CSIR-IICT
Biennial Report 2018-2020

सी एस आई आर - भारतीय रासायनिक प्रौद्योगिकी संस्थान
(वैज्ञानिक तथा औद्योगिक अनुसंधान परिषद्)
CSIR-INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY
(Council of Scientific & Industrial Research)
तारनाका, Tarnaka, Hyderabad-500 007, हैदराबाद - 500 007, भारत, INDIA

THE VISION

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

THE MISSION

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

KEY OBJECTIVES OF CSIR-IICT

- Partner the industry to develop cost efficient processes / technologies and materials, which are relevant to the industry
- Provide value added services, by way of Analytical and Consultancy services
- Support entrepreneurship in niche and upcoming areas by creating echo-system to support start-ups, incubations and spin-offs.
- Generate revenues from above to keep pace with self-sustenance goal of CSIR.
- Utilize public funds for enhancing the expertise in niche areas

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.

प्रस्तावना

संस्थान की द्विवार्षिक अवधि 2018-20 के दौरान सीएसआईआर-आईआईसीटी के अनुसंधान और विकास उत्पादन एवं संबंधित उपलब्धियों के विवरण की रिपोर्ट प्रस्तुत करते हुए मुझे खुशी हो रही है । संगठन के 75 वें वर्ष को चिह्नित करते हुए हमने 5 अगस्त 2018 को ऐतिहासिक कार्यक्रम प्लेटिनम जुबली के वर्षिक समारोह का उद्घाटन किया ।

विशेष रूप से बड़े पैमाने पर उद्योग और समाज के लाभ हेतु विज्ञान और प्रौद्योगिकी में अनुसंधान तथा विकास गतिविधियों और शोध के निष्कर्षों का ट्रांस्लेशन करना के बीच संतुलन बनाए रखने के लिए संस्थान का ध्यान केंद्रित किया गया है । अनुसंधान परिषद की सिफारिश के अनुसार, संस्थान में आठ विभागों और दो केंद्रों के उद्भव के साथ प्रभागों का पुनर्गठन किया गया । कई शैक्षणिक संस्थानों और विश्वविद्यालयों के साथ सहयोगात्मक अनुसंधान के लिए समझौता ज्ञापन पर हस्ताक्षर किए गए हैं । उद्योग द्वारा प्रायोजित और परामर्शी परियोजनाओं के साथ-साथ वैज्ञानिक पूरी तरह से सरकार द्वारा वित्त पोषित योजनाओं के साथ भी जुड़े हुए हैं । उल्लेखनीय है कि सन फार्मा ने पेटेंट के लिए वैश्विक लाइसेंसिंग समझौते पर हस्ताक्षर किया थे, जो बहुल लक्षणो से भरे संभावित चिकित्सीय गतिविधि से युक्त कुछ यौगिकों से संबंधित है । अपस्कूलिंग एपीआई, केएसएम और अन्य फार्मा उत्पादों के लिए, पद्म भूषण डॉ. ए. वी. रामा राव किलो लैब सुविधा उपलब्ध कराई गई थी और एक अत्याधुनिक पशु सदन (Animal House) सुविधा को भी पूर्ण परिचालन में लाया गया है। इसके अलावा, "कोई अवलोकन नहीं" के साथ यूएसएफडीए निरीक्षण ने संस्थान के एनएमआर परीक्षण सुविधा को मंजूरी दे दी ।

इस अवधि के अंत में, संपूर्ण मानव जाति कोविड-19 महामारी की चपेट में था और मेरे सहयोगियों सहित वैज्ञानिक समुदाय ने खुद को इस नई वायरल बीमारी को समझने और इससे निपटने के लिए उपाय खोजने के लिए समर्पित रहे।

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 चंद्रशेखर)

निदेशक

FOREWORD

I am happy to present the CSIR-IICT Biennial Report containing the Research & Development activities and the achievements during the period 2018-20. We celebrated a land mark event, the inauguration of the platinum Jubilee Year celebration on 5th August 2018 followed by a year-long events marking the 75th year.

The focus of the institute has been to strike a balance between R & D activities in science & technology and translating the research findings for the benefit of industry and the society at large. As per the recommendation of Research Council, the reorganisation was undertaken with emergence of eight departments and two centres. MoUs for collaborative research with several academic institutions and universities have been signed. The scientists have been fully engaged with Govt. funded as well as industry sponsored & consultancy projects. Noteworthy to mention that Sun Pharma entered into a global licensing agreement for patents related to certain compounds with potential therapeutic activity across multiple indications. Padma Bhushan Dr. A. V. Rama Rao kilo lab facility was made available for upscaling API, KSM and other pharma products and a State-of-the-Art Animal House facility was also brought into full operation. Further the NMR test facility of the institute cleared the USFDA inspection with "no observations".

Towards the end of this period, the whole humankind was under the grip of COVID 19 pandemic and the scientific community including my colleagues dedicated themselves to understand the new viral disease and also find solutions to combat.

I thank the Chairman and the Members of the Research Council and Management Council of the Institute for their valuable guidance.

(Dr. S. Chandrasekhar)

Director

RESEARCH COUNCIL

Chairman

Prof. Gautam R Desiraju
Solid State and Structural Chemistry Unit,
Indian Institute of Science,
Bengaluru

Members

Dr. R.K. Khandal
President R&D and Business Development
India Glycols Limited
Noida

Dr. T. Rajamannar

Director,
Sun Pharma Advanced Research Co. Ltd
(SPARC Ltd), Nima Compound,
Tandalja, Vadodara

Dr. S. Sivashankar

Chair Professor,
National Centre for Catalysis,
Indian Institute of Technology, Madras
Chennai

Dr. R.R. Hirwani
Former Head,
CSIR-URDIP
Pune

Dr. G.N. Qazi

(Former VC, Hamdard University)
Director General HIMSR
New Delhi

Dr. Samir P Dave

Director,
Aimco Pesticides Ltd
Mumbai

Dr. G.P. Singh

Sr. Vice President,
Lupin (R&D)
Mumbai

Dr. Ram Vishwakarma

Director,
CSIR-IIIM
Jammu

Dr. Ashwani Kumar Nangia

Director,
CSIR-NCL
Pune

Dr. Srivari Chandrasekhar

Director, CSIR-IICT
Hyderabad

Member Secretary

Dr. D. Shailaja
Chief Scientist
Head Business Development & Research
Management, CSIR-IICT
Hyderabad

MANAGEMENT COUNCIL

CHAIRMAN

Director
CSIR- IICT, Hyderabad

MEMBERS

Dr (Ms.) Prathama S Mainkar
Senior Principal Scientist,
CSIR-IICT

Dr. B. V. Subba Reddy
Chief Scientist,
CSIR-IICT

Dr. (Ms.) S. Sreelatha
Principal Scientist,
CSIR-IICT

Dr. N. Jagadeesh Babu
Sr. Scientist,
CSIR-IICT

Dr. Hafeez ur Rahman
Principal Technical Officer,
CSIR-IICT

Dr. V. M. Tiwari
Director,
CSIR-NGRI

Dr (Mrs) D. Shailaja
Chief Scientist
CSIR-IICT

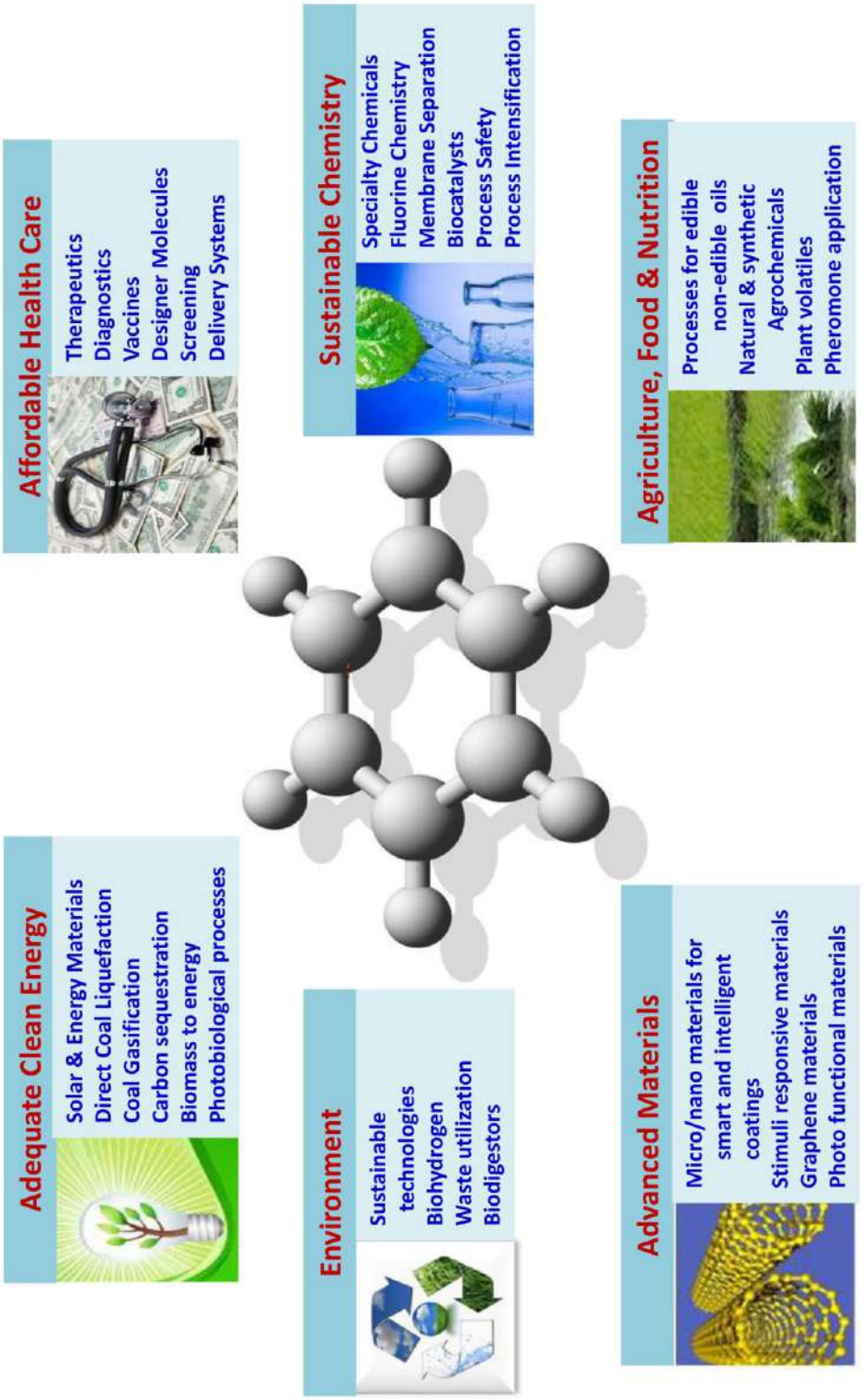
COFA / FA
CSIR-IICT, Hyderabad

MEMBER-SECRETARY
COA/AO, CSIR-IICT

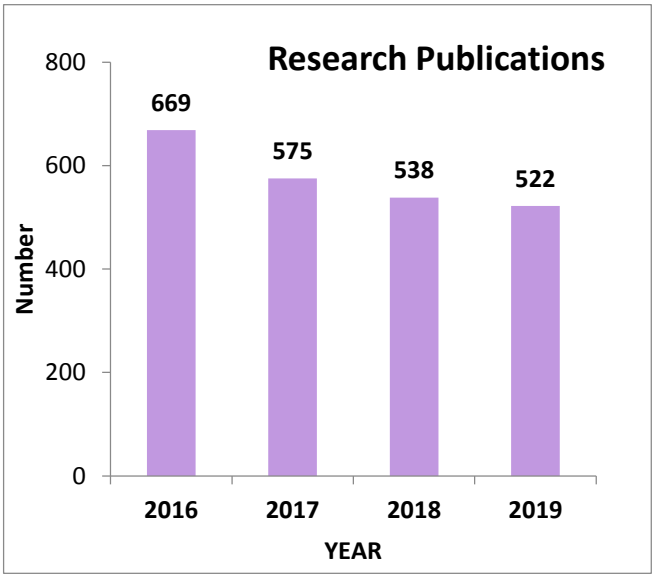
Research Council Meetings 2018 & 2019

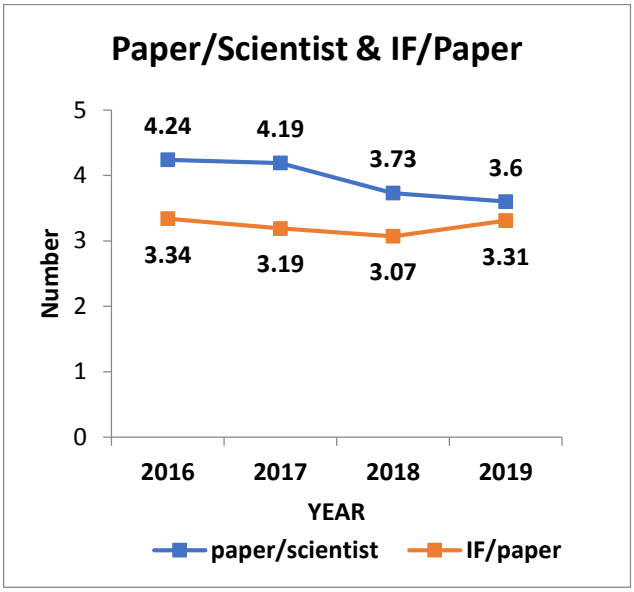
ORGANISATIONAL STRUCTURE

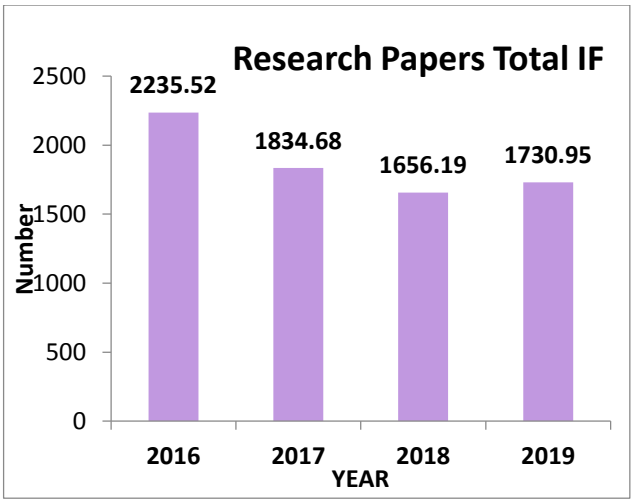
FOCUSED RESEARCH AREAS

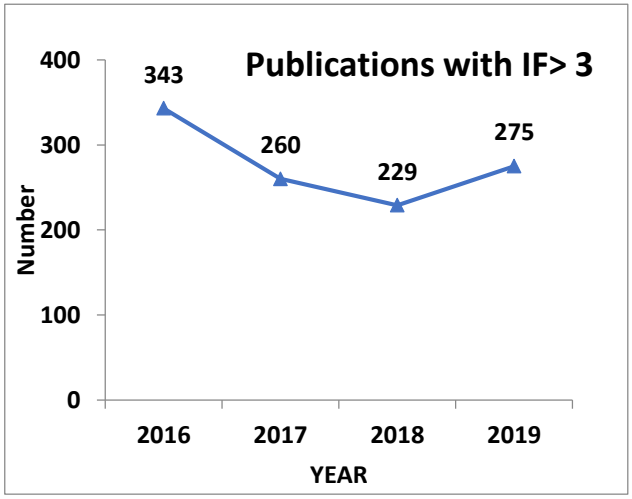


R & D Outputs

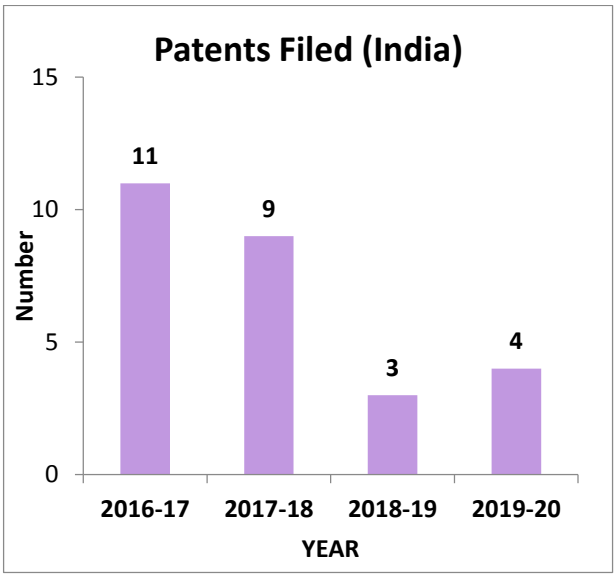

Research Publications
800
600
400
200
0
Number
669
575
538
522
2016
2017
2018
2019
YEAR

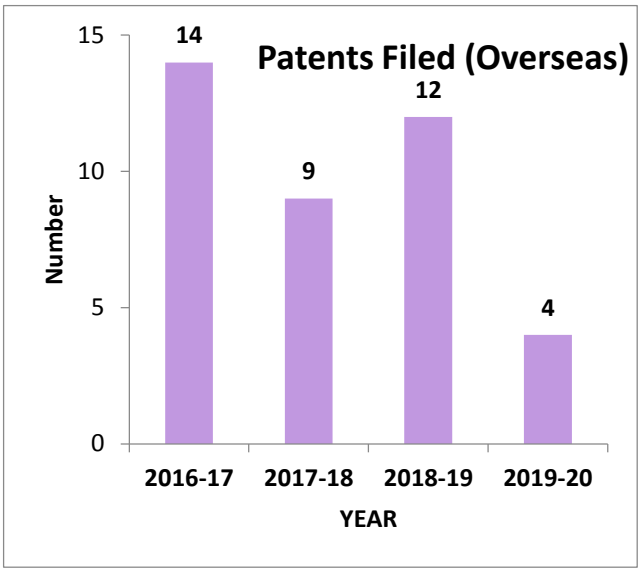

Paper/Scientist & IF/Paper
5
4
3
2
1
0
Number
4.24
4.19
3.73
3.6
3.34
3.19
3.07
3.31
2016
2017
2018
2019
YEAR
paper/scientist
IF/paper

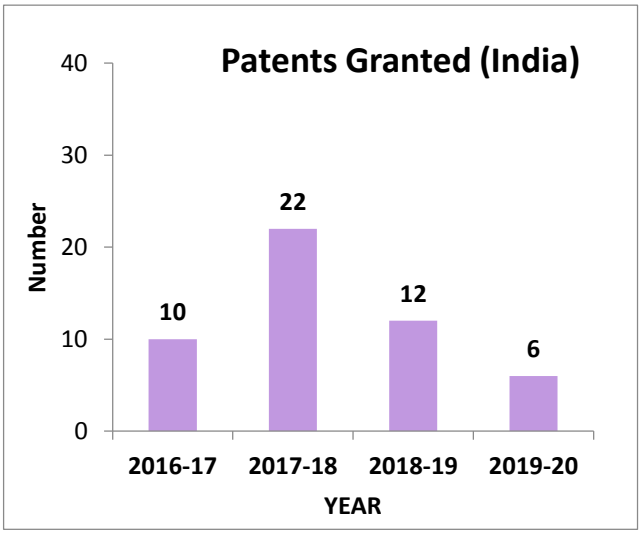

Research Papers Total IF
2500
2000
1500
1000
500
0
Number
2235.52
1834.68
1656.19
1730.95
2016
2017
2018
2019
YEAR

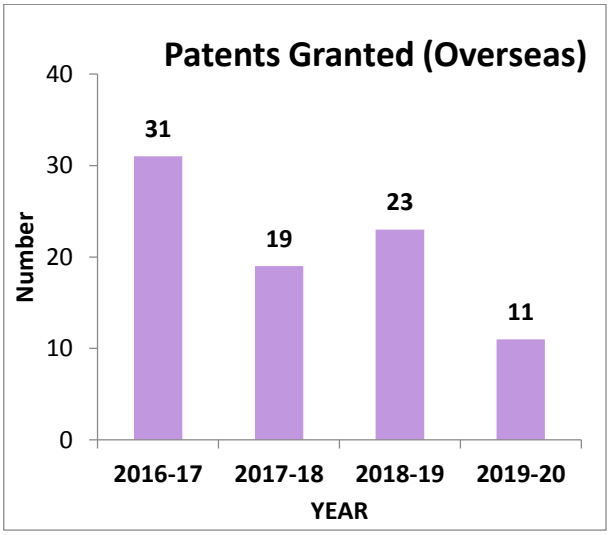

Publications with IF> 3
400
300
200
100
0
Number
343
260
229
275
2016
2017
2018
2019
YEAR

R & D Outputs

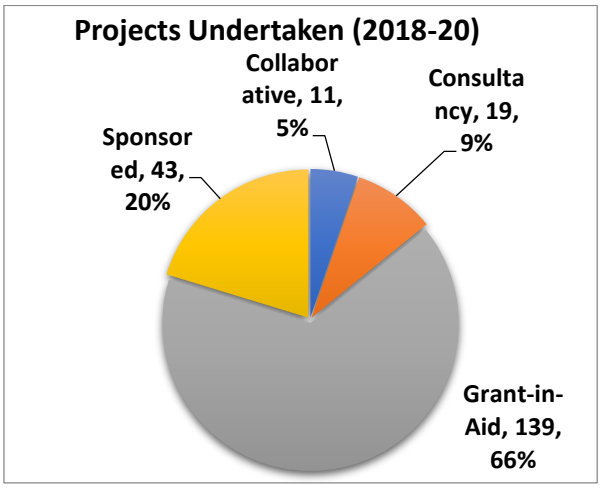

Patents Filed (India)
15
10
5
0
Number
11
9
3
4
2016-17
2017-18
2018-19
2019-20
YEAR

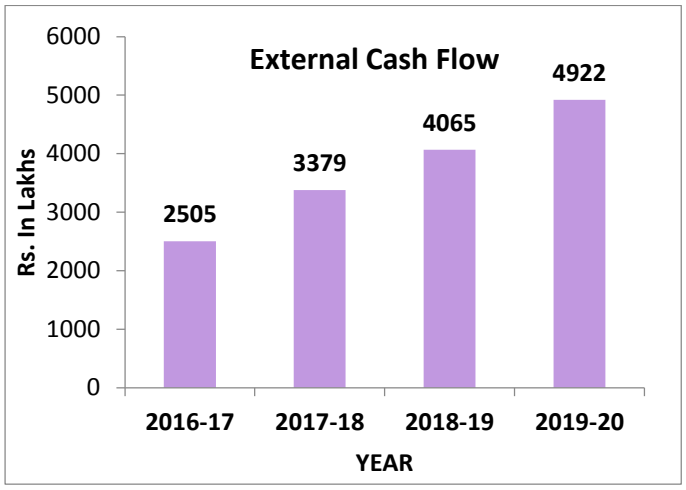

Patents Filed (Overseas)
15
10
5
0
Number
14
9
12
4
2016-17
2017-18
2018-19
2019-20
YEAR


Patents Granted (India)
40
30
20
10
0
Number
10
22
12
6
2016-17
2017-18
2018-19
2019-20
YEAR

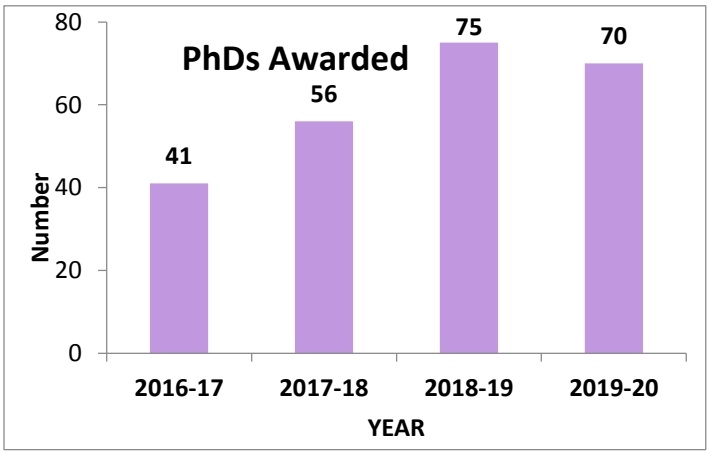

Patents Granted (Overseas)
40
30
20
10
0
Number
31
19
23
11
2016-17
2017-18
2018-19
2019-20
YEAR

R & D Outputs



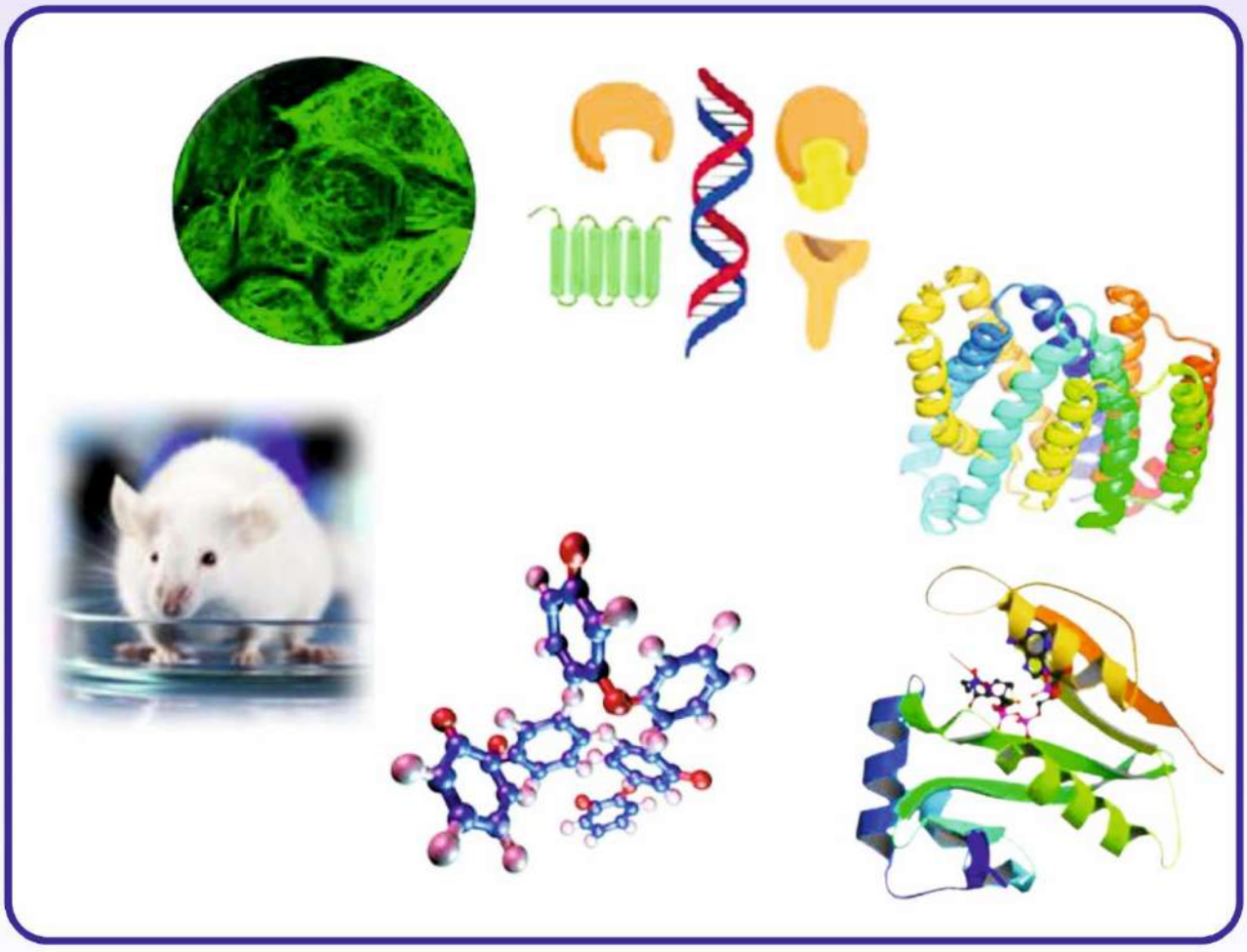


HUMAN RESOURCE BASE		
	2018-19	**2019-20**
TOTAL STAFF	**532**	**493**
***Total S & T Staff**		
Scientist (Group-IV)	150	153
Technical (Group-III)	107	99
Technical (Group-II & I)	126	110
***Total Administrative & Non-Technical**	149	131
***Research Scholars/Assts.**		
RA/NPDF/TWAS/WOS/I F etc…	137	112
SRF/JRF	396	360
Project Assistants	168	244



R & D PERFORMANCE

APPLIED BIOLOGY



APPLIED BIOLOGY

The Department of Applied Biology is actively pursuing research in various aspects of biology with major focus on disease areas such as cancer biology, neurobiology, metabolic disorders and infectious diseases. The core strength of chemistry of the Institute in designing and developing new molecules pertaining to the need of the society are fully explored at Applied Biology Department, with proficiency in multi disciplinary sciences encompassing biochemistry, genetics, structural and molecular cell biology. Applied biology is enriched with expertise in Toxicology, Pharmacological evaluation, Novel Drug Delivery Systems (NDDS), Entomology, mosquito borne disease and disease modelling, computational biology, big data analytics and Insilco studies. The focal point of Applied biology is in lead discovery, optimization and validation using suitable cell and animal models for obtaining proof of concept. Providing sustainable solutions to needs of the rural society is also an important arm of Applied Biology. The department undertakes evaluation of various materials for toxicity, bio-efficacy, Anti-cancer/microbial/termite/ rodent/ mosquito larvicidal activities to cater the industry and academia needs. The department has established Drug Testing Facility which is approved by Drugs Control Administration (DCA), Govt. of Telangana, Telangana state, in form 37 of Drugs and Cosmetics Act 1940 and Rules made there under for testing of APIs and finished dosage forms. Central Insecticides Board, Govt. of India, has recognized CSIR IICT for testing pesticidal activity on public health and agriculture pests.

Dept. of Applied Biology, CSIR-IICT contributes significantly in various inter-disciplinary research programs for awarding Ph.D degrees in the areas of Chemical Biology, Pharmacology, Nanomaterials and Drug Delivery. The research activities of division has broadly classified into following themes:

1) Cancer
2) Cardiovascular and metabolic disease research
3) Neurobiology research
4) Stem Cells and Regenerative Medicine
5) Antitubercular agents
6) Structural Biology
7) Drug Delivery and Nanomedicine Research
8) Pharmacology & Toxicology
9) Infectious Diseases & Computational Biology.
10) Liver Diseases
11) Biosensors

BASIC RESEARCH

1. Cancer:

- Pancreatic adenocarcinoma (PDAC) is one of the most aggressive malignant diseases with poorest prognoses (median survival time 6-12 months). Patients suffering from pancreatic cancer have the survival rate estimated to be less than 5% due to its aggressive growing nature, metastasis and chemoresistance. The major reason for the poor prognosis of pancreatic cancer patients is the failure of the tumor cells to undergo apoptosis due to intrinsic resistance to death receptor- and mitochondria-initiated apoptosis and therefore these patients do not respond to most conventional therapies, such as chemotherapy and radiotherapy. Further, oncogenic KRAS mutation is a driver mutation, which plays a central role in the control of pancreatic tumor metabolism and its progression thereby making it a signature genetic event in PDAC. But no effective treatments that target this mutant protein have reached the clinic making it an undruggable target. Gemcitabine is the current standard chemotherapy for pancreatic cancer. However, due to the complex tumor microenvironment and high metastatic property of pancreatic cancer the effectiveness of gemcitabine is un-satisfactory. Therefore,

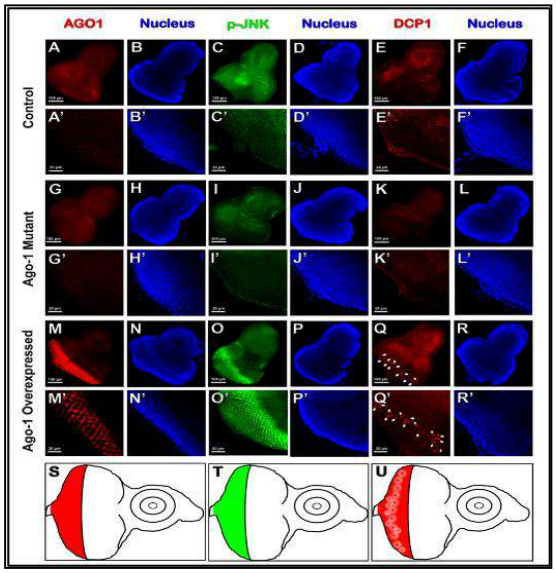
identification of the key targets and the development of sensitizing agents or molecules with new mechanisms of action to kill these chemoresistant cancer cells is a need of the hour. The research in our lab is focussed on understanding the role of autophagy in cell death and survival, epigenetics and role of cytoprotective enzymes towards chemo resistance and its implications in chemo therapy in pancreatic cancer by cell and molecular biology approaches. As a part of this endeavour we have explored the biological activity of some natural plant based as well as synthetic/ semisynthetic molecules in *in vitro* models of pancreatic cancer/others.

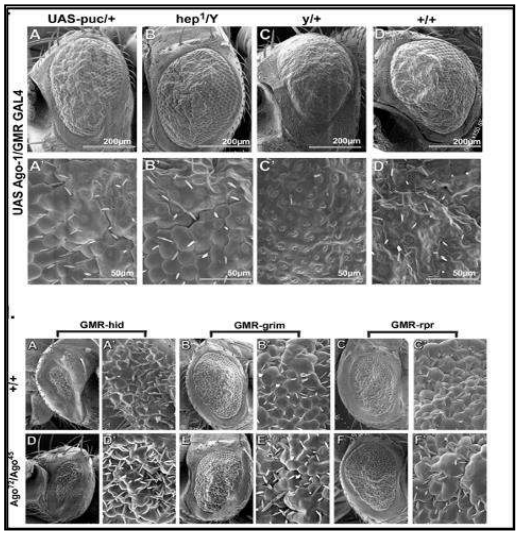
- The effect of hybrid-polar HDACI m-carboxycinnamic acid bishydroxyamide (CBHA) on the growth of human pancreatic adenocarcinoma cells, using MIA PaCa- 2 cell line as an *in vitro* model was investigated. Following CBHA treatment of the MIA PaCa-2 cells, the effect of CBHA was characterized by *in vitro* cytotoxicity evaluation, clonogenic assay, cell cycle analysis, immunoblotting for soluble and insoluble fractions of tubulin, immune fluorescence and caspase-3 assay. We observed that CBHA markedly impaired growth of the pancreatic cancer cells by resulting in dose-dependent G2/M arrest, disruption of microtubule organization, induction of caspase-mediated apoptosis and *in vitro* suppression of HDAC6. Together, our findings show that CBHA can be a potential plausible therapeutic that could be exploited for pancreatic cancer therapy (*ACAMC*., **2019**, 19: 750)
- Noscapine, a phthalideisoquinoline alkaloid isolated from the opium poppy Papaver somniferum, is traditionally being used as an anticough drug. Sincenoscapine and its analogues exhibit safe *in vitro* toxicological profile our study has led to the identification of noscapinoids which are more effective than parent noscapine against pancreatic cancer. These conjugates showed potent cytotoxicity with low IC50 values. Further, flow cytometry analysis revealed that MIA PaCa-2 cells treated with these compounds induced cell cycle G2/M-phase arrest. In addition, Western blot analysis revealed that the cells treated with these conjugates accumulate tubulin in the soluble fraction and also elevate cyclin-B1 protein expression levels. Moreover, the conjugates also increased the expression of caspase-3 and PARP levels which is indicative of apoptotic cell death. In silico molecular docking studies showed several noncovalent interactions like Van der Waals and hydrogen-bonding with tubulin protein and with good binding energy. The results indicated that these noscapine analogues may serve as novel compounds that can possibly inhibit tubulin protein and can be considered for further optimization as a clinical candidate for treating pancreatic cancer (*ACS Omega*, **2019**, 4 (21), 19382; *Chemistry Select*, **2019**, 4 (14), 4092)
- Antimicrobial and anticancer potential of low molecular weight polypeptides extracted and characterized from leaves of *Azadirachta indica* was studied. The total protein extracted was precipitated with 15% TCA-Acetone. The SDS-PAGE analysis identified the presence of eight low molecular weight polypeptides. The antimicrobial activity of the resolved bands was detected by Polyacrylamide gel-Agar overlay diffusion assay (PAG-ADA). The broad-spectrum bactericidal activity of these polypeptides was confirmed using the same technique and found three low molecular weight bands from 11 to 14 kDa collectively exhibiting superior bactericidal activity against the bacterial pathogens. Further, the purified protein extract was found to be active against HELA, BT-549 and Neuro-2a cell lines. The results of present

study indicate that these polypeptides exhibit broad spectrum antimicrobial and anticancer activity and can therefore be explored for their therapeutic potential. (*Int. J. Biol. Macromol*., **2018**, 114, 906)

- We explored the cellular mechanisms that regulate isocitrate dehydrogenase-1 and 2 (IDH1 and IDH2) enzymes in cells. IDH1 and IDH2 are frequently mutated in a spectrum of cancers; IDH1 is mutated more in solid tumors, whereas IDH2 is mutated in liquid tumors. Some of the mammalian and yeast enzymes which function in metabolisms show an cell cycle dependent expressions, as IDH1 and IDH2 are evolutionary conserved we elucidated their cell cycle dependencies. We found that IDH1 and IDH2 are expressed more in G2/M than other phases of cell cycle. In particular, we also observed that the G2/M specific transcription factor, FOXM1 regulates IDH1 gene and protein levels in G2/M. Blocking FOXM1 function using inhibitors, shRNA or CRISPR/Cas9 based genome editing inhibited IDH1 levels in G2/M. Further, in mutant IDH1 expressing cells, we showed that the oncometabolite termed as D-2HG levels were also high in G2/M. Thus, our work shows that IDH1 and IDH2 enzymes are high in G2/M and with their metabolite. The implications of our work can be extended to finding possible co-therapies, as specific small molecule inhibitors of IDH proteins are either in trials or in clinics co-treating them with mitotic blockers could lead to better regimens. We further delved into regulation of IDH proteins by identifying the kinases which can phosphorylate them in G2/M as well as the E3 ligases that are responsible for IDH ubiquitination. Also, we found a signalling pathway that elicits drug resistance to the existing mutant IDH1 inhibitors.
- To develop small molecule based protein degraders, we adopted the Protac strategy to develop molecules that can degrade mutant IDH1 proteins. Initially, to understand whether mutant IDH1 can be degraded by small molecules, we started off with a dTag system. In the dTag system, mutant IDH1 is expressed as a fusion protein with FKBP12 in cells either as an over-expressed protein or genetic knock-in of FKBP12 in IDH1 locus. After developing these fusion proteins, we plan to elucidate the degradation kinetics of mutant IDH1 using dTag 13, a hetero bifunctional molecule that binds to FKBP12 with high affinity in various model systems developed in our laboratory. Overall, we worked to identify the cellular mechanisms that govern IDH proteins and cause drug resistance, which lead us to develop novel molecules that can overcome drug resistance by degrading mutant IDH1 proteins.
- Understanding role of *DmArgonaute-1* on apoptosis: Argonaute family proteins are well conserved among all organisms. Its role in mitotic cell cycle progression and apoptotic cell elimination is poorly understood. Earlier we have established the contribution of Argonaute 1 (*Ago-1)* in cell cycle control related to G2/M cyclin in *Drosophila*. This study is focussed in understanding the relationship of *Ago-1* in regulating apoptosis during *Drosophila* development. Multifarious regulatory pathways control apoptosis during development among which highly conserved JNK (c-Jun N-terminal kinase) pathway play a crucial role. Over expression of *Ago-1* resulted in reduced number of ommatidia in the eye and produced smaller size brain in adult and larval *Drosophila*. A drastic reversal of the phenotype towards normal was observed upon introduction of a single copy of the dominant negative mutation of *basket* (*bsk*, *Drosophila* homolog of JNK)

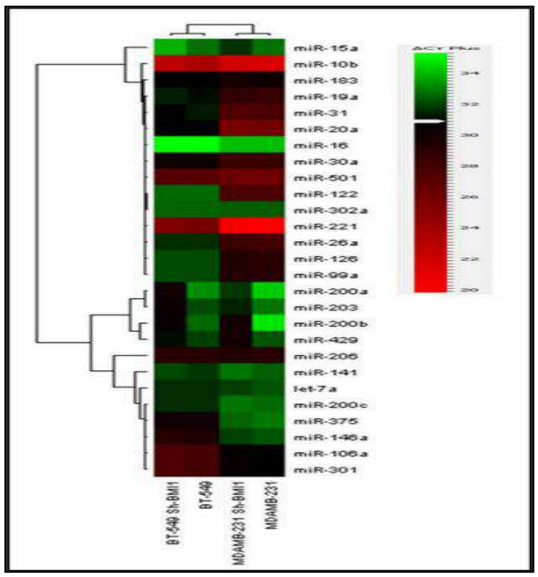
indicating an active and physical involvement of the *bsk* with *Ago-1* in inducing developmental apoptotic process. Study also showed that *Ago-1* stimulates phosphorylation of JNK through *transforming growth factor-β activated kinase 1-hemipterous (Tak1-hep)* axis of JNK pathway resulting in up regulation of pro-apoptotic genes *head involution defective (hid), grim* & *reaper (rpr)*, inturn leading to 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 (Death-associated inhibitor of apoptosis 1). Further, *Ago-1* also inhibited miR-14 expression to trigger apoptosis. Findings propose that *Ago-1* act 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*, **2018,** 13(1))





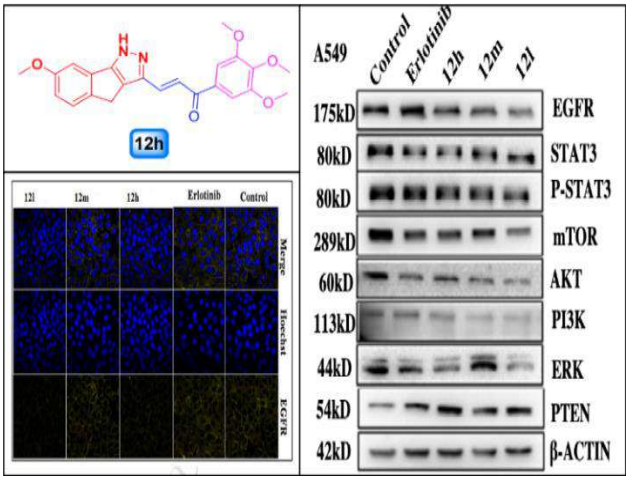
Regulating BMI1 Expression via Mirnas Promote Mesenchymal to Epithelial Transition (MET) and Sensitizes Breast Cancer Cell to Chemotherapeutic Drug: Polycomb group (PcG) proteinB lymphoma Mo-MLV insertion region 1 homolog (BMI1) is a transcriptional repressor that plays an important role in human carcinogenesis. Deregulation of the expression of small non-coding RNAs (miRNAs) has been implicated in tumorigenesis. Here, we have shown that knock-down ofBMI1increases the expression of tumor-suppressive miRNAs; miR-200a, miR-200b, miR-15a, miR-429, miR-203. Up-regulation of these miRNAs leads to down-regulation ofPRC1 group of proteins i.e. BMI1, RING1A, RING1B and Ub-H2A. Overexpression of miR-200a, miR-200b and miR-15aalso produced decreased BMI1 and Ub-H2A protein expression in the CD44+ Cancer Stem Cell population of MDAMB-231cells. Elevating the levels of BMI1 regulated miRNAs promoted Mesenchymal to Epithelial transition by regulating the expression of N-Cadherin, Vimentin, β-Catenin, Zeb, Snail thereby resulting in decreased invasion, migration and proliferation. Here, we also report that miR-200a, miR-200b, miR-203 accretes the sensitivity of MDAMB-231 cells to the histone deacetylase inhibitor (HDACi) SAHA and miR-15a sensitized breast cancer cells to the chemotherapeutic drug cisplatin leading to apoptosis. These findings suggest that

modulatingspecific miRNAs may serve as atherapeutic approach for the treatment of breast cancer. (*PloS one*, **2018,** 13(2))

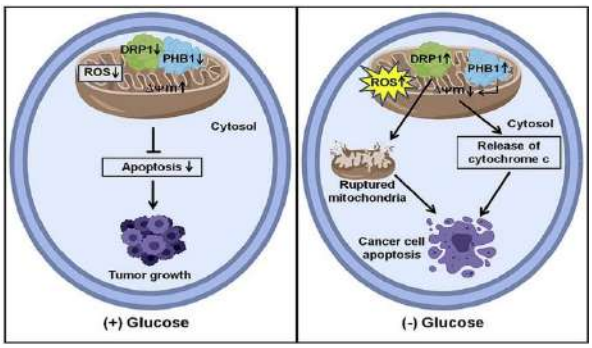


Design, Synthesis, *In Silico* Pharma cokinetics Prediction and Biological Evaluation of 1,4Dihydroindeno[1,2-C] Pyrazole Chalcone as EGFR /Akt Pathway Inhibitors

Conjugates of 1,4-dihydroindeno [1,2-c]pyrazole chalcone (12h, 12land 12m) when treated to a panel of human cancer cell lines showed a G2/M cell cycle arrest on A549 cell line with respect to the positive control. Furhter mechanistic studies showed inhibition of EGFR and Akt pathways. (*EJMC*, **2019**, 163, 636)



Glucose Starvation-Induced Oxidative Stress Cause Mitochondrial Dysfunction and Induces Apoptosis via Prohibitin 1 Upregulation in Human Breast Cancer Cells Alterations in mitochondrial bioenergetics and impaired mitochondrial function may serve as effective targeting strategies especially in triple-negative breast cancers (TNBC) where hormone receptors and endocrine therapy are absent. Therefore, in an attempt to understand how cell microenvironment might produce an effect on reprogramming cancer cells, triple-negative breast cancer (TNBC) cell line (MDA-MB-231) was exposed to glucose starved media for 24 and 48 hours. This led to change in the cell metabolism and reverted the cells towards apoptosis. Mechanistic studies showed that GS led to increase in mitochondrial ROS and upregulation of the pleiotropic protein, Prohibitin 1 (PHB1), leading to its dissociation from Dynamin-related protein 1 (DRP1), perturbance of mitochondrial membrane potential (MMP) and triggering of the apoptosis cascade. Also, glucose starvation (GS) of MDA-MB-231 showed decrease in mitochondrial Oxygen Consumption Rate (OCR), which was rescuable to control level through addition of exogenous antioxidant N-Acetyl Cysteine (NAC). We emphasize that glucose starvation remarkably sensitized the highly glycolytic metastatic TNBC cell line, MDA-MB-231 to apoptosis and decreased its migratory potential. Based on our findings, a nutritional paradigm be proposed for anticancer therapy. (*Free Rad. Biol. Med.*, **2019**, 145, 428)



Glutathione S-Transferase Omega 1 Inhibition Activates JNK-Mediated Apoptotic Response in Breast Cancer Stem Cells: Glutathione S-transferase omega 1 (GSTO1) contributes to the inactivation of a wide range of drug compounds via conjugation to glutathione during phasereactions. Chemotherapy-induced GSTO1 expression in breast cancer cellsleads to chemoresistance and promotes metastasis. In search of novel GSTO1 inhibitors, we identified S2E, a thia-Michael adduct of sulfonamide chalconewith low LC50 (3.75 ± 0.73 μM) that binds to the active site of GSTO1, asrevealed by molecular docking (glide score: -8.1), cellular thermal shift assayand fluorescence quenching assay (Kb ~ 10 × 105 mol. L-1). Docking studies confirmed molecular interactions between GSTO1 and S2E, and identified the hydrogen bond donor Val-72 (2.14 ˚A) and hydrogen bond acceptor Ser-86(2.77 ˚A). Best pharmacophore hypotheses could effectively map S2E and identifiedthe 4-methyl group of the benzene sulfonamide ring as crucial to its anticanceractivity. Lack of a thiophenyl group in another analog, 2e, reduced itsefficacy as observed by cytotoxicity and pharmacophore matching. Furthermore, GSTO1 inhibition by S2E, along with tamoxifen, led to a significant increase in apoptosis and decreased migration of aggressive MDA-MB-231cells, as well as significantly decreased migration, invasion and mammosphereformation in sorted breast cancer stem cells (CSCs, CD24-/CD44+). GSTO1 silencing in breast CSCs also significantly increased apoptosis and decreased migration. Mechanistically, GSTO1 inhibition activated the c-Jun N-terminalkinase stress kinase, inducing a mitochondrial apoptosis signaling pathway inbreast CSCs via the pro-apoptotic proteins BAX, cytochrome c and cleavedcaspase 3. Our study elucidated the role of the GSTO1 inhibitor S2E as apotential therapeutic strategy for preventing chemotherapy-induced breast CSC-mediated cancer metastasis and recurrence. (*The FEBS Journal*, **2019**, 286, 2167)

In Silico Design, Synthesis and Activity of Potential Drug-Like Chrysin Scaffold-Derivedselective EGFR Inhibitors as Anticancer Agents: Epidermal growth factor receptor (EGFR) signaling pathway is one of the promising andwell-established targets for anticancer therapy. The objective of the present study was to identify new EGFRinhibitors using ligand and structure-based drug designing methods, followed by a synthesis of selected inhibitorsand evaluation of their activity. A series of C-7-hydroxyproton substituted chrysin derivatives were virtually drawn to generate a small compound library that was screened using 3D QSAR model created from forty-two known EGFR tyrosine kinase inhibitors. Next, the obtained hits with fitness score ≥ 1.0 were subjected to molecular docking analysis. Basedon the predicted activity and XP glide score, three EGFR inhibitors were synthesized and characterized using ^{1}H NMR, ^{13}C-NMR and MS. Finally, comparative in vitro investigation of the biological activity of synthesizedinhibitors was performed with that of the parent molecule, chrysin. The data depicted a 3.2–fold enhanced cytotoxicity of chrysin derivative, CHM-04 against breast cancercells as compared with chrysin as well as its binding with EGFR protein. Furthermore, the biological activity ofCHM-04 was comparable to the standard EGFR inhibitor, AG1478 in increasing apoptosis and decreasing themigratory potential of triple-negative breast cancer cells as well as significantly lowering the mammosphereforming ability of breast cancer stem cells. The present study suggests CHM-04, an EGFR inhibitor possessing drug-like properties as a plausibletherapeutic candidate against breast cancer. (*Comp. Biol. Chem.*, **2019**, 83, 107156)

Doxorubicin Induces Prostate Cancer Drug Resistance by Upregulation of ABCG4 Through GSH Depletion and CREB Activation: Relevance of Statins in Chemosensitization: Multidrug resistance mediated by ATP-binding cassette (ABC) transporters remains a major impediment to cancer

chemotherapy. In the present study, we documented that doxorubicin (Dox) or cisplatin-induced prostate cancer (PCa) chemoresistance is predominantly mediated by the induction of ABCG4 in androgen-independent PCa cells. Treatment of DU-145 or PC-3 cells with Dox significantly enhanced the expression of ABCG4 that resulted in the efflux of intracellular Dox. However, incubation of cells with ABCG4 short hairpin RNA resulted in a significant accumulation of Dox and sensitized cells to Dox-induced cytotoxicity. Interestingly, simvastatin synergistically potentiated Dox-induced cytotoxicity by inhibiting ABCG4 in DU-145 and DU-145 Doxres cells. Mechanistically, ABCG4 expression was regulated redox-dependently by intracellular glutathione (GSH) levels. Treatment of cells with N-acetylcysteine or simvastatin restored Dox-induced depletion of GSH levels that in turn inhibited ABCG4 levels. In addition, a reduction in GSH levels by Dox caused a nuclear factor-κB dependent enhancement of c-Myc expression, which led to cAMP-regulatory element-binding protein (CREB) activation. Furthermore, chromatin immunoprecipitation experiments revealed that Dox-induced CREB activation transcriptionally upregulates ABCG4 expression. These results were further confirmed in an in vivo PCaxenograft mice model. Combination of simvastatin and Dox significantly regressed the tumor growth and size with no noticeable Dox-induced cardiotoxic side effects. Intriguingly, DU-145 cells with stably depleted ABCG4 levels not only significantly delayed the development of the tumor but also greatly sensitized the tumor to a low dose of Dox that resulted in complete tumor regression. Collectively, this data reinforces a novel function of ABCG4 in Dox-mediated chemoresistance, and as a potential therapeutic target in drug-induced PC achemo resistance. (*Mol Carcinog.*, **2019**, 58(7), 1118)

Dimethylarginine Dimethylaminohydrolase-1 (DDAH1) is Frequently Upregulated in Prostate Cancer and its Overexpression Conveys Tumor Growth and Angiogenesis by Metabolizing Asymmetric Dimethyl arginine (ADMA): Tissue microarray analysis confirmed higher Dimethylarginine dimethyl amino hydrolase-1 (DDAH-1) expression in prostate cancer (PCa) compared to benign and normal prostate tissues. DDAH1 regulates Nitric oxide (NO) production by degrading endogenous Nitric Oxide Synthase (NOS) inhibitor, Asymmetric Dimethylarginine (ADMA). This study examined whether DDAH1 has any physiological role in PCa progression. Using overexpression of DDAH1 in PCa (PC3 and LNCaP) cell lines, we found that DDAH1 promotes cell proliferation, migration and invasion by lowering ADMA levels, as well as increasing NO production. VEGF, HIF-1α and iNOS were upregulated in DDAH1 expressing cells as result of elevated NO. DDAH1 increased secretion of proangiogenic signals bFGF and IL-8, into conditioned media. Treatment of DDAH1 positive PCa cells with NOS inhibitors (L-NAME and 1400W) attenuated DDAH1 activity to promote cell growth. Xenografts derived from these cells grew significantly faster (> 2 fold) than those derived from control cells. Proliferation rate of cells stably expressing mutant DDAH1 was same as control cells unlike wild type DDAH1 positive PCa cells. Xenograft tumors derived from mutant positive cells did not differ from control tumors. VEGF, HIF-1α and iNOS expression did not differ in DDAH1 mutant positive tumours compared to control tumours but was upregulated in wild type DDAH1 overexpressing tumours. Furthermore, CD31 immunostaining on xenograft tissues demonstrated that DDAH1 tumours had high endothelial content than mutant DDAH1 tumours. These data suggest that DDAH1 is an important mediator of PCa progression and NO/DDAH pathway need to be considered in developing therapeutic strategies targeted at PCa. (*Angiogenesis*, **2018**, 21(1), 79)

Proteomic Analysis Reveals that Interleukin-6 Induces Expression of Valosin-Containing Protein

(VCP)/P97 Associated with Androgen-Independent Prostate Cancer Progression: Though Androgen deprivation therapy (ADT) is effective initially, numerous patients become resistant to it and develop castration resistant PCa (CRPC). Cytokines promotes ligand independent activation of AR. Interleukin-6 (IL-6) levels are elevated in CRPC patients and regulate AR activity. However, progression to CRPC is not fully understood. In this study, we analyzed differential protein expression in LNCaP cells treated with IL-6 using proteomics. Results revealed altered expression of 27 proteins and Valosin-containing protein (VCP) / p97 plays a predominant role in co-regulation of altered proteins. Interestingly, IL-6 induced VCP expression through Pim-1 via STAT3 is AR independent there by suggesting a role for VCP in CRPC. Transfection of LNCaP cells for VCP overexpression showed an increased cell proliferation, migration and invasion where as its inhibition by NMS-873 showed the reverse effect causing cell death. Mechanistic studies demonstrate that cell death occurs due to apoptosis by endoplasmic reticulum (ER) stress, elevated cell cycle inhibitors p21, p27kip1 and active PARP and reduced Bcl-2. VCP promotes cell invasion and migration by altering E-cadherin and Vimentin levels inversely triggering EMT of PCa cells. VCP immunostaining revealed no staining in BPH but strong staining in PCa. This study determines VCP may play an important role in progression to CRPC and it can be a favorable target with to develop new therapies to treat ADT resistant prostate cancer. (*J. Cellular physiol*., **2018**, 233(10), 7148)

Tumor Protein D52 (Isoform 3) Interacts with and Promotes Peroxidase Activity of Peroxiredoxin 1 in Prostate Cancer Cells Implicated in Cell Growth and Migration Tumor protein D52 (TPD52) is overexpressed in multiple cancers including prostate cancer due to gene amplification and investigations to understand its role in the pathophysiology of different cancers are continuing. GST pull-down assays and Tandem affinity purification of TPD52 as bait identified novel prey Peroxiredoxin 1 (PRDX1) in prostate cancer (PCa) cells. PRDX1 interaction with TPD52 was confirmed in immunoprecipitation and affinity interaction assays. Mapping of interaction domain indicated that PRDX1 interacts with C-terminal region of TPD52 containing PEST domain between 152-179 amino acids, a new binding region of TPD52. Here we show that TPD52 interaction with PRDX1 increased its peroxidase activity and ectopic expression of TPD52 induced dimerization of PRDX1 in PCa cells. Moreover, H_2O_2 exposure evoked the interaction between TPD52 and PRDX1 while depletion of both proteins led to the accumulation of H_2O_2 suggesting peroxidase activity is important to maintain oxidative capacity in PCa cells. We also observed that overexpression or downregulation of TPD52 and PRDX1 individually or together affecting PCa cells growth, survival, and migration. Altogether, our results show a novel interaction partner of TPD52 providing new insights of its functions and ascertain the role of TPD52-PRDX1 interaction in PCa progression. (*Biochim. Biophys. Acta: Mol. Cell Res*., **2019**, 1866(8), 1298)

Novel Cellularly Active Inhibitor Regresses DDAH1 Induced Prostate Tumor Growth by Restraining Tumor Angiogenesis Through Targeting DDAH1/ADMA/NOS Pathway: Dimethylarginine dimethylaminohydrolase1 (DDAH1) inhibitors are important therapeutics by virtue of their ability to control nitric oxide (NO) production by elevating asymmetric dimethylarginine (ADMA) levels. In a screening campaign, we identified that DD1E5 (3-amino-6-tert-butyl-N-(1,3-thiazol-2-yl)-4-(trifluoromethyl) thieno[2,3-b] pyridine-2- carbo xamide) inhibits the DDAH1 activity both *in vitro* and in cultured cells. Mechanistic studies found that DD1E5 is a competitive inhibitor (dissociation constant (K_i) of 2.05 ± 0.15 μM). Enzyme kinetic assays showed time and concentration dependent inhibition of DDAH1

with DD1E5, which shows tight binding with inactivation rate constant of 0.2756±0.015 $M^{-1}S^{-1}$. Treatment of cancer cells with DDAH1 inhibitors shows inhibition of cell proliferation and a subsequent decrease in NO production with ADMA accumulation. DD1E5 reversed the elevated VEGF, c-Myc, HIF-1α and iNOS levels induced by exogenous DDAH1 overexpression in PCa cells. Moreover, DD1E5 significantly increased intracellular levels of ADMA and reduced NO production suggesting its therapeutic potential for cancers in which DDAH1 is upregulated. In *in vitro* assays, DD1E5 abrogated the secretion of angiogenic factors (bFGF and IL-8) into conditional media indicating its anti-angiogenic potential. DD1E5 inhibited *in vivo* growth of xenograft tumors derived from PCa cells with DDAH1 overexpression, by reducing tumor endothelial content represented with low CD31 expression. VEGF, HIF-1α and iNOS expression were reversed in DD1E5 treated tumours compared to respective control tumours. In this work integrating multiple approaches shows DD1E5 is a promising tool for the study of methylarginine-mediated NO control and a potential therapeutic lead compound against pathological conditions with elevated NO production such as cancers and other diseases. (*ACS Comb. Sci*., **2019,** 00133)

2. Cardiovascular Research

Metformin Treatment Prevents SREBP2-Mediated Cholesterol Uptake and Improves Lipid Homeostasis During Oxidative Stress-Induced Atherosclerosis: Lipids are responsible for the atheromatous plaque formation during atherosclerosis by their deposition in the subendothelial intima of the aorta, leading to infarction. Sterol regulatory element-binding protein 2 (SREBP2), regulating cholesterol homeostasis, is suggested to play a pivotal role during the early incidence of atherosclerosis through dysregulation of lipid homeostasis. Here we demonstrate that oxidative stress stimulates SREBP2-mediated cholesterol uptake via low-density lipoprotein receptor (LDLR), rather than cholesterol synthesis, in mouse vascular aortic smooth muscle cells (MOVAS) and THP-1 monocytes. The enhancement of mature form of SREBP2 (SREBP2-M) during oxidative stress was associated with the inhibition of AMP-activated protein kinase (AMPK) activation. In contrast, inhibition of either SREBP2 by fatostatin or LDLR by siLDLR resulted in decreased cholesterol levels during oxidative stress. Thereby confirming the role of SREBP2 in cholesterol regulation via LDLR. Metformin-mediated activation of AMPK was able to significantly abrogate cholesterol uptake by inhibiting SREBP2-M. Interestingly, although metformin administration attenuated angiotensin (Ang)-II-impaired lipid homeo stasis in both aorta and liver tissues of $ApoE^{-/-}$ mice, the results indicate that SREBP2 through LDLR regulates lipid homeostasis in aorta but not in liver tissue. Taken together, AMPK activation inhibits oxidative stress-mediated SREBP2-dependent cholesterol uptake, and moreover, metformin-induced prevention of atheromatic events are in part due to its ability to regulate the SREBP2-LDLR axis. (*Free Rad. Biol. Med*., **2018**, 118, 85)

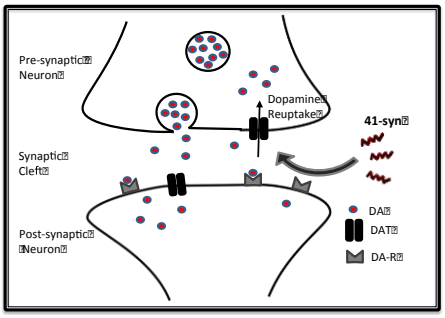
Metformin Regulates Mitochondrial Biogenesis and Senescence through AMPK Mediated H3K79 Methylation: Relevance in Age-Associated Vascular Dysfunction: Endothelial senescence in conjunction with mitochondrial dysfunction orchestrates age-associated cardiovascular disorders. In this study we investigated the causal link between these two processes and studied the molecular mechanisms by which metformin acts to coordinate the delay of endothelial senescence via enhancing mitochondrial biogenesis/function. AMPK activators metformin and AICAR delayed endothelial senescence via SIRT1-mediated upregulation of DOT1L, leading to increased trimethylation of H3K79 (H3K79me3). Treatment of cells with either

siAMPK or siSIRT1 repressed DOT1L-mediated enhancement of H3K79me3. Moreover, the increase in SIRT3 expression and mitochondrial biogenesis/function by AMPK activators was H3K79me-dependent as H3K79N mutant or siDOT1L abrogated these effects. This was confirmed by the enrichment of H3K79me3 in the SIRT3 promoter with AMPK activation. Intriguingly, enhanced PGC-1α expression by SIRT3 via AMPK activation was responsible for increased hTERT expression and delayed endothelial senescence. In contrast, SIRT3 knock down caused increased oxidative stress and premature senescence, possibly by depleting hTERT expression. Furthermore, a chronic low dose administration of metformin significantly attenuated vascular aging and inhibited age-associated atherosclerotic plaque formation in ApoE-/- mice. Overall, the results of this study show a novel regulation of mitochondrial biogenesis/function, and cellular senescence by H3K79me acting through SIRT3, thus providing a molecular basis for metformin-mediated age-delaying effects. (*Biochim. Biophys. Acta: Mol Basis Dis*., **2018**, 1864(4 Pt A), 1115)

3. Neurobiology Research

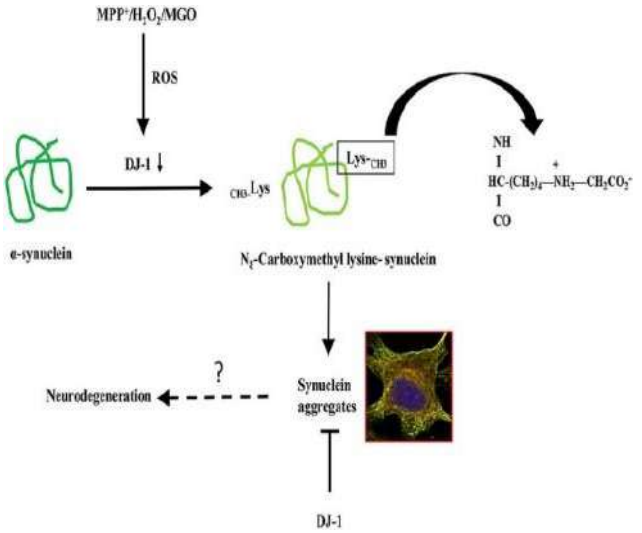
(A) Neurodegenerative Disease Mechanisms:

I. Identification of an Alternatively Spliced A-Synuclein Isoform that Generates A 41-Amino Acid N-Terminal Truncated Peptide, 41-Syn: Role in Dopamine Homeostasis: The presynaptic protein, α-synuclein (α-syn), has been shown to play a crucial role in multiple neurodegenerative diseases, such as Parkinson's disease (PD), Alzheimer's disease (AD), and dementia with Lewy bodies (DLB). The three major domains of α-syn protein were shown to govern its membrane interaction, protein fibrillation, and chaperone activity. So far, four different alternatively spliced isoforms of α-syn, which lack either exon 3 (syn-126) or exon 5 (syn-112) or both (syn-98) resulting in altered function of the proteins, have been identified. Very recently, we have identified the smallest isoform of α-syn due to the skipping of exons 3 and 4 generating a 238 bp transcript. Due to the presence of a premature stop codon, the 238 bp transcript generated a 41 aa N-terminal peptide instead of the 78 aa protein, which is secreted into the extracellular medium when over expressed in cells. The presence of 41-syn was initially noticed in the substantia nigra of PD autopsy tissues, as well as in cells undergoing oxidative stress. In vitro studies inferred that 41-syn neither aggregates nor alters the aggregation propensity of either WT or 112-syn. Overexpression of 41-syn or treatment of cells with 41-syn peptide did not affect cell viability. However, PC-12 cells treated with 41-syn exhibited a time and dose dependent enhancement in the cellular uptake of dopamine. Based on the physiological role of the N-terminal region of α-syn in modulating membrane trafficking events, we believe that the identification of 41-syn may provide novel impetus in unraveling the physiological basis of alternative splicing events in governing PD pathophysiology. (*ACS Chem. Neurosci*., **2018,** 9(12), 2948)



II. The Role of DJ-1/PARK7 in the Mechanisms Mediating Parkinson's Disease: Parkinson's disease (PD) is a progressive neurodegenerative disorder associated with the degeneration of dopamine neurons of the substantia nigra pars compacta (SNpc) and the presence of intra-neuronal aggregates of α-synuclein and its post-translational products. Based on emerging reports on the association between glycated α-synuclein and PD; and the newly identified deglycase activity of DJ-1, we have identified the relevance of deglycase activity of DJ-1 on glycation of α-synuclein and its plausible role in PD. Our results demonstrate that DJ-1 has a higher

affinity towards the substrate methylglyoxal (MGO) (Km = 900 mM) as compared to its familial mutant, L166P (Km = 1900 mM). Also, CML α-synuclein (CML-syn) served as a substrate for the deglycase activity of DJ-1. Treatment of cells with Parkinsonian mimetic, 1-methyl-4-phenyl pyridinium ion (MPP^+); oxidants, such as H_2O_2 and methylglyoxal (MGO) lead to a dose-dependent decrease in the levels of DJ-1 with a concomitant increase in CML-syn. Also, MGO induced cytosolic α-synuclein aggregates in cells which stained positive with the anti-CML antibody. Further, unilateral stereotaxic administration of MGO into the SNpc of mice induced α-synuclein aggregates and CML-syn with a concomitant reduction in the number of TH positive neurons, protein levels of TH and DJ-1 at the site of injection. Interestingly, overexpression of DJ-1 enhanced the clearance of preformed CML-syn in cells, mitigated MGO induced CML-syn and intracellular α-synuclein aggregates. Overall, the findings of our present study demonstrate that DJ-1 plays a pivotal role in the glycation and aggregation of α-synuclein. Reduced DJ-1 activity due to mutations or oxidative stress may lead to the accumulation of glycated α-synuclein and its aggregates. (*Free Rad. Biol. Med*., **2019**, 135, 28)



b) Neuropsychiatric and Neurologic Disorders

Neurologic disorders including Psychiatric involvements, contribute a large portion of the total disease and disability burden, worldwide. According to World Health Organization (WHO) report, 25% of the people in the world experience with various kind of mental disorders at some stages in their life. In order to getappropriate curative for these diseases several studies needed to add up in the proper understanding of the disease mechanisms. There is an urgent need of strong focus on developing drug for neurological and psychiatric disorders. In order to achieve a cost-effective vivo model is needed for screening new drug molecules as available rodent models are highly expensive to screen hundreds and thousands of compounds we have already developed a cost effective neuro disease vertebrate model (zebra fish) for better understanding of the disease mechanism and in identifying new drugs. Here, we also report the use of those models in that purpose

- Owing to the interesting structural and potent neurotrophic role of Fellutamide B (a lipopeptide aldehyde), we have demonstrated that the Fellutamide B synthetic path intermediates have potential neurotrophic, neurogenic, and mood-elevating effects and thus good prospect to be developed as potential therapeutics to treat psychiatric disorders. (*ACS Omega*, **2018**, 5(3), 10534)
- In another study, our results suggest that the novel carbazole-based HDAC inhibitors, crafted with vorinostat and tubastatin-A pharmacophoric moieties, have potent neurite outgrowth activity and potential to be developed as therapeutics to treat depression and related psychiatric disorders. (*ACS Omega*, **2019,** 4(17), 17279)
- In collaborative studies (with **CSIR-CCMB** and **NIN**, Hyderabad) we have elucidated the behavioural correlates of chronic severe and moderate vitamin B12 deficiency in C57BL/6 mouse model established by us earlier (*Nut. Neurosci.*, **2018**, 25,1); In two other collaborative studies (with **CSIR-CCMB**), first using transgenic mouse facility, we have demonstrated

that the partial deletion of the heterochromatin region of the Y chromosome may exhibit to the increased stress vulnerability and reduced new neuron formation in mice. (*Front Behav. Neurosci.*, **2018,** 12, 215); In another study, we also showed that miR-30 family miRNAs mediate chronic stress-induced depression-like phenotype by altering hippocampal neuro genesis and neuroplasticity via controlling the epigenetic and transcription regulators such as Mll3 and Runx1; and cell signaling regulators like Socs3, Ppp3r1, Gpr125, and Nrp1. (*Front. Mol. Neurosci.*, **2018,** *12,188*)

- As major focus of our lab (study of sex difference in neuro-diseases), we have uncovered cellular and molecular deference in sex-specific systemic responses during the post-hypoxia recovery using a novel zebrafish hypoxic model. This insight might help in devising better therapeutic strategy for stroke in female patient. (*Neurosci. Lett.*, **2019**, 10, 134492)

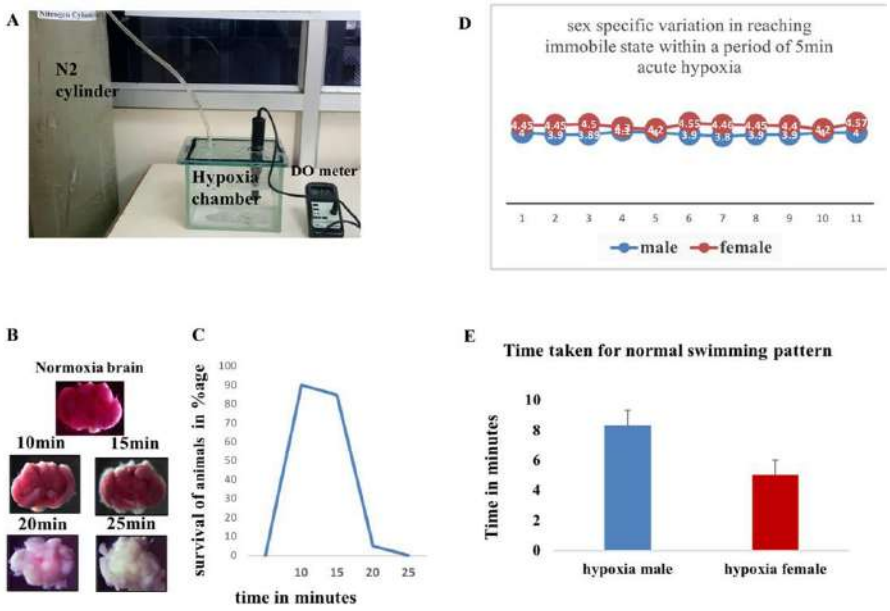
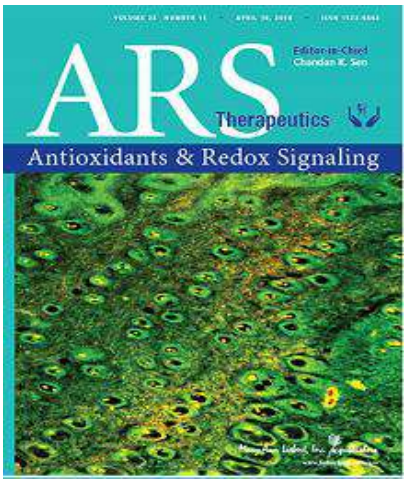


Fig**.** Image of hypoxia chamber connected with N_2 cylinder and DO meter (A). TTC staining showing infarcts in brain caused by hypoxic exposure for different time period (B). Graph showing survival of animals at different times post-hypoxia exposure (n=10) (C). Line graph showing the time taken by male and female zebrafish in reaching immobile state upon severe hypoxia exposure (DO =±0.6 mg/l) for 5 min (D). Bar graph showing the time taken by male and female zebrafish post-hypoxic exposure to regain normal swimming pattern (n=11) (E).

- By using our newly established mouse model of global ischemia mimicking cardiac arrest induced human stroke condition we have shown a region-specific temporal molecular response in the brain, which is uniquely important to get better insight into the pathophysiology since each region consists of different subsets of neurons that are having different susceptibility and tolerance pattern/level. (*J. Chem. Neuroanat.*, **2018,** 24(92), 1)
- Additionally, with our institutional biomaterial group, we also contributed in targeting brain-associated TAMs and tumor cells first time Folate Receptor-based nanodeliveryusing Glioma orthotopic mouse model to evaluate the efficacy of their formulations as glioma chemotherapy (*Nano scale Adv.*,**2019**,1,3555); whereas we also contributed to investigate the efficacy of lactoferrin nanoparticles (LfNPs) in delivering siRNA across the blood– brain barrier to treat

glioblastoma multiforme (GBM) and with an additional objective of potentiation of conventional temozolomide (TMZ) chemotherapy with CSIR-CCMB nano group. (*Nanomedicine(Lond)*, **2018,** 13(20), 2579)



4. Stem Cells and Regenerative Medicine

Low Oxidative Stress-Mediated Proliferation via JNK-FOXO3a-Catalase Signaling in Transplanted Adult Stem Cells Promotes Wound Tissue Regeneration: Stem cells exposed to pathological levels of reactive oxygen species (ROS) at wound sites fail to regenerate tissue. The molecular mechanism underlying differential levels of ROS-mediated regulation of stem cells remains elusive. This study elucidates the mechanistic role of catalase at 10 µM H_2O_2-induced proliferation of mouse bone marrow stromal (BMSC) and hematopoietic (HSPC) stem/progenitor cells. BMSCs and HSPCs depicted an increased growth rate and colony formation, in the presence of 10 µM but not 100 µM concentration of H_2O_2, an effect that was perturbed by Vit. C. Mechanistically, JNK activation–FOXO3a nuclear translocation and binding of FOXO3a to catalase promoter at 10 µM H_2O_2 led to an increased expression and activity of anti-oxidant gene, catalase. This was followed by an increased proliferative phenotype via the AKT-dependent pathway that was perturbed in the presence of catalase-inhibitor, 3-aminotriazole due to an increased ROS-mediated inactivation of AKT. Preclinically, 10 µM H_2O_2-mediatedpreconditioning of BMSCs/HSPCs transplantation accelerated wound closure, enhanced catalase expression, and decreased ROS levels at the wound site. Transplantation of male donor cells into female recipient mice or GFP-labeled BMSCs or HSPCs depicted an increased engraftment and proliferation in preconditioned cell transplanted groups as compared with the wound control. Wound healing occurred via keratinocyte generation and vascularization in preconditioned BMSCs, whereas only neo-vascularization occurred in the preconditioned HSPCs transplanted groups. Our study suggests a distinct role of catalase that protects BMSCs and HSPCs from low ROS and promotes proliferation. Transplantation of preconditioned stem cells enhanced wound tissue regeneration with a better antioxidant defense mechanism—as a therapeutic approach in stem cell transplantation-mediated tissue regeneration. (*Antioxid. Redox Signal*, **2018**, 28, 1047)

Cycloxygenase-2 Inhibition Potentiates Trans-Differentiation of Wharton's Jelly-Mesenchy mal Stromal Cells into Endothelial Cells: Transplantation Enhances Neovascular- ization-Mediated Wound Repair: Neo-vascularization, an indispensible phenomenon for tissue regeneration, facilitates repair and remodeling of wound tissues. This process is impaired in chronic wounds due to reduced number and recruitment of endothelial cells(ECs), thereby necessitating development of newer strategies to enhance the EC repertoire as a therapeutic approach. We explored the 'plasticity' of Wharton's jelly-derived mesenchymal stromal cells (WJ-MSCs) using an anti-inflammatory drug-mediated enhanced trans-differentiation into ECs, based on our observation of temporal decrease inCOX-2 expression during trans-differentiation of MSCs into ECs at day 7 and 14 along with mature ECs. At a physiological level, an increased DiI-labeled acetylated-low density lipoprotein (DiI-Ac-

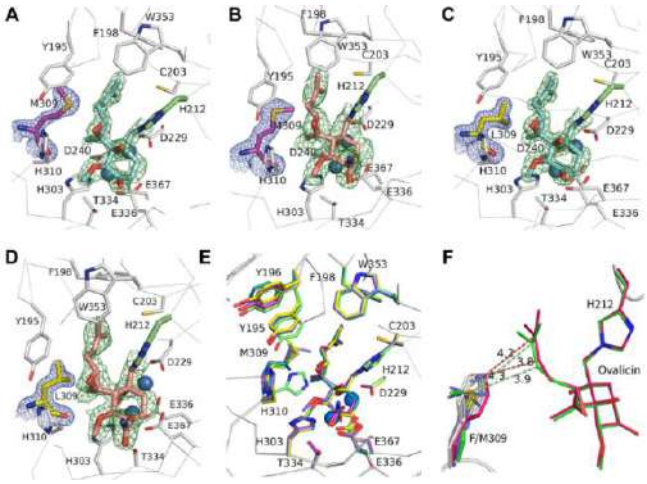
LDL) uptake, proliferation, migration and chick chorioallantoic membrane (CAM)-vasculogenesis occurred while at a molecular level significant up-regulation in messenger RNA (mRNA) and protein expression of endothelial-specific markers, Vegfr2, Pecam, eNOS, VE-Cadh and Tie-2, along with an activated p-VEGFR2 and its downstream mediators were observed in celecoxib-preconditioned ECs as compared with WJ-MSCs. Green fluorescent protein (GFP)-expressing stable WJ-MSCs and trans-differentiated EC-D14 in the absence/presence of celecoxib were generated using antibiotic selection for intradermal transplantation at the wound site on a murine 'excisional splinting wound' model. Engraftment of transplanted human cells in immunosuppressant-treated mice was confirmed by a significant increase in the expression levels of human gene-specific endothelial markers at the regenerated wound sites. Morphometrically, increased vascularity and percent wound closure were observed in regenerated wounds of mice transplanted with celecoxib-preconditioned-EC-D14. Cox-2 inhibition led to an enhanced trans-differentiation of WJ-MSCs into ECs that, when transplanted, accelerated the skin regeneration by engraftment and neo-vascularization at the wound bed, suggesting a plausible new therapeutic role of celecoxib. (*Cytotherapy*, **2019**; 21, 260)

Endothelial Progenitor Cell Therapy for Chronic Wound Tissue Regeneration: Despite advancements in wound care, healing of chronic diabetic wounds remains a great challenge for the clinical fraternity because of the intricacies of the healing process. Due to the limitations of existing treatment strategies for chronic wounds, stem/progenitor cell transplantation therapies have been explored as an alternative for tissue regeneration at the wound site. The non-healing phenotype of chronic wounds is directly associated with lack of vascularization. Therefore, endothelial progenitorcell (EPC) transplantation is proving to be a promising approach for the treatment of hypo-vascular chronic wounds. With the existing knowledge in EPC biology, significant efforts have been made to enrich EPCs at the chronic wound site, generating EPCs from somatic cells, induced pluripotent stem cells (iPSCs) using transcription factors, or from adult stem cells using chemicals/drugs for use in transplantation, as well as modulating the endogenous dysfunctional /compromised EPCs under diabetic conditions. This review mainly focuses on the pre-clinical and clinical approaches undertaken to date with EPC-based translational therapy for chronic diabetic as well as non-diabetic wounds to evaluate their vascularity-mediated regeneration potential. (*Cytotherapy,* **2019,** 21, 1137)

5. Structural Biology

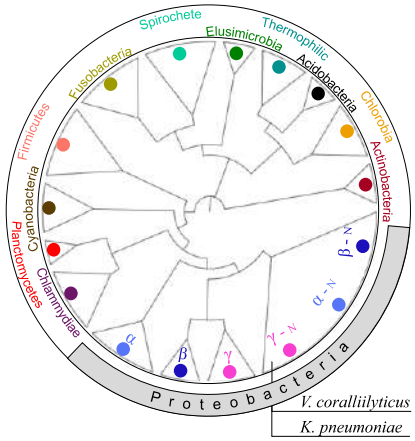
Discovery of Natural Product Ovalicin Sensitive Type 1 Methionine Amino peptidases: Molecular and Structural Basis: Natural product ovalicin and its synthetic derivative TNP-470 have been extensively studied for their anti-angiogenic property, and the later reached phase 3 clinical trials. They covalently modify the conserved histidine in Type 2 methionine aminopeptidases (MetAPs) at nanomolar concentrations. Even though a similar mechanism is possible in Type 1 human MetAP, it is inhibited only at millimolar concentration. In this study, we have discovered two Type 1 wild type MetAPs (*S. pneumoniae* and *E. faecalis*) that are inhibited at low micromolar to nanomolar concentrations, and established the molecular mechanism. F309 in the active site of human Type 1 MetAP (*Hs*MetAP1b) seems to be the key to the resistance, while newly identified ovalicin sensitive Type 1 MetAPs have a methionine or isoleucine at this position. Type 2 human MetAP (*Hs*MetAP2) also has an isoleucine (I338) in the analogous position. Ovalicin inhibited F309M and F309I mutants of human MetAP1b at low micromolar concentration. MD simulations suggest that ovalicin is not stably placed in the active site of wild type MetAP1b before the covalent modification. In the case of F309M mutant and

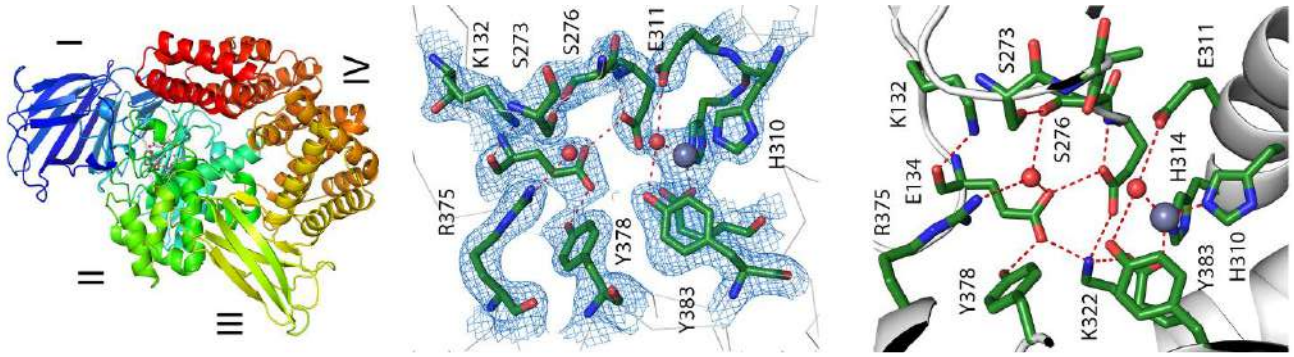
human Type 2 MetAP, molecule spends more time in the active site providing time for covalent modification. (*Biochem. J.*, **2019**, 476(6), 991)



Discovery of a New Class of Type 1 Methionine Aminopeptidases that have Relaxed Substrate Specificity: Methionine aminopeptidases (MetAPs) are a class of enzymes evolved to cleave initiator methionine in 60-70% of the total cellular proteins in all living cells. Based on their sequence differences, they are classified into Type 1 and Type 2. Type 1 is further divided into Type 1a, 1a', 1b, 1c and 1d. Irrespective of various classifications, all MetAPs reported till date displayed hydrolytic activity against peptides that contain only methionine on the N-terminus. A cysteine at the top of the active site in all the Type 1 structures is reported to be critical for the specificity. Mutation of this cysteine to serine or asparagine leads to loss of specificity. In the present study, we have identified a class of MetAPs in some of the proteobacteria that have an asparagine at this site. Most of the proteobacteria that contain MetAP1n are pathogenic in nature. Biochemical and structural studies on two proteins, one from each of *V. coralliilyticus* and *K. pneumoniae* confirm that these enzymes cleave leucine in addition to methionine. Crystallographic and homology modeling studies suggest that relaxed substrate specificity of this new class of enzymes could be due to the increased flexibility in the active site. Since this new class has an asparagine at the critical position that probably contributes for the relaxed substrate specificity and also differentiates them from other Type 1 MetAPs, we classified them as Type 1n. (*Int. J. Biol. Macromol*., **2019**, 129, 523)

Discovery, Structural and Biochemical Studies of a rare Glu/Asp Specific M1 Class Aminopeptidase from *Legionella pneumophila*: Aminopeptidases catalyze the hydrolysis of amino acids from the N-terminus of protein or peptide substrates. M1 family aminopeptidases are important for the pathogenicity of bacteria and play critical role in many physiological processes such as protein maturation, regulation of peptide hormone levels in humans. Most of the M1 family aminopeptidases reported till date display broad substrates specificity, mostly specific to basic and hydrophobic residues. In the current study we report the discovery of a novel M1 class aminopeptidase from *Legionella pneumophila* (*Le*PepA) which cleaves only acidic residues. Biochemical and structural studies reveal that the S1 pocket is polar and positively charged. Bioinformatic analysis suggests that such active site is unique to only *Legionella* species and probably evolved for special needs of the microbe. Given its specific activity, *Le*PepA could be useful in specific biotechnological applications. (*Int. J. Biol. Macro mol*., **2018**, 120, 1111)





6. Drug Delivery and Nanomedicine Research

a) In order to explore human clinical use of our previously developed glucocorticoid receptor (GR)-targeted nano-lipoplexes, we demonstrated herein how a structural change in lipid excipient, such as incorporation of a single unsaturation in one of the aliphatic chains of cationic lipid, can alter the anti-tumor response and genotoxicological profiling of the overall nano-lipoplex. One unsaturated bond in aliphatic chain of the lipid, where the aliphatic chain is only 1/6th of the total formulation component, induces markedly decreased lipoplex-mediated genotoxicity but increased anti-tumor response compared to lipoplex formulation carrying lipid of saturated aliphatic chains. This delineates the importance of carrying cationic lipids of one unsaturated aliphatic chain when anti-tumor lipoplexes yet exhibiting least genotoxicity are employed. (*Nanotoxicol.*, **2019**, 13(9), 1161)

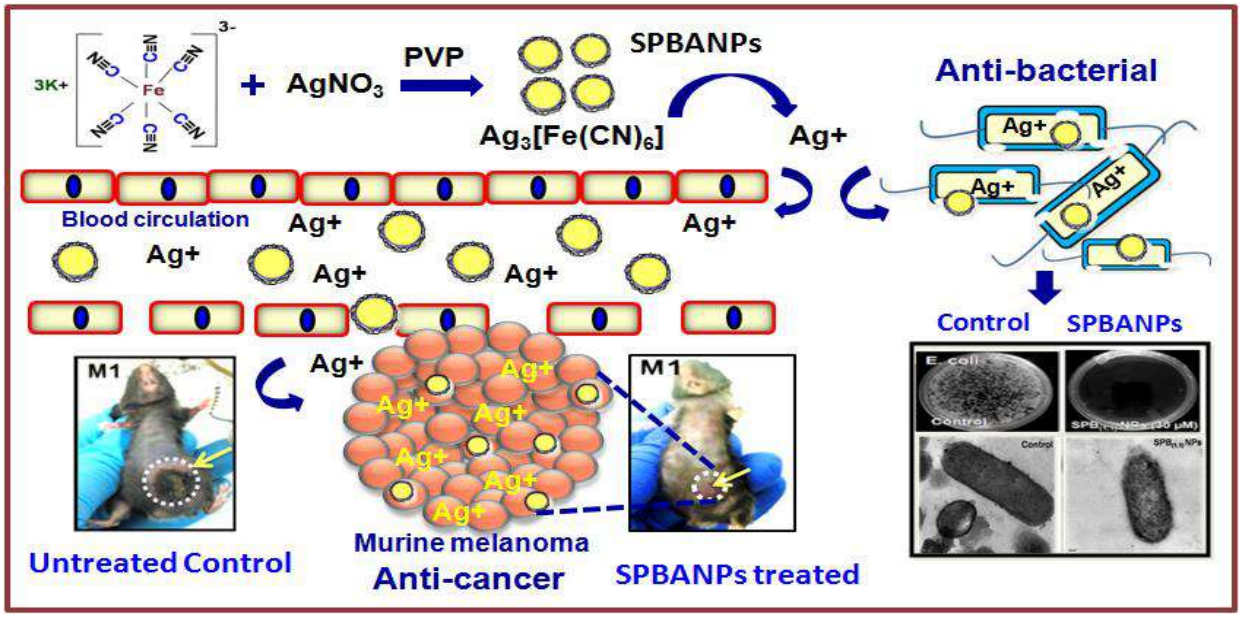
b) In collaboration with JNCASR, Bangalore, we developed a carbon nanosphere (CSP)-based delivery system that could dually target folate receptor (FR)-expressing glioma tumor-associated macrophages and tumor epithelial cells in the brain. CSP, originally developed by JNCASR, has its intrinsic property to glide through blood brain barrier (BBB) but lacks selective targeting ability to glioma lesions. Glioma tumor-associated epithelial cells and pro-tumorigenic M2 macrophages moderately express FR, thus are minimally targeted by conventional folate targeted formulations which could target only cells overtly expressing FR. Challenge to target FR-expressing cells, however is bigger if the cells are within brain. Using a special cationic folate-CSP nanoconjugate we accomplished in situ glioma tumor regression with increased survivability of mice**.** (*Nanoscale Adv.*, **2019**, 1, 3555 & India Patent Appln. No. 201841009113)

c) We explored the potential of an estrogen receptor (ER)-targeted liposomal formulation using an unique molecule, ESC10 as a ligand to target melanoma which avidly express ER. ESC10, an estrogen moiety conjugated with cationic lipid, is previously established as an anticancer agent against ER+ breast and skin cancer cells. Except for malignancies of gynaecological organs, as ER remains largely unutilized as a target to treat cancers of ER-expressing brain, prostate, skin etc., in this study we explored and demonstrated the targeting ability of ESC10 in a drug-carrying liposomal delivery system and additive anticancer effect along with drug cargo against melanoma model. (*J. Drug Target.*, **2018**, 26(5-6), 481)

7. Nanomedicine for Cancers:

- In one project, we have incorporated prussian blue (PB) and silver salts (silver nitrate) to develop silver prussian blue analogue nanoparticles (SPBANPs), a new nano medicine formulation as a safer and effective mode of treatment strategy (2-in-1) for both cancer and bacterial infections. The nanoparticles showed biocompatibility *in vivo*

in C57BL6/J mice that encouraged us to screen the nanoparticles for various biomedical applications. SPBANPs itself exhibited remarkable inhibition of cancer cell proliferation (B16F10, A549, MCF-7 and SK-OV-3) *in vitro*. Substantial inhibition of melanoma tumor growth was observed in C57BL6/J mouse model (aggressive murine melanoma model: B16F10) after intra peritonial administration of SPBANPs without any anti-cancer drug. Additionally, the SPBANPs exhibited excellent antibacterial activity in various Gram-negative (*E. coli*, *K. pneumonia* and *P. aeruginosa*) and Gram-positive (*B. subtilis*) bacteria. Interestingly, this nanoformulation itself works as a drug delivery vehicle, anti-cancer as well as an anti-bacterial agent. (*ACS Biomater. Sci. Eng.*, **2019**, 6, 690 & USA Patent Number: 10,231,996 (Date of Grant : March 19 2019)

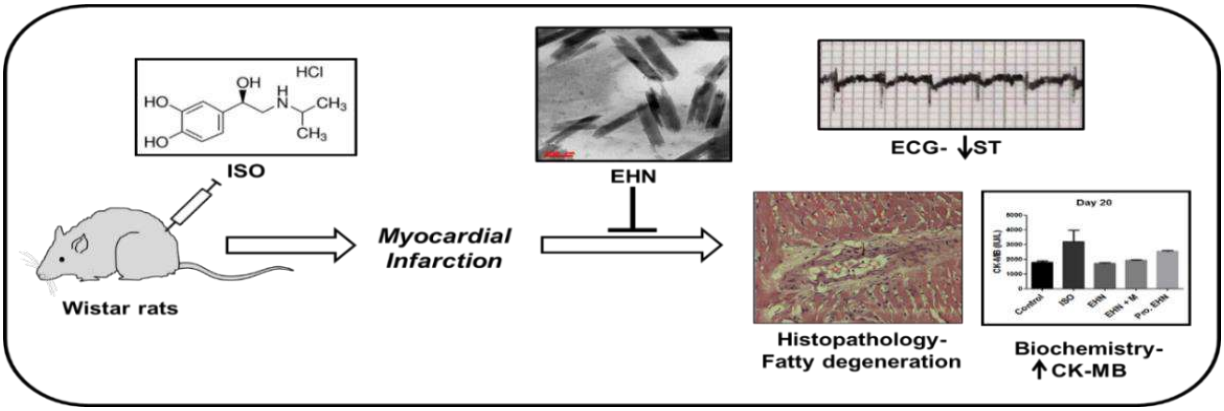


- We demonstrate the *Zinnia eligans*plant extract (abbreviated as ZE) assisted synthesis of highly biocompatible gold nanoparticles (AuZE) and their non-invasive bio-imaging applications in NIR region (red at 820nm emission: NIR region). After intraperitoneal administration of AuZE in C57BL6 mice, very interestingly, AuZE is distributed into the brain of C57BL6 mice without the need of any targeted ligand and exhibited bright red fluorescence at NIR region (710nm excitation, 820nm emission) as evidenced from non-invasive imaging as well as ICP-OES techniques. We further explored the activity of ZE and AuZE as cell labeling agents (B16F10 cells pre-incubated with AuZE and implanted into mice and the fluorescence was monitored) which could be applicable for graft transplantation biology. The present research on biosynthesized AuNPs open new directions for the future research to explore these latest observations in the field of disease diagnosis and therapy. (*ACS Biomater. Sci. Eng.*, **2019**, 5, 10, 5439)
- We have also demonstrated the restoration of p53 function in ovarian cancer mediated by gold nanoparticles based EGFR targeted gene delivery system (*ACS Biomater. Sci. Eng*., **2019**, 5(7), 3631). In another work, we demonstrated the

shikimoyl-ligand decorated gold nanoparticles induce anti-tumor immune response in dendritic cell-based DNA vaccination (*Nanoscale*, **2019,** 11, 7931). Similarly, we reported that Au-CGKRK nano conjugates for combating cancer through T cell driven therapeutic RNA interference (*ACS Omega*, **2018**, 3, 8663). We also demonstrated the design of DNA-intercalators based copper(II) complexes, investigation of their potential anti-cancer activity and sub-chronic toxicity. (*Mater. Sci. Engg. C.*, **2019,** 105, 110079)

Nanomedicine for Myocardial Infarction:

We have reported the the effect of the pro-angiogenic europium hydroxide nanorods (EHN) on the ischemic condition was validated using several assays which revealed that the ischemia and cardiotoxicity induced by isoproterenol was ameliorated by EHN in both H9C2 rat cardiomyocytes (in vitro) and Wistar rats (in vivo). The results shows that the EHN could be exploited as alternative treatment strategies for myocardial ischemia therapy and other ischemic diseases where angiogenesis plays a significant role in near future. (*ACS App. Bio Mat.*, **2019**, 2(3), 1078)



Nanomedicine for Wound Healing and Treatment of Microbial Infection:

We designed and synthesized silver nitroprusside complex nanoparticles (abbreviated as AgNNPs) using sodium nitroprusside and silver nitrate (both are FDA approved precursors. These nanoparticles show effective antibacterial activity against both Gram positive and Gram negative bacteria through membrane and DNA damage. Additionally, AgNNPs accelerate the wound healing in C57BL6 mice by altering the macrophages from M_1 to M_2. This study could be exploited for the development of new silver nano-complex nanomaterials that shows synergistic effect on anti-bacterial activity and wound healing (2-in-1-system). (*ACS Biomater. Sci. & Eng.*, **2018**, 4(9), 3434)

Nanomedicine and its Applications in Site Specific Drug Delivery:

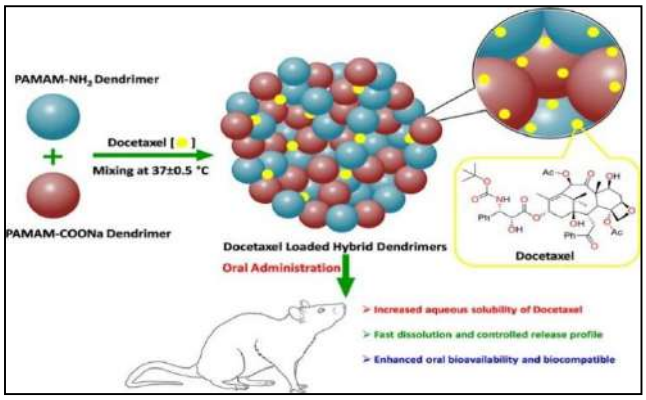
Crossing blood brain barrier is the main hurdle for many therapeutic CNS drugs against neurological or brain disorders including glioma. Glioblastoma multiforme (GBM) is one of the most encountered gliomas of the central nervous system. The chemotherapeutic drugs used in the treatment of GBM suffer from poor blood brain barrier penetration, severe systemic toxicities and lack of specificity towards tumor cells. Effective delivery would be the better approach to circumvent this obstacle and offer the therapeutic effect in brain. In this regard, we developed couple of delivery systems using Nanoparticles and dendrimers.

