Dt: 10-03-17 (WO)**

Synthesis and biological evaluation of mitochondria - targeted esculetin for its anti-atherosclerotic and age

delaying effects **Application No. 15/443538 Dt: 27-02-17 (US)**

Synthesis of N-((1-pheny1-9H-pyrido[3,4-b]indo1-3-y1) methy1)cinnamamides as potential Anticancer Agents **Application No. PCT/IN2017/050031 Dt: 20-01-17 (PCT)**

2017-18

A dewaxing aid for petroleum refining **Application No. 201741028218 Dt: 08-08-17 (India)**

An improved process for production of hydrazine hydrate **Application No. PCT/IN2017/0505431 Dt: 28-09-17 (PCT)**

C5, C6 substituted and/or fused oxindoles as anti-cancer agents and process for preparation thereof **Application No. 15/802003 Dt: 02-11-17 (US)**

Design of highly compact, low cost membrane system of high capacity for the production of ultrapure demineralized water **Application No. 201711037739 Dt: 25-10-17 (India)**

Donor-pie-acceptor based porphyrin sensitizers for dye-sensitized solar cells **Application No. 201711011999 Dt: 03-04-17 (India)**

Gold nanoparticles based new formulations for the delivery of drugs and nucleic acids for HER2+cancer therapy **Application No. PCT/IN2017/050488 Dt: 23-10-17 (PCT)**

Indole(sulfomyl) N-hydroxy benzamide derivatives as selective HDAC inhibitors **Application No. 201711042426 Dt: 27-11-17 (India)**

Nimbolide derivatives as Anticancer agents and preparation thereof **Application No. 201811000561 Dt: 05-01-18 (India)**

Novel Borondipyrromethene Fluorochromes Tailored with Phenoxymethylpyridine and Application thereof **Application No. 201711018190 Dt: 24-05-17 (India)**

Process for the preparation of novel propiolamides and pyrrolidine-2,5-diones and their use as potential pancreatic lipase inhibitors for the management of obesity **Application No. 15/831867 Dt: 05-12-17 (US)**

Process for the preparation of zafirlukast and analogs thereof **Application No. 201711046976 Dt: 28-12-17 (India)**

Progesterone-cationic lipid hybrid as anticancer agent and the process of synthesis thereof **Application No. 15/649832 Dt: 14-07-2017 (US); Application No. 17179456.3 Dt: 04-07-2017 (EP)**

Sequential High rate Acidogenic Anaerobic Reactor incorporating pre-treatment Process (SHAARP) for the generation of mixture of bio-ethanol and VFA from solid organic waste **Application No. 201711024332 Dt: 11-07-17 (India)**

Spirooxindole compounds as GSK3Â¿ inhibitors and process for preparation thereof **Application No. PCT/IN2018/050134 Dt: 09-03-18 (PCT)**

Sulfonyl substituted tetrazolones as anti-feedant, Acetylcholine esterase inhibitory and anti-microbial agents and process for preparation thereof **Application No. 201711043101 Dt: 01-12-17 (India)**

Synthesis and Biological evaluation of (Z)-3,4,5 - Trimethoxystyryl - benzene sulfonamides as potential anti cancer agents **Application No.15/523205 Dt:28-04-2017 (US); Application No.15808035.8 Dt: 15-05-2017 (EP)**

PATENTS GRANTED IN INDIA & OVERSEAS

2016-17

1,8-Imidazofused quinolone carboxamide **Patent No. 275174 Dt: 26-08-16 (India)**

3-[4-(1H-Benzo[d]imidazol-2-yl) phenyl]-5-phenyl-1,2,4-oxadiazole derivatives useful as potential anticancer agents and process for the preparation thereof **Patent No. 9522907 Dt: 20-12-20 (US); Patent No. 2966073 16 Dt: 14-12-2016 (Europe)**

A Chemoenzymatic process for the stereoselective preparation of (R)-gama-amino-beta-hydroxybutyric acid [(R)-GABOB] and (R) carnitine **Patent No. 276587 Dt: 26-10-16 (India)**