Lipid Nanoparticles:

Solid lipid nanoparticles (SLN) are biocompatible vehicle with less toxicity issues compared to other drug delivery systems and serve the purpose of obviating the limitations posed by existing anti-cancer drugs for GBM. In this study, angiopep-2, a ligand for the lipoprotein receptor related protein 1 (LRP 1) receptor over expressed in endothelial cells of both brain and glioma, was grafted on the surface of solid lipid nanoparticles for the delivery of docetaxel. The peptide grafted nanoparticles (A-SLN) showed increased cytotoxicity, enhanced cellular internalization and prominent apoptosis than that of unconjugated nanoparticles against U87MG human glioblastoma and GL261 mouse glioma cells. A significant dual targeting effect of A-SLN ($p < 0.0001$) was confirmed in in-vivo studies by real time fluorescence imaging studies in glioblastoma induced C57BL/6 mice model. Pharmacokinetic and tissue distribution studies showed selective targeting with higher accumulation of A-SLN in brain compared to Taxtotere, a marketed formulation of docetaxel. After treatment with A-SLN, the mean animal survival time of the animals was significantly enhanced to 39 days from 24 days of plain docetaxel. *(DOI: 10.1016/j.ejpb.2018.09.012)*

Dendrimers:

Dendrimers have proven to be effective for drug delivery and their biodisposition varies with change on their surface, generation and core. In an effort to understand the role of critical nanoscale design parameters, we developed a novel hybrid dendrimer approach to harness unique features of individual dendrimers and create a nano-assembly. We report an easy in situ method of creating hybrid dendrimer nano-assembly by mixing G4.0 PAMAM (-NH2) and G3.5 PAMAM (-COONa) dendrimers with a chemotherapeutic drug docetaxel (DTX). Cellular uptake, cytotoxicity, and flow cytometric analysis in human/mouse glioblastoma cells indicated the effectiveness of hybrid dendrimers. The oral administration of the hybrid dendrimers showed pharmacokinetic equivalence to intravenous injection of commercially available Taxotere®. Hybrid dendrimer concept provides much needed fine-tuning to create multistage next-generation dendritic platform in nanomedicine. *(https://doi.org/10.1016/j.nano.2019.102043)*



9. Pharmacology and Toxicology Group

Inauguration of Animal House Facility:

Animal experimentation plays an important role in understanding the human disease process and in improving the well being of humans. Many important medical advancements have been made by first employing animal models fo disease. CSIR Indian Institute of Chemical Technology, Hyderabad upgraded the animal house facility. This facility was inaugurated on 14th March 2018 by Dr R Hemalatha, Director, National Institute of Nutriton (ICMR), Hyderabad. The animal house was constructed with state of art facilities as per GLP norms and it caters the need of Pharma and Biotech industries.

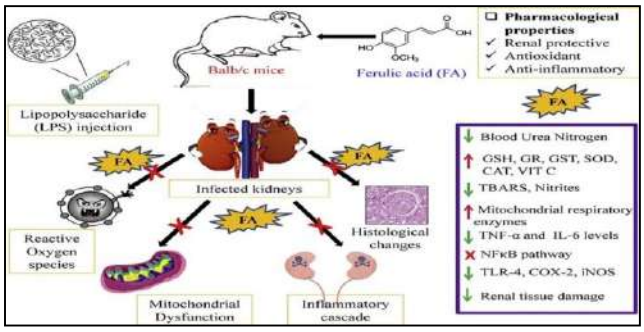
BASIC RESEARCH

Novel Small molecules or plant based chemicals are emerging to address the unmet medical needs. However; novel/authenticated models are required to test and validate these molecules before taking forward for clinical application. Here we have developed several animal models to validate the small molecules or phytochemicals against kidney, intestine, cardiovascular and pulmonary disorders. The details are presented in brief.

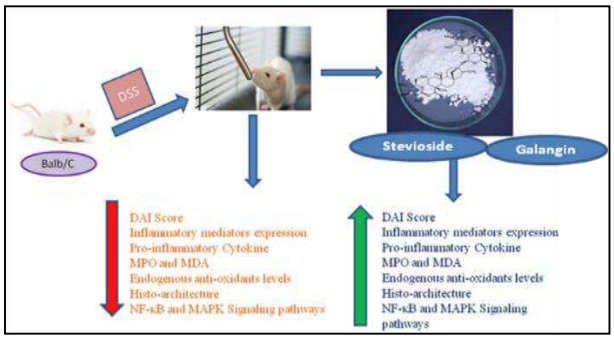
Inflammatory Pharmacology

Acute kidney injury (AKI) is a sudden episode of kidney failure or kidney damage that happens within a few hours or a few days. AKI causes a build-up of waste products in blood and makes it hard for kidneys to keep the right balance of fluid in the body. AKI can also affect other organs such as the brain, heart, and lungs. There are few models to test the AKI, here we developed the model using LPS and validated using Ferulic acid as model drug, against AKI. LPS induced oxidative stress, mitochondrial dysfunction and inflammatory events. Ferulic acid treatment restored levels of antioxidants and mitochondrial enzymes. Ferulic acid attenuated the TLR-4 receptor mediated activation of NF-κB pathway. Ferulic acid treatment reverted the LPS induced histological changes in kidney. Ferulic acid protected the LPS induced kidney injury by reducing the protein expression of TLR4 mediated NF-κB signaling pathway, up regulation of antioxidant defences and suppression of inflammatory events by inhibiting TLR-4 mediated NFκB activation. (PMID: 29448207 *DOI: 10.1016/j.biopha.2018. 01.169*)

Inflammatory bowel disease (IBD) is known to cause chronic inflammation in the digestive tract by the immune malfunction. Since most of the inflammatory medications in current use have several undesirable side-effects, we investigated the therapeutic effects of naturally occurring compounds such as stevioside and galangin. We demonstrated the protective effect of steveoside and galangin (GAL), against LPS-induced inflammation in cultured mouse macrophages (RAW 264.7) and the treatment of DSS-induced ulcerative colitis in Balb/c mice. Interestingly in both the studies, we observed that, treatment with Stevioside and galangin significantly reduced the LPS induced inflammatory cytokine levels.

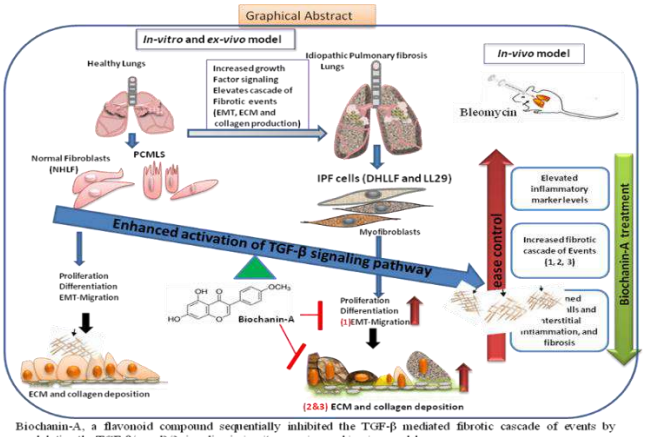


Stevioside and galangin have also been evaluated for their anti-inflammatory effect employing dextran sulfate sodium (DSS)-induced ulcerative colitis model in mice. Similar to in-vitro data, invivo data also revealed that, Stevioside and galangin (*Inflammation Research* volume 68, pages 691–704(2019)) significantly reduced the DSS induced abnormalities in balb/C mice. Study revealed that stevioside significantly suppressed NF-κB (p65) activation by abrogating IκB phosphory lation and attenuated the phosphorylation of p38, ERK and JNK proteins in colon tissues. The findings of the present study suggested that stevioside exhibited anti-inflammatory property by inhibiting NF-κB (p65) and MAPK pathways and can be employed as an adjunct in nutraceuticals to treat IBD. (*DOI: 10.1016/j. ejphar.2019.05.015*)



Pulmonary Research:

Idiopathic Pulmonary Fibrosis (IPF) is a progressive inflammatory disorder driven by fibrotic cascade of events such as epithelial to mesenchymal transition, extra cellular matrix production and collagen formation in the lungs in a sequential manner. IPF incidences were rising rapidly across the world. Till today, FDA approved two tyrosine kinase inhibitors (Pirfinidone and Nintedanib) to treat IPF, however, neither the quality of life nor survival rates have been improved because of non-selectivity, hitting multiple receptors simultaneously. Thus, development of novel therapeutic approaches targeting TGF-β mediated cascade of fibrotic events is urgently needed to improve the survival of the patients suffering from devastating disease. Here, we standardized the TGF-beta induced invitro models for pulmonary fibrosis using pulmonary fibrosis cells and Bleomycin induced pulmonary fibrosis model in rats. The therapeutic activity of Biochainin-A was determined in *in-vitro/ex-vivo* models by pretreatment of cells with BCA and exposure to recombinant-TGF-β to stimulate the fibrotic cascade of events. Pulmonary fibrosis was developed by intra-tracheal administration of bleomycin in rats. Our results revealed that, Biochainin-A treatment significantly (p <0.001) reduced the TGF-β elevated fibrotic genes/proteins expression levels (including their functions) which are involved in the events of fibrotic cascade. BCA treatment significantly reduced the bleomycin-induced inflammatory cell-infiltration, markers expression, collagen deposition and expression of fibrotic markers in lung tissues. In addition, BCA treatment significantly (p<0.001) attenuated the TGF-β1/BLM-mediated increase of TGF-β/Smad2/3 phosphorylation and resulted in the reduction of pathological abnormalities in lung tissues gauged by histopathology observations.



Biochanin-A, a flavonoid compound sequentially inhibited the TGF-β mediated fibrotic cascade of events by modulating the TGF-β/smad2/3 signaling in *in-vitro*, *ex-vivo* and *in-vivo* models.

Site-Specific Oral Delivery of Sorafenib:

Globally, one in six deaths is reported due to cancer suggesting the critical need for development of advanced treatment regimens. Efficient site specific delivery of the therapeutic compound would be the bottle-neck for effective treatment outcome. In this regards, solid lipid nanoparticles (SLN) were prepared and appended with polyethylene glycol (PEGylated) galactose and a multikinase inhibitor sorafenib (SRFB) was used as chemotherapeutic drug, for treating hepatocellular carcinoma (HCC). The nanoparticles were evaluated for in-vitro and in-vivo performances to showcase the targeting efficiency and therapeutic benefits of the sorafenib loaded ligand conjugated nanoparticles (GAL-SSLN). When compared with SRFB or Sorafenib loaded SLN, GAL-SSLN showed superior cytotoxicity and apoptosis in HepG2 (human hepatocellular carcinoma cells). In addition, in-vivo pharmacokinetics and real time biodistribution studies in BALB/c mice showed that the surface conjugation of nanoparticles with galactose resulted in better pharmacokinetic performance and targeted delivery of the nanoparticles to liver. Results indicated that GAL-SSLN showed promising attributes in terms of targeting sorafenib to liver and therapeutic efficacy

(*https://doi.org/10.1016/j.ejps.2019.104978*)

Inter Divisional Collaborations: Novel menadione compounds were evaluated for their anticancer activity against five selected cancer cell lines including lung (A549), prostate (DU-145), cervical (Hela), breast (MCF-7), and mouse melanoma (B-16) using MTT assay and concluded as lead molecule for further development as potent anticancer therapeutic agent. Myrrhanones A and B were isolated from the gum resin of *Commiphora mukul* and their analogues were evaluated for anti inflammatory activity and were found to be potent inhibitors of TNF-α and IL-1β. Sixteen novel orsellinic esters along with four lecanoric acid related depsides were evaluated for their *in vitro* α-glucosidase (*Saccharomyces cerevisiae*) inhibitory potential.

Standardization of in Vitro and Animal Models Pulmonary inflammation: Standardization of *in vitro* and *in vivo* techniques for pulmonary fibrosis: There are very few *in vitro* and ex-vivo techniques available for screening anti-fibrotic compounds against Idiopathic Pulmonary Fibrosis. We developed *in vitro* and ex-vivo methods to screen anti-fibrotic compounds. In addition to these methods we have also standardized in-vivo methods to validate the compounds.

I. Standardization of invitro method for testing anti-fibrotic compounds using LL29, NHLF and DHLF cell lines.
II. Optimization of precision-cut lung tissue culture method to test anti-fibrotic compounds against IPF
III. Standardization of Bleomycin induced pulmonary fibrosis in mice.

Prenatal Hyper Androgenised Polycystic Ovarian Syndrome Mice Models: We developed and validated the prenatal hyper androgenised polycystic ovarian syndrome mice models to test the compounds for reproductive diseases. The prenatal models are hyper androgenised by DHT and DHEA hormones in C57BL6/J inbred mice.

Efficient Anti-Tumor Nano-Lipoplexes With Unsaturated or Saturated Lipid Induce Differential Genotoxic Effects in Mice: In this study, (DXE nano-lipoplex), which carries cationic lipid of saturated twin aliphatic chains and an another nano-lipoplex (D1XE) group that carried cationic lipid with one of its aliphatic chain carrying unsaturation were used to assess the anti-tumor efficacy and genotoxicological profiling. Herein, we report that nanoplex with unsaturated cationic lipid (D1XE) exhibited better physical appearance with less flocculent behavior than nanoplex with saturated lipid (DXE). Upon multiple injections, D1XE nanoplex imparted better tumor regression but most importantly, exhibited much lower overall toxicity (e.g. genotoxicity, weight loss, etc.) than DXE nanoplex. With a higher antitumor effect but a lower genotoxic effect, D1XE is proved to be a better nanoplex than DXE for the potential clinical trial. Thus, this study clearly delineates the importance of incorporating a constituent lipid that carries a single unsaturated aliphatic chain toward developing efficient anti-tumor nano-lipoplexes with reduced genotoxicity. *(DOI: 10.1080/17435390.2019.1643049*)

Anti-Hyperglycemic and Genotoxic Studies of 1-O-Methyl Chrysophanol, A New Anthraquinone Isolated from Amycolatopsis Thermoflava Strain SFMA-103: The compound 1-O-methyl chrysophanol (OMC) which belongs to a class of hydroxyl anthraquinones was isolated from Amycolatopsis thermoflava strain SFMA-103 and studied for their anti-diabetic and genotoxicity properties. OMC demonstrated enzyme inhibitory activity towards a-amylase (IC50 3.4mg mL_1) and a-glucosidase (IC50 38.49 lg mL_1). In *in vivo* anti-diabetic activity, (oral dose in Wistar rats) revealed that OMC inhibited significantly the increase in glucose concentration at 100mg/kg as compared to starch control ($p<0.05$). Further, to understand the safety of OMC as a therapeutic agent, the genotoxic analysis was performed in both *in vitro* Chinese Hamster Ovary cells (250, 500, and 1000 mM/mL) and *in vivo* Swiss albino mice (250, 500, and 1000mg/kg). In vitro results showed that OMC concentration of up to 250 mM/mL did not elicit

significant changes in CAs, MI, and MN counts in CHO cells. Similarly, in mice experiments (i.p. injection), no significant changes in CAs, MI, and MN induction were observed till 500 mg/kg of OMC when compared with chrysophanic acid (Cy) (200 mg/kg). In addition, mice that received the OMC (250 mg/kg) did not show any histological changes in liver, kidney, and heart. The study concluded that OMC can be utilized against hyperglycemia with no genotoxic effects.

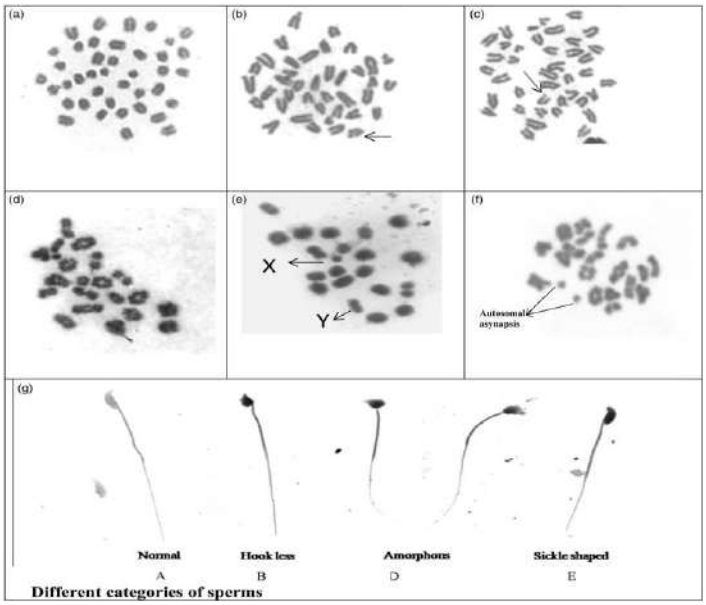
(https://doi.org/10.1080/01480545.2018.1551406)

Potential of the Bioinspired CaCO3 Microspheres Loaded with Tetracycline in Inducing Differential Cytotoxic Effects toward Noncancerous and Cancer Cells: A Cytogenetic Toxicity Assessment Using CHO Cells in Vitro: A bioinspired polypeptide- mediated calcium carbonate microspheres loaded with tetracycline ($CaCO_3$-TC) was developed to explore its safe application in cancer therapeutics. Its therapeutic application in cancer patients essentially demands its safety information on the normal cells. Herein our study presents the in vitro genetic toxicological information on $CaCO_3$-TC using noncancerous mammalian CHO cells in comparison to bare TC at three different concentrations (100, 200, and 300 μM) selected based on the cytotoxicity data (MTT). Assessment of various end points like chromosome aberrations, micronucleus, mitotic index and effects on cell cycle distribution after 24 h post-treatment demonstrates a significant reduction in clastogenic ($P < 0.001$), aneugenic potential ($P < 0.05$), and nonmitotoxic nature of $CaCO_3$-TC than that of bare TC. Noticeably, as inferred from the FACS analysis on cancer cells, G2/M phase accumulation in breast cancer cells (MDA-MB-231), and at G1 phase in cervical cancer cells (HeLa) reveal its potential anticancer property. On the other hand, the genotoxicity studies illustrate protective effects of CaCO3-TC on noncancerous cells. While the pH-dependent dissolution property of the CaCO3 matrix encasing tetracycline results in higher toxicity on cancer cells, the near neutral pH in the case of normal cells prevents complete dissolution of $CaCO_3$ thereby not allowing the encapsulated TC to adequately interact with the cells. Therefore, thus assembled $CaCO_3$ spheres not only provide a way for facile encapsulation of tetracycline under mild conditions but also result in an effective matrix for differential toxicity toward normal and cancer cells justifying its clinical development as a novel targetspecific drug in therapeutic applications for metastatic cancers. (*Chem. Res. Toxicol.*, **2018.** *31* (7), 629)

Zoledronic Acid Induces Micronuclei Formation, Mitochondrial-Mediated Apop tosis and Cytostasis in Kidney Cells, Cytogenetic Toxicity in Male Germline Cells of Swiss Albino Mice: Zoledronic acid (ZA), a FDA approved drug has used widely in the treatment of bone metastasis complications, has been linked to renal toxicity with unclear mechanism. The present study Vero and MDCK cells were used. The CBMN assay has shown prominent dose-dependent (IC_{10-50}) induction of micronuclei formation in both cells, indicating ZA's clastogenic and aneugenic potential. Further, the ZA treatment led the cells to apoptosis, evident from dose-dependent increase in the percentage of cells in sub G_1 phase and display of membranous phosphatidylserine translocation. Studies also confirmed apoptosis through mitochondria, evident from the prominent increase in BAX/Bcl-2 ratio, mitochondrial membrane depolarization and caspase-3/7 activity. In addition, ZA reduces cytokinetic activity of renal cells, evident from dose-wise lowered replicative indices. The study depict ZA's potential genotoxic effect along with cytotoxic effect in renal epithelial cells, could be key factors for the development of renal complications associated with it, which prompts renal safety measures in lieu with ZA usage.

The same ZA used to assess the cytogenetic toxicity in the male germline cells of Swiss albino mice.

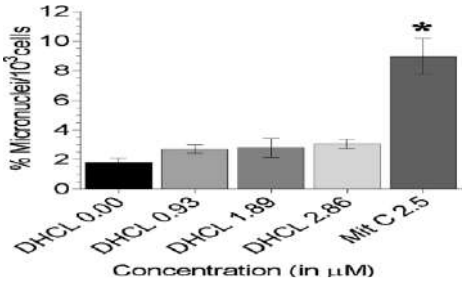
Three different doses of ZA (2, 4, and 8mg/kg body weight), were treated and toxicity was assessed by analyzing spermatogonial metaphase chromosome aberrations, aberrant primary spermatocytes, and abnormal spermatozoa. The results showed that there was a significant induction in the number of chromosomal aberrations especially at two doses of ZA (4 and 8 mg/kg) after 24 h in the spermatogonial cells ($p<0.001$) compared to vehicle control. The transmission genetic damages were noticed as aberrant spermatocytes with atypical bivalents (X-Y/autosomal asynapsis) at 4mg/kg of ZA ($p<0.01$) and at 8mg/kg of ZA ($p<0.001$) at week 4 posttreatment. A statistically significant higher number of abnormal spermatozoa (sperm) were also noticed at week 8 posttreatment of both at 4 and 8 mg/kg of ZA ($p<0.001$). Hence, from these *in vivo* genotoxicity studies, it can be concluded that ZA is genotoxic in male germline cells and has the potential of transmitting the genotoxic effects from spermatogonial cells to sperm in male Swiss mice. (*DOI:10.1080/01 480545. 2018.1455205*)



About figure: (a) Spermatogonial metaphase after 24 h post treatment; (b) normal; (c) with chromatid gap; (d–f) with chromatid break; (d) primary spermatocyte chromosomes spreads after week 4 posttreatment; (e) normal 20 bivalents; (f) 19 bivalentþX-Y univalents (asynapsis); (g) 19 bivalent þ2 univalents (autosomal asynapsis): (A) normal sperm: (B–E) types of aberrant sperms after week 8 posttreatment.

Dehydrocostus Lactone Induces Prominent Apoptosis in Kidney Distal Tubular Epithelial Cells and Interstitial Fibroblasts along with Cell Cycle Arrest in Ovarian Epithelial Cells: Dehydrocostus lactone (DHCL), a sesquiterpene lactone is well-known for its antiulcer, anti-hepatotoxic and anticancer activity. The present study is aimed at investigating the toxicity potential of DHCL in renal distal tubular and interstitial fibroblast cell lines (MDCK and NRK-49F cells, respectively), and also in ovarian epithelial cell line (CHO cells). Dehydrocostus lactone (DHCL) possesses potential cytotoxic activity against the kidney cell lines (MDCK, NRK-49F) and CHO cells. DHCL prominently causes apoptosis of all cell types. Among the various kinds of cells, the distal tubular epithelial (MDCK) cells are highly prone to DHCL's cytotoxic effect. DHCL induces ROS production in renal cell lines. The oxidative stress by DHCL in NRK-49F cells results due to cellular GSH depletion, which triggers apoptotic cell death in a mitochondrial mediated manner by altering the BAX and Bcl-2

protein levels, mitochondrial membrane permeability and caspase activity. Further, the CHO cells escalating sensitivity toward DHCL was reflected by the induction of mitotic arrest at sub-lethal concentrations (≤IC30) and prominent apoptosis at higher concentrations (≥IC50). The CHO cells have purposefully undergone mitotic arrest in response to the induced chromatid gaps by inhibiting the Cyclin B1 degradation. Due to the ability of CHO cells to switch to cell cycle arrest, they are able to tolerate DHCL exposure till certain concentration with negligible cell death, when compared to the renal cell lines. The observations of DHCL directed potential toxic effects toward kidney (MDCK and NRK-49F) cell lines, which are of normal tissue origin, leads to the suspicion of prominent renal toxicity. In the renal system, the damage of both distal tubular epithelial cells (DTEs) and interstitial fibroblasts could lead to serious renal complications. Hence, the study recommends in-depth investigations on DHCL usage concerning its safety in therapeutic applications. (*Biomedicine & Pharmacotherapy*, **2018,** 99, 956)



Comparative Study of Cyto and Genotoxic Potential with Mechanistic Insights of Tungsten Oxide Nano and Microparticles in Lung Carcinoma Cells: The exigency of semiconductor and super capacitor tungsten oxide nanoparticles (WO_3 NPs) is increasing in various sectors. However, limited information on their toxicity and biological interactions are available. Hence, we explored the underlying mechanisms of toxicity induced by WO_3 NPs and their microparticles (MPs) using different concentrations (0–300 µg ml^{-1}) in human lung carcinoma (A549) cells. The mean size of WO_3 NPs and MPs by transmission electron microscopy was 53.84 nm and 3.88 µm, respectively. WO_3 NPs induced reduction in cell viability, membrane damage and the degree of induction was size- and dose-dependent. There was a significant increase in the percentage tail DNA and micronuclei formation at 200 and 300 µg ml^{-1} after 24 hours of exposure. The DNA damage induced by WO_3 NPs could be attributed to increased oxidative stress and inflammation through reactive oxygen species generation, which correlated with the depletion of reduced glutathione content, catalase and an increase in malondialdehyde levels. Cellular uptake studies unveiled that both the particles were attached/surrounded to the cell membrane according to their size. In addition, NP inhibited the progression of the cell cycle in the G_2/M phase. Other studies such as caspase-9 and -3 and Annexin-V-fluorescein isothiocyanate revealed that NPs induced intrinsic apoptotic cell death at 200 and 300 µg ml^{-1} concentrations. However, in comparison to NPs, WO_3 MPs did not incite any toxic effects at the tested concentrations. Under these experimental conditions, the no-observed-significant-effect level of WO_3 NPs was determined to be ≤200 µg ml^{-1} in A549 cells. (*J. Appl. Toxicol.*, **2018**, 38(6), 896)

Comparative Study of Toxicological Assessment of Yttrium Oxide Nano- and Microparticles in Wistar Rats after 28 Days of Repeated Oral Administration: Despite their enormous advantages, nanoparticles (NPs) have elicited disquiet over their safety. Among the numerous NPs, yttrium oxide (Y2O3) NPs are utilised in many applications. However, knowledge about their toxicity is limited, and it is imperative to investigate their potential adverse effects. Therefore, this study explored the effect of 28 days of repeated oral exposure of Wistar rats to 30, 120 and 480 mg/kg body weight (bw) per day of Y2O3 NPs and microparticles (MPs). Before initiation of the study, characterisation of the

particles by transmission electron microscopy, dynamic light scattering, Brunauer–Emmett–Teller and laser Doppler velocimetry was undertaken. Genotoxicity was evaluated using the comet and micronucleus (MN) assays. Biochemical markers aspartate transaminase, alanine transaminase, alkaline phosphatase, malondialdehyde, superoxide dismutase, reduced glutathione, catalase and lactate dehydrogenase in serum, liver and kidney were determined. Bioaccumulation of the particles was analysed by inductively coupled plasma optical emission spectrometry. The results of the comet and MN assays showed significant differences between the control and groups treated with 120 and 480 mg/kg bw/day Y2O3 NPs. Significant biochemical alterations were also observed at 120 and 480 mg/kg bw/day. Haematological and histopathological changes were documented. Yttrium (Y) biodistribution was detected in liver, kidney, blood, intestine, lungs, spleen, heart and brain in a dose- and the organ-dependent manner in both the particles. Further, the highest levels of Y were found in the liver and the lowest in the brain of the treated rats. More of the Y from NPs was excreted in the urine than in the faeces. Furthermore, NP-treated rats exhibited much higher absorption and tissue accumulation. These interpretations furnish rudimentary data of the apparent genotoxicity of NPs and MPs of Y2O3 as well as the biodistribution of Y. A no-observed adverse effect level of 30 mg/kg bw/day was found after oral exposure of rats to Y2O3 NPs. (*Mutagenesis*, **2019**, 34, 181)

In Vitro Genotoxicity Assessment of Nickel(II) Oxide Nanoparticles on Lymphocytes of Human Peripheral Blood: Genotoxicity of Nickel (II) Oxide Nano particles on Human Lymphocytes: The current study was intended to elucidate the cytotoxicity, genotoxicity ability of nickel oxide (NiO) nanoparticles (NPs) and assessment of preliminary mechanism of the toxicity. Characterization studies showed that NiO-NPs have a particle size of 17.94 (±3.48) nm. The particle size of the NPs obtained by dynamic light scattering method in Milli-Q and RPMI 1640 media was 189.9 (±17.1) and 285.9 (±19.6) nm, respectively. The IC50 concentration for NiO-NPs after 24 hours of treatment was estimated as 23.58 µg/mL. Comet and cytokinesis-block micronucleus assays revealed a significant dose- and time-dependent genotoxic potential of NiO-NPs. Morphological assessment of the lymphocytes upon exposure to NiO-NPs showed that the mechanism of toxicity was apoptosis. Reactive oxygen species analysis and lipid peroxidation patterns were aligned with the cytotoxicity and genotoxicity endpoints. Thus, the preliminary mechanism of NiO-NPs for cytotoxicity on lymphocytes was assumed to be oxidative stress-mediated apoptosis and DNA damage. Furthermore, these NiO-NPs are considered a potentially hazardous substance at environmentally significant levels. Further investigations are suggested to understand the immunotoxic effects of NiO-NPs. (*J. Appl. Toxicol.*, **2019,** 39(3))

Toxicity Assessment of Magnesium Oxide Nano and Microparticles on Cancer and Non-Cancer Cell Lines: Testing of magnesium oxide nanoparticles (MgO NPs) on established cell lines at cellular levels using toxicological endpoints provide valuable information about their adverse effects upon exposure. In vitro toxicity assessment of MgO NPs and their microparticles was carried out at 50, 100, 200 and 400 µg/mL concentrations by using cytotoxicity, genotoxicity, oxidative stress, cellular apoptosis and cellular uptake studies in cancer (HepG2) and non-cancer (NRK 49F) cell lines after 24 h of treatment. IC50 concentration for MgO NPs was found to be > 400 µg/mL in both cell lines after 24 h treatment. A concentration dependent toxicity was noted in genotoxic studies and oxidative stress parameters. A significant increase in the comet tail DNA was recorded at 200 and 400 µg/mL concentrations of MgO NPs when compared with controls in HepG2 and NRK 49F cells. Exposure to MgO NPs led to an increase in the generation of reactive oxygen species (ROS) in both the cell types.

Genotoxicity results were further supported by apoptotic analysis. MgO particles were found adhered to the cell membrane when assayed by ICP-OES. The results of this study showed that the MgO NPs were toxic at high concentrations only. Furthermore, MgO NPs are more toxic to cancerous cells compared to non-cancerous cells. ROS mediated genotoxicity was observed when treated with MgO NPs. The current study adds to the information on MgO particles. The results of this investigation may help in advancement of understanding of toxicological nature of MgO NPs and aid in their use. (Nucleus (India), **2019**, 62(4))

Repeated Oral Dose Toxicity Study of Nickel Oxide Nanoparticles in Wistar Rats: A Histological and Biochemical Perspective: Despite the increasing use of nickel oxide (NiO) nanoparticles (NPs), limited information is available on their toxicological effects. Health consequences of 28 days repeated oral exposure to NiO NPs have not been explored thoroughly. Hence, toxicity investigations were performed after 28-day daily exposure in albino Wistar rats with NiO NPs following Organization for Economic Co-operation and Development test guideline 407. Histopathology, biochemical indices including oxidative stress and biodistribution patterns were evaluated to decipher the toxicological impact of NiO NPs. NiO NP characterization by transmission electron microscopy showed an average size of 12.9 (±3.4) nm. Histological studies depicted a prominent impact on the vital organs of the rats. A dose-dependent rise in both aminotransferase enzyme values was recorded in the homogenates of liver and kidney tissues. A significant decrease in superoxide dismutase activity and increase in catalase activity was noted. Further, a dose-dependent decrease in reduced glutathione content was recorded in rats, which suggested generation of reactive oxygen species and oxidative stress. Increase in the malondialdehyde levels was observed with an increase in the dose substantiating the antioxidant enzyme activity profiles. Biodistribution studies indicated maximum accumulation of Ni content in liver followed by kidney. Excretion of Ni was predominantly through feces and a little through renal clearance. Our study indicated that NiO NPs adversely alter the biochemical profile of the rats and cause histological damage. Further investigations are warranted to address the mechanism by which physiological path these NiO NPs exhibit their toxic nature in in vivo. (*J. Appl. Toxicol.*, **2019,** 39(7))

***Allium cepa* Root Tip Assay in Assessment of Toxicity of Magnesium Oxide Nanoparticles and Microparticles:** *Allium cepa* bioassay had been used from decades for the assessment of toxicants and their harmful effects on environment as well as human health. Magnesium oxide (MgO) particles are being utilized in different fields. However, reports on the adverse effects of MgO nanoparticles on the environment and mankind are scarce. Hence, the toxicity of MgO particles is of concern because of their increased utilization. In the current study, *A. cepa* was used as an indicator to assess the toxicological efficiency of MgO nano- and microparticles (NPs and MPs) at a range of exposure concentrations (12.5, 25, 50, and 100 µg/mL). The toxicity was evaluated by using various bioassays on *A. cepa* root tip cells such as comet assay, oxidative stress and their uptake/internalization profile. Results indicated a dose dependent increase in chromosomal aberrations and decrease in mitotic index (MI) when compared to control cells and the effect was more significant for NPs than MPs (at $p < 0.05$). Comet analysis revealed that the Deoxyribonucleic acid (DNA) damage in terms of percent tail DNA ranged from 6.8–30.1 over 12.5–100 µg/mL concentrations of MgO NPs and was found to be significant at the exposed concentrations. A significant increase in generation of hydrogen peroxide and superoxide radicals was observed in accordance with the lipid peroxidation profile in both MgO NPs and MPs

treated plants when compared with control. In conclusion, this investigation revealed that MgO NPs exposure exhibited greater toxicity on *A. cepa* than MPs. (*J. Environ. Sci.,* **2018**, 66, 125)

Toxicity Assessment of Magnesium Oxide Nano and Microparticles on Cancer and Non-Cancer Cell Lines: Testing of magnesium oxide nanoparticles (MgO NPs) on established cell lines at cellular levels using toxicological endpointsprovide valuable information about their adverse effects upon exposure. In vitro toxicity assessment of MgO NPs and their microparticles was carried out at 50, 100, 200 and 400 µg/mL concentrations by using cytotoxicity, genotoxicity, oxidative stress, cellular apoptosis and cellular uptake studies in cancer (HepG2) and non-cancer (NRK 49F) cell lines after 24 h of treatment. IC50 concentration for MgO NPs was found to be > 400 µg/mL in both cell lines after 24 h treatment. A concentration dependent toxicity was noted in genotoxic studies and oxidative stress parameters. A significant increase in the comet tail DNA was recorded at 200 and 400 µg/mL concentrations of MgO NPs when compared with controls in HepG2 and NRK. (*The Nucleus,* **2019,** 62(3), 227)

Genotoxicity, Biochemical and Biodistribution Studies of Magnesium Oxide Nano and Micro particles in Albino Wistar Rats after 28-Day Repeated Oral Exposure: Increased utilization and exposure levels of Magnesium oxide (MgO) nanoparticles (NPs) to humans and environment may raise unexpected consequences. The goal of this study was to evaluate the toxicological implications of MgO NPs and MPs after 28 day repeated oral administration in Wistar rats with three different doses (250, 500, and 1000 mg/kg). The MgO particles were characterised systematically in order to get more insights of the toxicological behaviour. MgO NPs induced significant DNA damage and aberrations in chromosomes. Moreover, hepatic enzymes released into the systemic circulation caused significant elevated levels of physiological enzymes in blood. NPs could interfere with proteins and enzymes and alter the redox balance in cell environment. Significant accumulation of Mg in all tissues and clearance via urine and faeces was noted in size dependent kinetics. (*Environ. Toxicol.,* **2018**, 33(4), 396)

Ecotoxicity Study of SSP Compounds from Industries

The acute ecotoxicity study of chemicals from industries has been carried in aquatic animal models using OECD guidelines. Acute toxicity of chemicals is determined for 48 hrs in daphnia and for 96 hrs in Zebrafish.

Test Animals

Daphnia, a genus of small planktonic crustacean and members of the sub-class Phyllopoda (some time called Branchiopoda) which are characterized by flattened leaf-like legs used to produce a water current for the filtering apparatus. Within the branchiopods, Daphnia belong to the Cladocera, whose bodies are enclosed by an uncalcified shell, known as the carapace.

Figure 1 Photographs of daphnia cultured in our laboratory

Zebrafish

Scientific name: *Danio rerio*

Common name: Zebrafish

The **zebrafish** (*Danio rerio*) is a freshwater fish belonging to the minnow family (Cyprinidae) of the order Cypriniformes.

8. Infectious Diseases & Computational Biology:

APPLIED RESEARCH

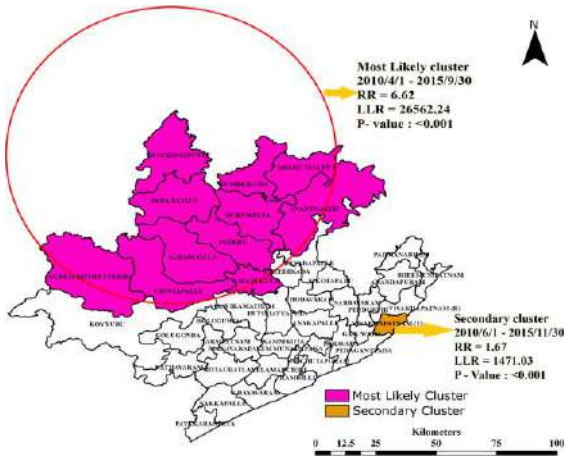
Mosquito borne diseases like malaria, dengue, Chikungunya and filariasis are major public health concern in India. CSIR-IICT is significantly contributing to control these diseases and also studying the impact climatic factors on these diseases. The Applied Biology division of CSIR-IICT has developed various predictive models and also identifies the disease hotspots in various regions of India.

Dengue

- Dengue is an emerging and re-emerging infectious disease, transmitted by mosquitoes. It is mostly prevalent in tropical and sub-tropical regions of the world, particularly, in Asia-Pacific region. To understand the epidemiology and spatial distribution of dengue, a retrospective surveillance study was conducted in the state of Andhra Pradesh, India during 2011–2013.

A district-wise disease endemicity levels were mapped through geographical information system (GIS) tools. Spatial statistical analysis such as Getis-OrdGi* was performed to identify hot spots and cold spots of dengue disease in Andhra Pradesh and Telangana. Similarly, self organizing maps (SOM), a datamining tool was also applied to understand the endemicity patterns in study areas. (*Parasite Epidemiology and Control*, **2018**, 3(1), 52)

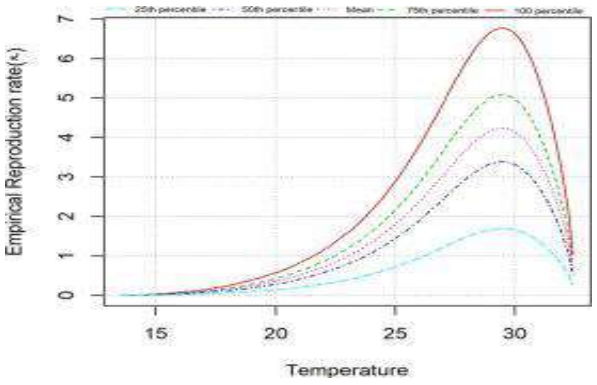
- The interaction between vector, host and pathogen is influenced by various climatic factors and the relationship between dengue and climatic conditions has been poorly explored in India. This study explores the relationship between El Niño Southern Oscillation (ENSO), the Indian Ocean Dipole (IOD) and dengue cases in India. Additionally, distributed lag non-linear model was used to assess the delayed effects of climatic factors on dengue cases from 2010–2017 were analysed. The study shows that dengue cases usually follow a seasonal pattern, with most cases reported in August and September. The precipitation shows the higher transmission risk of dengue was observed between 8 and 15 weeks of lag. The highest relative risk (RR) of dengue was observed at 60 mm rainfall with a 12-week lag period when compared with 40 and 80 mm rainfall. The RR of dengue tends to increase with increasing mean temperature above 24 °C. The largest transmission risk of dengue was observed at 30 °C with a 0–3 weeks of lag. Similarly, the transmission risk increases more than twofold when the minimum temperature reaches 26 °C with a 2-week lag period. The dengue cases and El Niño were positively correlated with a 3–6 months lag period. The significant correlation observed between the IOD and dengue cases was shown for a 0–2 months lag period. (*Epidemiology & Infection*., **2019**, 147)



Malaria

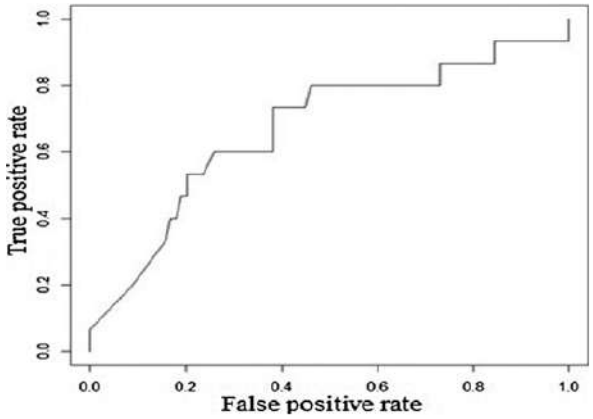
- Malaria is a major public health problem in Vishakhapatnam district of Andhra Pradesh, India. To understand malaria prevalence a retrospective surveillance study was conducted in the district from 1995 to 2015. A total of 204,229 malaria cases were reported from 1999 to 2015. *Plasmodium falciparum* and *Plasmodium vivax* are the major parasites that accounted for 66.8% and 33.2% of the total cases. Tribal population (67%) affected more than the coastal population (33%). Similarly, males were affected (56%) more than female (44%) populace and the highest prevalence was observed in > 15 years age group (83.74%). The spatial analysis reveals that the distribution of malaria i having high spatial autocorrelation (0.231 to 0.493) and scan statistics declare that the malaria cases were significantly clustered in spatial, temporal and spatiotemporal distribution. The most likely spatiotemporal cluster of malaria (LLR = 26, 562.24, RR = 6.62, P < 0.001) occurred in the Northern part of the district covering 11 mandals with the time frame from April 2010 to September 2015. The results confirm that the presence of spatial and space–time clusters concentrated in the North and North-eastern region of the district, which contribute for better understanding of disease spreading dynamics in high-risk areas for future

malaria prevention and control. (*Spatial Information Research*, **2019**, 27, 659)



Role of Climate on Chikungunya Transmission

Chikungunya is a major public health problem in tropical and subtropical countries of the world. During 2016, the National Capital Territory of Delhi experienced an epidemic caused by chikungunya virus with >12,000 cases. Similarly, other parts of India also reported a large number of chikungunya cases, highest incidence rate was observed during 2016 in comparison with last 10 years of epidemiological data. In the present study we exploited R_0 mathematical model to understand the transmission risk of chikungunya virus which is transmitted by *Aedes* vectors. This mechanistic transmission model is climate driven and it predicts how the probability and transmission risk of chikungunya occurs in India. The gridded temperature data from 1948 to 2016 shows that the mean temperatures are gradually increasing in South India from 1982 to 2016 when compared with data of 1948–1981 time scale. During 1982–2016 period many states have reported gradual increase in risk of chikungunya transmission when compared with the 1948–1981 period. The highest transmission risk of chikungunya in India due to favourable ecoclimatic conditions, increasing temperature leads to low extrinsic incubation period, mortality rates and high biting rate were predicted for the year 2016. The epidemics in 2010 and 2016 are also strongly connected to El Nino conditions which favours transmission of chikungunya in India. The study shows that transmission of chikungunya occurs between 20 and 34 °C but the peak transmission occurs at 29 °C. The infections of chikungunya in India are due to availability of vectors and optimum temperature conditions influence chikungunya transmission faster in India. This climate based empirical model helps the public health authorities to assess the risk of chikungunya and one can implement necessary control measures before onset of disease outbreak (*Science of the Total Environment*, **2019**, 647, 66)



Filariasis

Filariasis is one of the major public health concerns in India. Approximately 600 million people spread across 250 districts of India are at risk of filariasis. To predict this disease, a pilot scale study was carried out in 30 villages of Karimnagar district of Telangana from 2004 to 2007 to collect epidemiological and socio-economic data. The collected data are analysed by employing various machine learning techniques such as Naïve Bayes (NB), logistic model tree, probabilistic neural network, J48 (C4.5), classification and regression tree, JRip and gradient boosting machine. The performances of these algorithms are reported using sensitivity, specificity, accuracy and area under ROC curve (AUC). Among all employed classification methods, NB yielded the best AUC of 64% and was equally statistically

significant with the rest of the classifiers. Similarly, the J48 algorithm generated 23 decision rules that help in developing an early warning system to implement better prevention and control efforts in the management of filariasis. (*Epidemiology & Infection*, **2019**, 147)

New Generation of Anti-Tubercular Agents

CSIR-IICT has been involved in developing anti-tubercular agents with novel mode of action against virulence of pathogen. In this endeavour, CSIR-IICT partnered with Umea University, Sweden and the partnership was supported by Govt. of India and Innovation Council, Sweden.

Mycobacterium Tuberculosis Virulence Inhibitors Discovered by *Mycobacterium Marinum* High-Throughput Screening: High-throughput screening facilities do not generally support biosafety level 3 organisms such as Mycobacterium tuberculosis. To discover not only antibacterials, but also virulence inhibitors with either bacterial or host cell targets, an assay monitoring lung fibroblast survival upon infection was developed and optimized for 384-plate format and robotic liquid handling. By using Mycobacterium marinum as surrogate organism, 28,000 compounds were screened at biosafety level 2 classification, resulting in 49 primary hits. Exclusion of substances with unfavorable properties and known antimicrobials resulted in 11 validated hits of which 7 had virulence inhibiting properties and one had bactericidal effect also in wild type Mycobacterium tuberculosis. This strategy to discover virulence inhibitors using a model organism in high-throughput screening can be a valuable tool for other researchers working on drug discovery against tuberculosis and other biosafety level 3 infectious agents. (*Sci. Rep.*, **2019,** 9(1), 26)

Corticosteroids Protect Infected Cells against Mycobacterial Killing in Vitro: The effect of corticosteroids on human physiology is complex and their use in tuberculosis patients remains controversial. In a high-throughput screening approach designed to discover virulence inhibitors, several corticosteroids were found to prevent cytolysis of fibroblasts infected with mycobacteria. Further experiments with Mycobacterium tuberculosis showed anti-cytolytic activity in the 10 nM range, but no effect on bacterial growth or survival in the absence of host cells at 20 mM. The results from a panel of corticosteroids with various affinities to the glucocorticoid- and mineralocorticoid receptors indicate that the inhibition of cytolysis most likely is mediated through the glucocorticoid receptor. Using live-imaging of M. tuberculosis-infected human monocyte-derived macrophages, we also show that corticosteroids to some extent control intracellular bacteria. In vitro systems with reduced complexity are to further study and understand the interactions between bacterial infection, immune defense and cell signaling. (*Biochem. Biophys. Res. Commun*., **2019**, 511(1), 117)

9. Liver Diseases

Cellular Crosstalk Mediated by Platelet-Derived Growth Factor BB and Transforming Growth Factor During Hepatic Injury Activate Shepatic Stellate Cells: Apoptotic hepatocytes release factors that activate hepatic stellate cells (HSCs), hereby inducing hepatic fibrosis. In the present study, in vivo and in vitro injury models were established using acetaminophen, ethanol, carbon tetrachloride, orthioacetamide. Histology of hepatotoxicant-induced diseased hepatic tissue correlated with differential expression of fibrosis related genes. A marked increase in co-staining of transforming growth factor β receptor type II (TGFRIIβ) – desmin or α-smooth muscle actin – platelet-derived growth factor receptor β (PDGFRβ), markers of activated HSCs, in liver sections of these hepatotoxicant-treated mice also depicted an increase in Annexin V – cytokeratin expressing hepatocytes. To understand the molecular mechanisms of disease pathology, in vitro experiments were designed using the conditioned medium (CM) of hepatotoxicant-treated

HepG2 cells supplemented to HSCs. A significant increase in HSC proliferation, migration, and expression of fibrosis-related genes and protein was observed, thereby suggesting the characteristics of an activated phenotype. Treating HepG2 cells with hepatotoxicants resulted in a significant increase in mRNA expression of platelet-derived growth factor BB (PDGF-BB) and transforming growth factor β (TGFβ). CM supplemented to HSCs resulted in increased phosphorylation of PDGFRβ and TGFRIIβ along with its downstream effectors, extracellular signal-related kinase 1/2 and focal adhesion kinase. Neutralizing antibodies against PDGF-BB and TGFβ effectively perturbed the hepatotoxicant-treated HepG2 cell CM-induced activation of HSCs. This study suggests PDGF-BB and TGFβas potential molecular targets for developing anti-fibrotic therapeutics. (*Can. J. Physiol. Pharmacol.*, **2018**, 96(8), 728)

10. Biosensors:

Recent Trends in Electrochemical Biosensors of Superoxide Dismutases: Superoxide dismutases (SODs), a family of ubiquitous enzymes, provide essential protection to biological systems against uncontrolled reactions with oxygen- and nitrogen-based radical species. We review first the role of SODs in oxidative stress and the other biological functions such as peroxidase, nitrite oxidase, thiol oxidase activities etc., implicating its role in neuro degenerative, cardiovascular diseases, and ageing. Also, this review focuses on the development of electrochemical label-free immuno sensor for SOD1 and the recent advances in biosensing assay methods based on their catalytic and biological functions with various substrates including reactive oxygen species (superoxide anion radical, hydrogen peroxide), nitric oxide metabolites (nitrite, nitrate) and thiols using thiol oxidase activity. Furthermore, we emphasize the progress made in improving the detection performance through incorporation of the SOD into conducting polymers and nanocomposite matrices. In addition, we address the potential opportunities, challenges, advances in electrochemical-sensing platforms and development of portable analyzer for point-of-care applications. (*Biosens. Bioelectron.*, **2018**, 116, 89)

Toxicity Evaluation of Ayurvedic Herbometallic Preparations *(Funded by Ministry of AYUSH, GOI,* New Delhi): 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, elephant-tiasis, gout and tumors in man. The objectives of the study are as follows:

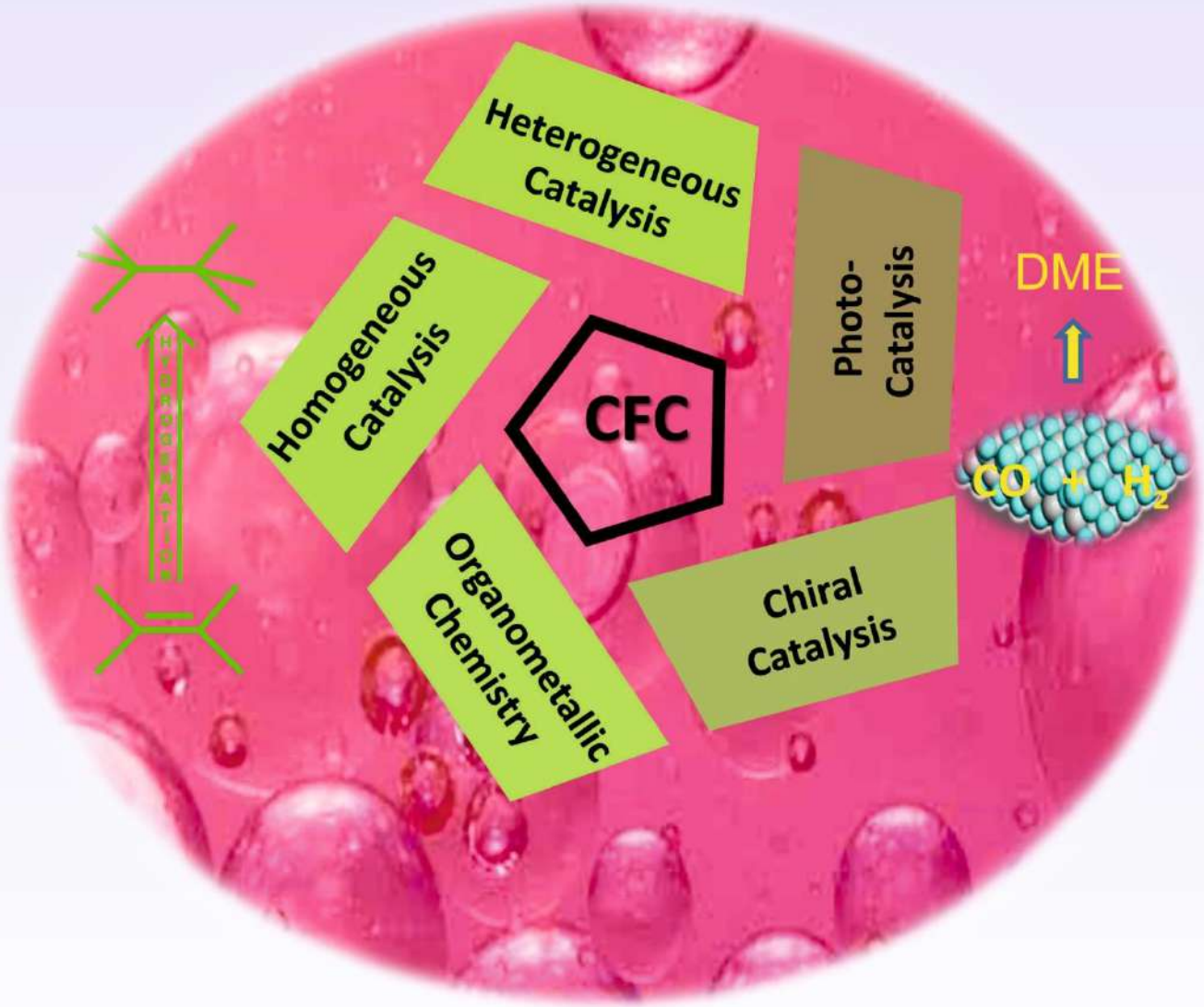
- To assess the genotoxic potential and the effect on the expression of ROS genes
- To estimate hematological and biochemical alterations
- To analyse the metals in HM drugs and their biodistribution in serum
- To perform the histopathological studies on the vital organs

Toxicological Assessment of Micro and Nano Plastics in Water Stored in Polyethylene Terephlate (PET) Bottles Using Plant and Animal Models. *CSIR HRDG (EMR -1)***:** In our studies, we have focused up on investigating water samples stored in PET bottles for physicochemical properties,

identification and quantification of Micro plastics (MPs) and Nanoparticles (NPs) by usingBio imaging techniques. The polymorphic content from bottled water and also in rat blood and their tissues will be measured using ICP-OES .The toxicity associated with bio-effects resulting after acute and 90 days repeated oral exposure will be assayed by using bio imaging techniques. The imaging of biological samples enables us to analyse tissues, cells and molecules without any physical hindrance and also non-invasively visualise biological processes in real time. Bio imaging also includes methods visualising biological material that has been fixed for observation. Within the last few years a strong interaction between Molecular Biology and Bio imaging has led to the design of an increasing number of nanosensors for many ions and metabolites. When expressed or incorporated in cells, these cells become self-reporting for the metabolites. Imaging techniques have their own strengths in terms of resolution, sensitivity and penetration depth — and it is tackling this variation in their application that has enabled materials science to come into its own within the field of bio imaging. More specifically, nanomaterials that can encapsulate or be functionalized with small molecules (for example fluorophores or radionuclides) have allowed the combination of several imaging techniques into one nanoscale platform together with the possibility of detection capabilities. The objectives of the study are as follows:

- How to detect and quantify the micro and nano plastics in PET bottled water
- Following ingestion does uptake of micro- and nano plastics occur?
- If uptake occurs, do proteins bind to the surface of the plastic particles to form a protein corona?
- If the micro and nano plastic particles get detected in visceral organ tissues, which type of imaging technique needs to be employed?

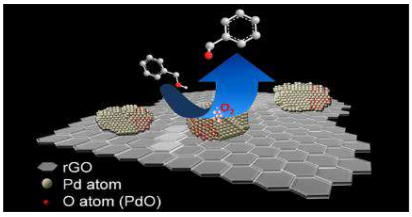
CATALYSIS AND FINE CHEMICALS



BASIC RESEARCH

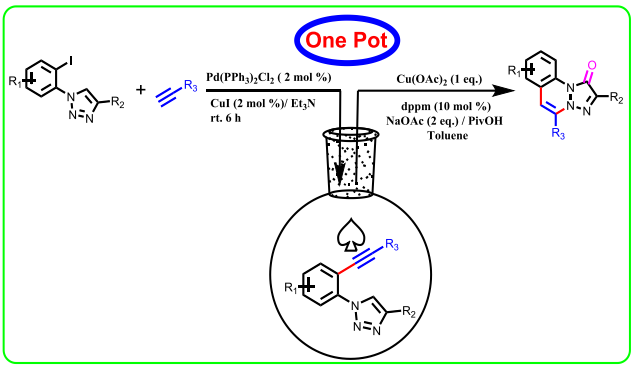
A Rational Design of a Pd-Based Catalyst with a Metal–Metal Oxide Interface Influencing Molecular Oxygen in the Aerobic Oxidation of Alcohols

In a green process for selective oxidation of alcohols utilizing molecular oxygen, it is demonstrated that the presence of both Pd^0 and Pd^{2+} species with a Pd–PdO interface stabilized on the surface of reduced graphene oxide (rGO) is important. With an optimum Pd^{2+}/Pd^0 ratio, the catalyst catalyzes the oxidation of benzyl alcohol in water with oxygen, resulting in a turnover frequency (TOF) of up to 18 000 h^{-1} with 98% selectivity towards the aldehyde. It is proposed that both metallic Pd and its oxide domains, when co-existing with a phase boundary between them, promote the activation of oxygen. On the other hand, rGO provides surface functionalities for the formation and stabilization of Pd–PdO nanoclusters enabling the catalyst to be both stable and reusable. Using histidine as a scavenger for singlet oxygen, we have also determined the importance of oxygen-activation in the reaction. Furthermore, the catalyst is capable of converting various other alcohols into the corresponding carbonyl compounds. Comparison of various catalysts shows that the Pd–PdO@rGO catalyst is the most efficient in terms of TOF, conversion and selectivity for the oxidation of benzyl alcohol using oxygen compared to the reported Pd-based catalysts, particularly when performed under milder reaction conditions. Therefore, the result on Pd-catalyst designing is believed to be of significance for the further developments in the environmentally benign oxidation processes involving molecular oxygen as the oxidant. (*Green Chem.*, **2019,** 21, 2494)



Unprecedented Synthesis of 1,2,3-Triazolocinnolinone via Sonogashira Coupling and Intra molecular Cyclization

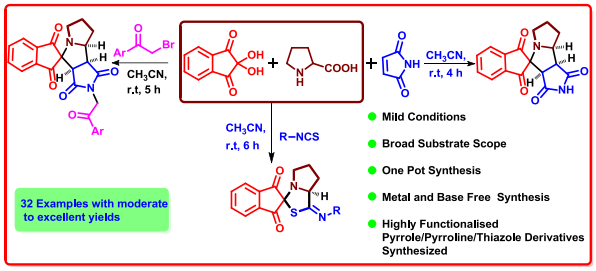
An unprecedented copper mediated one-pot sequential synthesis of 1,2,3-triazolo cinnolinone derivatives from 2-halo-phenyl triazoles and terminal alkynes has been reported. Under the optimized reaction conditions, a broad range of substituted triazoles and alkynes were found to participate in this transformation, thus affording unknown 1,2,3-triazolo cinnolinone derivatives in moderate to excellent yields. This method proceeds through sequential C–C coupling followed by an annulation cascade sequence in the same vessel under atmospheric air as the sole oxidant, thus representing a simple, efficient and atom economical approach for the synthesis of aza-cinnolinones. (*Org. Biomol. Chem.*, **2018**, 16, 4840)



Synthesis of New Spiro Pyrrole/Pyrrolizine/Thiazole Derivatives via (3+2) Cycloaddition Reaction

A new series of spiro pyrrole/pyrrolizine/thiazole compounds have been synthesized using (3+2) dipolar cycloaddition *via* three-component condensation reactions of ninhydrin and α-amino acids with different dipolarophiles such as maleimide, malic anhydride, 2-benzyl-2-methyl cyclopent-4-ene-1,3-dione and isothio cyanates. Another four-component protocol has been developed in which ninhydrin, proline, maleimide and phenacyl bromides are reacted to afford a novel library of pyrrolizine derivatives in good yields

without the use of catalyst. (*New J. Chem.*, **2018**, 42, 13819)



Transition-Metal-Free Approach for the Synthesis of 4-Aryl-quinolines from Alkynes and Anilines

An efficient and transition-metal-free approach for the synthesis of 4-arylquinolines from readily available anilines and alkynes in the presence of $K_2S_2O_8$ and DMSO has been developed. A variety of alkynes and anilines having a diverse range of substitution patterns can undergo the one-pot cascade process successfully. Effectively, this method uses DMSO as one carbon source, thus providing a highly atom-economical and environmentally benign approach for the synthesis of 4-arylquinolines. (*J. Org. Chem.*, **2018**, 83, 9137)

An Efficient Synthesis of Pyrrido[1,2-b]isoquinoline Derivatives via (3+2) Cycloaddition Multi-Component Reaction

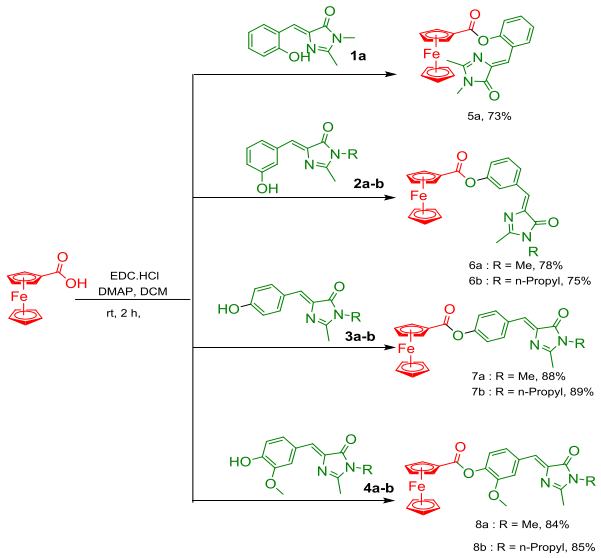
An efficient and one-pot tandem procedure for the synthesis of fused ethanopyrido [1,2-b] isoquinoline derivatives from ninhydrin, proline and alkynes has been developed. This strategy exhibits an un-precedented [3 + 2] cycloaddition reaction between alkynes and isoquinolinium ylide (1,3 dipole) gener-ated in situ from proline and ninhydrin. This newly developed methodology features simple operation and is metal free. In this methodology overall three new C–C bonds, two C–N bonds, and three new rings are formed in a single step process. (*Org. Biomol. Chem.*, **2018,** 17, 4121)

Oxyanion-Binding in a Bioinspired Nanoparticle-Assembled Hybrid Microsphere Structure: Effective Removal of Arsenate/Chromate from Water

A bioinspired assembly is demonstrated wherein the specific interaction of polyamines with multivalent anions allows the assembly of silica nanoparticles to generate hybrid microsphere structures while this very phenomenon further provides ways for the microspheres to adsorb oxyanions like arsenate and chromate. In a typical method based on the biomineralization of diatomaceous biosilica structure, thus produced nanoparticle-assembled microspheres with a porous structure and hybrid functionalities exhibit efficient adsorption and separation of these toxic anions from water. The adsorption follows Freundlich isotherm with an inference for stronger interaction between adsorbate and adsorbent with nonuniform distribution of adsorption affinities. The opportunities to tune the composition with respect to the multivalent anion and their interaction with the polyamine, charge ratio, and so forth, illustrate the design of bioinspired robust structures with efficient oxyanion-binding property and recyclability. The consequence of competing anions shows that the binding selectivity follows the Hofmeister series of counterion interaction. Interestingly, in accordance with a molecular imprinting mechanism, the silica nanoparticle-assembled structure stabilizes and preserves the polyamine-anion nanostructure creating cavities/voids complementary to the adsorbing ions in shape, size, and functional groups. As a result, the

polyamine with phosphate as the multivalent anion exhibits efficient binding and removal of these toxic contaminants, which is better than most of the other reported adsorbents. (*ACS Appl. Nano Mater*., **2019**, 2(3), 1525)

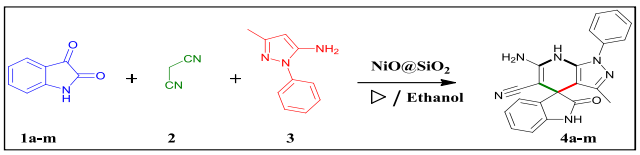
Facile Synthesis, Characterisation and Anti-Inflammatory Activities of Ferrocenyl Ester Derivatives of Arylidene-Imidazolinones



Herein, we describe the synthesis, optoelectronic properties and anti-inflammatory activities of a series of seven ferrocenyl ester linked arylidene imidazolinone conjugates. The structure of one of the conjugate was confirmed by single crystal X-ray diffraction study. ortho-, meta- and para- substituted ferrocenyl esters have been prepared and their UV-vis spectra and electrochemical studies are described. These conjugates exhibited moderate anti-inflammatory activities. (*Appl. Organomet. Chem*., **2018**, 4021)

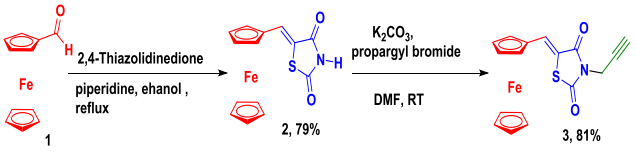
A Facile Ni@Sio$_2$catalyzed One-Pot Synthesis of Spirooxindole Fused Pyrazolo Pyridine Derivatives and their Antimicrobial Studies

An efficient one-pot synthesis of spiro [indoline-3, 4'pyrazolo [3,4-b] pyridine] derivatives using Ni@SiO_2 catalyst via three-component reaction of isatin, 5-amino-3-methylpyrazole, and malononitrile in ethanol is described. This green protocol has certain advantages such as multicomponent one pot procedure, good yield within shorter reaction time, a simple work-up coupled with recovery and reusability of solid acid heterogeneous catalyst. The characterization of the catalyst was performed by X-ray diffraction (XRD) study, surface area analysis (BET), transmission electron microscopy (TEM), scanning electron microscopy (SEM), XPS, UV-DRS and EDX. The new compounds were tested for in-vitro anti-microbial activity. (*Synth. Commun.*, **2018**, 48, 255)

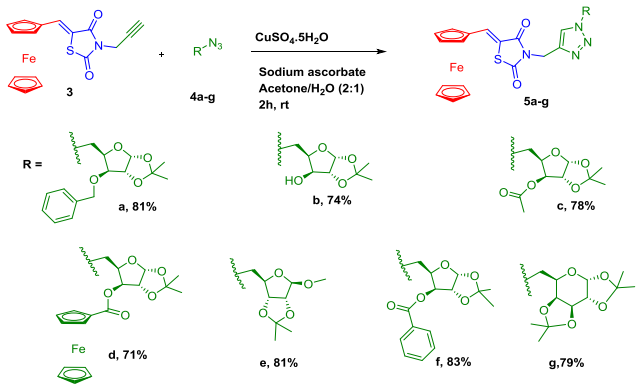


2,4-Thiazolidinedione as a Bioactive Linker for Ferrocenyl Sugar–Triazole Conjugates: Synthesis, Characterization and Biological Properties

A new series of ferrocenyl sugar triazole conjugates derived from D-Xylose, D-Ribose and D-Galactose linked via a 2,4-thiazolidinedione moiety has been prepared. A facile 1,3-dipolar-Huisgen coupling reaction of the respective sugar azides with the ferrocenyl 2,4-thiazolidinedione alkyne unit gave the corresponding conjugates. These conjugates have been characterized by various spectroscopic techniques including UV-visible spectroscopy. The electrochemical analysis exhibited one-electron quasi reversible oxidation behaviour. The single crystal X-ray diffraction study on two of the compounds 2 and 3 was performed to determine their structures. The 2,4-thiazolidinedione linked ferrocenyl sugar triazole conjugates exhibited moderate to good antibacterial and antidiabetic activities. (*Eur. J. Inorg. Chem*., **2018**, 1571)



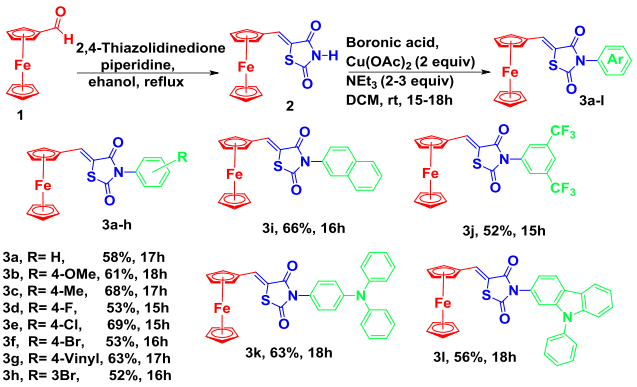
Synthesis of ferrocenyl 2,4-thiaolidinedione alkyne



Synthesis of ferrocenyl2, 4-thiazolidinedione - triazole sugar (5a-g)

N-Arylation of Ferrocenyl 2,4-Thiazolidinedione Conjugates via Copper-Catalysed Chan-Lam Cross Coupling Reaction with Aryl Boronic Acids and their Optoelectronic Properties

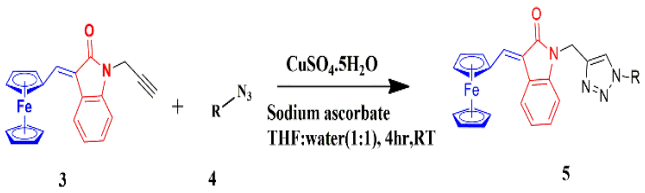
A coppercatalyzed Chan-Lam type N-arylation protocol has been applied to achieve moderate to good yields of N-arylated ferrocenyl 2,4 thiazolidinedione conjugates. A general and mild strategy has been developed for the cross-coupling of arylboronic acids and ferrocenyl 2,4 thiazoli dinedione conjugates. This coupling was achieved through the use of copper(II) acetate and screened for different bases, solvents and a variety of arylboronic acids including electron-withdrawing and electron-donating groups. All the new compounds were obtained as red crystalline solids. The solid state structure of (3b) was established by single crystal X-ray diffraction analysis. The all compounds were fully characterized by ^{1}H and ^{13}CNMR, FT-IR, ESI mass and UV-visible spectroscopy. Electrochemical studies (CV) exhibited reversible one-electron oxidation and the conjugates were found to be stable in organic solvents. (*New J. Chem.*, **2018**, 42, 12587)



Synthesis of ferrocenyl 2,4-thiazolidinedione N-aryl conjugates (3a-l)

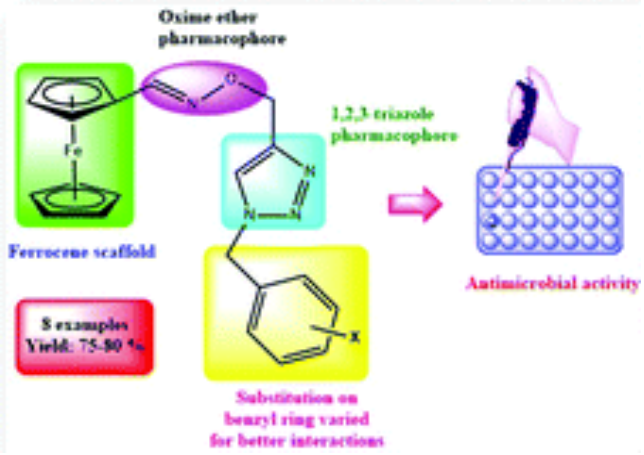
1,2, 3-Triazole Derivatives of 3-Ferrocenylidene-2-Oxindole: Synthesis, Characterization, Electro chemical and Antimicrobial Evaluation

A series of bioactive triazole linked benzyl, aryl, sugar and aliphatic conjugates of 3-ferrocenylidene-oxindole have been synthesized. A facile 1,3-dipolar-Huisgen coupling reaction of the respective aryl and sugar azides with the 3-ferrocenylidene-oxindole N-propargyl moiety (3) gave the corresponding conjugates (5a-n). All the newly synthesized compounds (5a-n) were characterized by ^{1}H NMR, ^{13}C NMR, HRMS, FT-IR spectroscopy and elemental analysis. The UV-vis and electrochemical studies of these compounds were performed in DMSO solutions. The single crystal X-ray diffraction study of the compound (3) was performed to determine its structure. These compounds exhibited moderate to good antimicrobial activity against gram positive and gram negative strains. *(Appl. Organomet. Chem.*, **2019**, 33, e4817)



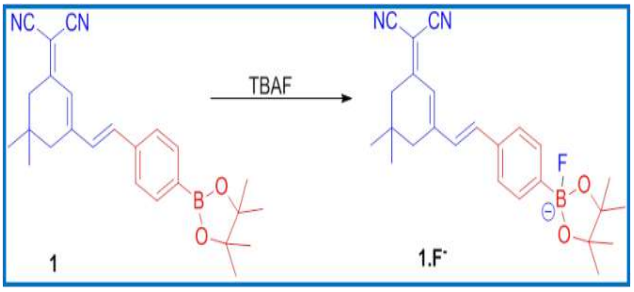
Synthesis, Characterization and Antimicrobial Evaluation of Ferrocene–Oxime Ether Benzyl 1*H*-1,2,3-Triazole Hybrids

A series of ferrocene–oxime ether benzyl 1H-1,2,3 triazole hybrids has been synthesized by employing Cu(I) catalyzedazide–alkyne [3+2] cycloaddition reaction and their antibacterial and antifungal activities are reported. (*New J. Chem.*, **2019**, 43, 8341)



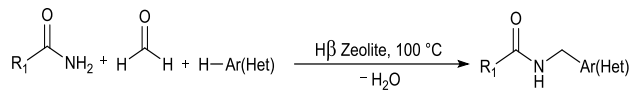
Isophorone-Boronate Ester: A Simple Chemosensor for Opticaldetection of Fluoride Anion

A highly selective isophorone-boronate ester based chemosensor, (1), having a dicyanovinyl moiety as a convenient colorimetric probe, has been designed. Different types of anionic analyte such as CH_3COO^-, ClO_4^-, Cl^-, F^-, PF_6^-, Br^- and HSO_4^- were tested and among them only highly nucleophilic F^- anion displayed significant response towards the sensor. Addition of the fluoride anion across the boron atom disrupts the π-conjugation thereby shifts the absorption wavelength towards the redshift region due to the decrease in the HOMO-LUMO energy gap and a colour change from yellow to blue is observed under visible light condition. The detection limit of this probe was calculated to be 3.25×10^{-8} M for fluoride anion. The binding constants and the detection limits of the sensor were calculated using absorption titration studies. The silica gel TLC strips dip-coated by the chemosensor (1) revealed a colour change from yellow to brick red to naked eye. (*Appl. Organomet. Chem.*, **2018,** 32, e4688)



Three-Component Synthesis of Amido methylarenes and -Heteroarenes over Hβ Zeolite under Solvent-Free Conditions

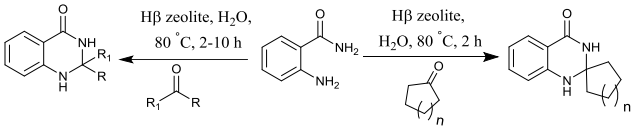
A highly efficient, and eco-friendly protocol has been developed for the synthesis of amidomethylarenes and -heteroarenes via one-pot three-component coupling reaction of amides, aldehydes and (hetero) arenes over heterogeneous catalyst (Hβ zeolite) in solvent-free conditions. The scope and limitations of this catalytic process are demonstrated with various amides and arenes, the corresponding amidoalkyl atedarene products were obtained in moderate to excellent yields. The preliminary mechanistic insight (control experiments) suggest that bisamide and/ or N-(hydroxymethyl)benzamide were found to be probable intermediates in this reaction. The noteworthy features of the present method are the use of non-hazardous and reusable catalysts, broad substrate scope, absence of solvent, higher yields of the desired products, high atom economy (only water as by-product), simple work-up procedure and mild reaction conditions, which make it an inexpensive and environmentally benign protocol. *(Catal. Commun.*, **2018**, 105, 20)



R1= Aryl/Akyl/
Hetero aryl

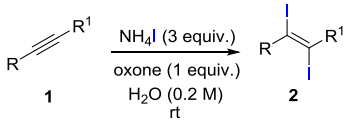
Synthesis of 2,3-Dihydroquinazolin-4(1H)-Ones from Anthranilamide and Ketones over Hβ Zeolite in Aqueous Media

A green and straightforward method for the synthesis of 2,3-dihydroquinazolin-4(1H)-ones involving the condensation of anthranilamide with ketones over Hβ zeolite in aqueous media was successfully developed. Broad substrate scope, water as a solvent, use of non-hazardous and reusable catalysts, higher yields of the desired products, and simple workup procedures are prominent advantages of this catalytic strategy. These findings highlight the potential of this protocol as an inexpensive and environmentally benign method. *(Synth. Commun.*, **2018**, 48, 2866)



An Aqueous Media-Controlled Stereospecific Oxidative Iodination of Alkynes: An Efficient Access to (E)-Diiodoalkene Derivatives

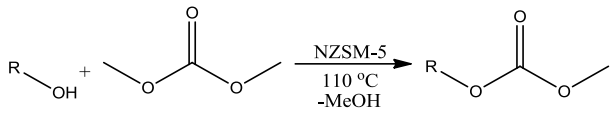
A new and versatile approach for the synthesis of trans-diiodoalkenes from alkynes using cheap, air stable and non-toxic reagents in aqueous media has been developed. This protocol is tolerant of various functional groups, provides a broad range of vicinal diiodoalkenes with exceptional E-selectivity under mild conditions. The scope of the reaction has been demonstrated with various alkynes such as aromatic, aliphatic and hetero aromatic alkynes. This method operates under mild conditions and employs cheap, commercially available and non-toxic inorganic salts as reagents and water as a green solvent. (*New J. Chem.*, **2018**, 42, 17879)



- *single product*
- *easy post-reaction purification*
- *broad scope*

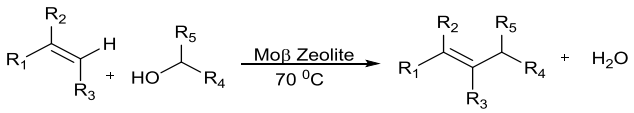
New Synthesis of Non-symmetrical Alkyl Carbonates from Alcohols and DMC over Nanocrystalline ZSM-5 Zeolite

A novel heterogeneous acid (nanocrystalline ZSM-5) catalyzed carboxymethylation of alcohols to non-symmetrical alkyl carbonates using DMC has been realized. Nanocrystalline ZSM-5 (NZSM-5) with crystal size of 20-30 nm was synthesized by hydrothermal crystallization. The present protocol provides an attractive approach to a variety of non-symmetrical alkyl carbonates in high yields. This method broadens the series of possible utilization for DMC in green chemistry. (*GREEN CHEM.*, **2019**, 21, 2938)



Synthesis of Internal Olefins by Direct Coupling of Alcohols and Olefins over Moβ Zeolite

An efficient and novel Moβ zeolite catalyzed sp^2-sp^3 C-C bond development reaction over the direct coupling of alcohols and alkenes has been performed in solvent free environment. The current method gives an attractive access to a wide variety of polysubstituted alkenes in good to excellent yields. *(Cataly. Commun.*, **2019**, 123, 114)

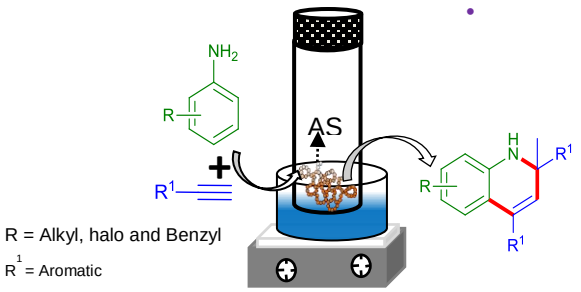


A Heterogeneous Catalytic and Solvent-Free Approach to 1,2-Dihydroquinoline Derivatives from Aromatic Amines and Alkynes by Tandem Hydroarylation-Hydroamination

Mesoporous aluminosilicate (ASM) catalyst-induced one-step synthesis of substituted dihydroquinolines through a hydroarylation/hydroamination cascade reaction under solvent-free conditions has been developed. A sol-gel method was utilized to prepare the ASM catalyst using tetraethyl orthosilicate

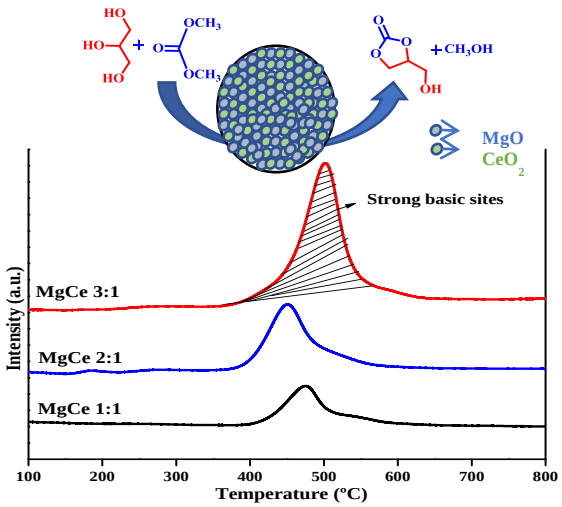
(TEOS) and aluminum nitrate ($Al(NO_3)_3.9H_2O$). The probability and limitations of the catalytic route are presented with a variety of aromatic amines and alkynes. The catalytic protocol, utilizing simple starting materials and a heterogeneous catalyst in a clean reaction environment, is considered an alternative and economically viable route to synthesize a wide range of 1,2-dihydroquinoline derivatives. *DOI:org/10.1016/j.catcom.2019.105888)*

- Solvent-free conditions
- Cascade reaction (tandem)
- Heterogeneous catalyst
- 22 entries, up to 90% yield



Biomass Utilization: Glycerol to Value Added Chemicals

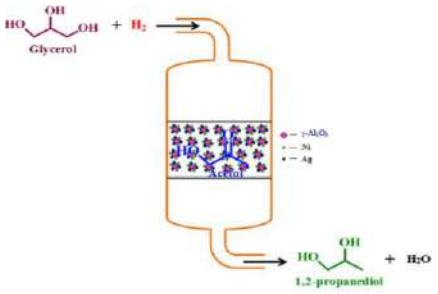
Glycerol, a byproduct in the preparation of biodiesel is used as feedstock to prepare different value added chemicals like 1,2-propanediol, glycerol carbonate and glycidol.



Glycerol to Glycerol Carbonate: Selective synthesis of glycerol carbonate from bio glycerol using urea or dimethyl carbonate as carbonating agent is taken up. In this work we developed both acid and base mixed oxide catalysts. MgO based mixed oxide catalysts are developed for the selective synthesis of glycerol carbonate from bio-glycerol. We established a continuous process to prepare glycerol carbonate using glycerol and dimethyl carbonate. (*Mol. Cataly.*, **2018**, 427, 135)

Glycerol to 1,2-Propanediol

Selective hydrogenolysis of glycerol is carried over Ni and Cu based supported catalysts for the preparation of ,2-propanediol. The activity of the catalysts depends on metal surface area, metal particle size and acidity of the support. Ni and Cu based catalysts are designed and studied for the preparation of 1,2-propoanediol and the mechanistic aspects of the catalysts for hydrogenolysis reaction is studied in detail. A continuous process in place of traditional batch mode hydrogenolyss is explored and obtained better activity towards the preparation of 1,2-pronediol. *(Cataly. Green Chem. Engg.*, **2018,** 1, 79)

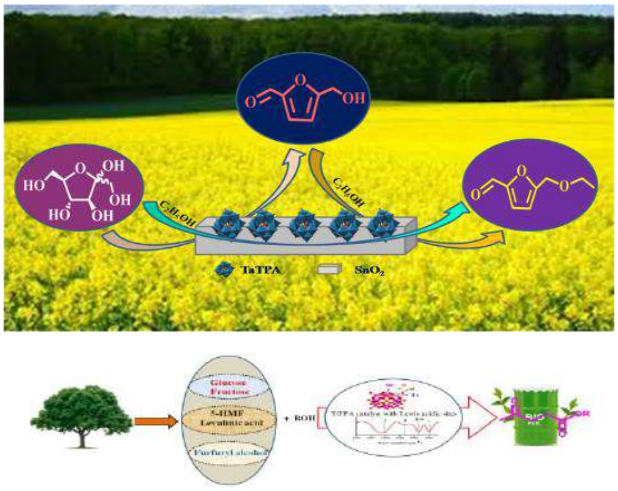


Biomass to Chemicals: Preparation of Fuel/Fuel Additives

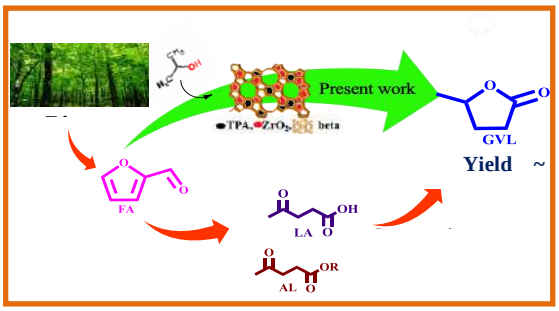
Biomass derived platform chemicals like carbohydrates, 5-hydroxyul methyl furfural (5-HMF) and furfural are converted to different value added chemicals. Fuels/fuel additives by employing different solid acid catalysts. A series of modified heteropoly acid catalysts are designed and used to prepares these chemicals by different processes like

hydrolysis, esterification, etherification, catalytic transfer hydrogenation etc.

Tungstophosphoric (TPA) supported on mesoporous usniobiu moxophosphate (NbP) and Ta exchanged TPA supported on tin oxide catalysts were prepared with different loadings. The synthesized materials employed as heterogeneous solid acid catalysts for selective etherification of 5-hydroxymethylfurfural to 5-ethoxymethylfurfural (EMF) and also directly from fructose to EMF.The activity of the catalysts depends on amount of TPA dispersed on NbP or content of exchangeable Ta in TA, which directs the overall acidity of the catalyst. The conversion and yields were also depend on the reaction temperature, reaction time and amount of catalyst. The catalysts are easy to recover and reusable without any loss in activity. *(Mol. Cataly.*, **2018,** 448, 108; *Cataly. Today*, **2018**, 309, 269; *Cataly. Today*, **2019**, 325, 53)

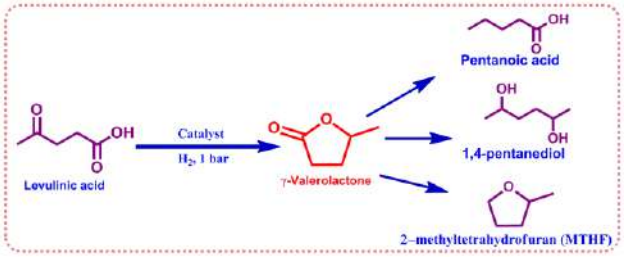


One pot selective conversion of furfural to γ-valerolactone: A series of metal oxide and tungsto phosphoric acid (TPA) supported on β-zeolite catalysts were prepared and evaluated for the one pot selective conversion of furfural (FA) to γ-valerolactone (GVL) using transfer hydrogenation approach. The yield of GVL is guided by metal oxide present in catalyst. The presence of Bronsted acidic TPA is essential for the conversion of intermediate FAL/FE to alkyl levulinates step. The presence of Lewis acidic sites and base sites in the catalysts was essential for efficient catalytic transfer hydrogenation to realize more GVL yield. *(Mol. Cataly.*, **2019**, 466, 52)



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. A: Gen.*, **2018**, 550, 142; *J. Phys. Chem. C*, **2018**, 122, 19670; *Cataly. Today*, **2019**, 325, 68)



Possible levulinic acid conversion strategies

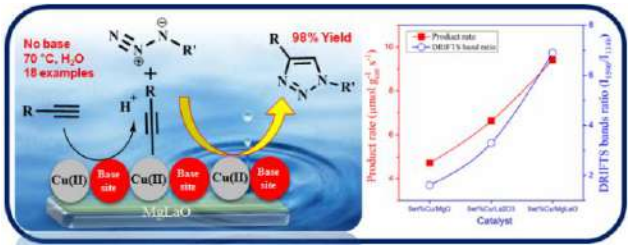
Catalytic CH_4 Decomposition to Produce Co_x Free Hydrogen over Ni-Based Catalysts

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

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 highquality carbon nano fibers/nanotubes over a decade. (*Energy Fuels*, **2018**, 32, 4008 & **2019**, 12, 12656)

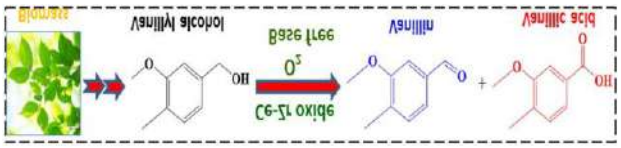
Strong Basic Sites are Selective for Regioselective Synthesis of Substituted Triazoles

Surface active sites examined by HCOOH-DRIFTS and N_2O titration techniques. MgLaO identified as a suitable support for Cu in Click reaction in the absence of base. (*Mol. Catal.*, **2018**, 445, 43 & **2019**, 476, 110523; *Ind. J. Chem. A*, **2018**, 57A, 1106)



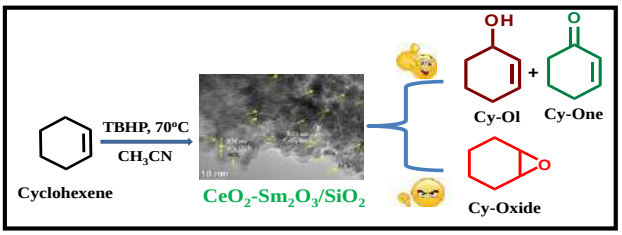
Selective Aerobic Oxidation of Vanillyl Alcohol to Vanillin Catalysed by Nano-Structured Ce-Zr-O Solid Solutions

A series of Ce_{1-x}–$ZrxO_2$ − δ (x = 0.2, 0.5, and 0.8) mixed oxides were explored for selective oxidation of vanillyl alcohol employing O_2 in liquid phase. the $Ce0.8Zr0.2O_2$ combination exhibited a high catalytic activity with ~ 98% conversion and ~ 99% selectivity to vanillin. Smaller crystallite size, large BET surface area, more number of oxygen vacancies, improved redox properties, and strong synergetic interaction are found to be the key factors to promote the oxidation ability of $Ce0.8Zr0.2O_2$ catalysts towards vanillyl alcohol oxidation. (*Cataly. Lett.*, **2019**, 149, 533)



Selective Allylic Oxidation of Cyclohexene over a Novel Nanostructured Ceo_2-Sm_2O_3/Sio_2 Catalyst

CeO_2, CeO_2/SiO_2, and CeO_2-Sm_2O_3/SiO_2 catalysts are explored for liquid phase selective allylic oxidation of cyclohexene using TBHP and acetonitrile as oxidant and solvent respectively. Allylic products such as 2-cyclohexene-1-ol and 2-cyclohexene-1-one are crucial intermediates in the manufacture of spices, medication, pesticides, and insect pheromones. The achieved cyclohexene conversions over developed catalysts are as follows: CeO_2-Sm_2O_3/SiO_2>CeO_2/SiO_2> CeO_2. Irrespective of the catalyst tested, a high selectivity towards allylic products, namely, 2-cyclohexen-1-one and 2-cyclohexen-1-ol were found compared to epoxidation product (cyclohexene oxide). *(Re. Chem. Intermed.*, **2018**, 44, 6151)



Metal-Free Cross-Dehydrogenative Coupling Approach for C-H Bond Functionalization of 2-Phenyl Pyridine Derivatives in Water

Cross-dehydrogenative coupling (CDC) has emerged as one of the most efficient and atom economical strategies for direct conversion of two different C-H bonds into C-C bonds. We have developed a simple $K_2S_2O_8$-mediated C-H bond functionalization of 2-phenyl pyridines (C-2 position) with ethers involving C(sp2)-C(sp3) cross-dehydrogenative coupling. The reaction does not require metal catalysts nor visible light and operates under mild conditions. Furthermore, the protocol is easily scalable and extendable to a wide range of pyridine derivatives. (*Heteroatom Chem.*, **2018**)

Ru Nanoparticle-Decorated Porous Organic Network for Direct Hydrodeoxygenation of Long Chain Fatty Acids to Alkanes

We present the design, synthesis, and characterization of a new porous organic network (Tp-PON) through acid-catalyzed condensation of 1,3,5-triformylphloroglucinol (Tp) and triphenyl amine (TPA). Ru^0 nanoparticles are successfully fabricated at the porous surface of Tp-PON to obtain a novel catalytic system Ru@TpPON, which exhibits

excellent catalytic performance together with outstanding stability for the hydrodeoxygenation of various vegetable oils to long-chain alkanes in water, and thus TpPON has wide potential for large-scale biodiesel production from renewable resources. (*ACS Sust. Chem. Engg.*, **2018**, 6, 1610)

Cu–Pd Bimetallic Nanoalloy Anchored on a N-Rich Porous Organic Polymer for High-Performance Hydrodeoxygenation of Biomass-Derived Vanillin

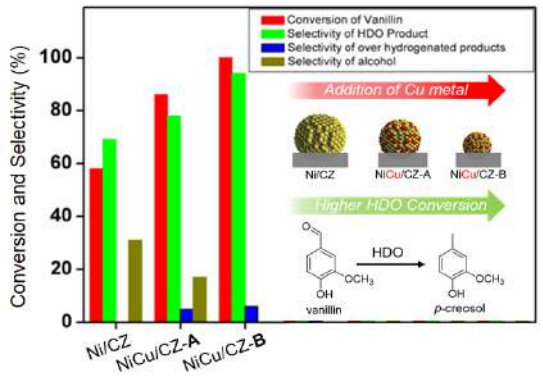
In this present investigation, we have synthesized a novel nanocatalyst based on a bimetallic CuPd nanoalloy anchored on a porous organic polymer (BBA- 1) and related Cu and Pd based catalysts with varying metallic molar ratios by a polyol method using $NaBH_4$ as a strong reducing agent. In particular, bimetallic Pd–Cu nanocatalysts composed of Cu_3Pd@BBA-1 exhibited the highest catalytic activity towards a vanillin conversion of 99.3% with exclusive selectivity (93.6%) for the hydrogenolysis product 2-methoxy- 4-methylphenol. Detailed characterization techniques including XPS and XAFS analysis experimentally evidenced that the superior activity of the bimetallic Cu–Pd catalyst compared with monometallic counterparts could be attributed to the intrinsic synergistic effects caused by the modulation of the electronic structure involved in the Cu–Pd bimetallic interfaces. *(Cataly. Sci. Technol.*, **2018**, 8, 2195)

Unraveling the Structural Properties and Reactivity Trends of Cu–Ni Bimetallic Nanoalloy Catalysts for Biomass-Derived Levulinic Acid Hydrogenation

We have developed a series of silica nanosphere supported CuNi bimetallic nanoalloy catalysts via solvothermal, impregnation and co-precipitation methods and evaluated their catalytic performance for thehydrogenation of levulinic acid, a key platform molecule in many biorefinery schemes, into γ-valerolactone.The resultant catalyst as developed by animpregnation method presents enhanced catalytic performance compared with other catalysts,providing 99.3% conversion of levulinic acid with 96.8% selectivity of γ-valerolactone in 13 h at 120^0C. Comparing catalytic experiments between bimetallic Cu–Ni and monometallic Cu catalysts demonstrated that the outstandingly improved catalyst activity and stability could be ascribed to themodulation of the electronic properties of the active sites and inhibition of metal particles with theintroduction of another metal promoter, with good recyclability after ten recycles without notable loss inthe activity. *(Sust. Energy Fuels*, **2018**, 2, 1516)

Design of Efficient Noble Metal Free Copper-Promoted Nickel-Ceria- Zirconia Nano catalyst for Bio-Fuel Upgrading

A new series of noble metal free bimetallic Cu@Ni supported ceria-zirconia catalysts (Cu@Ni/CZ) has been developed with various Cu/Ni ratios by a simple co-precipitation/impregnation method. Aqueous-phase hydrodeoxygenation (HDO) of vanillin a typical compound of lignin-derived bio-oil, in promoting biomass refining was carried out to investigate catalytic performances under 25 bar of H_2 pressure at 160°C. It was found that 15 wt% Cu on Ni/CZ (Cu@Ni/CZ@B) nanocomposite enhanced activity significantly in comparison with other bimetallic or monometallic catalysts, exhibiting ~98% of vanillin conversion and ~94% of selectivity toward 2-methoxy-4-methylphenol as a desired product. The superior catalytic performance with improved stability were explained by synergistic effects at the interfaces of each species, in which electron interactions between Ni, Cu, and ceria-zirconia support generated novel active sites. (*ChemistrySelect*, **2018**, 3, 6174)



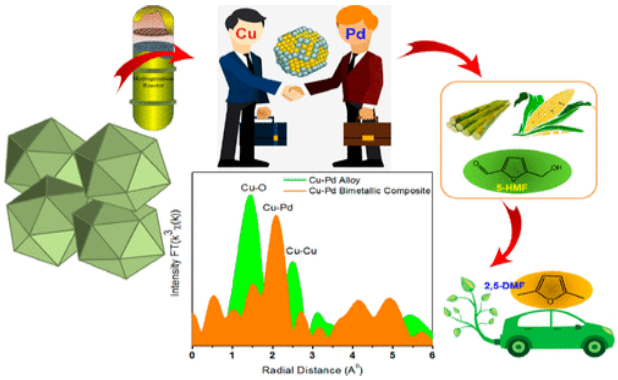
Metal–Organic-Framework Derived Co–Pd Bond is Preferred over Fe–Pd for Reductive Upgrading of Furfural to Tetrahydrofurfuryl Alcohol

Combined noble-transition metal catalysts have been used to produce a wide range of important nonpetroleum-based chemicals from biomass-derived furfural (as a platform molecule) and have garnered colossal research interest due to the urgent demand for sustainable and clean fuels. Herein, we report the palladium-modified metal organic-framework (MOF) assisted preparation of $PdCo_3O_4$ and $PdFe_3O_4$ nanoparticles encapsulated in a graphitic N-doped carbon (NC) matrix via facile in situ thermolysis. This provides a change in selectivity with superior catalytic activity for the reductive upgrading of biomassderived furfural (FA). Under the optimized reaction conditions, the newly designed $PdCo_3O_4$@NC catalyst exhibited highly efficient catalytic performance in the hydrogenation of furfural, providing 100% furfural conversion with 95% yield of tetrahydrofurfuryl alcohol (THFAL). (*Dalton Transact.*, **2019**, 48, 8791)

Integration of Interfacial and Alloy Effects to Modulate Catalytic Performance of Metal–Organic-Framework-Derived Cu–Pd Nano crystals toward Hydrogenolysis of 5-Hydroxymethylfurfural

Selective formation of 2,5-dimethylfuran (DMF) by hydrogenolysis of lignocellulosic biomass-derived 5-hydroxymethylfurfural (HMF) is highly desirable for renewable liquid biofuel production. Here we have synthesized Cu–Pd bimetallic nanoparticles embedded in carbon matrix (Cu–Pd@C) by simple pyrolysis of Pd-impregnated Cu-based metal–organic frameworks (MOFs) followed by conventional hydrogenation route. It was found that Cu–Pd@C-B (solid–gas-phase hydrogenation route) with Cu–Pd bimetallic alloying exhibited brilliant catalytic performance at 120 °C under 15 bar H2 pressure to produce liquid DMF biofuel with 96.5% yield from HMF as compared with the Cu–Pd@C-A catalyst

(liquid phase hydrogenation route), which gave 46.4% yield under the same conditions. (*ACS Sust. Chem. Engg.*, **2019**, 7, 12, 10349)

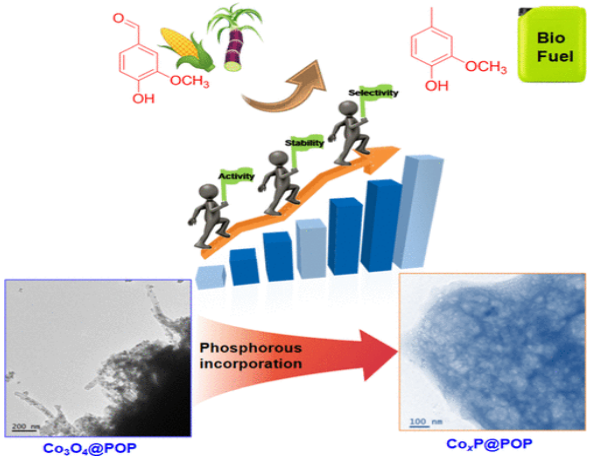


Interface Engineering of Graphene-Supported Cu Nanoparticles Encapsulated by Mesoporous Silica for Size Dependent Catalytic Oxidative Coupling of Aromatic Amines

In this study, graphene nanosheet-supported ultrafine Cu nanoparticles (NPs) encapsulated with thin mesoporous silica (Cu−GO@m- SiO2) materials are fabricated with particle sizes ranging from 60 to 7.8 nm and are systematically investigated for the oxidative coupling of amines to produce biologically and pharmaceutically important imine derivatives. Catalytic activity remarkably increased from 76.5% conversion of benzyl amine for 60 nm NPs to 99.3% conversion and exclusive selectivity of N-benzylidene-1-phenylmethanamine for 7.8 nm NPs. The superior catalytic performance along with the outstanding catalyst stability of newly designed catalysts are attributed to the easy diffusion of organic molecules through the porous channel of mesoporous SiO2 layers, which not only restricts the restacking of the graphene nanosheets but also prevents the sintering and leaching of metal NPs to an extreme extent through the nanoconfinement effect. Density functional theory calculations were performed to shed light on the reaction mechanism and to give insight into the trend of catalytic activity observed. *(ACS Appl. Mat. Interf.*, **2019**, 11, 11722)

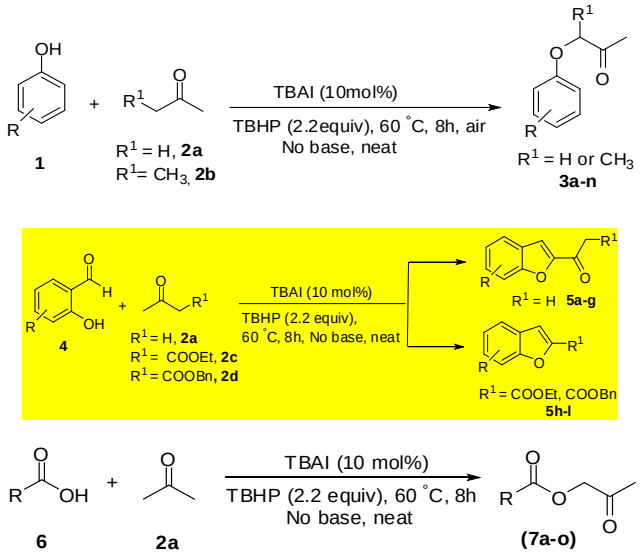
Porous Organic Polymer-Driven Evolution of High-Performance Cobalt Phosphide Hybrid Nanosheets as Vanillin Hydrodeoxygenation Catalyst

Hydrodeoxygenation (HDO) is a promising route for the upgrading of bio-oils to eco-friendly biofuel produced from lignocellulose. Herein, we report the sequential synthesis of a hybrid nanocatalystCo_xP@POP, where substoichiometricCo_xP nanoparticles are distributed in a porous organic polymer (POP) via solid-state phosphidation of the Co_3O_4@POP nanohybrid system. We also explored the catalytic activity of the above two nanohybrids toward the HDO of vanillin, a typical compound of lignin-derived bio-oil to 2-methoxy-4-methylphenol, which is a promising future biofuel. The Co_xP@POP exhibited superior catalytic activity and selectivity toward desired product with improved stability compared to the Co_3O_4@POP. *(ACS Appl. Mat. Interf.*, **2019,** 11, 27, 24140)



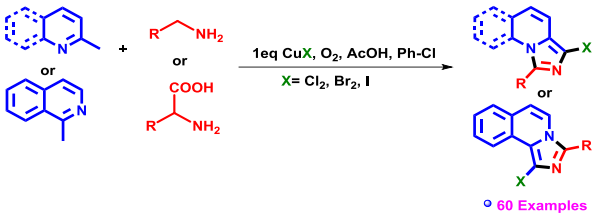
TBAI/TBHP Mediated Oxidative Cross Coupling of Ketones with Phenols and Carboxylic Acids: Direct access to Benzofurans

TBAI/TBHP mediated oxidative cross coupling of phenols and carboxylic acids with ketones has been reported under metal-free, base free, solvent free conditions enabling environmentally benign synthesis of aryloxyketones, acyloxy ketones and benzofurans. Phenoxyketones and acyloxylcarbonyl compounds were synthesized in good to high yields, where as benzofurans were synthesiszed in moderate yields. This method is operationally simple, works under mild conditions, using commercially available as well as inexpensive TBAI and an oxidant TBHP. (Tetrahedron Lett., **2018**, 59, 33)



Direct Access to Halogenated Fused Imidazo[1,5-a] N-heteroaromatics through Copper-Promoted Double Oxidative C–H Amination and Halogenation

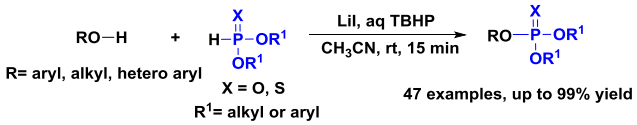
An aerobic copper promoted double oxidative C-H amination and 50alogenations tandem reaction of 2-methylazarenes with aliphatic amines or amino acids have been developed, by employing copper salts as catalysts as well as halogen sources and molecular oxygen as a sole oxidant. This protocol is operationally simple and enables the direct access to functionalized fused imidazoles in one pot operation with good functional group tolerance. The synthetic utility of the method has been tested for Suzuki cross coupling reaction and the product obtained in good yield. (*Eur. J. Org. Chem.*, **2018**, 3036)



- Good functional group tolerance
- Broad substrate scope
- Yields upto 85%
- Well tolerated simple aliphatic amines
- Extended to 2-methyl pyridine derivatives
- Phenyl glycine as an aliphatic amine source
- Gram scale applicability

LiI/TBHP Mediated Dehydrogenative Cross Coupling between Phenol Derivatives and H-Phosphonates: Direct Access for the Synthesis of Organophosphates

An efficient and mild method for the direct phosphorylation of phenol derivatives has been reported by LiI/TBHP mediated dehydrogenative cross coupling reaction. Furthermore, this method is extended to the synthesis of organopesticides such as paraoxon, cyanophos and methyl parathion. The phosphorylation of hydroxylated napthyls and heteroarene derivatives also been achieved using this method. (*Eur. J. Org. Chem.*, **2019**, 7463)

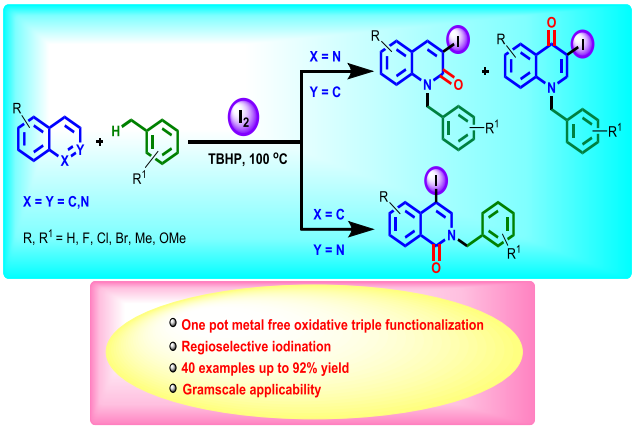


- broad substrate scope and mild conditions
- base free and no additives
- quick reaction time

Metal Free, One-Pot Oxidative Triple Functionalization of Azaarenes with Methyl Arenes Mediated by Molecular Iodine/TBHP: Synthesis of 1-Benzyl-3-Iodoquinolinones and 2-Benzyl-4-Iodoisoquinolin-1(2H)-Ones

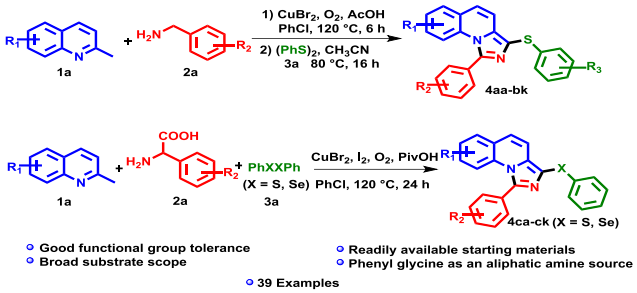
An efficient metal free one-pot triple functionalization of azaarenes has been developed via a successive regioselective iodination, N-benzylation

and amidation by using readily available methylarenes in presence of molecular iodine and TBHP. This method avoids the use of expensive noble metal catalysts and multi-step conversions. Moreover, we have shown the synthetic utility of the iodo functionality with traditional cross-coupling reactions (like Suzuki, Heck and Sonogashira) and the corresponding products were obtained in good yields. (*Asian J. Org. Chem.*, **2019**, 8, 2162)



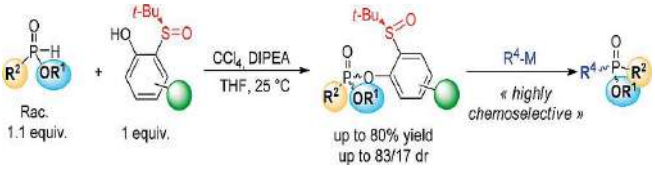
One-Pot Synthesis of 3-Sulfenyl/ Selenylimidazo [1,5-a]quinolines from 2-Methylquinolines, Aliphatic amines/ Amino acids and Dichalco genides

One-pot sulfenylation/selenylation reaction have been developed to access 3-sulfenyl/ selenyl imidazo[1,5-a]quinolines from 2-methyl quinolines, aliphatic amines/ aminoacids and dichalcogenides. This developed method gives direct access to 3-chalcogenylimidazo[1,5-a]quinolines in moderate to good yields with good functional group tolerance from readily available starting materials. Moreover, this protocol can avoid the prior synthesis of fused imidazoles as starting materials for the synthesis of 3-chalcogenylimidazo[1,5-a]quinolines. Further, we have shown synthetic utility of 3-sulfenyl imidazo[1,5-a]quinolines with m-CPBA to afford corresponding sulfones in good to excellent yields. *(Eur. J. Org. Chem.*, **2019**, 6122)



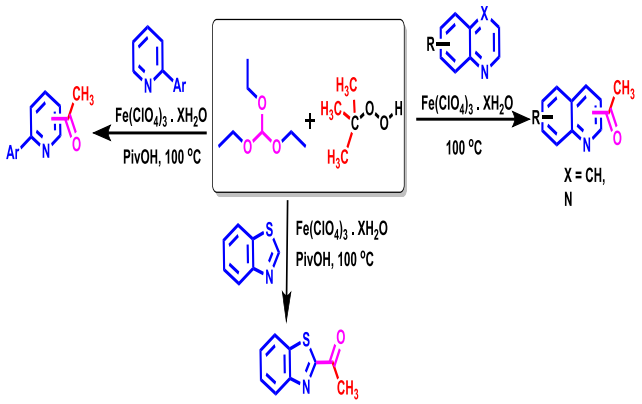
P-Stereogenic Phosphonates via Dynamic Kinetic Resolution: A Route towards Enantiopure Tertiary Phosphine Oxides

Asymmetric synthesis of P-stereogenic phosphonates presents a great challenge. Following this target we disclose herein a DKR strategy towards the O–P coupling reaction between an easily accessible enantiopure phenol bearing a chiral sulfinyl auxiliary and a commercially available or easily accessible racemic H-phosphinate. Although moderate to high chiral induction is achieved, several diastereopure phosphonates can be afforded either by crystallization or flash chromatography. Thus accessed optically pure P-stereogenic precursors may be used as appealing building blocks to rapidly assembly original privileged scaffolds as illustrated via the synthesis of a chiral ligand such as PAMPO. *(Eur. J. Org. Chem.*, **2019**, 7836)



Iron Catalyzed Minisci Type Acetylation of N-Heteroarenes Mediated by $CH(OEt)_3$/TBHP

Iron catalysed acetylation of electron deficient N-heteroareneshas been reported using triethylortho formate/TBHP as a novel, robust and inexpensive acetyl source. This new method is successfully applied for the acetylation of quinolines, isoquinoline, quinoxalines, arylpyridines, bipyridines and benzothiazole. *(Eur. J. Org. Chem.*, **2019**, 1815)



Copper-Catalyzed C-H activation

Activation of C-H bonds and their application in cross coupling chemistry has received a wider interest in recent years. The conventional strategy in cross coupling reaction involves the pre-functionalization step of coupling reactants such as organic halides, pseudohalides and organometallic reagents. The C-H activation facilitates a simple and straight forward approach devoid of pre-functionalization step. Overview of our group work with the collaborators in this area is summarized and manuscript is under view process. (*Chem. Rec.* **2019**, 19, 1302)

APPLIED RESEARCH

Process Development for Paracetamol using Acetic Acid as Acetylating Agent (*Sponsored by M/s Bharat Chemical, Mumbai*)

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 present process for acylation of para-aminophenol (PAP) is carried out using acetic acid and toluene as solvent. The demonstration at 500 mL size reactor is completed.

Process Development for Lily Aldehyde (Condensation and Hydrogenation process) at 100g Scale (*Sponsored by M/s VOL, Mumbai*)

Lily aldehyde is commonly used as a perfume in cosmetic preparations and laundry powders. The commonly adopted synthetic procedure for the preparation of lilial is aldol condensation of two aldehydes followed by hydrogenation. The present process involves the improvement in conversion and yields of aldol condensation as well as in hydrogenation process. The design for commercial scale of the process is under progress.

Process Development for Avobenzone using Methyl Ester of Para-Tert Butyl Benzoic Acid and Para-Methoxy Acetophenone (*Sponsored by M/s VOL, Mumbai*)

The base catalysed condensation reaction ofmethyl ester of para-tert butyl benzoic acid and para-methoxy acetophenone is known to produce avobenzone. Avobenzone is known as an active ingredient in preparation of sun screen products. The present process involves the application of inexpensive base and achieves improvement in conversion and yields of aldol condensation as well as in hydrogenation process. The design for commercial scale of the process is under progress.

Process Development for Para Methoxy Acetophenone from Anisole (Pilot Scale Reactor Studies in Progress) (*Sponsored by M/s VOL, Mumbai*)

para-methoxy acetophenone (PMAP) is widely used as a fragrance, and a flavouring in food. The preparation of the PMAP is carried out in batch mode using heterogeneous catalysts. The processes suffer from high temperatures with low selectivity towards PMAP. The process developed by IICT is a continuous process with exclusive selectivity of PMAP with high conversion. The catalyst used is in-expensive catalyst.

Process Development and Data Generation for the Oxidation of Toluene to Benzaldehyde (*Sponsored by M/s VOL, Mumbai*)

The air oxidation of toluene is the source of most of the world's synthetic benzaldehyde. Both vapour and liquid-phase air oxidation processes have been used. IICT has developed catalytic route for the oxidation of toluene using air as an oxidant and recyclable catalyst with 65% conversion and 35% selectivity. The demonstration of this process at bench scale is completed and design for the intermediate scale (semi pilot scale) is submitted to client.

Dicyanadiamide (DCDA)(To Develop a Process for Producing Dicyanadiamide through the Calcium Carbide Route, Reaction Parameters Optimization)

DCDA is the raw material for Metformin drug, primary drug for diabetes. DCDA is not manufactured in India and being imported mainly from China, the other major producers are U.S.A., Germany, Canada and Japan. The calcium carbide to calcium cyanamide route is world-wide accepted route for the commercial production of DCDA. Calcium cyanamide is the main starting material for the production of dicyandiamide and is also not produced in India.

To develop the process for DCDA under MAKE IN INDIA flagship program and to reduce the dependency on Chinese supplier, Research Council Chairman suggested to establish two independent routes for the production of DCDA at 500 gm scale to CSIR-IICT, Hyderabad and CSIR-NCL, Pune.

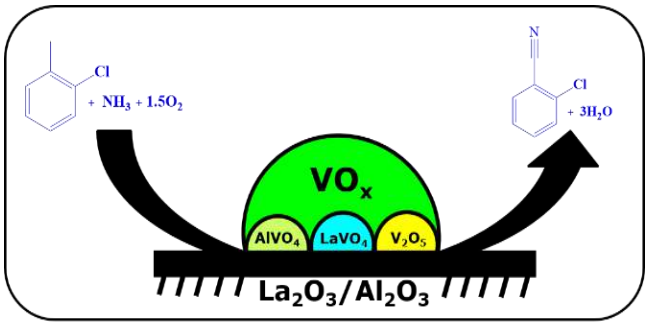
Process Development for Dibromomethane from bromomethane (*Sponsored by M/s Intech Organics, Vadodara*)

Dibromomethane is used as a solvent, gauge fluid, and in organic synthesis. It is a convenient agent for converting catechols totheir methylenedioxy derivati ves.

IICT has developed thermal process for preparation of dibromomethane from bromomethane and bromine. The process demonstrated to the client under continuous mode and isolated the product after down streaming.

Ammoxidation: Preparation of O-Chloro Benzo nitrile from O-Chlorotoluene

We have been developing vanadia based catalysts for the vapour phase ammoxidation of alkyl aromatics to prepare corresponding aromatic nitriles. A series of La2O3 modified Al2O3 supported V2O5 catalysts were prepared and evaluated for ammoxidation of 2-chlorotoluene to 2-chlorobenzonitrile. Well dispersed tetrahedrally coordinated isolated surface and polymeric vanadia species were responsible for the ammoxidation activity. Small proportions of crystalline V2O5, AlVO4and LaVO4 species are also beneficial to obtain high catalytic activity. (*New J. Chem*., **2018**, **42,** 1892)



Development of Catalytic Process for Benzene Hydroxylation to Phenol with Molecular Oxygen (*Sponsored by M/S SABIC R&D*)

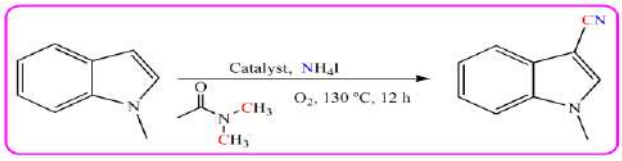
Selective hydroxylation of benzene to phenol is a challenge reaction in petrochemical industry as phenol has wide range of applications. Conventional phenol sysnthesis is from Cumene oxidation, which is a multi step process with high acetone production as a co-product, conversions are kept low at every 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. Vapor phase air oxidation of benzene is the suitable and economically valuable process if one can develop an active and selective catalyst. We developed few lead catalysts for the high conversion of benzene with reasonable selectivity towards phenol.

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

Highlights of this work:

- A reusable Cu/SBA-15 catalyst identified for regioselective C3-cyanation of indole
- DRIFTS studies emphasized the role of surface Lewis acid sites on cyanation activity

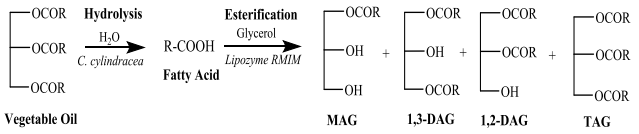


Cyanation of N-methylindole

CENTRE FOR LIPID SCIENCE & TECHNOLOGY

BASIC RESEARCH

Nutritionally Enriched 1,3-Diacylglycerol-Rich Oil: Low Calorie Fat with Hypolipidemic Effects in Rats: An enzymatic process was developed for the preparation of a nutritionally enriched 1,3-diacylglycerol(DAG)-rich oil from a blend of refined sunflower and rice bran oils. The process involves hydrolysis of vegetable oil blend using *Candida cylindracea* followed by esterification with glycerol using *Lipozyme* RMIM. The resultant DAG-rich oil contains 84% of DAG (66% of 1,3-DAG, 18% of 1,2-DAG) and 16% of triacylglycerol (TAG) along with micro nutrients like γ-oryzanol, tocotrienols, tocopherols and phytosterols. Nutritional studies of the DAG-rich oil were conducted in rats and compared with sunflower oil (SFO). The calorific value of the DAG-rich oil was estimated to be 6.45 Kcals/g as against 9.25 Kcals/g for SFO. The serum and liver cholesterol and TAG levels in rats fed with 1,3-DAG-rich oil were found to be significantly reduced as compared to SFO. We conclude that 1,3-DAG-rich oil is a low calorie fat and exhibits hypolipidemic effects. (Food *Chem.*, **2018**, 248, 210)



Scheme 1: Preparation of nutritionally enriched 1,3-DAG-rich oil

Design, Synthesis, and Cytotoxicity Evaluation of Threonine-Based Galacto ceramide with Aromatic Groups and Various Fatty-Acyl Side Chains: The synthesis of threonine-based β-galactoceramide was carried out and its derivatives were prepared by modifying the fatty-acyl group on amide moiety with different unusual, branched, saturated, and unsaturated fatty-acyl moieties and aromatic acids employing trichloroacetimidate methodology. Further, all the synthesized compounds were evaluated for in vitro cytotoxicity and all these compounds exhibited good to moderate cytotoxicity against all the tested cancer cell lines with IC50 values ranging between 14.08 to 64.05 μM. Based on structure–activity relationship, aromatic-acid derivatives exhibited promising activity as compared to fatty-acid derivatives. Further, the compounds bearing longer spacer chain length between aromatic residue and amide functional group, methoxy substituents on aryl group compounds, terminal unsaturation of fatty-acid compounds and branching chain compounds showed good cytotoxicity when compared to their respective counterparts. (*Med. Chem. Res*., **2018,** 27, 285)

Synthesis and Biological Evaluation of 3,6-Dialkylsubstituted-[1,2,4] Triazolo[3,4-B][1,3,4] Thiadiazoles: A series of di-alkyl 1,2,4-triazolo [3,4-b] [1,3,4] thiadiazoles were synthesized and their antimicrobial activity and cytotoxicity were investigated. It was observed that, butyl, hexyl and lauryl derivatives exhibited good antimicrobial activities. Butyl analogue showed potent minimum bactericidal concentration activity. Hexyl, decyl, undecenyl, lauryl, myristyl, palmityl, stearyl and oleyl-based derivatives exhibited significant activities against SKOV3 and MCF-7 cell lines. (*J. Chem. Sci*., **2018,** 130 (3), Article ID 0023)

Synthesis and Cytotoxic Evaluation of Cholesteryl 6-*O*-Acyl-β-D- Galacto Pyranosides: Cholesteryl 6-*O*-acyl-β-D-galacto pyranosides were synthesized with unusual, short, medium, long and unsaturated fatty acids using trichloroacetimidate methodology. Cholesteryl β-D-galactopyranoside was selectively esterified at C-6 position employing EDC.HCl coupling reagent. All the compounds were evaluated for cytotoxicity against four cancer and one normal cell lines namely, SKOV3, HeLa, MDA-MB-231, DU145, CHO-K1 cell lines. Among all the tested compounds long chain saturated palmitic and stearic acid derivatives exhibited significant cytotoxicity against cervical cancer cell line. However, all the tested compounds did not show any toxicity towards normal CHO-K1 cell line. (*Ind. J. Chem B*., **2018**, 57 B, 91)

Synthesis and Cytotoxicity Evaluation of Unusual Mixture Acid Acetate-Protected Monogalacto syldiacylglycerols: Unusual fatty acid and aromatic acid (cinnamic acid)-based, acetate-protected monogalactosyldiacylglycerol were synthesized employing trichloroacetimidate methodology. All the synthesized glycoglycerolipids were examined for cytotoxicity against four cancer cell lines and one normal cell line. Based on the results, it could be concluded that the combination of oleic acid with aromatic acid (cinnamic acid type) and other saturated fatty acids enhances the cytotoxicity of glycoglycerolipids. (*Ind. J. Pharm. Sci*., **2018,** 80, 1143)

Chemical Composition and Antioxidant Activity of *Syzygium Aromaticum* and *Monodora Myristica* Essential Oils from Cameroon: The objective of this study was to evaluate the chemical composition and antioxidant activity of *Monodora myristica* and *Syzygium aromaticum* essential oils. The oils were extracted by hydro distillation and their chemical composition determined by gas-chromatography coupled to a mass spectrometer detector. The antioxidant activity of the oils was evaluated through the following tests: DPPH radical scavenging activity; the ferric reducing antioxidant power, the metal chelation and finally the hydroxyl radical scavenging activity. Results showed that alpha-phellandrene (52.2%) and (p)-cymene (13.1%) were the most represented compounds in the essence of *Monodora myristica* while Eugenol (59.5%) and (E)-Caryophyllene (23%) were the most abundant molecules in that of *Syzygium aromaticum.* The evaluation of the antioxidant activity showed that the oil of *Syzygium aromaticum* has good antioxidant activity compared to that of *Monodora myristica.* (*J. Food Stability*, **2018**, 1, 1)

Effect of Boiling and Roasting on Lipid Quality, Proximate Composition and Mineral Content of Walnut Seeds (*Tetracarpidium Conophorum*) Produced and Commercialized in Kumba, South-West Region Cameroon: The effect of boiling and roasting on the lipid quality, proximate composition, and mineral content of African walnut seeds (*Tetracarpidium conophorum*) was assessed. Results indicated that the quality of walnut oil significantly ($p < .05$) reduces with the treatments. Oils extracted from *DBWN* 60 min (Dried and boiled walnuts 60 min) and *FBWN* 60 min (Boiled fresh walnuts 60 min) were the most altered. The proximate composition and mineral content of walnut seeds was also significantly affected ($p < .05$) by the treatments. This study reveals that, thermal processing has significant effects on the nutrients and quality of lipids of walnut oil. *DTRWN* 60 min (Dried and traditionally roasted walnuts 60 min), *DORWN* 60 min (Dried and oven roasted walnuts 60 min), and *TRFWN* 30 min (traditionally roasted fresh nuts 30 min) are the best methods for cooking walnut because they preserve the quality of its lipids and some of the nutrients. (*Food Sci. Nut.*, **2018**, 6 (2), 417)

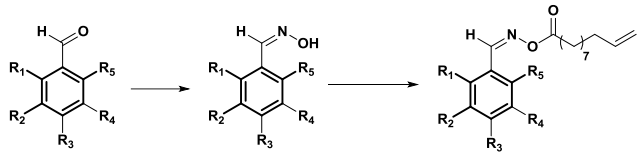
Optimization of the Extraction of Natural Antioxidants from *Coffea Robusta* Leaves and Evaluation of their Ability to Preserve Palm Olein from Oxidation During Accelerated Storage: Response surface methodology (RSM) was used to optimize the extraction of pheonolic antioxidants of *Coffea robusta* leaves and to evaluate the effect of optimized extract and storage time on the stability of palm olein. The optimization of the extraction process was conducted, and the total polyphenol value of 127.06 mg GAE/g and scavenging activity of 90.65% were obtained under optimal extraction conditions. The phenolic antioxidants of the optimized extract and their thermal stability were determined using HPLC-DAD (high-performance liquid chromatography-diode array detector) and Rancimat test, respectively. The effect of concentration of the optimized extract and storage time on the stability of palm olein was also evaluated. Results showed that the optimized extract contains gallic acid, vanillic acid, cafeic acid and was efficient

in retarding palm olein oxidation during 32 months at room temperature. *Coffea robusta* can be recommended as good source of antioxidants for stabilization of palm olein. (*Food Sci. Nut.*, **2018,** 6, 1751)

Role of Ferulic Acid in Protecting Lipopoly sachharised-Induced Acute Kidney Injury: Ferulic acid (FA), a natural phenolic compound is known for its role in renal protection in several induced model. However, its role in lipopolysaccharide (LPS) induced acute kidney injury AKI) is not known. Looking at the high mortality rate (70-80%) of sepsis-induced AKI due to elevated level of endotoxin LPS, it was planned to check the efficacy of FA on LPS induced AKI in mice model and also to understand the mechanism behind it. Balb/c mice were treated with FA at 50 mg/kg and 100 mg/kg dosages after LPS stimulation (10 mg/kg). At the end of the intervention, the concentrations of serum creatinine and blood urea nitrogen, inflammatory cytokines and histopathological changes in animals were determined. Also, the relative protein expression level of TLR4 mediated NF-κB signaling pathway were studied in kidney tissues. FA treated animals showed upregulation of antioxidant defences and suppression of inflammatory events by inhibiting TLR-4 mediated NFκB activation. However, LPS alone administered group, resulted in rapid renal damage with increased levels of blood urea nitrogen and modest increase in creatinine; decreased antioxidant defences and release of inflammatory cytokines. The histopathological analysis also revealed the protective action of the FA against sepsis induced fibrosis and renal damage. Our findings demonstrated that FA exhibits marked protective effects on LPS-induced AKI in mice suggesting its chemo-potential role for treating AKI in humans. (*Biomed. Pharmacoth.*, **2018,** 100, 304)

Dietary Supplementation of Avenanthramide-Rich Oat Extract Protects Alcohol-Induced Acute Liver Injury: In our earlier study we have found enrichment of avenanthramide in the ethyl acetate (EA)-soluble part of polar crude extract of oat. There are no reports on prophylactic role of oat extract against acute liver injury. In the present study, we hypothesized that oat extract may play a protective role against alcohol-induced acute liver injury in a mouse model. To test this hypothesis, male C57BL/6 mice were pretreated with phenolic-enriched EA fraction of oats at dosages of 125 and 250 mg/Kg body weight/day for 12 consecutive days. Acute liver injury was induced by administering 5 doses of 50% ethanol intragastrically (10 g/kg body weight) to mice at an interval of 12 hours. The alcohol-induced liver injury was evaluated by measuring serum levels of alanine aminotransferase, aspartate aminotransferase, lactate dehydrogenase, antioxidant parameters, mitochondrial function, and histology of liver tissue. Our results demonstrated that pretreatment with EA fraction at 250 mg/Kg/day significantly ($P < 0.001$ for aspartate aminotransferase, alanine amino transferase, and thiobarbituric acid–reactive species and $P < 0.01$ for lactate dehydrogenase and nitrites) reduced the levels of liver injury markers and significantly increased the levels of antioxidant defences. Furthermore, EA-pretreated mice showed mechanistic inhibition of nuclear factor κB signaling pathway through decreased phosphorylation and degradation of IκBα. Thus, avenanthramide enriched EA fraction of oats has the potential to serve as dietary intervention against alcohol-induced liver damage. (*Nut. Res.*, **2018,** 54, 80)

Synthesis and Cytotoxic Evaluation of Undecenoic Acid Based Oxime Esters: Undecenoic acid based aldoxime esters were synthesized employing substituted benzaldehydes and 10-undecenoic acid. About nineteen compounds were synthesized and screened for cytotoxicity assay against five cell lines where most of the compounds exhibited activity. Among the synthesized derivatives, 2,3-dimethoxy and 2-methoxy substituted compounds exhibited promising activity against few cell lines and were non-toxic towards normal cell lines. (*Ind. J. Chem. B*, **2018**, 57, 1015)



Scheme 2: Synthesis of undecenoic acid based oxime esters

Synthesis and Self-Assembly Properties of Glycolipid Amphiphiles: Employing simple synthetic strategy a new type of glycolipid amphiphiles were synthesized and investigated for their self-assembly properties. Incorporation of amino acid successfully increased the solubility of the surfactant. The results show the branched nonionic surfactants molecular geometry influence the surface and micellar properties in aqueous solution. The presence of the hydrophilic groups, such as aspartic acid increases the intermolecular attraction between the headgroup and reduces the water penetration inside the micelle, but the orientation of chiral glucamine unit is not suitable for further supramolecular aggregation. Surprisingly, the dicephalic head group has a pronounced reduction in A_{min} (29.212 $Å^2$/molecule) while Langmuir monolayer formation at the air-water interface. The packing parameter, and anisotropy obtained for dicephalic headgroup lead to a bilayer aggregate, whereas our aggregation number and DLS studies suggest for spherical micelle. Further TEM study confirms the distorted micelle of 9 nm size for the dicephalic glycolipid. The intramolecular attractions between the highly branched headgroup lead to highly ordered micellar core (r_{ss} = 0.151) with exceptionally high microviscosity of 63.7 MPa s. The orientation of chiral glucamine unit and intermolecular interactions facilitated the formation of fibrillar helical aggregates in the linear glycolipid which undergoes time dependence aggregation behavior at 25°C. The self-assembly studies and cytotoxicity data suggests that the amphiphiles may have potential use as solubilizers and drug delivery vehicles in the pharmaceutical industry. Further surface active studies were executed on the above nine glycolipids with headgroup and chain length variation. SFT, IFT, foaming, wetting, emulsification, and solubilization studies were performed as a function of glycolipid concentration. SFT and IFT studies exhibited strong headgroup dependence as well as hydrophobic chain length. The surface and interfacial activities of glycolipids with big headgroup size loosing at very higher chain lengths. Results obtained from foaming, wetting, and emulsification reflected similar trend as observed in SFT and IFT studies of glycolipids. Glycolipids having good foamability and foam stability exhibited chromium removal efficiency in presence of sunlight. Glycolipid having two glucamine units with good foamability showed excellent chromium removal capacity (231.3 milligram of chromium per one gram of glycolipid). These glycolipids are capable to form stable emulsions with sunflower and water. Emulsification power of the glycolipids was increased with alkyl chain length and in few cases they are capable to form stable gel-emulsions. Additionally, emulsions prepared with glycolipids are able to encapsulate water and oil soluble bioactives. Obtained formulation exhibited enzyme triggered release behavior and the release rates are decreased with increase in hydrophobic chain length of glycolipids and decrease in ϕ_w values of the corresponding glycolipid emulsion. Finally the studies on glycolipids with different headgroup size and chain length were useful to understand the structural activity on amphiphilic properties of glycolipid and these glycolipids finds numerous industrial applications. (*Langmuir*, **2018**, 34, 8875; *Langmuir*, **2018**, 34, 14347; *Colloids Surf A: Physicochem. Eng. Asp*, **2019**, 563, 226)

Synthesis and Gelation Properties of Phenoxy-Alkyl Maleate-Based Amphiphiles: A new series of phenoxy-alkyl maleate based amphiphiles were synthesized using cost effective starting materials and tested for hydrogelation property in phosphate buffer solution at pH 8. These amphiphiles formed stable and thermoreversibility hydrogels. FE-SEM analysis

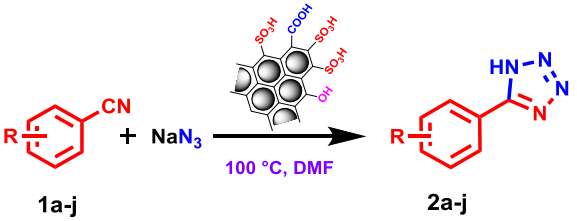
suggests hierarchical structure such as flower bunch and leaf vein structures. Encapsulation of curcumin (1%) in the hydrophobic pockets of hydrogel was achieved. Trapped hydrophobic drug was released from gel network structure by the lipozyme enzyme. Herein, ester bond between phenoxy alkanol and maleic anhydride was hydrolysed by the enzyme. Hydrolysis of gelator molecule leads to gel degradation and subsequent release of curcumin from gel networks. In addition, when the curcumin trapped hydrogel was exposed to acidic pH, the curcumin was efficiently released within 55 min. Based on the output of this present work; we anticipate that these hydrogels will find applications as the drug carrier agent in the pharmaceutical field. Further these phenoxy-alkyl maleate gelators gelate a variety of edible oil with high oleogelation capacity. Notably, the best gelation ability was observed in case of 12-chain gelator molecules. The 12-chain gelator showed low MGC (19 mg/mL) value in sunflower oil among the all edible oils. From the results of tube inversion method as well as DSC experiment, we observed that the thermal stability of oleogels increased with increasing alkyl chain length of gelator molecules. Self-assembled sheet like network was the main factor for the oleogel formation as evidenced from FE-SEM study. Furthermore, the gelators are showed phase-selective gelation behavior with edible oils in the biphasic mixture of oil and water. After phase selective gelation, the edible oil can be recovered quantitatively (>95%) through simple vacuum distillation. The main advantage of these molecular gelators is easy preparation and reusability. The molecular gelators may hold future promise for remediation of an oil spill. (*New J. Chem.*, **2019**, 43(14), 5559; *Eur. J. Lipid Sci. Tech.*, **2019**, 121, 1800364)

Synthesis, Cytotoxic Evaluation of Substituted Cinnamic Acid-Based 1,2,4-Triazolo Thiadiazoles: A series of substituted cinnamic-based 1,2,4-triazolo [3,4-*b*] [1,3,4] thiadiazoles were synthesized. All the synthesized compounds were evaluated for their cytotoxic activities. 2,3-dimethoxy and 4-trifluoro methyl derivatives exhibited promising activities against HeLa and SKOV3 cell lines. Most of the compounds were nontoxic against the normal cell line (Chinese hamster ovary cell, CHO-K1). (*Ind. J. Chem B*, **2019,** 58 B, 475)

Synthesis and Cytotoxic Studies of Undecenoic Acid-Based Schiff's Base Derivatives Bearing 1,2,4-Triazole Moiety: A series of novel 1,2,4-triazole-based schiff's base heterocycles were synthesized. All the synthesized compounds were evaluated for their cytotoxicity against three cancer cells and a normal cell line. In this study, 4-bromo, 4-chloro, 4-fluoro, 5-chloro-2-nitro, 2-nitro and 2-fluoro substitution-based schiff's base derivatives exhibited significant cytotoxicity; however, 4-bromo derivative exhibited promising cytotoxicity to cancer cells. Majority of these active compounds were non-toxic towards the normal cells which supports their therapeutic applications. Taken together, the observations of cytotoxic nature of these compounds against cancer cells, supports their preliminary anticancer properties. (*Ind. J. Pharm. Sci*., **2019**, 81(4), 737)

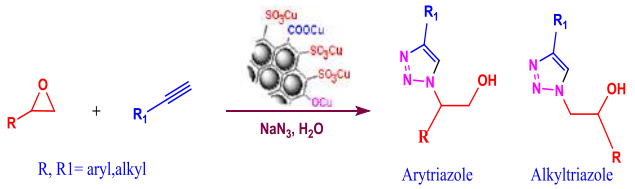
Benign Synthesis of 5-Substituted 1*H*-Tetrazoles Via [3+2] Cycloaddition of Nitriles and Sodium Azide Employing SO_3H-Carbon as an Efficient Heterogeneous Catalyst: A novel and green methodology was developed for the synthesis of 5-substituted 1-*H*-tetrazoles by [3+2] cycloaddition of nitriles with sodium azide in DMF at 100 ºC in the presence of highly stable, water resistant and recyclable nonmetallic SO_3H-carbon catalyst derived from glycerol. The methodology was extended for the preparation of different 5-substituted1-*H*-tetrazoles from arylnitriles having electron donating as well as electron releasing groups on the arene nucleus in good to excellent yields (85-95%) under optimum conditions. The catalyst was recovered by simple filtration and reused for five cycles without any loss of activity. The main advantages of this methodology are moderate temperature, easy

purification of products, easy recovery and reusability of the catalyst. (*Asian J. Green Chem.*, **2019**, 3(2), 125)



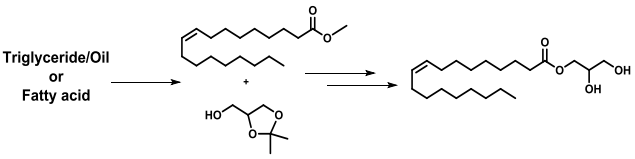
Scheme 3: Synthesis of 5-substituted 1*H*-tetrazoles using SO_3H-Carbon

SO_3Cu-Carbon: A Novel Heterogeneous Catalyst for the Synthesis of β-Hydroxy 1,2,3-Triazoles by One Pot Cycloaddition Reaction: Developed a novel, highly stable and water resistant heterogeneous SO_3Cu-carbon catalyst by modifying the SO_3H-carbon derived from glycerol by treatment with 10% aqueous $CuCl_2$ solution under controlled conditions for the first time. The catalytic activity of the SO_3Cu-carbon was investigated for the synthesis of β-hydroxy 1,2,3-triazoles by one-pot 'click' reaction of three component (epoxide, sodium azide and terminal alkyne) azide–alkyne cycloaddition in aqueous medium at 60 °C. The catalytic activity of the SO_3Cu-carbon catalyst was demonstrated for the one pot 'click' reaction of epoxide, sodium azide and terminal alkyne in water at 60 °C for the synthesis of β-hydroxy 1,2,3-triazoles in excellent yields (89-94%) without any additives. The formation of the product proceeds in one pot through a mechanism that involves *in situ* generation of organic azide intermediate followed by rapid ring closure with alkynes. The catalyst was easily recovered by simple filtration and reused for 5 cycles without any leaching and deactivation thus exhibiting its excellent stability and reusability. Moreover, the cascade reaction was best performed in water at moderate temperature, rendering all the processes truly green. (*Chemistry Select*, **2019**, 4, 10133)



Scheme 4: Synthesis of β-hydroxy 1,2,3-triazoles using SO_3Cu-Carbon

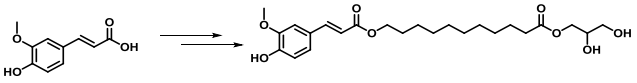
Synthesis, Characterization & Evaluation of Structured Lipids for Potential Bioactive Applications *(GAP-0664; Sponsored by Science & Engineering Research Board (SERB), New Delhi, India)***:** Several monoacylglycerols varying in chain length, unsaturation and functional groups were synthesized and screened for antimicrobial activity. In first part, synthesis of 1-monoacylglycerols of selected unsaturated fatty acids and their antimicrobial and cytotoxicity activity was carried out. The monoacylglycerols of fatty acids like undecenoic, oleic, linoleic and erucic acids were prepared by chemical esterification with solketal followed by deprotection (Scheme 1). The antimicrobial activity revealed that the monoacylglycerol of gamma linolenic acid was the most effective antibacterial followed by the monoacylglycerols of undecenoic and alpha linolenic acids. In the cytotoxicity assay against five cell lines, all the monoacylglycerols exhibited moderate anticancer activity. (*Grasas Aceites*, **2019**, 70 (4), e325)



Scheme 5: Synthetic route for 1-monoacylglycerols

A chemo enzymatic pathway was designed for the synthesis of naturally isolated monoacylglycerol, 1-[11-(ferulyloxy) undecanoyl)] glycerol for the first time where two out of four steps were carried out using lipase as catalyst. Synthesis started from ferulic acid as the primary component which was converted to vinyl ferulate and esterified using lipase with 11-

hydroxy undecanoic acid (Scheme 2). This fatty acid was transesterified using lipase and resulting acetonide was deprotected to yield the final product. (*Biotech. Reports*, **2019**, 24, e00375)



Scheme 6: Synthetic route of 1- [11-(ferulyloxy)unde canoyl)] glycerol

Influence of Flour Type on Physico-Chemical Characteristics during Deep Frying: The study focused on understanding the influence of nutrients on frying oil degradation as well as its role in oil uptake by the fried substrate. Raw substrates were prepared taking refined wheat flour (rich in carbohydrate), soy flour (rich in protein) and gram flour (with both in a definite proportion) which were subjected to frying in sunflower oil at 185–200 °C. Analysis of the fried oil, substrate and fried product was carried out. Increase in acid value with respect to the composition of the flour was not significant. Higher rate of oxidation and peroxide value were observed in the oil used for gram flour snacks, which could be due to significant amounts of sodium and potassium salts. Fried oil with soy flour based snack showed higher total polar material which could be due to accelerated oxidation. Oil absorption was promoted by starch and gluten and controlled by protein and insoluble fiber. Oil absorbed by refined-wheat flour and soy flour based snack was 30% and 9.33% whereas gram flour-based snack absorbed 4.52% oil with superior oil quality comparatively. (*J. Food Sci. Tech.*, **2019**, 56 (7), 3471)

Effect Boiling and Roasting on the Physico chemical Properties of Djansang Seeds (*Ricinodendron Heudelotii*): This study was aimed at determining the effect of boiling and roasting on physicochemical properties of Djansang seeds. Dried Djansang seeds were divided into three groups: one group was boiled for 5, 10, and 15 min; another group was traditionally roasted for 5, 10, and 15 min, and the last group was left unprocessed and served as the control. Polyphenols were extracted from the processed seeds using the maceration method, and their content and antioxidant activity were evaluated. Oils were extracted from the dried seeds by Maceration method, and the quality was analyzed by determining their peroxide value (PV), thiobarbituric acid value (TBA), iodine value (IV), and acid value (AV). The changes in proximate composition and mineral content of the processed samples were also evaluated using standard methods. Results showed that traditional roasting significantly decreases ($p < .05$) the polyphenol content and antioxidant activity of Djansang seeds as compared to boiling. The analysis of oil showed that traditional roasting and boiling significantly reduce the quality of Djansang seed oil and that traditionally roasted samples were the most affected. The proximate and mineral composition of Djansang was also affected during processing. Boiling for 5 and 10 min (*BNS* 5 min and 10 min) and traditional roasting for 5 min (*TRNS* 5 min) appear to be the best processing methods of Djansang for production of Djansang-based foods like Djansang sauce. (*Food Sci. Nut.*, **2019**, 7, 3425)

Effect of Sunlight on the Physico-Chemical Properties of Refined Bleached and Deodorized Palm Olein: In this study, the effect of sunlight on the quality of palm olein was assessed. Palm olein samples were subjected to sunlight (34-40°C) and ambient storage (~24°C) for 90 days. Oil samples were collected at 30 days intervals for quality analysis. At the beginning of the experiment, the peroxide (PV), *p*-anisidine (p-AnV), total oxidation (TOTOX), thiobarbituric acid (TBA) and free fatty acid (FFA) values of palm olein were 2.67 ppm, 0.68, 6.02, 0.69 and 0.07% respectively; color 1R, 6Y and induction time (IT) 23.89 and 26.55 h for oil-containing antioxidant and oil without antioxidants respectively. After 90 days storage at room temperature, the PV, *p*-An-V, TOTOX, TBA and FFA values were respectively ranged between 5.19-7.13 ppm, 1.27-2.99, 11.65-17.25, 0.97-1.73 ppm and

0.11-0.12%; the color in the red and yellow unit 1.17-1.19R and 6.00-6.10Y respectively; and the induction time 22.82-25.77 h. However, the same parameters after 90 days of exposure to sunlight were ranged in the same order, between 34.11-36.50 ppm, 28.22-29.65, 96.44-102.65, 5.38-5.44 ppm and 0.63-0.67% respectively; the color in the red and yellow units 0.20R and 0.77-0.80Y respectively; and the induction time 0.01 h. Results showed that sunlight significantly reduced the quality of palm olein, even with the presence of antioxidants. (*Food Research*, **2019,** 3 (1), 49)

Kinetics of the Enzymatic Hydrolysis of Flax Seed Oil Methyl Ester: Enzymatic hydrolysis of flax seed oil methyl ester was performed in this study using *Rhizomucor miehei*. The work focused on the optimization of hydrolysis carried out by varying the temperature (30-60°C) and enzyme load (2-5%). The optimal conditions for the system were found to be 50 °C, 6 h reaction time, buffer to flax seed oil methyl ester ratio 1.5:1(v/w) and 4% enzyme load to achieve a maximum hydrolysis conversion of 97.56%. The effect of temperature on the reaction rate constant and equilibrium constant has been determined using Arrhenius equation. The heat of reaction was found to be 14.516 KJ/mol. (*J. Lip. Sci.Tech*., **2019**, 51(2), 50)

APPLIED RESEARCH

Synthetic Aviation Lubricants (SAL) Phase-II *(GAP-0564, Sponsored by Centre for High Technology (CHT), Ministry of Petroleum & Natural Gas, Govt. of India, New Delhi*): SAL Phase II involves Ground & In-flight Tests with indigenously developed Synthetic Aviation Lubricants on TV2 Aero Engine by Indian Air Force at 3BRD, Chandigarh. The main objectives are: a) To prepare 500 kg each of the base oils for SVS-11 and SVS-21 lubricants at CSIR-IICT and carryout preliminary testing. b) Formulation of the SVS-11 & SVS-21 lubricants and their physico-chemical testing at HPCL - R&D. c) Testing of both the lubricants for compatibility with elastomers and for ground test in Aero engines on test bed and In-flight testing by IAF and CEMILAC. During this period, CSIR-IICT prepared SVS-21 and SVS-11 lubricant base oil (500 lts each). HPLC completed the formulation and physiochemical (including lubricity and rubber seal compatibility) tests and tribology tests with both the developed synthetic aviation lubricants SVS-21 & SVS-11. 3BRD completed the engine bed tests for about 50 hours with proven oil (OX-38) and with SVS-21 oil SVS 21 oil in TV2 aero engine. CEMILAC approved the SVS-21 oil for its commercial exploitation by HPCL. Engine testing of SVS-11 oil on TV-3 aero engine test bed at 3BRD & In-flight test schedule and flight trails after ground tests of SVS-11 at 3 BRD, IAF is in progress. After completion of these activities, HPCL will take up the commercialization of the developed two Aviation Lubricants.

Preparation of Edible Oil Blends of Palmolein and Palm Stearin with Indigenous Edible Oils for Cooking and Trans-Free Solid Fat Formulation Applications *(GAP-0727; Sponsored by Malaysian Palm Oil Board (MPOB), Malaysia):* The main objective of the project was to prepare different palmolein blends with indigenous edible oils to obtain blends with balanced fatty acid profile and enriched nutraceuticals like tocopherols, tocotrienols, carotenoids, oryzanol, lignans etc. Another objective was preparation of selected blends followed by interesterification to obtain new structured lipids and study their oxidative stability. Palmolein with iodine value in range of 56-68 was employed to prepare blends with indigenous edible oils like sunflower, soybean oils, etc oils to obtain blends with balanced fatty acid profile. Initially various blends were prepared in small scale to observe the blend which is close to the recommended fatty acid ratio. Later selected blends with desired fatty acid ratios were prepared in large scale for storage studies. Further frying of the selected blends was initiated taking

popular snacks for data generation on physico-chemical characteristics.

Development of Process for the Preparation of Rice Bran Lecithin from Crude Rice Bran Gums *(GAP-0797 Sponsored by BIRAC-SBIRI):* The aim of the project is to develop processes for preparation of rice bran lecithin from crude rice bran gums supplied by Ms AP Organics Ltd., Punjab. Also, to prepare PC-enriched lecithin (30 & 50% PC enriched lecithin) and modified lecithins such as acetylated, hydroxylated lecithins using the refined rice bran lecithin. Optimization of bleaching experiments was carried out using H_2O_2, benzoyl peroxide and sodium chlorite bleaching agents. Color reduction was better in case of bleaching using H_2O_2 and benzoyl peroxide agents (18+ to 16+ Gardner units). Optimization of conditions to prepare PC-enriched rice bran lecithin was carried out using ethanol fractionation method. Enrichment to an extent of 40% was achieved. Work is in progress to further optimize the bleaching conditions and also to further enrich lecithin with PC.

Central Sector Scheme for the Upgradation of National Referral Laboratory *(GAP-00639; Sponsored by Food Safety and Standard Authority of India (FSSAI))*: Food Safety and Standards Authority of India (FSSAI) has recognized Centre for Lipid Science and Technology of CSIR-IICT as "National Referral Laboratory (NRL) for Oils & Fats" in 2014. As a part of NRL lab, FSSAI, sponsored a project under Central Sector Scheme with the aim of upgradation of the testing facility as a NRL for edible oils & fats. CSIR-IICT purchased three equipments namely AAS, GC-MS & HPLC with FLD detector. As a part of National Referral Laboratory for vegetable oils and fats, helping FSSAI in testing and analysis of surveillance samples of various vegetable oils to check and maintain the quality and standard specifications of the products. The main objectives of this proposal are: Making available the upgraded laboratory for imparting training for other states/FSSAI notified labs in the state/region, beside ensuring participation of the laboratory personnel in the training program to be organized by FSSAI; Open to the inspection/ audit of the laboratory by FSSAI during the process of up gradation & obtaining NABL Accreditation for the lab. Hence, CSIR-IICT obtained NABL Accreditation for Oils & Fats Testing Facility at CLST. During this period, scope of work on oils & fats covering all the physico-chemical parameters, tocols analysis by HPLC, fatty acid composition by GC-FID and pesticide and heavy metal contaminants analysis in oils & fats by GC-MS/MS & ICP-OES respectively as per FSSAI specifications was finalized and the final draft was submitted along with other scope of Analytical Department of CSIR-IICT for NABL accreditation in the month of April 2018. After the Assessment by NABL accreditation team during 8-9th September 2018, the Oils & Fats testing facility covering all the physico-chemical parameters, tocols analysis by HPLC, fatty acid composition by GC-FID was NABL Accredited in accordance with the standard "ISO/IEC 17025:2005" in November 2018.

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 *(GAP-0598; Sponsored by Food Safety and Standard Authority of India (FSSAI))*: Adulteration is done mainly for economic reason, by mixing cheap oil or used oil with good oil. Most of the time adulteration is done in a manner with overlapping physicochemical properties. Such economically motivated adulteration is difficult to detect and quantify by available methods. The proposed project is focused on generating data base on triacylglycerol (TAG) molecular species of all edible oils. Each oil has characteristic TAG structure based on types and number of fatty acids present in it. Triolein in olive oil, triricinolein in castor oil, trilinolein in safflower, sunflower and soybean are some of the very specific symmetrical TAG molecular species. As part of the project fingerprinting TAG molecular species of all commonly consumed edible oil in India has been

accomplished. Different combinations of 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 etc.) has been studied. Based on HPLC data, detection index for each combination of oil has been identified for quantification of low cost minor oil in expensive major oil. Developed method was validated by adopting some of the edible oils at different ratios of blending. Developed method also successfully tested on several blended oil available in the market in ascertaining their ratio.

Generation of Data on Pesticide Residues and Metal Contaminants in Edible Vegetable Oils of Different Regions *(GAP-0599; Sponsored by Food Safety and Standard Authority of India (FSSAI))*: The aim of generation of data on pesticide residues and metal contaminants in Indigenous edible oils to help in fixing the detection and specification limits by FSSAI. The final completion report was submitted to FSSAI during January 2019 and the output achievements of the project are: Presently, no maximal residue limits (MRLs) are available for most of the pesticide residues and metal contaminants for edible vegetable oils. Collected 131 edible oil samples of Sunflower, Groundnut, Soybean, Coconut, Cottonseed, Rice bran, Palm, Mustard, Rapeseed, Sesame, Palm Kernel, Vanaspati and Olive oils (crude and refined) from different regions. Standardized the analytical and extraction protocols for the analysis of 51 pesticides by GC-MS/MS and LC-MS and also validated the methodology. Most of the refined oils were found to be free from pesticide residues and some of them were found to contain much below than the MRL levels. None of the oils contains- trifluralin, chlorothalanil, dichlorvos, cartap hydrochloride, aluminium phosphide, carbendazim, chlorantraniliprole, paraquat dichloride, metolachlor, mancozeb, lufenuron, fenobucarb and difenthiuron pesticides. Standardized the protocol for the determination of selected metal contaminants namely, Cu, Sn, Zn, Cd, Cr, Fe, Ni, Pb, Hg. As in the edible vegetable oils by ICP-OES using the standard ASTM methods. Analyzed 57 different crude and refined edible oil samples for the presence of metal contaminants and no heavy metal (As, Hg, Pb, Cd & Sn) contamination was observed in most of the refined oils that are studied except in refined sunflower, soybean and palm oils. From this study, it is clear that the pesticide residues and metal contaminants that are detected in most of the crude oils in higher levels were found to be absent or detected in negligible levels in the corresponding refined oils, which may be perhaps are getting eliminated during refining process.

CSIR Mission Mode Programme on Food and Consumer Safety Solutions *(HCP-0016, Sponsored by CSIR under FOCUS Mission):* Considering the national priority of safe food for all, CSIR initiated a mission project to develop new methods and technologies to assure better human health through safe food commodities from field to consumer end. This culminated into the conceptualization of a mission mode program on "Food and Consumer Safety Solutions". Food and Consumer Safety Solutions (FOCUS) has 6 work packages i.e. 1. Milk and Milk Products, 2. Beverages and Packaged Foods, 3. Ghee and Edible oils, 4. Safety systems for post-harvest produce, 5. Development of multi-analyte detection methods & 6. Digital Food Safety Portal. These work packages of FOCUS mission has strong relevance to Make in India, Swasth Bharat, Swachh Bharat, Innovate in India, Skill India and Startup India. The participating CSIR institutes are, CSIR-CEERI, CSIR-CGCRI, CSIR-CSIO, CSIR-IICT, CSIR-IITR, CSIR-NIIST. As part of the consortium of this mission project, CSIR-IICT was involved in WP- 3, Ghee and Edible oils along with CEERI & CSIO [WP-3.1- Spectral Systems for Detection of Adulteration in Ghee and Edible Oils (CSIR-CEERI and CSIR-IICT) & WP-3.2- Rancidity Indicator Strip for Edible Oils (CSIR-CSIO & CSIR-IICT)]. In WP 3.1, CSIR-IICT's role was to assist

CSIR-CEERI in developing and validating NIR-based technique to detect adulteration of edible oil and ghee. CSIR-IICT generated database of physicochemical properties of several edible oils and ghee samples available in the market and shared with CSIR-CEERI. Generated database helped CEERI to categorize each oil and correlate with their FTIR spectra and accordingly develop chemometric models and algorithms to detect adulteration. In WP 3.2, CSIR-IICT's role was to assist CSIR-CSIO in developing rancidity indicator strip to detect oxidative degradation of edible oil during frying. During the execution of the project, CSIO sent several neat and fried oil samples, especially mustard and soybean oil. All these samples were analysed for acid value, peroxide value, p-anisidine value, iodine value and total polar matter (TPM) by TESTO method and the data was shared with CSIO in validating their indicator strip.

Indigenous Enzymes for Degumming of Rice Bran Oil and other Vegetable oils *(MLP-036, Sponsored by CSIR under Agriculture Nutrition Biotechnology theme):* CSIR-IICT has developed enzymatic degumming technology for rice bran oil using commercially available phospholipase A1 enzyme from Novozymes and the technology was licensed to 29 industries including 8 project engineering companies. However, the industries were totally dependent on imported enzymes. It was, therefore, decided to develop indigenous phospholipase enzyme to get import substitutes. The process was optimized for the codon of the phospholipase A1 clone for soluble production of protein in *E. coli* and *P. pastoris*. Expression was optimized in five different bacterial strains and one strain of *P. pastoris*. Using both the expression systems, a minimum of five batches of soluble protein at the lab scale was prepared. These enzymes were tested for degumming of rice bran oil. The recombinant enzyme purified at CSIR-IICT shows comparable activity with the commercial enzyme. After degumming, bleaching and dewaxing the phosphorus content of the oil samples were found to be less than 5 ppm using selected recombinant enzymes. CSIR-IICT will look forward to collaboration with suitable industrial partner.

Vegetable Oil-based Gels as Trans Free Fat (Oleogel) *(MLP-0045 Sponsored by CSIR under Agriculture Nutrition Biotechnology theme): Trans* fats increase the risk of coronary heart disease by raising LDL level and lowering HDL level. FDA has declared partially hydrogenated oils must phase out by 2018. Similarly, FSSAI restrict the trans fatty acid content to less than 2% by 2020. Structuring of edible oil with a gelator (mostly agricultural by-products) in the form of oleogel for the replacement of Trans fats may be a suitable alternative. Hence the objective of the project proposal is to develop novel trans-free oleogels for cooking, margarine, spreads and confectionary applications. An attempt has been made to analyze the oleogels on the aspects of melting profile, oil migration, solid fat content, rheological properties, etc on plant based oleogelators such as rice bran wax and sunflower wax. Wax based oleogels of 24 variants were prepared using Rice bran/Sunflower wax and eight available edible oils (Ground nut oil, Rice bran oil, Sunflower oil, Soyabean oil, Mustard oil, Palm oil, Sesame oil and Coconut oil). These oleogels were compared with the commercial food spread and margarine with respect to their physical/mechanical/thermal properties which is at par with the commercial sample. Based on the mechanical/thermal performances sunflower wax based oleogel was identified for process optimization and scale up to 1 kg/batch.

Development of Hybrid Flocculants at 100 G Scale for Selective Adsorption of Low Grade Iron Ore Slimes and Fines to Recover Iron Ore More Than 80% (HYBFLOC) *(MLP-0044 Sponsored by CSIR under Mining, Minerals, Metals and Materials (4M) theme):* The conventional mineral beneficiation techniques are generally ineffective in treating the ultra-fine particles. In order to recover values from ultra-fines, several industries are employing selective

flocculation technique to treat fines and slimes generated during mining and processing of the ore. Based on the knowledge available in the literature the proposed project will be dealt with selective flocculation of typical iron ore tailings employing hybrid flocculants. In order to address the challenges in handling ultra fines of iron ore samples in the mineral beneficiation process, 41 numbers of formulations were prepared and screened for iron ore fines settling. Out of the 41 formulations, 4 formulations have shown selective flocculation of iron ore fines. Optimization of the process was done at 1 L/batch scale at CSIR-IICT. Pilot scale efficacy for one formulation was studied in a column of 100 mm diameter and 2 m height at CSIR-IMMT.

Preparation of 1, 20-Eicosadioic Acid *(M/s Sun Pharma Advanced Research Co. Ltd., Vadodara):* The compound was prepared employing a two step procedure. The first step involved self metathesis of undecenoic acid employing Grubbs First Generation catalyst. The mixture was stirred mechanically and heated at 45°C, and after ~5 min of reaction a white precipitate was observed. After 72 h of the reaction a small amount of the crude product was removed from the reaction mixture and analyzed by GC and GC/MS. The reaction mixture was quenched with ethyl vinyl ether and unreacted ether was removed under reduced pressure. The residue was recrystallized twice using chilled methanol to give pure 1,20-eicos-10-enedioic acid. The 10-enedioic acid was hydrogenated using 10% Pd/C to obtain 1,20-Eicosadioic Acid. The product was characterized using ^{1}H and ^{13}C NMR. About 50 g of 1,20-Eicosadioic acid was sent to M/s Sun Pharma.

Development of Process Know-How for the Alcohol Based Hand Sanitizer Formulation *(SSP-0764, Sponsored by M/s Sante Triumph LLP, Rajasthan):* A process for preparation of alcohol based hand sanitizer gel as per CDC and WHO guidelines was successfully developed at 10 L per batch scale. The process know was transferred to Rajasthan based MSME on non-exclusive basis and also provided advisory consultancy during the commercialization of the process.

Supercritical Carbon Dioxide Extraction of Wheat Germ Oil: The most common solvent used for extraction of vegetable oils is hexane. Recently, hexane is declared as hazardous air pollutant by US EPA. Researchers are trying to find alternatives to hexane. Supercritical carbon dioxide (SC-CO_2) has been projected as one of the best alternatives. However, limited data are available on process optimization for this green extraction technique. Not only the higher initial investment, but also the scarcity of engineering data is causing slow growth of this technique. Optimization studies were carried out by CSIR-IICT to extract the oil from wheat germ by varying operating conditions such as pressure, temperature and CO_2 flow rate with an objective to get high oil yield with rich tocols content (vitamin E) and low phosphorous content. The process parameters were maintained between 300 to 500 bar of pressure, 40 to 60 °C of temperature and 10 to 30 g min^{-1} of CO_2 flow rate. Under the optimum conditions, experimental oil yield, phosphorous content and tocols content were found to be 8.68%, 42.5 ppm and 2057.3 ppm respectively. These data will be very useful in designing SC-CO_2 extraction of oils having higher nutritional values like wheat germ oil. (*Grasas Aceites*, **2018,** 69)

A 9,10,12-Trihydroxy Octadecanoic Acid Alkyl Ester and 9,10,12-Triacyloxy Octadecanoic Acid Alkyl Ester Rich Fatty Acid Alkyl Esters Mixture and a Process for Preparation Thereof: The present invention relates to modification of the chemical structure of ricinoleic acid, which is present to an extent of 85-90% in castor oil into triacyloxy alkyl ester derivatives. Accordingly, 9,10,12-trihydroxy octadecanoic acid rich fatty acid mixture was prepared from castor oil and converted to their alkyl esters followed by acylation of hydroxy groups to get 9,10,12-triacyloxy octadecanoic acid alkyl ester rich fatty, acid alkyl esters mixture. The 9,10,12-triacyloxy octadecanoic acid alkyl esters

were purified from the crude product and characterized by ^{1}H NMR studies. The crude products were also evaluated for acid value, hydroxyl value, iodine value, viscosity, viscosity index, pour point, flash point and copper strip corrosion and found to be potential base stocks for hydraulic, metal working fluids and other industrial fluids (*Brazil Patent* No. BRPI091306-6, **2018)**

A Process for the Preparation of Karanja Oil-based Epoxy and Acyloxy Compounds as Lubricant Base-stocks: The present invention relates to preparation of epoxy karanja oil, epoxy karanja fatty acid methyl esters and their acylated derivatives. Accordingly, karanja oil and karanja fatty acid methyl esters were epoxidised using performic acid method. Karanja oil and its fatty acid methyl esters were also hydroxylated to prepare their acyloxy derivatives (C_3, C_4 &C_6). Both the epoxy and acyloxy derivatives of karanja oil and its methyl esters were characterized by ^{1}H NMR and IR studies. The products were evaluated for acid value, hydroxyl value, iodine value, viscosity, viscosity index, pour point., flash point and copper strip corrosion and lubricant properties like oxidation stability, air release value, evaporation loss, rust prevention characteristics, hydrolytic stability, foam stability and load carrying capacity and found to be potential base stocks for hydraulic, metal working fluids and other industrial fluids (*Australian Patent* No. 2013288213, **2018**)

Study of Erucic Acid-Based Polyol Esters as Industrial Gear Oils: The growing environmental concern increased the exploitation of renewable materials for the development of biobased lubricants. Synthetic and vegetable oil-based esters offer the best choice in formulating environmentally friendly lubricants. In the present study, erucic acid-based polyol esters were prepared and characterized using IR, ^{1}H NMR, ^{13}C NMR and mass spectral techniques and evaluated for lubricant properties namely kinematic viscosity, viscosity index, oxidation stability, wear, weld load and copper corrosion value. The products were compared with industrial gear oils of VG-68 and VG-100 grade. The products were found to have good potential for use as basestocks for formulation as extreme pressure type of industrial gear oils. *(J. Lipid Sci. Tech.,* **2018**, 50(1) 15)

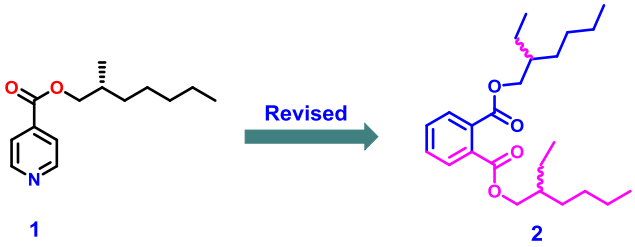
Tribological Studies of α-Lipoic Acid Esters as Effective Multifunctional Lubricant Additives: Enzymatic synthesis of six esters of α-lipoic acid with different fatty alcohols and diols was carried out to produce novel compounds with lubricant additive properties. The synthetic route was mild and efficient with good yields. The synthesized compounds were characterized by IR, NMR and mass spectral studies and screened for their thermal stability, antiwear, extreme pressure and antioxidant properties. The tribo tests in a synthetic base fluid indicated that all the synthesized compounds act as antiwear and extreme pressure additives. All the prepared esters exhibited very good thermal stability and excellent antioxidant properties by exhibiting better performance compared to commercial antioxidant BHT as determined by differential scanning calorimetry. (*Energy Sources Part A: Rec. Utilizat. Environ. Effects*, **2018,** 41(6), 700)

Utilization of Bhallataka (*Semecarpus Anacardium*)-Residue Oil in the Development of Biolubricant Base-Stock: Bhallataka kernel residue oil (BO) was explored for its use as a feedstock for biolubricants. Epoxidized bhallataka kernel residue oil (EBO) was prepared by peroxyformic acid generated *in situ* by reacting formic acid and hydrogen peroxide in the presence of sulphuric acid as catalyst with oxirane value 3.77. EBO was characterized using IR, ^{1}H & ^{13}C NMR, GC and GC-MS spectral techniques and evaluated for lubricant properties namely kinematic viscosity, viscosity index, copper corrosion, pour and flash point, wear, oxidation and thermal stability using standard ASTM and IP methods. EBO exhibited superior oxidation and thermal stability and enhanced viscosity compared to BO. The lubricating properties of EBO matched well with other epoxy oil properties. Hence, EBO can be projected as a potential source of high temperature applications. *(J. Lipid Sci.Tech.,* **2019**, 51(3) 99)

CENTRE FOR NATURAL PRODUCTS AND TRADITIONAL KNOWLEDGE

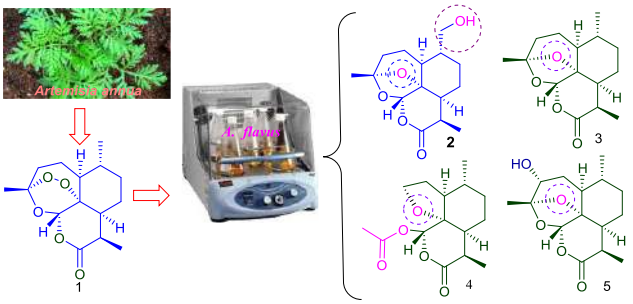
On the Structural Solution of (*R*)-2- Methylheptyl Isonicotinate: Evidence for the Structure Solution from Total Synthesis

The controversial molecular identification of (*R*)-2-methylheptyl isonicotinate (**1**) has been settled. Despite its significance as a potent anti-microbial agent against several clinically relevant pathogens, the structure of natural product is uncertain so far due to controversial reports. Its structure has been resolved as bis (2-ethylhexyl) phthalate (**2**) by total syntheses of chain isomers. In addition, we have also revised bis (2-methylheptyl) phthalate (**3**) as (**2**) in some reports. (*Nat. Prod. Commun.*, **2018,** 13, 335)



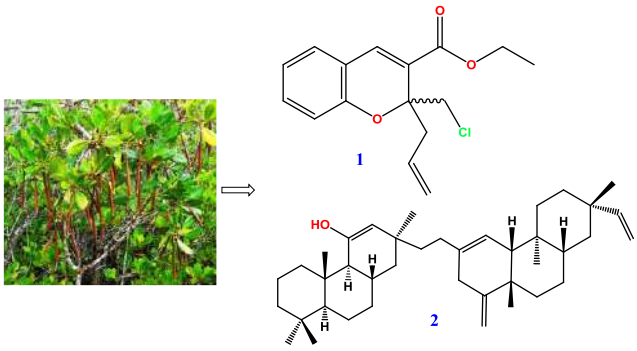
Biotransformation of Artemisinin to 14-hydroxy deoxyartemisinin: C-14 hydroxylation by *Aspergillus flavus*

The biotransformation of the front-line antimalarial drug, artemisinin (1) by the filamentous fungus *Aspergillus flavus* MTCC-9167 was investigated. Incubation of compound 1 with *A. flavus* afforded a new hydroxy derivative (**2**) along with three known metabolites (3-5). The new compound was characterized as 14-hydroxydeoxyartemisinin (**2**) by extensive spectroscopic data analysis (IR, ^{1}H, ^{13}C NMR, HSQC, HMBC, COSY, NOESY and HR-ESIMS). The known metabolites were identified as deoxyartemisinin (3), artemisinin G (4), and 4α-hydroxydeoxyartemisinin (5). This is the first report of hydroxylation of a secondary methyl of artemisinin at C-14 by the fungus *A. flavus*, which is synthetically not accessible. In addition, these compounds were evaluated for their *in vitro* anti-plasmodial activity. Artemisinin G (4) exhibited IC_{50} values in submicromolar concentration compared to non-peroxidic metabolites. (*J. Agric. Food Chem.*, **2018,** 66, 10490)



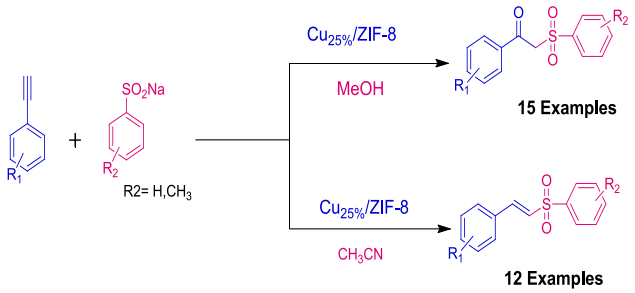
Two New Cerioptins (A-B) from the Mangrove *Ceriops Tagal*

Two novel compounds (1-2), cerioptins A-B, along with seven known compounds were isolated from the mangrove, *Ceriops tagal*. These new compounds were characterized as a rare ethyl-[(2-allyl-2-chloromethyl)-2H-1-benzopyran]-3-carboxylate (1) and a novel tetraterpenoid congener of heterodimeric diterpenoid, pimara-11-enol-(16→2')-dolabra-1,4 (18), 15-triene (2) by extensive modern spectro scopic 2D NMR [COSY (correlation spectroscopy), NOESY (Nuclear Overhauser Effect Spectroscopy), HSQC (heteronuclear single-quantum correlation), HMBC (heteronuclear multiple bond correlation)], IR (infrared) and mass data analysis. The naturally occurring new heterodimeric diterpene is derived from two new diterpenes as pimara-11-enol and dolabra-1,4(18),15-triene. (*Chemistry Select*, **2018,** 3, 8926)



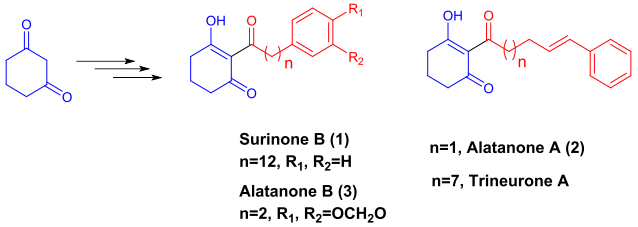
Cu-Doped Zeolitic Imidazolate Framework Catalysed Highly Selective Conversion of Alkynes to B-Keto and Vinyl Sulfones using Sodium Sulfinates

Cu^{2+}-doped zeolitic imidazolate framework-8 (ZIF-8) catalyzed one-pot procedure to synthesize β-keto and vinyl sulfones by the direct oxysulfonylation and hydrosulfonylation of alkynes via radical reaction under mild conditions were described. The advantages of this protocol included broad substrate scope and excellent β-keto and E-stereoselectivity. The Cu/ZIF-8 particles not only exhibit excellent performances but also had a great stability in the reaction, succesfully allowing their reuse up to 5 recycles. This efficient Cu/ZIF-8 heterogeneous catalyst is explored first time for C-S bond formation. (*J. Chem. Sci.*, **2019**, 131, 1)



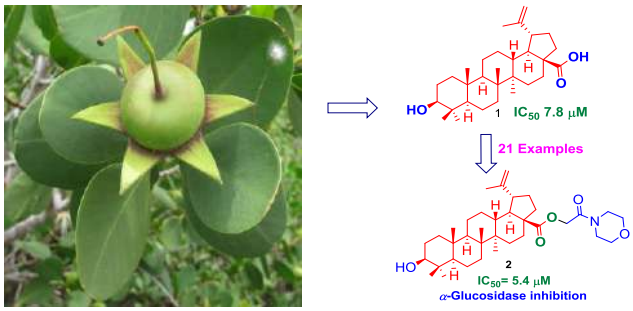
Total Syntheses of Surinone B, Alatanones A-B and Trineurone A

The total syntheses of four polyketides, surinone B (**1**), alatanones A–B (**2**–**3**), and trineurone A (**4**) were accomplished through an efficient and unified strategy via one-pot C-acylation reaction coupling 1,3-cyclohexadiones with EDC-activated acids under mild conditions. Alatanone A (**2**) was found to be a potent anti-microbial agent against Gram-positive and Gram-negative bacteria with MIC 31.25 µg/ml while alatanone B (**3**) was found to be a potent anti-fungal agent against *Cladosporium cladospori oides* with MIC 62.5 µg/ml compared to cycloheximide MIC 125 µg/ml. Our methodology allows performing kilogram scale of these scarce polyketides for the development of new antimicrobials. (*J. Asian Nat. Prod. Res.*, **2019,** 31, 262)



Betulinic Acid Derivatives: A New Class of A-Glucosidase Inhibitors and LPS-Stimulated Nitric Oxide Production Inhibition on Mouse Macro phage RAW 264.7 Cells

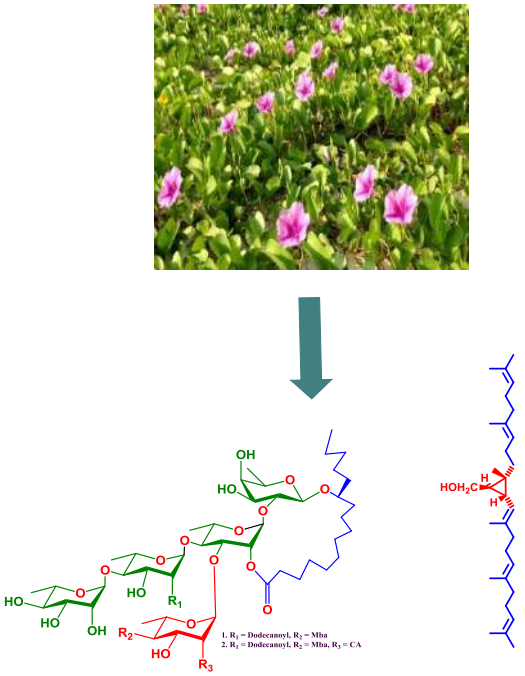
Chemical manipulation studies were conducted on betulinic acid (**1**), twenty-one new rationally designed analogues of **1** with modifications at C-28 were synthesized for their evaluation of inhibitory effects on α-glucosidase and LPS-stimulated nitric oxide production in mouse macrophage RAW 264.7 cells. Compound **2** (IC_{50} = 5.4 µM) exhibited an almost 1.4-fold increase in α-glucosidase inhibitory activity on yeast α-glucosidase while analogues **5** (IC50 16.4 µM) and **11** (IC50 16.6 µM) exhibited a 2-fold enhanced inhibitory activity on NO-production than betulinic acid. (*Nat. Prod. Res.*, **2019**, 33, 2618)



Ipomeolides A and B, Resin Glycosides from *Ipomoea pes-caprae* and Combination Therapy of Ipomeolide A with Doxorubicin

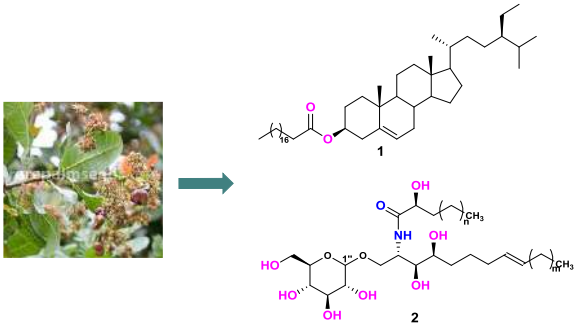
Two new resin glycosides, ipomeolides A (**1**) and B (**2**), both with an unusual non-linear heteropenta saccharide core along with five known compounds were isolated from the *n*-hexane:$CHCl_3$ (1:1) extract of the aerial parts of *Ipomoea pes-caprae*.