Benzophenone-piperazine linked pyrrolo [2,1-c][1,4] benzodiazepine hybrids as potential anticancer agents and process for the preparation there of **Patent No. 280843 Dt: 28-02-17 (India)**

Biological evaluation of 4-aza-2,3-didehydropodophyllotoxin analogues possessing potent antitumour activity **Patent No. EP2649078 Dt: 27-07-2016 (EP); Patent No. 2649078 Dt: 27-07-2016 (France, Germany, GB)**

C2-Fluoro subsituted piperazine linked pyrrolo [2,1-C][1,4] benzodiazepine dimers and a process for the preparation thereof **Patent No. 278139 Dt: 14-12-16 (India)**

Castor oil fatty acid based estolide esters and their acetates as potential lubricant base stocks **Patent No. 281351 Dt: 15-03-17 (India)**

Castor oil fatty acid based estolide esters and their acetates as potential lubricant base stocks **Patent No. ZL200980123247.X Dt: 08-02-17 (China)**

Deacidification of Jatropha and Karanja oils and purification of crude biodiesel by liquid-liquid extraction **Patent No. 2215195 Dt: 13-07-16 (Britain, Europe, France, Germany)**

Glucocorticoid receptor targeting formulates for delivering genes to cancer cells **Patent No. 9364566 Dt: 14-06-16 (US)**

Isoxazole / isoxazoline / combretastatin linked dihydroquinazolinone hybrids a potential anticancer agents and process for the preparation thereof **Patent No. 2350030 Dt: 20-04-16 (Britain, Europe, France, Germany)**

Microbial process preparation of Acrylic acid from Acrylonitrile **Patent No. 273667 Dt: 22-06-16 (India)**

N-((1-Benzyl-1H-1,2,3-triazol-4-yl) methyl)arylamide derivatives as potential anticancer agents and process for the preparation there of **Patent No. 9309225 Dt: 12-04-16 (US)**

Novel integrin binding RGD-Lipopeptides with gene transfer activities **Patent No. 9403869 Dt: 02-08-16 (US)**

Novel phenanthrylphenol linked pyrrole [2,1-C][1,4] benzodiazepine hybrids as potential antitumour agents and process for the preparation there of **Patent No. 282164 Dt: 31-03-17 (India)**

Polyol esters of undecenoic and undecanoic acids as potential lubricant base stocks **Patent No. 278776 Dt: 30-12-16 (India)**

Process for synthesizing histidinylated cationic amphiphiles, a new class of anti- cancer compounds **Patent No. 2928871 Dt: 01-02-17 (Britain, Europe, France, Germany)**

Process for the preparation of polythiophene and its co-polymer dispersions with reactive surfactants **Patent No. 9428603 Dt: 30-08-16 (US)**

Pyridopyrimidine and Indolizine based derivatives useful as potential phosphodiesterase 3 (PDE 3) inhibitors and a process for the preparation thereof **Patent No. 9562045 Dt: 07-02-17 (USA)**

Pyridopyrimidine based derivatives useful as potential phosphodiesterase 3 (PDE 3) inhibitors and a process for the preparation thereof **Patent No. 9505760 Dt: 29-11-16 (USA)**

Pyrrolo[2,1-c][1,4] benzodiazepine linked imidazo[1,5-a] pyridine conjugates as potential antitumour agents and process for the preparation thereof **Patent No. 5941058 Dt: 27-05-16 (Japan)**

Quinazolinone linked pyrrolo [2,1-C][1,4] benzodiazepine hybrids as potential anticancer agents and process for the preparation thereof **Patent No. 275269 Dt: 30-08-16 (India)**

Self mixed anaerobic digester for the treatment of

organic solid waste **Patent No. IDP000043500 Dt: 24-11-16 (Indonesia)**

Synthesis and biological evaluation of 3,4,5-trimethoxy styrylarylamino Propenone as potential anticancer agents **Patent No. 9487482 Dt: 08-11-16 (US)**