Ipomeolides A (**1**) and B (**2**) are macrolactone analogues of the rare (11*R*)-jalapinolic acid and macrolactonization occurred at C-2 of the second saccharide moiety. Compounds **1** and **2** show structural variation even in the pentasaccharide core. The structures of **1** and **2** were established by a combination of spectroscopic techniques as well as chemical modifications such as acetyl and acetonide derivatives as well as hydrolysis products. The new glycosidic acid was named ipomeic acid (**1c**). Compounds **1**, **1b,** and **2b** were evaluated for cytotoxicity against human tumor cell lines. Compounds **1b** and **2b** were not effective on epithelial cells, but affected survival of K-562, which is of hematopoietic origin. Sub lethal concentration of compound **1** (4 μM) when used in combination with 1 μM doxorubicin, an anticancer agent significantly enhanced cytotoxicity to tumor cells. Such combined synergistic potency against leukemia cells and the absence of effects on epithelial cells may be beneficial for chemotherapy with minimal side effects to treat CML (Chronic Myeloid Leukemia) malignancies. (*J. Nat. Prod.*, **2019**, 82, 1292)



New *n*-Nonadecanoyl-β-sitosterol and other Constituents from the Stem-bark of *Anacardium occidentale*

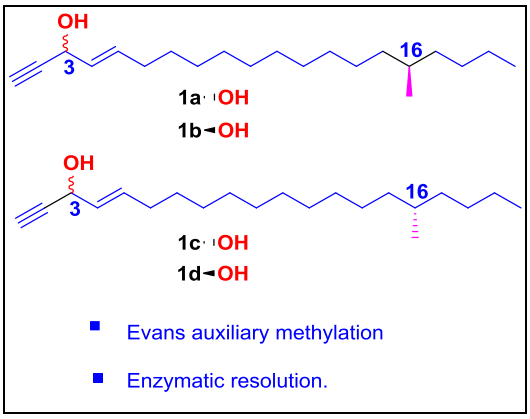
A new steroidal ester bearing *n*-nonadecanoyl moiety (**1**) and a mixture of isomeric cerebrosides (**2**) along with two known compounds were isolated from the methanol extract of the stem-bark of *Anacardium occidentale*. The structure of the new steroidal ester was determined as 3-*n*-nonadecanoyl-β-sitosterol on the basis of modern spectroscopic techniques (IR, ESI-MS, HR-ESIMS, 1D and 2D NMR) and chemical degradation studies. The structures of the known compounds were identified as gallic acid and tanacetene by comparison of the spectroscopic data with those of reported data. The mixture of cerebrosides was confirmed based on the analysis of 1D and 2D NMR. These compounds were evaluated for cytotoxicity against human cancer cell lines A549, SCOV3 and rat normal cell line NRK49f. (*https://doi.org/10.1080/14786419.2019.1650353*)



Asymmetric Total Synthesis of 16-Methyleicos-(4*E*)-en-1-yn-3-ol from the Marine Sponge *Cribrochalina vasculum*: Establishment of Absolute Configuration of Chiral Centers

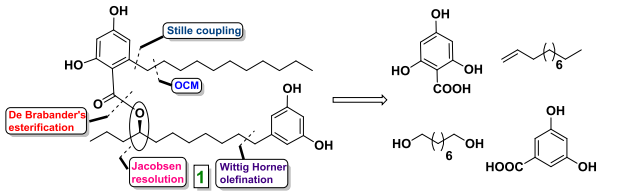
The first total synthesis of 16-Methyleicos-(4*E*)-en-1-yn-3-ol, a bioactive component of the marine sponge *Cribrochalina vasculum* was achieved by Evans auxiliary methylation followed by resolution of the corresponding racemates using lipase formulation Novozyme 435 and Mosher's ester method. We report the asymmetric syntheses of four diastereomers (**1a-d**) of the natural compound **1** and

established the absolute configuration of chiral centers, leading to the revision of the natural product configuration from 3 *S* to 3 *R*. (*Chemistry Select*, **2019**, 4, 399)



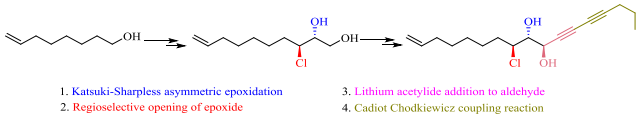
Bioinspired First Stereoselective Total Synthesis of Spinosulfate B

An efficient bioinspired stereoselective first total synthesis of spinosulfate B has been accomplished following Jacobsen's hydrolytic kinetic resolution, Stille coupling, olefin-cross metathesis (OCM), Wittig Horner olefination, and De Brabander's esterification as key steps. (*Chemistry Select*, **2019**, *4*, 8911)



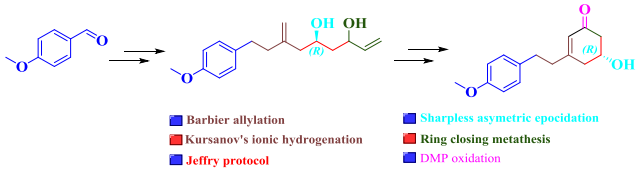
First Stereoselective Total Synthesis of Ciryneol C

The acetylene derivative ciryneol c was isolated from the roots of c. Japonicum. The asymmetric total synthesis of ciryneol c was achieved in seven steps, with horner–wittig olefination, regioselective epoxide opening, and cadiot–chodkiewicz coupling reactions being the key steps. (*SynOpen*, **2019,** 03(02), 59)



A Stereoselective Synthesis of (R)-5-hydroxy-3-(4-methoxyphenethyl) Cyclohex-2-enone, towards Total Synthesis of Prelunularin

A first chiral strategy for synthesis of (R)-5-hydroxy-3-(4-methoxyphenethyl) cyclohex-2-enone reported. Key transformation includes Barbier allylation, ionic hydrogenation, Jeffery reaction, Katsuki Sharpless asymmetric epoxidation, reductive opening of epoxide and ring closing metathesis. (*Tetrahedron Lett.*, **2019,** 60 (41)**,** 151134)



Synthesis and Biological Evaluation of Schizandrin Derivatives as Potential Anti-Cancer Agents: A new series of Schizandrin (1) derivatives were synthesized utilizing the C-9 position of the Schizandrin core and evaluated for their cytotoxic activities against HeLa (cervical cancer), A549 (lung cancer), MCF-7 (breast cancer) and DU-145 (prostate cancer) cell lines. Among the synthesized series, 4e, 4f, 4g and 5 showed potent activities against tested cell lines. More significantly, compound 5 exhibited most potent cytotoxic activity against DU-145 with an IC50 value of 1.38 µM which is comparable to the standard agent, doxorubicin. Further, flow cytometry analysis indicated that **5** arrested cells in G2/M phase and consequently leading to apoptosis. Molecular docking analysis showed that **5** occupied the colchicine binding pocket of tubulin. Overall, the present study demonstrates that **5**, as a mitotic-agent. (*https://doi.org/10.1016/j.ejmech.2018.02.066*)

Pharmacokinetic Study on Piplartine and Piperine after Oral Administration of *Piper Chaba* Root by Liquid Chromatography-Mass Spectrometry/ Mass Spectrometry: Background: Piperaceae family are a well-known source of structurally diverse amides with the wide range of bioactivities

such as cytotoxic, stomach aches, insect repellents, anti-inflammatory, insecticidal, and antifeedant activities. It has been reported that piplartine and piperine, alkaloid/amide compounds from *Piper* species, show antitumor activities. **Objective:** A rapid, sensitive liquid chromatography-tandem mass spectrometry method has been developed and validated for the determination of piplartine and piperine from *Piper chaba* extract. **Materials and Methods:** The two analytes, together with internal standard (IS, trichostachine), were separated on a Waters Acquity ethylene bridged hybrid C_{18}(2.1 mm × 100 mm, 1.9 μ) column using a mobile phase of acetonitrile with 0.1% formic acid and water with 0.1% formic acid (70:30, v/v) with isocratic elution. The detection was performed using the positive ion electrospray ionization in multiple reaction monitoring mode with transitions at m/z 318→221 for piplartine, m/z 286→201 for piperine, and m/z 272→201 for the IS. **Results:** The calibration curves were both linear (r^2 > 0.995) over a concentration range of 1.0–2000 ng/mL; the lower limit of detection quantification was 1.0 ng/mL for both piplartine and piperine. The intra-day and inter-day precisions (relative standard deviation %) were <10.9%, and recoveries ranged from 90.3% to 103.0%. **Conclusions:** The analytes were proven stable in the short-term, long-term, and after three freeze-thaw cycles. The method was successfully applied to pharmacokinetic studies of piplartine and piperine in rats after oral administration of *P. chaba* extract. **Abbreviations used:** AUC: Area under the curve; BEH: Ethylene bridged hybrid; CDER: Centre for drug evaluation and research; CID: Collision-induced dissociation; C_{max}: Maximum concentration; CTO: Column Temperature Oven; DGU: Degassing Unit; ESI: Electrospray ionization; eV: Electron volt; FCV: Flow control valve; HPLC: High-pressure liquid chromatography; HPTLC: High performance thin layer chromatography; IS: Internal standard; LLOQ: Lower limit of quantitation; LC: Liquid chromatography; LC-MS: Liquid chromatography-Mass Spectrometry; LC-MS/MS: Liquid chromatography-Mass Spectrometry/Mass Spectrometry; LC-HRMS: Liquid chromatography-High resolution mass Spectrometry; LC-NMR-MS: Liquid chromatography-Nuclear magnetic resonance-Mass Spectrometry; MRM: Multiple reaction monitoring; MC: Methyl cellulose; N_2: Nitrogen; RSD: Relative standard deviation; RE: Relative error; r^2: Regression coefficient; $t_{1/2}$: Half-life; T_{max}: Time to maximum effect; QC: Quality control; UFLC: Ultrafast liquid chromatography; UPLC-qTOF-MS: Ultra pressure liquid chromatography-Time of flight-Mass spectrometry; USFDA: United states Food and Drug Administration. (*Pharmacog. Magazine*, **2018**, 14(55), 161)

UPLC–MS/MS Quantitative Analysis and Structural Fragmentation Study of five Parmotrema Lichens from the Eastern Ghats: Comparative phytochemical analysis of five lichen species [Parmotrema tinctorum (Delise ex Nyl.) Hale, P. andinum (Mull. Arg.) Hale, P. praesorediosum (Nyl.) Hale, P. grayanum (Hue) Hale, P. austrosinense (Zahlbr.) Hale] of Parmotrema genus were performed using two complementary UPLC-MS systems. The first system consists of high resolution UPLC-QToF-MS/MS spectrometer and the second system consisted of UPLC-MS/MS in Multiple Reaction Monitoring (MRM) mode for quantitative analysis of major constituents in the selected lichen species. The individual compounds (47 compounds) were identified using Q-ToF-MS/MS, via comparison of the exact molecular masses from their MS/MS spectra, the comparison of literature data and retention times to those of standard compounds which were isolated from crude extract of abundant lichen, P. tinctorum. The analysis also allowed us to identify unknown peaks/compounds, which were further characterized by their mass fragmentation studies. The quantitative MRM analysis was useful to have a better discrimination of species according to their chemical profile. Moreover, the determination of antioxidant activities ($ABTS^+$ inhibition) and

Advance Glycation Endproducts (AGEs) inhibition carried out for the crude extracts revealed a potential antiglycaemic activity to be confirmed for P. austrosinense.
(*https://doi.org/10.1016/j.jpba.2018.04.017*)

***Diospyros melanoxylon* (Roxb.): A Tribal Fruit that Maintains Euglycemic State after Consumption and Cools Oxidative Stress:** Tendu, *Diospyros melanoxylon* Roxb. (Family: Ebenaceae) fruit is indigenous to the Indian subcontinent. The ripe fruit of tendu is eaten by tribal people. Both, unripe, as well as ripe fruits, have been used in folk-medicine by tribal communities. Aqueous methanol extract of unripe fruit displayed potent free radicals scavenging properties and also mitigated free radicals induced DNA damage. Furthermore, this extract also alleviated the development of oxidative stress induced due to a hyper physiological concentration of H_2O_2 and glucose in NIH 3T3 cells. FACS analysis revealed that extracts significantly (p <0.001) prevented the build-up of reactive oxygen species in NIH 3T3 cells generated due to a hyper physiological concentration of H_2O_2. Total polyphenols, flavonoids, and anthocyanins were present in unripe fruit were observed radically decreased when the fruit ripened. Presence of pancreatic α-amylase, intestinal α-glucosidase, and pancreatic lipase inhibitory activities in fruit extracts were also recorded. Postprandial glycemic excursion of unripe as well as ripe fruits pulp were significantly (p <0.05) less than that induced due to oral sucrose administration. Results suggest for the first time that fruit of *D. melanoxylon* may become an economic beverage fully equipped to counter free radicals and resultant oxidative stress. Furthermore, fruit may serve as a true euglycemic sweetener against sucrose. (*http://nopr.niscair.res.in/handle/123456789/45557*)

A One-pot Facile Construction of 1*H*-1,2,3-Triazolyl1,2-Dihydropyridyl Derivatives and Evaluation of Bioactivity Profile: A one-pot, facile method has been established for the preparation of 1*H*-1,2,3-triazolyl 1,2-dihydro pyridyl derivatives **6 a-y**. The ring opening of the chromone and cyclo addition are the notable reactions to achieve the target compounds **6 a-y**. All the compounds were screened for their antiproliferative, free radical scavenging (DPPH,$ABTS^{\cdot+}$), α-glucosidase inhibitory and anti-inflammatory activities. The bioactivity profile revealed that the compounds 6 **x-y** were shown potent antiproliferative activity against HeLa cell line, while compounds 6 **e-h and 6 w** identified as potent $ABTS^{+\cdot}$ and **6n** identified as potent DPPH free radical scavenger. Compounds **6 h-i, 6 p-r, 6 u** and **6 w** denoted promising anti- inflammatory activity. (*Chemistry Select*, **2018**, 3, 13729)

Administration of Roasted Barley and Roasted Horse Gram Powders Pacified Chronic Sucrose-Induced Dysglycemia and Dyslipidemia in Rats and Exerted in Vitro Potent Antioxidative Stress Effect: Background: Sugar-enriched diets/beverages consumption aggravates dysglycemia, dyslipidemia, insulin resistance, glucose intolerance, and weight gain. If unchecked, these disturbances culminate into diabetes. Indian medical classics advise consumption of roasted barley (BR) and roasted horse gram (HG) to resolve such issues. **Objective:** To investigate impact of BR and HG in chronic sucrose-induced dysglycemic rats. **Materials and Methods:** Dysglycemia was induced in rats by oral feeding of 40% sucrose solution continuously for 2 months. Later, rats were treated with test samples at a dose of 4 g/kg body weight twice a day for 1 month after withdrawal of sucrose feeding. Oral glucose tolerance test was performed at the end of experimental period. Biochemical and hematological parameters were analyzed accordingly. Nutritional contents and antioxidative stress activities in food grain powders were evaluated. **Results:** Chronic sucrose feeding induced glucose intolerance and weight gain. Mere sucrose withdrawal in the absence of supportive

therapy aggravated glucose intolerance. Increase in plasma triglycerides, aspartate transaminase, and alanine transaminase and disturbances in hematological parameters were also observed. BR and HG treatment pacified sucrose-induced biochemical metabolic disturbances and improved hematological parameters. BR was superior in normalizing disturbances than horse gram. These grains possess potent antioxidant activities and antioxidative stress properties and are rich source of micronutrient vitamins, minerals, essential amino acids, and fatty acids. **Conclusion:** Consumption of these food grains may resolve and normalize sucrose-induced metabolic, biochemical, and hematological disturbances. Multiple therapeutic properties originating through phytochemicals, vitamins, minerals, amino acids, and fatty acids in totality may be responsible for observed beneficial effects. (*Pharmacog. Magazine*, **2018,** 14(59) Supplement 3, 578)

Anti-Hyperglycemic and Genotoxic Studies of 1-O-Methyl Chrysophanol, A New Anthraquinone Isolated from *Amycolatopsis Thermoflava* Strain SFMA-103: The compound 1-O-methyl chryso phanol (OMC) which belongs to a class of hydroxyl anthraquinones was isolated from Amycolatopsis thermoflava strain SFMA-103 and studied for their anti-diabetic properties. OMC was evaluated as an anti-diabetic agent based on in silico studies which initially predicted the binding energy with α-amylase (-188.81 KJ mol^{-1}) and with α-glucosidase (70.53 KJ mol^{-1}). Further, these results were validated based on enzyme inhibition assays where OMC demonstrated enzyme inhibitory activity towards α-amylase (IC_{50} 3.4 mg mL^{-1}) and α-glucosidase (IC_{50} 38.49 µg mL^{-1}). To confirm the anti-diabetic activity, in vivo studies (oral dose in Wistar rats) revealed that OMC inhibited significantly the increase in glucose concentration at 100 mg/kg as compared to starch control ($p < 0.05$). Further, to understand the safety of OMC as a therapeutic agent, the genotoxic analysis was performed in both in vitro Chinese Hamster Ovary cells (250, 500, and 1000 µM/mL) and in vivo Swiss albino mice (250, 500, and 1000 mg/kg). In vitro results showed that OMC concentration of up to 250 µM/mL did not elicit significant changes in CAs, MI, and MN counts in CHO cells. Similarly, in mice experiments (i.p. injection), no significant changes in CAs, MI, and MN induction were observed till 500 mg/kg of OMC when compared with chrysophanic acid (Cy) (200 mg/kg). In addition, mice that received the lowest dose of OMC (250 mg/kg) did not show any histological changes in liver, kidney, and heart. The study concluded that five times higher therapeutic dose (100 mg/kg) of OMC can be utilized against hyperglycemia with no genotoxic effects. (*doi.org/10.1080/01480545.2018.1551406*)

***Raphanus Sativus* (Linn.) Fresh Juice Priming Moderates Sucrose-Induced Postprandial Glycemia as well as Postprandial Glycemic Excursion in Rats:** Consumption of sugar sweetened beverages increase individual's susceptibility towards weight gain, development of Type 2 diabetes mellitus, hypertension, cardiovascular disorders and number of chronic illnesses. Extended postprandial hyperglycemic rise and larger postprandial glycemic spikes following sugar ingestion in diabetic as well as non-diabetic individuals relate with the onset of cardiovascular complications and development of atherosclerosis. Oxidative stress induced due to prolonged postprandial hyperglycemia further aggravates development of diabetic complications. Influence of *Raphanus sativus* leaf and root juice on sucrose induced postprandial glycemic rise and postprandial glycemic spikes in rats was evaluated in this research. It was observed that priming rats with *R. sativus* leaf and root juice assuaged sucrose induced postprandial glycemic rise and postprandial glycemic excursions. The juice of *R. sativus* leaf was found superior than root juice in achieving these results. Similarly, the juice of leaves was more potent ($p<0.01$) in decreasing sucrose induced postprandial

glycemic load than the juice of root. Acidic in nature, juice of *R. sativus* leaf and root was rich source of polyphenol, flavonoid and displayed potent free radical scavenging activity. Additionally, juices also mitigated formation of advance glycation end-products and glycation of hemoglobin under hyperglycemic environment. (*Ind. J. Trad. Knowledge*, **2019,** 18(2), 339)

Synthesis, Free Radical Scavenging and A-Glucosidase Inhibitory Activities of 2*H*-Chromenylphenyloxazolones: A series of 2*H*-chromenylphenyloxazolones have been prepared starting from 2*H*-chromene-3-carbaldehydes. The compounds have been evaluated for their DPPH, $ABTS^{\cdot+}$ free radical scavenging and α-glucosidase inhibitory activities. Compound 4**g** has been identified as the most potent $ABTS^{\cdot+}$ free radical scavenger when compared to the standard drug. The compounds **4k**, **5a-c** and **5g** are identified as potent $ABTS^{\cdot+}$ free radical scavengers in the present series of the compounds. Compound **5g** has been identified as a promising α-glucosidase inhibitor. Molecular modeling studies have been carried out for compound **5g** to explain the molecular basis of α-glucosidase inhibition. (*http://nopr.niscair.res.in/handle/123456789/48239*)

Comprehensive Analysis of Secondary Metabolites in Usnea longissima (Lichenized Ascomycetes, Parmeliaceae) Using UPLC-ESI-QTOF-MS/MS and Pro-Apoptotic Activity of Barbatic Acid: Considering the importance of ultra-performance liquid chromatography-electrospray ionization-quadrupole time of flight-tandem mass spectrometry(UPLC-ESI-QTOF-MS/MS) hyphenated techniques for analysis of secondary metabolites from crude extracts, the present study was aimed at identification of secondary metabolites in acetone extract of the lichen *Usnea longissima*. From our study, 19 compounds were tentatively identified through comparison of exact molecular masses from their MS/MS spectra, mass fragmentation studies and comparison with literature data. In addition, potent cytotoxic activity of *U. longissima* extract prompted us to isolate four compounds, 18*R*-hydroxy-dihydroalloprotolichester inic acid (**19**), neuropogolic acid (**20**), barbatic acid (**21**)**,** and usnic acid (**22**) from this extract which were adequately identified through mass spectrometry and NMR spectroscopy. All four compounds displayed cytotoxic activity. Barbatic acid (**21**) manifested doxorubicin equivalent activity against A549 lung cancer cell line with IC_{50} of 1.78 µM and strong G0/G1 accumulation of cells. Poly ADP-ribose polymerase (PARP) cleavage confirmed that it induced cytotoxic activity via apoptosis. Finally, our work has discerned the depside, barbatic acid (**21**) from crude extract as a candidate anti-cancer molecule, which induces cell death by stepping up apoptosis. *(Molecules*, **2019**, 24, 2270)

Isolation, Semi-Synthesis, Free-Radicals Scavenging and Advanced Glycation End Products Formation Inhibitory Constituents from *Parmotrema Tinctorum*: Bioassay-guided separation of acetone extract from lichen *Parmotrema tinctorum* (Delise ex Nyl.) Hale led to the isolation of six major phenolic constituents (**1-6**). Compounds structures were established using NMR and mass spectral techniques. Further, to develop libraries on these scaffolds, a series of semi-synthetic derivatives were prepared (**1a-1f, 2a-2b, 3a, 5a**) and investigated for their free-radicals (2,2-diphenyl-1-picrylhydrazyl and 2,2'-azinobis(3-ethylbenz thiazoline-6-sulfonic acid) (ABTS)) scavenging and advanced glycation end products (AGEs) formation inhibitory activities. Amongst tested derivatives, **1a, 1d, 1e, 2a**, and **5a** showed strong ABTS scavenging potentials comparable to Trolox. In addition, these derivatives also manifested moderate AGEs formation inhibitory activities. (*doi.org/10.1080/10286020.2019.1628024*)

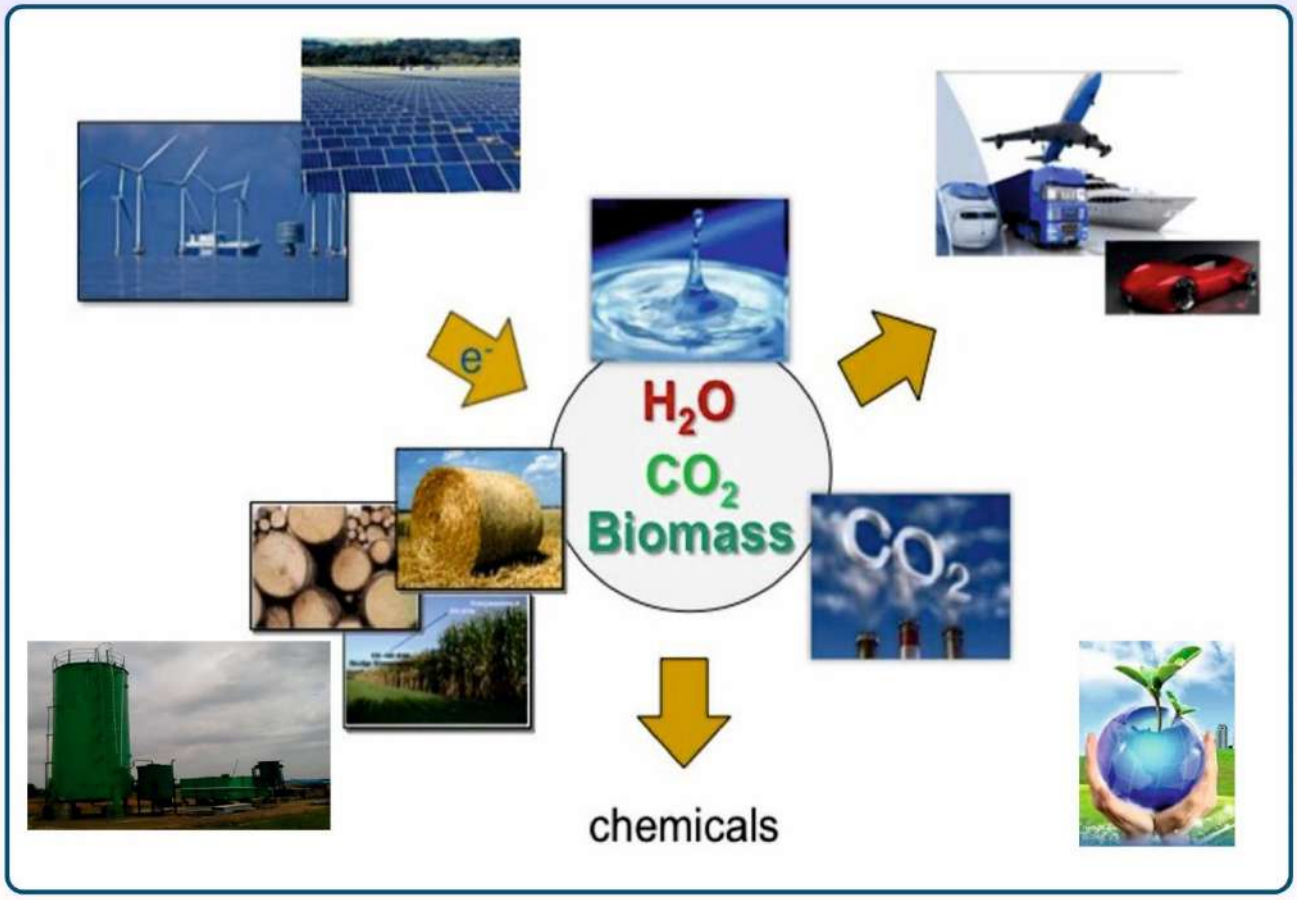
Nutritional Composition and Antioxidative Stress Properties in Boiled Tuberous Rhizome of Neel Kamal (Nymphaea Nouchali Burm. F.): *Nymphaea nouchali* (Burm. f.) is known as *Neel Kamal*,

Utpal, *Kumud* and *Indeevar* in India. Its tuberous rhizome is used for the preparation of various vegetable items, curries and pickles, and is also consumed boiled or roasted. It finds application in folk medicine for the treatment of a number of disease conditions. In this research macro- and micronutrients profiling along with phytochemical analysis of the boiled tuberous rhizome of *N.nouchali* was carried out. Furthermore, antioxidant activities and antioxidative stress potentials of aqueous methanol extract of boiled tuber were also evaluated. Boiled tuber presents a rich source of carbohydrate, protein, fat, fibres, essential amino acids and fatty acids. Simultaneously, vitamins and minerals were also present in ample amounts. The aqueous methanol extract of boiled tuber contains potent antioxidant phytochemicals. *In vitro* analysis on HEK-293, CHO and NIH 3T3 cell lines reveal that it effectively quashes H_2O_2 induced oxidative stress and protects DNA against free radical-induced damage. This research demonstrates that *N. nouchali* tuber can become an economical dietary adjunct and functional food full of macro- and micronutrient that can help fight against oxidative stress originating due to modern lifestyle induced metabolic disorders. This is the first report presenting nutritional composition and antioxidative stress properties in the boiled tuber of *N. nouc.* *(http://nopr.niscair.res.in/handle/123456789/50425*)

Synthesis and Biological Evaluation of Bergenin-1,2,3-Triazole Hybrids as Novel Class of Anti-Mitotic Agents: In continuation of our investigation of pharmacologically-motivated natural products, we have isolated bergenin (**1**) as a major compound from *Mallotus philippensis*, which is deployed in different Indian traditional systems of medicine. Here, a series of bergenin-1,2,3-triazole hybrids were synthesized and evaluated for their potentials against a panel of cancer cell lines. Several of the hybrid derivatives were found more potent in comparison to parent compound bergenin (**1**). Among them, **4j** demonstrated potent activity against A-549 and HeLa cell lines with IC_{50} values of **1.86** µM and **1.33** µM, respectively, and was equipotent to doxorubicin. Cell cycle analysis showed that **4j** arrested HeLa cells at G2/M phase and lead to accumulation of Cyclin B1 protein. Cell based tubulin polymerization assays and docking studies demonstrated that **4j** disrupts tubulin assembly by occupying colchicine binding pocket of tubulin. (*Bioorg. Chem.*, **2019**, 91, 103161)

Estimation of Boswellic Acids in Herbal Formulations Containing Boswellia Serrata Extract and Comprehensive Characterization of Secondary Metabolites Using UPLC-Q-Tof-Mse: *Boswellia serrata* is a widely used herb in Indian systems of medicine and is well known for its potential medicinal properties. A chromatographic method was developed for the analysis and quantification of six boswellic acid marker compounds, i.e., keto boswellic acid (**1**), 3-O-Acetyl 11-keto β-boswellic acid (**2**), α-Boswellic acid (**3**), β-Boswellic acid (**4**), 3-O-Acetyl-α-boswellic acid (**5**) and 3-O-Acetyl-β-boswellic acid (**6**) in commercial herbal products containing *B. serrata* as an ingredient. Combining UPLC with Q-Tof-MS/MS makes the better identification of secondary metabolites and adulterants in the herbal formulations containing *B. serrata* in rapid time using fragmentation approach than the traditional approaches. In this study quantification of boswellic acids with UPLC-PDA method was performed as per the pharmacopeia guidelines. Furthermore, minor phytochemical constituents were identified and characterized with the help of LC-Q-Tof-MS/MS fragmentation data and various isoforms of boswellic acids and tirucallic acids in *B. serrata* oleo-gum-resin extract were identified. (*J. Pharm. Analy.*, **2019**, 9(6), 414)

ENERGY & ENVIRONMENTAL ENGINEERING



BASIC RESEARCH

Solid Waste Treatment and Management

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 Bio Manure

The objective of the present study is to assess the impact of TS concentration, substratemixing ratio (co digestion) and thermal pretreatment on biogas production, methane yield, VSreduction (%) 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 biomanureof 0.18 and 0.21 m3CH4/(kg VS reduced) and 3.15 and 2.8 kg/kg waste was obtained from FW atTS of 25 % and 30 % at an HRT of 41 and 31 days respectively whereas it was 0.32 and 0.43m^3CH4/(kg VS reduced) and 2.2 and 1.15 kg/kg waste from pretreated FW at an HRT of 16 and20 days correspondingly. Improvement of methane from 62 – 81 % was obtained due to thermalpretreatment. The highest nutrient recovery in terms of N, P, K was found to be 5.14, 2.6 and 3.2respectively. The results revealed that by increasing TS concentration from 25% to 30%, the biogasproduction improved in the range of 70-85% whereas the methane content in biogas increasedfrom 62 to 81 %. It was observed that the VS reduction (%) obtained in DAD reactors rangedbetween 72 % and 89 %. Highest methane yield of 0.43 CH4/(kg VS reduced) was obtained withpretreated FW co digested with CM at TS of 30%. The quality and quantity of biomanureobtained in DAD systems is noteworthy with highest nutrients recovery i.e. N, P, K values of5.14, 2.6 and 3.2 respectively (Fig. 1). (*Bioresource Tech.,* **2018**, 253, 273)

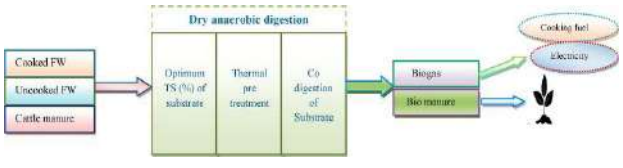


Fig. 1. Schematics experimental methodology of anaerobic co-digestion

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

This work aims to evaluate the impact of pH and initial organic load (IOL) in terms of Chemical Oxygen Demand (COD) of landfill leachate for the production of value added products during single and two stage anaerobic digestion (AD). It was observed that at an optimal IOL of 48 g/L, acetic acid was dominant at pH 5.5 whereas it was butyric acid at pH of 5.5–6.0 and 10–11. The yield of Volatile Fatty Acids (VFA) was dependent on IOL and it was in the range of 0.26 to 0.36 g VFA/(g COD removed). Methane was also harvested during single and two stage AD and found that it was varying in the range of 0.21–0.34 L CH_4/(g COD removed) and 0.2–0.32 L CH4/(g COD removed) respectively. An overall increase of 21% COD removal was noticed in two stage AD in comparison to single stage (Fig. 2). (*Bioresource Tech.,* **2018**, 251, 364)

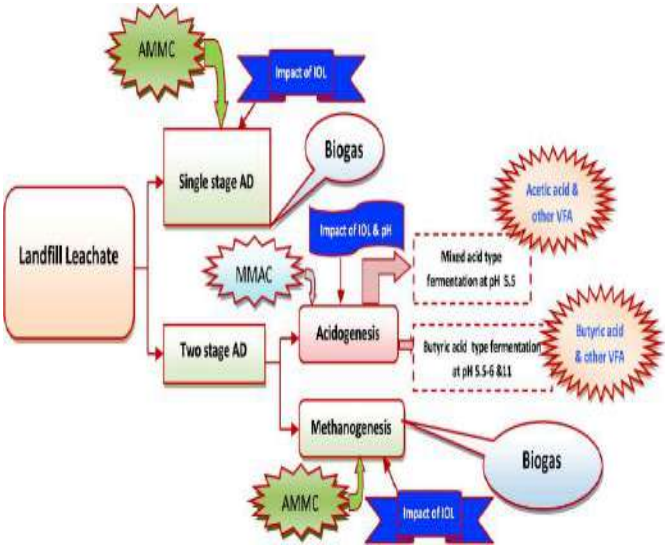


Fig. 2. Schematics experimental methodology of single and two stage anaerobic digestion

Microbial Electrochemical Technology

Microbial Electro-Hydrolysis of Sewage Sludge for Enhancing Acidogenic Production of

Biohydrogen and Volatile Fatty Acids Along with Struvite

Synergy of multi-biological unit operations was studied to maximize the resource recovery with biorefinery approach using sewage sludge (SS) as primary feedstock. Microbial electro-hydrolysis systems (MES) were used as a pretreatment system with *ex situ* and *in situ* potentials to enhance the SS solubilization against non-electrochemical control (AnT) under alkaline conditions. Subsequently, the resulting organic and nutrient-rich hydrolysates were acidogenically fermented for volatile fatty acids (VFA: C_2–C_5), biohydrogen (Bio-H_2) and struvite production. Comparatively, applied potential MES (polarized) resulted in high SS solubilization (27.5%) than MES-closed circuit (21.5%) and MES-open circuit (14.8%). In contrast, low SS solubilization was found in AnT (8.8%). SS pretreatment with alkali MES improved sludge flocs disintegration with increase in SCOD solubilization. Voltammograms of MES showed involvement redox mediators like cytochrome-c and cytochrome-b_c during SS solubilization, which play a major role in electron transport chain, specifically under microbial electro-catalyzed conditions. FE-SEM showed degradation of SS structures with MES-AP pretreatment, while FE-SEM-EDX spectrum also showed changes in elemental composition. Subsequent utilization of organic-rich hydrolysate in acidogenic fermentation (AFR) resulted in high VFA (4.65 g/L) and Bio-H_2 (21%) production. Relatively, MES-AP-hydrolysate resulted in high VFA production with maximum acidification degree. Rich nutrient content of SS hydrolysate resulted in good struvite precipitation (phosphate fertilizer), which was confirmed with structural morphology and crystalline nature (Fig. 3). The findings concluded on the alliance of multiple biological systems for sewage sludge (SS) valorization towards VFA, Bio-H_2 and struvite production. *(Chem. Engg. J.*, **2019**, 374, 1264*)*

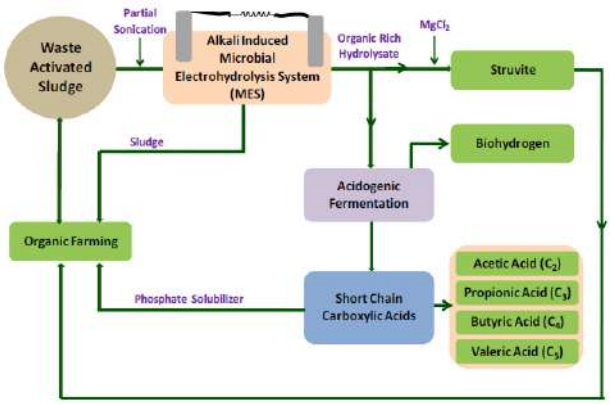


Fig. 3. Schematics experimental methodology designed in a closed loop approach

Bio-Compatible Electrodes for Microbial Fuel Cell

Graphene Modified Electrodes for Microbial Fuel Cell

Potential reduced graphene oxide electrodes were fabricated using dip-coating method followed by electrochemical reduction for microbial fuel cell (MFC) applications. The physical characterization and formation of graphene oxide (GO) and electrochemically reduced graphene oxide (ERGO) was validated using X-ray diffraction (XRD) and Raman spectroscopy techniques. Electrochemical characterization of electrodes using cyclic voltammetry and electrochemical impedance spectroscopy, showed improved properties of ERGO with high current response, enhanced charge storing capacity and less charge-transfer resistance. The MFC with ERGO-modified anode improved the power density by 17.5- and 8.75-times compared to CC and GO, respectively. Higher open circuit potential of ERGO (0.75 V) suggests higher electrogenic activity at anode, while cyclic voltammetry depicted more intense redox peaks for ERGO that highlight higher catalytic activity and rapid electron transfer. The high performance of ERGO electrodes is attributed to the large specific surface area and efficient charge transfer process. It demonstrated fabrication of efficient and cost-effective ERGO electrodes by the simple technique with their application in MFC to achieve increased power production (Fig. 4). Synergistic effect of the

large surface area for bacterial colonization and high conductivity of ERGO is responsible for its superior performance. (*J. Mat. Sci.*, **2019**, 54(17), 11604)

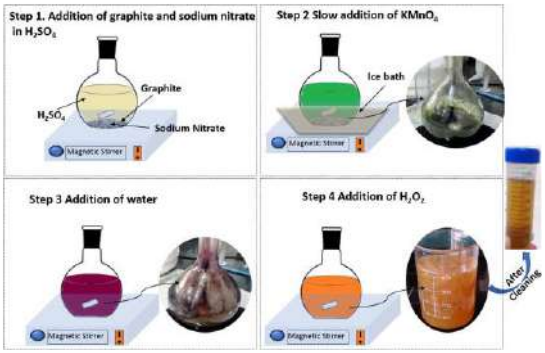


Fig. 4. Schematic showing stepwise synthesis of graphene oxide by modified Hummers' method

Modified Conductive Polyaniline-Carbon Nanotube Composite Electrodes for Microbial Fuel Cell

Anode with specifically good electrocatalytic capabilities is required to reduce ohmic losses during microbial fuel cell (MFC) operation. Highly conductive polymers viz., Polyaniline (PANi) and Polyaniline/Carbon nanotube (PANi/CNT) composite were prepared by *in situ* oxidative chemical polymerization method. Electrodes were fabricated as coatings on stainless steel mess (SSM) as anode and evaluated against SSM as cathode and operated in MFC. The nanocomposite electrodes, initially characterized by analytical techniques, were evaluated as anode in MFC towards bioelectricity production and wastewater treatment. Charge-transfer capacity of materials was confirmed using cyclic voltammetry and impedance spectroscopy. The SSM-PANi/CNT showed maximum PD of 48 mW/m^2 followed by SSM-PANi (38 mW/m^2) and SSM (28 mW/m^2). It highlights synthesis of efficient, hybrid and cost-effective PANi/CNT electrodes for MFC application to achieve increased power production and wastewater treatment compared to PANi and SSM (Fig. 5). It inferred modified composites to be highly conductive with higher surface area, influencing the microbe-electrode interactions towards greater electrocatalytic activity. (*Bioresource Tech.*, **2019**, 284, 148)

Biobased Chemicals/Fuels (from Waste)

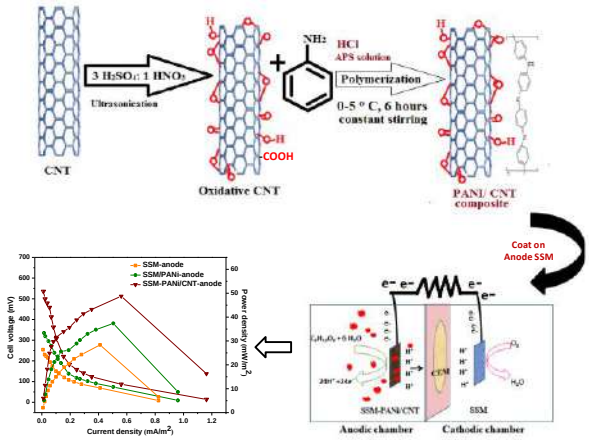


Fig. 5. Schematic showing stepwise synthesis of PANi and PANi/CNT composites by *in situ* oxidative chemical polymerization methodand operation as anode in MFC

Selective Control of Volatile Fatty Acids Production from Food Waste by Regulating Biosystem Buffering

The investigation of the role of different buffering/neutralizing agents viz., sodium hydroxide (NaOH), sodium carbonate (Na_2CO_3), calcium carbonate ($CaCO_3$) and calcium hydroxide [$Ca(OH)_2$] was evaluated towards selective production of acetic (H_{Ac}), butyric (H_{Bu}) and propionic (H_{Pr}) acid from food waste fermentation. Experiments were performed in two approaches, where systems were buffered initially (IBS) and regularly in controlled mode (CBS) with the respective studied buffering/neutralizing agent. Higher selective H_{Ac}production was observed with Na_2CO_3 CBS (5.85±0.29 g VFA/L) followed by NaOH CBS (4.2±0.12 g VFA/L) while highest H_{Bu} production (2.62±0.13 g VFA/L) followed by 1.55 ±0.04g VFA/L was achieved with the CBS and IBS operated with the combination of NaOH+$CaCO_3$ (1:2) respectively. Highest total VFA productivity was achieved with NaOH CBS (11.4±0.34 g VFA/L) followed by Na_2CO_3 CBS (10.02±0.3 g VFA/L) and

least with $Ca(OH)_2$ CBS (4.35±0.13g VFA/L). A higher degree of acidification was observed in the NaOH CBS (34.98%) while higher buffering and biohydrogen production (54±2.6%) was achieved with systems operated with Na_2CO_3 CBS and IBS respectively. Buffering intensity graphs revealed the role of supplemented and *in situ* developed carbonic acid, bicarbonate (p^{Ka} 6.35), carbonate (p^{Ka} 10.33), ammonium (p^{Ka} 9.25) and equilibrium between these buffers towards the selective VFA production (Fig. 6). The results illustrated the specific role of buffering/neutralizing agents towards enhanced and selective VFA production. (*Chem. Engg. J.*, **2019**, 357, 787)

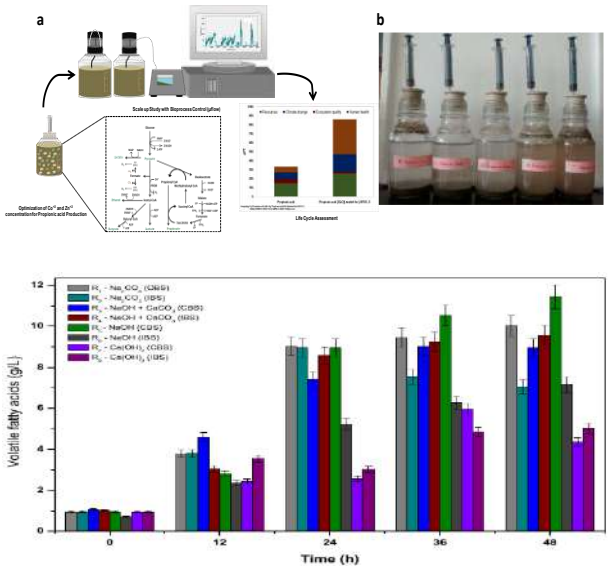


Fig. 6. Schematic of volatile fatty acids production from food waste; b) Biosystems; c) Total volatile fatty acids production with the experimental variations

Single Pot Bioprocessing for Ethanol Production from Biogenic Municipal Solid Waste

Single pot bioprocessing (SPB) strategy employing in-house laccase, cellulase plus xylanase and amylase along with hexose and pentose sugar fermenting yeasts (*Saccharomyces cerevisiae* and *Pichia stipitis*) is designed for ethanol production from biogenic municipal solid waste (BMSW). BMSW when subjected to simultaneous pretreatment and saccharification (SPS) resulted in 79.69% enzymatic digestibility and fared better compared to alkali pretreated counterparts (14.03%–51.10%). The maximum total sugar release of SPS was 146.9 g/L in 24 h. The synergism of lignin degrading laccase, hydrolytic enzymes viz., cellulase, xylanase and amylase, and *S. cerevisiae* and *P. stipitis* used for SPB of BMSWP6 at 25% (w/v) solid loading resulted in a maximum ethanol of 5.24% (v/v) in 30 h with a net bioconversion of 26.61% (g/g). Whereas, BMSWP7 subjected to 0.5% NaOH pretreatment followed by SSCF using same hydrolytic enzymes and fermenting microorganisms resulted in 5.1% (v/v) ethanol in 36 h with a bioconversion yield of 25.85% (g/g). SPB for ethanol production from BMSW is an interesting and effective alternative to MSW going to landfill or incineration with an added perk of waste to wealth conversion (Fig. 7). The research illustrates SPB as an effective resource recovering strategy from BMSW at higher feed concentration in shorter incubation time through simple and eco-friendly SPB approach. (*Bioresource Tech.*, **2019**, 283, 159)

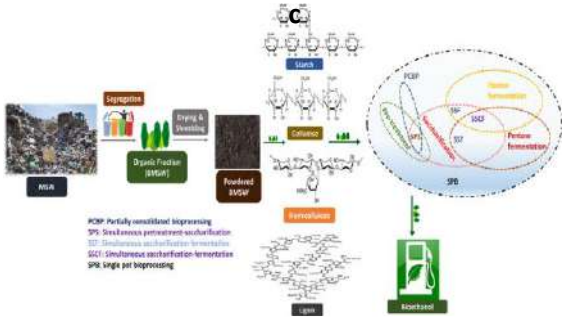


Fig. 7. Schematic representation of bioethanol production from MSW using SPB

Co-digestion of Food and Vegetable Waste Using Three Stage Integrated Bioprocess

During two-stage (Acidogenesis-Methanogenesis) process, solid organics and gaseous by-products are usually left unused. To increase resource recovery efficiency, a three-stage process (Hydrolysis/ Acidogenesis-Methanogenesis-Composting) was designed. Initially, co-digestion of food waste (FW) and vegetable waste (VW) was carried out in Leach

Bed Reactor (LBR) for hydrolysis and acidogenesis, followed by airlift reactor (ALR) for methanogenesis for 21 days using two different feedstocks [2:3 FW:VW~FVW; FW alone]. The diversion of the gaseous by-products (H_2 and CO_2) from the first stage of the LBR to the second stage of the ALR was also studied for the combined benefits of wet AD, biogas circulation and composting process to enhance methane recovery. Results depicted co-digestion of FW and VW influenced leachate characteristics and VFA dynamics leading to an increase in H_2 and CH_4 recovery from FVW and VFA and H_2 from FW. Three different functional zones in three separate chambers significantly accelerated organic removal rate while gas diversion increased overall methane recovery. Gas transfer from LBR to ALR promoted hydrogenotrophicmethanogenesis in ALR during two-stage AD process. In third stage, residual solid organic matter from LBR was subjected to aerobic composting and compost with N (%): 2.90 and 2.76; C/N ratio: 18.2 and 20.8 for FVW and FW was recovered. Integrating three processes enhanced "C" recovery where residual organic fraction in LBR was utilized and established as model for Zero discharge into environment (Fig. 8).

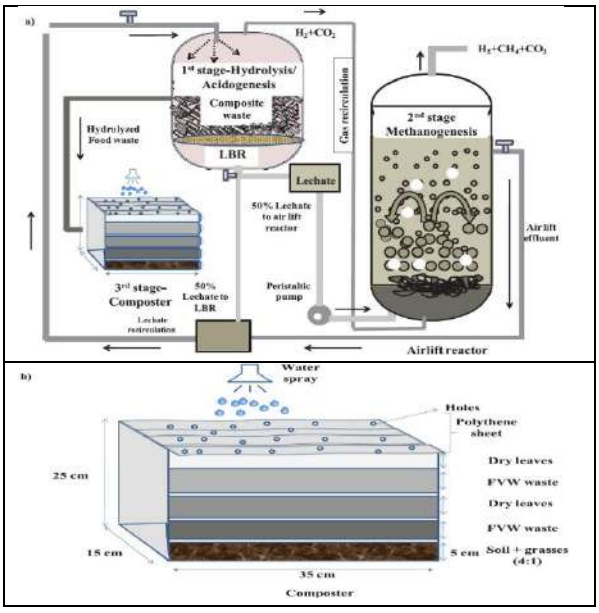


Fig. 8. (a) Three-stage (Hydrolysis/Acidogenesis-Methano genesis-Composting) reactor; (b) composter

The three-stage process has advantages of zero waste generation and overall process stability, accounting for resource efficient circular loop. Novel compact three-stage anaerobic digester (LBR Air lift-Composting) increases process stability and resource recovery efficiency. (*Bioresource Tech.*, **2019**, 284, 373)

Non-Lethal Nitrate Supplementation Enhances Photosystem II Efficiency in Mixotrophic Microalgae towards the Synthesis of Lipids and Proteins

Understanding the effect of two different concentrations of nitrate ($NaNO_3$) i.e., 2.94 mM (1X) and 8.82 mM (3X) on the productivity of *Scenedesmus* sp. in terms photosynthetic efficiency, growth, biomass and protein/lipid synthesis was evaluated. Experiments were conducted by growing the microalgae in mixotrophic mode with a fixed dissolved organic carbon (110 mM). The growth kinetics in lieu with biomass production, chlorophyll content, carbohydrate, protein and lipid accumulation were studied under mixotrophic growth cultivation. Chlorophyll a fluorescence fast kinetics parameter such as F_V/F_M, F_M/F_O, Pi-Abs, TRo/RC and ABS/RC depicted an improved PSII efficiency in 3X conditions when compared to 1X cultures thereby improving the overall growth and biomass. Results clearly indicated that higher nitrate concentration in BBM medium favored better assimilation of chlorophyll pigments, carbohydrates (160 mg/g), proteins (524 mg/g) and total lipids along with higher biomass (11.4 g/L) (Fig. 9). Microalgae cell growth, biomass and biochemical composition are significantly influenced by excess nitrates supplementation in growth medium. (*Bioresource Tech.*, **2019**, 283, 373)

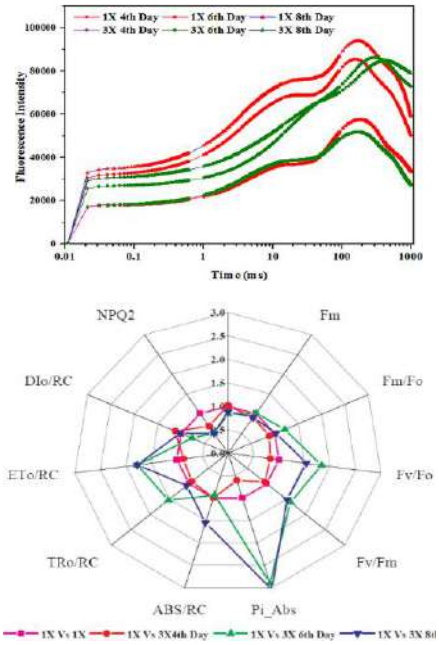


Fig. 9. (a) OJIP curves showing Chlorophyll-a fluore scence intensity;(b) JIP parameters showing PSII efficiency of Scenedesmus sp. under 1X and 3X nitrates treatment in mixotrophic conditions

CO_2 Bio-Sequestration to Chemicals

Capacitive Biocathodes Driving Electrotrophy Towards Enhanced CO_2 Reduction for Microbial Electrosynthesis of Fatty Acids

Electron transfer towards biocathode is a rate limiting step for CO_2 reduction during microbial electrosynthesis (MES). Understanding on electrotrophy using four different electrode materials viz., carbon cloth (CC), stainless-steel mesh (SS), combination of both (CC-SS) and a hybrid material (CC-SS-AC with activated carbon (AC)) as capacitive biocathodes for MES was evaluated. Key functioning abilities of electrode materials as biocathodes in terms of electrotrophy, catalytic currents, electrochemical impedance, reductive behavior, etc., were performed. Non turn-over and turn-over electrochemical investigations revealed electrode properties to be relatively higher with CC-SS-AC and CC-SS. Acetic acid was higher in CC-SS-AC (4.31 g/l) than CC-SS (4.21 g/l), CC (3.5 g/l) and SS (2.83 g/l) along with ethanol in all biocathodes except SS. Interestingly, long-term operation of all biocathodes witnessed reduction in resistance visualized through Nyquist impedance spectra relatively efficient with CC-SS-AC. Biocompatible property of CC-SS- AC with increased surface area was presumed to be critical factor for enhancing electrotrophy linked with capacitive nature of biocathode towards enhanced bioelectrochemical CO_2 reduction (Fig. 10). Potential of MES in not only synthesizing multi-carbon biobased products, but also efficient electrotrophy deciphering role of electrode materials as capacitive biocathodes towards enhanced product synthesis was established. (*Bioresource Tech.*, **2019**, 294, 122181)

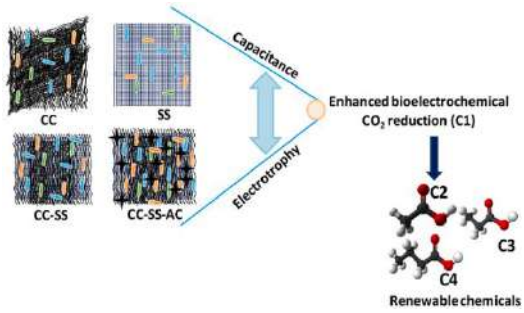


Fig. 10. Four electrode materials used as biocathodes in MES for bioelectrochemicalreduction of CO_2

Bio-succinic Acid Production:

Electron Donor and Redox Microenvironment Regulates CO_2 Fixation for Biosuccinic Acid Production in *Citrobacteramalonaticus*

Succinic acid (SA) a dicarboxylic acid is produced as an intermediate in the tricarboxylic acid (TCA) cycle has numerous applications in the agriculture, food, chemical, pharmaceutical and plastics industries. Production of biobased-SA through CO_2 fixation is considered to be sustainable. Biological sequestration of CO_2 for succinic acid (SA) production was evaluated using isolated strain more closely related to *Citrobacteramalonaticus* (IICTSVMSA1), by considering critical process parameters viz., different carbon sources at various initial concentrations, buffering agent ($NaHCO_3$) concentrations and different pH conditions. Effect of H_2 as electron donor and CO_2 availability during SA production was also evaluated. Regulatory role of CO_2 and H_2 during

SA fermentation was observed in *Citrobactera malonaticus* (IICTSVMSA1). Sucrose at an initial concentration of 30 gL^{-1} at pH 7, buffering agent concentration of 10 gL^{-1} and CO_2 partial pressure of 1 bar depicted SA yield of 48.57% with 80% H_2 consumption, 69.63 mL L^{-1} h^{-1} of CO_2 fixation rate and SA productivity of 0.36 gL^{-1}. Incorporation of CO_2 and H_2 not only enhanced the SA production but also affected the total acids profile favoring the SA production over lactic, formic and acetic acids. Redox potential maintained by the supply of H_2 enhanced SA production, indicating that control of redox potential can be applied in other anaerobic fermentation processes and in industrial production of reduced biobased chemicals. The isolated strain depicted the ability to utilize diverse carbon sources towards good SA production with sucrose as substrate, indicating that reduced carbon substrates help in maximizing redox potential (Fig. 11). Positive effect of CO_2 for SA production provides scope for sustainable integration of SA and CO_2-generating biofuel industries or industrial side streams. (*Sci. Total Environ.*, **2019**, 695, 133838)

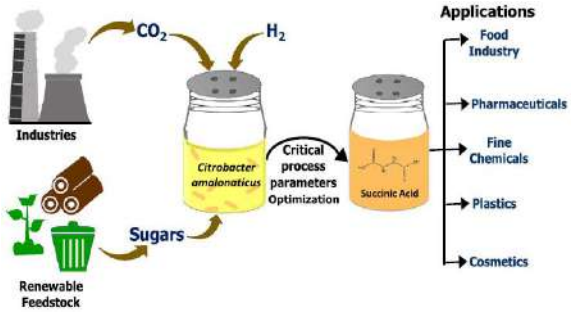


Fig. 11. Flow chart depicting the experimental methodology and applications

Circular Economy and Biorefinery

Self-Sustainable Biosystem with Circularity

Design of Self-Sustainable Azolla-Biorefinery Platform for Valorization of Various Biobased Products with Circular Cascading Design

A self-sustainable biorefinery model using azolla cultivation was designed at the focal point of a circular loop. This model is aimed to enable a cascading valorization of bio-based products through a series of sequentially integrated biological/thermal unit operations. *Azollapinnata* with an inherent ability to sequester CO_2 along with simultaneous nitrogen fixation capability serves as a potential and renewable carbon resource (feedstock) for the integrated unit operations viz., acidogenesis, photosynthesis, hydrolysis, and pyrolysis. The cascading loop is initiated by acidogenesis of spent wash (distillery wastewater-DSW) in a semi pilot scale bioreactor for the production of biohydrogen and volatile fatty acids (VFA). Treated spent wash after acidogenesis (TSW) was used as feed for *Azollapinnata* cultivation, which eventually depicted good COD and nitrates removal efficiency. Harvested *A. pinnata* biomass (AB) showed presence of good amount of carbohydrates (237 mg/g) and proteins (160 mg/g) along with 11% of lipids (composed of 22% omega fatty acids) thus making it a good nutritional feed for livestock. AB after lipid extraction was subjected to mild acid-hydrolysis and the hydrolysate was used as substrate for acidogenesis to facilitate circular/closed loop operation (Fig. 12). The techno-economics of biorefinery process evaluated using SuperPro Designer software depicted the feasibility of the integrated strategy. This study extended the scope of biobased platform with self-sustainability as core objective. (*Chem. Engg. J.*, **2019**, 373, 1042)

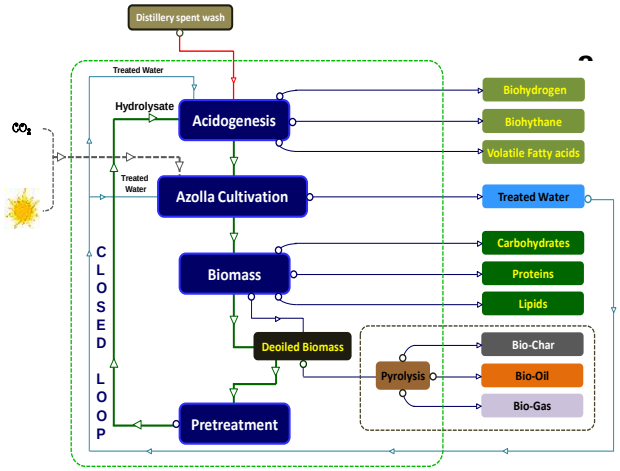


Fig. 12. Self-sustained Azolla integrated biorefinery in a circular loop framework

Azolla Derived Bioelectrode as Anode and Hydrolysate as Substrate for Electro-Fermentation Applicationsin Biorefinery Framework

This work is in continuation with the above discussed self-sustainable azollabiorefinery closed loop approach. This research focused on the use of pyrolyzeddeoiledAzolla biomass (P-DAB) as an electrode and hydrolyzed deoiledAzolla biomass (H-DAB) as substrate in MFC application for bioelectricity production. It involves P-DAB and H-DAB in double chambered MFC as biotic electrode (BE) and substrate at anode under two circuitry operations viz., open (OC) and closed-circuit (CC). The biochar obtained from pyrolyzed DAB (P-DAB) was characterized for structural and elemental functionalities using SEM, XRD and Raman spectroscopy whereas reducing sugar-rich hydrolysate obtained from hydrolyzed DAB (H-DAB) was analyzed for its composition. Experimental results indicated that at 3 g/L reducing sugar concentration, voltage of 382 mV was observed with reduction of sugars upto 43.4% (OC) and 65.6% (CC). Electrochemical characterization depicted maximum oxidative and reductive peak currents of 3.42 mA and -4.0 mA. Electrode stability was measured which showed to be stable for almost 60 days. Microbial diversity showed clear dominance of *Proteobacteria*, a phylum known for exo-electrogenic bacterial species indicating effective utilization of *Azolla*hydrolysate as substrate in MFC for power production. The DAB-derived products account to environmental sustainability and support circular bioeconomy in an integrated biorefinery mode. Self-sustained azollabiorefinery (SSAB) in a closed loop coupled with integration of various bioprocesses addresses the key challenges of current environmental/economic issues (Fig. 13). As SSAB includes valorization of liquid and solid waste in generating valuable products, it can be considered as a solution to 3R's (reduce, recycle and reuse) which reduces waste generation favoring bioeconomy. (*Sci. Total Environ.*, **2019**, 707, 135851)

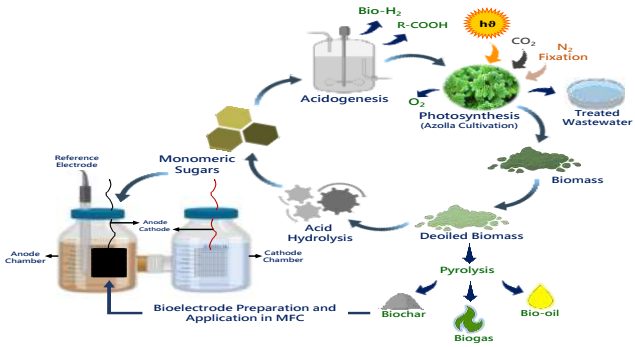


Fig. 13. Schematic of self-sustained azolla biorefinery loop utilizing the DAB in MFC

Microalgae-Biorefinery with Cascading Resource Recovery Design Associated to Dairy Wastewater Treatment

Experiments were designed and conducted in three stage process integration including photosynthesis, hydrolysis and fermentation to maximize resource recovery in a biorefinery framework. The potential of microalgae for the treatment of dairy wastewater (DWW) was studied by integrating with bioethanol production. Raw dairy wastewater (DWW) [TDS−894 ppm, Chemical oxygen demand (COD)−1746 mgL^{-1}, Nitrates−62.7 mgL^{-1}, Phosphates−152 mgL^{-1}, Sulphates−13 mgL^{-1}, pH-7.4] was collected from Telangana State Dairy Development Cooperative Federation Ltd., Hyderabad was used for the treatment using mixed microalgae. Biomass concentration was observed to increase from 3rd day and reached a maximum of 1.4 g L^{-1} by end of cycle. Organic carbon removal was observed to be 90% with simultaneous removal of nutrients. The biomolecular composition of microalgae comprised of 38% carbohydrates, 15% proteins and 22% lipids. Composition of microalgae cultivated using DWW showed higher fraction of carbohydrates and lipids than proteins. Defatted biomass load, conditions for pretreatment and fermentation need to be optimized to achieve higher ethanol production (Fig. 14). The results obtained

indicate potential of microalgae to treat dairy wastewater with simultaneous production of biomass for its use in production of multiple biobased products in a biorefinery framework. (*Bioresource Tech.*, **2019**, 284, 424)

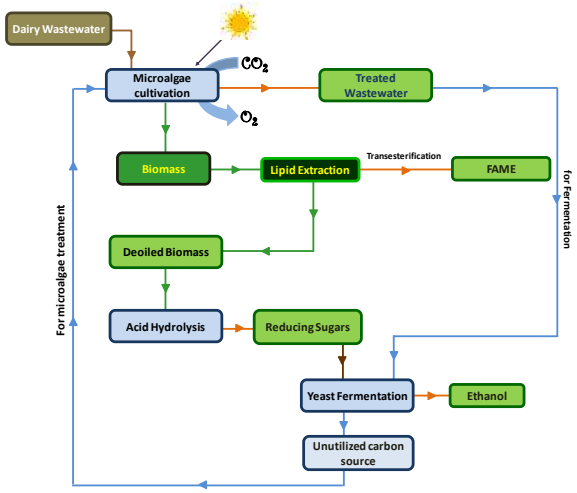


Fig. 14. Self-sustainable Algal cultivation integrated with diary wastewater treatment in closed loop biorefinery format

Ecological Engineered Wetland (Tri-phasic) Treatment System

Treatment of Azo Dye-Based Wastewater

Synthetic dyes are a major class of compounds used in the textile industry. Effluents from these industries are carcinogenic and mutagenic and pose threat to all life forms. A novel tri-phasic engineered flow-through wetland system (TEWS) with three specific microenvironments (tri-phasic aquatic systems) integrated in defined sequence was designed, to effectively treat azo dye-based textile wastewater. Tank 1 with free-floating macrophytes (*Eichhor niacrassipes*) helps to maintain anoxic microenvironment, Tank 2 with slender, submerged, perennial aquatic herbs (*Hydrillaverticillata*) helps to maintain aerobic condition by respiring underwater. Tank 3 is designed to have *Pistia stratiotes* (water cabbage) along with fish (*Gambusiaaffinis*) and snails (*Cornuaspersum*), which enables final water polishing by filter-feeding action of snails and fish and consume bacteria/planktons to remove suspended solids and colour, as well as residual carbon. Results from TEWS depicted sustainable solution for effective azo dye-based wastewater treatment, employing synergism of anaerobic and aerobic microenvironment simulated with near-natural conditions. Essential part of study contributes significantly to color and COD removal, which is supported by FT-IR and UV–Vis spectra. An overall efficiency of 76% of dye removal was achieved, with individual tanks removal efficiency accounting to 62%, 25%, and 17% in Tank 1, Tank 2, and Tank 3, respectively. Strategically designed TEWS attributes to 76%/87% of dye/COD removal. Morphological toxicity test of plants and fishes illustrate the non-toxic nature of treated effluents. TEWS not only decolorizes azo dye but also removes its toxic and mutagenic components. TEWS has the advantage of tri-phasic microenvironment and flow connections that mineralize azo dye by sequential redox reactions with anoxic, aerobic and filtering mechanisms. (*NPJ Clean Water*, **2019**, 2(1), 1)

APPLIED RESEARCH

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 m^3/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 Plants Based on AGR Technology for the Treatment of Food Waste

Food Waste (Cooked and Uncooked) as Feedstock

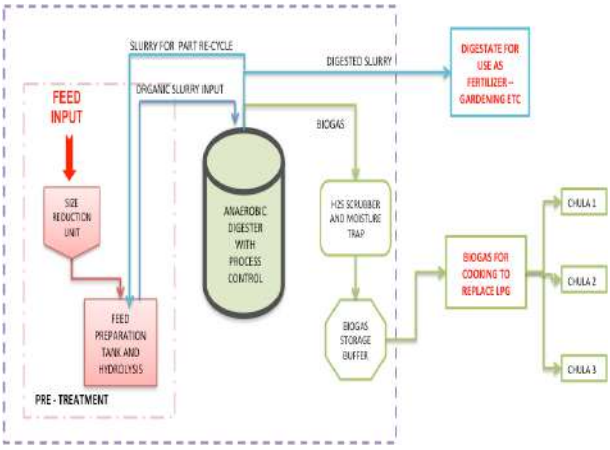
Currently, food waste across our cities and towns is rapidly increasing along with human population. Cooked and uncooked food waste collected from households, restaurants, institutional canteens etc. constitutes the food waste and it is known as organic fraction of MSW (OFMSW). Instead of land filling, 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:

Beneficiary-I:

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.

Biomethanation Process Flow



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.

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

Beneficiary-II: M/s Hyderabad Integrated MSW Limited (A Joint Venture of GHMC and M/s Ramky)

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 bio methanation 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. UpendraTripathy 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)

Beneficiary-III: The Agriculture Market Committee (AMC), Kurnool, Government of AP

One plant is installed for the treatment of 500 kg/day of market & vegetable waste at Kurnool market yard.

The biogas generated from the plant (70 to 75 m^3/day) is being used for cooking food (replacing LPG of 25 to 30 kg/day) and the same is served for approximately 500 farmers in the same market yard. Bio manure is being given free of cost to the farmers visiting the market yard.

Beneficiary-IV: Ministry of Agriculture, Govt. of Telangana

One plant is installed for the treatment of 10,000 kg/day of market & vegetable waste at Bowenpally vegetable market yard. The plant is under construction. The biogas generated from the plant (1,000 to 1,200 m^3/day) would be used for power generation (11,000 to 13,000 kWh) and the same will be used by beneficiary for replacing convention grid power. Bio manure will also be sold to customers.

Beneficiary-V: CVR Engineering College (Hyderabad)

Replacing LPG consumption (approximately 2cylinders, 14.2 kg each) with biogas (70-75 m^3/day of biogas) for decentralized cooking applications at the kitchen of College along with 75- 100 kg/day of bio manure is utilized as fertilizer in the garden.

Beneficiary-VI: CSIR-IICT, Hyderabad

Replacing LPG consumption (approximately 1 cylinder, 14.2 kg each) with biogas (30-35 m^3/day of biogas) for decentralized cooking applications at the kitchen of College along with 40- 50 kg/day of bio manure is utilized as fertilizer in the garden.

Beneficiary-VII: University College of Engineering, Osmania University (Hyderabad)

Replacing LPG consumption (approximately 2cylinders, 14.2 kg each) with biogas (70-75 m^3/day of biogas) for decentralized cooking applications at the kitchen of College along with 75- 100 kg/day of bio manure is utilized as fertilizer in the garden.

Beneficiary-VIII: Capgemini, Hyderabad

Replacing LPG consumption (approximately 2cylinders, 14.2 kg each) with biogas (70-75 m^3/day of biogas) for decentralized cooking applications at the kitchen of College along with 75- 100 kg/day of bio manure is utilized as fertilizer in the garden.

Full scale biogas plant for the treatment of poultry litter based on AGR at Tooparan, Telangana

Full scale biogas plant for the treatment of food waste based on AGR at Bellary, Karnataka

Full scale biogas plant for the treatment of food waste based on AGR at Ahmadabad, Gujarat

Full scale biogas plant for the treatment of food waste based on AGR at Hubli, Karnataka

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

Biogas plant for the treatment of 5000 kg/day of organic fraction of MSW, installed at Jawahar Nagar, MSW Processing Site, Hyderabad

Full scale biogas plant for the treatment of food waste based on AGR at Rourkela, Odisha

Full scale biogas plant for the treatment of food waste based on AGR at Kurnool, AP

Full scale biogas plant for the treatment of food waste based on AGR at Capgemini, Hyderabad

Full scale biogas plant for the treatment of vegetable and market waste on AGR Technology, Bowenpally vegetable market yard-Hyderabad

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 kg/day	Type of substrate	Biogas generation (m^3/day)	Biogas utilization	Bio manure generation (kg/day)	Year of Installation
1.	Bellary (Karnataka)	1000	Food waste	120 - 150	LPG replacement (55 – 60 kg/day)	100 - 150	2015
2.	Hubli (Karnataka)	1000	Food waste	120 - 150	LPG replacement (55 – 60 kg/day)	100 - 150	2016
3.	Ahmadabad (Gujarat)	1000	Food waste	120 - 150	LPG replacement (55 – 60 kg/day)	100 - 150	2015
4.	Surat (Gujarat)	1000	Food waste	120 - 150	LPG replacement (55 – 60 kg/day)	100 - 150	2017
5.	Bhavnagar (Gujarat)	500	Food waste	55 - 70	LPG replacement (25 – 30 kg/day)	50 - 70	2017
6.	CSIR-IICT, Hyderabad	250	Food waste	25 - 40	LPG replacement (14 – 18 kg/day)	20 - 30	2017
7.	Vrindavan (UP)	1000	Food waste	120 - 150	LPG replacement (55 – 60 kg/day)	100 - 150	2017
8.	Rourkela (Odisha)	500	Food waste	55 - 70	LPG replacement (25 – 30 kg/day)	50 - 70	2017
9.	Jawahar Nagar (Hyderabad)	3,000 – 5,000	Organic fraction of MSW	210 - 350	Electricity generation (231 – 385 kWh/day)	300 - 50	2017
10.	Bowenapally Vegetable market yard, (Hyderabad)	10,000	Vegetable and market waste	800-850	Electricity generation (800 – 835 kWh/day)	1000-1050	2020
11.	Vegetable market yard (Kurnool)	500	Vegetable and market waste	55 - 70	LPG replacement (25 – 30 kg/day)	50 - 70	2018
12.	Capgemini (Hyderabad)	300	Food waste	25 - 40	LPG replacement (14 – 18 kg/day)	20 - 30	2018
13	CVR Engineering College (Hyderabad)	300	Food waste	25 - 40	LPG replacement (14 – 18 kg/day)	20 - 30	2018
14	University College of Engineering, Osmania University (Hyderabad)	300	Food waste	25-40	LPG replacement (14 – 18 kg/day)	20 - 30	2019
15	M/s AESPL	100	Poultry Litter	75 – 100	Electricity generation (80 – 100 kWh/day)	200 - 250	2013
16	Bhuj (Gujarat)	750	Food waste	80-85	LPG replacement (30 – 34 kg/day)	75 - 90	Under installation
17	Pondicherry	750	Food waste	80-85	LPG replacement (30 – 34 kg/day)	75 - 90	Under installation

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

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 Kapralake, Hyderabad and its conversion to organic fertilizer. The same is being sold in the market as soil conditioner.

Waste to Wealth Stake holders of the project of the conversion of Water Hyacinth from Kapra lake to Organic Soil Conditioner

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 m^3biofilter 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 17m^3biofilter 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 KondapallyEnvirotech Private Limited, Vijayawada.
- Commercialization of **Bio-filter** Technology for the removal of odour and VOC from chemical and allied sectors and a 17 m^3biofilter 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 m^3 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. 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.

SPONSORED RESEARCH

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 10 Ton/Day Vegetable and Market Waste 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 Department of Agricultural and marketing committee for the installation of 10 ton/day of vegentabke and market waste for the 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.

Integrated and Sustainable Treatment of Sewage and Organic Solid Waste for Decentralized Applications

Department of Science and Technology (DST) has awarded a project entitled "Integrated and sustainable treatment of sewage and organic solid waste for decentralized applications". To establish an integrated and sustainable technology incorporating Nano filtration for sewage (50-100 m^3/day) treatment and anaerobic digestion for organic solid waste for the generation of biogas (combined heat and power applications) and bio manure for decentralized applications. The project include transformation of sewage to recyclable water and organic solid waste to biogas and bio manure through Nano filtration (NF) (Aerobic Moving Bed Bioreactor (MBBR) + side stream NF integrated process) and high rate biomethanation process developed by CSIR-IICT for the concomitant generation of biogas and bio manure.

Aerobic Moving Bed Bioreactor (AMBBR) + side stream NF

Aerobic Moving Bed Bioreactor (AMBBR) + side stream NF

Aerobic Moving Bed Bioreactor (AMBBR) + side stream NF unit integrated with anaerobic gas lift reactor (AGR)

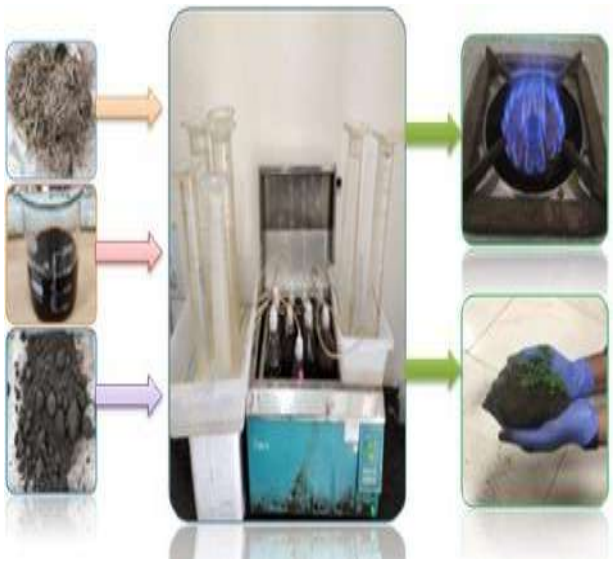
Global Change and Climate Programmes

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.

Development of High Rate Biomethanation Technology for the Combined Distillery Waste (Spent Wash, Bagasse and Press Mud)

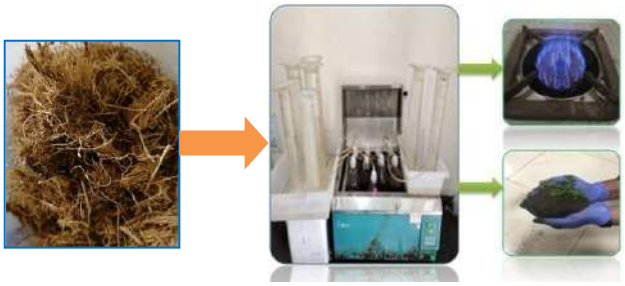
M/s Spectrum Renewable Energy Private Limited (SREL) sponsored a project to CSIR-IICT to understand the biogas generation potential of mixed distillery wastes (bagasse, press mud and spent wash) generated from an integrated sugar mill and distillery. The project is for the duration of six months starting from April 2019. M/s SREL had sent all the samples of bagasse, press mud and spent wash to CSIR-IICT to carry out the experiments. The project staff of BEES lab in CSIR-IICT had immediately characterized all the samples and organised anaerobic batch experiments in anaerobic batch reactors (ABR's). CSIR-IICT had accomplished the assignment, documented the results and this is the final project completion report being submitted by CSIR-IICT to M/s SREL. The biomethanation potential (BMP) of bagasse, press mud and spent wash was carried out for 60 days in batch reactors under anaerobic conditions.



Biomethanation potential experiments for distillery waste

Development of High Rate Bio Methanation Technology for Palm Oil Empty Fruit Bunches and Palm Oil Waste

M/s Global Environmental Services Private Limited (GESPL), Hyderabad, Telangana State, India, is a professionally managed company working in the interface of energy and environment. GESPL is very active in the area of palm oil related subject and they could envisage, great potential in generating renewable energy from palm oil empty bunches (PEFB). Presently PFEB are being used as a fuel in boilers of respective palm oil processing mills. However, in the recent past Bio-CNG is emerging rapidly in India and GESPL is very much keen in entering into the business domain of Bio-CNG. In this regard, they could foresee great future for the generation of biogas followed by Bio-CNG from PEFB. Therefore, M/s GESPL is interested in detailed studies to understated the biogas generation potential of PEFB and the same work was awarded to CSIR-IICT through a MoU.



Biomethanation potential of Palm oil empty fruit bunch waste

Laboratory Scale Investigation on Chemical Treatment of Subsurface Lignite Deposits to Enhance the Conversion of Lignite to Methane

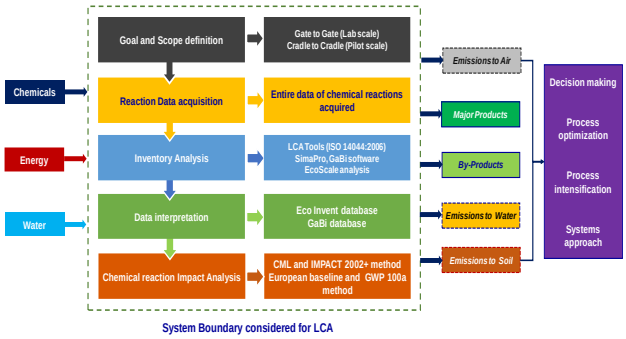
The main objective of the project is chemical treatment of subsurface lignite deposit samples in a laboratory scale reactor to understand the methane generation potential of lignite.Initial characterization of specific chemical constituents of lignite using latest analytical techniques along with Feasibility studies on chemical treatment of the lignite with acids, bases, reductants, solvents, chemicals etc.Identification of suitable chemical treatment for possible generation of methane from lignite. Analysis of lignite sample before and after chemical treatment for porosity (pore size distribution and surface area measurement).

Laboratory scale high pressure reactor

Sustainable Development of Process through Life Cycle Assessment Tools

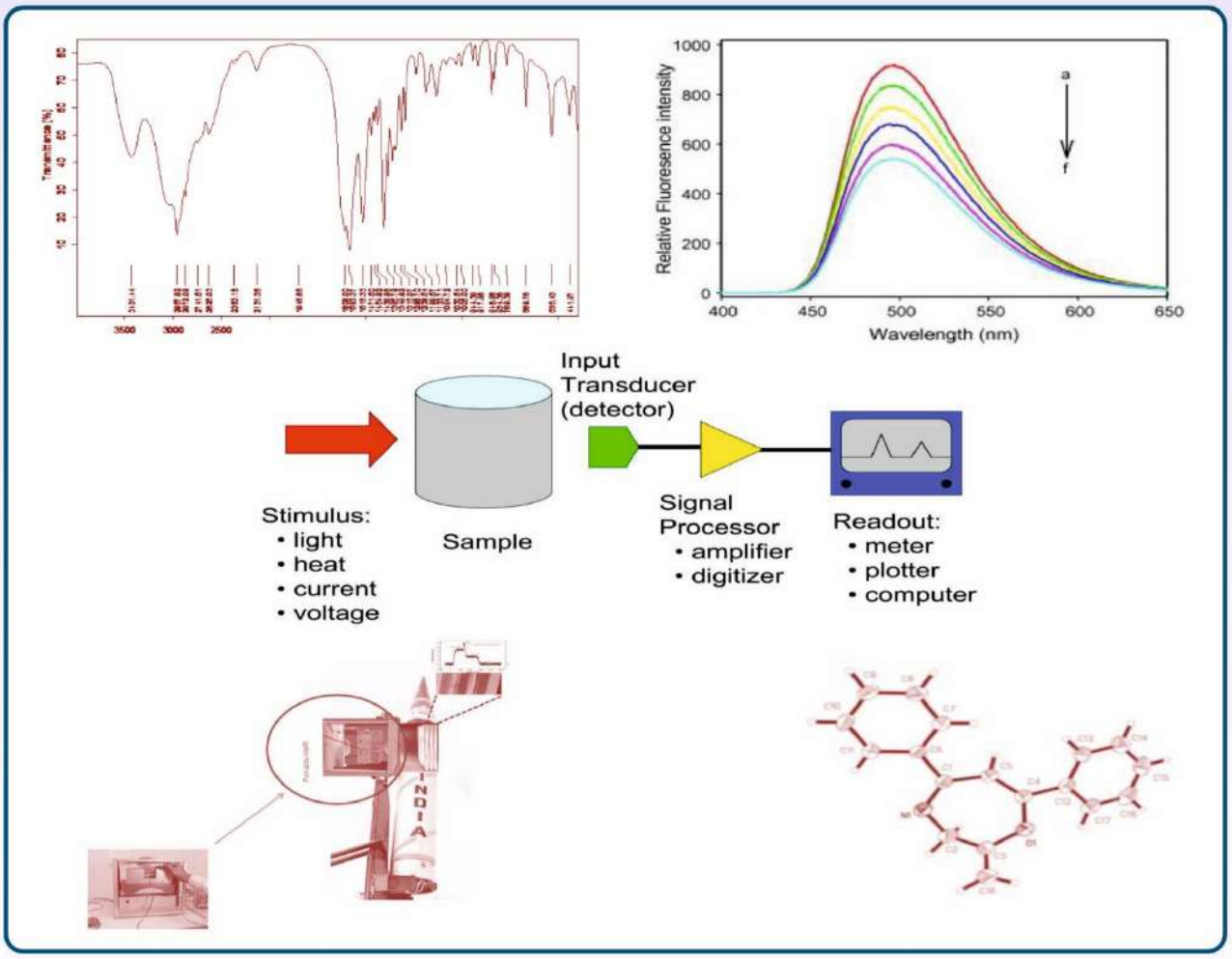
The sustainability analysis tool (SAT) adopting Life cycle assessment (LCA) was designed and applied during the production and scale-up of active pharmaceutical ingredient (APIs) prepared by CSIR-IICT and CSIR sister laboratories to assess the impact of the process on the environment and to identify specific hotspots sthat need to be optimized. SAT was designed with three steps to study- mass balance and associated emissions (GaBi software), EcoScale score, and understand the contribution of the process inputs on various impacts categories (SimaPro). The system boundary for LCA analysis was fixed as per the gate-to-gate approach. Sustainability analysis was performed to understand the impact of API processes on several categories viz., global warming, ozone depletion, human toxicity, acidification, eutrophication, resource depletion, and ecotoxicity. The data pertaining to raw materials, chemicals, water, and energy along with outputs such as the targeted products (API)/by-products and emissions to the environment at each step of the processes were acquired from the Ecoinvent v3.5 database. The primary data pertaining to electricity requirements for different unit operations such as heating, mixing, filtration, autoclave, etc., chemicals and water consumed in the process was provided to the software, whereas, the secondary data for the processes such as the production of electricity, chemicals, solvents, and water was considered from Ecoinvent v3.5 database. The impact assessment was processed using Impact 2002+ LCIA and IPCC GWP 100a methods to evaluate the influence of a product/process on impact categories. Impact 2002+ LCIA method was employed to study the LCA results with reference to 14 midpoint categories and 4 endpoint damage categories. Sankey diagrams was executed (IPCC GWP 100a method) to understand the contribution of the particular input of the process

on global warming. The data quality was addressed as per the guidelines of ISO 14044:2006. The functional unit of the study was set as one-kilogram (kg) of each API and offers a reference to which the inputs and outputs are associated. Sustainability analysis was performed for α-lipoic acid, Daclatasvir, Ledipasvir, Nilotinib, Paracetamol, Azelaic acid, Pregabalin and Sitagliptin synthesis pathways and identified the impact on the environment.

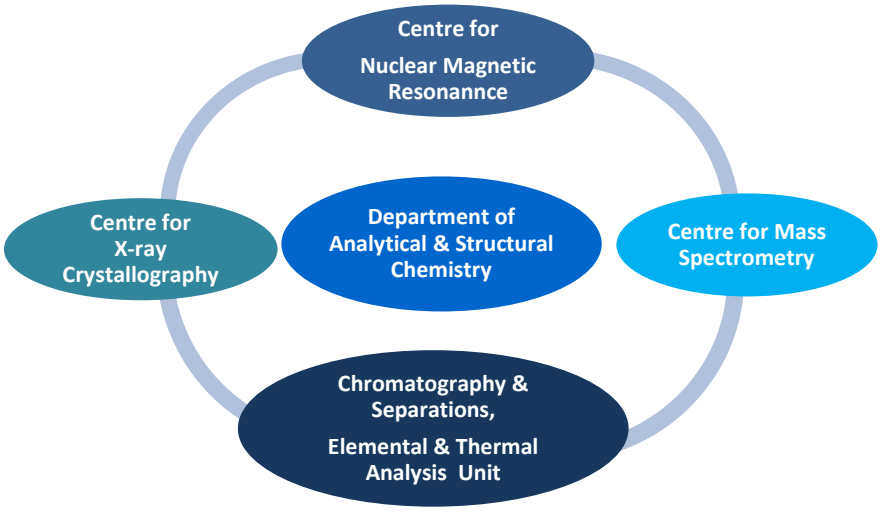


System boundary, goal and scope considered for SAT analysis

ANALYTICAL & STRUCTURAL CHEMISTRY



Analytical & Structural Chemistry Department of CSIR-IICT is the unique department in the country that carry advanced basic and applied research programs using latest sophisticated analytical instruments such as NMR spectrometers, Mass Spectrometers, X-Ray, HPLCs, ICP-OES, GPC, SEM, TEM, UV, IR etc. The department is a consortium of specialized in-house analytical research centers as shown below.



Research interests and Core Competencies

Core strength of the department is the well expertise and competent scientific and technical staff with several years of experience in the relevant fields. The staff has been engaged in diverse research programs of integrated and independent projects. The department is instrumental in developing various approaches in the identification, characterization and quantification of analytes of interests. The department has core competencies, expertise and state-of-the-art equipment (21CFR-part 11) in the following areas.

- *Structural Characterization***:** High resolution NMR (USFDA inspected facility), XRD (powder and single-crystal), High Resolution Mass Spectrometry, tandem mass spectrometry (MS/MS) and FTIR studies of APIs, Intermediates, Drug Polymorphism, Co-crystals, Peptides and Biosimilars
- *Analytical Method Development &Validation*
- *Mass Spectrometry & Chromatography based Qualitative and Quantitative Analysis*: Impurity profiling of APIs and Agrochemicals, Stability of APIs, Residual solvents, Contaminants, Genotoxic impurities, Metabolomics, Lipidomics, Chemical toxins, Protein/peptide analysis, Multi-class nutrients etc.
- *Morphology & Surface Analysis:* FE-SEM, TEM, Particle size analysis
- *Thermal and Elemental Analysis:* DSC, TGA, ICP-OES and CHNSO
- *Pharmacokinetic Studies*
- *Analytical Skill Development Programs*

The department is also the backbone for our institute's research programs. In addition, the staff is also capable of providing quick and value based analytical solutions to industries and academic/government agencies.

The department has NABL (ISO/IEC 17025) accredited facilities for testing drugs and pharmaceuticals and chemical warfare agents. Centre for Analysis of Chemical Toxins is a dedicated facility for off-site analysis of chemicals related to chemical weapons convention (CWC) by mass spectrometry. The centre has been participating in the international official OPCW proficiency tests every

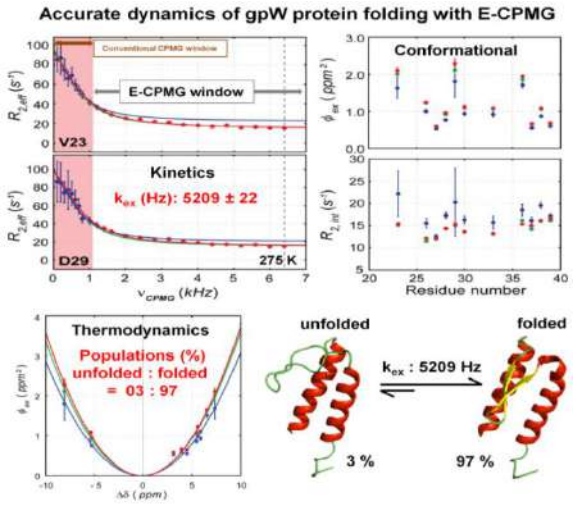
year. This laboratory is contributing to the mission of OPCW and NACWC, New Delhi in achieving the common goal for a world free of chemical weapons.

The department is continuing to focus on the following areas:

(A) Basic/Applied Research
(B) Collaborative Research
(C) Analytical Solutions

A. BASIC /APPLIED RESEARCH

1) Peptides by NMR: The peptides and proteins, derived from α-amino acids, adopt specific folding pattern and conformations which are responsible for their function. The inherent differences that are associated with the synthesis of peptides from α-amino acids such as a solubility, permeability, stability and others, prompted us to undertake investigation on the on the use of non-natural amino acids partly or fully in the peptide design. In this study a new 10/12 mixed helix is observed for the first time in the peptides containing homoleucine and has not reported earlier.



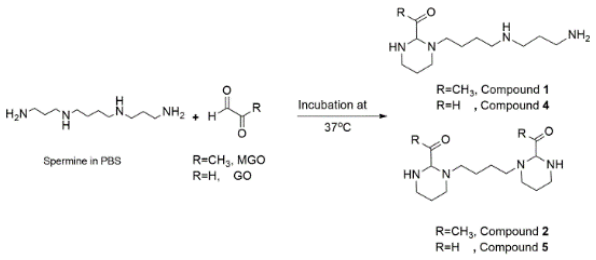
2) Simultaneous Determination of Fast and Slow Dynamics in Molecules Using Extreme CPMG Relaxation Dispersion Experiments: Molecular dynamics play a significant role in how molecules perform their function. A critical method that provides information on dynamics, at the atomic level, is NMR-based relaxation dispersion (RD) experiments. RD experiments have been utilized for understanding multiple biological processes occurring at micro-to-millisecond time, such as enzyme catalysis, molecular recognition, ligand binding and protein folding. Here, we applied the recently developed high-power RD concept to the Carr–Purcell–Meiboom–Gill sequence (extreme CPMG; E-CPMG) for the simultaneous detection of fast and slow dynamics. Using a fast folding protein, gpW, we have shown that previously inaccessible kinetics can be accessed with the improved precision and efficiency of the measurement by using this experiment. (*J. Biomol. NMR*, **2018**, 70(1), 01)

3) Characterization of N-methyl Amino Acids by ESI-MS/MS for Metabolomic Studies: Methylation is one of the important post translational modifications of biological systems: A few of the methylated amino acids are identified and have been proved as potential biomarkers for several metabolic disorders by using mass spectrometry based metabolomics workstation. As it is possible to encounter all the *N*-methyl forms of the proteinogenic amino acids in plant/biological systems, it is essential to have analytical data of all *N*-methyl amino acids for their detection and identification. In our earlier studies, ESI-MS/MS data of all methylated proteinogenic amino acids, except that of mono-*N*-methyl amino acids. In this study, the *N*-methyl amino acids of all the amino acids (**1-21**; including one isomeric pair) were synthesized and characterized by ESI-MS/MS, LC/MS/MS and HRMS.

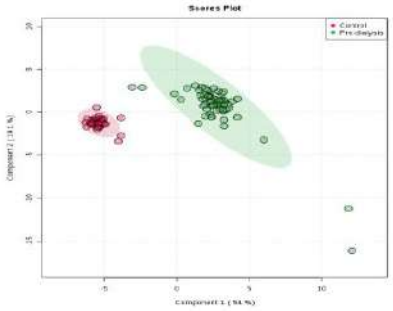
4) **Shotgun Metabolomics for the Analysis of Plasma Metabolites in CKD Patients on Maintenance Hemodialysis**: Hemodialysis process is being used to clear uremic toxins in the renal failure of CKD patients. We aimed to study the plasma metabolites and their relative quantities among three different groups (pre-hemodialysis, post-hemodialysis and healthy controls) to study

uremic toxins present in hemodialysis patients. A Direct-ESI-HRMS (Orbitrap) based shotgun metabolomics technique was successfully applied. Univariate and multivariate statistical methods were applied to visualize the metabolite changes among the PRE-HD, POST-HD and HC groups. A typical PLS-DA score plot of metabolites is shown in figure. (Green=Pre-Hemodialysis; Red=Healthy controls)

5. Identification and Characterization of Reaction Products of Spermine/Spermidine with Methylglyoxal and Glyoxal by LC/MS/MS: Reactive carbonyl species, such as methylglyoxal (MGO) and glyoxal (GO), are potent agents to form AGEs in vitro and in vivo by reacting with amino group containing molecules in the body. In this study, interaction of GO/MGO with spermine/spermidine was studied under physiological condition (PBS buffer at pH 7.4). The reaction of spermine with MGO/GO resulted in two reaction products, that of spermidine in a single product. The reaction products were successfully identified and characterized by high resolution LC/MS and LC/MS/MS.

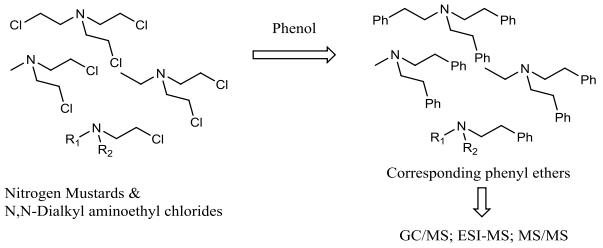


6. Degradation/Reaction Products of Chemical Warfare Agents: As the part of the verification process of the chemical weapons convention (CWC), it is essential to detect and identify the CWC related scheduled chemicals and their precursors/ degradation/reaction products in suspected environmental samples. The mass spectrometry (GC/MS and LC/MS) techniques are widely used for this purpose, but authentic samples or library data is required for confirmation of the degradation/reaction products. In these lines, our research group has been working on synthesis of all possible degradation/ reaction products (through different safe synthetic routes), and generating library data, as well as the data is published in the literature for benefit of other groups who involve in the analysis of CWC related chemicals.



a) Reaction Products of Nitrogen Mustards or N,N-Dialkyl Aminoethyl-2-Chlorides with Phenol

In this work, reaction products of nitrogen mustards or N,N-dialkyl aminoethyl-2-chlorides with phenol were studied. The selected CWC chemicals react with phenols during decontamination process and form corresponding phenyl ethers. The reactions products were characterized by GC/MS (EI and CI), GC/RI, and ESI-MS/MS data. With this data, it is possible to detect and identify the reaction products of nitrogen mustards with phenol.



b) Trace Level Identification of Acidic Hydrolysis Products of Chemicals Related to Chemical Weapons Convention

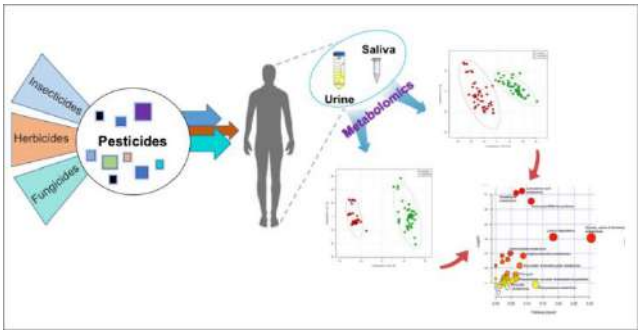
Majority of the CWC related chemicals are organophosphonates, mustards and psychotomimetic agents. The chemicals are unstable in nature and degrade under environmental and biological conditions to their corresponding acidic hydrolysis products. Identification of these products from the environmental samples is a challenging process and

needs simple, sensitive and specific methods. A trace level identification method with insitubutylation derivatization method was developed from aqueous and soil samples. The method has sensitivity in parts per billion levels and is suitable for the OPCW proficiency tests (*J. Sep. Sci*., **2018**, 41(3), 689)

7. Identification of Metabolic Changes in Artificially Ripened Fruits: Artificial Ripening is a major concern around the world due to irregular, unauthorized and unethical ways of ripening. Artificial ripening is being carried out due to the reduced shelf life and problems in transportation of fully ripened fruits. Artificial ripening is a faster ripening process when compared to the natural phenomenon which can lead to changes in the composition of various metabolites. Presently the studies are being carried out on the metabolic changes in mango, banana and Sapota fruits ripened with ethylene, ethephon and calcium carbide ripeners. The studies were mainly focused on the variation of phenolic metabolites, amino acids, volatiles and sugars. New analytical methods for identification residues of artificial ripeners are in the development stage.

8. Quantiative Evaluation of Endocrine Disrupting Phthalates and Bisphenols from Packaged Drinking Water Samples: Sensitive and specific LC-MS/MS and GC-MS based analytical methods were developed for trace level quantification 8 phthalates and 3 bisphenols from packaged drinking water samples. The samples were incubated at various temperatures (low, room temperature, elevated temperatures) and the leaching from the packaging material was studied. A total of 350 samples were analysed.

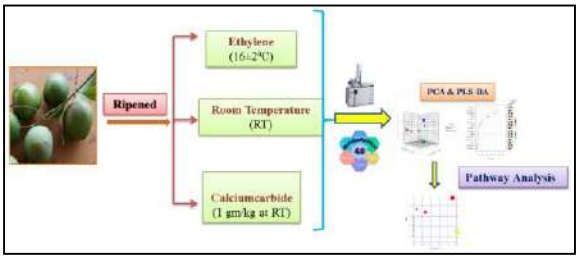
9. Understanding the Metabolic Perturbations in the Saliva and Urine Samples of Male Farmers Exposed to Pesticides Sprayed for Agriculture Applications: A study to understand the metabolic perturbations in the saliva and urine of farmers exposed to pesticides during their spray for agricultural applications using mass spectrometry-based metabolomics.



The main aim of the study is to establish non-invasive matrices (saliva and urine) as alternative diagnostics to evaluate the occupational exposure. Thirteen metabolites of urine samples and sixteen metabolites of saliva samples were altered significantly due to pesticide exposure. The amino acid metabolism, energy metabolism (glycolysis and TCA cycle) and glutathione metabolism (oxidative stress) were found to affect in the pesticide exposed population. The study reveals that GC-MS based metabolomics can be a potential tool to evaluate the metabolic perturbations in humans exposed to pesticides.

(Chemosphere, **2019**, 226, 636)

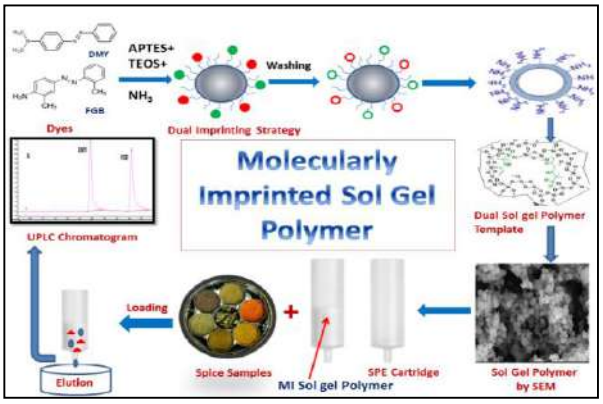
10. GC-MS Based Metabolomics to Evaluate the Effect of Various Ripening Agents/Practices on Mango (*Mangifera Indica*):



Mango said to be king of the fruits has been widely taken by the consumers, due to which, many ripening agents were used to make it ready-to-eat fruit. A study to evaluate the metabolic disturbances in the mango fruits after ripening with ethylene, calcium

carbide and room temperature ripening was performed using GC-MS based metabolomics. The study has identified 16 differential metabolites belongs to classes of amino acids, fatty acids, sugars, and polyols in the mango samples ripened with ethylene and calcium carbide. Fructose, Glucose, and Galactose were found to be significantly up-regulated due to calcium carbide ripening in comparison to other ripening agents/processes. Thus, mass spectrometry-based metabolomics has potential to evaluate the fruit quality and safety with respect to consumer health. *(J. Sep. Sci.*, **2019**, 42(19), 3086)

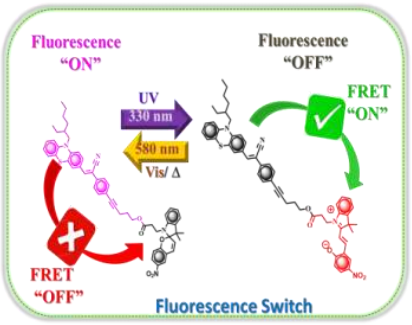
11. Synthesis and Application of Molecularly Imprinted Sol-Gels Coupled with UHPLC for Selective Extraction and Analysis of Dyes from Spices:



The dual imprinted sol-gel was prepared for the simultaneous extraction of dimethyl yellow (DMY) and fast garnet base (FGB) from the spices followed by UHPLC analysis. The surface and binding characterizations of the prepared sol-gel was found to exhibit higher binding affinity in comparison to non-imprinted sol gel. The developed method has shown LOD and LOQ of 0.029 ng/g and 0.097 ng/g for FGB and 0.021 ng/g and 0.070 ng/g for DMY respectively. The accuracy in terms of percent recovery was found to be 80–91%. (*Sep. Sci. Plus*, **2019**, 2, 160)

12. Ultrafast Photochemistry

We developed and explored the ultrafast relaxation pertaining to charge / electron / energy transfer



dynamics of functional materials of different categories comprising bi-stable fluorescence switch molecules and functional organic molecule-quantum dot composite materials.

Fluorescence Switch Molecule

Stimuli response FRET induced reversible fluorescence modulation in a newly synthesized fluorophore-photochrome like dyad molecules comprisingphenothiazine derivative and spiropyran is explored which manifests the implications for the design of molecular switching devices.

Femto-Chemistry/Relaxation Dynamics

We successfully delineate that H-bonded phenols covalently linked to porphyrins shows PCET where electron transfer from H-bonded phenol to the excited singlet porphyrin macrocycle was coupled with the movement of the bound proton to the pyridine. Such movement of the proton lowered phenol oxidation potential and was consistent with electron movement. Demonstrated results will aid in understanding of PCET reactions in biological processes and other systems as well.

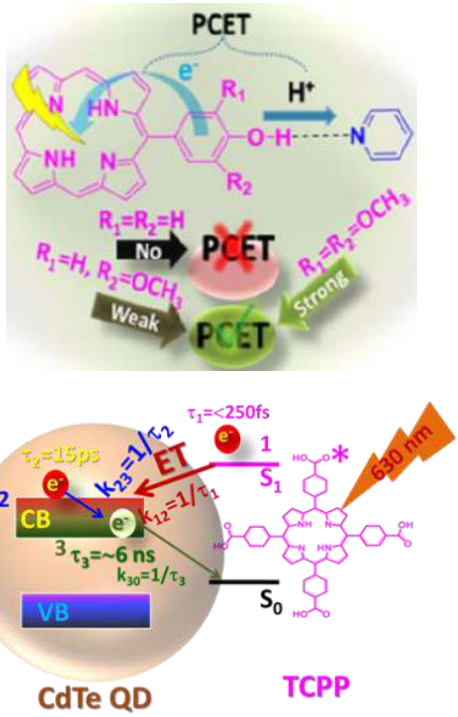
Relaxation mechanism of hot exciton, band edge exciton, and charge carriers are explored for multidimensional un-doped and doped perovskite materials were explored. Energy-transfer dynamics were explored in Mn^{2+}-Doped $(C_4H_9NH_3)_2PbBr_4$ Two-Dimensional (2D)Layered Perovskite. Energy transfer dynamics of highly stable Fe^{3+} Doped $CsPbCl_3$ perovskite quantum dot with dual-color emission is explored. The charge separation and

charge recombination dynamics in CdTe QD and carboxyl phenyl linked porphyrin composite systems are explored in details. The fundamental understanding of this photo-induced electron transfer dynamics in CdTe QD-TCPP composite opens up new possibilities to design an efficient light-harvesting system based on inorganic-organic hybrid systems.

B) COLLABORATIVE RESEARCH

1. Induction of Apoptosis in Lung Carcinoma Cells by Antiproliferative Cyclic Lipopeptides from Marine Algicolous Isolate Bacillus Atrophaeus Strain AKLSR1

In the present study, an exopolymeric biosurfactant composed of lipoheptapeptides was isolated and identified from a marine algicolous bacterial isolate, Bacillus atrophaeus strain AKLSR1, endophytic to Padina tetrastromatica.



The lipopeptides were characterized by using FT-IR, NMR, GC–MS and UPLC-ESI-Q-Tof-MS/MS spectroscopic studies. Structural analysis unveiled five CLP variants that formed one major polymeric lipopeptide. This is the first report on the complete structural characterization of new cyclic lipopeptide isoforms from a marine algicolous B. atrophaeus and also their application as an anticancer agent. (*Process Biochem*., 2018, 79, 142)

2. Evolvement of Nutraceutical Onion Plants Engineered for Resveratrol Biosynthetic Pathway

The present study reports the development of nutraceutical onion by engineering Resveratrol biosynthetic pathway. LC-ESI-HRMS analysis revealed the accumulation of variable quantities of RV (24.98-50.18 µg/g FW) and its glycosylated form polydatin (33.6-67.15 µg/g FW) in both leaves and bulbs, respectively, indicating the successful engineering of RV biosynthetic pathway into onion. This is a collaboration study with centre for plant molecular biology, Osmania University. (*Plant Cell Report*, 2019, 38, 1127)

3. Binding Preference of Nitroimidazolic Radiosensitizers to Nucleobases and Nucleosides Probed by Electrospray Ionization Mass Spectrometry and Density Functional Theory

Nitroimidazolic radiosensitizers are used in radiation therapy to selectively sensitize cancer cells deprived of oxygen, and the actual mechanism of radiosensitization is still not understood. Here, we have selected popularly used radiosensitizers (1-methyl-5-nitroimidazole, ronidazole, ornidazole, metronidazole, and nimorazole) with a common 5-nitroimidazolic ring with different substitutions at N1 and C2 positions of the imidazole moiety, and investigate their binding to nucleobases (A, T, G, and C) and nucleosides (As, Td, Gs, and Cd) via the positive electrospray ionization mass spectrometry experiments. In addition, quantum chemical calculations at the M062x/6-311+G (d,p) level of theory and basis set were used to determine binding energies of the proton bound dimers of a radiosensitizer and a nucleobase. This study can pave a way to understand basic mechanism of the

radiosensitizers in order to develop new and efficient drugs and also useful to know potential of radiation to be used to treat a patient. I have shared my knowledge while executing this work using mass spectral techniques. (*J. Chem. Phys*. **2019**, 150(1), 014302)

4. *In Vitro* and *In Vivo* Investigation of Metabolic Fate of Riociguat by HPLC-QTOF/MS/MS and *In Silico* Evaluation of the Metabolites by ADMET Predictor™

Riociguat, a guanyl cyclase inhibitor, is one of its kind drug regimen approved for management of pulmonary arterial hypertension and chronic thromboembolism pulmonary hypertension. Extensive literature review indicates lack of comprehensive reports on its metabolic fate. The present study reports the *in vivo* and *in vitro* identification and characterization of metabolites of riociguat, using LC-HRMS and MS/MS. *In vitro studies* were conducted by incubating the drug in human and rat liver microsomes in presence of respective cofactors. *In vivo* studies were undertaken by oral administration of suspension of drug to male Sprague–Dawley rats followed by collection of urine, feces and blood at specific intervals. we have identified a total of 18 metabolites in *in vivo* and *in vitro* matrices which includes hydroxyl, N-oxide, desmethyl, defluorinated hydroxyl, glucuronides and N-acetyl cysteine conjugates. Presence of N-acetyl cysteine conjugates strongly points towards the formation of a reactive metabolite intermediate trapped through N-acetyl cysteine and can be considered a matter of concern as the reactive metabolites have been known to manifest toxicities. Their presence was mimicked in *in vitro* samples as well. The toxicological properties of drug and metabolites were evaluated by using ADMET Predictor™ softwar. In this study, I was involved in the identification of metabolites by using mass spectrometry technique. *(J. Pharm. Biomed. Anal.*, **2019**, 164, 326)

5. Leishmania Donovani Molecules Recognized by Sera of Filaria Infected Host Facilitate Filarial Infection

Lymphatic filariasis (LF) caused by the nematode parasites *Wuchereria bancrofti*, *Brugia malayi*,and *B. timori* and visceral leishmaniasis (VL) caused by the protozoan parasite *Leishmania donovani* pose serious public health problems in several tropical and subtropical countries, including India. Over 120 million people suffer from LF which causes the debilitating "elephantiasis" whereas the lifethreatening VL affects about 1 million people and more are at risk of the infection. VL is a serious problem in India and LF and VL co-infections are reported in India and in Mali. However, whether coexisting VL and LF infections facilitate or limit one another or influence disease manifestations is not known. This knowledge is important because studies in patients harboring closely related co-infections such as cutaneous leishmaniasis (CL; caused by L. braziliensis) and intestinal helminth infections of Ancylostoma duodenale, Ascaris lumbricoides, Trichuris trichiura, and Schistosoma mansoni showed altered immune responses to CL and delayed healing of cutaneous wounds. In the present study, we identified a 52.9–93.6 kDa fraction Ld1 from soluble *L. donovani* extract (SLD) that strongly reacted with sera of *B. malayi* infected *Mastomys coucha* and investigated the following: (1) the effect of Ld1 fraction on *B. malayi* infection and host's immune responses (cell proliferation, release of NO and cytokines, and IgG and its subclasses), (2) the status of phagocytic activity, MHC class-I, MHC class-II, and FceR1 in peritoneal macrophages, and relative distribution of CD4+, CD8+, and CD19+ cells in splenocytes to identify immunomodulation by Ld1, and (3) the identity of proteins in Ld1 fraction by two-dimensional electrophoresis (2-DE) and matrix-assisted laser desorption ionization–time of flight-mass spectrometry (MALDI-TOFMS) analysis. In this work, I was involved in the identification of eight

proteins by using MALDI-MS analysis. (*Parasitol Res*. **2018**, 117, 2901)

6. Xenobiotic Binding Domain of Glutathione S-Transferase has Cryptic Antimicrobial Peptides

Antimicrobial peptides are one of the important components of innate immune defense system and play a critical role in controlling infections. Although vast sequence and structural diversities exist, AMPs share several common features like cationicity, amphipathicity and membrane permeabilisation as mode of action. In this study, a moderately short cationic and hydrophobic peptides derived from the conserved domains of human glutathione S-transferase (GST) have been shown to have antimicrobial activity against *Staphylococcus aureus* ATCC 29213 and *Klebsiella pneumoniae* ATCC 7637 in physiological conditions without any toxicity issues. We further shown here that human GST, a C-terminal region which showed the higher antimicrobial activity, is conserved in the vertebrates. Our results demonstrate the potential of human GST derived peptides as a template for the development of anti-infective therapeutics. In this study, I have performed peptide sequence analysis by using MADI-MS technique. (*Int. J. Pept. Res. Ther*., **2019**, 25, 1477)

C) VALUE ADDED ANALYTICAL SOLUTIONS AND SERVICES

i) Analytical Services to In-House Projects of IICT

NMR Centre of Department of Analytical & SC, 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 multinuclear and 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. The centre provides services to various departments in CSIR-IICT for both in liquid as well as solid state NMR. The three new Bruker AVANCE III HD 400 MHz NMR and Bruker AVANCE III HD 500 MHz NMR spectrometers were like work horses to meet the requirements of the institute.

Bruker AVANCE III HD 500 MHz

Bruker AVANCE NEO 600 MHz

Bruker AVANCE III 700 MHz

ii) 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. One great achievement of the centre is recent successful FDA inspection without any observations. For many APIs and drugs, NMR based

analytical methods have been established at our centre and are routinely characterized.

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.

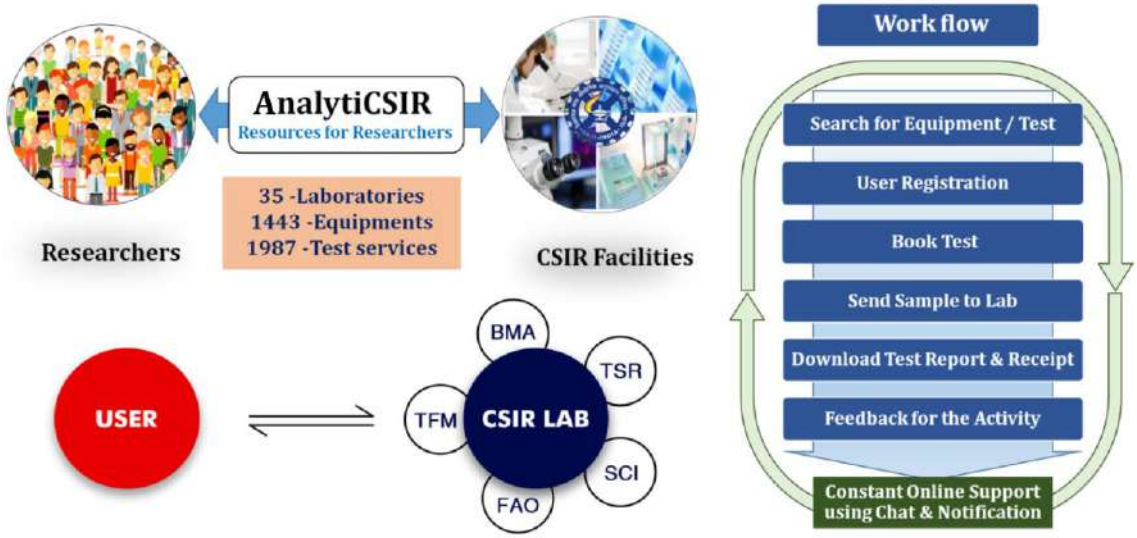
A total number of 8472 powder samples were analysed and 482 crystal structures have been elucidated during the above said period.

AnalytiCSIR: An Online Platform Providing Access to Analytical and R&D Facilities of CSIR Laboratories across the Country

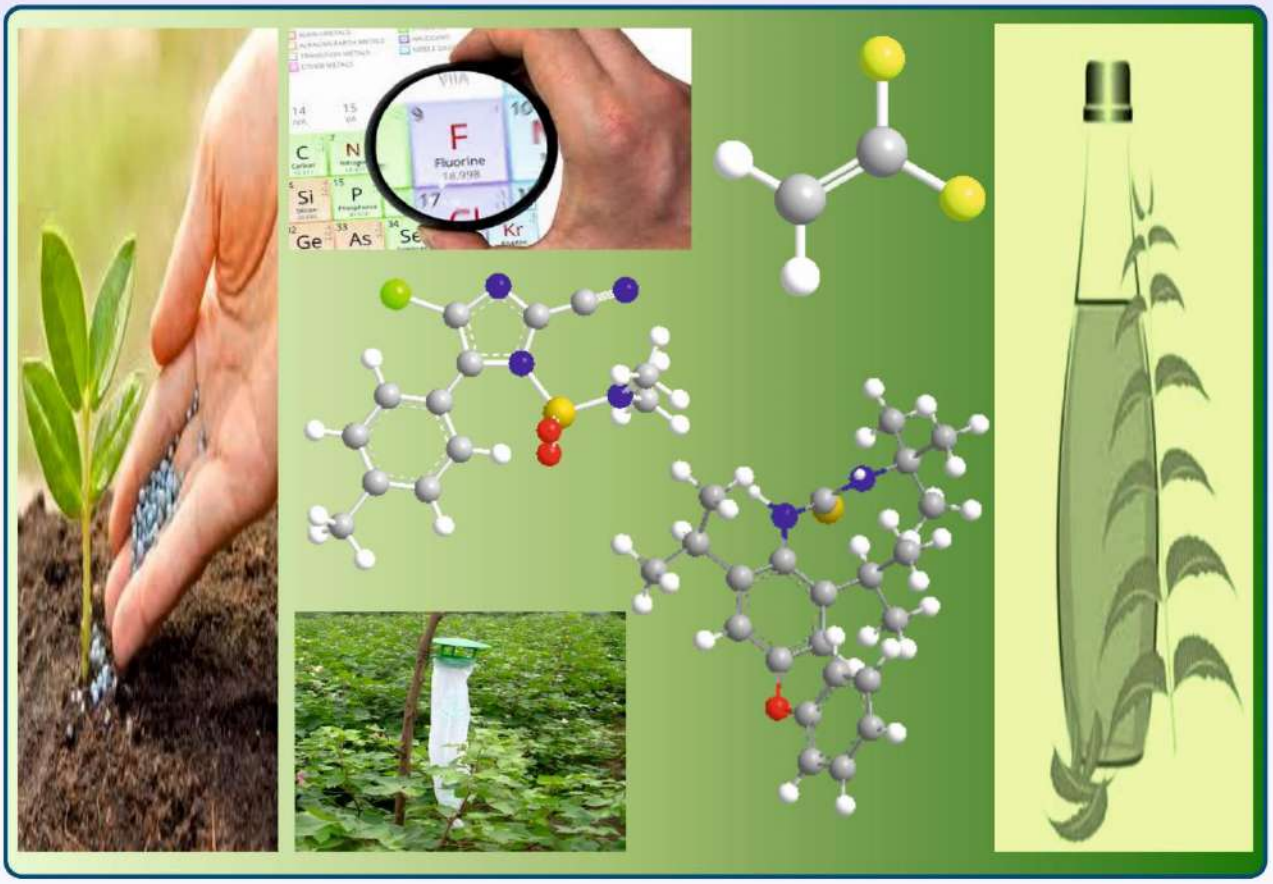
CSIR has taken a new initiative to share its analytical and research facilities located at various CSIR-laboratories across the country, with academic, industrial and other researchers who do not have required sophisticated scientific equipment to carry out their research programs on par with the developments happening globally.

AnalytiCSIR, an online web portal, has been developed under the chairmanship of Dr S Chandrasekhar, Director, CSIR-IICT. CSIR-IICT, Hyderabad has carried out the design, development, and execution of the AnalytiCSIR Web portal. AnalytiCSIR provides an easy online access for researchers to locate the nearest, desired state-of-the-art R&D facility available at CSIR laboratories and reserve for their research activities. It aims to help and guide users online to get quality and reliable R&D services / solutions through the scientific expertise available at CSIR laboratories across the country.

Presently the portal includes 1443 equipments at 35 CSIR labs across India and offers 1987 tests. The portal contains dashboards covering sample & test management, payment confirmation and test reporting, monitoring of lab-wise test bookings and earnings. AnalytiCSIR e-portal was pre launched by DGCSIR on 9th February 2019, during the Director's Conference in Dhanbad, which was initially limited for the intra and inter-lab usage. Soon after the process is streamlined and found robust in intra/inter-lab usage, it will be extended to all students/ academia/ industries/other public sector laboratories within the country.

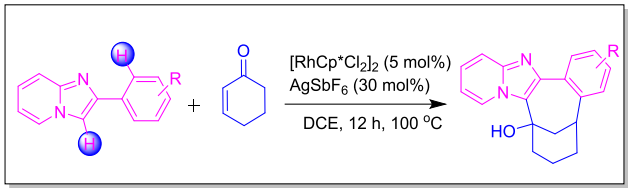


FLUORO AND AGROCHEMICALS



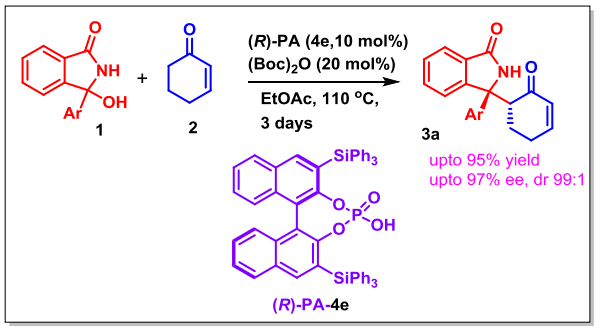
BASIC RESEARCH

Rh(III)-Catalyzed Tandem Bicyclization of 2-Arylimidazo[1,2-A]Pyridines With Cyclic Enones for the Construction of Bridged Scaffolds



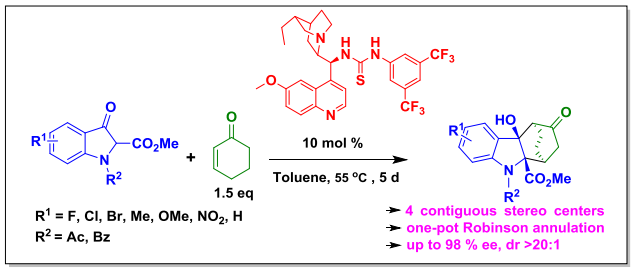
An efficient Rh(III)-catalyzed bicyclization of 2-arylimidazo[1,2-*a*]pyridine with cyclic enones has been developed for the synthesis of bridged imidazopyridine derivatives in excellent yields up to 95%. The reaction proceeds *through* a sequential conjugate addition of *ortho*-C-H bond of aryl group followed by an intramolecular C3-alkylation of imidazopyridine ring in a highly regioselective manner. This protocol provides a wide range of bicyclic scaffolds in a single step process. This is the first report on the bicyclization of imidazopyridines with cyclic enones. (*Org. Lett.*, **2019**, 21, 8548)

BINOL Phosphoric Acid-Catalyzed Asymmetric Mannich Reaction of Cyclic *N* -Acyl Ketimines with Cyclic Enones



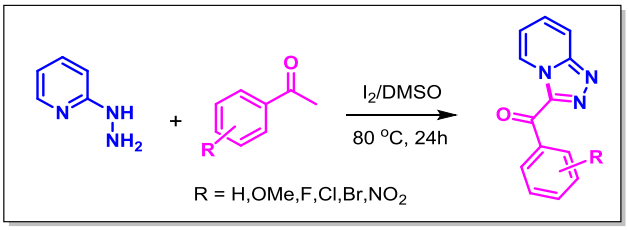
A highly enantio- and diastereoselective Mannich reaction of cyclic *N* -acyl ketimines generated in situ from 3-hydroxyisoindolin-1-ones with cyclic enones has been accomplished using a chiral phosphoric acid catalyst to afford the chiral isoindalinone derivatives in high yields with excellent enantioselectivities (upto 97 % *ee*). This is the first report on the synthesis of chiral isoindolin-1-ones bearing adjacent quaternary and tertiary stereogenic centers. (*Chem Asian J.*, **2019**, 14, 2958)

Asymmetric Robinson Annulation of 3-Indolinone -2-carboxylates with Cyclohexenone: Access to Chiral Bridged Tricyclic Hydrocarbazoles



The chiral bifuntional thiourea catalyzed diastereo- and enantioselective Michael addition followed by intramolecular Aldol reaction of 3-indolinone-2-carboxylates with cyclohexenone has been accomplished using 10 mol% chiral thiourea catalyst. It is a novel strategy for the construction of chiral bridged tricyclic hydrocarbazole derivatives bearing four contiguous stereocenters with excellent diastereo- and enantioselectivity. (*Org. Lett.*, **2018**, 20, 4195)

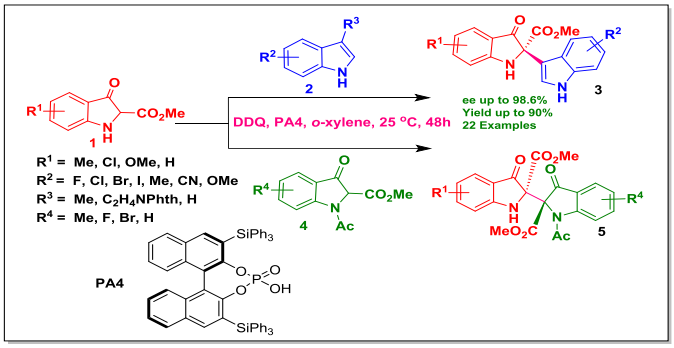
Metal-free One-Pot Synthesis of 1,2,4-Triazolo [4,3-a]Pyridines from 2-Hydrazinylpyridines



A metal-free one-pot strategy has been developed for the synthesis of 3-aryl[1,2,4]triazolo[4,3-*a*]pyridines through an oxidative cyclization of 2-(2-arylidenehydrazinyl)pyridines by utilizing molecular iodine in DMSO. This is the first report on the synthesis of 3-aroyl[1,2,4]triazolo[4,3-*a*]pyridines directly from α-aryl methyl ketones or ethyl benzoylacetate or styrenes or phenylacetylenes and 2-hydrazinylpyridines *via* iodine promoted oxidative cyclization. The catalytic use of iodine makes this method quite simple, more convenient and

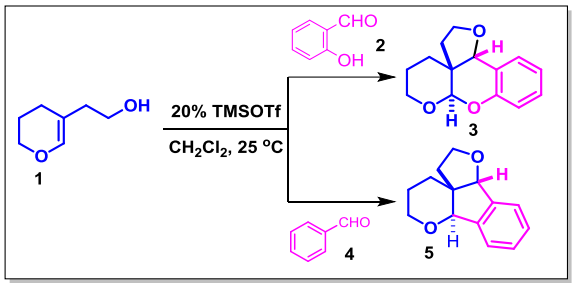
economical. Moreover, this protocol showed broad substrate scope under mild reaction conditions and could override the usage of hazardous metal reagents. (*Adv. Synth. Catal.*, **2018**, 360, 3069)

Oxidative Asymmetric Aza-Friedel-Crafts Alkylation of Indoles with 3-Indolinone-2-carboxylates Catalyzed by a BINOL Phosphoric Acid and Promoted by DDQ



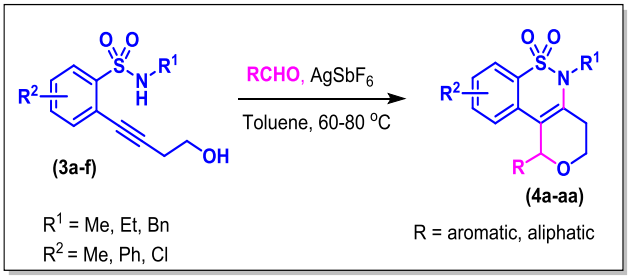
An asymmetric aza-Friedel-Crafts alkylation has been developed using a catalytic amount of 3,3′-bis(triphenylsilyl)-1,1′-binaphthyl-2,2′-diyl hydrogen phosphate through the addition of indoles to indolenines derived in situ from 3-indolinone-2-carboxylates by DDQ. Similarly, the addition of indoline-3-ones to indolenines provides heterodimers with *vicinal*-chiral quaternary centers. (*Chem Asian J.*, **2018**, 13, 1327)

Tandem Prins-Type Cyclization for the Stereoselective Construction of Fused Polycyclic Ring Systems



A novel cascade process has been developed for the stereoselective synthesis of fused tetrahydrofuro[3,2-*c*]pyrano[2,3-*b*]chromene derivatives through the condensation of 2-(3,4-dihydro-2H-pyran-5-yl)ethan-1-ol with 2-hydroxybenzaldehydes in the presence of 20 mol% TMSOTf in dichloromethane at 25 °C. Similarly, the condensation of 2-(3,4-dihydro-2*H*-pyran-5-yl)ethan-1-ol with aromatic aldehydes provides the corresponding hexahydro-4*H*-furo[3',2':2,3]indeno[1,2-*b*]pyran derivatives in good yields with high diastereoselectivity. It is a modular approach for the rapid construction of polycyclic architectures in a single-step. These cyclic frameworks are an integral part of the structure of many natural products. (*Org. Chem. Front.*, **2018,** 5, 1320)

Silver(I)-Catalyzed Sequential Hydroamination and Prins Type Cyclization for the Synthesis of Fused Benzo-Delta-Sultams

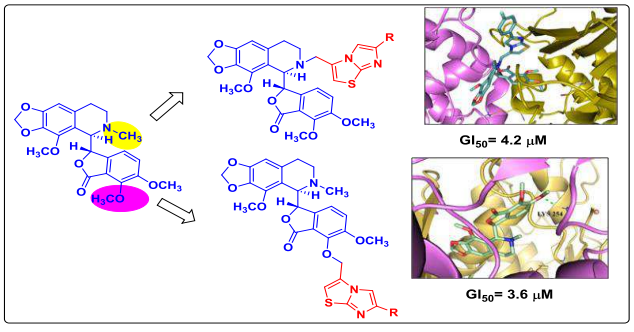


An intramolecular annulation strategy has been developed for the synthesis of tetrahydro benzo [*e*]pyrano[4,3-*c*][1,2]thiazine derivatives by means of coupling of aldehydes with 2-(4-hydroxybut-1-yn-1-yl)-*N*-arylsulfonamides using a catalytic amount of silver hexafluoro antimonate in toluene at 80 °C. This is the first report on the synthesis of fused benzo-δ-sultam derivatives through C-N, C-O, and C-C bond formations. The reaction proceeds through a cascade of hydroamination and Prins type cyclization. (*Org. Biomol. Chem.*, **2018**, 16, 5163)

Chemicals in Crop Care: Yesterday, Today and Tomorrow

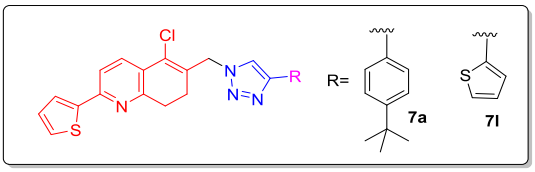
Crop protection in some form or the other has been routinely used ever since humankind started practising agriculture. Chemical crop protection ensures higher yields, better quality of produce, thereby an assured food supply and reliability of harvest dependent livelihoods. Crop protection chemicals or agrochemicals that restrain thousands of pests and weeds have been major contributors to the green revolution and surplus produce all over the world. However, the quest for research and development efforts towards discovery of newer products remains unabated due to multiple reasons. The article scans through the history and significance of agrochemicals; complexities of new agrochemical discovery and Indian scenario in the sector. (*Chem. Indust. Dig.*, **2019**, 45)

Imidazo[2,1-b]thiazole-Coupled Natural Noscapine Derivatives as Anticancer Agents



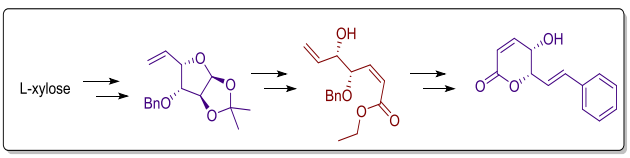
A series of noscapine–imidazothiazole conjugates linked at 5′-N and 7-O positions, respectively, were synthesized and evaluated as anticancer agents. Among the synthesized set of noscapinoids, it was interesting to note that initial intermediate compounds were found to be active. Among which 5′-N derived imidazo thiazole was found to be the most potent among the series. Six compounds were found to be potent in the cytotoxicity studies, and the same was corroborated with the molecular modelling studies where the binding energies were found to be in accordance with the activities observed. Cell cycle analysis revealed that these molecules were active in the G_2/M phase of the cell cycle via induction of apoptosis, inhibiting caspase-3 and increasing the levels of cyclin-B1 and CDK-1. (*ACS Omega*, **2019**, *4(21)*, 19382)

5-Chloro-2-Thiophenyl-1,2,3-Triazolylmethyl Dihydroquinolines as Dual inhibitors of Myco bacterium Tuberculosis and Influenza Virus: Synthesis and Evaluation



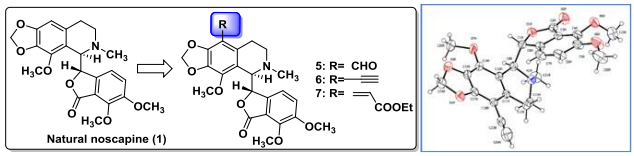
A series of novel dihydroquinoline-1,2,3-triazole conjugates have been synthesized *via* click reaction in good to excellent yields and were evaluated for their *in vitro* antimycobacterial activity against *M. tuberculosis* H37Rv (*Mtb*). Among the compounds screened for the virus-inhibiting activity against influenza virus A/Puerto Rico/8/34 (H1N1), almost all fifteen analogues were found to be moderate, and among them the compound **7l**, bearing thiophene moiety appeared the most active with good selectivity index (IC_{50}=19.5 μg/mL; SI=15). The results described here demonstrate the potential utility of dihydroquinoline-1,2,3-triazoles as antitubercular and antiviral agents. (*Bioorg. Med. Chem. Lett.*, **2019**, *29(18)*, 2664)

Total Synthesis of 5-Hydroxygoniothalamin



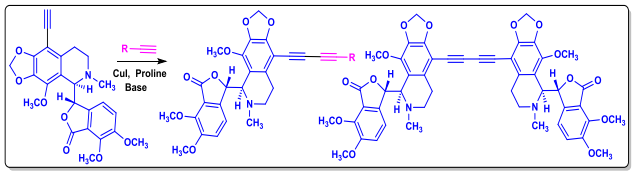
Total synthesis of 5-hydoxygoniothalamin has been achieved from commercially available L-xylose. The α, β-unsaturated-δ-lactone core was constructed in very good yields by utilizing one carbon and two carbon *cis*-Wittig olefinations and δ-lactonization using Yamaguchi conditions. Grubbs cross metathesis followed by desilylation resulted 5-hydoxygoniothalamin. (*Synthesis*, **2019**, *51(03)*, 780)

Synthesis and Antiproliferative Activity of 9-Formyl and 9-Ethynyl Noscapines



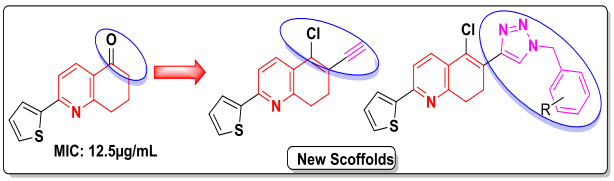
Appending functional groups to the core skeleton of natural α-noscapine, an FDA approved cough medicine, resulted in analogs with anticancer activity. In this study, we synthesized and evaluated antiproliferative activity of 9-formyl and 9-ethynylnoscapines. 9-Formylnoscapine **5** was synthesized from 9-bromonoscapine *via* a three-step reaction sequence involving palladium catalysed Heck reaction with ethyl acrylate leading to noscapinoid **7**, dihydroxylation of **7** with OsO_4 and oxidative cleavage of diol. Further, Seyferth-Gilbert homologation of 9-formylnoscapine using *Bestmann-Ohira* reagent resulted in 9-ethynylnoscapine **6** in excellent yield. Antiproliferative activity screening of new noscapinoids **5-7** against NCI60 human tumor cell lines resulted in 9-ethynylnoscapine **6** as a potent anticancer agent with the lowest mean percentage growth against the full 60-cell line panel. (*ChemistrySelect*, **2019**, *4*, 4092)

Copper-Catalysed Glaser-Hey-Type Cross Coupling of 9-Ethynyl-α-Noscapine Leading to Unsymmetrical 1,3-Diynyl Noscapinoids



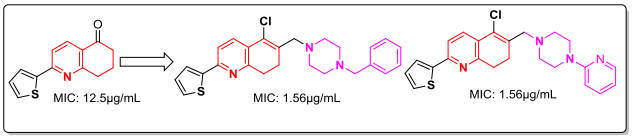
Cu(I) catalyzed Glaser-Hey type cross coupling of 9-ethynylnoscapine with terminal alkynes is described, which enables synthesis of unsymmetrical noscapine 1,3-diynes in very good yields in the presence of base and amines as ligands. The symmetrical dimer of 9-ethynylnoscapine was also isolated as by-product. Outcome of these couplings critically depends on the choice of ligands and base as well as employed reaction conditions. The synthesized 1,3-diyne analogues were evaluated for their anti-proliferative activity. (*Asian J. Org. Chem.*, **2019**, *8(8)*, 1495)

Synthesis and Evaluation of Novel Substituted 1,2,3-Triazolyldihydro Quinolines as Promising Antitubercular Agents



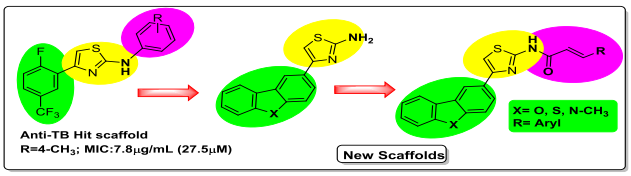
A series of novel substituted 1,2,3-triazolyldihydroquinolines was designed and synthesized from 2-acetylthiophene in five-step reaction sequence involving modified Boltzmann-Rahtz reaction of β-Enaminone; Vilsmeier-Haack chloro formylation using DMF/$POCl_3$; Ohira-Bestmann homologation of aldehyde to alkyne as key steps. The reaction of alkyne with various aryl azides in the presence of copper sulfate and sodium ascorbate resulted desired new 1,2,3-triazolyldihydroquinolines in excellent yields. *In vitro* screening of new compounds for anti-mycobacterial activity against *Mycobacterium tuberculosis H37Rv* (*Mtb*), resulted in three derivatives as promising antitubercular agents with lower cytotoxicity profiles. (*Bioorg. Med. Chem. Lett.*, **2019**, *29*, 529)

Synthesis of Novel Morpholine, Thiomorpholine and N-Substituted Pipe razine Coupled 2-(Thiophen-2-Yl)Dihydro quinolines as Potent Inhibitors of *Myco bacterium Tuberculosis*



A series of novel morpholine, thiomorpholine and N-substituted piperazine coupled 2-(thiophen-2-yl)dihydroquinolines was designed and synthesized from 2-acetyl thiophene in six step reaction sequence involving modified Bohlmann-Rahtz and Vilsmeier-Haack-Arnold reactions as key transformations. 2-(Thiophen-2-yl)dihydroquinoline was formylated using DMF-$POCl_3$, the resulting aldehyde was reduced to give an alcohol and then converted to bromide using PBr_3. Further coupling with morpholine, thiomorpholine and N-substituted piperazines resulted in the desired quinolines in very good yields. All the new derivatives were characterized by their NMR and mass spectral analysis. *In vitro* screening of new compounds for antimycobacterial activity against *Mycobacterium tuberculosis* H37Rv (MTB), resulted in two derivatives as most potent antitubercular agents (MIC:1.56 µg/mL) with lower cytotoxicity profiles. (*Eur. J. Med. Chem.*, **2019**, *164*, 171)

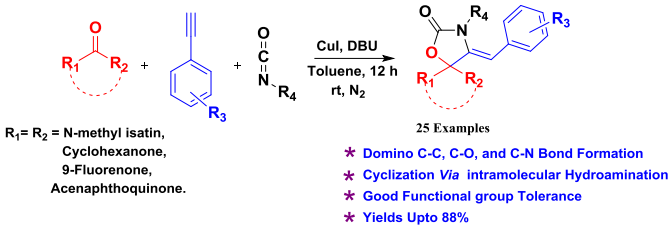
Dibenzofuran, Dibenzothiophene and N-Methyl Carbazole Tethered 2-Aminothiazoles and their Cinnamamides as Potent Inhibitors of *Mycobacterium Tuberculosis*



Herein described the design, synthesis and antitubercular evaluation of novel series of dibenzofuran, dibenzothiophene and *N*-methyl carbazole tethered 2-aminothiazoles and their cinnamamide analogs. One pot condensation of *N*-methyl carbazole, dibenzofuran and dibenzothiophene methyl ketones with thiourea in the presence of Iodine and CuO gave respective 2-aminothiazoles in very good yields. Aminothiazoles were further coupled with substituted cinnamic acids using **acid-amine coupling conditions to give desired** cinnamamide **analogs.** All the newly synthesized compounds were fully characterized by their NMR and mass spectral analysis. *In vitro* screening of new derivatives against *Mycobacterium tuberculosis* H37Rv (*Mtb*) resulted three analogs (MIC: 0.78 µg/ mL) and two 2-aminothiazoles (MIC: 1.56 µg/ mL) as potent compounds with lower cytotoxicity profile. (*Bioorg. Med. Chem. Lett.*, **2018**, *28(9)*, 1610)

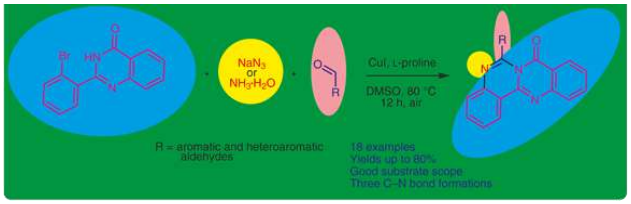
Copper-Catalyzed Domino Addition, Hydro amination, and Cyclization: A Multi component Approach to Spiro Oxazolidinone Derivatives

A copper-catalyzed one-pot multicomponent protocol has been developed for construction of spiro heterocycles. The domino approach leads to the synthesis of spiro oxazolidinones starting from ketones, arylacetylenes, and isocyanates via catalytic addition, hydroamination, and cyclization involving consecutive C–C, C–O, and C–N bond formations. (*J. Org. Chem.*, **2018**, 83, 15186)



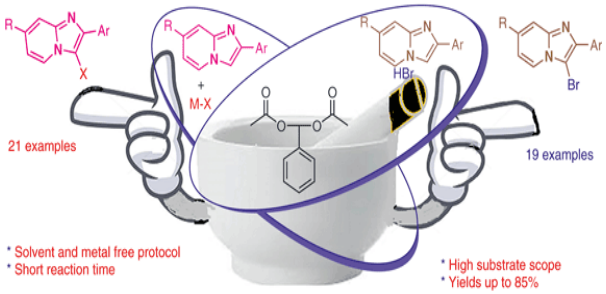
An Efficient One-Pot Multicomponent Synthesis of Tetracyclic Quinazolino[4,3-b] quinazolines by Sequential C–N Bond Formation and Copper-Mediated Aerobic Oxidative Cyclization

An efficient one-pot synthesis of quinazolino [4,3-b]quinazoline derivatives has been accomplished, starting from 2-(2-bromophenyl) quinazolin-4(3H)-one, aldehydes, and various nitrogen sources under aerobic conditions. The multicomponent protocol is mediated by copper(I) salts and involves amination of 2-(2-bromophenyl)quinazolin 4(3H)-one, followed by condensation with the aldehyde and an oxidative cyclization to give the target compounds in moderate to good yields. (*Synlett*, **2018**, 29, 1717)



Hypervalent Iodine Mediated Efficient Solvent Regioselective Halogenation and Thiocyation of fused N-Heterocycles

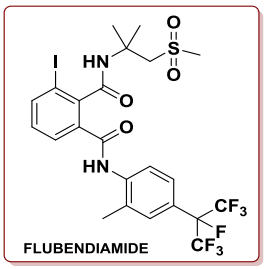
A facile, rapid, metal-free regioselective halogenation and thiocyanation of imidazo[1,2-a]pyridine/pyrimidine heterocycles has been achieved under solvent-free reaction conditions. Halogenations and thiocyanation of the heterocycles could be accomplished by simple grinding of reactants and hypervalent iodine reagents with the corresponding alkali metal or ammonium salts. The method has been extrapolated to a cleaner synthesis of brominated imidazo[1,2-a]pyridine/pyrimidine derivatives, starting from the corresponding heterocyclic amines and substituted α-bromoketones, utilising HBr generated in situ as the source of bromine. *(Synlett*, **2019**, 30(13), 1573)



Agro Mission:

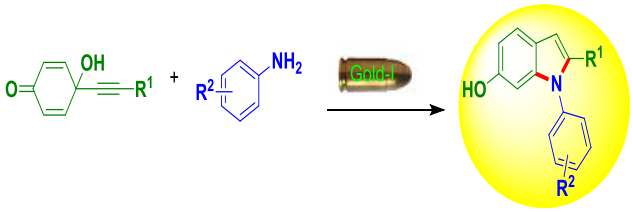
Process Development of Flubendiamide:

As part of CSIR agro mission, CSIR-IICT as a nodal laboratory, taken up the process development of three molecules i.e. Flubendiamide, Prothioconazole and Tembotrione. Accordingly, process development of Flubendiamide, first representative of phthalic acid diamide insecticide with the mode of action by activating Ryanodine receptors (RyRS) was taken-up. An economically viable route was devised starting from Pthalic anhydride and experimental studies are being carried out simultaneously to prepare key starting materials as well. Work is in progress at a steady pace in order to meet March, 2020 the completion target.



Gold-Catalyzed Synthesis of 6-Hydroxyindoles from Alkynylcyclohexadienones and Substituted Amines

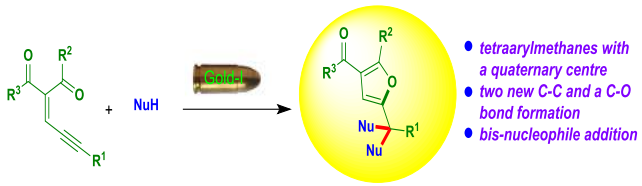
An efficient gold-catalyzed formation of 6-hydroxyindoles from substituted alkynylcyclo hexadienones and amines have been developed. In this reaction two new C−N bonds were formed, and moderate to very good yields of the 6-hydroxyindole derivatives were obtained in one pot. This organic transformation tolerates a range of substituted alkynylcyclo hexadienones and amines, which resulted in 6-hydroxyindole derivatives selectively. *(J. Org. Chem.*, **2019**, 84, 12228)



Gold–Carbene Assisted Formation of Tetraarylmethane Derivatives: Double X–H Activation by Gold

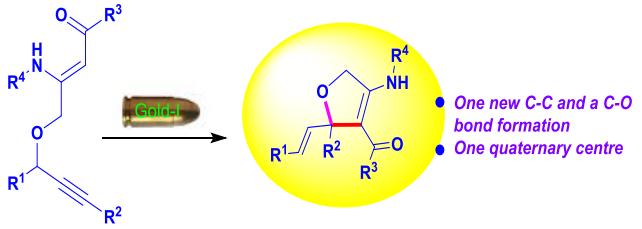
An efficient gold-carbene promoted synthesis of tetraarylmethane derivatives from enynones and indoles was accomplished by formation of a new C-O and two C-C bonds. It is significant that (2-furyl) gold-carbene assisted addition of two nucleophiles resulted the formation of tetraarylmethane derivatives with a quaternary

centre in moderate to good yields in one-pot. (*Org. Biomol. Chem.*, **2019**, 17, 4856)



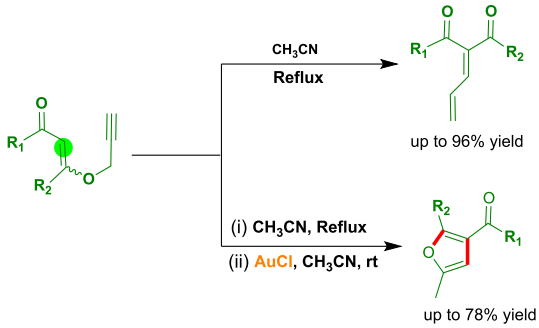
Gold-Catalyzed Facile Intramolecular Rearrangement and Cyclization Sequance for Synthesis of 2,5-Dihydrofurans

An efficient gold-catalyzed intramolecular rearrangement and cyclization protocol was developed for synthesis of 2,5-dihydrofuran derivatives from *O*-propargyl *β*-enaminones. In this organic transformation a new C-C and C-O bonds are formed with a quaternary centre under mild reaction conditions. Very good yields of substituted 2,5-dihydrofuran derivatives are obtained in one-pot synthesis. (*Org. Biomol. Chem.*, **2019**, 17, 6015)



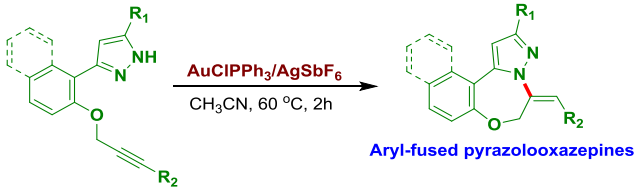
Conversion of *O*-Propargyl *B*-Enones to 2-Allylidene 1,3-Diones *via* [3,3]-Sigmatropic Rearrangement and Formation of Substituted Furans under Gold-Catalysis

An efficient synthetic protocol was developed for the formation of 2-allylidene 1,3-diones in very good yields *via* [3,3]-sigmatropic rearrangement of *O*-propargyl *β*-enones. Good yields of highly functionalized substituted furan derivatives were synthesized from *O*-propargyl *β*-enones under gold-catalysis *via* intramolecular cycloisomerization. In this organic transformation a new C-C and C-O bond formation was occurred in one pot synthesis. (*Chemistry Select*, **2019**, 4, 2053)



Gold-Catalyzed Formation of Aryl-Fused Pyrazolooxazepines via Intramolecular Regioselective 7-*Exo-Dig* Cyclization

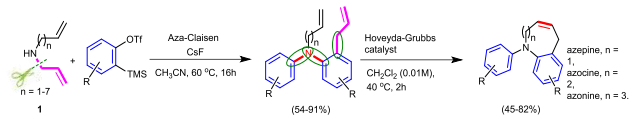
We have established an efficient synthetic protocol for the formation of substituted pyrazolo benzooxazepines and pyrazolo naphthoxazepines from substituted *ortho*-*O*-propargyl aryl pyrazoles. Significantly, this gold-catalyzed regioselective organic transformation takes place *via* *7-exo-dig* cyclization. The title compounds were obtained in moderate to good yields. (*Org. Biomol. Chem.*, **2019**, 17, 2809)



Synthesis of Medium-Sized Aryl-Fused Nitrogenous Heterocycles *via* Sequential Aryne Aza-Claisen Rearrangement/ Ring-Closing Metathesis

The reaction of arynes and secondary allylamines furnished ortho-allyl-substituted N-arylanilines *via* an aza-Claisen rearrangement. In this transformation, the sequential formation of C–C and C–N bonds occurred by involving two aryne molecules under metal-free reaction conditions to provide moderate to good yields of the products. The obtained ortho-allyl-substituted N-arylaniline derivatives were further converted into aryl-fused medium-sized (7-9) nitrogenous heterocyclic molecules such as azepines,

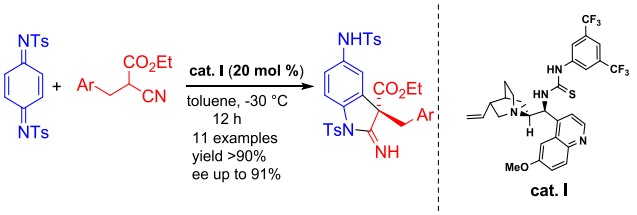
azocines and azonines *via* ring-closing metathesis (RCM). (*Org. Biomol. Chem.*, **2018**, 16, 2134)



Asymmetric Organocatalysis and Organometallic Catalysis:

BASIC RESEARCH

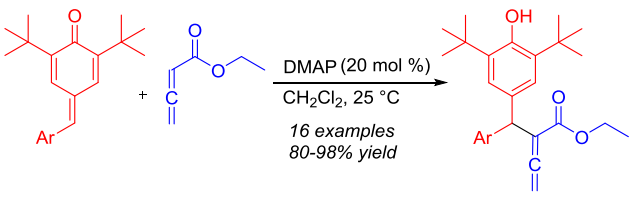
Ia. Asymmetric Reaction of *Para*-Quinone Diimide: Organocatalyzed Michael Addition of α-Cyanoacetates



Scheme 1

Hitherto unknown catalytic enantioselective transformation of *p*-quinone diimides is achieved using chiral bifunctional organic molecules. Bifunctional thiourea compounds catalyze the Michael addition of cyanoacetates with excellent yields and enantioselectivities. The initially formed Michael adducts undergo cyclization to yield functionally rich, fused cyclic imidine, bearing a quaternary benzylic chiral center (Scheme 1). Density functional theory calculations of the competing transition states (TSs) were carried out to explain the observed stereochemical outcome. (*Org. Lett.*, **2018**, 20(9), 2572)

Ib. DMAP Catalysed Vinylogous Rauhut–Currier Reaction of Allenoates with *Para*-Quinone Methides

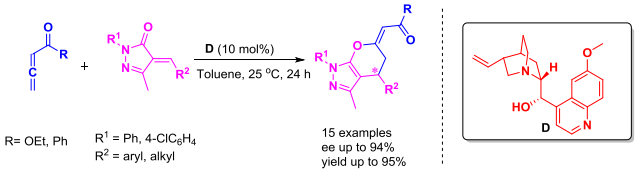


Scheme 2

We have identified that DMAP efficiently catalyses the vinylogous Rauhut–Currier reaction of allenoate esters with *para*-quinone methides affording the adducts in high to excellent yields. It is noteworthy that the vinylogous Rauhut–Currier reaction of allenoates are so far unknown in the literature. Under the reaction conditions identified, allenoate ketones failed to react with *p*-QM(Scheme 2). Unfortunately, our initial efforts towards achieving enantiocontrol by employing chiral bases were unsuccessful.

Ic. Direct Catalytic Asymmetric Method for the Synthesis of Tetrahydropyranopyrazoles through Allene Zwitterion Chemistry

The enantioselective synthesis of the tetrahydropyranopyrazole scaffold has been achieved. The quinidine catalyzed reaction of allenoates with arylidenepyrazolonesproceeds with high enantio- and diastereoselectivity affording the target structures, while the reaction of alkylidenepyrazolonesare less efficient. Allene ketones also afforded the tetrahydropyranopyrazolederivatives in high yields, however with only moderate enantioselectivity (Scheme 3). The primary adduct undergoes further functional group transformations without effecting the initially formed chiral centre.

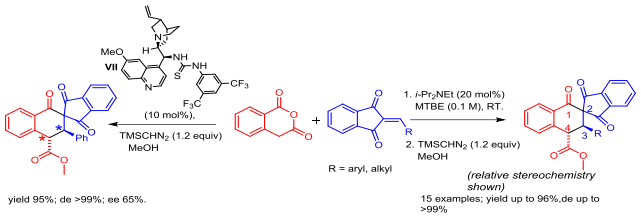


Scheme 3

1d. Base Catalysed Diastereoselective Tamura Cycloaddition of Vinylidene Indanediones

The base catalysed Tamura cycloaddition reaction of vinylidene indanediones afforded the corresponding spiro[indane-1,3-dione-1-tetralone] structures as single diastereomers in excellent yields. Chiral bifunctional hydrogen bonding thiourea catalysts rendered the reaction enantioselective (Scheme 4). However, the selectivity observed was moderate with

Soós catalyst providing an enantiomeric ratio of 82.5:17.5



Scheme 4

1e. Gold-catalysed regioselective cascade cyclo isomerisation reactions of aza-enediynes for the synthesis of substituted benzoisoquinoline derivatives

Aza-enediynes underwent a facile, regioselective gold-catalysed cascade cycloisomerisation to furnish dihydrobenzo[*f*]isoquinoline derivatives in excellent yields. The aza-enediynes were conveniently prepared *via* a formal vinylic displacement reaction of allyl bromosulfones (Scheme 5). The latter functioned as a stable and easily accessible synthetic equivalent of allenyl sulfone.

Scheme 5

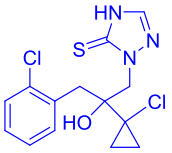
APPLIED RESEARCH

CSIR agromission program in developing processes for new generation agrochemicals. The project proposal was flouted, defended, got necessary approvals and implemented in 2018-19.

Concept note on agromission 2 submitted.

Process Development:

Prothioconazole:



Prothioconazole is a systemic demethylation inhibitor fungicide of the triazolinthione chemical class. It has demonstrated protective, curative and eradicative action against plant diseases caused by ascomycetes, basidiomycetes, and deuteromycetes fungi in many crops, and is intended to be used for the control of fusarium head blight and reduction of deoxynivalenol levels in barley and wheat.

The product has good sales though not launched in India. This can be seen from the export licenses given in India to many companies. However, no Indian manufacturing or import licenses are found. Hence, the product has good export potential immediately in US and in 2019 in Europe. So process chemistry has been designed and developed for this molecule.

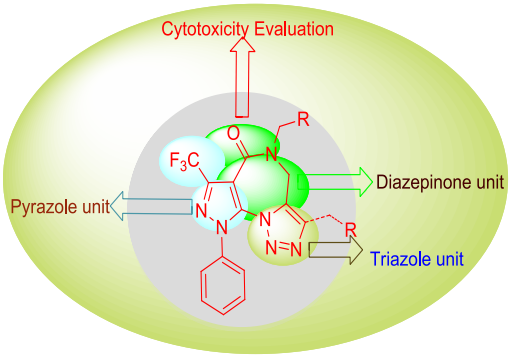
New Chemical Entities:

As a part industry sponsored program, multiple new scaffolds have been prepared and submitted for evaluation to IIL, Delhi. Some promising results obtained.

Synthesis and Cytotoxicity Evaluation of Novel Tricyclic Dihydropyrazolo [4,3-*f*][1,2,3]triazolo Diazepines

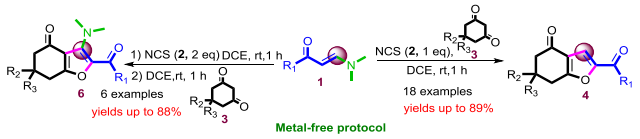
Number of novel fluorinated 4,5-dihydropyrazolo [4,3-*f*][1,2,3] triazolo diazepines (**9-11**) have been accomplished starting from 1-phenyl-3-trifluoromethyl pyrazole-5-one (**3**) in a multistep synthesis. Thus obtained compound **9** was converted into corresponding 5-aryl /alkyl fluorinated 4,5-dihydropyrazolo [4,3-*f*][1,2,3]triazolo diazepinones **10a-j** and also 3,5-diaryl /dialkyl fluorinated 4,5-dihydropyrazolo [4,3-*f*][1,2,3]triazolo diazepinones **11a-c** and all the compounds **9-11** were evaluated for *in vitro* cytotoxic activities. The outcome of the study showed that compounds **9**, **10c**, **11a** showed very promising activity against MCF7, HeLa, Neuro2a and A549 cell lines. Further, compound **10g** showed good activity against HeLa, Neuro2a and A549 cell lines whereas **10f** and **11c** showed good activity

against A549 cell line. (*Lett. Drug. Des. Discov.*, **2018,** 15, 1020)



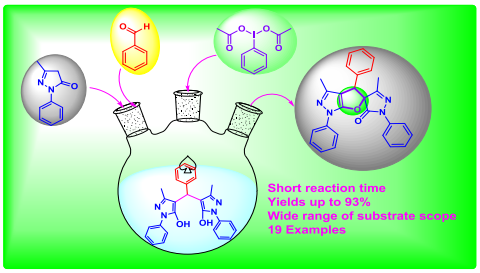
Regioselective Synthesis of 2-Carbonyl Furans in a One Pot Three Component Reaction

Regioselective synthesis of 2-benzoyl-6,6-dimethyl-6,7-dihydrobenzofuran-4(5H)-ones have been accomplished through a novel protocol involving b-amino enone, N-chlorosuccinimide and dimedone in a one pot catalyst-free reaction at an ambient temperature. On the other hand, the same reaction when conducted with two equivalents of N-chlorosuccinimide under similar reaction conditions, exclusive formation of 2-benzoyl-3-(dimethylamino)-6,6-dimethyl-6,7-dihydrobenzofuran-4(5H)-ones were observed. Simple and metal-free reaction conditions, selective product formation and excellent yields are the advantages of this protocol. (*Tetrahedron Lett.*, **2018,** 59, 4168)



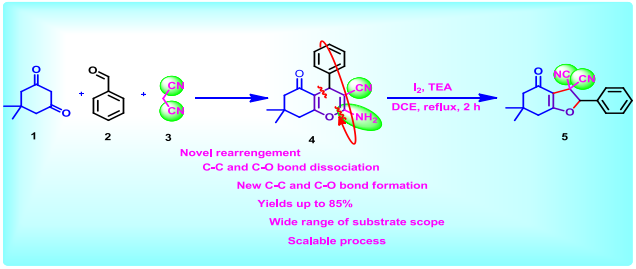
Synthesis of Dihydrospiro Furo[2,3-C]Pyrazoles Promoted by Hypervalent Iodine in Water

A simple, green protocol has been accomplished for synthesis of dihydrospiro furo[2,3-*c*]pyrazoles (4) in water medium involving pyrazolone (1) and aldehydes (2) in a one pot reaction promoted by bis (acetoxy) iodobenzene (BAIB) at ambient temperature. The protocol presented herein, is for the first time, via a novel transformation where two moles of pyrazolone react with aldehyde in a Knoevenagel followed by Michael fashion and the resulting dienol was rearranged to the title compound 4. High compatibility, easy work-up and excellent yields are the advantages of this protocol. *(Synlett*, **2018**, 29, 1037)



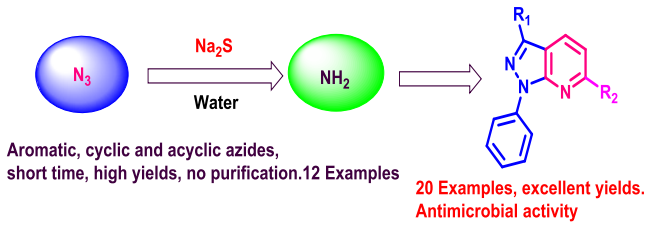
Molecular Iodine Promoted Synthesis of 3,3-Dicarbonitrile Dihydrobenzofurans through a Novel Rearrangement

Synthesis of title compounds accomplished through a novel protocol involving 5,5-dimethylcyclohexane-1,3-dione (**1**), aromatic aldehydes (**2**) and malononitrile (**3**) via 2-amino-7,7-dimethyl-5-oxo-4-phenyl-5,6,7,8-tetrahydro-4H-chromene-3 carbo-nitrile (**4**) promoted by molecular iodine in basic medium. The protocol presented herein, for the first time, through a novel rearrangement where the 4H-chromene fragment dissociates into cyclopropane moiety and re-arranges to five membered 6,6-di methyl-4-oxo-2-phenyl-4,5,6,7-tetrahydro benzo furan-3,3(2H)-dicarbonitrile (**5**). Simple reaction conditions, excellent yields and high compatibility are the advantages of this protocol. (*Synlett*, **2019,** 30, 293)



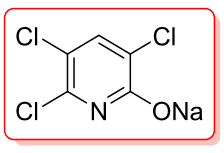
Na_2S Promoted Reduction of Azides in Water: Synthesis of Pyrazolopyridines in One Pot and Evaluation of Antimicrobial Activity

Reduction of various azides using Na_2S has been accomplished in water and the *in situ* resulted amine on reaction with various ketones lead to pyrazolo[3,4-*b*]pyridines in one pot. Thus, a number of new trifluoromethyl substituted pyrazolo[3,4-*b*]pyridine compounds have been prepared and screened for antimicrobial activity against different Gram-positive & Gram-negative strains. A good number of compounds were found to posses promising activity. Notably, Na_2S up on hydrolysis in water generating H_2S and NaOH which are facilitating the reduction of azides followed by intramolecular cyclization leading to title compounds. To the best of our knowledge, this is the first report to synthesize the title compounds in aqueous medium in a one pot reaction (*Org. Biomol. Chem.*, **2019**, **17,** 3186)



Process Development of Na-TCP

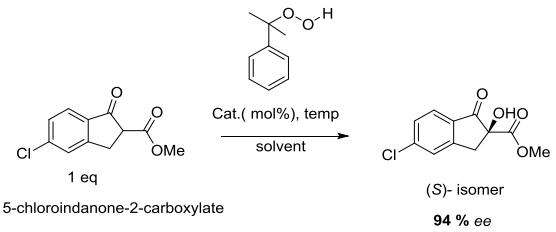
Sodium salt of 3,5,6-trichloro-2-pyridinol (NaTCP) is a high volume import chemical and *n-1* compound in the manufacture of "Chlorpyriphos". Re-investigation studies on the process of NaTCP was conducted and an alternate route with economic competitiveness is developed. Thus, developed process was successfully demonstrated**.**



Sodium salt of TCP

Towards the Chiral Synthesis of M-240: Enantioselective Hydroxylation of 5-Chloroindanone-2-Carboxylate

In agrochemicals having at least one chiral center, most often available commercially as racemic mixtures, the activity is associated with one of the stereoisomers. Indoxacarb, a highly useful insecticide is also marketed as a racemate, although the (*S*)-isomer is found to be the active enantiomer. The critical intermediate for the preparation of (*S*)-indoxacarb is the (*S*)-5-chloro-2-hydroxy-indanone-2-carboxylate, which is obtained by the hydroxylation of 5-chloroindanone-2-carboxylate. We have successfully carried out the enantioselective hydroxylation of 5-chloroindanone-2-carboxylate with up to 94 % enantiomeric excess and demonstrated the laboratory scale process to ADAMA India Pvt. Ltd (SSP 0737) as shown in Scheme 6.



Scheme 6

Pheromone Application Technology for Sustainable Agriculture

Pheromones are the chemicals that are released by the insects for their own communication. Isolation, identification and synthesis of those chemicals and using their synthetic mimics in the field to manage/control them (pests) itself is PAT. It is a well-established and accepted agro-practice all over the world. But, PAT in India is still in primitive stage. Farmers are not fully aware of the potentiality and versatility of this eco-friendly and environmentally safe technology. Especially PAT is highly suitable for the control of Insect pests with internal feeding habit/borer category that damage economically important crops. Incidentally such

internally feeding insects/pests cannot be controlled by conventional pesticide application.

Methods/Techniques in PAT

PAT is a unique agro practice

- To estimate the density of the pests. MONITORING
- To trap out pests in large numbers. MASS TRAPPING
- To prevent males in locating females. MATING DISRUPTION
- To confuse males by males AUTO-CONFUSION

The following pheromone technologies are readily available for the implementation in various crops.

1	Maize/Corn	Fall armyworm (Spodoptera frugiperda)	(*Z*)-11-Hexadecen-1-yl acetate: (*Z*)-9-Tetradecen-1-yl acetate: (*Z*)-7-Dodecen-1-yl acetate
2	Cotton	Pink bollworm (Pectinophora gassypiella)	(*Z*,*E*)-7,11-Hexadecadien-1-yl acetate: (*Z*,*Z*)-7,11-Hexadecadien-1-yl acetate
3	Rice	Yellow stem borer (Scirpophaga incertulas)	(*Z*)-11-Hexadecenal: (*Z*)-9-Hexadecenal
4	Brinjal	Leucinodes orbonalis (Brinjal shoot and fruit borer)	(Z)-11-Hexadecenyl acetate: (Z)-11-Hexadecenol
5	Mango, Guava, Sapota, Papaya	Bactrocera dorsalis (Oriental fruit fly)	Methyl eugenol
6	Bitter gourd, Ridge gourd, Bottle gourd, Cucumber, Pumpkin, Tindora, Teasel gourd, Musk melon, Watermelon, Gherkin	Bactrocera cucurbite (Melon fly)	Cue-Lure

Training for the Formulation of Pheromone Lures

The training component would cover the following aspects:

- Pheromone extraction methodologies
- Microfiltration techniques
- Purification of the ovipositor/gland extracts by HPLC
- Electrophysiological recording from the sensory receptors on the antennae commonly referred to as Electroantennogram Recording Technique (EAG):
- Gas Chromatograph coupled to Electro antennogram (GC-EAG) technique
- Detection of the Behavioral Activity in the laboratory using Wind tunnel /olfactometer
- Dispenser Pre-treatment procedures
- Pheromone blend impregnation methodologies
- Analysis of pheromone blend
- Quantification of the blend

I) CSIR-IICT has Expertise in the Pheromone Technology for the Supply of Pheromone Lures/Traps for Monitoring and Mass-Trapping Adult Pests for the Below Crops

1) During the Kharif Season 2018, CSIR-IICT has supplied pheromone lures and traps to Department of Agriculture, TELANGANA for monitoring and mass trapping PINK BOLLWORM (PBW), which is a major damaging pest in COTTON to cover 25000 ACRES.

❖ During this season CSIR-IICT distributed Pink Bollworm Lures and Traps in mandal level in Nine Districts and earned Rs 66,00,000/-.

Table: Distribution of Pheromone Lures & Traps in 32 Mandals of Nine Districts

Name of the District	Name of the Mandal	Pheramone Traps Supplied	Lures Supplied
Adilabad	Thalamadugu	19900	19900
	Mavala	2000	2000
	Gudihatnoor	13700	13700
	Boath	19700	19700
	Bazarhatnoor	14800	14800
	Total	70100	70100
Khammam	Enkoor/VAIRA	4600	4600
	Kusumanchi	5000	5000
	Tirumalaipalem	4900	4900
	Mudigonda	3600	3600
	Total	18100	18100
Warangal®	Nekonda*	[13,700+ 34,500]= 48200	48200
	Wardhannapet	3510	3510
	Duggondi	3510	3510
	Chennaraopet	2410	2410
	Total	**57630**	**57630**
Warangal(U)	Khila Warangal	940	940
	Total	**940**	**940**
Nalgonda	Kattangur	2650	2650
	Thipparthy	3400	3400
	Nalgonda	7000	7000
	Munugodu	8900	8900
	Total	**21950**	**21950**
Nirmal	Kuber	2700	2700
	Tanoor	1950	1950
	Basar	900	900
	Dilwarpur	900	900
	Sarangapur	1110	1110
	Total	**7560**	**7560**
Asifabad	Tiryani	2300	2300
	Wankidi	3700	3700
	Kagaznagar	2100	2100
	Sirpur-T	2200	2200
	Total	**10300**	**10300**
Karimnagar	Jammikunta	3800	3800
	Ramadugu	3500	3500
	Karimnagar	1600	1600
	Total	**8900**	**8900**
Rajanna Siricilla	Vemulawada(R)	3500	3500
	Vemulawada(U)	1900	1900
	Total	**5400**	**5400**
	Grand Total	**201,250**	**201,250**

2) During the Kharif Season 2019, CSIR-IICT has supplied pheromone lures and traps to Department of Agriculture, TELANGANA for monitoring and mass trapping FALL ARMYWORM (FAW), which is a devastating pest in MAIZE/CORN to cover 42440 ACRES in 120 mandals of 28 districts.

During this season CSIR-IICT distributed Fall Armyworm Lures and Traps in 120 mandal of 31 Districts and earned Rs 1,69,76,000/- in the months of July to August 2019 in two phases.

Table: Distribution of Pheromone Lures & Traps in 120 Mandals of 31 Districts

Pheromone Traps and Lures for Management of FAW in Maize for Kharif 2019			
S.No	**DISTRICT**	**Number of Pheromone Lures**	**Pheromone Traps**
1	**Adilabad**	1000	**2000**
2	**Badradri Kothagudem**	2000	4000
3	**Jagtiyal**	26442	52884
5	**Janagoan**	1448	2896
6	**Jayashanker**	1000	2000
7	**Gadwal (Jogulamba)**	12600	25200
8	**Kamareddy**	4160	8320
9	**Karimnagar**	2000	4000
10	**Khammam**	1000	2000
11	**Mahabubnagar**	4520	9040
12	**Mancherial**	1000	2000
13	**Medak**	2400	4800
16	**Mehababad**	3000	6000
17	**Mulugu**	1000	2000
18	**Nagarkurnool**	6000	12000
19	**Narayanpet**	1000	2000
20	**Nirmal**	2000	4000
21	**Nizamabad**	2820	5640
22	**Peddapalli**	1000	2000
23	**Rajanna Siricilla**	2000	4000
24	**Rangareddy**	3500	7000
25	**Sangareddy**	5080	10160
26	**Siddipet**	245952	491904
27	**Vikarabad**	5780	11560
28	**Wanaparthy**	1000	2000
29	**Warangal (Rural)**	5000	2000
30	**Warangal Urban)**	2184	4368
31	**Yadadri**	1000	2000
	Grand Total	**3,39,517**	**6,79,034**

- During the Kharif Season 2019, CSIR-IICT has supplied pheromone lures and traps to Department of Agriculture, ANDHRA PRADESH, for monitoring PINK BOLLWORM (PBW), which is a major damaging pest in COTTON to cover 62400 HECTARES (156000 Acres) over 9 districts.
- During this period earned Rs. 2,18,40,000/-

Pheromone Traps and Lures for Management of PBW in Maize for Kharif 2019			
S.No	**District**	**Number of Pheromone Lures**	**Pheromone Traps**
1	**Ananthapuram**	**51,000**	**51,000**
2	**East Godavari**	**16,000**	**16,000**
3	**Guntur**	**1,81,000**	**1,81,000**
4	**Krishna**	**48,000**	**48,000**
5	**Kurnool**	**2,40,000**	**2,40,000**
6	**Prakaham**	**43,000**	**43,000**
7	**Srikakulam**	**7000**	**7000**
8	**Vizayanagaram**	**14,000**	**14,000**
9	**YSR Kadapa**	**24,000**	**24,000**
		6,24,000	**6,24,000**

Demonstration Photos in the field :

Distribution and Demonstration Program about Pheromone Lures & Traps to Farmers at Adilabad District by CSIR-IICT Team

Distribution and Awareness Program to Farmers at Markook Mandal Siddipet District by CSIR-IICT Team

Distribution and Demonstration about Pheromone Traps to Farmers at Wardannapet mandal, Warangal District by CSIR-IICT Team

Handing Over of Pheromone Lures to Agriculture Officer at Kurnool Man District by CSIR-IICT Team

Distribution and Demonstration about Pheromone Traps to Farmers at Dubbaka mandal, Siddipet District by CSIR-IICT Team

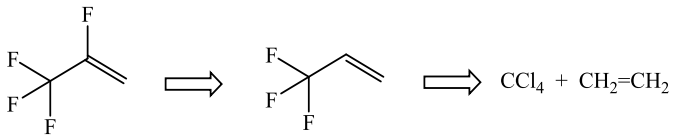
Distribution and Demonstration about Pheromone Traps to Farmers at Mulugu mandal, Siddipet District by CSIR-IICT Team

A Joint awareness Program on importance and uses about Pheromone Lures & Traps to farmers at Vemuluripadu Village, Phirangipuram Mandal, Guntur Dist by CSIR-IICT Team and Spl Commissioner to Department of Agriculture, Govt of Andhra Pradesh Shri H. Arun Kumar IAS & their team.

Our research group focuses on controlled radical polymerization processes such as atom transfer radical polymerization and reversible addition-fragmentation chain transfer polymerization are adopted to obtain controlled molecular weights of the targeted fluoro/(meth)acrylate-based macromolecular architectures for strategic, solar cell, membrane, and biomedical applications.

Development of polymeric additives for petroleum refining, and petrochemical processes is a key component of research for downstream hydrocarbon processing technologies. The efforts are discharging in the area of dewaxing of lube molecules to produce cold flow property boosters. We involved in developing novel and cost effective propane dewaxing aid polymers for M/s Hindustan Petroleum Corporation Limited (M/s HPCL), Bangalore. Moreover, most of the available dewaxing aids preparation procedures are patented and the availability is restricted. Companies which used to supply dewaxing aids to the M/s HPCL have stopped their production and alternative dewaxing aids are very expensive. Hence there is an enormous and immediate need for development of indigenous dewaxing aids. We come up with indigenous materials and technology and going to be employed these materials at Mumbai Refinery, India. We successfully, synthesized novel polymers including polyalkyl-(meth)acrylates as dewaxing aids (DWAs) and evaluated the performance of the developed polymers and identified right DWAs that closely match the performance of benchmark samples. We have scaled up for commercial trails up to 5 L batch size.

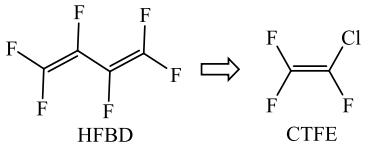
Development of Process for New Generation Refrigerant HFO-1234yf: HFO-123yf (2,3,3,3-tetrafluoropropene) is a environmentally safe refrigerant with zero ozone depletion potential, negligible global warming potential and very low atmospheric life when compared to currently widely used refrigerants HFC-134a and R22. It is a near drop-in replacement to HFC-134a. DST and MoEF sponsored this project and studies on development of an industrially viable multi-step process using inexpensive and readily available raw materials, carbon tetrachloride and ethylene via 3,3,3-trifluoropropene is in progress.



HFO-1234yf

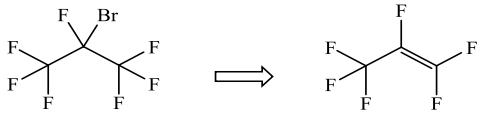
Development of Process for Hexafluoro-1,3-butadiene(HFBD): It is a new plasma etching gas used in semiconductor industry. Unlike other commonly used etchants such as SF6, NF3, chlorine and tetrafluoromethane, HFBD is environmentally non-corrosive, non-ozone depleting and

environmentally safe. Semiconductor Laboratory (SCL), Mohali sponsored project for development of a process. Several routes were studied and identified a viable and scalable method for preparation of hexafluoro-1,3-butadiene starting from chloro trifluoroethylene via 1,2,3,4-tetrachlorohexa fluoro butane. Process optimization studies are in progress.



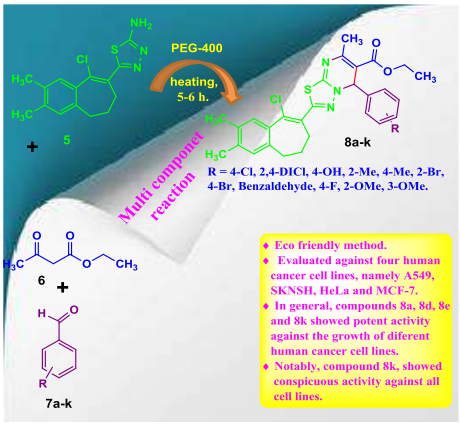
Development of a Process for 1-Iodo-2,2,2-trifluoroethane: This project was sponsored by CFEES(DRDO) seeking process development at bench scale for this molecule starting from 1-chloro-2,2,2-trifluoroethane (HFC-133a). This process development was completed and demonstrated at 100g/batch scale.

Development of Process for 2-bromohepta fluoropropane: This compound is a key intermediate for preparation of pesticide Flubendiamide. A scalable two-step process was developed for this molecule from hexafluoropropene as a part of CSIR-Agro Mission project.



A Green Protocol for One Pot Synthesis of Benzosuberone Tethered Thiadiazolo pyrimidine-6-Carboxylates Using PEG-400 as Potent Anti-Proliferative Agents

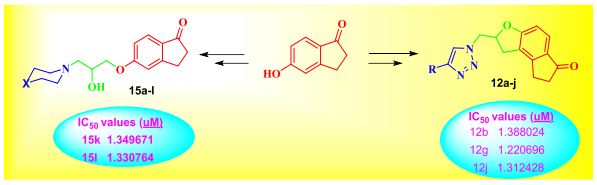
A new concise and facile method was explored to synthesize a collection of new benzosuberone based thiadiazolo[3,2-*a*]pyrimidine-6-carboxy lates using polyethylene glycol (PEG), which could be regarded as the derivatives of the hybrid scaffolds of bioactive natural benzosuberone and heterocyclic thiadiazolo[3,2-*a*]pyrimidine. The structures of the synthesized compounds were characterized by ^{1}H, ^{13}C NMR, MS and IR; and their anti-proliferative activity was evaluated against four human cancer cell lines; A549, SKNSH, HeLa and MCF-7. Among the tested compounds, compound **8k** showed the most prominent activity against all the cell lines and these results may lay the foundation for further design of novel anti-proliferative agents. (*Tetrahedron Lett.*, **2018**, *59*, 3015)



Potent ACE inhibitors from 5-Hydroxy Indanone Derivatives

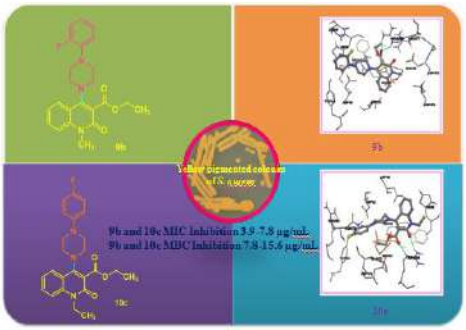
A novel triazole derivatives(±)-2-(hydroxyl methyl)-7,8-dihydro-1*H*-indeno[5,4-b]furan-6 (2*H*)-one (**12a-j**) were designed and synthesized by the reaction between racemic azide and terminal acetylenes under click chemistry reaction conditions followed by biological evaluation as angiotensin converting enzyme (ACE) inhibitors. *β*-Amino alcohol derivatives of 1-indanone (**15a-l**) were synthesized from 5-hydroxy indanone, it was reacted with epichlorohydrin and followed by oxirane ring opening with various piperazine derivatives. Among the newly synthesized compounds **12b** (IC_{50}: 1.388024 µM), **12g** (IC_{50}: 1.220696 µM),**12j** (IC_{50}: 1.312428 µM) and **15k** (IC_{50}: 1.349671 μM) and **15l** (IC_{50}: 1.330764 μM) emerged as most active non-carboxylic acid ACE inhibitors with

minimal toxicity comparable to clinical drug Lisinopril. *(Bioorg. Chem.*, **2018**, 77, 660)



A Novel Templates of Piperazinyl-1,2-Dihydro quinoline-3-Carboxylates: Synthesis, Anti-Micro bial Evaluation and Molecular Docking Studies

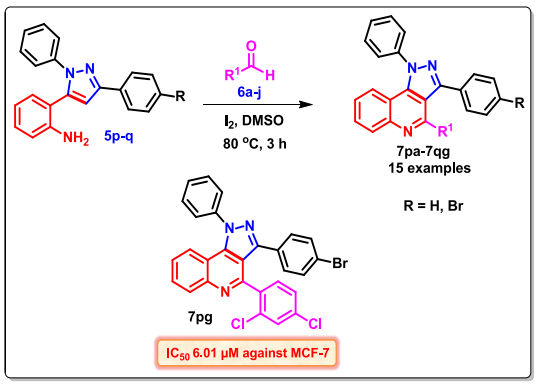
A series of piperazinyl-1,2-dihydroquinoline carboxylates were synthesized by the reaction of ethyl4-chloro-1-methyl-2-oxo-1,2-dihydroquino line-3-carboxylates with various pipera zines and their structures were confirmed by ^{1}H NMR, ^{13}C NMR, IR and mass spectral analysis. All the synthesized compounds were screened for their *in vitro* antimicrobial activities. Further, the *in silico* molecular docking studies of the active compounds was performed to explore the binding interactions between piperazinyl-1,2-dihydroquinoline carboxylate derivatives and the active site of the *Staphylococcus aureus* (CrtM) dehydrosqualene synthase (PDB ID: 2ZCQ).



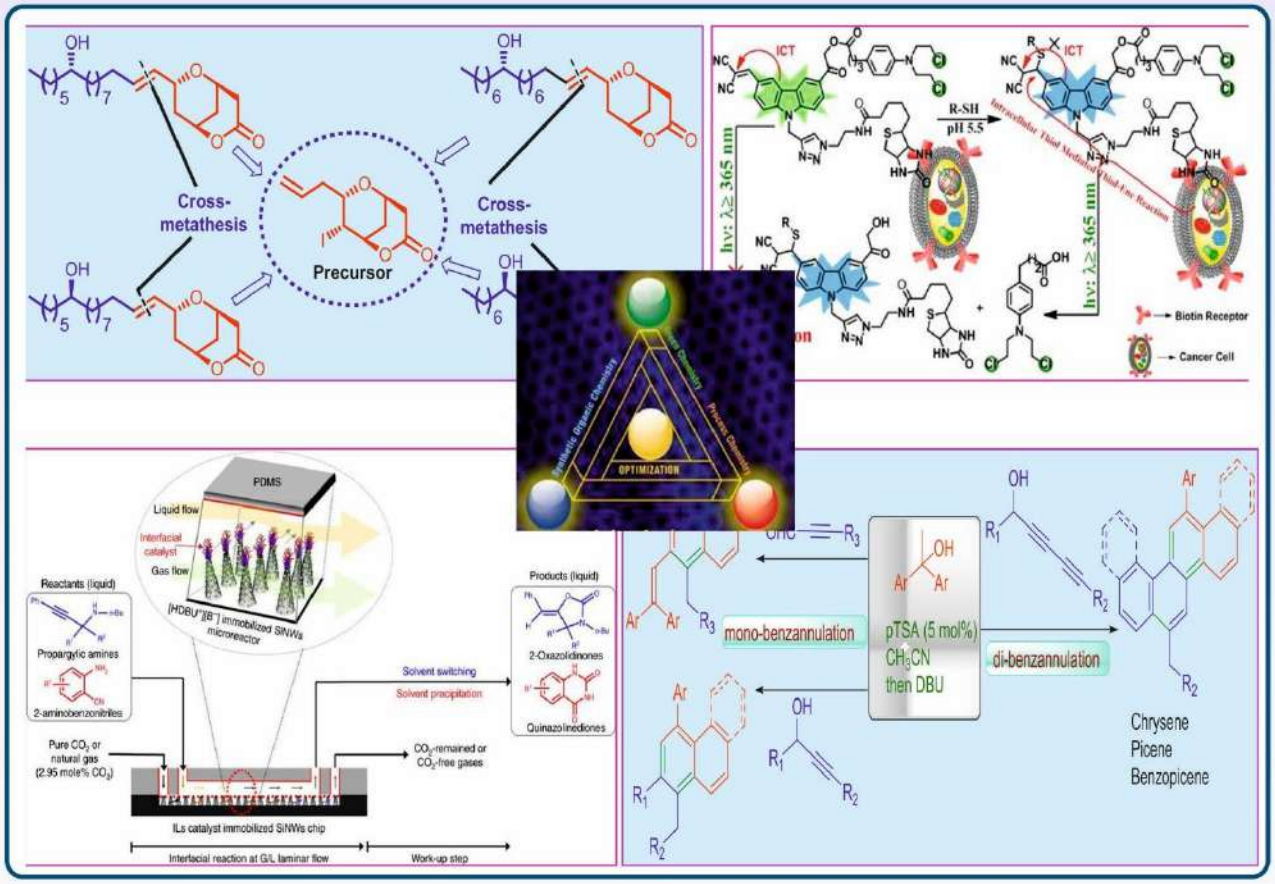
The docking studies revealed that the synthesized derivatives showed high binding energies and strong H-bond interactions with the dehydrosqualene synthase validating the observed antimicrobial activity data. Based on antimicrobial activity and docking studies, the compounds **9b** and **10c** were identified as promising antimicrobial lead molecules. This study might provide insights to identify new drug candidates that target the *S. aureus* virulence factor, dehydrosqualene synthase. *(Bioorg. Med. Chem. Lett.*, **2018**, 28, 1166)

Iodine Mediated Pyrazolo-Quinoline Derivatives as Potent Anti-Proliferative Agents

A novel series of substituted pyrazolo-quinoline derivatives **7pa-7qg** were synthesized efficiently by using molecular iodine in DMSO and further characterized based on ^{1}H NMR, ^{13}C NMR, IR and HRMS spectral studies. All the synthesized derivatives were screened for their *in vitro* cytotoxic activity against a panel of five different cancer cell lines such as A549, HeLa, SKNSH, HepG2 and MCF7. The compounds **7pc, 7pd, and 7pj** exhibited considerable to promising anti-proliferative activity with IC_{50} values of 3.76, 3.87 and 3.83 μM against SKNSH cancer cell line. It was revealed that the compounds **7pa** and **7pg** have shown very close IC_{50} values of 2.43 and 6.01 μM, against A549 and MCF7 cancer cell lines respectively, which compared to positive control of Doxorubicin. This is the first report on the synthesis and *in vitro* anti-proliferative evaluation of pyrazolo-quinoline derivatives. *(Bioorg. Med. Chem. Lett.*, **2018**, 28, 664)



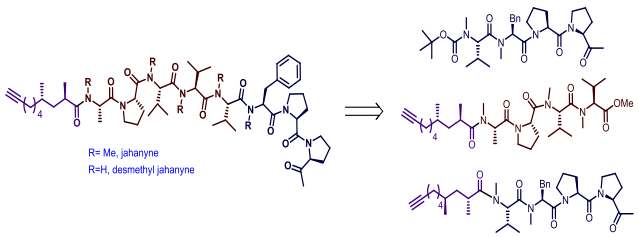
ORGANIC SYNTHESIS AND PROCESS CHEMISTRY



BASIC RESEARCH

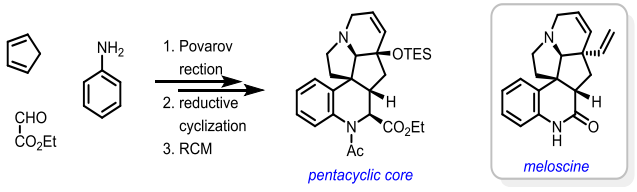
1. Total Synthesis of Desmethyl Jahanyne and Its Lipo-Tetrapeptide Conjugates Derived from Parent Skeleton as BCL-2-Mediated Apoptosis-Inducing Agents

The total synthesis of highly potent and scarcely available marine natural product (−)-jahanyne was attempted resulting in a solution-phase synthesis of pruned versions with comparable activity. A simple and facile synthetic route was employed for the preparation of pruned congeners and would be scalable. The lipophilic tail of the natural product was synthesized from *R*-(+)-citronellol, utilizing easily available chemicals. All the synthesized compounds were screened for apoptotic activity against a panel of cell lines. These compounds depicted marked binding to B cell lymphoma 2 till 50 °C in cellular thermal shift analysis. *(ACS Omega*, **2018**, 3(1), 63)



2. Synthetic Strategy towards the Pentacyclic Core of Melodinus Alkaloids

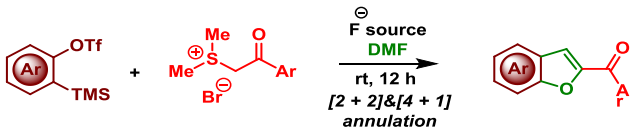
The three-component Povarov reaction is efficiently utilized for construction of the pentacyclic framework of complex *Melodinus* alkaloids, which is amenable to expansion to other complex natural products. The key steps were Povarov reaction, one-pot reductive cyclization, and ring-closing metathesis (RCM) reaction. *(J. Org. Chem.*, **2018**, 83(4), 2244)



3. Syntheses of 2-Aroyl Benzofurans through Cascade Annulation on Arynes

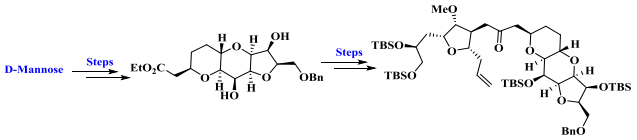
The highly efficient and expedient route for the syntheses of 2-aroyl benzofurans has been developed via the cascade [2+2] followed by a [4+1] annulation on arynes. The overall transformation proceeded through the formation of *ortho*-quinone methide by the insertion of transient aryne into *N*,*N*-dimethyl formamide and subsequent trapping with sulfur ylide. Moreover, this transformation has a broad range of substrate scope with a high functional-group tolerance. This new reaction was successfully utilized in the synthesis of the potent CYP19 aromatase inhibitor and late-stage functionalization on the bioactive complex estrone.