Synthesis and biological evaluation of benzophenone hybrids as potential anticancer agents **Patent No. 2682384 Dt: 10-05-16 (Canada)**

Synthesis and biological evaluation of mitochondria - targeted esculetin for its anti-atherosclerotic and age delaying effects **Patent No. 9580452 Dt: 28-02-17 (US)**

Synthesis and biological evaluation of pyrazolochalcone derivatives as potential anticancer agents **Patent No. 9604933 Dt: 28-03-17(US)**

Synthesis of hexadecyl cis-9-tetra decenoate and hexadecyl cis-10-tetradecenoate and their evaluation for anti arthritis properties in rats **Patent No. 281062 Dt: 06-03-17 (India)**

2017-18

1,8-Imidazofused quinolone carboxamide **Patent No. 285017 Dt: 10-07-17 (India)**

2-Phenyl benzothiazole linked imidazole compounds as potential anticancer agents **Patent No. 290369 Dt: 07-12-17 (India)**

3-Arylethynyl substituted quinazolinone compounds useful as potential anticancer agents **Patent No. 2501403 Dt: 21-02-18 (Britain)**

9,10,12-Tricycloxy ocetadecanoic acid alkyl esters as potential lubricant base stocks **Patent No. 288753 Dt: 26-10-17 (India)**

A New Porous Polymer Scaffold for On-site delivery of Stem Cells: Neo-vascularization Potentiates Tissue Regenaration while Protecting from Oxidative Stress by Enhanced Engraftment **Patent No. 9925298 Dt: 27-03-18 (US)**

A novel electrodialysis - distillation hybrid process for the recovery of dimethylsulfoxide (DMSO) solvent from pharmaceutical industrial effluent **Patent No. 289556 Dt: 14-11-17 (India)**

A novel electrodialysis - distillation hybrid process for the recovery of dimethylsulfoxide (DMSO) solvent from pharmaceutical industrial effluent **Patent No. 2779656 Dt: 02-01-18 (Canada)**

A Rapid and continuous transesterification process for biodiesel from crude jatropha oil **Patent No. 283102 Dt: 04-05-17 (India)**

Alkyl 11-anilino-10-hydroxy undecanoates as potential antioxidants **Patent No. 282411 Dt: 07-04-17 (India)**

Anti Cancer gene-associated Cat-ionic Lipid and estrogenic drug formulation for the treatment of aggressive pancreatic cancer and breast cancer stem (CSC)- like cells **Patent No. 9861653 Dt: 09-01-18 (US)**

Benzylidineanthracenone linked pyrrolobenzodiazepine hybrids useful as anti cancer agents and the process for preparation thereof **Patent No. 290366 Dt: 07-12-17 (India)**

Chalcone linked imidazolones as potential anticancer agents and process for the preparation thereof **Patent No. 291423 Dt: 05-01-18 (India)**

Cinnamide-pyrrolo [2,1-C] [1,4] benzodiazepines as potential anticancer agents and process for the preparation thereof **Patent No. 285045 Dt: 11-07-17 (India)**

Development of new catalyst for preparation of 1,1,1-trifluoroethane (HFC-143a) **Patent No. 188022 Dt: 03-10-17 (India)**

Isoxazoline linked pyrrolo[2,1-C][1,4] bezodiazepine hybrids as potential anticancer agents and the process for the preparation thereof **Patent No. 284169 Dt: 13-06-17 (India)**

Karanja oil based epoxy and acylory based derivatives as lubricant Basestocks **Patent No. 2013288213 Dt: 22-03-18 (Australia)**

Multifunctional calcium carbonate microstructures useful in encapsulation applications and a process for the preparation thereof **Patent No. 283280 Dt: 11-05-17 (India)**

N-((3,4,5 - Trimethoxystyryl)aryl) cinnamamide derivatives as potential anticancer agents **Patent No. 9878977 Dt: 30-01-18 (US)**