(*J. Org. Chem.*, **2018**, 83(6), 3325)



4. Stereoselective Synthesis of Northern Fragment of Eribulin Mesylate from D-Mannose

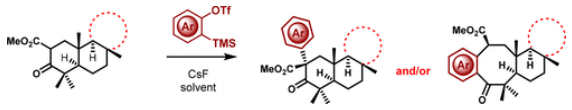
Stereoselective synthesis of northern fragment of eribulin mesylate is reported by coupling of C1-C13 fragment with C28-C35 fragment. The key steps involved in this synthesis are *n*-BuLi facilitated coupling between sulfone and aldehyde, then DMP oxidation followed by samarium(II) iodide mediated desulfonylation. (*Synthesis*, **2018**, 50(9), 1901)



5. Benzyne Insertion onto β-Keto Esters of Polycyclic Natural Products: Synthesis of Benzo Octacyclo Scaffolds

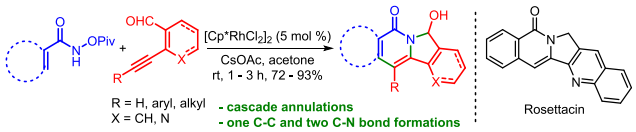
Benzyne insertion to build the privileged scaffold of a [6.8.6]-tricyclic framework on polycyclic and sp3 -rich natural products has been developed. The formation of the [6.8.6]-tricyclic ring system is

solvent dependent. , in the case of aliphatic β-keto esters, the major product on the arylation is the ring expansion product, whereas in the case of polycyclic compounds C-arylation is the major product in acetonitrile. (*Org. Lett.*, **2018**, 20(22), 7121)



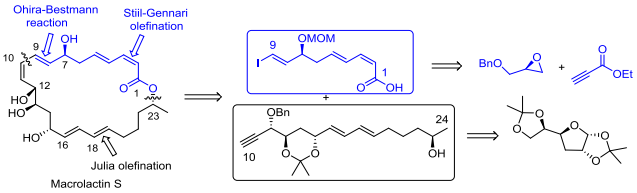
6. Rh(III)-Catalyzed Cascade Annulations to Access Isoindolo[2,1-*b*]isoquinolin-5(7*H*)-ones *via* C−H Activation: Synthesis of Rosettacin

A one-pot efficient method for the synthesis of 7-hydroxy isoindolo[2,1-b]isoquinolin-5(7*H*)-ones from *N*-(pivaloyloxy) amides and 2-alkynyl aldehydes by Rh(III)-catalyzed C−H functionalization has been developed. The established reactions are first examples of cascade Rh(III)-catalyzed alkyne insertion/intramolecular amide nitrogen addition to aldehydes. The significance of the products having aminal functionality was shown by further diversification through substitutions in the five-membered ring. Additionally, the application of this method in a short synthesis of rosettacin and topoisomerase I inhibitor was also demonstrated. The flexibility and the extensive scope of this cascade annulation approach should find applications in the synthesis bio-active natural product-like molecules. (*Org. Lett.*, **2018**, 20(1), 150)



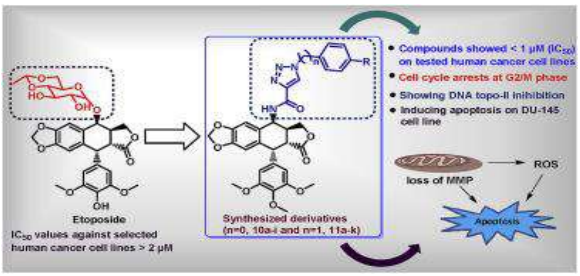
7. Studies on the Total Synthesis of Antibiotic Macrolactin S: A Conventional Approach for the Synthesis of the C1–C9 and C10–C24 Fragments

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*, **2018**, 50(3), 663)



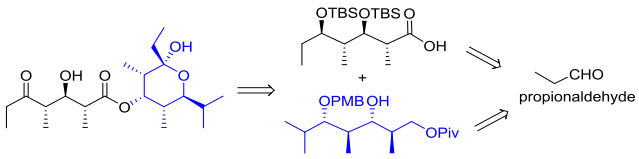
8. 4β-Amidotriazole Linked Podophyllotoxin Congeners: DNA Topoisomerase-Iia Inhibition and Potential Anticancer Agents for Prostate Cancer

Topoisomerases (topo-I and topo-II) have occupied a significant role in DNA replication, transcription, and are a promising set of antitumor targets. In the present approach, a series of new 4b-amidotriazole linked podophyllotoxin derivatives (10a-i and 11a-k) were designed, synthesized by employing the click chemistry and their biological activities were evaluated. The majority of derivatives showed promising antiproliferative activity with IC_{50} values ranging from 1 to 10 mM on the six human cancer cell lines; cervical (HeLa), breast (MCF-7), prostate (DU-145), lung (A549), liver (HepG2) and colon (HT-29). Among them, some of the congeners 10b, 10g and 10i have shown remarkable cytotoxicity with IC50 values of, < 1 mM against the tested cancer cell lines and found to be more active than etoposide. Topoisomerase- mediated DNA relaxation assay results showed that the derivatives could efficiently inhibit the activity of topoisomerase-II. In addition, flow cytometry analysis on DU-145 cells revealed that these compounds arrest G2/M phase of cell cycle. Further apoptotic studies were also performed on these DU-145 cells, which showed that this class of compounds could induce apoptosis effectively. (*Eur. J. Med. Chem.*, **2018**, 144, 595)



9. Stereoselective Total Synthesis of the Non-Contiguous Polyketide Natural Product (–)-Dolabriferol

The stereoselective total synthesis of the non-contiguous polypropionate dolabriferol has been accomplished in 17 steps, by an approach that is both divergent and convergent. The key reactions involved are enantioselective cross-aldol coupling, aldol dimerisation of propionaldehyde, Sharpless asymmetric epoxidation, regioselective epoxide opening and Yama guchi esterification. The effects of the protecting groups on the alcohol substrate on differential reactivity in Yamaguchi esterification were noteworthy. (*Eur. J. Org. Chem.*, **2018**, 2018(10), 1230)

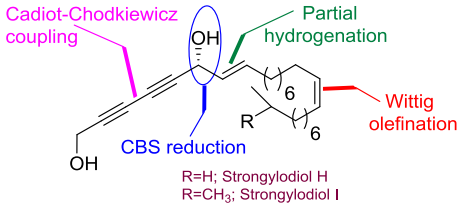


10. Synthesis and Biological Evaluation of 12-, 13-, 14-Membered Macrolides and Open Chain 2,6-Trans-Disubstituted Dihydropyran Analogues for Aspergillides

Stereoselective synthesis of twenty (three 12-, five 13- and twelve 14-membered) macrolides and seventeen functionalized 2,6-trans-disubstituted dihydropyran derivatives have been achieved. The key reactions include an Achmatowicz rearrangement, Ferrier-type alkynylation, Yamaguchi macrolactonization and Lindlar's hydrogenation. Biological screening of the synthesised compounds showed moderate activity against human cancer cell-lines. (*Tetrahedron Lett.*, **2018**, 59(26), 2570)

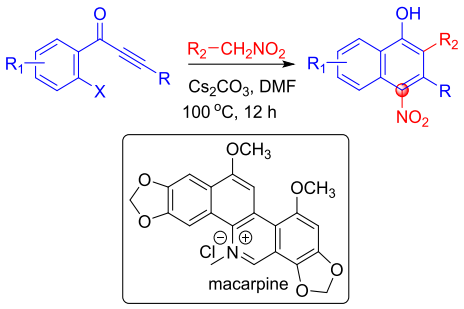
11. Stereoselective Total Synthesis and Structural Revision of the Diacetylenic Diol Natural Products Strongylodiols H And I

The stereoselective total synthesis of strongylodiol H and I has been accomplished. The synthetic procedure comprised the stereoselective reduction of a ketone functionality in an eneyne–one employing CBS as a catalyst and a Cadiot–Chodkiewicz coupling reaction as the key reaction steps. A common aldehyde intermediate has been used for the synthesis of both strongylodiols. *(Beilstein J. Org. Chem.*, **2018**, 14, 2313)



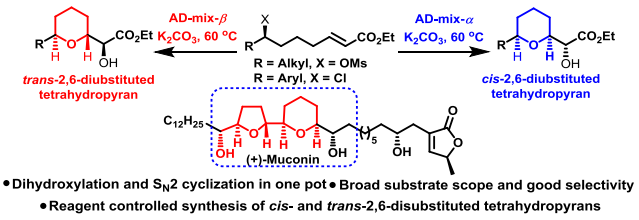
12. Nitromethane as a Carbanion Source for Domino Benzoannulation with Ynones: One-Pot Synthesis of Polyfunctional Naphthalenes and a Total Synthesis of Macarpine

A one-pot, transition-metal-free, domino Michael/ S_NAr protocol of general applicability has been devised for the regioselective synthesis of polyfunctional naphthalenes by employing nitromethane and ortho-haloaryl ynones. Utilization of nitromethane as a one carbon carbanion source that is incorporated into a variety of ynones, ends up as an aromatic nitro substituent. The application of this domino process towards a total synthesis of the polycyclic alkaloid macarpine demonstrate for the efficacy of this methodology. The conceptually simple approach to affect regioselective, multifunctional benzoannulation of ynones displays wide substrate scope and functional-group tolerance and has been implemented with substituted nitromethanes, as well as with alicyclic o-haloynones. (*Angew. Chem. Int. Ed.*, **2018**, 57(51), 16847)



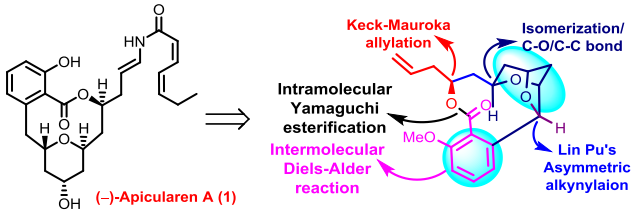
13. A General Diastereoselective Strategy for Both cis- and trans-2,6-Disubsttuted Tetrahydro pyrans: Formal Total Synthesis of (+)-Muconin

An anti-Markovnikov-type highly regioselective and an extremely mild protocol is described using gold as the catalyst for different types of γ-acetoxy aryl alkynes by the assistance of a neighboring carbonyl group to access two different types of acyloins in good to excellent yields. The reaction procedure operates under room temperature conditions with broad functional group tolerance in presence of more than stoichiometric amount of water. Acetate protected acyloins were produced from primary and secondary substrates, while tertiary ones react differently to give free-acyloins under identical condition, pathways for such divergent functionalization were deduced from isotopic mechanistic results. (*Org. Lett.*, **2018**, 20(21), 6810)



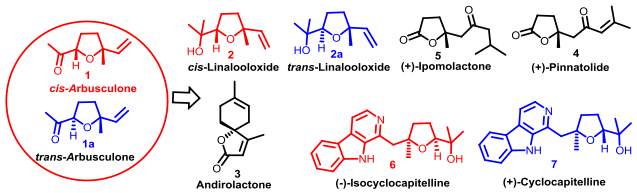
14. A Synthetic Study toward the Core Structure of (−)-Apicularen A

A concise synthetic strategy towards the core structure of (−)-apicularen A has been described in an 11 step synthetic sequence from a known intermediate. The key steps include tandem isomerization followed by C-O and C-C bond-forming reactions and iodocyclization strategies for the synthesis of the bicyclic ether embedded in the macrolactone ring. The applied reagent-controlled Keck-Maruoka allylation, Lin Pu alkynylation and Ricket-Diels-Alder reactions were used to simplify the synthetic sequence of related natural products. An intramolecular Yamaguchi lactonization constructed the macrolactone core, while the attempt to install the C11 hydroxyl chiral centre either under catalytic hydrogenation conditions or oxidative conditions was not successful. (*Org. Biomol. Chem.*, **2018**, 16(45), 8110)



15. A Protecting-Group-Free Synthesis of Arbusculone, Andirolactone, Pinnatolide, Ipomo lactone, Cyclocapitelline and isocycloca pitelline

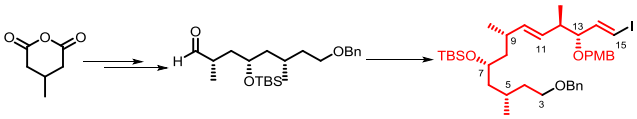
A general approach for a collective synthesis of natural products containing substituted THF ring is described. In this paper, Arbusculone, a small molecule natural product accomplished using a short route, is used as the key intermediate to achieve the total synthesis of Andirolactone, Pinnatolide, Ipomolactone, Cyclocapitelline, Isocyclocapitelline and their two isomers in less than ten steps. The present effort highlights protecting-group-free total syntheses and the shortest route to access these natural products from commercially available cheap starting materials. (*Tetrahedron Lett.*, **2018**, 59(47), 4172)



16. Stereoselective Synthesis of the C3-C15 Fragment of Callyspongiolide

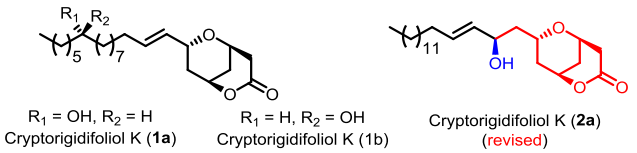
A general approach for a collective synthesis of natural products containing substituted THF ring is described. In this paper, Arbusculone, a small

molecule natural product accomplished using a short route, is used as the key intermediate to achieve the total synthesis of Andirolactone, Pinnatolide, Ipomolactone, Cyclocapitelline, Isocyclocapitelline and their two isomers in less than ten steps. The present effort highlights protecting-group-free total syntheses and the shortest route to access these natural products from commercially available cheap starting materials. (*Tetrahedron Lett.*, **2018**, 59(39), 3579)



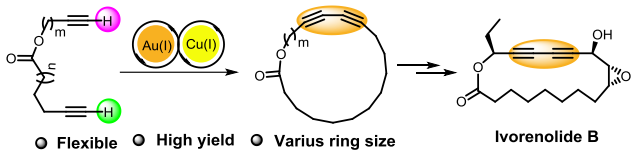
17. Total Synthesis of Cryptorigidifoliol K: Confirmation of Structure and Absolute Configuration

The first total synthesis of the revised Cryptorigidifoliol K and 2′-*epi*-Cryptorigidifoliol K was accomplished. Salient features of the synthesis involve tandem isomerization followed by C-O and C-C bond forming reaction, iodolactonization and Nozaki-Hiyama-Kishi reaction. The synthesis allowed for confirmation of the structure as well as the elucidation of the unassigned stereocenter present in the side chain of the revised structure by correlating the spectral and analytical data of the synthetic cryptorigidifoliol K and 2′-*epi*-cryptorigidifoliol K with the natural product data, which was found to be 1*S*,5*R*,7*S*,2′*R*,3′*E*. (*Asian J. Org. Chem.*, **2018**, 7(12)2504)



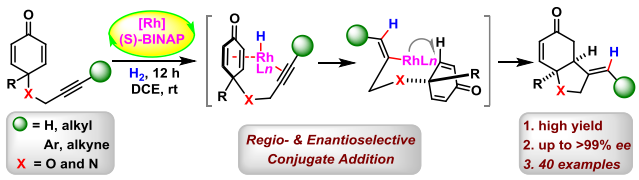
18. Synergistic Gold and Copper Dual Catalysis for Intramolecular Glaser-Hay Coupling: Rapid Total Synthesis of Ivorenolide B

A synergistic dual catalysis approach involving gold and copper catalysts for the synthesis of macrolactones bearing 1,3-butadiynes through an intramolecular Glaser-Hay coupling reaction in good yield is described. This dual catalytic system exhibited good selectivity, reactivity and functional group tolerance. This unique process offers a paradigm shift: the potential as well as the versatility of this novel method is not only exemplified for the synthesis of macrolactones of different ring size but also for the rapid total synthesis of ivorenolide B, a new class of macrolides endowed with conjugated 1,3-diyne motif, having impressive immuno suppressive activities. (*Eur. J. Org. Chem.*, **2018**, 2018(32), 4376)



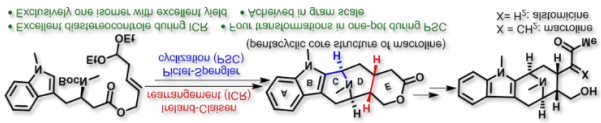
19. Rhodium-Catalyzed Highly Regio- and Enantioselective Reductive Cyclization of Alkyne-Tethered Cyclohexadienones

Rhodium-catalyzed asymmetric hydrogenation of alkyne-tethered cyclohexadienones enables highly regio- and enantioselective reductive cyclization to afford cis-hydrobenzofurans and cis-hydroindoles in high yields. Desymmetrization of 1,3-diyne-tethered cyclohexadienones was also explored, wherein the intramolecular coordination of a Rh-complex with the cyclohexadienone ring induces exclusive region selectivity. Mechanistic studies including hydrogen-deuterium crossover experiments suggested that hydrogen activation is the rate-determining step for tandem reductive cyclization. Moreover, this highly practical and atom-economical transformation has tolerance to many functional-groups with a broad range of substrate scope, allowing further transformations to expand the structural complexity. *(ACS Catal.*, **2018**, 8(2), 1440)



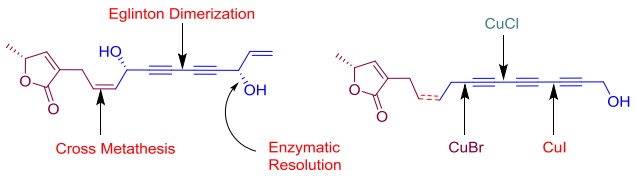
20. Stereoselective Access to the Core Structure of Macroline-type Indole Alkaloids: Total Synthesis of Macroline and Alstomicine

Rapid synthesis of the pentacyclic core structure of macroline-type indole alkaloids, and its application in the total synthesis of macroline, and alstomicine is described. The core structure was accomplished in a highly stereocontrolled manner *via* two key steps, Ireland-Claisen rearrangement, and Pictet-Spengler cyclization, commencing from a readily available starting material L-tryptophan, which obviated the need of a particular chiral source as an external catalyst, reagent or internal auxiliary. (*Org. Lett.*, **2018**, 20(16), 4782)



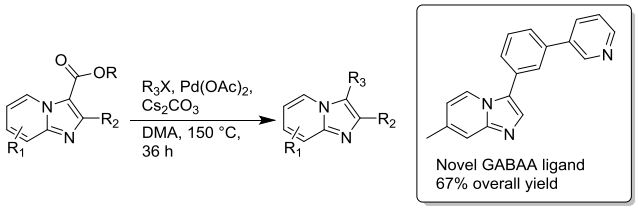
21. Studies towards the Synthesis of Trochelio phorolides

Total synthesis of trocheliophorolide C epimer is reported. The synthetic strategy involves generation of lactone skeleton and preparation of unsaturated side chain followed by cross-metathesis. The Eglinton oxidative coupling, Cadiot-Chodkiewicz cross-coupling and cross-metathesis are the key reactions used in the synthesis. We also attempted the synthesis of trocheliophorolide D epimer, which includes Cu catalyzed various cross-coupling reactions. (*Tetrahedron Lett.*, **2018**, 59(22), 2157)



22. Palladium (II) Acetate/Base-Catalyzed Inter molecular Coupling of Imidazo[1,2-*A*] Pyridine Esters with Aryl Halides

The combination of Cs_2CO_3 and $Pd(OAc)_2$ enables the coupling of imidazo[1,2-*a*]pyridine esters and aryl halides, allowing an easy access to generate 3-aryl imidazo[1,2-*a*]pyridine. The reaction pathway involves a Cs_2CO_3-mediated ester hydrolysis followed by a palladium (II) acetate-catalyzed decarboxylative arylation. The method is comparable with direct arylation of imidazo[1,2-*a*]pyridine and aryl halides. The synthetic utility of this relay reaction resulted in the generation of novel GABAA ligand and potent kinase inhibitor in high overall yields. (*ChemistrySelect*, **2018**, 3(20), 5639)



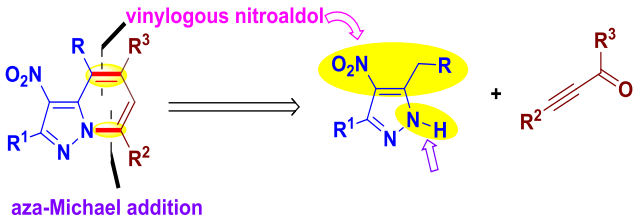
23. Crosslinked Enzyme Aggregates (CLEA) Of Phytase with Soymilk Proteins

Crosslinked Enzyme Aggregates (CLEA) of phytase (E.C. 3.1.3.8) have been successfully prepared using soymilk as protein feeder. Compared to total initial activity of 4428 units used for immobilization, the recovered activity in the CLEA is enhanced to 8000 units. The CLEA retained 100% phytase activity up to 50 °C and 70% activity at 70 °C after 6 h incubation while soluble enzyme lost 50% activity at 50 °C and 80% at 70 °C. Soluble phytase has an optimum pH of 2.1 while immobilized enzyme maintains high level of activity in a broad pH range of 1–6. CLEA also retain 80% activity upon proteolytic hydrolysis with pepsin, pancreatin, trypsin and chymotrypsin, while soluble enzyme loses 40% activity under same conditions. Phytase CLEA were recycled for 5 times without loss in activity using a stirred basket reactor. (*J. Biotechnol.*, **2018**, 282, 67)

24. Tandem Aza Michael Addition−Vinylogous Nitroaldol Condensation: Construction of Highly Substituted *N*-Fused 3-Nitropyrazolopyridines

A base-mediated tandem aza-Michael addition − vinylogous nitroaldol condensation has been

described between 3,5-dialkyl 4-nitropyrazoles and alkynyl ketones/aldehydes. This transition metal-free atom economical transformation occurred *via* C−N and C=C bond formations in one step with the elimination of water. The construction of a variety of highly substituted *N*-fused 3-nitropyrazolopyridine derivatives has been demonstrated with good yields. Good to excellent regioselectivities have been achieved with unsymmetrically substituted 4-nitropyrazoles. (*J. Org. Chem.*, **2018**, 83(12), 6454)

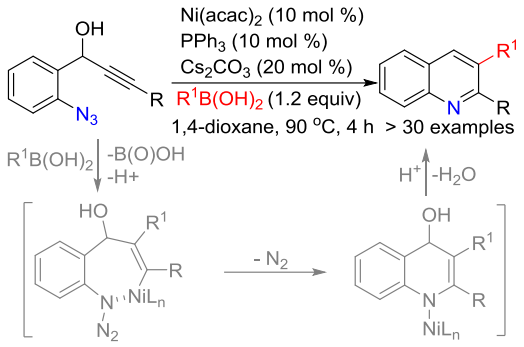


25. Stereoselective Carbon–Carbon Bond Formation Via 1,2-Asymmetric Induction by A B-Substituent in the Reaction of A-Chloro Sulfides with Organozinc Reagents was Investigated

The stereoselectivity of C–C bond formation in the reaction of α-chlorosulfides with a variety of organozinc reagents has been investigated. The study reveals excellent 1,2-asymmetric induction by a β-siloxy substituent and moderate 1,2-induction by the β-methyl substituent. The stereoselectivity is a function of the size of the organozinc reagents. (*Indian J. Chem.B*, **2018**, 57B(3), 327)

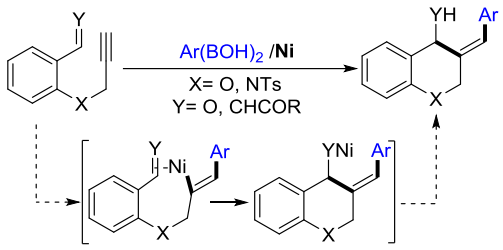
26. A Nickel-Catalyzed anti-Carbometallative Cyclization of Alkyne-Azides with Organoboronic Acids: Synthesis of 2,3-Diarylquinolines

An anti-carbonickelative cyclization via reversible alkenylnickel E/Z isomerization of 2-azido phenyl propargyl alcohols with aryl boronic acids is achieved using Ni(acac)2 as the catalyst to access 2,3-diaryl quinolines. It represents a rare example of trapping the vinyl metal intermediate with a nitrogen center, a non-carbon center electrophile. (*Chem. Commun.*, **2018**, 54(7), 759)



27. Nickel Catalyzed Syn Selective Aryl-Nickelation and Cyclization of Aldehyde/Enone-Tethered Terminal Alkynes with Arylboronic Acids

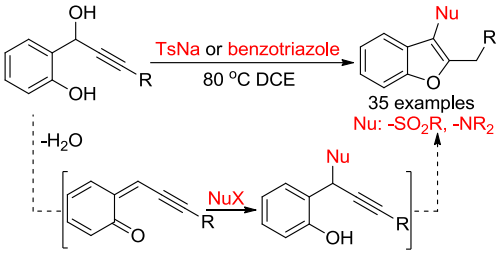
A syn arylative nickelation followed by nucleophilic syn selective cyclization of o-propargyloxy benzaldehydes is achieved towards the synthesis of chromanol skeletons with alkenyl substitution at C3. The capture of the intermediate vinyl nickel in its cis geometry is done also with Michael acceptor to synthesize 4-alkylated derivatives. This protocol is equally applicable to o-propargylamino benzalde hydes to access 3,4-disubstituted tetrahydro-hydro quinolines. (*J. Org. Chem.*, **2018**, 83(24), 15361)



28. 3-Heterosubstituted Benzofurans from Hydroxyphenyl Propargyl Alcohols via Ortho-Quinone Methide through a Metal/Catalyst free Conjugate Addition/Oxy-Cyclization

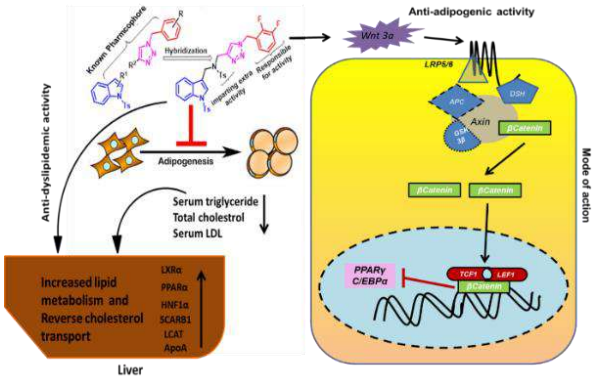
A facile route to 3-sulfonylated and 3-(1-benzotriazolyl)-benzofurans is achieved from readily available o-hydroxyphenyl propargyl alcohols (o-HPPAs) and bench top sodium sulfonylates and benzotriazoles with no assistance of any reagent or catalyst. Bi-functional o-quinone methides (o-QMs) were the putative reaction intermediates ensued from

dehydration of o-HPPA. Our study revealed that the o-QM was so choosy in selection of the nucleophiles for the key Michael addition reaction. (*ACS Omega*, **2018**, 3(12), 17155)



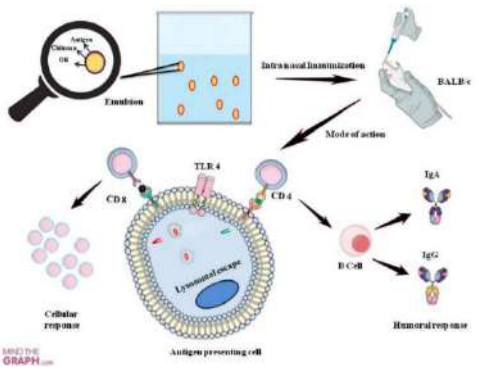
29. Novel Indole and Triazole Based Hybrid Molecules Exhibit Potent Anti-Adipogenic and Antidyslipidemic Activity by Activating Wnt3a/B-Catenin Pathway

Obesity and dyslipidemia are the two facet of metabolic syndrome, which needs further attention. Recent studies indicate triazole and indole derivatives have remarkable anti-obesity/antidyslipidemic activity. To harness the above-mentioned potential, a series of novel triazole clubbed indole derivatives were prepared using click chemistry and evaluated for anti-adipogenic activity. Based on the structure-activity relationship, essential functional groups which potentiate anti-adipogenic activity were identified. The lead compound 13m exhibited potent anti-adipogenic activity compared to its parent compounds with the IC-50 value of 1.67 µM. Further evaluation of anti-adipogenic activity was conducted in different cell lines such as C3H10T1/2 and hMSC with excellent results. The anti-adipogenic effect of compound 13m was most prominent in the early phase of adipogenesis, which is driven by the G1 to S phase cell cycle arrest during mitotic clonal expansion. The mechanistic study suggests that compound 13m exhibit anti-adipogenic property by activating wnt3a/β catenin pathway, a known suppressor of key adipogenic genes PPARγ and C/EBPα. It is noteworthy that the compound 13m also reduced serum triglyceride, LDL and total cholesterol in Syrian golden Hamster Model of dyslipidemia. The anti-adipogenic activity of compound 13m can also be correlated with decreased expression of PPARγ and increased expression β-catenine in vivo. The compound 13m also increased the expression genes involved in reverse cholesterol transport (RCT) such as PPARα and LXR1α indicating another mechanism by which compound 13m ameliorates dyslipidemia in Syrian golden hamster model. Overall this study provides a unique perspective into the anti-adipogenic/antidyslipidemic property of triazole and indole hybrids molecules with further scope to increase the anti-adipogenic potency for therapeutic intervention of obesity and metabolic syndrome. (*Eur. J. Med. Chem.*, **2018**, 143, 1360-1346)



30. Chitosan Stabilized Nasal Emulsion Delivery System for Effective Humoral and Cellular Response against Recombinant Tetravalent Dengue Antigen

Novel oleic acid emulsion was designed that activates the innate (TLR 4) and adaptive immune systems apart from performing its antigen delivery function, when immunized along with recombinant tetravalent dengue antigen which elicited a profound antigen specific humoral and cellular response. This significant humoral and cellular response elicited proves the suitability of this emulsion system for enhancing the protective effect of vaccines against various intracellular pathogens. (*Carbohydr Polym.*, **2018**, 190, 129)



31. What has come out from Phytomedicines and Herbal Edibles for the Treatment of Cancer?

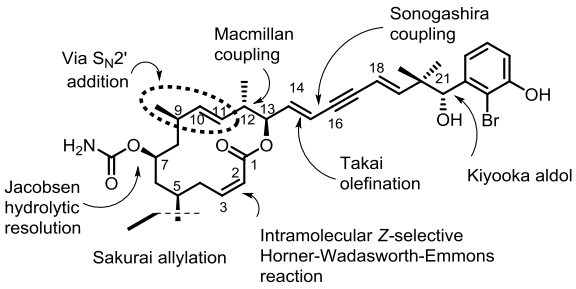
The focus of this article is to present an update of medicinal plants and their bioactive compounds, or mere changes in the bioactive compounds, and herbal edibles, which display efficacy against diverse cancer cells and in anticancer therapy. It describes the basic mechanism(s) of action of phytochemicals used either alone or in combo therapy with other phytochemicals/herbal edibles. The anticancer phytochemicals used in clinical research are also described and further, we stated our own experience related to semi synthetic derivatives, which are developed based on the phytochemicals. Overall, this compilation aims at facilitating research and development projects on phytopharmaceuticals for successful anticancer drug discovery. (*ChemMedChem*, **2018**, 13(18), 1854)

32. Anti-Proliferative and Anti-Malarial Activities of Spiroisoxazoline Analogues of Artemisinin

A series of spiroisoxazoline analogues of artemisinin was synthesized and evaluated for their anti-proliferative and anti-malarial activities. Compound 11a demonstrated anti-proliferative activities against the human cancer cell line HCT-15 and compound 11b showed excellent anti-plasmodial activity. Molecular docking studies of 11b suggest that this class of compounds binds differently to cysteine proteases compared to the C-10 modified analogs. (*Arch. Pharm.*, **2018**, e1800192)

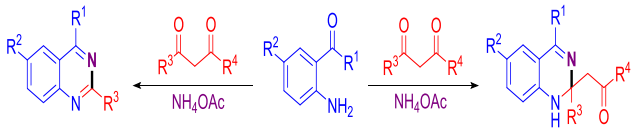
33. Total Synthesis of Callyspongioide: An Anticancer Marine Natural Product

The stereoselective total synthesis of cytotoxic marine macrolide callyspongiolide has been reported. The 14-membered macrolactone ring along with *Z*-olefin in the molecule was constructed via an intramolecular Horner–Wadsworth–Emmons olefination in a *Z*-selective fashion. The other *E*-olefinic moiety as well as the C9 stereocenter was introduced via stereoselective addition of the methyl group in an S_N2' fashion. The C5 stereocenter was installed via Sakurai allylation, whereas the C7 center was fixed by Jacobsen hydrolytic kinetic resolution. The C12 methyl and C13 hydroxy centers were fixed via Macmillan coupling reaction. The macrolactone core with a vinyl iodide side chain was coupled with the known alkyne fragment to complete the synthesis. (*ACS Omega*, **2018**, 3(12), 16563)



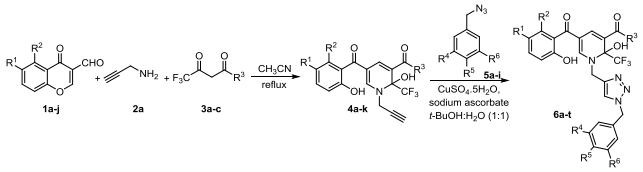
34. A Selective Three-Component, One-Pot Approach for the Synthesis of 1,2-Dihydroquinazolines and Quinazolines

A facile and selective method has been developed for the preparation of 1,2-dihydroquinazolines 3a-u, quinazolines 5a-f and spiro cyclohexane-1,2-quinazolines 7a-d by the reaction of 2-aminoacetophenones, benzophenones with β-ketoesters, 1,3-diketones and cyclic ketones in the presence of ammonium salts for the first time. (*Chemistry Select*, **2018,** 3(32), 9388)



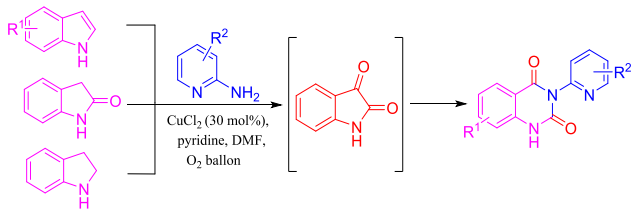
35. A One-pot Facile Construction of 1*H*-1,2,3-Triazolyl 1,2-Dihydropyridyl Derivatives and Evaluation of Bioactivity Profile

A one-pot, facile method has been established for the preparation of 1H-1,2,3-triazolyl 1,2-dihydropyridyl derivatives 6a-y. The ring openings of the chromone and cyclo addition are the notable reactions to achieve the target compounds 6a-y. All the compounds were screened for their antiproliferative, free radical scavenging (DPPH, $ABTS^{\cdot+}$), α-glucosidase inhibitory and anti-inflammatory activities. (*ChemistrySelect*, **2018,** 3(48), 13729)



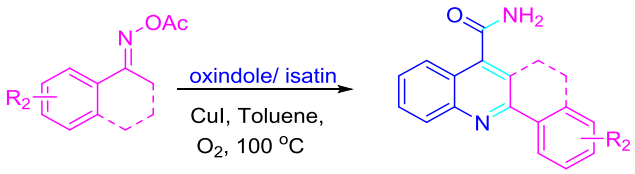
36. Copper-Catalyzed Domino CC Bond Cleavage of 2,3- Unsubstituted Indoles/Indolines and Oxindoles via Oxidation and Directed Insertion of 2-Aminopyridines: Direct Access to Quinazolinediones

In this project development of a novel copper-catalyzed domino C-C bond cleavage of 2,3-unsubstituted Indole/Indolines and Oxindoles through oxygenation followed by insertion of 2-aminopyridine has been described. This method implies the formation of two new C-N andC-O bonds using molecular oxygen as a sole oxidant for construction of highly valuable Quinazoline-2,4(1H,3H)-dione derivatives from readilyavailable substrates. (*Adv. Synth. Catal.*, **2018**, 360(16), 3009)



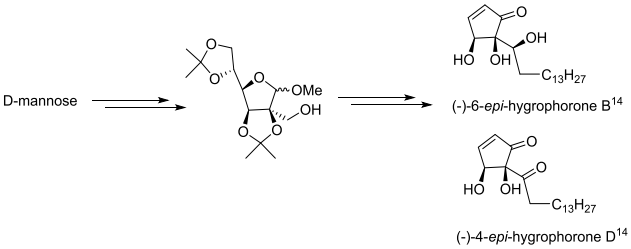
37. Cu-Catalyzed Coupling of *O*-Acyl Oximes with Isatins: Domino Rearrangement Strategy for Direct Access to Quinoline-4-Carboxamides by C–N Bond Cleavage

A mild domino rearrangement strategy for the direct access to substituted quinoline-4-carboxamides has been developed. This copper-catalyzed coupling reaction of *O*-acyl oximes with isatins in the presence of molecular oxygen as the sole oxidizing agent proceeds through a ring expansion of the isatins through cleavage of the two C–N bonds. (*Eur. J. Org. Chem.*, **2018**, 2018(23), 2963)



38. Stereo Selective Total Synthesis of (–)–6–epi–Hygrophorone B14 and (–)–4–epi–Hygrophorone D14

Total synthesis of (–)–6–epi–hygrophorones B14 and (–)–4–epi– hygrophorone D14 was achieved using stereo selective Grignard reaction, Bernet–Vasella protocol and Ring closing metathesis, starting from D–mannose. (*ChemistrySelect*, **2018**, 3(33), 9596)



39. Recent Advances in the Development of Pharmaceutical Agents for Metabolic Disorders: A Computational Perspective

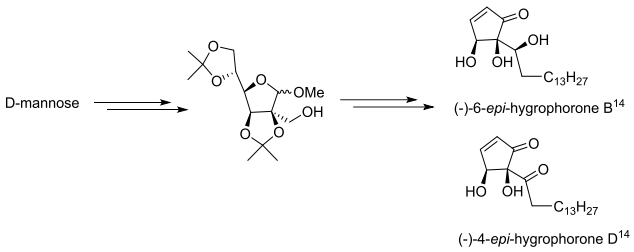
The recent advances of developing pharmaceutical agents for various metabolic disorders by considering their pathogenesis, mechanisms of action, therapeutic and adverse effects have been summarized. We have highlighted the role of computational techniques, drug repurposing, and network-based polypharma cological approaches in the identification of new/existing medicines with improved drug-likeness properties for the rare metabolic disorders. (*Curr. Med. Chem.*, **2018**, 25(39), 5432)

40. Design, Synthesis and Biological Evaluation of 1, 4-Dihydro Indeno[1,2-C] Pyrazole Linked Oxindole Analogues as Potential Anticancer Agents Targeting Tubulin and Inducing P53 Dependent Apoptosis

1, 4-dihydroindeno-[1,2-c] pyrazole linked oxindole conjugates were synthesized by using Knoevenagel condensation method and further evaluated for their antiproliferative activity against HeLa, A549 and MDA-MB-231 human cancer cell lines along with HEK-293 (normal human embryonic kidney cells). Among the derivatives, some compounds showed excellent cytotoxicity with IC_{50} values ranging between 1.33 to 4.33 mM. Detailed biological assays showed that there was accumulation of mitotic cells in G2/M phase, disruption of microtubule network and increase in the G2/M checkpoint proteins (Cyclin B1 and CDK1). One promising compound with IC_{50} value of 1.33 mM showed significant upregulation of tumor suppressor proteins like p53, p21 and pro-apoptotic Bax. Molecular docking analysis demonstrated that these conjugates occupy the colchicine binding pocket of tubulin. (*Eur. J. Med. Chem.*, **2018**, 144, 104)

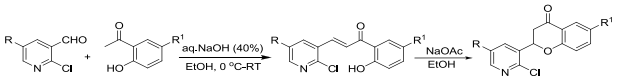
41. Synthesis and Anti-Proliferative Activity of 4*H*-Chromone based Phenylhydrazones, Pyrazole carboxylates and Pyrazolylmethanones

Series of 4*H*-chromone based hydrazones, pyrazolecarboxylates and pyrazolylmethanones are prepared and screened for their anti-proliferative activity on A549, HeLa, DU145 and MDAMB 231 cell lines. The hydrazone compound with chloro substitution on chromanone and methoxy on phenyl displayed promising activity on A549, HeLa and DU145 cell lines. The compound with bromo substitution on chromanone and methyl substitution on phenyl displayed potent activity on DU145. Furo pyrazolecarboxylate methyl substitution on phenyl displayed potent activity on HeLa cell line. The pyrazolylmethanone with fluoro substitution on phenyl and compound has methyl substitution on chromanone and methoxy on phenyl shown promising anti-proliferative activity on HeLa cell line. (*Acta Chim. Slov.*, **2018,** 65(1), 34)



42. Anti-Proliferative, Structure-Activity Relation ship of Pyridinylchalcones and Chromanones

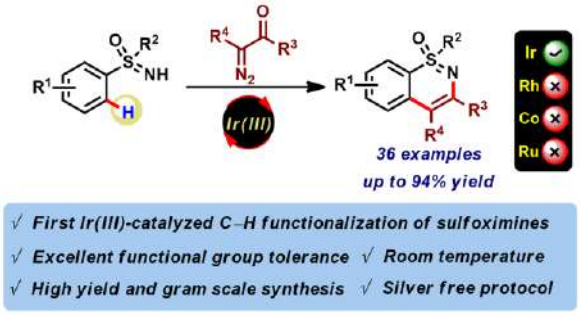
A series of pyridinylchalcones, chromanones were prepared and screened for their *in vitro* anti-proliferative activity against four human cancer cell lines *viz*., cervical (HeLa), lung adenocarcinoma (A549), prostate (DU-145) and breast (MDA-MB-231). Pyridinylchalcones and chromanones exhibited IC_{50} values in the range of 5.9-289 µM. (*E*)-3-(2-chloro-5-phenylpyridin-3-yl)-1-(2-hydroxy-5-methyl phenyl)prop-2-en-1-oneexhibited an IC_{50} of 5.9 µM and also increased caspase-3 activity to ~2.7-fold at 10 µM concentration in HeLa cell line. Cell cycle analysis further confirmed the apoptotic effects of (*E*)-3-(2-chloro-5-phenylpyridin-3-yl)-1-(2-hydroxy-5-methylphenyl)prop-2-en-1-one due to a substantial increase in cells arrested at sub-G1 phase of cell cycle. (*Med. Chem. Res*., **2018**, 27(1), 80)



43. Cp*Ir(III)-Catalyzed C−H/N−H Function alization of Sulfoximines for the Synthesis of 1,2-Benzothiazines at Room Temperature

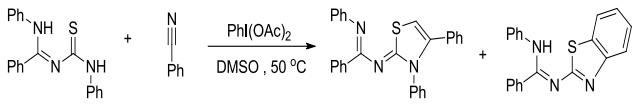
First Cp*Ir(III)-catalyzed C−H/N−H bond functionalization of sulfoximines with α-diazocarbonyl compounds has been developed for the synthesis of 1,2-benzothaizines under redox-neutral conditions. The reactions proceed at room temperature with excellent functional group tolerance

and high yields without requirement of any silver additive. (*Chem. Commun*. **2018**, 54(49), 6288)



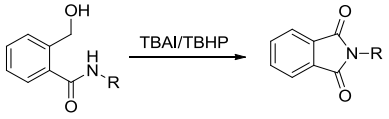
44. Hypervalent Iodine(III)-Mediated Solvent-Free, Regioselective Synthesis of 3,4-Disubstituted 5-Imino-1,2,4-thiadiazoles and 2- Aminobenzo [*d*]thiazoles

A convenient approach for the synthesis of 3,4-disubstituted 5-imino-1,2,4-thiadiazoles and 2 aminobenzo[*d*]thiazoles has been developed using phenyliodine diacetate (PIDA). This approach involves a metal-free oxidative C-N, N-S and C-S bond formations under neat conditions. High regioselectivity, solvent-free conditions, short reaction time and broad functional group compatibility are the notable features of this report. (*Adv. Synth. Catal*., **2018**, 360(15), 2806)



45. Synthesis of Phthalimides: A New Entry via TBAI Catalyzed Intramolecular Cyclization of 2 (Hydroxymethyl)benzamides

Herein we report an unprecedented metal-free TBAI/TBHP mediated C–N bond formation via intramolecular cyclization of 2-(hydroxymethyl) benzamides to furnish N-substituted phthalimides in excellent yields. (*SynOpen*, **2018**, 2(02), 145)

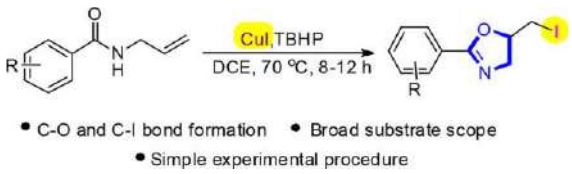


46. I_2-Mediated Oxidative C−N and N−S Bond Formation in Water: A Metal-Free Synthesis of 4,5-Disubstituted/N-Fused 3-Amino-1,2,4-triazoles and 3-Substituted 5-Amino-1,2,4-thiadiazoles

An environmentally benign and convenient strategy for the synthesis of 4,5-disubstituted/N-fused 3-amino-1,2,4- triazoles and 3-substituted 5-amino-1,2,4-thiadiazoles from isothiocyanates has been developed. This metal-free method involves I2-mediated oxidative C−N and N−S bond formations in water. Furthermore, this facile protocol exhibited excellent substrate tolerance in good to high yields and scalable fashion. (*J. Org. Chem.*, **2018**, 83(10), 5715)

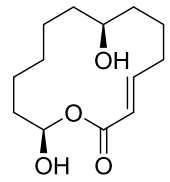
47. CuI/TBHP: A Versatile Reagent System for the Synthesis of 5-Iodomethyl-2-Aryl-4,5-Dihydrooxazoles from N-Allylarylamides

A novel reagent system using CuI/TBHP is described for the facile conversion of easily accessible *N*-allylarylamides into 5- iodomethyl-2-aryl-4,5-dihydrooxazoles in moderate to good yields. In this communication we describe CuI as the iodine source for the first time towards the intramolecular iodooxygenation of *N*-allylarylamides. (*Synth.Commun.*, **2018**, 48(9), 1001)



48. A Concise and Stereoselective Total Synthesis of Pestalotioprolide-C Using Ring-Closing Metathesis

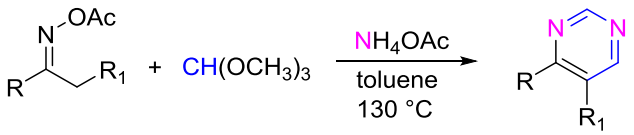
The stereoselective total synthesis of the pestalotioprolide C is disclosed in 13 linear steps in 4% overall yield. The key steps in this approach are a ring-closing-metathesis protocol for the construction of the 14-membered macrolide with *E*-olefinic bond, a Keck allylation, and a Sharpless kinetic resolution for the installation of desired stereocenters at C4 and C7. (*Synthesis*, **2018,** 50(05), 1152)



Pestalotioprolide-C

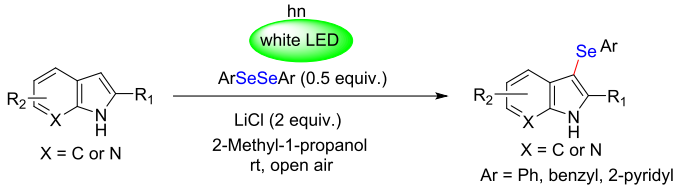
49. Catalyst Free Synthesis of Mono and Di Substituted Pyrimidines from O-Acyl Oximes

Transition-metal or iodine catalyzed transformations of *O*-acyl oximes to various *N*-heterocycles are well established. Herein, we report a catalyst free, oxime carboxylate based, three-component condensation method to access mono- and disubstituted pyrimidines. A broad range of substituted pyrimidines were prepared in moderate to excellent yields. Control experiments reveal that *in situ* generated formamidine is the key intermediate. *(Tetrahedron Lett.,* **2018**, 59(25), 2430)



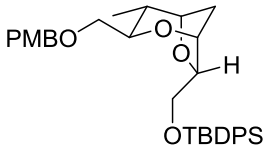
50. Catalyst and Sensitizer-Free Visible Light Induced C(SP^2)-H Chalcogenation of Arenes/ Heteroarenes with Dichalogenides

We have developed a direct regioselective C(sp^2)-H selenation of variously substituted indoles, imidazopyridines, and electron-rich aryl substrates under neutral conditions. Importantly, this C(sp^2)-H selenation method is atom-economical, and it requires no sensitizer and catalyst. This reaction proceeds at ambient temperature with the illumination of day-white LED lamp eliminating the blue lamp source. The interesting feature of this sustainable protocol is i) use of recoverable eco-friendly benign alcohol solvent as a reaction medium ii) a half equivalent of diorganyl diselenide iii) high regioselectivity along with high yields of the respective products. (*Asian J. Org. Chem.*, **2018**, 7(8), 1689)



51. Synthesis of the Dioxabicylooctane Subunit of Sorangicin

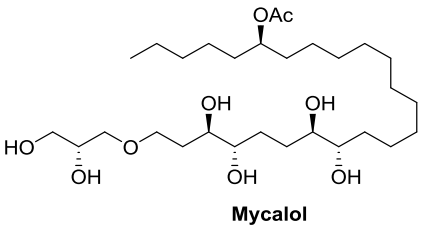
The synthesis of the dioxabicyclo [3.2.1]octane subunit of the potent antibiotic sorangicin A has been developed. The synthesis was achieved in a convergent manner in 8 steps. Regio- and stereoselective intermolecular epoxide opening, ring-closing metathesis and iodo-etherification are key steps. cis-2-Butene diol has been employed as a common staring material. (*Tetrahedron*, **2018**, 74(10), 1071)



Dioxabicyclooctane subunit of Sorangicin

52. Total Synthesis of the Anticancer Marine Natural Product Mycalol

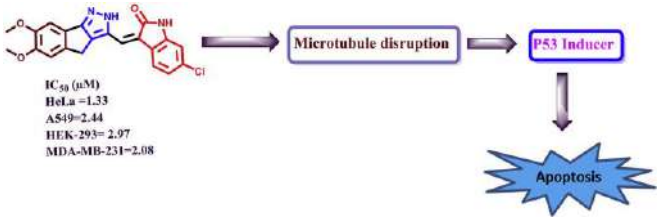
Asymmetric total synthesis of mycalol, a cytotoxic marine natural product has been achieved. All the stereocenter except one, have been created via asymmetric transformation. Key reactions used in the synthesis are Corey-Chaykovsky epoxidation, Keck asymmetric allylation, Alkyn Zipper reaction, asymmetric transfer hydrogenation (Noyori reduction). (Eur. J. Org. Chem., **2018**, *2018(3), 398)*



Mycalol

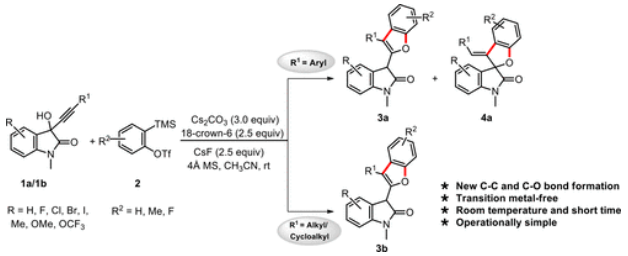
53. Design, Synthesis and Biological Evaluation of 1, 4-dihydro indeno[1,2-c] Pyrazole Linked Oxindole Analogues as Potential Anticancer Agents Targeting Tubulin and Inducing p53 Dependent Apoptosis

A series of 1, 4-dihydroindeno-[1,2-c] pyrazole linked oxindole conjugates have been synthesized by using Knoevenagel condensation method and further evaluated for their antiproliferative activity against HeLa, A549 and MDA-MB-231 human cancer cell lines along with HEK-293 (normal human embryonic kidney cells). Among the derivatives, compounds 12a, 12b, and 12d showed excellent cytotoxicity with IC_{50} values ranging between 1.33 to 4.33 μM. Furthermore, detailed biological assays showed that there was accumulation of mitotic cells in G2/M phase, disruption of microtubule network and increase in the G2/M checkpoint proteins (Cyclin B1 and CDK1). Moreover, compound 12d with IC_{50} value of 1.33 μM showed significant upregulation of tumor suppressor proteins like p53, p21 and pro-apoptotic Bax. The molecular docking analysis demonstrated that these congeners occupy the colchicine binding pocket of the tubulin. (*Eur. J. Med. Chem*., **2018**, 144, 104)



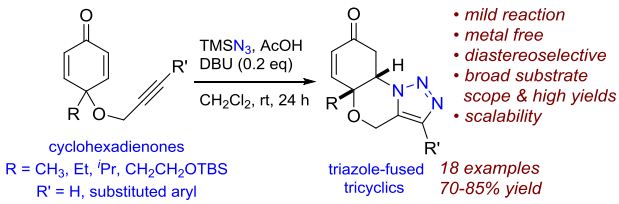
54. Transition-Metal-Free Cyclization of Propargylic Alcohols with Aryne: Synthesis of 3-Benzofuranyl-2-oxindole and 3-Spirooxindole Benzofuran Derivatives

An unprecedented base-mediated cyclization of propargylic alcohols with aryne is reported, providing a novel method for the synthesis of 3-benzofuranyl-2-oxindole and 3-spirooxindole benzofuran scaffolds via a propargyl Claisen rearrangement/cycloaddition pathway. The nature of the substituent on acetylene group of propargylic alcohol influences the outcome of the reaction. The protocol offers a transition-metal-free and operationally simple methodology with broad substrate scope as a ready access to complex oxindole-linked heterocyclic compounds. (*Org. Lett*., **2018**, 20(13), 3824)



55. Metal Free Domino β-Azidation/[3 + 2] Cycloaddition Reaction for the Synthesis of 1,2,3-Triazole-Fused Dihydrobenzoxazinones

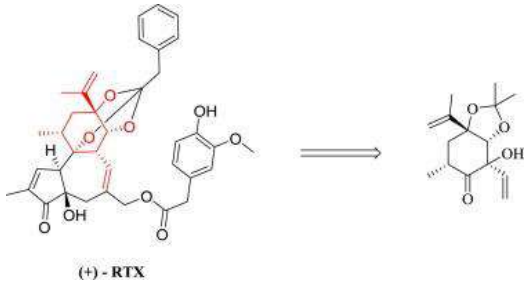
A metal free DBU catalyzed synthesis of 1,2,3-triazole-fused dihydrobenzoxazinone derivatives by tandem *β*-azidation/[3+2] cycloaddition reaction has been developed under mild condition. The methodological studies offer a broad scope and proceed well with a wide range of alkynylated cyclohexa 2,5-dienones giving new *cis*-triazole-fused tricyclic scaffolds. (*J. Org. Chem.*, **2019**, 84(16), 10546)



56. Chiron Approach to Fully Functionalized Cyclohexane Frame of (+)-Resiniferatoxin

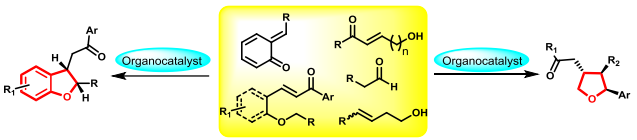
The commercially available (−)-Shikimic acid is used to construct the fully functionalised cyclohexane

frame (C-ring) of (+)-Resiniferatoxin. The key reactions involve stereo-selective epoxide opening with trimethylaluminium and vinyl Grignard reaction. (*Tetrahedron Lett*., **2019**, 60(41), 151133)



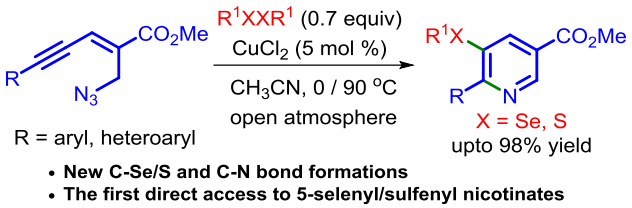
57. Organocatalytic Asymmetric Synthesis of Tetrahydrofuran and1,2-Dihydrobenzofuran Scaffolds

Asymmetric synthesis of substituted tetrahydrofurans and dibenzofurans is emerging as a challenging field. Use of organocatalysis has been explored extensively to achieve the asymmetry involves mild conditions and control over enantio- and diastereo-selectivity for the synthesis of substituted THF and DHB. A review of various conditions and catalysts developed so far towards synthesis of substituted tetrahydrofuran and dibenzofuran are presented here. (*Eur. J. Org. Chem.*, **2019**, 2019(41), 6890)



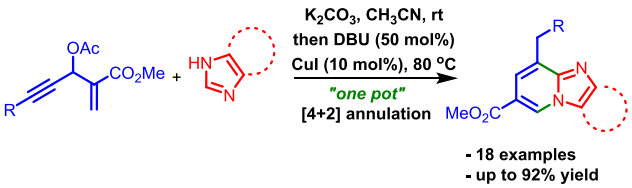
58. Copper-Catalyzed Intramolecular Chalcogeno amination of Enynyl Azides: Synthesis of 5-Selenyl/Sulfenyl Nicotinates

A novel methodology for the synthesis of 5-selenyl/sulfenyl nicotinates involving copper-catalyzed organochalcogenyl *aza*-annulation of enynyl azide with diorganyl-dichalcogenides has been described. This method offers difunctionalization of alkynes *via* regioselective intramolecular chalcogenoamination in one-pot to provide substituted 5-chalcogenyl nicotinates in good to excellent yields. The resulting nicotinates provide access to their oxides, sulfones and acid derivatives. (*Org. Lett.*, **2019**, 21(3), 623)



59. [4+2]-Annulation of MBH-Acetates of Acetylenic Aldehydes with Imidazoles/ Benzimidazoles to Access Imidazo[1,2-*a*]pyridines/ Benzimidazo[1,2-*a*]pyridines

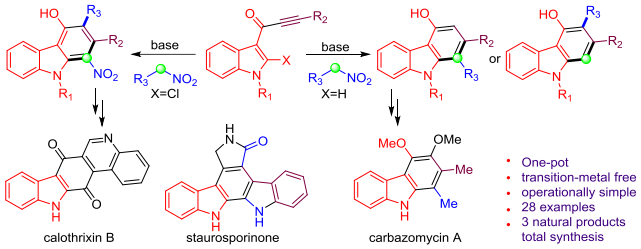
A new strategy for the synthesis of distinctively substituted imidazo[1,2-*a*]pyridines that relies on the use of simple imidazole as a reaction partner with Morita-Baylis-Hillman acetates of acetylenic aldehydes has been developed. This [4+2] annulation approach was further extended using 1*H*-Benzo[*d*]imidazoles to access benzo[4,5]imidazo[1,2-*a*]pyridine derivatives. Having notable features such as readily accessible substrates, mild reaction conditions, handy synthetic procedure and atom economy, the described one-pot reaction is expected to find wide applications in the efficient construction of pharmacologically valued products. (*J. Org. Chem.*, **2019**, 84(14), 9169)



60. A General Carbazole Synthesis via Stitching of Indole−Ynones with Nitromethanes: Application to Total Synthesis of Carbazomycin A, Calothrixin B, and Staurosporinone

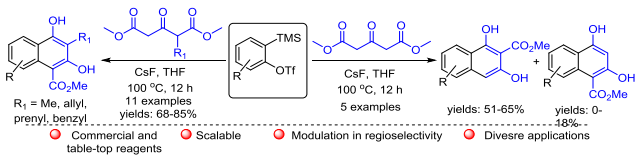
A new, one-pot domino benzannulation reaction between indole-3-ynones and various nitromethane derivatives has been explored for a general entry to diversely functionalized carbazole frameworks (28 examples). The scope of this new benzannulation has been extended to variants like 2-chloroindole-3-ynones to eventuate in chemo-differentiated 1,2,3,4-tetrasub- stituted carbazoles with retention of the

nitro group. The efficacy of this strategy has been demonstrated through concise total synthesis of natural products, viz. carbazomycin A, calothrixin B, and staurosporinone (K252c). (*Org. Lett*., **2019**, 21(9), 3372)



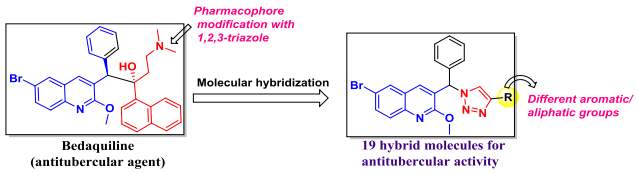
61. Benzannulation of Arynes with Dimethyl acetonedicarboxylates via an Insertion-Fragmentation-Dieckman-Aromatization Cascade: Expeditious Entry to Naphtho resorcinols and Binaphthoresorcinols

Aryne insertions into 1,3,5-tricarbonyl bearing dimethylacetonedicarboxylate (DMAD) proceeds through a 4-step cascade process to eventuate in a versatile one pot synthesis of functionally embellished naphthoresorcinols. Functional group amplifications and transformations on these entities have been explored with the intent to apply them for natural products syntheses and to access other interesting scaffolds. (*Tetrahedron*, **2019**, 75(21), 2923)



62. Synthesis and Evaluation of Novel Quinoline-Triazole Analogs for Antitubercular Properties via Molecular Hybridization Approach

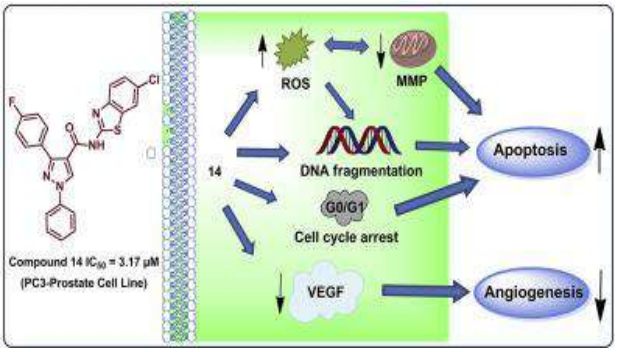
Towards a quest for establishing new antitubercular agents, we have designed new quinoline–triazole hybrid analogs in a six-step reaction sequence involving versatile reactions like Vilsmeier–Haack and click reaction protocol. The design is based on the structural modification of bedaquiline moiety and involves molecular hybridization approach. The structure of the synthesized product was elucidated by single crystal X-ray diffraction study. The synthesized target compounds were screened for their antitubercular activity against *Mycobacterium bovis*. Interestingly, two compounds of the series showed significant inhibition with MIC of 31.5 and 34.8 µM. Compounds bearing 3-fluoro phenyl and *n*-octyl groups on the 1,2,3-triazole ring emerged as the most potent leads among the compounds tested. Further these hit compounds were also screened for their cytotoxic effect on human embryonic kidney 293 (HEK293) cells and other cancer cell lines such as HeLa (Cervical), PC3 (Prostate), Panc-1 (Pancreatic) and SKOV3 (Ovarian) indicating to be safer with the minimal cytotoxicity. (*Bioorg. Med. Chem. Lett*., **2019**, 29(20), 126671)



63. Pyrazolo-Benzothiazole Hybrids: Synthesis, Anticancer Properties and Evaluation of Antiangiogenic Activity Using In Vitro VEGFR-2 Kinase and In Vivo Transgenic Zebrafish Model

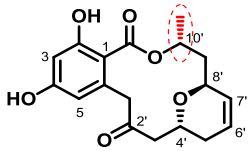
A series of new pyrazolo-benzothiazole hybrids (7e26) were synthesised and screened for their cytotoxic activity towards several cancer cell lines [colon (HT-29), prostate (PC-3), lung (A549), glioblastoma (U87MG)] and normal human embryonic kidney cell line (Hek-293T). These compounds displayed significant activity, with one of the hit compound being particularly potent towards all the tested cancer cell lines with IC_{50} values in the range 3.17-6.77 mM, even better than reference drug axitinib (4.88-21.7 mM). This compound also showed the strongest growth inhibition in 3D multicellular spheroids of PC-3 and U87MG cells. The mechanism of cellular toxicity in PC-3 cells was found to be cell cycle arrest and apoptosis induction

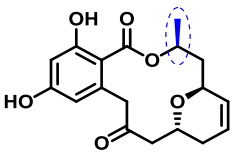
through depolarisation of mitochondrial membrane potential, increased ROS production and subsequent DNA damage. Further, the compound also displayed significant in vitro (VEGFR-2 inhibition) and in vivo [transgenic zebrafish Tg(flila:EGFP) model] antiangiogenic properties. Overall, these results provide strong evidence that the present hit compound could be considered for a lead candidate in anticancer and antiangiogenic drug discovery. (*Eur. J. Med. Chem.*, **2019**, 182, 111609)



64. Total Synthesis and Structural Revision of Monocillin VII

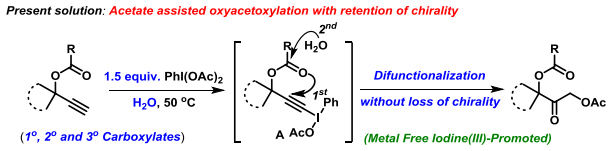
The first asymmetric total synthesis of macrolactone monocillin VII and its C-10′ epimer was achieved starting from a known chiral pure epoxide in 16 longest linear sequences. The present synthesis highlights the macrolactone formation involving an alkyne-dicobalt carbonyl complex under De Brabander's conditions followed by an unexpected regioselective hydration. The asymmetric total synthesis resulted in the revision of the configuration at C10′ and reassignment of the absolute configuration of the natural product. (*Org. Lett.*, **2019**, 21(15), 5152)





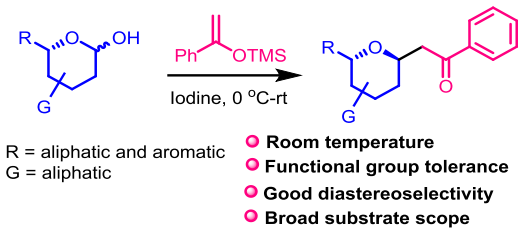
65. Neighboring Carbonyl Group Assisted Oxyacetoxylation of Propargylic Carboxylates with Retention of Chirality under Metal Free Conditions

A metal-free oxyacetoxylation method of primary, secondary and tertiary propargylic acetates with retention of chirality was presented. The reaction proceeds through the intramolecular nucleophilic attack of the neighboring carbonyl group on an alkynyliodonium intermediate. The process is general with broad substrate scope and is amenable for application to a variety of propargyl carboxylates including those obtained from natural products. Insight into the mechanistic pathway by isotopic labelling (using H_2O^{18} and D_2O) and controlled experiments confirmed. (*Adv. Synth. Catalys.*, **2019**, 361(15), 3605)



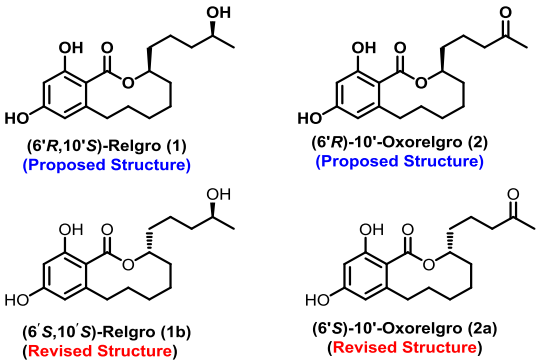
66. The Mukaiyama Type Aldol Reaction for the Synthesis of Trans-2,6-Disubstituted Tetra hydropyrans: Synthesis of Diospongin A And B

An efficient synthetic protocol for the preparation of *trans*-2,6-disubstituted tetrahydropyrans by the reaction of 1-phenyl-1-triemthylsiloxyethylene with six membered cyclic hemiacetals in the presence of iodine is developed. This reaction proceeds smoothly under mild conditions employing a catalytic amount of molecular iodine. The feature of this novel conversion includes milder reaction conditions, broader substrate scope, functional group tolerance and good diastereoselectivity. The efficiency and practicality of this current method was successfully displayed in the total synthesis of diospongin A and B in good yields. (*Org. Biomol. Chem.*, **2019**, 17(41), 9169)



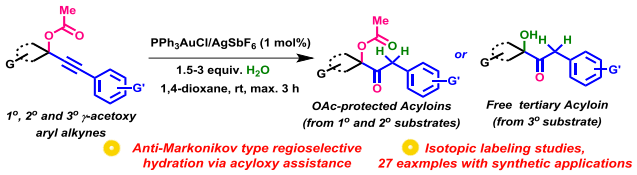
67. Total Synthesis and Stereochemical Revision of Relgro and 10′-Oxorelgro

The first asymmetric total synthesis and stereochemical assignment of 10-membered macrolactones relgro and 10′-oxorelgro are disclosed. To this end, palladium-catalyzed Stille coupling, Mitsunobu reaction, ring-closing metathesis, EDCI promoted coupling and Jacobsen hydrolytic kinetic resolution used as key steps. The total synthesis followed by thorough evaluation of the optical rotation and CD spectral data led to the revision of the absolute configuration at C-6′ for both relgro and 10′-oxorelgro. Moreover, the ^{1}H as well as ^{13}C NMR data is reported first time for relgro. (*Org. Biomol. Chem.*, **2019**, 17(22), 5601)



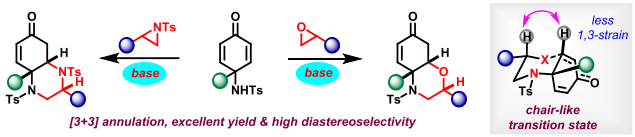
68. Neighboring Carbonyl Group Assisted Hydration of Unsymmetrical Aryl Alkynes Overriding Regular Selectivity

An anti-Markovnikov-type highly regioselective and an extremely mild protocol is described using gold as the catalyst for different types of γ-acetoxy aryl alkynes by the assistance of a neighboring carbonyl group to access two different types of acyloins in good to excellent yields. The reaction procedure operates under room temperature conditions with broad functional group tolerance in presence of more than stoichiometric amount of water. Acetate protected acyloins were produced from primary and secondary substrates, while tertiary ones react differently to give free-acyloins under identical condition, pathways for such divergent functionalization were deduced from isotopic mechanistic results. (*Eur. J. Org. Chem.*, **2019**, 2019(33), 5787)



69. Diastereoselective Desymmetrization of Para-Quinamines through Regioselective Ring Opening of Epoxides and Aziridines

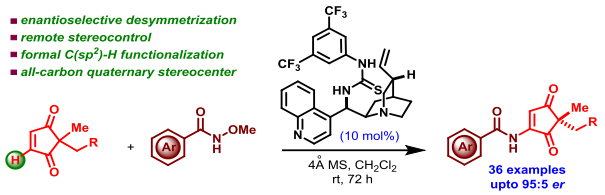
A highly diastereoselective desymmetrization of p-quinamines via regioselective ring opening of epoxides and aziridines under mild conditions has been developed. A chair-like six-membered transition state with minimized 1,3-diaxial interac-tions explains the relative stereoselectivity of the cycli¬zation reaction. This transition-metal free [3+3] annulation reaction provides rapid access to fused bicyclic morpholines and piperazines with a tetrasubstituted carbon center in high yields. In addition, it also allows the synthesis of enantioenriched products by using easily accessible chiral non-racemic epoxides and aziridines. (*Org. Lett.*, **2019**, 21(24), 10115)



70. Enantioselective Desymmetrization of Prochiral Cyclopentene-1,3-diones Triggered by Remote C(sp2)−N Bond Formation

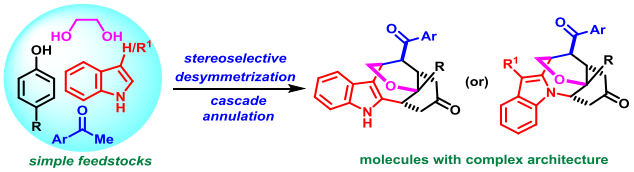
The enantioselective desymmetrization via remote C(sp2)−H amidation of prochiral 2,2-disubstituted cyclopentene-1,3-dione with N-methoxybenzamide

has been developed. The overall process was catalyzed by a chiral bifunctional thiourea catalyst through a sequential conjugate-addition—elimination—tautomerization. This strategy provides rapid access to highly functionalized five-membered carbocycles bearing an all-carbon quaternary stereogenic center through remote stereocontrol in high yields with moderate to excellent enantioselectivities. (*J. Org. Chem.*, **2019**, 84(23), 15735**)**



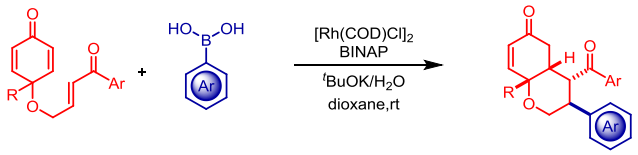
71. Stereoselective Desymmetrization of Cyclo hexadienone-Tethered Enones: Efficient Access to Highly Strained Polycyclic Indoles

A highly regio- and stereoselective cascade annulation of indoles with C2-symmetric enone tethered-cyclohexadienones provides rapid access to complex indole alkaloid-like scaffolds in high yields. Interestingly, a different reaction course was observed with 3-substituted indoles giving C-2/N annulation products with similar complexity via intramolecular aza-Michael addition. This desymmetrization approach is highly practical and allows atom-economical synthesis of natural product-like molecules containing several contiguous stereocenters with broad range of substrate scope and high functional-group tolerance. The synthetic utility of the products was demonstrated with various chemo-, regio- and diastereoselective transformations on the highly strained polycyclic indoles to elaborate the value of this tandem reaction. (*ACS Catal.*, **2019**, 9(11), 10012)



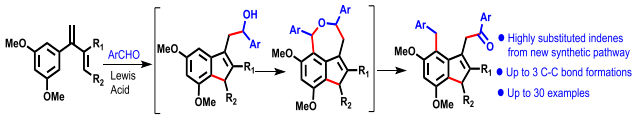
72. Rh-Catalyzed Diastereoselective Desymmetrization of Enone Tethered Cyclo hexadienone via Tandem Arylative Cyclization

The rhodium-catalyzed arylative cyclization of enone tethered-cyclohexadienone has been developed with high efficiency, thus providing cis-fused bicyclic enones in good yields and excellent diastereo selectivities. Furthermore, this mild transformation has broad range of substrate scope and excellent functional group tolerance. In addition, bicyclic products have enone functionality, which can be synthetically valuable handle for further transformations. (*Org. Biomol. Chem.*, **2019**, 17(7), 1937)



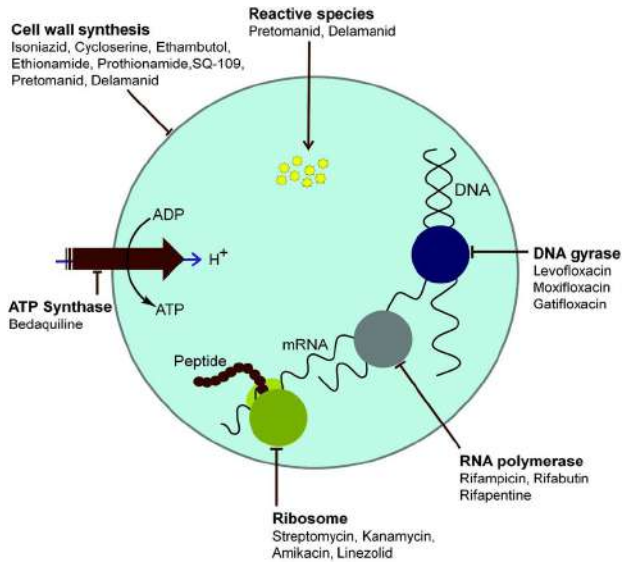
73. Tandem Addition/Electrocyclization/ Benzylation of Alkyl Aryl-1,3-dienes and Aromatic Aldehydes: Access to Highly Substituted Indenes

$BF_3.Et_2O$ mediated synthesis of multisubstituted indenes from alkyl aryl-1,3-dienes and aromatic aldehydes through tandem addition/4π-electro cyclization/ and benzylation *via* tetrahydroindeno-oxepine/quinone methide followed by the intramolecular 1,6-hydride transfer is described. This novel reaction pathway was established by the isolation of potential intermediates and with the support of deuterium labelling studies. In addition, the generality of this method has been demonstrated by reacting various aromatic aldehydes, which ascertained the role of aldehyde's electronic effect on the formation of indene derivatives and tetrahydro indeno-oxepines. (*J. Org. Chem.*, **2019**, 84(12), 7815)



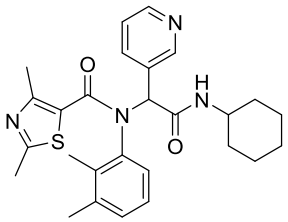
74. Strategies towards the Synthesis of Anti-Tuberculosis Drugs

Antituberculosis drugs have captured the attention of the scientific community due to the emergence of drug resistance. Hence, the development of new analogs and new drugs which can treat drug-resistant tuberculosis is required. In this report, we reviewed the strategies towards the synthesis of antituberculosis drugs. These strategies include semisynthetic approaches, resolution based strategies, microbial transformations, solid phase synthesis, and asymmetric synthesis. As stereochemistry is an important hallmark of many drugs, the strategies based on asymmetric synthesis are described in detail. The emphasis on semisynthetic approaches is given for aminoglycoside antibiotics. (*Org. Biomol. Chem.*, **2019**, 17(22), 5428)



75. Synthesis and Evaluation of A-Aminoacyl Amides as Antitubercular Agents Effective on Drug Resistant Tuberculosis

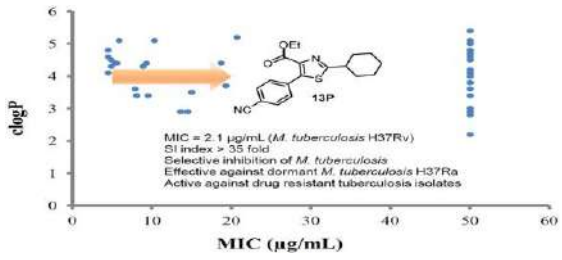
The development of an effective antitubercular agent is a challenge due to the complex nature of tuberculosis. Herein, we report the synthesis and evaluation of α-aminoacyl amides as antitubercular agents. The systematic medicinal chemistry approach led to identification of optimal substitutions required for the activity. Compound 11l was identified as antitubercular lead with drug like properties. Further, 11l selectively inhibited *M. tuberculosis* H37Rv with MIC value of 0.78 μM and was found to be non-toxic to CHOK1 cells. The lead compound inhibited multidrug resistant and Pre-Extensively drug resistant strains of Mycobacterium at 2 μg/mL and 8 μg/mL respectively. (*Eur. J. Med. Chem.*, **2019**, 164, 665)



11l

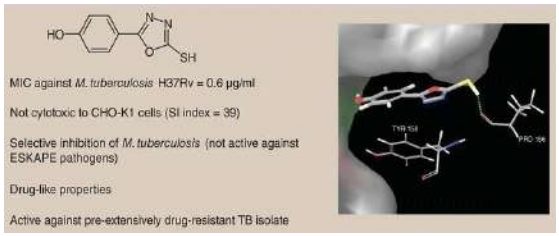
76. Synthesis and Biological Evaluation of 2,4,5-Trisubstituted Thiazoles as Antituberculosis Agents Effective Against Drug-Resistant Tuberculosis

The dormant and resistant form of Mycobacterium tuberculosis presents a challenge in developing new anti-tubercular drugs. Herein, we report the synthesis and evaluation of trisubstituted thiazoles as antituberculosis agents. The SAR study has identified a requirement of hydrophobic substituent at C2, ester functionality at C4, and various groups with hydrogen bond acceptor character at C5 of thiazole scaffold. This has led to the identification of 13h and 13p as lead compounds. These compounds inhibited the dormant Mycobacterium tuberculosis H37Ra strain and M. tuberculosis H37Rv selectively. Importantly, 13h and 13p were non-toxic to CHO cells. The 13p showed activity against multidrug-resistant tuberculosis isolates. (*Eur. J. Med. Chem.*, **2019**, 178, 315)



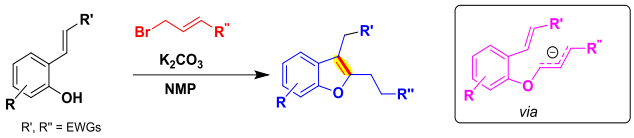
77. Novel 1,3,4-Oxadiazoles as Antitubercular agents with Limited Activity Against Drug-Resistant Tuberculosis

In recent times, heterocyclic chemotypes are being explored for the development of new antimycobacterials that target the drug-resistant tuberculosis. Here, we are disclosing the 5-substitued 2-mercapto-1,3,4-oxadiazoles as potent antitubercular agents. A small library of 2-mercapto-1,3,4-oxadiazoles was synthesized using various acids. The compounds were evaluated for antituberculosis activity against *M. tuberculosis* H37Rv. Compound 8j was identified as antitubercular lead with MIC of 0.6 µg/ml against *M. tuberculosis* H37Rv. This compound was nontoxic to CHO-K1 cells and showed selectivity index of 39. Of note, 8j showed antitubercular activity against pre-extensively drug-resistant clinical isolate of *Mycobacterium* with MIC of 2 µg/ml. This study provides potent antitubercular agent which can be further optimized to discover novel antibiotics. (*Fut. Med. Chem.*, **2019**, 11(6), 499)



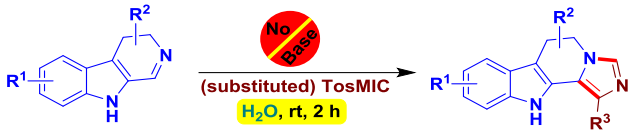
78. One-Pot Allylation–Intramolecular Vinylogous Michael Addition–Isomerization Cascade of *o*-Hydroxycinnamates and Congeners: Synthesis of Substituted Benzofuran Derivatives

A unique intramolecular vinylogous Michael addition leading to the synthesis of heterocycles has been disclosed. Base-promoted one-pot sequential O-allylation of *o*-hydroxy-cinnamates or -cinnamonitrile or -chalcones with γ-bromocrotonates followed by an intramolecular conjugate addition of vinylogous Michael donors resulted in the formation of highly substituted benzofuran derivatives in good to excellent yields. The intramolecular event followed by two [1,3]-H shifts leading to aromatization appears to be the key to the success of this unprecedented transformation. (*Org. Lett.*, **2019**, 21(6), 1823)



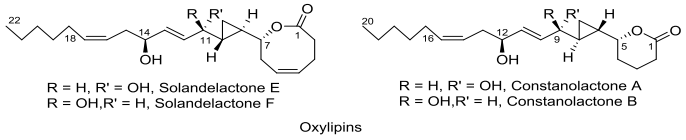
79. The Base-Free van Leusen Reaction of Cyclic Imines on Water: Synthesis of *N*-Fused Imidazo 6,11-Dihydro β-Carboline Derivatives

Construction of imidazoles has been demonstrated on water under base-free conditions. The reaction of dihydro β-carboline imines and p-toluenesulfonylmethyl isocyanides furnished the corresponding substituted *N*-fused imidazo 6,11-dihydro β-carboline derivatives in very good yields under ambient conditions. The use of deuterium oxide (D_2O) as a solvent enabled the incorporation of deuterium isotopes in the imidazole ring. (*Org. Biomol. Chem.*, **2019**, 17(21), 5234)

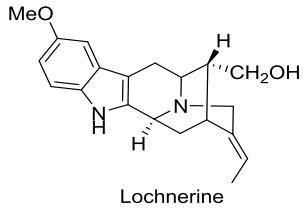


80. Efforts towards the Synthesis of Lochnerine

The stereoselective synthesis of (+)-lochnerine, a sarpagine alkaloid was undertaken. The synthesis was designed utilizing an intramolecular catalytic hydroamination of an alkene by an oxazolidine, derived in situ from an unsaturated aldehyde, as the key step. The other key steps of the sequence include substrate-controlled, Lewis acid promoted C3 allylation to secure the C3/C5 *syn* disubstituted product, Kulinkovich and ring-closing metathesis reactions. (*ChemistrySelect*, **2019**, 4(14), 4203)



81. Synthesis of Solandelactone F, Constanolactone A and an advanced intermediate towards Solandelactone E

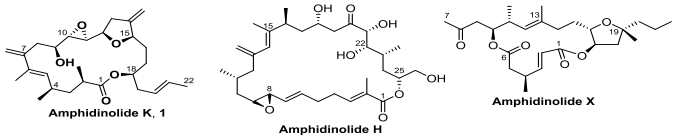


Lochnerine

The stereoselective synthesis of solandelactone F and constanolactone A from a common synthetic intermediate has been developed. The propargylic sulfide stereocenter is created stereoselectively via carbon-carbon bond formation in the reaction of α-chloro sulfides with alkynylzinc reagents via 1,2-asymmetric induction by a β-siloxy group. The characteristic 1,4-diol motif of the natural products is introduced by a [2,3] sigmatropic rearrangement of an allylic sulfoxide or by Mislow-Evans-Braverman rearrangement of a propargylic sulfoxide followed by stereoselective reduction of the ensuing α, β-unsaturated ketone. Unlike earlier reports, the C11/C9 carbinol center is created with excellent stereocontrol and derivatives of natural products differing at C14/C12 can be readily obtained. Catalytic asymmetric protocols and substrate-controlled asymmetric induction is utilized for the efficient introduction of the stereogenic centers. (*Org. Biomol. Chem.*, **2019**, 17(18), 4572)

82. Stereoselective Synthesis of the C1-C22 Carbon Framework of (-)-Amphidinolide K

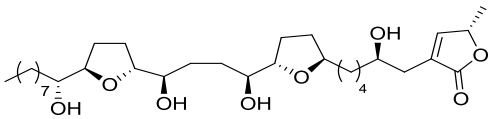
Two stereoselective routes to the C7-C22 subunit of amphidinolide K have been elaborated. Jacobsen's hydrolytic kinetic resolution and Sharpless' asymmetric dihydroxylation reactions have been employed for the construction of the THF ring. The C10-C11, C16-C17, C9-O and C18-O bonds have been created using α-chloro sulfide intermediates and [2,3] sigmatropic rearrangement. Marshall's propargylation protocol is utilized to create the C4 stereogenic center and regioselective hydrozirconation/iodine quench afforded an alkenyl iodide which is employed in the NHK coupling with the C7-C22 subunit. Oxonia-Cope rearrangement resulted in the creation of the C18 carbinol stereogenic center and chain elongation. (*J. Org. Chem.*, **2019**, 84(15), 9584)



Representative Amphidinolides

83. Stereoselective Synthesis of C3–C17 and C18–C34 subunits of Bullatanocin

A convergent synthesis of bullatanocin was envisaged by the union of C18-C34, C3-C17 and the butenolide subunits. The synthesis of the C3-C17 and C18-C34 subunits takes advantage of the chirality of tartaric acid for 1,2-asymmetric induction, chloro sulfides for carbon chain elongation and [2,3] sigmatropic shift for the preparation of 1,4-diol moiety via efficient 1,3-chirality transfer. The THF ring is elaborated by intramolecular displacement. (*Tetrahedron Lett.*, **2019**, 60 (41), 151132)

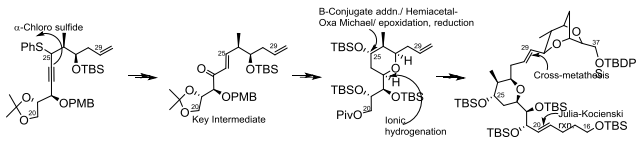


Bullatanocin

84. Convergent Stereoselective Synthesis of the C16-C37 Subunit of Sorangicin A

A convergent stereoselective route to the C16-C37 fragment of sorangicin A has been developed using an α-chloro sulfide for C-C bond formation. The key intermediate, an α,β-unsaturated ketone, is revealed by a [2,3] sigmatropic rearrangement of a propargylic sulfoxide. Three disparate approaches are detailed to create the C25 carbinol stereocenter. The *cis* 2,6-disubstitution of the THP ring is secured by ionic hydrogenation. A cross-metathesis reaction and Julia-Kocienski olefination to furnish the C16-C37

fragment of sorangicin A. (*Org. Lett.*, **2019**, 21(19), 7778)

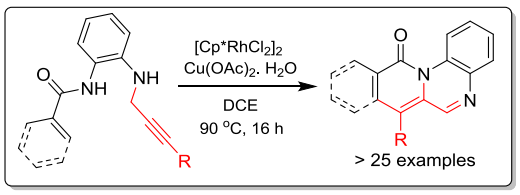


85. Stereoselective Synthesis of the A,E-ring Bicyclic Core of Calyciphylline B

A stereoselective synthesis of the bicyclic unit constituting the A,E rings of calyciphylline B type alkaloids is elaborated. The propionate ester of (*R*)-cyclohexenol, obtained by enzymatic resolution, is subjected to Ireland-Claisen rearrangement. Further reduction of the acid, Mitsunobu reaction to introduce the nitrogen functionality, oxidative cleavage to a dialdehyde followed by intramolecular aldol and aza-Michael reaction afforded the bicyclic subunit. (*Synlett*, **2019**, 30(19), 2157)

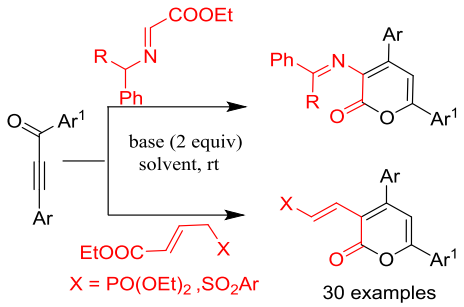
86. Rh(III)-Catalyzed Intramolecular Oxidative Annulation of Propargyl Amino Phenyl Benzamides to Access Pyrido/ Isoquinolino Quinoxalinones

A rhodium catalyzed copper mediated double oxidative annulation of propargylamino phenyl benzamides is developed. A quick assembly of tri, tetra and penta cyclic pyrido/isoquinolo-quinoxilines are thus achieved from readily available linear substrates. The reaction is shown to be very general by accommodating a large variety of substrates in the transformation. A mechanism through an amide directed C-H bond activation followed by an intramolecular alkyne activation/annulation followed by an oxidation is postulated. (*Adv. Synth. Catal.*, **2019**, 361(20), 4825)



87. Base Mediated Tandem Vinylogous Addition and Cyclization of γ-Phosphonyl/Sulfonyl Crotonates and Ynones: Synthesis of Functionalized 2-Pyrones