New - 4 beta-[4"-(1"-3"-subsituted benzothiazole-2"-yl) anilino podophyllotoxin analogues as antitumour agents **Patent No. 291453 Dt: 05-01-18 (India)**

New Intestinal alpha-glucosidase inhibitors from natural source and use thereof **Patent No. 1986670 Dt: 28-06-17 (EP)**

Novel 4 beta-polyarylamine podophyllotoxin analogues as potential anticancer agents **Patent No. 282325 Dt: 05-04-17 (India)**

Novel benzimidazole linked pyrrolo [2,1-C][1,4] benzodiazepine hybrids as potential anticancer agents and process for the preparation thereof **Patent No. 284153 Dt: 12-06-17 (India)**

Novel Glycerol-based heterogeneous carbon base catalyst useful for the transesterification of vegetable oils to biodiesel a process and use thereof **Patent No. 290563 Dt: 13-12-17 (India)**

Novel Napthalimide-benzimidazole hybrids as potential anticancer agents and process for the preparation thereof **Patent No. 283471 Dt: 23-05-17 (India)**

Novel Thiolactomycin based congeners as potential anti-tubercular agents **Patent No. 285763 Dt: 28-07-17 (India)**

Preparation of solid heterogeneous acid catalyst from crude glycerol and other organic compounds and their application in the esterification of fatty acids for the preparation of biodiesel (alkyl esters of fatty acids) **Patent No. 112007003607 Dt: 17-08-17 (Germany)**

Process for preparation of (2S,3S)-Taxifolin-6-C-Â-D-Glucopyranoside(ulmoside A) AND (2R,3R)-Taxifolin-6-C-Â¿-D-Glucopyranoside **Patent No. 9611255 Dt: 04-04-17 (US)**

Process for Synthesis of novel Mannose-Receptor selective lysinylated cationic amphiphile for invivo delivery of DNA Vaccines **Patent No. 9840530 Dt: 12-12-17 (US)**

Pyrrolo[2,1-c][1,4]naphthodiazepine linked substituted piperazine conjugates as potential antitumour agents and process for the preparation thereof **Patent No. 112012000807 Dt: 04-01-2018 (Germany); Patent No. 2499154 Dt: 21/02/2018 (Britain)**

Self mixed anaerobic digester for the treatment of organic solid waste **Patent No. 289243 Dt: 06-11-17 (India)**

Specific Rice bran-Glycolipid and Phospholipids Associated cationic Lipid Formulations: A Potent Carrier to Deliver Genes & Bioactive compounds to Breast and lung cancer cells **Patent No. 9763881 Dt: 19-09-17 (USA)**

Synthesis and biological evaluation of 3-(4-ethynyl phenyl) pyrido-pyrimidinone compounds as potential anticancer agents **Patent No. 9783537 Dt: 10-10-17 (US)**

Synthesis and biological evaluation of 3,4,5-trimethoxy styrylarylamino Propenone as potential anticancer agents **Patent No. 2942345 Dt: 28-03-18 (Britain, EP, France, Germany)**

Synthesis and biological evaluation of anthranilic acid hybrids as potential anti cancer agents **Patent No. 285450 Dt: 20-07-17 (India)**

Synthesis of highly efficient nano-structured photo-catalysts for hydrogen production under solar light irradiation **Patent No. 9776162 Dt: 03-10-17 (US)**

Synthesis of new 4beeta-acrylamidopodophyllotoxin congeners as antitumour antibiotics and the process for preparation thereof **Patent No. 293591 Dt: 28-02-18(India)**

Undecenoic acid based dimer acid esters as potential biolubricant base oils **Patent No. 289111 Dt: 02-11-17 (India)**

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- Adiyala, Praveen Reddy; Borra, Satheesh; Kamal, Ahmed; Maurya, Ram Awatar; Access to Imidazole Derivatives by Silver(I) Carbonate Mediated Coupling of Vinyl Azides with Secondary Amines, **European Journal of Organic Chemistry, 1269-1273, (7) 2016**
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VISITORS GALLERY