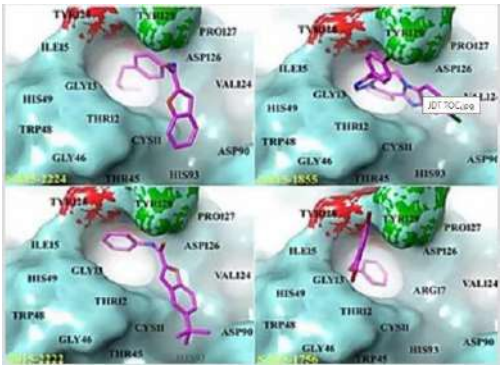
A general method for highly functionalized 2-pyrones via a base mediated sequential vinylogous addition and a cyclization of γ-phosphonyl/sulfonyl crotonates and ynones is described. An exclusive E-geometry with respect to the newly generated olefin substituent at C3 of pyrone was observed. Imino glyoxalates and glycine imines similarly reacted with ynones to deliver 3-imino pyrones. (*ACS Omega*, **2019**, 4(20), 18846)



88. Mycobacterial Protein Tyrosine Kinase a Augments the Secretion of Ptpa by Phosphory lation at Tyrosine Residues and the Mechanism is Stalled by Benzylbenzofurans and Benzofuran amides

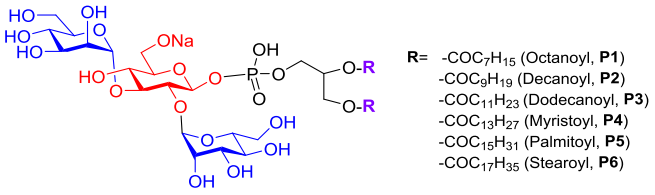
Phosphorylation and dephosphorylation are the key mechanisms for mycobacterial physiology and play critical roles in mycobacterial survival and in the pathogenesis. Mycobacteria evade host immune mechanism by inhibiting phagosome – lysosome fusion in which mycobacterial protein tyrosine phosphatase A (TP) plays an indispensable role. Tyrosine kinase (TK) activated by autophosphorylating; phosphorylates TP, which subsequently leads to increase in its phosphatase activity. The activated TP after getting phosphorylated is secreted in phagosome of macrophage. In present study we have shown that the phosphorylation at two sites of TP; Y128 and Y129 are critical for TK mediated TP secretion and its

phosphatase activity. The disruption of this interaction between TK and TP inhibits activation of later which further leads to the decrease in its secretion and in intracellular survival of mycobacteria. Further, the experiments have shown that Benzylbenzofurans and Benzofuranamides which inhibit the growth of mycobacteria, associate with the functional sites of TP and contend with the TK. This binding was further restated by looking at the anchorage of protein-protein and the protein-inhibitor complexes in the homology based structure models. *(J. Drug. Targeting*, **2019**, 27(1), 51)



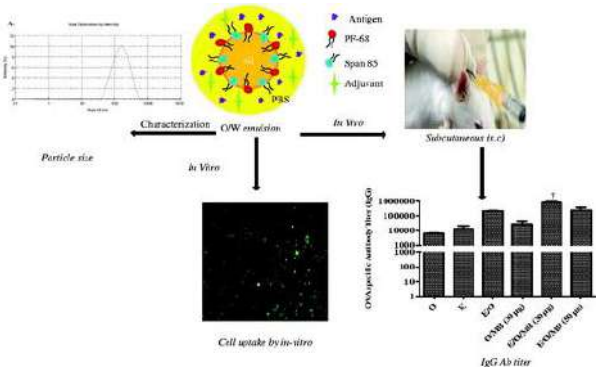
89. Novel Trisaccharide Based Phospholipids as Immunomodulators

A focused library of novel mannosylated glycophospholipids was synthesized employing imidate coupling and H-phosphate phosphorylation methods. All novel glycophospholipids were evaluated for their receptor interactions by molecular docking studies. Docking studies revealed dendritic cell-specific intercellular adhesion molecule-3-grabbing non-integrin (DC-SIGN) specific interaction of the glycophospholipid ligand P4 acts, which was further confirmed by in vitro DC-SIGN expression on monocyte-derived dendritic cells (MoDCs). Further, in vitro and in vivo immune modulatory activity among the six compounds (P1-P6) examined, compound P4 displayed good immunopotentiation and adjuvant properties as indicated by the induced cytokine expression and enhanced ovalbumin (OVA) specific antibody (IgG) titers. *(Int. Immunopharmacol.*, **2019**, 74, 105684)



90. Squalane-Based Emulsion Vaccine Delivery System: Composition with Murabutide Activate Th1 Response

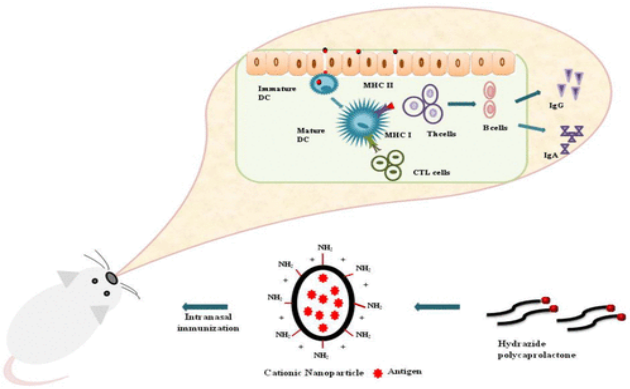
Novel squalane-based emulsion was formulated using surfactants viz., Pluronic F68, Span 85 along with Murabutide (MB) as immunepotentiator. The in vivo subcutaneous studies involving measurement of OVA-specific IgG antibody titers, Th1/Th2 cytokines were performed and a marked up regulation in IL-2, IL-12 and IFN-γ cytokines indicate Th1 immune response. Results supported that the squalane-based delivery system enhanced the uptake of the antigen by immune cells and elicited humoral as well as cell-mediated immune response in mice. (*Pharm. Dev. Technol*., **2019**, 24(3), 269)



91. Cationic pH-Responsive Polycaprolactone Nanoparticles as Intranasal Antigen Delivery System for Potent Humoral and Cellular Immunity against Recombinant Tetravalent Dengue Antigen

A novel polycaprolactone based nanoparticulate delivery system conjugated with hydrazine has been developed and tested for its intranasal vaccine

delivery capability andimmunogenicity. In vitro assays for antigen colocalization and cross-presentation have revealed that the modified polymers could effectively execute the anticipated function. In vivo evaluation in BALB/c mice using recombinant dengue antigen for intranasal immunization affirmed that the modified polymer having 457 μM/mg of free amine groups effectively stimulated humoral and potent cellular immune response. The overall data suggests that the modified polymeric nanoparticles—with their cationic, pH-responsive, and adjuvanting characteristics—proved to be a versatile system for effective mucosal antigen delivery. (*ACS Appl. Bio Mater*., **2019**, 2, 11, 4837)

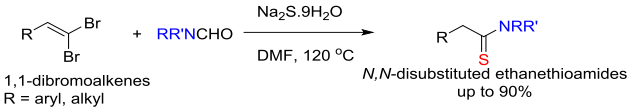


92. Secophragmalin-Type Limonoids from Trichilia connaroides Isolation and Their Cytotoxic Activities

Two new secophragmalin-type limonoids, secotrichagmalins B (1) and C (2) along with two known compounds were isolated from the fruits of Trichilia connaroides. In addition, semisynthetic derivatives (2a–2l) were efficiently synthesized and evaluated for their in vitro cytotoxicity along with the isolated limonoids against a panel of human cancer cell lines. The results indicated that new analogues 2a, 2d, and 2e showed cytotoxicity on the DU145 cell line with IC50 values of 3.6, 4.2, and 5.2 μM, respectively. Flow cytometric analysis revealed that these analogues arrested the cell cycle in the G0/G1 phase and markedly induced apoptosis. (*J. Nat. Prod*., **2019**, 82(10), 2731)

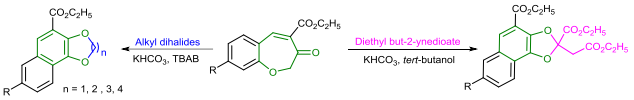
93. Synthesis of Substituted Thioamides from *Gem*-Dibromoalkenes and Sodiumsulfide

A three-component reaction of 1,1-dibromoalkenes, sodium sulfide, and *N*-substituted formamide for the synthesis of disubstituted thioamides has been developed. Various dibromoalkenes were found to be compatible under these conditions and gave corresponding thioamides in good to excellent yields. (*Eur. J. Org. Chem*., **2019**, 2019(42), 7159)



94. A Facile Construction of Oxygen Heterocycles by the Reaction of Benzoxepine-4-Carboxylates with Dihaloalkanes and Activated Alkynes

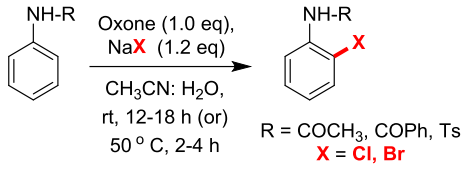
This work describes the preparation of heterocyclic compounds such as naphtho[1,3]-dioxoles, [1,4]-dioxines, [1,4]-dioxepines, [1,4]-dioxocines and diethyl 2-(2-ethoxy-2-oxoethyl)naphtho[1,3]dioxoles. These heterocyclic compounds have been achieved by the reaction of benzoxepine-4-carboxylates with dihaloalkanes and activated alkyne for the first time. This work represents the first example for the construction of utile oxygen heterocycles by the formation of C-C and C-O bonds in one step process. (*Org. Biomol. Chem.*, **2019,** 17(27) 6645)



95. A Green and Sustainable Approach for Selective Halogenation of Anilides, Benzanilides, Sulphonamides and Heterocycles

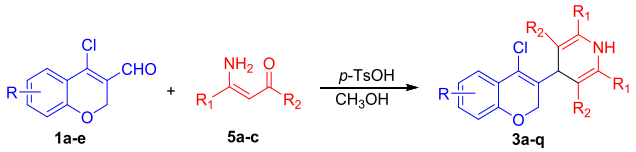
An efficient green sustainable protocol has been devised for selective oxidative halogenation of acetanilides, benzanilides, sulphonamides and heterocyclic compounds using easily available NaX as halogen source and Oxone as powerful oxidant. Reaction products are analyzed by GC-MS. Defined experimental conditions provided the mono and

dihalo compounds. The present protocol is simple and environmentally benign to conduct the laboratory scale halogenations and can be extended to prepare industrially important compounds. (*Asian J. Org. Chem.*, **2019,** 8(8), 1380)



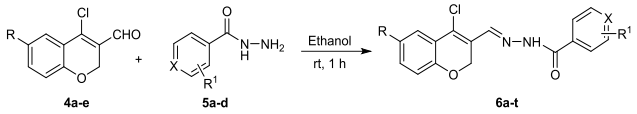
96. Condensation of 4-Chloro-2H-Chromene-3-Carbaldehydes and Ethyl-3-Aminocrotonates with *P*-Tsoh: A Facile Approach for the Synthesis of Chromenyldihydropyridines

The investigated reaction of 4-chloro-2*H*-chromene-3-carbaldehyde 1a with ethyl 3-oxobutanoate 2a in the presence of ammonium acetate provided two compounds, 2H-chromenyl dihydropyridine dicarboxylate 3a and chromenopyridine carboxylate 4a. However, the reaction of 1a with ethyl-3-aminocrotonate 5a in the presence of p-TsOH provided selectively 2H-chromenyldihydropyridine dicarboxylate 3a with very good yield. The established method was applied for the preparation of series of 2*H*-chromenyldihydropyridine dicarboxy lates 3a-q. (*Synth. Commun.*, **2019**, 49(19), 2538*)*



97. Synthesis and Anti-Microbial Activity of 2*H*-Chromenylmethylene Benzohydrazides

2*H*-Chromenylmethylene benzohydrazides **6a-t** have been prepared by the reaction of 2*H*-chromene-3-carbaldehydes **4a-e** with benzohydrizides **5a-c** and isonicotinohydrazide **5d** in ethyl alcohol at room temperature. All the synthesized compounds have been evaluated for their anti-microbial activity. Compounds **6a**, **6f**, **6p** and **6t** have potent anti-bacterial activity. Compounds **6a** and **6f** are highly potent and **6l**, **6p** and **6t** have equi potent anti-fungal activity. (*Ind. J. Chem. B*, **2019**, 58B, 497)

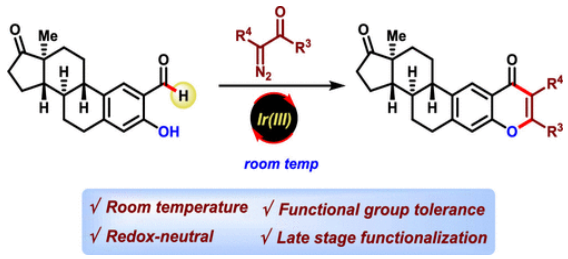


98. Catalyst- and Reagent-Free 1,6-Hydrophosphonylation of *P*-Quinone Methides: A Practical Approach for the Synthesis of Diarylmethyl Phosphine Oxides

We developed a catalyst-, reagent-, and additive-free protocol with 100% atom economy for the synthesis of diarylmethyl phosphine oxides via 1,6-hydrophosphonylation of p-quinone methides using water as a green solvent. The reaction showed broad scope with excellent functional group tolerance. The practicability of this method was demonstrated by carrying out the reaction on the gram scale whereby product was obtained in high yield by the filtration technique avoiding chromatographic purification. (*Org. Biomol. Chem.*, **2019**, 7(32), 7536)

99. Cp* Ir (III)-Catalyzed C–H/O–H Functional ization of Salicylaldehydes for the Synthesis of Chromones at Room Temperature

We report Cp*Ir(III)-catalyzed C–H/O–H-bond functionalization of salicylaldehydes with α-diazocarbonyl compounds for the synthesis of chromones under redox-neutral conditions. The reaction proceeds at room temperature and displays excellent functional group tolerance along with high yields of the corresponding products. The developed reaction protocol was successfully applied for the late-stage functionalization of estrone derivative. (*J. Org. Chem.*, **2019**, 84(14), 9188)



100. An Overview on the Synthetic and Medicinal Perspectives of Indenopyrazoles

Indenopyrazole is emerging as one of the most promising and privileged scaffold in medicinal chemistry. This scaffold have been investigated for the development of novel derivatives and hybrids with other moieties and substituents exhibiting a wide range of medicinal properties like antimycobacterial, antipsychotic, antihypertensive, cannabinoid receptor affinity, anti-tumor, antimicrobial, etc. Furthermore, indenopyrazoles function as inhibitors in various mechanistic pathways which has been well established based on its anticancer potential. This review illustrates various strategies adopted and reveals the extensive significant biological properties of indenopyrazoles. Furthermore, ample scope is available for this scaffold which needs to be explored by medicinal chemists for the development of new potential drug candidates. (*Eur. J. Med. Chem*., **2019**, 178, 1)

101. Phenazine-1-Carboxamide Functionalized Mesoporous Silica Nanoparticles as Antimicrobial Coatings on Silicone Urethral Catheters

Microbial infections due to biofilms on medical implants can be prevented by antimicrobial coatings on biomaterial surfaces. Mesoporous silica nanoparticles (MSNPs) were synthesized via base-catalyzed sol-gel process at room temperature, functionalized with phenazine-1-carboxamide (PCN) and characterized by UV-visible, FT-IR, DLS, XRD spectroscopic techniques, SEM, TEM, TGA and BET analysis. Native MSNPs, PCN and PCN-MSNPs were evaluated for anti-Candida minimum inhibitory concentration (MIC), minimum fungicidal concentration (MFC), Candida albicans (C. albicans) biofilms and C. albicans-Staphylococcus aureus (S. aureus) polymicrobial biofilm inhibition. PCN-MSNPs were four-fold effective (MIC 3.9 µg mL^{-1}; 17.47 µM) and MFC (7.8 µg mL^{-1}; 34.94 µM) as compared to pure PCN (MIC 15.6 µg mL^{-1}; 69.88 µM) and MFC (31.2 µg mL^{-1}; 139.76 µM). PCN-MSNPs inhibited in vitro C. albicans MTCC 227-S. aureus MTCC 96 biofilms at very low concentration (10 µg mL^{-1}; 44.79 µM) as compared to pure PCN (40 µg mL^{-1}; 179.18 µM). Mechanistic studies revealed that PCN induced intracellular ROS accumulation in C. albicans MTCC 227, S. aureus MTCC 96 and S. aureus MLS-16 MTCC 2940, reduction in total ergosterol content, membrane permeability, disruption of ionic homeostasis followed by Na^+, K^+ and Ca^{2+} leakage leading to cell death in C. albicans MTCC 227 as confirmed by confocal laser scanning micrographs. The silicone urethral catheters coated with PCN-MSNPs (500 µg mL^{-1}; 2.23 mM) exhibited no formation of C. albicans MTCC 227 - S. aureus MTCC 96 and C. albicans MTCC 227 - S. aureus MLS -16 MTCC 2940 biofilms. This is the first report on PCN-MSNPs for use as antimicrobial coatings against microbial adhesion and biofilm formation on silicone urethral catheters. (*Sci. Rep*., **2019**, 9(1), 6198)

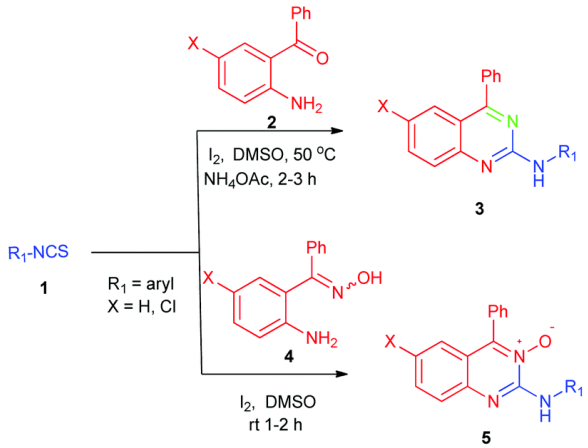
102. Design, Synthesis, in Silico Pharmacokinetics Prediction and Biological Evaluation of 1,4-Dihydroindeno[1,2-C]Pyrazole Chalcone as EGFR /Akt Pathway Inhibitors

In an attempt to develop potent and selective anticancer agents, a series of 15 conjugates of 1,4-dihydroindeno[1,2-c]pyrazole chalcone (12a-o) were designed, synthesized and evaluated for their antiproliferative activity against MCF7, A549, MDA-MB-231, HCT116 and SKBR3 human cancer cell lines. Among them, 12h, 12l and 12m showed IC_{50} values: 3.82, 5.33 and 4.21 µM, respectively, on A549 cell with respect to the positive control, Erlotinib (IC_{50} value: 10.26 µM). Detailed biological

assays showed accumulation of mitotic cells in G2/M phase. In addition, Western blot analysis and immunofluorescence study revealed inhibition of EGFR and Akt pathways. In silico computational studies were also carried out to predict the binding modes and pharmacokinetic parameters of these conjugates. (*Eur. J. Med. Chem*., **2019**, 163, 636)

103. I_2-Catalyzed Oxidative Synthesis Of *N*,4-Disubstituted Quinazolines and Quinazoline Oxides

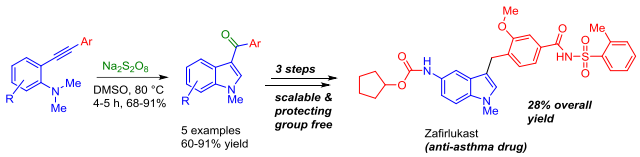
An easy and efficient approach to the synthesis of *N*,4-disubstituted quinazoline-2-amine and oxides is described. This transformation proceeds smoothly in the presence of molecular iodine. The metal-free protocol presented here is insensitive to air moisture and operationally simple. This versatile and synthetic methodology is broadly applicable to a variety of *N*,4-disubstituted quinazoline-2-amines and oxides, which are synthesized in good to excellent yields starting from readily available inexpensive precursors. (*Org. Biomol. Chem*., **2019**, 17(15), 3714)



APPLIED RESEARCH

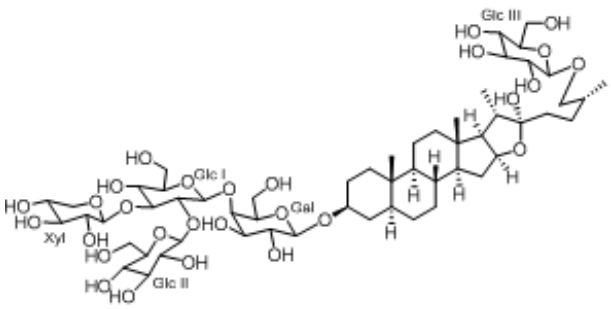
1. Synthesis of Asthma Drug Zafirlukast (Accolate) Using Intramolecular Oxidative Coupling via sp^3 C–H Bond Activation

The FDA-approved drug for the treatment of asthma, zafirlukast, is synthesized engaging multiple catalytic reactions including a new method for the construction of 3-aroylindoles via oxidative cyclization. The highlights include transition-metal and peroxide free C–H bond activation using the stoichiometric amount of sodium persulfate as an oxidizing agent in the construction of 3-aroylindole, avoiding transition metal, with over 28% overall yield. The complete process has a turnaround time of 28 h to get the target molecule starting from substituted aniline, with practically no protecting groups. (*ACS Omega*, **2018,** 3(4), 4289)

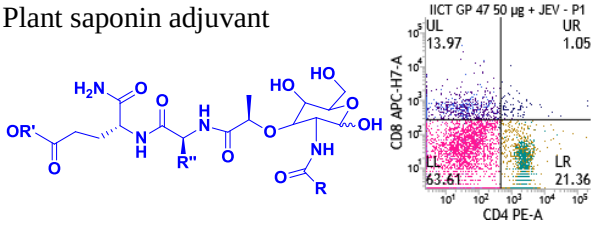


2. Identification of Muramyld Dipeptide NOD2 Agonistic Adjuvant & Saponin Agonist

During the reporting period, we have taken up immunopharmacological screening of focused library so new adjuvant entities belonging to muramyld dipeptide (NOD2 agonist) and Pam3cys (TLR2agonist) structural class. Identified potential adjuvant leads based on in vivo evaluation and in vitro tox studies. Also, we have identified a potential plant based saponin adjuvant as viable alternative to generic adjuvant QS21. (Muramyl peptide derivative compound, synthesis and uses thereof US10576147B2, US20180371023A1) & (A plant saponin based immune-adjuvant/potentiator composition and process for preparation thereof" Indian patent, date of filing: 13th Nov 2018, Application No. : **201811042595**).



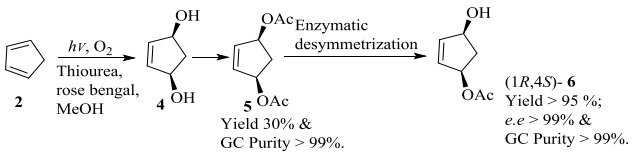
Plant saponin adjuvant

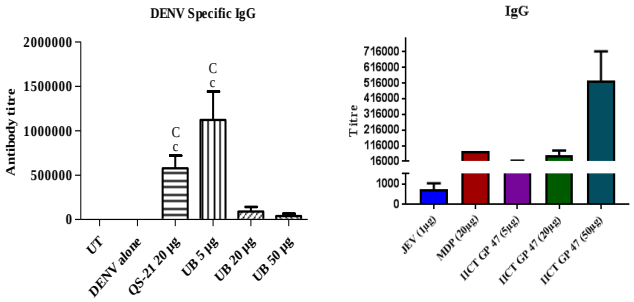


MDP analogue as NOD2 agonistic adjuvant

3. Preparation of (1*R*, 4*S*)-4-Hydroxycyclopent-2-En-1-Yl Acetate via Novozym-435® Catalyzed Desymmetrization of *Cis*-3,5-Diacetoxy-1-Cyclopentene

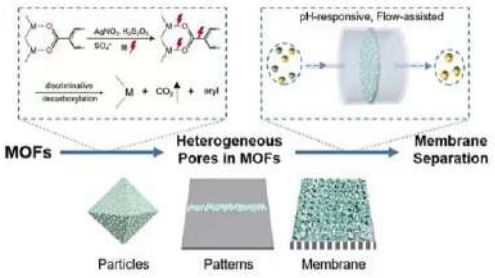
Photooxidation of cyclopentadiene has been carried out in methanol using white light of LED lamp, rose bengal as photo initiator, and compressed air at 0 □C. Under conditions of [thiourea] >> [cyclopentadiene], the consumption of thiourea follows a pseudo-first-order reaction kinetics with half life of 75±10 min; corr. coeff. r = 0.989. Slow addition of the monomer and maintaining excess thiourea concentration in reaction mass improves the yield. *cis*-1,3-Cyclopentene diol is acetylated without isolation o obtain *cis*-1,3-cyclopentene diacetate of high purity (>99%) with overall isolated yield of 30%. Desymmetrization of the diacetate to (1*R*,4*S*)-4-hydroxycyclopent-2-en-1-yl acetate has been carried out via enzymatic *trans*-esterification with methanol in methyl *tert*.butyl ether (MTBE) at 5°C using Novozyme-435. The enantiomerically pure monoacetate (*e.e.*>99%) was obtained in 95% isolated yield. The recovered enzyme was reused for more than 10 times without loss in yield and selectivity. The entire protocol does not require purification of final product by chromatography. (*Tetrahedron*, **2018**, 74(46), 6673)





4. Metal-Organic Framework Patterns and Membrane with Heterogeneous Pores for Flow-assisted Switchable Separation

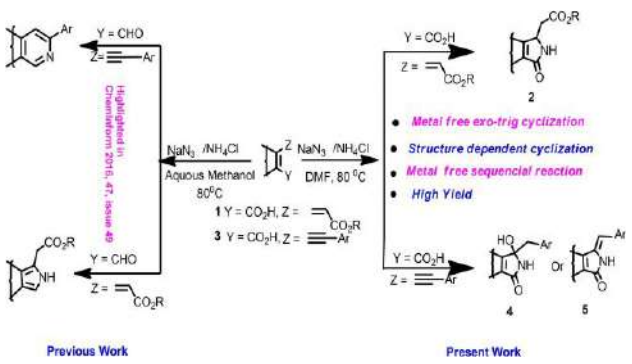
Tailoring Multi-Scale Porosity in MOF Particles, Films, and Membranes via Discriminative Etching Method and Its Nano-filter Application: We envision that our facile method to make these unique construct allows using multi-scale pores cooperatively to overcome the challenges existing in the fields of complex and largely organic, inorganic, and biological molecules. (*Nat. Commun.* **2018**, 9(1), 3968)



5. NaN_3/NH_4Cl-Promoted Aza-Cyclization: A Convenient Route for Bio-Active Diverse Isoindolinone Derivatives

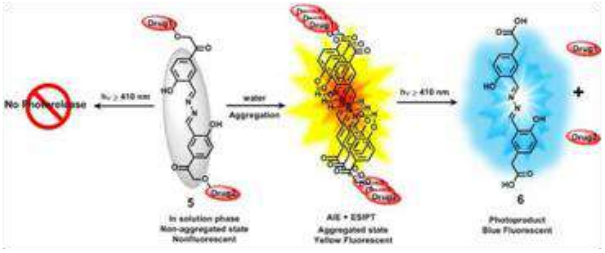
An efficient substrate dependent NaN_3/NH_4Cl promoted azacyclization was developed *via* metal free cascade transformation. A wide variety of bicyclic/tricyclic isoindolinone derivative was achieved with excellent diastereoselectivity from achiral reagent system. This protocol also provided synthetic route of dopamine D4 receptor in short way. The bio-imaging study towards CHO cell line with our isoindolinone embedded new fluorophore

was also demonstrated. (*ChemistrySelect*, **2018**, 3(42), 11950)



6. 'AIE + ESIPT' Assisted Photorelease: Fluorescent Organic Nanoparticles for Dual Anticancer Drug Delivery with Real-Time Monitoring Ability

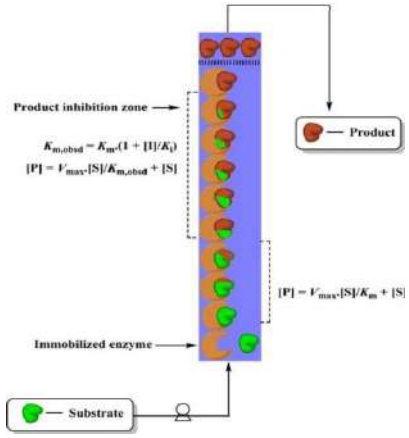
We have designed a photoresponsive drug delivery system, which exhibits both aggregation induced emission (AIE) and excited state intramolecular proton transfer (ESIPT) phenomena, by simple incorporation of a salicylaldazine moiety to a p-hydroxy phenacyl (pHP) phototrigger. The presence of AIE enables the DDS to photorelease and ESIPT makes the release more efficient. The newly developed photoresponsive DDS has the ability to release two different drugs sequentially so that it can be used effectively in the area of combination chemotherapy. (*Chem. Comm.* **2018**, 54(2), 168)



Schematic presentation of the AIE + ESIPT' assisted photorelease of dual anticancer drug with real-time monitoring ability

7. Ammonolysis of (5*S*)-N-(*tert*-Butoxycarbonyl)-5-(Methoxycarbonyl)-2-Pyrroline with Immobilized Candida Antarctica Lipase B (CAL B) in a Packed Bed Reactor

Conversion of (5*S*)-*N*-(tert-Butoxycarbonyl)-5-(methoxycarbonyl)-2-pyrroline to its corresponding amide, an important intermediate in the synthesis of the dipeptidyl peptidase IV (DPP4) inhibitor Saxagliptin, was carried out by ammonolysis reaction catalyzed by immobilized *Candida antarctica* lipase B (CAL B) in a packed bed reactor. The reaction proceeds smoothly at 50 °C in anhydrous *tert*-butanol containing 1.25 M ammonia and follows typical Michaelis-Menten kinetics with competitive product inhibition. The estimated kinetic parameters were V_{max} 40 ± 4.4 mM $h^{-1}g^{-1}$, K_m (216 ± 22 mM) and K_i 303 ± 31 mM. At substrate concentration of 30 mg/mL (132 mM) and flow rate of 0.1 mL/min, the product is obtained in > 98% yield and 98.5 % purity at steady state in a column (100 cm x 1.2 cm) packed with 40 g immobilized CAL B. (*Process Biochem.*, **2018,** 65, 109)



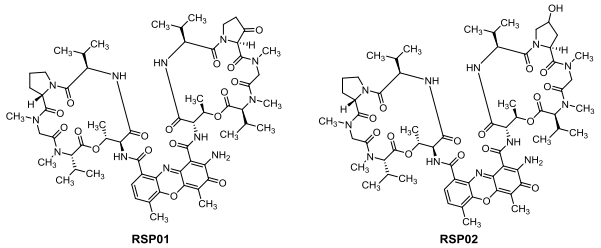
8. Polyhydroxy-*N*-Alkyl-2-Pyrrolidinones as a New Class of Glycolipid Analogues with Immune Modulation Potential

A focused library of novel N-alkyl-2-pyrrolidinone derivatives 3a–e was synthesized from d-galactose employing a multistep Chiron approach. These novel glycolipid analogues exhibited lipopolysaccharide-mediated splenocyte proliferation with no apparent toxicity against murine splenocytes. Various immunological assays on dendritic cells, macrophages, and

human peripheral blood mononuclear cells have ascertained the immunostimulatory activity of these new glycolipid analogues. (*J. Carbohydr. Chem.*, **2018**, 37(1), 1)

9. Novel Actinomycin Group Compound from Newly Isolated *Streptomyces* Sp. RAB12: Isolation, Characterization and Evaluation of Antimicrobial Potential

A *Streptomyces* sp. RAB12 having potential to produce novel actinomycin group compounds was isolated from soil samples collected from IICT garden premises using ISP protocol. The 16S rRNA sequence of the strain RAB12 exhibited identity with *Streptomyces* sp. 13647M and the sequence was deposited in NCBI under the accession number KY 203650. Cell free extract of this novel strain revealed two bioactive principles viz., RSP 01 and RSP 02. HR-MS analysis indicated a molecular mass of 1269.61 and 1270.63 m/z g/mole for RSP 01 and RSP 02, respectively. Proton ^{1}H, ^{13}C NMR, 2D NMR and mass spectroscopy analysis revealed similar fingerprint to that actinomycin D except peak at δH3.59 *J* (^{1}H NMR) and δ 208.88 (^{13}C NMR) for RSP 01 compound suggesting presence of keto carbonyl at 5-oxo position on the proline moiety which is absent in actinomycin D. Purified RSP 02 depicted similarity with RSP 01 except a peak in the ^{1}H proton NMR at δH 3.81 *J*. HR-ESI mass spectra confirmed the molecular formulae for RSP 01 and RSP 02 as $C_{62}H_{84}N_{12}O_{17}$ and $C_{62}H_{86}N_{12}O_{17}$, respectively. Antimicrobial activity profile revealed higher antimicrobial activity against bacterial strains (*P. aeruginosa, M. luteus, S. aureus, S. typhi* and *B. subtilis)* and *C. albicans* compared to standard Actinomycin D. MIC and MBC for RSP01 were observed to be 0.0039 and 0.0078 (µg/ml) against *C. albicans* while for actinomycin D it was found to be 0.031 and 0.62 (µg/ml), respectively indicating a ten-fold higher potency**.** Thus these RSP 01 and RSP 02 compounds from *Streptomyces* sp. RAB12 may be a promising candidate for industrial and clinical applications. (*Appl. Microbiol. Biotechnol.*, **2018**, 102(3), 1241)



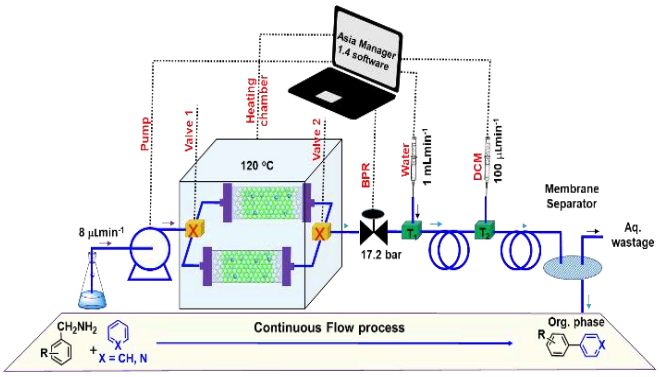
10. Biofilm Inhibition and Anti-Candida Activity of A Cationic Lipo-Benzamide Molecule with Twin-Nonyl Chain

A series of cationic lipo-benzamide compounds with varying lengths of hydrocarbon chains (C2M–C18M) were evaluated for anti-Candida activity. Four compounds harbouring 8–11 hydrocarbon chains demonstrated concentration-dependent inhibition of fungal cell growth with Minimum Inhibitory Concentration (MIC) of ≤6.2 mg ml^{-1}. The most active compound (C9M) inhibited growth of both Candida albicans and non-albicans strains and is equally active against pairs of azole sensitive and resistant clinical isolates of C. albicans. Compound C9M also inhibited different stages of Candida biofilms. Scanning Electron Microscopy (SEM) of Candida cells after C9M treatment was also done and no significant cell lysis was observed. Hemolysis assay was performed and only 2.5% haemolysis was observed at MIC concentration. (*Bioorg. Med. Chem. Lett.*, **2018**, 28(10), 1776)

11. Synthesis of bi(hetero)aryls via Sequential Oxidation and Decarboxylation of Benzyl Amines in a Batch/Fully Automated Continuous Flow Process

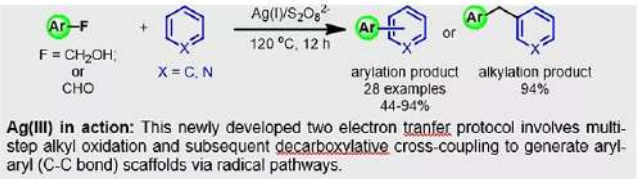
Catalytic dehydrogenative cross-coupling of two C−H bonds represents a green strategy in view of the atom- and step-economy. However, the challenge is to discover a new innovative bond

strategy, especially for the direct coupling between Csp^2-H and benzyl amines (BzAs). A series of biaryls and bi(hetero)aryls were prepared from commercially available substituted BzAs, $AgNO_3$, cheap $K_2S_2O_8$ as anoxidant and benzene/pyridines as the coupling source in batch and flow process. In batch reaction is somewhat problematic in terms of safety (peroxide in organic environment, high temperature above the boiling point of the solvent and substrate, pressure, toxic pyridines), we havechosen a convincing automated flow-setup to perform it in a controlled and safe manner to one-pot synthesis of biaryls. The mechanistic studies revealed that the current protocol involves radical-initiation, multi-step BzA oxidation and subsequent decarboxylative coupling for the generation of biaryls. (*Eur. J. Org. Chem.*, **2018**, 2018(22), 2831)



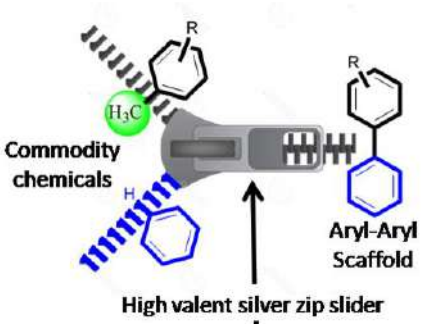
12. Silver-Catalyzed Arylation of (Hetero) Arenes via Oxidative Benzylic C−C Bond Cleavage of Benzyl Alcohols/ Benzaldehyde

We have developed a direct oxidative arylation of benzyl alcohol using tandem catalytic platform for the synthesis of aryl-aryl scaffolds from various arenes and pyridine as coupling partners. (*ChemistrySelect*, **2018**, 3(43), 12336)



13. Direct Aryl-Aryl Coupling without Pre-Functionalization Enabled by Excessive Oxidation of Two-Electron Ag(I)/Ag(III) Catalyst

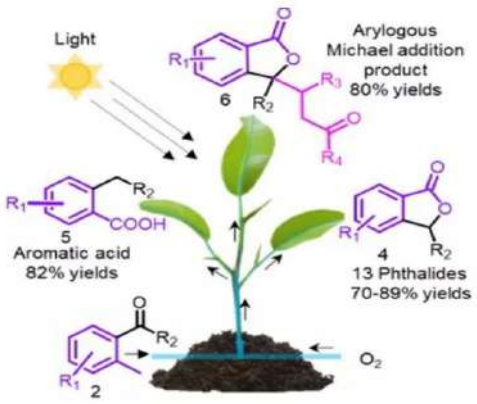
Reported herein is a catalytic platform for formation of unsymmetrical biaryls by the coupling between inert Csp^2-CH_3 and Csp^2-H via a tandem catalytic strategy. The platform utilizes traditional $AgNO_3$ catalyst and excess amount of $K_2S_2O_8$ oxidant. The excessive oxidant present converts the traditional one-electron Ag(I)/Ag(II) chemistry to two-electron Ag(I)/Ag(III) one, enabling one-pot synthesis of aryl-aryl scaffolds by using unactivated cheap commodity chemicals. (*Adv. Synth. Catal.*, **2018**, 360(10), 2032)



14. Controlled Photo-Flow Oxidative Reaction (UV-FOR) Platform for Ultra-Fast Phthalide and API Synthesis

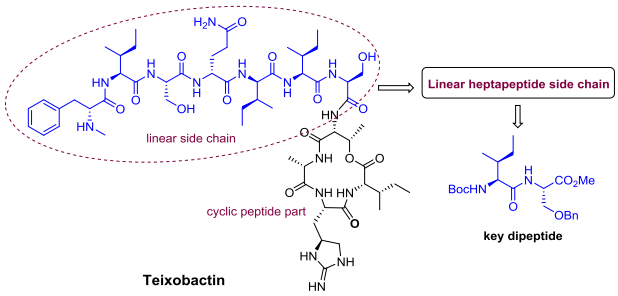
An integrated photo-flow oxidative reaction (UV-FOR) platform approach is presented for the synthesis of phthalides. The current protocol is catalyst-free, and uses economical and abundant hydro-carbons and hydrocarbon derivatives such as benzoic acid, benzene, and xylene, as starting materials. The reaction is performed using oxygen as a green oxidant in a time- and labour-efficient manner. This integrated approach has been shown to be successful in making a UV-FOR platform suitable for the on-demand synthesis of phthalides and their further syntheses to 2-arylmethylbenzoic acids and arylogous Michael addition products under relatively mild conditions. The current protocol was further extended to the gram scale synthesis of an ischemic

stroke-relevant active pharmaceutical ingredient (API), 3-N-butylphthalide (NBP), in a continuous flow process. (*Green Chem*., **2018**, 20, 4584)



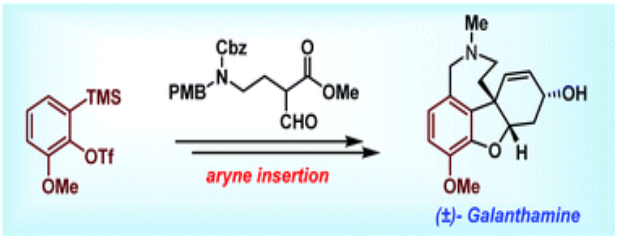
15. Gram Scale Solution-Phase Synthesis of Heptapeptide Side Chain of Teixobactin

A scalable synthesis of linear heptapeptide side chain of the depsipeptide natural product teixobactin through solution-phase has been reported. The synthesis of heptapeptide was achieved through an efficient coupling of suitably protected tripeptide and tetrapeptide comprising of three D-amino acids and four usual L-amino acid sub-units. (*Synlett*, **2019**, 30(20), 2268)



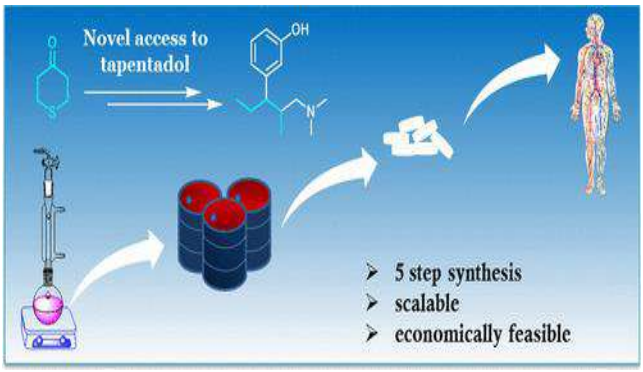
16. Total Synthesis of (±)-Galanthamine from GABA through Regioselective Aryne Insertion

The total synthesis of (±)-galanthamine is achieved in ~5% overall yield using a key regioselective aryne insertion reaction into a GABA (γ-amino butyric acid) derivative. The strategy presented involves only two sub-critical temperature reactions and less than five chromatographic purifications to achieve the synthesis of galanthamine. (*Org. Biomol. Chem*., **2019**, 17(8), 2192)



17. Tetrahydrothiopyran-4-one as Five-Carbon Source for Scalable Synthesis of (±)-Tapentadol

The improved process for the synthesis of (±)-tapentadol, the FDA-approved analgesic drug, is achieved from tetrahydrothiopyran-4-one as the five-carbon source. *(Org. Process Res. Dev.*, **2019**, 23(7), 1369)

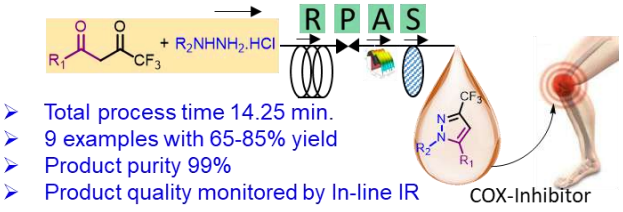


18. Integrated Continuous Flow/Batch Protocol for the Photoreduction of *Ortho*-Methyl Phenyl Ketones using Water as Hydrogen Source

Direct utilization of the abundant hydrogen in water for transfer hydrogenation reaction (THR) is very attractive and challenging research area. Herein, we report the first integrated photo- transfer hydrogenation reaction (PTHR) platform for the synthesis of benzhydrol derivatives (26 examples, 33-89% yields) with water as a green reducing agent. This transformation is time, labor-efficient, catalyst-free, economical and utilizes readily available hydrocarbon(s) (o-methyl phenyl ketones) as starting materials. (*React. Chem. Eng.*, **2019**, 4, 812)

19. An Integrated Continuous Flow Micro-Total Ultrafast Process System (μ-TUFPS) for the Synthesis of Celecoxib and Other Cyclooxygenase Inhibitors

Integrated continuous manufacturing has emerged as a promising device for the rapid manufacturing of active pharmaceutical ingredients (APIs). We herein report a newly designed continuous flow micro-total process system platform for the rapid manufacturing of celecoxib, a selective nonsteroidal anti-inflammatory drug. This approach has been proven generally for the synthesis of several alkyl and aryl substituted pyrazoles. In order to minimize the tedious work-up process of potential reaction intermediates/products, we have developed a continuous flow extraction and separation platform to carry out the entire reaction sequence resulting in a short residence time with good yield. The present process was further extended to gram- scale synthesis of the COX-2-related API, viz. celecoxib, in the continuous flow process. (*Org. Process Res. Dev.*, **2019**, 23(9), 1892)



R = Reaction; P = Pressure; A = Analysis; S = Separation

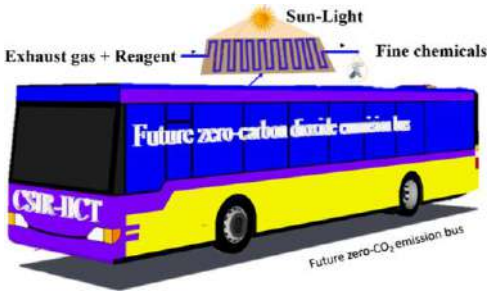
20. Micro-Electro-Flow Reactor (L-EFR) System for Ultra-Fast Arene Synthesis and Manufacture of Daclatasvir

The World Health Organization (WHO) has listed daclatasvir (DCV), symmetrical arene, as one of the essential medicines for human health. DCV manufacturing is usually carried out in a non-continuous or ‘‘batch’’ approach over multiple locations and is severely limited by long production times (3–10 days), resulting in non-affordability (highly expensive) and disruption of the potential chain supply. Here, we report the total process system including the development of a novel electro-flow reactor containing patterned electrodeposited Ni or Pt nanoparticles over a copper electrode for a C–C coupling reaction in a co-reductant/oxidant-free, ultra-fast process for sym- metrical substituted/unsubstituted biphenyl synthesis. This method was further extended to a new generation commercial batch synthetic route for continuous flow ultra-fast daclatasvir synthesis in 33.2 min. We envisage that this micro-electro-flow reactor (l-EFR) system platform will substantially enable advances in continuous-l-flow fine chemical manufacturing, multistep reaction sequences, reaction devising equipment, and real-time extraction. (*Chem. Commun.*, **2019**, 55(79), 11852)

21. Integrated Microfluidic Photo-Flow Process (μ-PFP) for Direct Upconversion of Exhaust Gas to Value-Added Chemicals

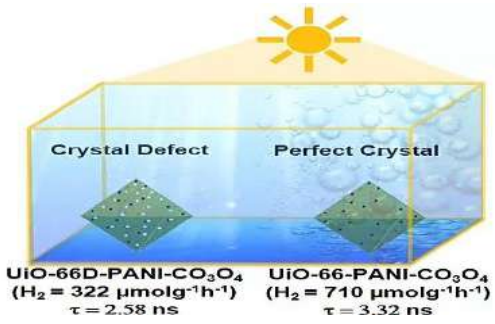
Exhaust gas emission globally continues to increase, with the burning of billions of tons of fossil carbon each year. Exploration and expansion of the

chemistries involving exhaust gas as a chemical resource are severely limited by the mixed composition of the gases, the low reactivity of CO_2, and immature recycling technologies. Herein, we present a micro-photo- flow process (μ-PFP) involving an automated platform for direct capture and photochemical conversion of CO_2 from the exhaust gas to a valuable mixture of chemicals such as carboxylic acid and phthalides. The current protocol was further extended to the automated serial work-up platform to obtain the highly pure product without laborious extraction and work-up platform. *(ACS Sustain. Chem. Eng.*, **2019**, *7*(24), 19605)



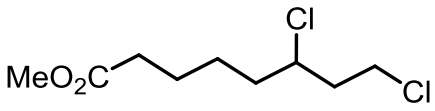
22. Noble Metal-Free Integrated UiO-66-PANI-Co3O4 Catalyst for Visible-Light-Induced H_2 Production

A viable route for the simple yet effective modification of UiO-66 by implanting PANI and cobalt oxide was demonstrated for the development of a series of UiO-66-based catalysts. The UiO-66-PANI-Co_3O_4 catalyst showed staggeringly enhanced photocatalytic activity, which was 24 times that of the pristine UiO-66(Zr). *(Chem. Commun.*, **2019**, 55(96), 14494)



23. Process Developed of Lipoic Acid Key Intermediate "Ethyl 6,8-Dichlorooctanoate"

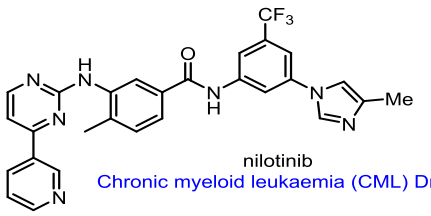
Dichlorooctanoic acid is key raw material for α-Lipoic Acid synthesis. Our pharmaceutical companies depend on China to import this key material. However, they are facing problems with unexpected price variations and time limit. Manufacturers are looking for strong support from research organization for process development of Dichlorooctanoic acid. Here, we have developed process technology for the Kg scale synthesis of dichlorooctanoate from adipic acid as starting material.



Methyl 6,8-dichlorooctanoate

24. Process Development of the Second-Generation Tyrosinekinase Inhibitor, Nilotinib (*CSIR-INPROTICS Project)*

Large scale synthesis of key intermediates of Nilotinib and process technology of Nilotinib have been developed in multi-gram scale. Alternative route have been also established for the synthesis of Nilotinib. Higher regioselectivity for N-arylation has been achieved compared to the commercial route using less expensive ligand.



nilotinib
Chronic myeloid leukaemia (CML) Drug

25. Bacterial Biosynthesis of Nanosilver: A Green Catalyst for the Synthesis of (Amino Pyrazolo) - (Phenyl) Methyl Naphth-2-Ol Derivatives and their Antimicrobial Potential

There has been growing interest in the use of silver nanoparticles in various fields like medicine,

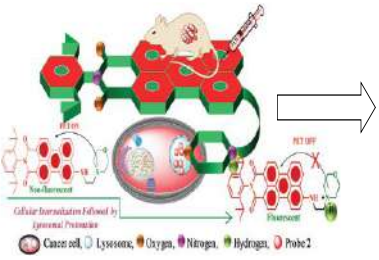
agriculture and food industry. In addition to these, recently, the silver nanoparticles have also demonstrated their catalytic properties in various applications like synthesis of pharmaceutical compounds and natural products. The use of silver nanoparticles as catalysts has gained more importance due to their stability, unique reactivity and recyclability. In the present study, heterogeneous silver nanoparticles, produced from isolated strain *Streptomyces* sp. RAB10, were used as catalysts in a three-component reaction of aryl aldehydes, 5-amino-3-methyl pyrazole and β-naphthol for the synthesis of naphthalene-2-derivatives in an aqueous media. The synthesized compounds were characterized using ^{1}H NMR, ^{13}C NMR, Mass spectroscopy and FT-IR. Some of the advantages of the multi-component one-pot protocol used in the study include shorter reaction time, good yield, ease of recoverability and reuse of the silver nanoparticles as catalysts. The biosynthesised AgNPs as well as the naphthalene-2-derivatives exhibited moderate to good anti-microbial activity.

26. Mutanase Enzyme from Paracoccus Mutanolyticus RSP02: Characterization and Application as a Biocontrol Agent

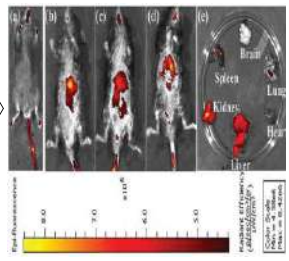
Mutanases are enzymes that have the ability to cleave α-1,3 linkages in glucan polymer. In the present investigation, mutanase enzyme purified from the culture filtrate of *Paracoccus mutanolyticus* was evaluated for *Streptococcal* biofilm degradation and antimicrobial activity against pathogenic fungi along with enzyme kinetics, activation energies, pH and thermal stability. Biochemical and molecular characterization depicted that the enzyme showed optimum activity at pH 5.5 and at 50ºC. It displayed Michaelis-Menten behaviour with a K_m of 1.263±0.03 (mg/ml), V_{max} of 2.712±0.15 U/ mg protein. Thermal stability studies denoted that it required 55.46 and 135.43 KJ mol^{-1} of energy for activation and deactivation in the temperature range of 30 to 50ºC and 50 to 70ºC respectively. Mutanase activity was enhanced ~50 and 75% by Fe^{2+} and EDTA, respectively, while presence of Hg^{2+} and Mn^{2+} inhibit > 90% of its activity. This enzyme has a molecular mass of 138 kDa and showed monomeric nature by Zymography. Scanning electron microscopy (SEM) analysis of mutanase treated *Streptococcal* cells revealed cleavage of linkages among the cells and complete separation of cells, indicating its potential in dentistry as an anticaries agent in the prophylaxis and therapy of dental caries. In addition, antifungal activity of mutanase against *Colletotrichum capsici* MTCC 10147 and *Cladosporium cladosporioide* MTCC 7371 revealed that the enzyme has potential towards biological control of phytopathogens which could be used as an alternative bio-control agent against chemical pesticides in the future.

27. Lysosome Specific Near-Infrared Fluorescent Probe for the in vitro Cancer Cell Detection and Non-Invasive in vivo Imaging

Near-infrared (NIR) fluorescent probes have been developed as potential bio-materials having profound applications in diagnosis and clinical practice. We have developed a perylene monoimide (PeIm)-based new NIR fluorescent probe, which could selectively and non-invasively detect and sense cancer cells over noncancerous cells *in vitro* and could also be a practical tool for in *vivo deep* tissue NIR imaging. *(Chem. Comm.*, **2019**, 55(94), 14182)



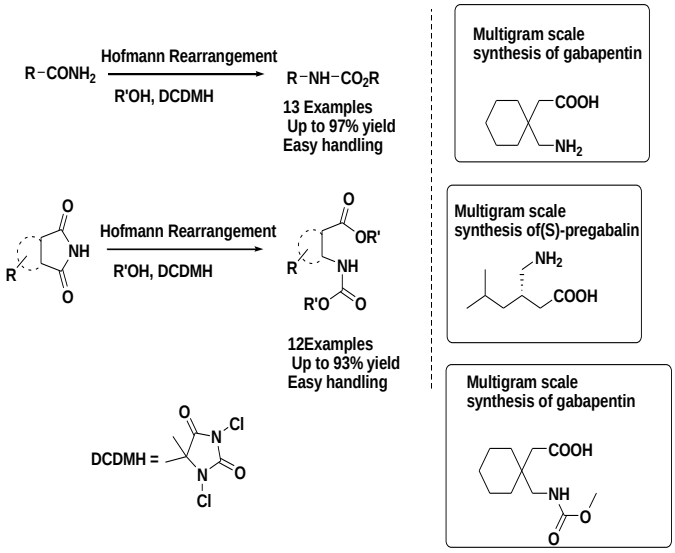
Schematic of the perylene monoimide (PeIm)-based NIR probe for in vitro and *in vivo* bio-imaging



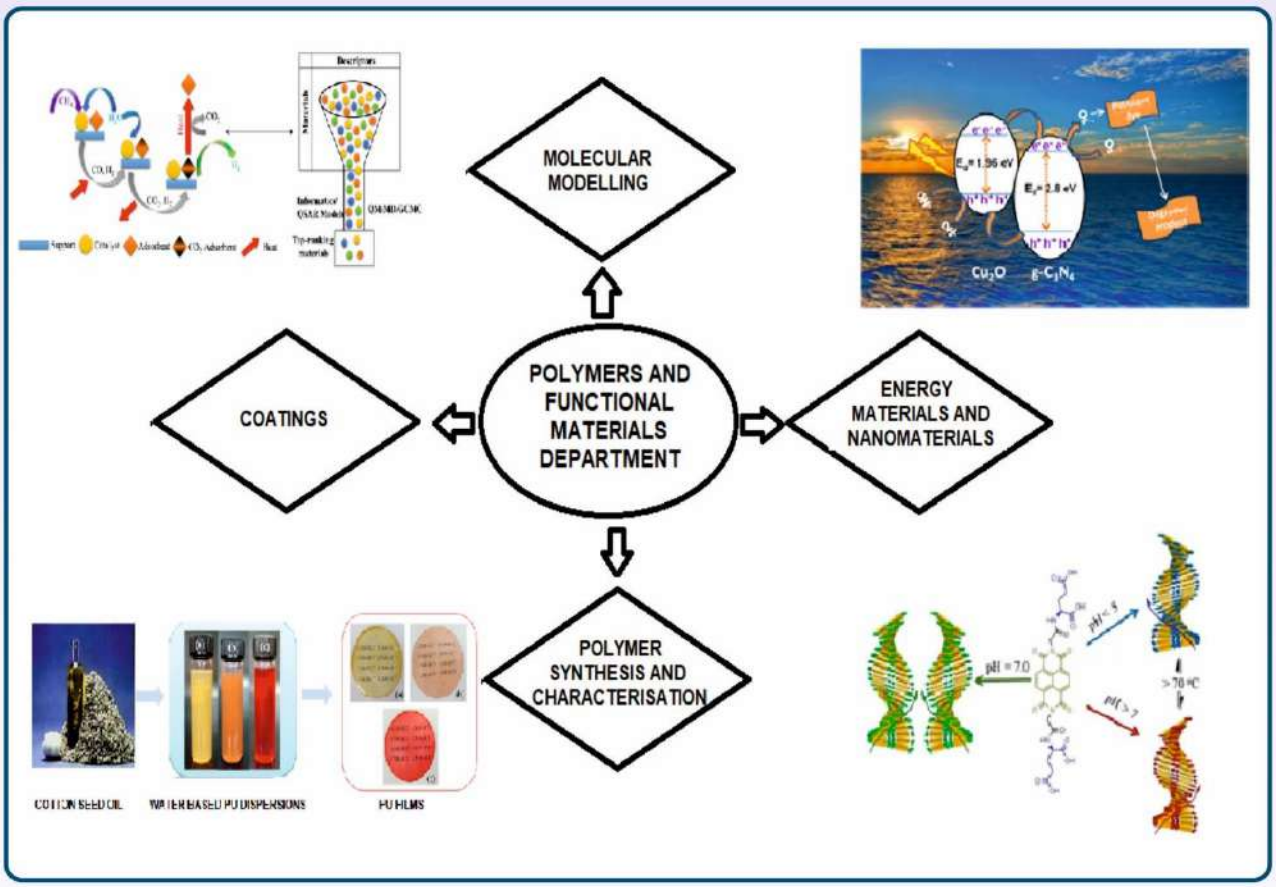
In vivo NIR imaging of the perylene monoimide (PeIm)-based NIR dye in female C57BL/6J mice: (a) after 0 h, (b) 8 h, (c) 16 h, and (d) 24 h of i.v. of probe **2**. (e) *Ex vivo* images of different organs after 24 h.

28. Hofmann Rearrangement of Primary Carboxamides and Cyclic Imides Using DCDMH and Application to the Synthesis of Gabapentin and its Potential Peptide Prodrugs

Two protocols for the efficient transformation of aromatic as well as aliphatic primary carboxamides to the corresponding carbamates and aromatic as well as aliphatic cyclic imides to the corresponding anthranilic acid derivatives & amino acid derivatives, respectively, are described. We also developed a novel methodology to the multigram scale synthesis of gabapentin and (S)-pregabalin. The gabapentin methyl carbamate was converted to novel potential peptide prodrugs of gabapentin. (*Tetrahedron Lett.*, **2019**, 60(7), 552)



POLYMERS AND FUNCTIONAL MATERIALS



BASIC RESEARCH

Energy

High-Performance Supercapacitor Coin-cell

The electrochemical performance of polyaniline was improved *via*. fabricating asymmetric cell of polyaniline and nitrogen and sulfur doped activated carbon in coin cell(fig.1). This cell showed better performances, i.e., V = 1.4 against 0.8 V of polyaniline with a high specific capacitance of 592 F g-1 and a high energy density of 80 W h kg^{-1} at a power density of 500 W kg^{-1}.(*J Solid State Electro.*, **2019**, 23(1), 295)

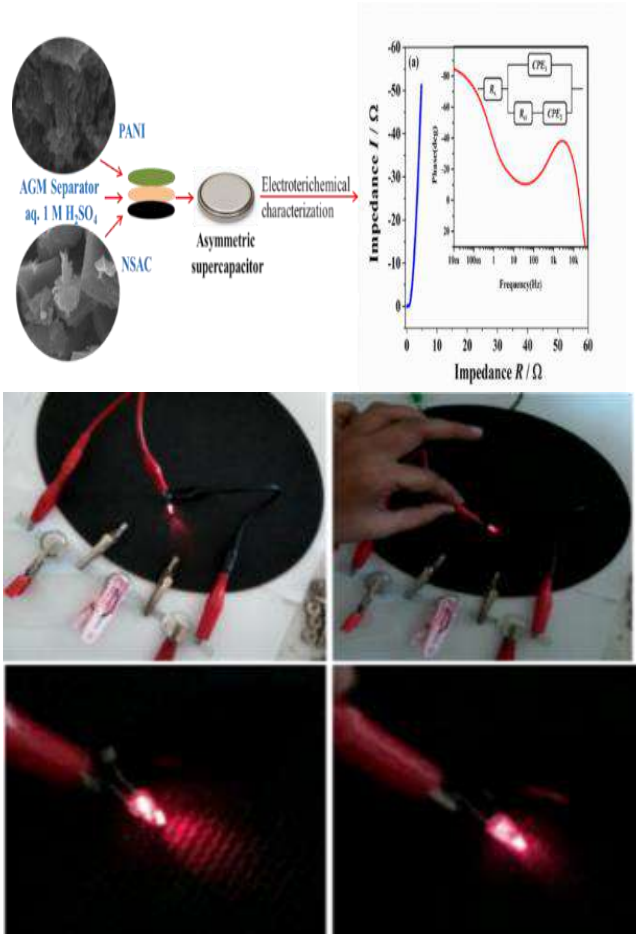


Fig. 1 Coin cell fabrication

Hybrid Polyurethane

A conducting hybrid polyurethanes from novel tetraaniline- diol as Gly-TAni (glycidol with TAni) has been synthesized and explored for its applications. A new diol Gly-TAni is synthesized in a simple process using tetraaniline (TAni) and glycidol via SN2 reaction in a single-step process. The asymmetric diol (Gly-TAni) and polyols (PTMEG and TMP) were reacted with isophorone diisocyanate to obtain —NCO terminated hybrid polyurethanes. These were subjected for curing under atmospheric moisture to obtain conducting polyurethane-urea coatings. All these conducting coatings films showed excellent corrosion resistance (on mild steel electrode) with an increase in the percentage of Gly-TANi (5 to 15 wt%). The films of these hybrid polyurethanes containing pendent tetraanilines showed good surface conductivity in the range of 3.69×10^{-4} to 2.21×10^{-3} S/cm. The electrochemical investigation showed 2 single electron oxidation and 2 single reductions reversibly, centred around tetraaniline segments present in the polymer. (*Polym. Advan. Technol*., **2018**, 29, 1620)

Electrically conducting Schiff bases :

Small molecules possessing –C=N- functional groups which are exploited for coordinating inorganic cations to form stable complexes which play the critical role in catalysis called Schiff base molecule (SBM) synthesised by condensation of terephthalaldehyde and conjugated dianiline. This Schiff base molecule (SBM) can be oxidized with ammonium peroxodisulfate in presence of 1 M HCl solution into emeraldine base form (O-SBM). Interestingly, the O-SBM molecule exhibits electrical conductivity after doping. The oxidized state (O-SBM) is dopable with 1 M HCl, to give better electrically conducting material than few oligoanilines such as trianiline, tetraaniline and pentaaniline. The electrical conductivity of O-SBM is 4.5×10^{-2} S/cm at room temperature. (*Synth. Met.*, **2019**, 247, 240)

Small Molecule Electron Donors

We have designed and synthesized two novel small molecule donor materials namely Si-PT2 and Ge-PT2 (fig 1.) with D-A-D-A-D molecular architecture. The two donors have the same electron-rich end group's

thienothiophene (TT) and similar electron-poor pyridal [2, 1, 3] thiadiazole (PT) subbunits but different central electron-rich cores dithienosilole (DTSi) and dithienogermole (DTGe). (*J. Mater. Chem. A*, **2018**, 6, 383)

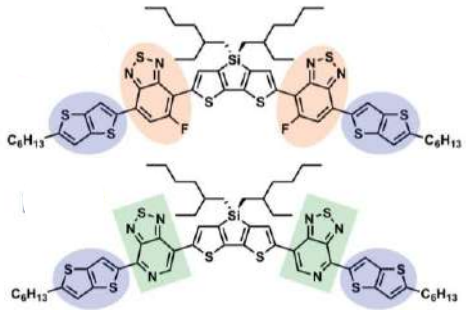


Fig. 2 Structure of small molecule electron donors - Si-PT2 and Ge-PT2

Non-fullerene Electron Acceptor

A small molecule non-fullerene electron acceptor (SMNFEA) bearing furan π-spacer and dicyano-*n*-hexyl rhodanine as flanking groups show in fig.3 was designed and synthesized for organic solar cell applications. Organic photovoltaic device based on $FRdCN_2$ and PTB7-Th polymer donor exhibited highly improved efficient power conversion efficiency of 10.7%, which is highest so far for OSCs fabricated from fluorene core based SMNFAs. *(Chem. Comm.*, **2018,** 54, 4001)

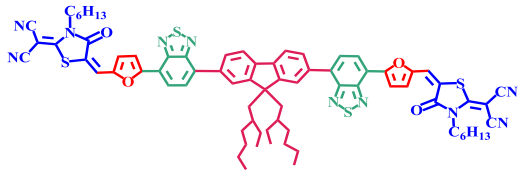


Fig. 3 Structure of non fullerene electron acceptor (SMNFEA)

Small Molecules Semiconductor *via* C-H Activation for Photovoltaic Applications

The first methodology of ruthenium carboxylate-catalysed single step oxidative cross coupling that challenges the conventional Stille and Suzuki coupling reactions, affording BT and MFBT derivatives(fig. 4) in absence of protecting groups. Both mono and bi-arylated derivatives are formed in moderate to high yields (30-75%). Innately high selectivity, low catalyst loading and lack of formation of regio-isomers ensures the large-scale synthesis of various photonic and electronic materials employing this method. (*Chem. Comm.*, **2018**, 54, 7322)

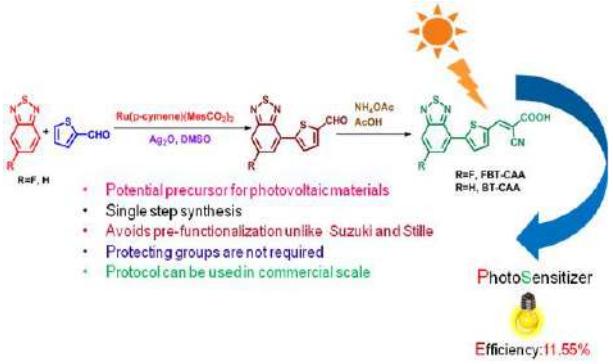


Fig. 4 Ruthenium carboxylate catalysed oxidative cross coupling reaction

Polymer Electrolyte Integrated Quasi Solid-State Dye Sensitized Solar Cells and Electrochromic Devices Endow Enhanced Stability

We have showcased the ease and feasibility of integrating a quasi-solid semi-IPN electrolyte supporting ionic conduction paired with photoanodes fabricated employing titania nanocuboids and electrochromic nanostructured WO_3 electrodes (fig.5), respectively to achieve functional devices with impressive performance and stability. It is understood, active electrode layer thickness as well as morphology has a crucial role to play on the device performance. The stability tests carried out on the DSSCs stored under ambient conditions demonstrate that these solid-state devices can retain Appxm.80% of their initial efficiency for at least 2600 h under the experimental conditions, which is devoid of hermetic sealing. For electrochromic devices, display a considerably high coloration efficiency of ~134 cm^2C^{-1}, an appreciably fast switching response (<2 s), full coloration/bleaching at competitive time scales of 5.9 s and 5.1 s, respectively, along with device reversibility of ~97% underlined the viability of electrode architecture and polymer electrolyte combination. Redox efficiency and reversibility >2000 cycles indicates a stable electrode-electrolyte interface and device performance. (*Solar Energy*, **2018**, 169, 159; *ChemNanoMat.*, **2018**, 4, 203)

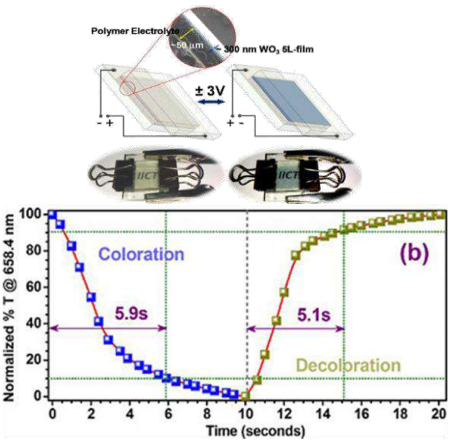


Fig. 5 Quasi-solid semi-IPN electrolyte paired with photoanodes employing titania nanocuboids and WO_3 electrodes

Napthalenedimide Based Small Molecules for Solar Cells

Novel dithiafulvenyl (DTF)-naphthalenediimide (NDI) derivatives DS1 and DS2 has been designed, synthesized and characterized to replace the costly PCBM. DS1 and DS2 were employed as electron transport layers (ETL) to fabricate inverted PSCs based on $CH_3NH_3PbI_{3-x}Cl_x$ as shown in fig.6. The best power conversion efficiencies (PCEs) of inverted PSCs based on DS1 and DS2 exhibit 9.6% and 11.4%, respectively. The difference in PCE values revealed that DS2 bearing two DTF moieties on NDI core could enhance the PCE compared to DS1 containing one DTF moiety. (*Asian J. Org. Chem*., **2018**, 7, 2294)

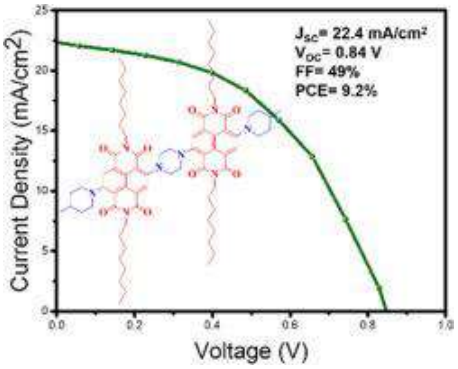


Fig. 6 Inverted PSCs based on $CH_3NH_3PbI_{3-x}Cl_x$

Two novel naphthalenediimide (NDI)-based electron transporting materials (4,4′-(piperazine-1,4-diyl)bis(2,7-dioctylbenzo[lmn]-[3,8]phenanthroline-1,3,6,8(2 H,7 H)-tetraone) **(PDPT**) and 9,9′-(piperazine-1,4-diyl) bis(4-(4-methylpiperidin-1-yl)-2,7 dioctylbenzo [lmn]-[3,8]phenanthroline-1,3,6,8 (2H, 7H)-tetraone) (**PMDPT**)), (fig.7) were synthesized and found that the inverted perovskite solar cells with **PMDPT** as an electron transporting layer can reach a power conversion efficiency up to 9.2% while the efficiency of PSCs based on **PDPT** can only approach 7.6%. (*J. Solid State Chem*., **2019**, 270, 51)

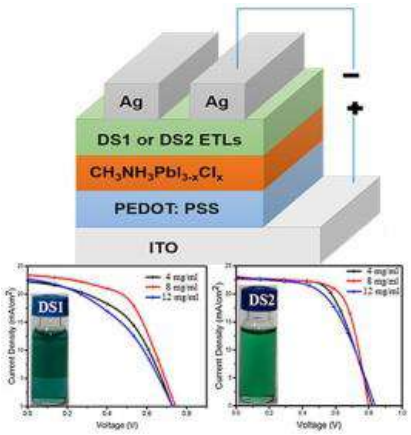


Fig. 7 Novel naphthalenediimide (NDI)-based electron transporting materials

Two simple semiconducting acceptor-acceptor$_1$-donor-acceptor (A-A$_1$-D-A) modular, small molecule non-fullerene electron acceptors, **NDICz-5** and **NDICz-6,** were designed, synthesized and characterized for application in solution-processable bulk-heterojunction solar cells. The optoelectronic and photovoltaic properties of **NDICz-5** and **NDICz-6** were directly compared with those of a structural analogue, **NDICz-4,** which was designed based on an A-D-A format. All of these new materials (shown in fig. 8) were designed to be V-shaped and comprised an electron rich carbazole donor core (D) together with electron deficient naphthalene diimide terminal core (A). Solution-processable bulk-heterojunction devices were fabricated with **NDICz-4, NDICz-5** and **NDICz-6** as non-fullerene electron acceptors. Studies on the photovoltaic properties revealed that the best P3HT: **NDI-Cz6**-based device showed an impressive enhanced power conversion efficiency of

7.58%, an increase of around two-fold with respect to as-cast blend, after solvent vapor annealing using carbon disulfide.(*Dyes Pigments*, **2019**, 171, 107677)

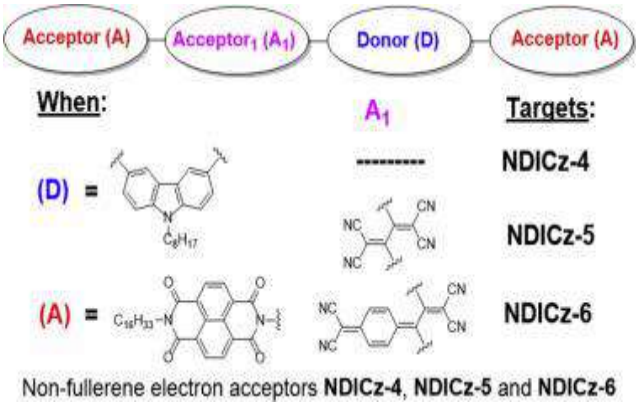


Fig. 8 Non-fullerene electron acceptors based on naphthalene dimidies

Two naphthalenediimide (NDI) derivatives (NDI-BTH1 and NDI-BTH2) were designed synthesised and it was found that introduction of 2-(benzo[*d*]thiazol-2-yl) acetonitrile groups at the NDI core position gave the lowest unoccupied molecular orbital (LUMO; −4.326 eV) and displayed strong electron affinities, suggesting that NDI-BTH1 might be a promising electron-transporting material (i.e., n-type semiconductor), whereas NDI-BTH2 bearing bis(benzo[*d*]thiazol-2-yl)methane at the NDI core with a LUMO of −4.243 eV was demonstrated to be an ambipolar material. OFETs based on NDI-BTH1 and NDI-BTH2 have been fabricated, and the electron mobilities of NDI-BTH1 and NDI-BTH2 are 14.00×10^{-5} and 8.64×10^{-4} $cm^2/V{\cdot}s$, respectively, and the hole mobility of NDI-BTH2 is 1.68×10^{-4} $cm^2/V{\cdot}s$. We further successfully employed NDI-BTH1 and NDI-BTH2 as electron transport layer (ETL) materials in inverted perovskite solar cells (PSCs). The PSC performance exhibits that NDI-BTH2 as the ETL material gave higher power conversion efficiency as compared to NDI-BTH1, that is, NDI-BTH2 produces 15.4%, while NDI-BTH1 gives 13.7%. The PSC performance is comparable with the results obtained from OFETs. (*ACS Appl. Mat. Interfac*., **2019**, 11, 44487)

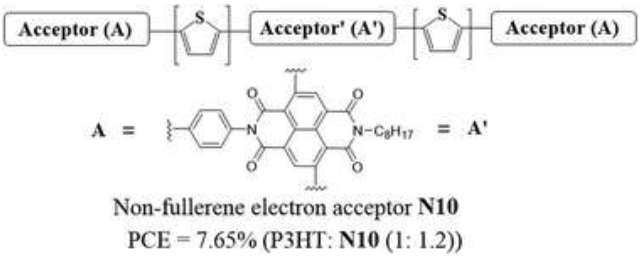


Fig 9. NDI-BTH1 and NDI-BTH2 as electron transport layer (ETL) materials in inverted perovskite solar cells

An Efficient Non-Fullerene Acceptor Based on Central and Peripheral Naphthalene Diimides

Through the coupling of central and terminal naphthalene diimide functionalities, a unique non-fullerene electron acceptor, coded as N10(fig.10), was designed, synthesized, characterized and applied in solution-processable bulk-heterojunction devices. The target N10 displayed good solubility, excellent thermal stability and energy levels complementing those of the conventional donor polymer poly(3-hexyl thiophene) (P3HT). An excellent power conversion efficiency of 7.65% was obtained in simple BHJ devices (P3HT : N10 1 : 1.2), which is the highest observed so far for NDI core-based non-fullerene acceptors. (***Chem. Commun.*, 2018, 54,** 5062)

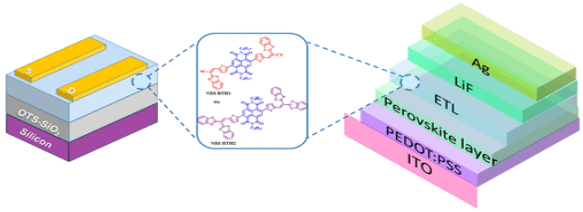


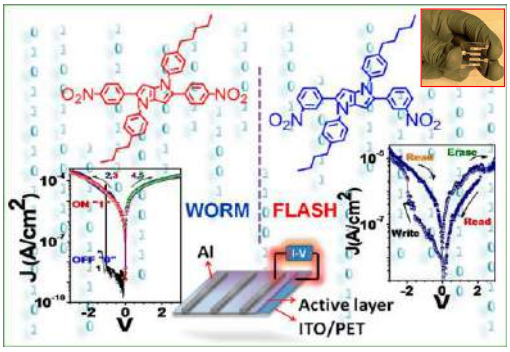
Fig. 10 Non-fullerene electron acceptor, coded as N10

Functional Materials

Quadrupolar Organic Moieties for Encoding Nano "Bits" – Nanostructured Fused Pyrrole Core as Potential Resistive Memory Elements

A series of 1,4-dihydropyrrolo[3,2-b]pyrrole derivatives synthesized were evaluated for their feasibility as resistive memory elements and elucidate the structure-property relationship. Smart

modifications through judicious choice of functional groups was carried out to establish a rationale between molecular framework in a quadrupolar A-π-D-π-A configuration and its influence on the resultant electronic and opto-electronic properties. A comprehensive understanding of resistive switching phenomenon and its dependence on molecular structure is established. The fabricated ORM devices display switching characteristics with an appreciable $I_{ON/OFF}$ ratio of ≈10^5. Studies employing conductive atomic force microscopy (C-AFM) demonstrate that the thin films can be electrically written to a "0" or "1" state under extremely low compliance currents of ±250 pA. Conservative estimates for the switching area of ≈150 nm^2 with energy as low as 15 fJ to induce a switching event underscore the possibility of nanoscale data storage with high areal density. (*Adv. Electron. Mater*., **2018**, 1700626; *Int. J. Mater. Eng. Resour*., **2018**, 23, 229)



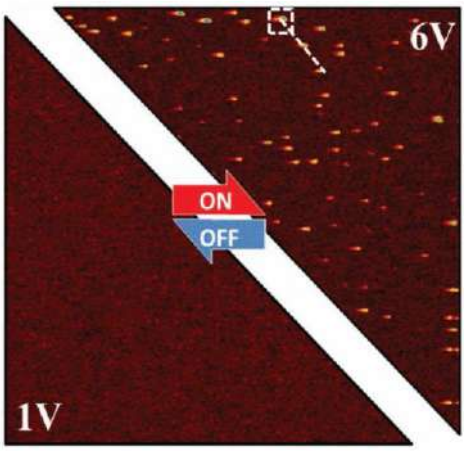


Fig. 11 Resistive memory elements based on 1,4-dihydropyrrolo[3,2-b]pyrrole derivatives

Aniline-Nonamer Segmented Electroactive Polyurea

An unprecedented A-B-A type block copolymer electroactive polyurea (EPU) is designed and synthesized with tetraaniline dimer and 1,4-phenylenediamine via an oxidative coupling, where aniline–nonamer and hexamethylene di-urea constitute two segments. EPU reorganizes into core–shell microcapsules(fig.12) in presence of aqueous acetic acid/n-octane interface. These microcapsules exhibited a wide range of pH responses in their absorption spectrum (UV–vis). The EPU is modified as carbon paste electrode which exhibits a remarkable electrocatalytic oxidation of ascorbic acid (AA, Vitamin C) in 0.2 M and pH 7.0 phosphate buffer solution. The carbon paste electrode is useful in sensing as low as 50 mM of ascorbic acid (*J. Appl. Polym. Sci*., **2018**, 135, 46630)

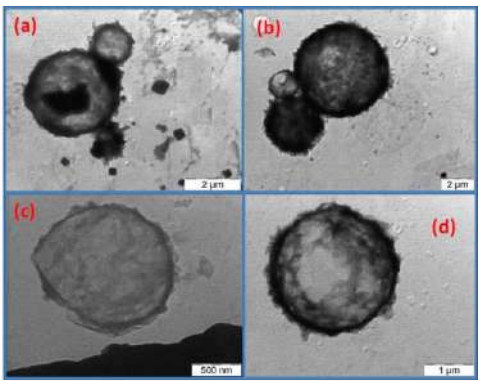


Fig. 12 TEM pictures of core–shell microspheres/ capsules

Catalytically Active Star Shaped Aniline Oligomer

Electrochemically active and star shaped aniline oligomer (SAO) has been prepared from N-phenyl-1,4-phenylenediamine and phloroglucinol in a simple synthetic route. The as prepared SAO is in its LEB state, this is the first time in the literature that an oligomer of this structure is used as support for Pt and Pt-Au nanoparticles for the methanol oxidation. Reduction of platinum for Pt/SAO and Pt-Au/SAO nanocatalysts has been achieved by formic acid. Extremely low amount of loading of catalyst (0.1 mg@3 mm GC electrode) is used. The bimetallic systems Pt-Au/SAO gave better current density

towards methanol oxidation than single metallic systems Pt/SAO (*Int. J. Hydrogen Energ*., **2019**, 44, 11066)

Naphthalenediimide appended L-glutamate (NDI-L-Glu) self-assembled into chiral supramolecular structures under physiological conditions and NDI-L-Glu shows a mixture of left- and right-handed helices under physiological conditions(fig.13). Any deviation from the ambient biochemical environment has a remarkable influence on the chirality of these structures. For instance, acidic environments shift the helicity to left-handedness while the alkaline conditions reversed the helical structures to right-handedness, thereby mimicking the molecular virulence mechanism of tobacco mosaic virus (TMV). The chirality of these supramolecular assemblies can also be controllably tuned by using temperature as an external stimulus, allowing reversible flip of helicity. (*Asian J. Org. Chem*., **2018**, 7, 2294)

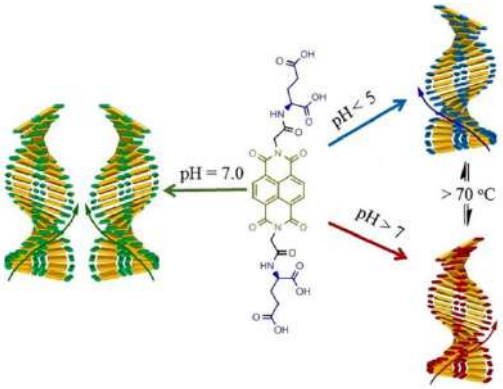


Fig.13 Self assembled napthalenediimide appended L glutamate

Naphthalenediimide-tetraphenylethylene conjugates with an alanine spacer (coded as: NDI-(Ala-TPE)$_2$) were synthesized to study the influence of the chirality of the amino acid spacer on its self-assemblies. NDI-Ala-TPE bearing L-alanine gives left-handed (M-type) helical superstructure, while D-alanine produces right-handed (P-type) helical ribbons in THF:H_2O at 40:60 % v/v ratio as shown in fig.14. However, particular aggregates were observed at 20:80 % v/v ratio. *(Chem- Asian J*, **2018**, 13, 3947)

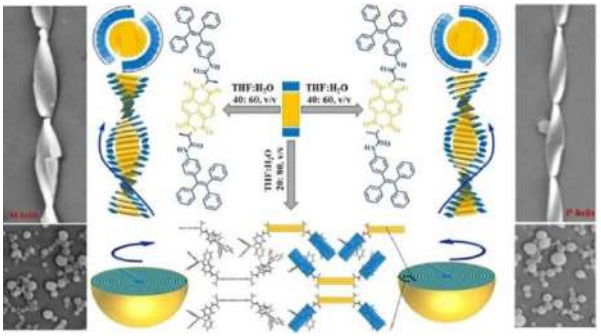


Fig. 14Naphthalenediimide-tetraphenylethylene conjugates with an alanine spacer

A naphthalene diimide (NDI) derivative bearing four carbamate groups (coded as: W2) was synthesised using a multistep strategy, and utilizing solvophobic effects, the self-assembly of this molecule was studied using solvent mixtures. Self-assembly led to a variety of controllable morphologies of supramolecular structures on both the micro and nanoscale. Nanobelts, nanospheres, nano-corals, microflowers and nanograss-like morphologies (fig.15) were obtained in DMF, MCH, $CHCl_3$, THF, water and MeOH solvent mixtures. The polarity of the solvent mixtures used directed the self-organisation of W2 by driving the π–π stacking interaction between NDI cores, and the H-bonding between the carbamate moieties. (*New J. Chem*., **2018**, 42, 6785)

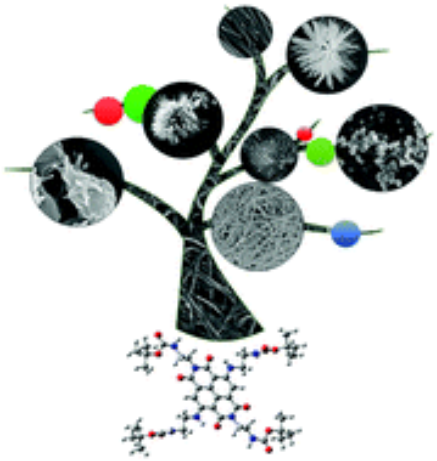


Fig.15 Controllable morphologies of supramolecular structures based on NDI carbamates

Two achiral naphthalene diimides (NDIs), in which phenyl moieties are linked to the NDI core via a urea subunit, leading to chiral supramolecular assemblies

in THF/methylcyclohexane were also synthesised. Circular dichroism spectroscopic analysis of twisted ribbons deposited from solutions indicated a mixture of left- and right-handed nanostructures for one NDI, whereas only left-handed structures were observed for the other one. Furthermore, this study also shows the effect of large atoms such as iodine on the self-assembly process, which governs and controls the helicity of the produced microstructures(fig.16). (*Chem-Asian J*, **2018**, 13, 3268)

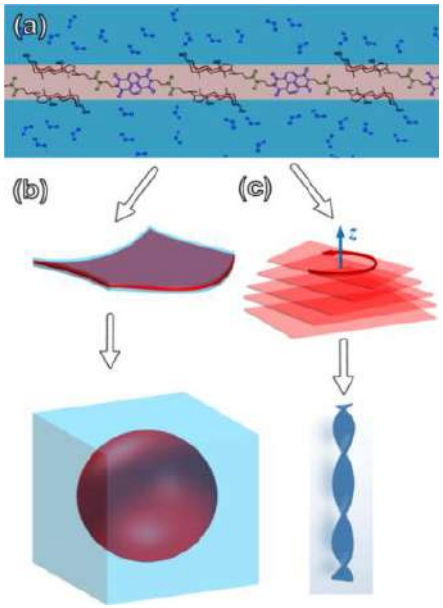


Fig.16 Iodine atom governing the self assembly and helicity of self assembled NDI moleceules

Self-assembled helical super-structure produced *via* facial stacking of a bile acid bolaamphiphile derivative with a naphthalene diimide core (NDI-DCA), driven by solvophobic effects in THF–H_2O solvent mixtures is reported. The chirality of the helical microstructure is directed by the multiple chiral centres in the precursor molecule. The chirality of the hierarchical assemblies was observed using circular dichroism (CD), Scanning electron microscopy (SEM) and transmission electron microscopy (TEM) measurements. We propose that the NDI-DCA super-structures(fig.17) are formed *via* similar interactions and mechanisms to those observed in biological molecules such as proteins and DNA. (*Sci. Rep.*, **2019**, *9*, 12825)

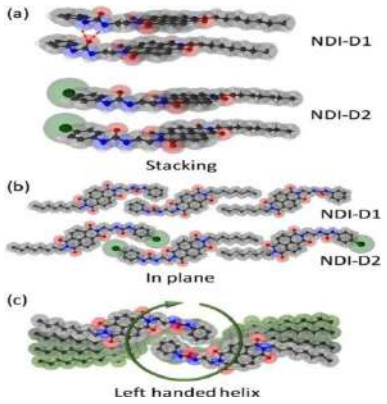


Fig.17 Stacking of bile acid derived bolaamphiphiles with NDI core

We also report the design and synthesis of a new naphthalimide-benzothiazole conjugate and its ability to sense various nitrophenols by means of its colorimetric and fluorescent characteristics. Under long-range UV light (365 nm), displayed a color change of its solution from bluish to colorless only upon addition of 2,4,6-trinitrophenol (TNP). Photoluminescence spectroscopy showed quantitative fluorescence quenching by TNP of the emission peaks at 398 nm and 418 nm due to donor–acceptor electron transfer. The interaction with TNP was via a cooperative, non-covalent hydrogen-bonding interaction(fig.18). Receptor exhibited high sensitivity and selectivity towards TNP over various aromatic nitro analytes. The binding constant (K) and Stern–Volmer constant (K_{sv}) between and TNP were found to be 5.332×10^{-5} M and 2.271×10^{6} M^{-1}, respectively. Furthermore, the limit of detection was calculated and found to be as low as 1.613×10^{-10} M. (*Chemosensors*, **2019**, *7*, 38)

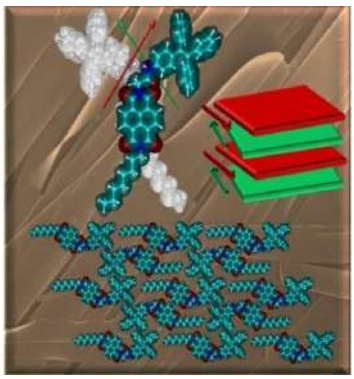


Fig.18 Interaction of naphthalimide-benzothiazole conjugate with TNP

Naphthalenediimide (NDI)-tetraphenylethene (TPE) conjugates with l-alanine (coded as: **1**) and d-alanine (coded as: **2**) exhibited self assembly. Mixtures of THF–water was used to fine tune the solvophobic effect leading to microbelt for both **1** and **2** in 40% *v/v* of THF in H_2O, while microbelt and particulate microsphere supramolecular structures were observed in 20%, *v/v* THF in H_2O. When 10% THF in H_2O was employed derivative **1** produces belt-like structures, however, **2** produces micro sphere. Less uniformly defined microstructure morphologies of **1** and **2** were formed in THF/hexane and DCM/hexane. DFT (density functional theory) and TD-DFT (time dependent density functional theory) molecular modelling(fig 19) support the hypothesis. (*Chemistry Select*, **2019**, 4, 2626)

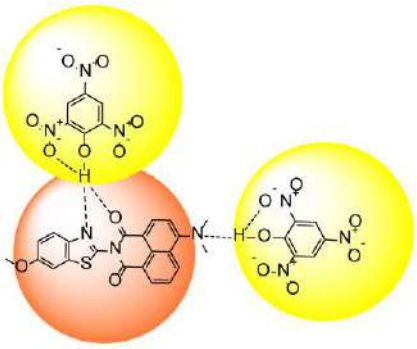


Fig.19 Naphthalenediimide (NDI)-tetraphenylethene (TPE) conjugates with l-alanine-molecular modelling

Spermine-Directed Supramolecular Self-Assembly of Water-Soluble AIE-Active Tetraphenylethylene

Tetrasulfonate-tetraphenylethylene (Su-TPE, fig.20) is non-emissive in water and upon addition of a good solvent such as THF (f_{THF} = 95%) it displays strong fluorescence emission with a quantum yield of 6.33%. In the presence of spermine, emission of Su-TPE produces higher quantum yields *i.e.* 1 : 48 molecular ratio gives 7.21%. Furthermore, interaction of spermine with Su-TPE is also shown to be pH dependent. Scanning electron microscopy (SEM) of Su-TPE molecule self-assemblies demonstrates that it produces various supramolecular structures at different Su-TPE : spermine molecular ratios. Nanobelts were obtained at 1 : 12, evolving into microsheets at 1 : 24, microglobular morphology at 1 : 36 and microtubes at 1 : 48 molecular ratios, respectively. Additionally, enhanced fluorescence emission was observed upon increasing the molar ratio of spermine with Su-TPE at pH 7. *New J. Chem.*, **2018**, 42, 15379)

Fig.20. Nanobelts, microsheets, globules and microtubes of self assembled Su-TPE

Merocyanine-Benzothiazole Chromophore-Based Sensor for Selective Picric Acid Detection

We report synthesis of (2E,4E)-2-(benzo[d] thiazol-2-yl)-4-(1,3,3-trim ethylindolin-2-ylidene) but-2-enenitrile (MC-BTH-1) chromophore and employed for picric acid sensing. MC-BTH-1 was prepared by Knoevenagel condensation of 2-(benzo [d]thiazol-2-yl) acetonitrile and (Z)-2-(1,3,3-trimethylindolin-2-ylidene) acetaldehyde in the presence of catalytic amount of piperidine in dry ethanol. The MC-BTH-1 conjugate displayed a remarkable sensing property towards picric acid in presence of interfering nitroaromatic compounds (fig.21). The sensing of nitroaromatic compounds was investigated by means of UV-vis absorption, fluorescence and ^{1}H NMR spectroscopic. Further more, colorimetric visualization of receptor MC-BTH-1 with the addition of various analytes under 365 nm UV light shows only color change from green to dark green for 2,4,6-trinitrophenol (TNP) and no significant color change was observed for other analytes. Under optimized condition the detection limit towards TNP and 2,4-dinitrophenol (DNP) are 1.58×10^{-9} M and 1.48×10^{-9} M, respectively. (*Chemistry Select*, **2019**, *9*, 10013)

Fig. 21 MC-BTH-1 conjugate displaying sensing property towards picric acid

Triphenylamine-Merocyanine-Based D1-A1-π-A2/A3-D2 Chromophore System: Synthesis, Optoelectronic, and Theoretical Studies. Donor–acceptor–π–acceptor–donor (D1-A1-π-A2/A3-D2)-type small molecules, such TPA-MC-2 and TPA-MC-3, were designed and synthesized starting from donor-substituted alkynes (TPA-MC-1) via [2 + 2] cycloaddition−retroelectrocyclization reaction with tetracyanoethylene (TCNE) and 7,7,8,8-tetracyano quinodimethane (TCNQ) units, respectively. TPA-MC-2 and TPA-MC-3 chromophores(fig22) differ on the A2/A3 acceptor subunit, which is 1,1,4,4-tetracyanobutadiene (TCBD) and a dicyanoquino dicyanomethane (DCQDCM), respectively. Both the derivative bearing same donors D1 (triphenylamine) and D2 (trimethylindolinm) and also same A1 (monocyano) as an acceptor, tetracyano with an aryl rings as the π-bridging moiety. The incorporation of TCNE and TCNQ as strong electron withdrawing units led to strong intramolecular charge-transfer (ICT) interactions, resulting in lower LUMO energy levels. (*Int. J. Mol. Sci*., **2019**, *20*, 1621)

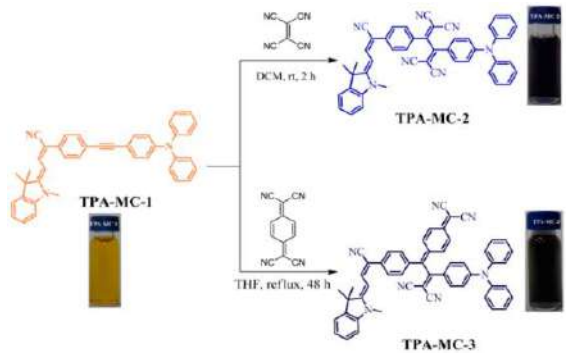


Fig. 22 Triphenylamine-Merocyanine-Based D1-A1-π-A2/A3-D2 Chromophores

Antenna-Like Ring Structures Via Self-Assembly of Octaphosphonatetetraphenylporphyrin with Nucleobases

Supramolecular self-assembly of an octaphosphona tetetraphenylporphyrin with three different nucleobases (adenine, cytosine, and thymine) was studied. Porphyrin with 8 and 10 equiv of cytosine produces light-harvesting ring-like structures, that is, architectures similar to those observed in natural light-harvesting antenna. However, porphyrin assembled with adenine or thymine resulted in prisms and microrods(shown in fig.23), respectively. UV–vis absorption, fluorescence, and dynamic light scattering were used to determine the mode of aggregation in solution. Scanning electron microscopy and X-ray diffraction spectroscopy used to visualize the self-assembled nanostructures and their behavior in the solid state, respectively. *(ACS Omega*, **2019**, 4, 11408)

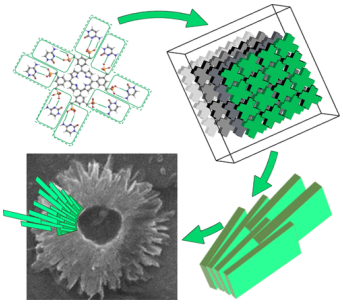


Fig. 23 Prisms and microrods octaphosphonatetetra phenylporphyrin

$Cu_2O@TiO_2$: A Nanocomposite Catalyst for Enhanced Visible Light Driven photocatalysis

The photocatalytic performance of Cu_2O, a p-type semiconducting oxide with a band gap in the visible region of the solar spectrum is improved by the presence of TiO_2 on its surface. It is observed that the photocatalytic activity is dependent on density of heterojunctions formed in the photo-system which the nano-crystalline TiO_2 , has very effectively created on the Cu_2O surface, which are responsible for the improved photocatalytic response. This work establishes that the in-situ creation of $Cu_2O@TiO_2$ (Fig. 24) is effective in creating p-n heterojunctions at the $Cu_2O@TiO_2$ interface, which result in arresting

the recombination processes, leading to improved photocatalytic performance. (*Chemistry Select*, **2019**, 4, 2249)

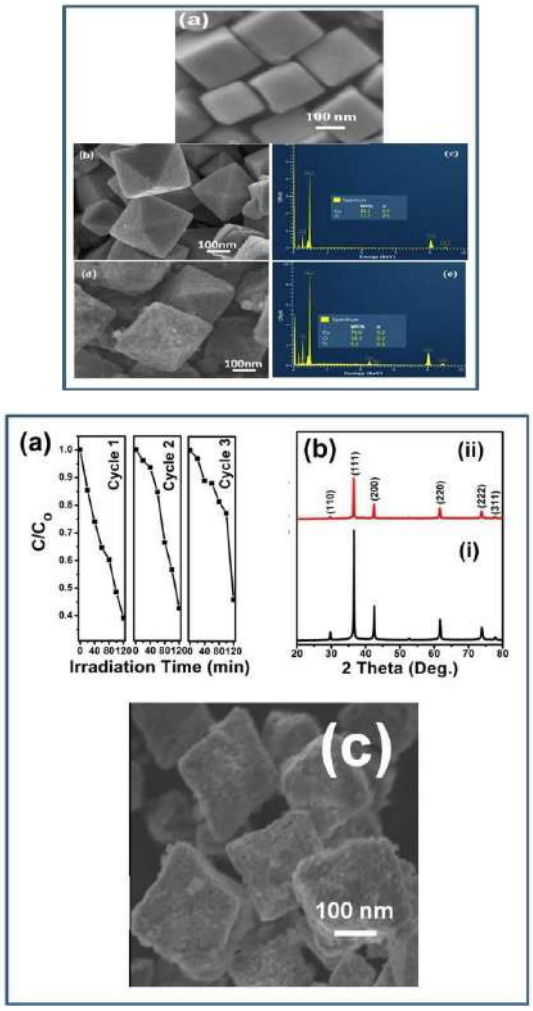


Fig. 24 $Cu_2O@TiO_2$ nanocrystals showing photocatalytic activity

Environment

Development of Eco-Friendly, Cost-Effective Adsorbents for the Selective Capture of Air-Pollutants by Employing Computational Screening and Molecular Engineering Approaches

The findings of studies carried out in the group has provided fundamental insights into the nature and relevance of various interactions at different molecular dimensions and time scales by using various computational methodologies.[1-4] Developed novel adsorbents based on metal oxides for the CO_2 capture from industrial flue gases.[1] These materials are based on non-volatile amino acids and alkanol amines that are chemically grafted on TiO_2 surface. The study explores the possibility of using f-TiO_2 surface as a potential solid adsorbent to capture CO_2 at much reduced cost. Recently an integrated Quantum Mechanical (QM) and Artificial Intelligence (AI) approach that bypasses the need for high throughput screening, narrows down the range of candidates has been widely implemented in the group. For example, in design and development of heterogeneous dual functional materials with combined catalytic activity and CO_2 sorption ability, shown schematically in Figure 25. (*J. Phys. Chem. C*, **2019**, 123, 3491; *J. Mol. Mod.*, **2018**, 24 (12), 341)

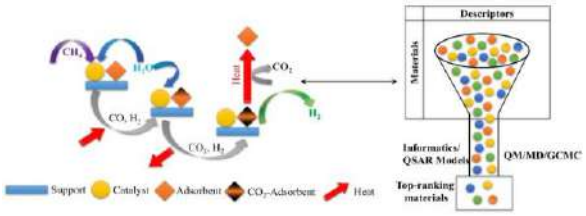


Fig. 25 Heterogeneous dual functional materials with combined catalytic activity and CO_2 sorption ability

Porous Composites with Improved Visible Light Photocatalytic Degradation of Organic Dyes

A highly porous architecture of graphitic carbon nitride g-C_3N_4/Cu_2O nanocomposite in the form of cubes with a side length of ≈1 μm, large pores of 1.5 nm, and a high surface area of 9.12 m^2/g was realized by an optimized in situ synthesis protocol. Detailed structural and morphological evaluations by powder X-ray diffraction and field emission scanning electron microscopy revealed the presence of highly exfoliated g-C_3N_4, which is responsible for the formation of the porous architecture in the cube like assembly of the composite. The micrographs (fig.26) clearly reveal the porous structure of the composite that retains the cubic shape of Cu_2O, and the energy-dispersive spectroscopy supports the presence of g-C_3N_4 within the cubic morphology.