A high level delegation from Republic of Belarus comprising Mr. Andrew Kosovsky, First Vice-Chairman of the State Committee on Science and Technology of the Republic of Belarus, Mr. Konstantin Maerovich, Deputy Director of International Science, Technology & Innovation Cooperation Department, State Committee on Science and Technology of the Republic of Belarus, Acad. Pyotr A. Vityaz, Presidium of the National Academy of Sciences of Belarus and Mr. Igor Pilipenko, Embassy of Belarus in India, New Delhi visited the institute in **April 2016** in connection with Indo-Belarus joint committee meeting on Science and Technology cooperation.

Dr. V K Subburaj, IAS, Secretary to Government of India, Department of Pharmaceuticals, Ministry of Chemicals and Fertilizers was being felicitated by Director, S Chandrasekhar on the National Technology Day on **10th May 2016**. He delivered the A V RAMA RAO TECHNOLOGY AWARD LECTURE on "Drugs and Diseases: An overview".

On the occasion of 73rd Foundation Day on **5th August 2016**, the institute organized a National Seminar on Chemical Bonding followed by the Foundation Lecture by Bharat Ratna Prof. C N R Rao. Director S. Chandrasekhar is seen welcoming him.

Dr. S. Chandrasekhar honoring Police Commissioner, Rachakonda, Shri Mahesh Muralidhar Bhagawat at "SHE for HER-II" orientation program for girl students on **03rd October 2016**.

Experts from industry and apex management officials of the industry participated in the Industry meet on **18th October 2016** at Hotel Park Hyatt.

Dr. G. Anupama, Joint Secretary, CSIR-Administration is seen along with Director, S Chandrasekhar inaugurating AAU facility on **11th November 2016**.

A monumental flag was hoisted on the occasion of Platinum Jubilee year of Council of Scientific and Industrial Research at Indian Institute of Chemical Technology on **26th November 2016**. Dr. Girish Sahni, Director General of CSIR and Secretary, DSIR, Govt. of India hoisted the tri-colour flag.

Hon'ble Minister, Shri K. T. Rama Rao, former DG Dr. R. A. Mashelkar, Shri Y S Chowdary, Hon'ble Minister of State for S & T and Earth Sciences, Director, Dr. S. Chandrasekhar at the inauguration of Research & Innovative Circle of Hyderabad (RICH) on **24th February 2017**.

A French delegation visited CSIR-IICT on **09th March 2017** to update themselves with the progress of the Indo-French project at the institute.

Director, S. Chandrasekhar welcoming Prof. K.C. Nicolaou, Department of Chemistry, Rice University, USA for Noble Lecture on **30th March 2017**.

Director, S. Chandrasekhar welcoming Padma Shri A. S. Kiran Kumar, Chairman ISRO on the occasion of National Technology Day on **12th May 2017**.

Scientific delegates visited X-Ray Division on **12th June 2017**. Director, Dr. S. Chandrasekhar and Dr. Ravi Kumar is seen interacting with them.

A scientific delegation from Ethiopia visited the Institute on **17th June 2017** for discussion on possibility of twinning programme on various areas of R&D.

Visitors from The National Dong Hwa University, Taiwan in Eastern Taiwan visited the Institute on **30th November 2017**.

Dr. S. Chandrasekhar, Director, and Professor Peter Coloe, Pro Vice-Chancellor and Vice-President, Professor Suresh K Bhargava, Deputy Pro Vice Chancellor (Intl) and Director, CAMIC, RMIT University at the extension of CSIR-IICT and RMIT exchange program on **21st January 2018**.

Inauguration of Photo Gallery on works and life of Pandit Deendayal Upadhyaya in museum hall by Chief Guest Shri. A. Jayakumar, General Secretary of Vijnana Bharati (VIBHA) on Pandit Deendayal Upadhyaya's Birth anniversary on **26th February 2018**.

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सीएसआईआर–भारतीय रासायनिक प्रौद्योगिकी संस्थान
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