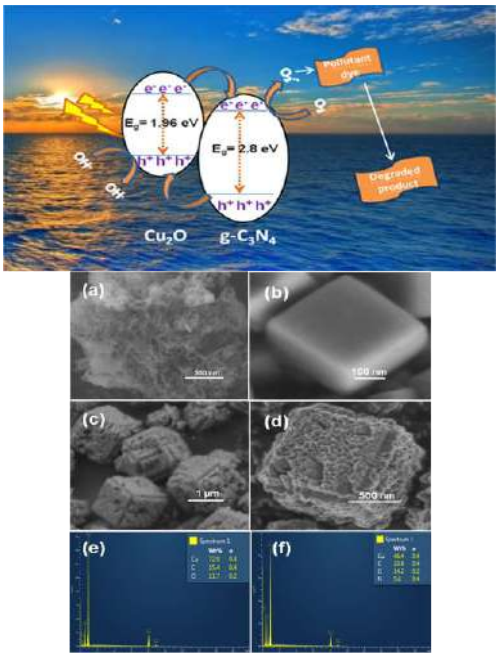


Fig. 26 Porous graphitic carbon nitride g-C_3N_4/Cu_2O nanocomposite

The improved photocatalytic performance of the composite could be attributed to the highly porous morphology along with the suitable optical band gap in the visible region of the solar spectrum. The optimized composite, CN/Cu-5, demonstrates a visible light degradation of 81% for Methylene Blue (MB) and 85.3% for Rhodamine-B (RhB) in 120 min. The decrease in the catalyst performance even after three repeated cycles is less than 5% for both MB and RhB dyes. The rate constant for MB and RhB degradation is six and eight times higher with CN/Cu-5 when compared with the pure Cu_2O catalyst. To validate our claim that the dye degradation is not merely decolorization, liquid chromatography−mass spectroscopy studies were carried out, and the end products of the degraded dyes were identified. (*ACS Omega*, **2019**, 4, 17301)

Novel, Eco-Friendly, Cost-Effective n-MO_3/p-NiO Nanocomposite for Selective Detection of CO_2 Gas

In our study, noble metal (Pd) incorporated n-MO_3/p-NiO was synthesized, characterized and gas sensing application was carried out toward CO_2 gas and prototype of the sensor (shown in fig.27) developed.

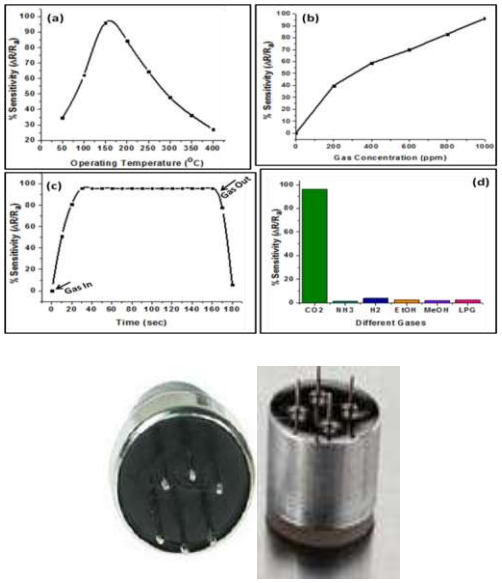


Fig. 27 Sensor response of MoO_3: NiO: Pd nanocomposite Fabricated prototypes Sensitivity as a function of (a) Operating temperature developed for CO_2 gas Sensor(b) Gas concentrations, (c) Response and Recovery Times (d) Different gases

MoO_3: NiO:Pd (0.1%Pd) nanocomposite exhibits higher sensitivity of S=96.16% at a lower operating temperature of 150°C towards CO_2 gas. There is increase in sensor response(fig 32) with increase in gas concentration and reaches a maximum at 1000ppm. It is also seen that the sensor is sensitive to low concentration of 200ppm CO_2 gas with response (T_r) and recovery (T_d) time of 30s & 20s and Selective to CO_2 gas compared to other interfering gases. (*J. Adv. Phys.*, **2018**, 7, 70; *J. Nanomat. Mol. Nanotech.*, **2018**, 6(7), 264; *Int. J. New Technol. Sci. Engg.*, **2018**, 43; *Mat. Res. Express*, **2019**, 6, (12), 125041:1)

Eco Friendly Castor Oil Derivatives *Organogels*

Bio-based N-(2-hydroxyethyl) ricinoleic amide (NHRA) a derivative of castor oil, exhibited thermoreversible gelation in specific tested organic solvents such as aniline and 1,4 dioxane. The synthesized organogel acts as a host for anions that change the physical state from gel to sol by disruption of intermolecular hydrogen-bonding

interactions as shown in figure 28. The propensity of the material to exhibit anion-responsive behavior is attributed to the presence of amide linkages, under which deprotonation of N–H fragments occur upon the addition of anions, as confirmed by ^{19}F NMR and FT-IR spectroscopy. These results indicate that NHRA gelator can be prospective candidate for sensing applications. (*Colloid polym. sci.*, **2019**, 297(11), 1411)

Fig. 28 Biobased organogel exhibiting anion tuning property

Co-Plasticizer in PVC Processing

An acidic cation exchange resin has been used to prepare epoxidised castor oil (ECO, fig. 29) having a high oxirane oxygen content which was used as a co-plasticizer with epoxidised soyabean oil (ESBO) for processing polyvinyl chloride (PVC). PVC/ (ESBO&ECO) blends were prepared by melt mixing and compression molded into sheets. The specimens were evaluated for tensile properties, impact strength and hardness. While the tensile strength did not vary much, the elongation reduced with the replacement of ESBO with ECO. Dynamic mechanical studies revealed that the glass transition temperature increased with incorporation of ECO. Replacing 20% of ESBO with ECO resulted in blends with desired thermal and mechanical properties without affecting the processability of PVC. (*J. Renew Mater.*, **2019**, 7(8),775)

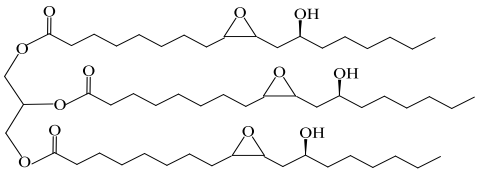


Fig. 29 Structure of epoxidised castor oil

Health Care

First High Affinity Neutral Fluorophores for Mitochondrial Tracking

The current report illustrates the development of neutral BODIPY-based non-toxic, stable, and highly efficient fluorophore (fig.30) which has exclusive affinity towards mitochondria. To the best of our knowledge, this is the first high affinity neutral fluorophore for mitochondrial tracking.

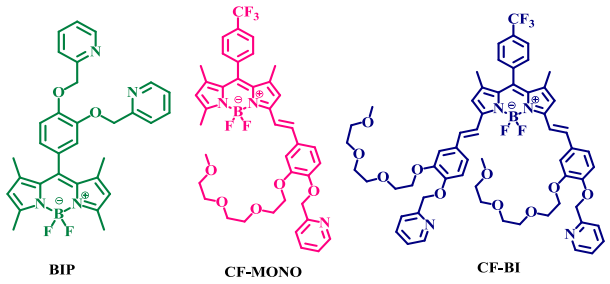


Fig.30. BODIPY based fluorophore

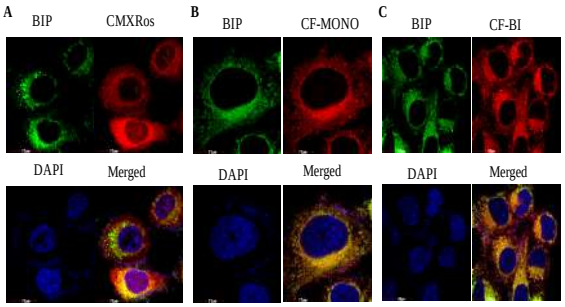


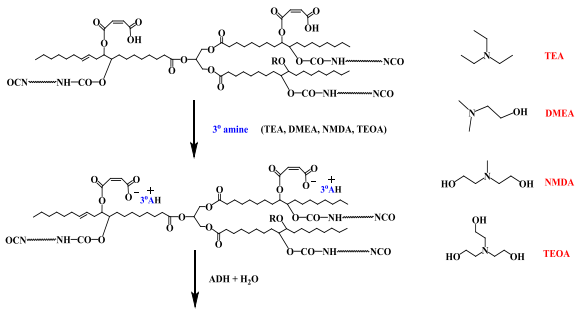
Fig. 31 Mitochondrial staining by BODIPY dyes in HeLa cells

A) Green fluorescence indicates mitochondrial staining of BIP compound by confocal microscopy using FITC filter. Red fluorescence indicates mitochondrial staining of mitotracker red CMXRos (Invitrogen) by confocal microscopy by using rhodamine filter. Blue fluorescence indicates nuclear staining by DAPI. B) Same as A, except that red fluorescence indicates mitochondrial staining of CF-MONO compound by confocal microscopy by using rhodamine filter. C) Same as *A*, except that red fluorescence indicates mitochondrial staining of CF-BI compound by confocal microscopy by using rhodamine filter (refer fig.31). (*ACS Med. Chem. Lett.*, **2018**, 9, 618)

Coatings

Anionic Waterborne Polyurethane Dispersions from Cottonseed Oil Based Polyol - Effect of Counterion

A series of maleated cottonseed oil polyol (MAHCSO) based, DMPA (dimethylol propionic acid) free, catalyst free waterborne polyurethane dispersions (PUDs) were synthesized. Four different tertiary amines (figure 32), were employed as neutralizing agents to investigate the role of countercation on the physico-chemical properties of PUDs and their corresponding cured films. It was found that the waterborne PUD with countercation having more number of hydroxy alkyl chains exhibit larger particle size, a less negative zeta potential, higher viscosity and lower storage stability, where as the corresponding cured film possesses lower thermal stability, mechanical strength and poor surface properties. (*J. Polym. Res*. **2018**, 25, 186)

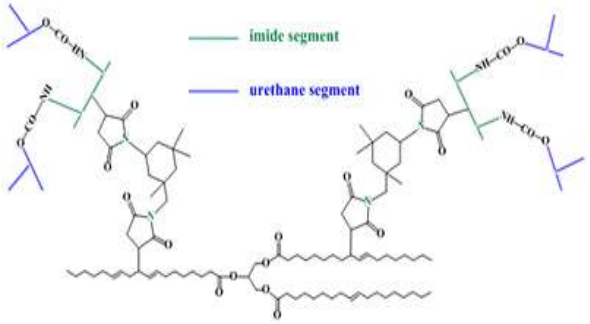


Waterborne polyurethane dispersion

Fig. 32 Anionic polyurethane dispersion

Bioased Polyurethane-Imides from Maleinized Cottonseed Oil and Castor Oil

Cotton seed oil was functionalized with maleic anhydride by 'ene' reaction to give maleinized cottonseed oil, the anhydride groups were reacted with isocyanates to yield –NCO terminated polyurethane prepolymer. The prepolymer was further chain extended with hydroxyl groups of castor oil to give polyurethane-imides as shown in figure 33. The crosslinked films thus obtained had good mechanical properties and the imide groups in the backbone improved the corrosion resistance of PUIs as revealed by potentiodynamic polarization study. With increasing content of MACSO, thermal stability, glass transition temperatures (Tg), tensile strength and corrosion resistance of resulting PUIs significantly increased. (*Polym. Adv. Technol.*, **2019**, 30(11), 2742)



Polyurethane-imide

Fig. 33 Structure of PUI derived from cotton seed and castor oil

APPLIED RESEARCH

Laboratory Process for Polychlorotrifluoro ethylene (PCTFE)

PCTFE is a fluorine rich engineering thermoplastic with outstanding physical and mechanical properties. Its non flammability, chemical resistance, near zero moisture absorption and excellent electrical properties make it a unique polymer, even within fluoropolymer family. Its ability to function in the temperature range of -240^{0}C to 200^{0}C makes it a specialty polymer. It is widely used in protection of sensitive electronic equipment, pharmaceutical blister packaging, chemical tank liners, O-rings, seals, gaskets etc.

A project was undertaken to develop an economically viable, laboratory scale process for synthesis of a high performance grade PCTFE. Polymerization of CTFE was systematically investigated using generic emulsion and suspension polymerization procedures and a highly reproducible process that provided a polymer that matched the bench mark in thermo-mechanical properties was developed in more than 75% conversion. This Process know how was transferred successfully to client.

PROCESS ENGINEERING & TECHNOLOGY TRANSFER

BASIC RESEARCH

Thermodynamic Properties Estimation for Important Industrial Streams:

Measurement and Modelingfor Para-Methoxyphenylacetic Acid Solubility in Mixed Solvents

The solubility of para-methoxyphenylacetic acid in different solvents is of critical significance for the design and optimization of its purification process via crystallization. The present study illustrates new solid–liquid phase equilibrium data of para-methoxy phenyl acetic acid in water, acetonitrile, propan-2-ol, morpholine, toluene, anisole, and binary (propan-2-ol + water, propan-2-ol + toluene) mixed solvents using a static analytical method from 283.15 to 323.15 K at atmospheric pressure. The highest solubility of para-methoxyphenylacetic acid was observed in propan-2-ol and lowest in water, with the maximum solubility effect for propan-2-ol + toluene binary system obtained at 0.5001 solute-free mole fraction of propan-2-ol. The modified Apelblat equation, λh (Buchowski) equation, and non-random two-liquid (NRTL) activity coefficient model were used to correlate the experimental solubility data in pure solvents, whereas the binary solvent systems were modeled using the van't Hoff–Jouyban–Acree, Apelblat–Jouyban–Acree, and NRTL models, among which the NRTL model exhibited better goodness of fit. Also, for insight into the molecular interactions in the solvent systems, the enthalpy of dissolution has been being evaluated.

Measurement and Correlation of Phase Equilibria and Thermo-Physical Properties of 4-Tert-Butylbenzaldehyde

This study reports the vapor pressure data and thermophysical properties of 4-*tert*-butylbenzaldehyde, a fine chemical that is widely used in the manufacturing of fragrances and agricultural chemicals. The saturated vapor pressure was measured at isobaric condition 1.48–33 kPa using a modified Swietoslawski-type ebulliometer and the data was correlated with Antoine and Clark-Glew equation where Antonie equation exhibited less deviation as compared to the Clark-Glew equation. Moreover, the critical properties were estimated based on Joback, Constantinou and Gani and Y. Nannoolal et al. methods. The boiling points computed using Constantinou and Gani method were in close approximation to the Antonie and Clark-Glew equations. The normal boiling point of 4-*tert*-butylbenzaldehyde was 523.9 K with an acentric factor of 0.4. The thermophysical properties i.e., refractive index, density, viscosity and surface tension of 4-*tert*-butylbenzaldehyde were measured at different temperatures 293.15–328.15 K. The density data was correlated with the Rackett equation with group contribution critical parameters. Amidst these contribution methods, Joback was found to exhibit the least relative average deviation (RAD) of 1.29. Further, the viscosity and surface tension were measured using Mansingh Survismeter and viscosity was fitted to the Vogel–Tamman–Fulcher equation with a RAD = 1.05, respectively. The surface tension data was predicated using Brock and Bird method with different group contribution critical parameters. Among the investigated models, Nanoolal method-based parameters showed the least RAD. Additionally, the Friccohesity parameter, which deals with frictional and cohesive forces was estimated from the experimental surface tension data. It can be concluded from the present study that none of the prediction methods (group contribution) was able to correctly predict the thermophysical properties of 4-*tert*-butyl benzaldehyde, hence necessitates the findings of the experimental data.

Measurement and Modeling of Solid–Liquid Equilibria of l-Glutamic Acid in Binary Mixtures

The experimental solubility data of l-glutamic acid in pure water, formic acid, methanol, 1-propanol, 2-propanol, acetonitrile, and binary mixtures (formic acid + water, methanol + water, 2-propanol + water, acetonitrile + water) with different compositions were carried out at temperatures ranging from

(283.15 to 328.15) K by the static analytic method. The solubility measurements showed that formic acid and its aqueous mixtures recorded a higher solubility than methanol + water, 2-propanol + water, and acetonitrile + water for the same composition at each temperature. Moreover, except formic acid the addition of methanol, 2-propanol, and acetonitrile to its aqueous mixtures resulted in the decrease in solubility of l-glutamic acid. The experimental data was fitted using different thermodynamic models such as the Buchowski–Ksiazczak equation, the Van't Hoff equation, the modified Apelblat equation, and the NRTL model, and the optimum values of the regressed parameters were obtained.The modified Apelblat equation, Buchowski–Ksiazczak equation, and NRTL activity coefficient model were fitted to the pure solvents solubility data, while the modified Apelblat, modified Apelblat–Jouyban–Acree, and NRTL models were used for the binary solvent systems. The results demonstrated formic acid as a cosolvent in the dissolution of l-glutamic acid in formic acid + water binary mixtures, while others exhibited an antisolvent effect on the solubilization of l-glutamic acid in their respective aqueous mixtures.

Thermo-Chemical Conversion and Value-Added Products:

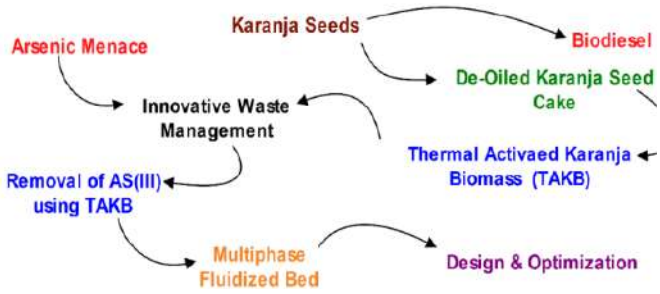
A Non-Edible Waste as A Potential Sorptive Media for Removal of Herbicide from the Watershed

A non-edible waste, from biodiesel processing industry is being turned to carbonaceous material (biochar) using slow pyrolysis. The material was found to be amorphous with hydroxyl, methyl, carbonyl and carboxyl functional groups onto the surface. The influencing parameters, namely adsorbate concentration (0.05-5 mg/l), biochar loading (0.02-0.4 g), pH(3–12) and particle sizes (0.03-0.13 mm) were studied to observe the effect on the sorption of simazine using biochar. A multivariate optimization using central composite design in response surface methodology was performed employing desirability function. The optimized biosorption efficiency (B%) and capacity qe was found to be 91.98 % and 0.83 mg/g respectively with the optimized parameters as 3.76 mg/l of adsorbate concentration, 0.12 g of biochar loading, pH of 5.26 and 0.0535 mm of particle size. The simazine adsorption phenomena were found to be multilayer heterogeneous sorption based on Langmuir and Freundlich models. The kinetics investigation shows that chemisorption was involved for the transfer of simazaine to the surface of biochar with three distinct intra particulate diffusional zones. An adsorption process requires activation energy of 11.27 kJ/mol and the negative magnitude of ΔH^* indicates the exothermicity involved in the process.

Application of an Agro-Industrial Waste for the Removal of As(III) in a Counter-Current Fluidized Bed

Arsenic pollution in groundwater has been identified as a major hazard in developing countries. In this purview, Karanja or Pongamia pinnata seed cake, a biodiesel residue has been proposed to being utilized to curb the arsenic menace using an agro-industrial waste. The study investigates the biosorption of As(III) onto thermally activated de-oiled karanja seed cake (TAKB) with a surface area of 19.8 m^2/g in a counter-current multiphase fluidized bed column. Experiments were designed with the aid of a full factorial central composite design to study the effect of fivedifferent process variables on the percentage adsorption of As(III). The maximum uptake capacity of the biosorbent was obtained to be 0.226 mg/g which was comparable to other reported biosorbents. Multiple regression analysis was used to derive a quadratic polynomial that developed a correlation between the independent process parameters and the percentage removal of As(III) together the analysis of variance. The optimum parameters for maximum percentage removal of As (III) were determined to be

an initial As (III) concentration of 0.378 mg/L, gas and liquid flow rates of 0.224 and 0.074 L/min, respectively, static bed height of 0.069 m and the average particle size of the biosorbent as 1.73 mm. Isotherm studies based on Langmuir and Freundlich models were also conducted in order to estimate the maximum sorption capacity of TAKB. A confirmatory test with groundwater at optimum conditions for real-time application was performed, and 93.17% As (III) removal was attained.



Overall strategy for the sorption of Arsenic from waste streams

Translation of Lignocellulosic Waste to Mesoporous Solid Acid Catalyst and its Efficacy in Esterification of Volatile Fatty Acid

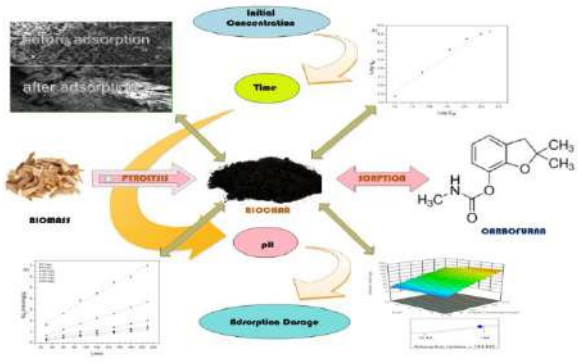
The growing environmental concern seeks global attention to minimize the contamination, especially for the disposal of solid wastes. In this preview, a lignocellulosic waste, de-oiled Pongamia pinnata seed cake is converted to a carbonaceous solid by incomplete carbon ization and subsequent sulfonation to obtain a mesoporous solid acid catalyst. The physico-chemical properties, surface morphology and molecular structure of the different stages involved in the preparation of the solid acid catalyst was carried out through Elemental analysis, Fourier Transform Infrared Spectroscopy, Scanning Electron Microscopy, X-Ray Diffraction, Brunauer-Emmett-Teller (BET) surface area and Thermogravimetric analysis. The characterization results validate the induced catalytic property in the carbonaceous solid with pore diameter of 3.96 nm. The appropriate testification of the catalyst performance was conducted through esterification of lactic acid with n-butanol. In the experimental design based on Taguchi optimization the process parameters catalyst loading, feed molar ratio and temperature effects were investigated. The optimized results suggested a 7 wt % catalyst loading, 1:1.5 molar ratio of acid to alcohol and temperature of 115 °C for the effective conversion of volatile fatty acid. The efficacy of lignocellulosic waste catalyst was compared with other commercial catalysts; sulphuric acid, methane sulfonic acid and Amberlyst-15. Thereby, the study provides an insightful knowledge on the resourceful transformation of a non-edible solid waste precursor to an industrially applicable solid acid catalyst.

Applicability of an Agro-Industrial Waste to Engineered Biochar for Fluoride Sorption

A potential feedstock, de-oiled *Pongamia-pinnata* seed cake is used to prepare engineered Biochar (EBC) for the removal of fluoride from ground water. EBC was characterized and batch biosorption studies were conducted at different initial fluoride concentrations, EBC dosages and pH values. A maximum fluoride adsorption occurred at pH-7 with an equilibrium time of 90 min and EBC dosage of 10 mg/L. Different isotherm models were investigated, among which Langmuir was found to best fit with a maximum adsorption capacity of 0.985 ± 0.025 mg/g. The chemisorption was defined by Ritchie-pseudo-second-order kinetics with intra-particle diffusion contributing to the rate determining step. Column studies with variable operating conditions (initial fluoride concentration, bed depth, flow rate) and modeling of the break through curves showed modified dose response model in excellent agreement with a maximum uptake of 1.12 ± 0.025 mg/g. EBC regeneration, comparison with contemporary sorbents and its real time application are also explored in the present study.

Torrefied and Unmodified Capsicum Annuum Biochar for the Removal of Synthetic Hazardous Pesticide (Carbofuran) from Watershed

The present study explored the applicability of torrefied and unmodified Capsicum Annuam biochar (CABC) for the removal of carbofuran from its aqueous streams. The developed biochar at low temperature pyrolysis (300°C) attained a surface area and pore volume of 32.07 m^2/g and 0.064 cm^3, respectively. The biochar was characterized for its physico-chemical transformation. It was observed that aromatic and hydroxyl groups present in the CABC were responsible for the sorption of carbofuran. The efficacy of carbofuran removal was examined by varying the process variables such as carbofuran concentration, sorption time, pH and adsorbent dosage. The investigation on isothermal models suggested a monolayer adsorption of carbofuran onto homogeneous surface of CABC. While the sorption kinetics is chemical rate controlling mechanism with abundant sorption sites available on the surface and the initial concentration of carbofuran is low compared to the sorption capacities of the CABC. The mass transfer mechanism was studied. The optimization of parameters with central composite design in response surface method-ology showed an optimum adsorption uptake value obtained is 134.84 ⁄ with a desirability value 0.98 with initial concentration as the most influencing parameter.



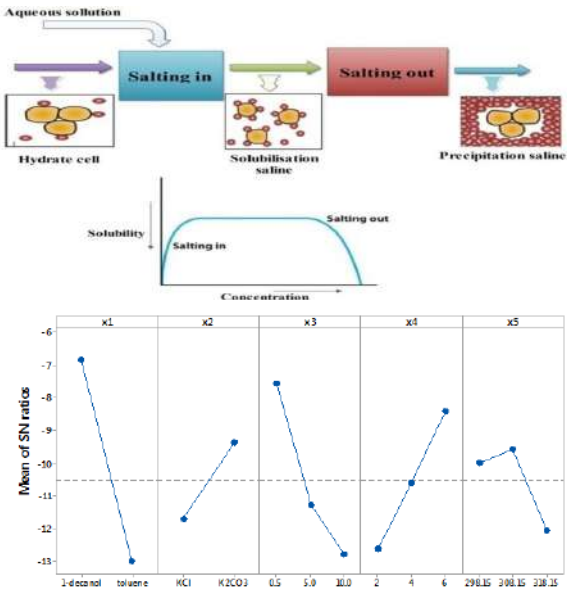
Pictorial Representation of Carbofuran Removal Using Chilli Stalk Biochar

Process Design, Modeling, Intensification, Simulation and Optimization:

Salting-Out Assisted Liquid-Liquid Extraction (SALLE) for the Separation of Morpholine from Aqueous Stream

In the present study, enhanced liquid-liquid extraction i.e., salting-out assisted liquid-liquid extraction (SALLE) was explored for the separation of morpholine from the aqueous stream. The salting out capacities of two kosmotropes K_2CO_3 and KCl with solvents (1-decanol and toluene) was investigated within its solubility limit. A Taguchi optimization technique was investigated to obtain the optimum combination of parameters employing a mixed array design (23×22). The results demonstrated that the salting-out effect of K_2CO_3 in combination with 1-decanol was more pronounced than KCl and thereby the tie-line data was generated for this quaternary system comprising water + morpholine + K_2CO_3 + 1-decanol at various temperatures (293.15–313.15 K). As the CO_3^{2-} anion shows the more negative value of Gibb's free energy of hydration, ΔGhyd than Cl− revealed the better salting-out ability of CO_3^{2-} ion. In other terms, the B-coefficients of the constituent anions (CO_3^{2-} and Cl^-) have been discussed further, which is related to the salt kosmotropicity, revealed the interactions between water molecules and electrolyte ions and their effect on the water lattice around the solute particles. Also, the critical concentration of K_2CO_3 required to form two phases is reduced with a rise in temperature. Further, the process parameters influencing the extraction efficiency, such as tie-line length, (TLL) of the quaternary system was also evaluated and data fitted to the Eisen-Joffe model to perform the consistency test in respect of the overall concentration of salt to water in each phase. The Eisen-Joffe salt parameter, Ks which signifies the reliability of the tie-line data, was obtained in the range of 1.71–5.93 and the tie-line data was also accurately predicted by the NRTL activity coefficient model. The applicability of the SALLE was finally

investigated in the continuous counter-current extraction column indicating the SALLE to show good performance on the separation efficiency of morpholine.



Salting Out Mechanism of Morpholine and the Parameters Effect on the Extraction of Morpholine

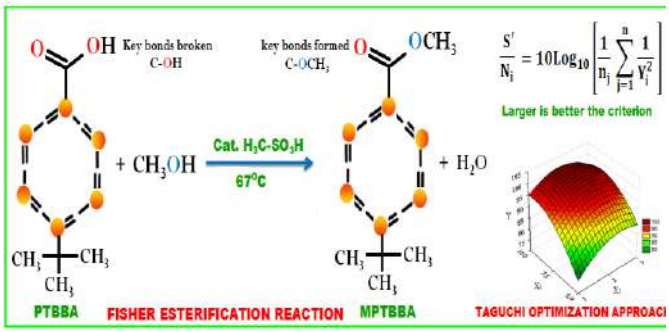
Economic and Environmental Impact Assessment of Extractive Distillation for Reprocessing Aq. 2-Propanol

Recently, in manufacturing industries innovative green and smart designs are being proposed that considers the minimal and efficient usage of resources including materials, energy, and effort which are environmentally safe. Accordingly, an enhanced purification methodology, extractive distillation (ED) has been investigated for the reprocessing of 2-Propanol (IPA) with three renewable entrainers viz. conventional solvent: **glycerol**, saline entrainer: glycerol + $MgCl_2$ and deep eutectic solvent (DES): choline chloride-glycerol based on the exponential surge in the production of glycerol over the past decade. The systematic assessment of the three processes includes investigating the experimental feasibility observed through phase equilibrium studies, thermodynamic modeling followed by process design and optimization. A sequential strategy defining desired objectives has been used for the parametric optimization with the key performance indicators including Total Annual Cost (TAC), Specific Energy Consumption (SEC), entrainer quantity and CO_2 emissions to comprehend the overall efficiency of each process. The results revealed that the saline entrainer based ED process as most reliable with substantial reduction of 32.5% and 21.4% in TAC together with 33.9% and 24.1% decline in the SEC and 34.2% and 24.4% lower CO_2 emissions compared to the conventional and DES based processes respectively.

Parametric Optimization and Rate Laws Determination for the Conversion of 4-Tert-Butylbenzoic Acid to Methyl 4-Tert-Butylbenzoate

The esterification of *4-tert*-butylbenzoic acid has been studied to produce methyl *4-tert*-butylbenzoate, having its widespread applications in the pharmaceuticals, perfumes, flavour, cosmetics, and fragrance industries. The limiting nature of the reaction is catalyzed with methane sulphonic acid, a green catalyst. The study focused on optimization of the experimental parameters to achieve higher conversion of acid with the aid of statistical analysis based on the Taguchi technique. An L_9 array, S/N ratios, and ANOVA have been used with catalyst concentration, molar ratio, and time as the process parameters with acid conversion as the response variable. Parametric optimization based on Taguchi method suggest a combination of optimal parameters as 10% catalyst concentration, 5:1 methanol to acid molar ratio and 2 h at a refluxing temperature of 67°C. A kinetic investigation for the esterification is also conducted to define the rate equations that govern the overall progress of reaction and the results established that the reaction follows irreversible pseudo second order rate in the initial phase followed by the reversible second order rate. The proposed

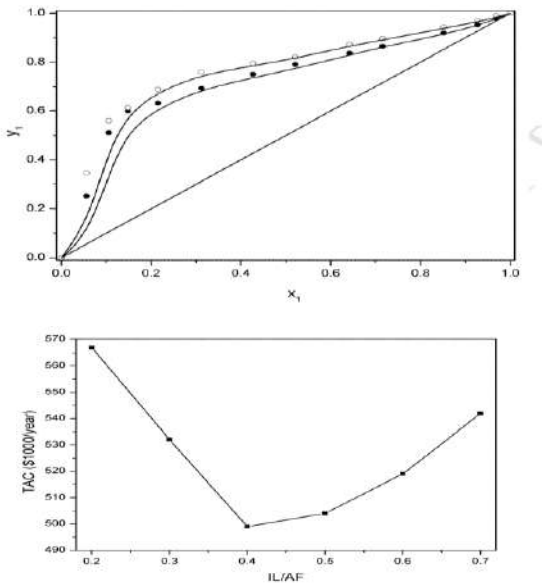
model is found to be in good agreement with the experimental results.



Reaction Scheme for Esterification of PTBBA

A Techno-Economic Assessment, Design and Operation of Extractive Distillation Systems

The 21st century beholds interest in biofuels, leading to a key challenge being the production of fuel grade '*tert* butyl alcohol' (TBA) with reduced economics. As a consequent step in the investigation with a different class of entrainer for TBA dehydration through extractive distillation (ED), the present study explores the utilization of ionic liquid [emim][Cl] and inorganic salt [$MgCl_2$] as a potent entrainer. A comprehensive approach is proposed with phase-equilibrium measurements, thermodynamic modeling, design and process optimization. A techno-economic assessment of all the investigated processes (conventional solvents: CSED, solvent + salt: SEED, designer solvents or ionic liquids: DEED and ionic liquid + salt: DSEED) concluded SEED process to be the most promising with 6%, 18% and 37% savings in TAC and 9%, 23% and 41% savings in SEC as compared to the DSEED, DEED and CSED processes respectively. Further, retrofits (heat integration and thermally coupled schemes) demonstrated 13% and 6% reduction in specific energy consumption respectively thus improving the energy efficiency of ED systems. Heat integration brought in 12% savings in TAC over SEED process. However, thermally coupled schemes resulted in marginal benefit (2% savings) in terms of TAC over SEED process.

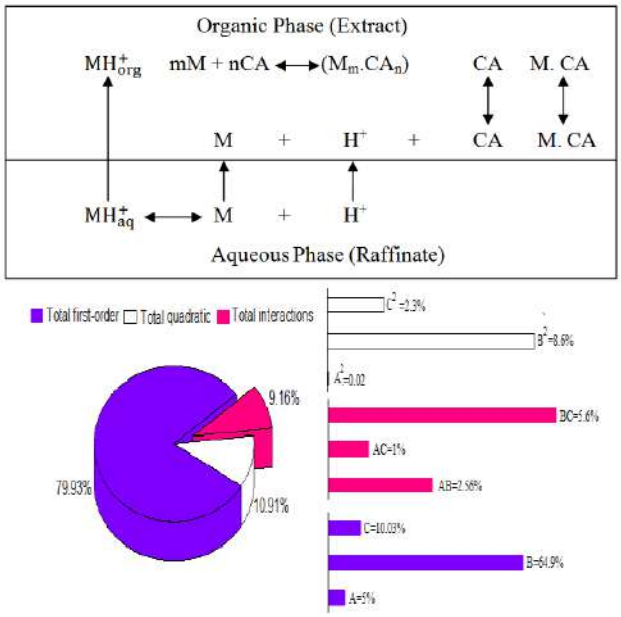


Exp data of (●) TBA (1) + water (2) + [emim][Cl] (3) and experimental quaternary (○) TBA (1) + water (2) + [emim][Cl] (3) + $MgCl_2$ (4) for IL/AF = 0.2 and TAC results based on optimization strategy.

Equilibrium and Kinetics of Morpholine Extraction from Aqueous Stream with CA in Toluene

The present study explores the equilibrium and kinetics for the reactive extraction of morpholine, an important industrial reagent from its aqueous stream using capric acid, CA (extractant) in toluene (diluent). An equilibrium model that employs the mass action law was also developed to evaluate the optimum apparent equilibrium constants (K_E), stoichiometric ratio (m) and physical constant (S). Equilibrium model was valid in representing the mechanism of morpholine extraction. Moreover, for the first time the study availed the simultaneous optimization of two significant response characteristics: extraction efficiency (%E) and loading ratio (Z) using Box–Behnken design (3^3) employing multivariate desirability function. The statistical models predicted %E of 80.2 and Z of 0.64 for the optimum combination of process parameters as follows: C_{MO} = 5%, C_{CAO} = 5% and T = 303.15 K with the desirability of 0.947. Further, the intrinsic

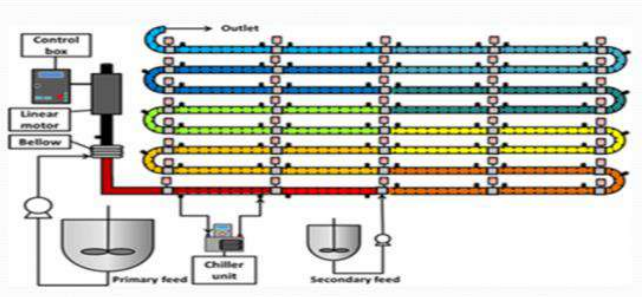
kinetics of the extraction model demonstrated that the reactions between morpholine and CA fall in regime 3 (fast chemical reaction in diffusion film), follows first order kinetics with respect to morpholine and displays exothermicity of the process as revealed from thermodynamic studies. The equilibrium and kinetic data are useful for the development, design and reliable scale-up of the extraction process.



Mechanism of reactive extraction of morpholine with capric acid and Schematic representation of % contribution to loading ratio, z.

Process Intensification: Design of Modular Reactors – Integration of Oscillatory Baffled / Flow Reactors with Fluidic Oscillators

Oscillatory Flow Reactors offer near plug flow pattern even in laminar flow rate which is stillunachievable in the case of conventional tubular reactors. These reactors have been gaining popularityin continuous synthesis of products. Fluidic Oscillator is a device which will produce self-sustaining periodic oscillatory flow at its outlet without any moving parts based on intrinsic flow instabilitymechanism. Current research activity focuses on the design and development of integrated FluidicOscillator with Oscillatory Flow / Baffled reactor, based on Computational Fluid Dynamics and rigorousexperimentation (One project titled "Intensified Continuous Crystallizer for APIs: Design and Development"sanctioned (**2019**) by SERB under SRG scheme.



Oscillatory Flow Reactor

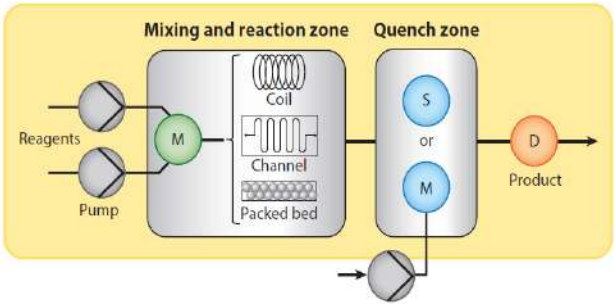
Flow Processes including Downstream Processes for Integrated Continuous Manufacturing

Continuous flow micro reactor technology has attracted a lot of attention from chemical, pharmaceutical, and agrochemical industries. In this context, research activity is directed in converting certain batch processes of industrial interest into continuous processes and thus scaling up to cater to the plant scales. Reactions such as esterification (trichloro acetyl chloride), trans-esterification, emulsion polymerization, hydroxylation, acetylation have been carried out. Given beneath are some of the case studies attempted in the recent time period.

Flow Process for Alpha-Lipoic Acid

This work is a part of Mission Mode project (INPROTICS), involving the Departments of OSPC and PETT at IICT. Main objective of the project is to develop a sustainable flow process for the synthesis of α-lipoic acid ((1,2-dithiolan-3-yl) pentanoic acid). α-lipoic acid recognized as a B-vitamin involved in the biochemical decarboxylation of of α-keto acids and as a growth factor for certain micro-organisms is one of the industrially relevant Pharmaceutical compound. Though batch process is established, it is of interest to explore the feasibility of improving the process yield and selectivity by adopting a flow process. Several experiments were carried out to

establish the sustainable flow process for the synthesis of α-lipoic acid in continuous mode of operation. A reproducible yield of 65% could be obtained in flow process. This process could also be numbered up to three times. Design of enhancer and reducer for efficient mixing played a vital role in improving the conversion along with yield.In addition to these, flow processes for reactions such as Trans-esterification (Biodiesel production), Acetylation (glycerol acetylation to tri-acetin), Esterification are carried out in flow reactors assembled in-house. (*Translational Research Trends In Process Engineering (TRTPE),* **2019**)



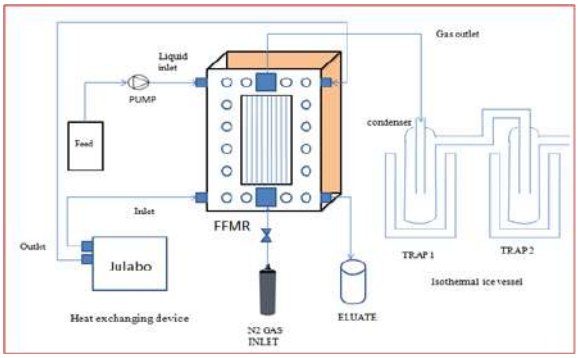
Assembled Flow Reactors

Continuous Emulsion Polymerization

Emulsion polymerization is the method of conducting the polymerization of a monomer in a dispersing medium (usually water) that leads to the formation of polymer dispersion with particles of a colloidal degree of dispersity. Continuous manufacturing of emulsion polymers has gained a great focus in industrial manufacturing, especially in paint industry. Currently studies are going on with micro and mini emulsions. Although there are some drawbacks with continuous polymerizations while performing in micro reactors like clogging of the reactor, fouling; these issues are handled in a different way by providing oscillations, pulsations etc. In the present work we have taken up the case study of homo polymerization of vinyl acetate which is exothermic in nature. (*International conference on advances and challenges for sustainable ecosystem (IASCE),* **2018***; Translational Research Trends in Process Engineering (TRTPE),* **2019**)

Downstream Processing in MRT (Micro-Distillation and Continuous Crystallization)

Many common chemical separation processes, including distillation, rely on mass transfer across a gas–liquid interface, and one of the major challenges for successful miniaturization, is the establishment of such an interface. Another key issue is the hydrodynamics in the micro separators. The scope of this research activity is to develop a table top end to end continuous process thus including distillation and crystallization. During distillation at micro scale, surface tension of the liquid often dominates over gravitational force, and hydrodynamics becomes the major challenge. The crucial issue for this design is the way the gas–liquid interface is stabilized. In this research activity, we are trying to develop contactor based micro distillation device. As a base study 'Falling Film Micro-Reactor (FFMR)' is being used. Experiments are being carried out with combinations of solvent mixture to explore the capability of FFMR to be used as a microstructured contactor for the separation of binary mixtures. (*Translational Research Trends In Process Engineering (TRTPE),* **2019**)



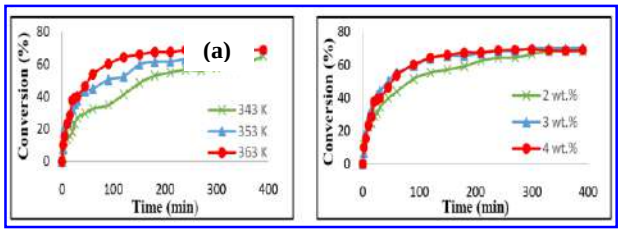
Falling Film Micro-Reactor

Process Systems Engineering: Modeling, Simulation, Optimization, Monitoring and Control of Chemical / Biochemical Processes

Kinetic and Thermodynamic Modeling and Process Design for Separation Processes

Development of A Kinetic Model for Esterification of Acrylic Acid with N-Butanol using Heterogeneous Catalyst from P-Toluene Sulfonic Acid

n- Butyl acrylate is an industrially important chemical as it is used as a raw material for fiber processing agents, adhesives, coatings, plastics, acrylic rubber, and emulsions. As reported in literature, it has been prepared by the esterification of acrylic acid with n- butanol using ion exchange resins as catalyst. Commonly used resin is Amberlyst for which kinetic models have been reported. In this study, liquid phase esterification of acrylic acid with n-butanol for the production of n-butyl acrylate has been studied in the presence of a heterogeneous catalyst derived from p-Toluene sulfonic acid, which has been developed in earlier work and was found to be highly efficient for other esterification reactions. Experiments are carried out in a stirred batch reactor with an equimolar feed to study the effects of temperature in the range of 343 – 363 K and catalyst loading varied from 2.0 – 4.0 weight % (based on the total mass of feed mixture) on the progress of acrylic acid reaction. It is observed that with increase in temperature and catalyst loading, the rate of reaction increases. This reversible reaction is considered to be of second order and a suitable kinetic model is developed. (*Proc. Intern. Conf. Sustainable Chemistry for Health, Environment and Materials (SUCHEM-2018),* **2018**)



(a) Effect of temperature on conversion of acrylic acid at 4wt. % catalyst loading, and (b) Effect of catalyst loading on conversion of acrylic acid at 363 K

Design and Analysis of Energy and Cost Effective Continuous Reactive Distillation Process for the Production of N-Butyl Acetate

Butyl acetate is widely used in Paints, Coatings, Semiconductor, Perfumes, Flavours, and Pharmaceutical industry. Esterification reaction for production of butyl acetate is an equilibrium reaction with limited conversion in a batch reactor and requires several downstream operations to obtain the product with desired purity. In this study, a continuous reactive distillation (RD) column is designed and analysed to produce n-butyl acetate in an energy and cost effective manner. In a RD column, reaction and separation occurs in the same unit. All the simulations are performed in Aspen plus (*Aspen One 8.8 academic version*) using sequential modular approach. The effect of reactive zone position in the RD column is studied by considering three cases i.e., (1) all stages are considered as reactive stages, (2) top part of the column as reactive zone and (3) reactive zone in the middle section with top and bottom as rectifying and stripping sections respectively. Highest conversion of 99.37 % and product purity of 99.5% are achieved in the third case where reactive zone is in middle of the column. Sensitivity analysis is carried out to find the optimal feed stage and reboiler duty for case three. Further, energy requirement and cost are determined for the optimal configuration. The column with reactive zone in the middle and mixed feed on top of the reactive zone proved to be an energy efficient and cost effective process. (*Proc. Su-CHEM Yuva,* **2019**)

Design and Analysis of Energy-Efficient Distillation (b) niques for Production of Anisole by O-Methylation Process

Anisole is produced at large scale by several chemical process routes, out of which O-methylation of phenol with dimethyl carbonate is the most promising technology because of its low temperature requirement, complete conversion, invaluable methanol production, absence of side reactions, and

its being a greener process. At the end of the reaction, the product contains multi-component mixture of anisole, methanol, CO_2 and unreacted phenol. Separation of pure components from multi-component mixture using conventional distillation sequence is energy intensive due to the use of multiple distillation columns. To address this issue, energy efficient distillation techniques such as fractional distillation column and fully thermally coupled distillation column (FTCDC)/ Petlyuk column configurations are proposed to replace conventional distillation sequences (CDS). In the present study, three different distillation configurations i.e. CDS, single fractional distillation column (MultiFrac) and FTCDC are compared in terms of energy efficiency and cost savings for the separation of the above mentioned multi-component mixture with high purity products. The proposed three configurations are simulated in Aspen plus (*Aspen One 8.8 academic version*) using sequential modular approach, and sensitivity analysis is carried out to find the optimal operating and design parameters. Optimal feed stage location, number of stages, and molar reflux ratio for the three configurations are calculated by considering product purity as target. Further, optimal results for the three alternatives are analyzed in terms of energy and total annual cost. The optimal results indicate that single fractional distillation column and Petlyuk column configuration/ FTCDC alternatives reduce the energy requirement by 9.31% and 21.23 % respectively, and the total annual cost by 32.49% and 19.94% respectively, compared to conventional distillation columns arrangement. (*Proc. TRTPE,* **2019**)

Thermodynamic Models for Prediction of Sorption Behavior in Pervaporation

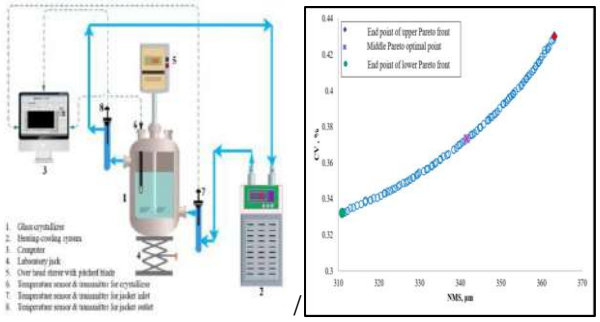
The main focus of this study is thermodynamic modelling of sorption behavior of single component/binary mixture mass transport through polymeric membranes in pervaporation (PV) process. Sorption and diffusion are the rate-limiting steps in the mass transport through PV process; therefore, it is necessary to develop accurate mathematical models for PV to identify the accurate mass transport mechanism for these steps. Sorption step has a dominant effect on the selectivity and efficiency of PV process. In our work, several thermodynamic models i.e. Flory-Huggins models, modified Flory-Huggins models, UNIQUAC, UNIQUAC-HB, and modified-NRTL (M-NRTL) models are reported with detailed derivation for prediction of sorption levels of single liquid/binary liquid into a polymer matrix. Further, the computational procedure for all the above models is explained through algorithms and step-wise calculations. Finally, with the help of a case study of binary ethanol/water mixture sorption in a PDMS polymer, the computational procedure using Flory-Huggins and modified Flory-Huggins models is illustrated, and the results of prediction of the sorption levels are compared with the reported experimental results.Comparison of experimental and simulated sorption levels for ethanol and water in PDMS polymer at 298K using modified Flory-Huggins model is illustrated. (*Adv. Memb. Proc.*, **2018**, 169)

Chemical Process Modeling, Optimization and Control:

Multi Objective Optimization and Experimental Validation for Batch Cooling Crystallization of Citric Acid Anhydrate

Multi Objective Optimization (MOO) of crystallization systems is gaining importance due to its ability to handle multiple conflicting objectives together for finding optimal operating policies. The present study focuses on batch cooling crystallization of citric acid. Among the two forms of citric acid, citric acid anhydride (CAA) is chosen for experimentation as no such study is available. Different operating policies are considered and compared through simulation for better product crystal size distribution. MOO is carried out to seek

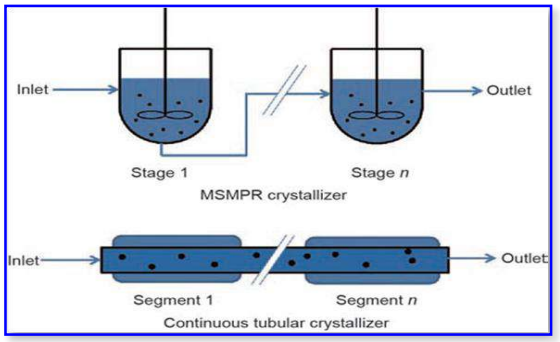
optimal cooling policy for unseeded cooling crystallization of CAA to maximize mean crystal size while minimizing variance in size. In this procedure, temperature is discretized using piecewise constant-control vector parameterization which is simple and convenient for practical implementation. One of the optimal solutions from the Pareto solution set is implemented through experimentation successfully and the measured product crystal properties are comparable to the predicted results obtained through optimization. (*Comp. Chem. Eng.*, **2018**, 112, 292)



(a) Experimental setup for cooling crystallization of CAA, (b) Pareto solution set obtained through MOO

Recent Advances in Engineering Aspects of Pharmaceutical Crystallization

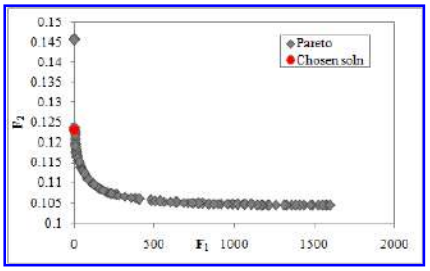
Crystallization, the most important separation and purification process in pharmaceutical industry has contributed to significant improvements in building efficient manufacturing practices for production of APIs. Past few decades have seen continuous rise in research and development activities in both coming up with novel approaches for deeper understanding of the process as well combining experimental and modelling methods for more robust and unified approaches in the monitoring, control as well as design and scale-up of industrial crystallization processes. This article summarizes recent developments from an engineering perspective in the key aspects of crystallization process such as thermodynamics, kinetics, design & scale-up, monitoring and control as well as a step forward towards continuous manufacturing using crystallization. This article puts forward certain future directions based on the advances in recent decades. (*Chem. Indus. Dig.*, **2018**, 31(8), 66; **2018**, 31(9), 48)



Different types of Crystallizers

Modelling of Semi-Batch Salicylic Acid Reactive Crystallization Process

Reactive crystallization has paramount importance in the production and separation of high value added chemicals like pharma ceuticals, polymers, catalysts, photographic materials etc. Modelling of reactive crystallization processes is complex as it involves both reaction and crystallization steps. In the present work, reactive crystallization of salicylic acid is carried out experimentally by adding sulphuric acid to sodium salicylate solution in semi-batch mode for moderately low initial supersaturation ratio. In a single feed semi-batch mode of operation, supersaturation can be controlled during crystallization which can lead to increased average crystal size compared to batch mode. Nucleation and growth parameters are estimated through multi-objective optimization considering minimization of deviation of final average crystal size and solution concentration profile from the experimental measurements. It is observed that the obtained crystallization kinetics is found to represent the process well, as the predicted average crystal size and solution concentration throughout the process using the developed model match very well with the experimentally measured data. (*Proc.- ICACSE-***2018**)



Pareto Solution Set Obtained Through MOO

Robust Trajectory Tracking in a Reactive Batch Distillation Process using Multi rate Nonlinear Internal Model Control

Operating a reactive batch distillation (RBD) process in an optimal manner is of paramount importance for improving product quality and profitability in the face of changing market conditions. However, implementation of an open loop optimal control policy may lead to significant reduction in yield and amount of desired product produced when unmeasured disturbances occur during operation. In this work, an observer error feedback-based multi rate Nonlinear Internal Model Control (NIMC) scheme is developed for optimal trajectory tracking in the face of unmeasured disturbances. In particular, mismatch in the initial conditions and process parameter variations that can occur during RBD operation are considered. To reduce the time required for online computations, a recently proposed reduced order RBD model is used for the controller synthesis. Because the thermodynamic model associated with the RBD process has discontinuities, a multi rate version of unscented Kalman filter (UKF) has been developed on the basis of the reduced order model for solving the state estimation problem associated with the proposed NIMC formulation. The efficacy of the proposed approach has been demonstrated by simulating an optimal trajectory tracking problem in the RBD process involving production of butyl acetate. The proposed multi rate NIMC formulation is found to be computationally efficient and work reasonably well when tested on the RBD process for solving the set point tracking problem in the presence of unmeasured disturbances. In particular, it is advantageous to operate the RBD process using the proposed UKF-NIMC scheme when the system is subjected to unmeasured disturbances. (*Ind. Eng. Chem. Res.*, **2019**, 58(26), 11364)

Molecular Weight Control in Semi Batch Copolymerization Reactor through Temperature Tracking: Evaluation of Control Strategies

Molecular weight is one of the influential attributes in a polymerization process and its control in semi-batch operation poses considerable difficulty due to complexities of the process. The present study focuses on the development of different control strategies for controlling the molecular weight by tracking reactor temperature and composition control using jacket temperature and feed flow rate as manipulated variables. The copolymerization of styrene acrylonitrile with xylene as solvent and AIBN as initiator is considered for the present study. The control strategies evaluated are Multi-loop-proportional integral (PI) control, multi variable-PI control and nonlinear generic model control (GMC). The present study showed that control of temperature and composition has resulted in achieving the desired molecular weight. Nonlinear GMC control is able achieve targeted molecular weight closely even in the presence of unmeasured load disturbances in the monomer feed concentration and initial initiator concentration, whereas multi-loop and multi-variable PI controllers resulted in some offset. (*Fifth Indian Cont. Conf. (ICC), IEEE Xplore,* **2019**, 213)

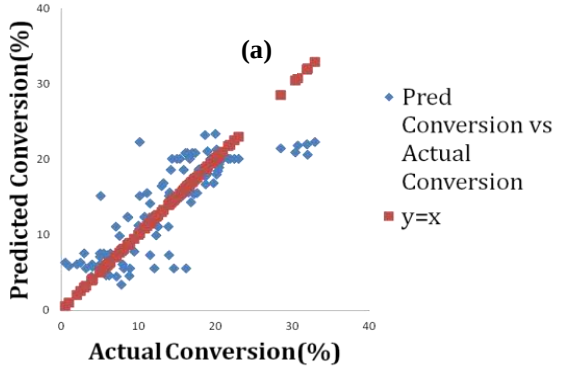
Artificial Intelligence and Machine Learning for Chemical Product Design:

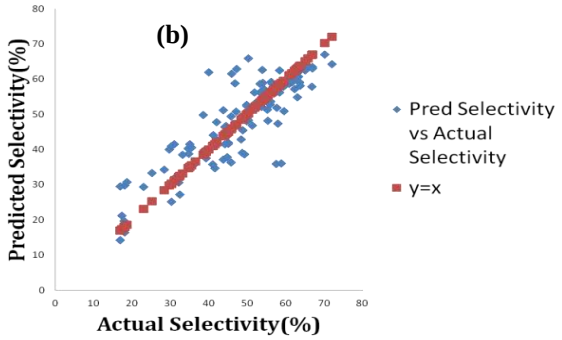
Catalyst Selection for CO_2 Hydrogenation based on Machine Learning

The climatic changes are majorly caused by Carbon dioxide, and this is a widely accepted fact. Hydrogenation of carbon dioxide into compounds like methane, methanol, formic acid, etc. is the

simplest way to use CO_2. Current day research is heavily focused on hydrogenation of CO_2 to methanol; given the importance of methanol for the organic chemical industry as well as its capability of replacing fossil fuels. The development of catalyst with high selectivity and high conversion is a multi-disciplinary and a complex research area especially for reactions like hydrogenation of CO_2 because of high operating conditions (220-300˚C and 50-100 bars) and chemical inertness of CO_2.

In this study, it is attempted to compile data available in the literature on several catalysts and operating conditions during methanol formation, and develop a data-driven model relating the input attributes to the conversion and selectivity towards methanol during CO_2 hydrogenation. The input attributes include reaction temperature, pressure, GHSV, calcination temperature and duration, S_{BET} and copper (wt.%), zinc(wt.%), aluminium(wt.%), zirconium(wt.%), titanium (wt.%) in catalyst. Firstly, multi-linear regression models are developed for conversion and selectivity considering all the input attributes which are found to result in R-Square value of 0.6435 and 0.733 respectively. ANOVA analysis is carried out, and significant terms are identified for both the models. These models are further modified by addition of quadratic terms for selected input attributes resulting in slight improvement in model prediction for conversion with R-Square value as 0.6883. The absolute mean deviation was found to be 7.756 for selectivity and 15.4 for conversion with the developed models.





Pareto plots: (a) Conversion and (b) Selectivity

Further, the developed models are used to find the optimum input attributes resulting in maximum selectivity with constraints on minimum conversion. The data reported shows that maximum selectivity of 72% is achieved with a conversion of 6.4%, while maximum conversion of 32.9% is achieved at a selectivity of 45.8%. The results obtained in this study through machine learning predict maximum selectivity close to 100% with a conversion of 25.773%. The optimum input attributions are 70.1(wt. %) of Cu, 67% (wt.%) of Zn, 31.62(wt.%) of Ti, reaction temperature as 214.43ºC, 7.52MPa pressure, 8527.28h^{-1} GHSV, 2.3 m^2/g-cat $S_{BET,}$800ºC as calcination temperature and calcination duration of 3.5 hrs. Experimentation is necessary to validate the results. (*Inter. Con. Adv. Catalysis: Indus. Outlook,* **2019)**

Development of Novel Pattern Recognition Methodologies for On-Line Disease Diagnosis

In this project, novel and efficient pattern recognition approaches have been developed for the diagnosis of critical diseases such as Parkinson, fetus heart anomalies, various types of cancers etc through the analysis of complex multivariate signals biomedical from instruments. To address the issue of PD diagnosis, it is proposed to develop efficient pattern recognition methods that utilize the dysphonic measurement data collected from the healthy as well as diseased people. Off-line multi variate models will be built using the historic dysphonia measurement data collected from people with Parkinson's (PWP), which serves as reference models representing the

disease condition. Further, respective multivariate Hotelling's T^2 and square prediction error (*SPE*) statistics will be derived and their 99% confidence limits will be established. On-line disease diagnosis can be performed by computing and monitoring the T^2 and *SPE* statistics. The ability of the proposed methods is compared with each other as well as with the recently reported methods. The application of proposed approaches can be easily extended to the diagnosis of any other disease.

Improved Fault Diagnosis of Overlapping Faults Using Dynamic Self Organizing Maps

Early detection and isolation of faults/abnormal events is an important task to maintain the productivity, safety and operability of any complex nonlinear process concerned to modern chemical industry. Abnormal event management (AEM) typically consists of the steps of on-line detection, diagnosis followed by timely correction of faults. The present work is focused towards the development of improved fault diagnosis methodology for the isolation of overlapping type of data and the application has been demonstrated on Tennessee Eastman Challenge Process (TEP). Dynamic self-organizing maps (DSOM) based diagnosis methodology is proposed, SOM is an unsupervised technique in which high dimensional data is projected on to a two-dimensional space and based on the similarity, data is clustered. However, it cannot address the auto correlations existing in data. DSOM extends the application of SOM to time varying processes by incorporating the variable delays to capture both static relationships and dynamical structure of the data. The application of proposed DSOM was demonstrated for the isolation of overlapping type of faults (F4, F9 and F11) of TEP. The results on comparison revealed that proposed DSOM has exhibited nearly 12% improved diagnostic efficiency as compared to the existing SOM. The average classification results of test data achieved with SOM and DSOM are 79.7 % and 91.9 % respectively.

Microbial Synthesis, Process Optimization and Kinetics Evaluation of Lipase Enzyme

Lipases are the industrially important biocatalysts, which are envisioned to have tremendous applications in the manufacture of a wide range of products. Their unique properties such as better stability, selectivity and substrate specificity position them as the most expansively used industrial enzymes. The research on production and applications of lipases is ever growing and there exists a need to have a latest review on the research findings of lipases. A review paper has been published that covers the latest and broadest overall picture of research and development on lipases by including the current studies and progressions not only in the diverse industrial application fields of lipases, but also with regard to its structure, classification and sources. Further, lipase enzyme has been synthesized from candida antarctica and the process has been optimized to improve the lipase activity. Also models have been developed representing microbial as well as enzyme kinetics of lipase. This work will be very useful for the researchers from both industry as well as academia in promoting lipolysis as the most promising approaches to intensified, greener and sustainable processes. (*Biotechnol. Prog.*, **2018**, 34, 5)

Process Optimization and Development of Kinetic Models for Heterogeneous Catalytic Processes

Selective Transesterification of Glycerol to Glycerol Carbonate Sro-Zro2 Base Catalysts

Glycerol carbonate was prepared selectively by transesterification of glycerol with dimethyl carbonate over heterogeneous strontium-zirconium mixed oxide base catalysts. These catalysts were prepared by coprecipitation method with varying Sr to Zr molar ratio and characterized by Brunauer-Emmett-Teller (BET) surface area, X-ray diffraction, and temperature programmed desorption of CO2. The catalysts' activity was varied with variation in the Sr to Zr ratio and the catalysts with the ratio of 3:1

exhibited the highest activity towards glycerol carbonate. The characterization results suggested that the activity of the catalysts depended on the amount of basic sites present in the catalysts and the basicity was dependent on the Sr to Zr ratio and treatment temperature. The effect of reaction parameters on the yield of glycerol carbonate was studied and also the kinetic expression was derived. The catalyst showed consistent activity upon reuse. (*Cataly. Green Chem. Engg.*, **2018**, 1, 79)

Tungstophosphoric Acid Supported on Meso porouusniobiumoxophosphate: An Efficient Solid Acid Catalyst for Ether ification of 5-Hydroxy methylfurfural to 5-Ethoxy methyl furfural

Tungstophosphoric (TPA) supported on meso porouusniobiumoxophosphate (NbP) catalysts were prepared with different loadings. The synthesized materials employed as hetero geneous solid acid catalysts for selective etherification of 5-hydroxymethylfurfural to 5-ethoxymethylfurfural. Physico-chemical properties of the catalysts were obtained by different spectroscopic techniques and their results exposed that TPA was a highly dispersed state on NbP and acidity of the catalyst enhanced due to its dispersion. The higher catalytic performance can be allied to the total acidity of the catalysts with appropriate number of Brønsted-Lewis acid sites which were directed by the contact and dispersion of TPA on support. Different reaction parameters were premeditated and 25 wt% TPA/NbP catalyst exhibited highest catalytic activity with 95% of HMF conversion and 89% of EMF yield. The catalyst is reusable without noticeable turn down in catalytic performance up to five cycles. A kinetic model for etherification of HMF was also derived. (*Cataly. Today*, **2019**, 325, 53)

Hydrodynamic Cavitation Based Advanced Oxidation Technology

Advanced oxidation technology have gained the prime focus over the conventional techniques of water treatment as the suitable method for the complete mineralization of organic compounds. Among different AOPs, most of the processes like UV, Fenton, electrochemical oxidation, photocatalysis are restricted by high operating cost and involve complicated set-up. Alternatively, cavitation is an emerging domain with huge potential inherent in the process for treating such pollutants at better energy efficiency and also requires simple set up and less maintenance to carry out the experiments. Basic research has been carried out on different applications of hydrodynamic cavitation (HC) as mentioned below:

Degradation of Sodium Dodecyl Sulphate: Surfactant degradation is a challenging problem related to wastewater treatment. The possibility of treating surfactant (sodium dodecyl sulphate, SDS) laden wastewater using hydrodynamic cavitation (HC) technology was investigated for the first time. The studies were conducted in a systematic approach by selecting the optimum geometrical configuration (Orifice diameter) followed by the experimental operating parameters (Solution pH, inlet pressure, concentration variation). It was found that (i) 1.6 mm was the optimum orifice diameter for carrying out HC, (ii) pH = 2 and pressure = 5 bar were the optimized operating conditions for HC. Further studies were conducted using HC coupled with other oxidizing agents. The kinetic studies revealed that the degradation of surfactant followed first order kinetics. Around 56% degradation was achieved in 1 hour using HC alone, which was further accelerated to more than 80% degradation using the integration approach. Encouraging results at the lab scale and further investigation provided the route for scale up studies.

Degradation of Organic Micropollutants: Studies were conducted to understand the performance efficiency of HC technology in physico-chemical degradation of common antibiotics ***ciprofloxacin***, ***cefixime*** and an organophosphorus insecticide, ***profenofos***. As the conventional water treatments methods are only capable of separating the pollutants from one phase to another rather than degrading or mineralizing them, complete degradation by HC were

the prime focus of these experiments. Also initial studies were conducted to understand the optimum geometrical parameter of the cavitating device and operating conditions. The optimum conditions resulted in a maximum reduction of 65.23,44.28 and 71.95% in Total Organic Carbon (TOC) for ciprofloxacin, cefixime and profenofos, respectively. The synergistic effects were also studied using HC coupled with ozone, hydrogen peroxide and Fenton's reagent. Keeping in mind the energetics and economics of the process, the integrated approach of (HC+H_2O_2) was identified as the most suitable one for complete mineralization of such compounds. The optimum conditions in this integrated process resulted in a degradation of 71.48, 62.31 and 87.48% of TOC for ciprofloxacin, cefixime and profenofos, respectively.

***Degradation of Dye*:** Degradation of Methylene Blue (MB), an azo dye, was investigated using hydrodynamic cavitation (HC) alone as well as integrated with other Advanced Oxidation Processes (AOP). Orifice plate was used as the cavitating device in the HC reactor. Under optimized geometrical and operating conditions of 1.6mm orifice plate opening, inlet pressure and pH of 5 bar and 2, standalone HC resulted in a degradation of 23.49% within 120 min. Improvement in the performance of HC was carried out using hybrid schemes and the maximum degradation of 91.45% was achieved.

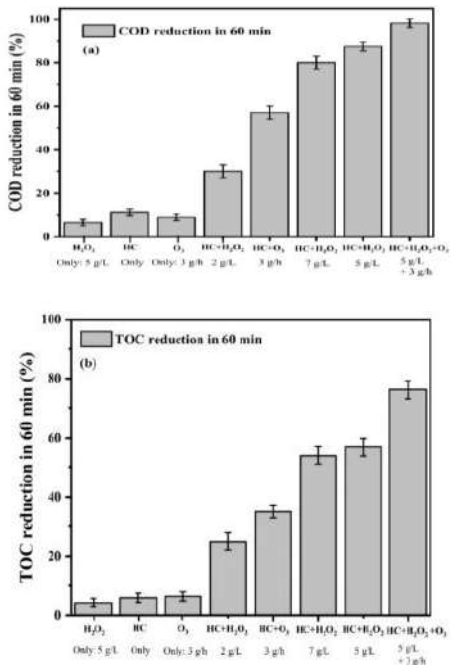
Ozonation: An Advanced Oxidation Process

The growing popularity of AOP's, experiments were carried out with ozonation to check for the performance efficiency as well as the energetics in comparison to the cavitation technology described above. Below discussed are few basic research carried out with ozonation.

***Degradation of Organic Micropollutants*:** Studies similar to cavitation were performed on the degradation of propenofos and cefixime with standalone ozonation. It was observed that profenofos degradation was found to be instantaneous with 38% TOC reduction and no further degradation was observed till 2 h of ozone treatment at 3 $g.h^{-1}$ dosage. Similar conclusions were arrived with the degradation of cefixime. It was also found that the energetics of standalone ozonation was very high compared to hydrodynamic cavitation technology aiming complete mineralization. Due to higher energetics, the cost consideration of the entire process too boosts up, concluding to the fact that standalone ozonation is not a feasible process for degradation of micropollutants, whereas integrating it with other AOP's is a fruitful process.

Grey Water Treatment

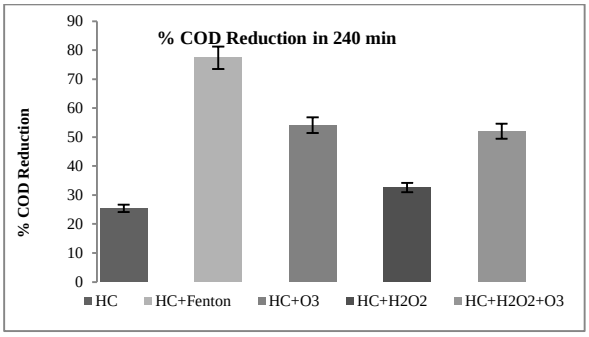
Experiments have been performed using Hydrodynamic Cavitation based Advanced Oxidation Technology for treatment of real life grey water streams. As understood from the basic research, operating parameters plays a dominant role in the cavitation phenomena and following Figs provides an insight into the effects of solution pH and inlet pressure on the COD and TOC content of the greywater. Experiments involving the addition of different oxidizing agents have also been performed and their efficiency on COD and TOC reduction has been calculated.



(a)% COD reduction and (b) % TOC reduction using O_3, H_2O_2, HC, HC + O_3, HC + H_2O_2 and HC + H_2O_2 + O_3

Textile Effluent Treatment

Lab scale organic degradation studies have been performed with a textile dye effluent solution using Hydrodynamic Cavitation based Advanced Oxidation Technology. The effects of orifice opening, feed concentration, pH, cavitation number and electrolyte on % dye effluent degradation have been studied to understand the feasibility of the process. The hybrid process integrated with Fenton reagent exhibited reduction in process operational cost as compared to conventional effluent treatment techniques.



% COD reduction in Dye effluent by lab scale orifice based hybrid hydrodynamic cavitation treatment

APPLIED RESEARCH

Design of Highly Compact Vertical Modular Nanofiltration System for Water Purification

The designed nanofiltration (NF) unit is suitable for treatment of moderate total dissolved solids (TDS) ground water ≤ 800 ppm and surface water of 150–400 ppm. The plant can effectively remove suspended solids, hardness, turbidity and disease causing microbes in a single step.

S & T Details:

- The highly compact skid mounted NF system costs only Rs. 3.5 Lakhs and runs on electric power to provide 1200 L/h of water at a low operating pressure of 6 bar.
- This plant removes all impurities in a single step including excess TDS, salinity, hardness, turbidity, heavy metals and microbial content.
- Greater water recovery of 70-80% with lower reject volume can be achieved. The reject water can be reused for washing water, laundry and other purposes.
- Retention of sufficient mineral content such as Ca, Mg, P, Na, K essential for human consumption and health.
- The operating cost is about 3-5 Paise per L of purified water generated.
- Highly compact nature of the design enables its portability to remote villages. The unit requires smaller footprint for installation.

Commercialized/Launched In Market:

The system is fully commercialized. The details of installations of NF water plant of 1200 L/h capacity are given below:

- Mogallu Village School, Bhimavaram Taluk in West Godavari District of Andhra Pradesh for surface water purification.
- Gandhi hospital, Hyderabad, Telangana for providing free drinking water to patients, staff and public.
- CSIR-IICT campus for providing drinking water to staff and students and for cooking purpose at IICT canteen.
- Nanofiltration Pilot Plant of 30,000 L/day based on an indigenously developed hydrophilised polyamide membrane which provides high water recovery at low applied pressure has been installed at Gandhi Hospital, Hyderabad. The water consumption was 2000 L/day during the first week of plant installation, whereas, the quantity of consumption got increased to 5000 L/day from second week onwards, which ensures intake by 10,000 poor people each day.

Nanofiltration pilot plant of 1000 L/h capacity installed at Gandhi Hospital, Hyderabad

Flood water treatment through hand operated NF hollow fibre membrane systemsat Kerala flood affected areas

Membrane Based Mini Pilot Plant for Schools, Hostels and Hospitals and Free Water Camps in Summer

Technology: The cost effective moderate capacity reverse osmosis plant is useful for the treatment of water containing high TDS, fluoride, suspended solids, turbidity, bacteria, pathogens etc. Ultrafiltration can be effectively used for clarification and disinfection of municipal water or surface water.

S & T Details:

- The unit is highly flexible, portable in nature and easy to use.
- The design has a feasibility to incorporate more than one membrane modules.
- The taste of the water is enhanced by post treatment using granulated activated carbon filter whereas the provision made for TDS controller in permeate line remineralize the water by providing sufficient minerals.
- The product is designed flexible for incorporation of either Reverse Osmosis or nanofiltration membrane.
- The system with different capacities ranging from 100 - 300 L/h are designed depending on the product water consumption.
- The UV lamp incorporated disinfects the permeate water making the product water safe for human consumption.
- The operational cost for drinking water production is 5-7 Paise per L of water produced.

Commercialized/Launched in Market:

The developed technology is deployed at both rural and urban areas in villages, schools, hostels and small hamlets. More than 20 such compact systems have been installed. Many of the installations were made in fluoride worst hit villages of Nalgonda District, Telangana.

Packaged Drinking Water Facility

Technology: Innovative low cost technology for chemical conversion of reverse osmosis membranes into nanofiltration can produce water with essential minerals for human consumption.

S & T Details:

- Innovative low cost technology for conversion of commercial reverse osmosis membranes into nanofiltration membrane using a proprietary reagent.
- The system removes all impurities in a single step including excess total dissolved solids, salinity, hardness, turbidity, heavy metals & pathogens.
- The membrane allows passage of 80 to 120 ppm of TDS comprised of Ca, Mg, P, Na, K and other minerals essential for human health.
- The highly compact skid mounted Nanofiltration system costs Rs. 3.5 Lakhs with water recovery of 70-80% in comparison to just 50% in conventional RO systems.

Commercialized/Launched in Market:

The Membrane team of CSIR-IICT developed an innovative low cost technology for conversion of commercial reverse osmosis membranes into nanofiltration membrane using a proprietary oxidizing reagent. The remineralized water generated from the unit meets the specified quality standards and certified by BIS and FSSAI. IICT has transferred technology to Hindustan Petroleum Corporation Limited (HPCL) for production of mineral rich water of good taste and neutral pH since most of the packaged drinking water available in the market has revealed acidic pH or low levels of TDS.

Technology Transfers: 3 (Navaratna company and 2 start-up companies)

Bottle Capacities: 20 L, 1 L, 0.5 L and 200 ml

Contribution to Make in India: Produced 20,000 no: of 20 L packaged bubble top water cans and One Lakh plus 1 L, 0.5 L packaged drinking water bottles.

Indigenous pilot scale membrane system of 1200 L/h capacity

Pilot scale water bottling unit of 1000 bottles per hr capacity

Atmospheric Water Generator (AWG) with Automated Remineralization

The unit captures moisture from humid air to get water. Dosing salt mixture is used to remineralize the water produced from atmospheric water generator.

S & T Details:

- The device takes advantage of relative humidity (RH > 25%) and temperature (20 ^{o}C) to produce drinking water for remote villages, coastal regions, border areas
- Developed a novel remineralisation technology using an automated system for dosing a proprietary salt mixture.
- Post treatment by novel indigenous high flux polyethersulfone based ultrafiltration membrane and ozonation / UV light produces clarified and disinfected water.
- Capital Investment Rs.10 Lakhs.
- Cost per Liter of potable water is Rs 3.5/- which may reduce to Rs 1.5/- using solar power.
- Design of Solar powered AWG unit reduces cost per liter production of potable water.

Atmospheric Water Generator Demonstration Unit of 1000 Lit/day capacity installed by CSIR-IICT & Maitri Aquatech Pvt. Ltd. at IICT campus

1000 L/day Atmospheric Water Generator Machine installation at Secunderabad Station

Inexpensive Import Substitute for Production of Ultrapure Medical Grade Water for Dialysis and Biochemical Applications

Technology: Demineralized water is used for preparation of saline water, dialysis water in hospitals, microbial culture preparation in biotech industries and laboratories, Water for soil test kits etc.

S & T Details:

- Cascaded compact reverse osmosis system of 25-40 L/h costs Rs. 80000/- only and 500 L/h costs Rs. 2.5 lakhs only as compared to Rs. 5 – 10 Lakhs charged by MNCs
- Novel polyether ureas reverse osmosis membrane that provides high TDS rejection.
- The system can produce Type-2 water of conductivity < 1 µS/cm at an operating cost of 30 Paisa per Liter.
- Maintenance free compared to multinational companies that charge Rs 1 lakh per annum.

Commercialized/Launched in Market:

The membrane based demineralized water technology developed by CSIR-IICT, Hyderabad is deployed successfully at Plantris Ventures Pvt. Ltd, New Delhi, Care Hospital, Nephroplus Hospital, NIPER, Hyd., JNTU, Kakinada, Osmania University, Hyderabad and in different divisions in IICT including Chemical Biology, Polymers & Fine Coatings, Bio-Engineering and Environmental Center and Nanomaterials Laboratory.

Beneficiaries: Automobile industries, biotech industries, caustic soda plants, R&D laboratories, hospitals etc.

DM water system of 200-500 L/h (left) and 40-60 L/h capacity (right)

Design and Development of Highly Compact Minipilot Scale Nanofiltration System for Surface Water Purification for Community Based Installation in Schools

The Low cost nanofiltration (NF) system is suitable to enrich the natural minerals essential to the human body by treatment of moderate total dissolved solids (TDS) ground water ≤ 800 ppm. The plant can effectively filters the ground water in a single step to produce drinking water TDS up to 150–200 ppm.

S & T Details:

- The highly compact skid mounted NF system costs only Rs. 1.5 Lakhs and runs on electric power to provide 300 L/h of water at a low operating pressure of 6 bar.
- This plant removes all impurities in a single step such as hardness, turbidity, heavy metals and microbial content etc., and moderately lowers the TDS to maintain the essential minerals in the permeate water.

- Lower reject volume can be achieved that can be reused for washing water, laundry and other purposes.
- The operating cost is about 2 - 4 Paise per L of purified water generated.
- Highly compact nature of the design enables its portability to remote villages. The unit requires smaller footprint for installation.

Commercialized/Launched in Market: The system is fully commercialized. NF water plant of 300 L/h capacity has been installed at Zilla Parishad High School, Vendra in West Godavari District of Andhra Pradesh for surface water purification.

Alkaline Water Cell as Immunity Booster for Disease Prevention

The device disclosed in this invention is pump free and requires tap water connection to the inlets of the anode and cathode chamber continuously and it works on the principle of electrolysis.

S & T Details:

- The low cost electrodes and highly selective indigenous polymeric composite UF 5kDa membrane aided alkaline water system produces 50 Lit/h alkaline ionized water at 24 V
- Alkaline ionized water production of pH ranging from 8 – 10 applicable for drinking and biomedical purpose.
- The produced alkaline ionized water is rich in minerals such as Ca, Mg, and K and provides enduring health benefits, which helps in prevention of various diseases like hyperacidity, arthritis, diabetes, and cancer.
- Daily intake will boost the immune system, inactivates the virus and also naturally neutralizes the free radicals, thereby cleansing the toxins present in the body.
- The advantage of this system is its low designing cost which makes the system reasonably prized when compared to other commercially available ionizers.

Membrane aided Alkaline Water System

Agreement with Micro Engineers

Commercialized/Launched in Market:

Installations are planned in health care centre's such as hospitals.

Beneficiaries: Hospitals, Health Care Centre's, Patients, Common People etc.

Technology Transfer: Micro engineers, Ghaziabad, Uttar Pradesh, India.

Salient Features:

- The low cost electrodes and indigenous cation transfer membrane aided alkaline water system produces 50 Lit/h alkaline ionized water at 16 V

- Alkaline ionized water production of pH ranging from 8 – 10 applicable for drinking and biomedical purpose.
- The produced alkaline ionized water is rich in minerals such as Ca, Mg, and K and provides enduring health benefits, which helps in prevention of various diseases like hyperacidity, arthritis, diabetes, and cancer.
- Daily intake will boost the immune system, inactivates the virus and also naturally neutralizes the free radicals, thereby cleansing the toxins present in the body.
- The advantage of this system is its low designing cost which makes the system reasonably prized when compared to other commercially available ionizers.

Defluoridation or Ground and Surface Water at Khammam District (*DBT Sponsored Project*)

The fluoride in the raw water varies from 2.5 to 3.6 ppm and is brought down to a concentration of less than 0.5 ppm as per WHO standards of potability. The salient design features of the plants are effective pretreatment through sand filtration, activated carbon treatment, anti-scalant dosing and micron cartridge filtration besides post treatment by UV radiation and ozonation for long term storage. Moreover, the option of blending the permeate (product water) with a small fraction of raw water is also made available to maintain a total dissolved solids (TDS) level of at least 60 ppm to ensure sufficient supply of minerals for human consumption. The reject (waste water or concentrate) is presently being treated in a sump by lime-alum mixture for recycle to non-edible plantations such as teak or cotton seed or washrooms in schools. the IICT membrane separation team installed the defluoridation plant in telangana State of 500 -1200 L/h for the fluoride-affected Tippanaputtuga Village and Upper Primary School, desinenipalem, Khammam District with a comprehensive scheme for proper treatment and reuse of the reject water. The plant was assembled at an economical capital investment of only Rs. 2.5 Lacs and is serving a population of 3500. The plant reduces the fluoride concentration from 2 ppm to less than 0.5 ppm.

Water Purification Plant (1000 Lit/hr) Installed by IICT at Upper Primary School, Desinenipalem, Khammam District

The water is being provided at the door step at a low cost of Rs 5/- per can of 20 Liters. The reject water from the plant is being recycled for domestic purposes, other than drinking, including school toilets to ensure zero water wastage and safe disposal of fluoride. Figures of defluoridization plant are shown below at different villages. Raw Water: TDS 2400 ppm ; Fluoride: 2.92 ppm Product Water: TDS 93 ; Fluoride: < 0.5 ppm;

Integrated Pilot Plant for Arsenic and Silica Removal at Srikakulam District

Installed a unique ultrafiltration + reverse osmosis (RO) integrated pilot plant for brackish water purification at Tippanaputtuga Village in Sompeta Mandal at Srikakulam district. The UF + RO integrated pilot plant for brackish water purification at Tippanaputtuga Village enables production of 750 L/h. The UF system removes colloidal silica, which is one of the causes of kidney ailments, along with turbidity, whereas the RO membrane removes impurities such as heavy metals (arsenic, mercury, lead and cadmium), excess hardness, nitrate and lithium. The purified water is remineralized online to a TDS level of 55 ppm for consumption using rock salt.

UF + RO Pilot Plant of 750 LPH capacity at Tippanaputtuga Village, Sompeta Mandal, Srikakulam District, A.P.

Ultrafiltration Plant with Hand Operated Pump System at Maharastra Flood Affected Areas

The flood affected regions will be lack of fresh water and there is plenty dirty water which can be clarified using ultrafiltration membrane as waterborne pathogens cause different type of diseases. In order to treat this water hand operated hollow fibre UF membrane systems were deployed and installed in several flood affected places such as such as Gokak taluk and Ramdurg, Karnataka State and Sangli, Maharastra for providing safe and clean drinking water to peoples as shown in Figure below. This set up can treat surface water and is capable to remove viruses, bacteria and suspended solids from the surface water. In this system surface water is needed to be pumped into the UF system and thereafter due to applied pressure the water will pass to the ultrafiltration module to produce purified drinking water.

Compact UF plant at Sangli , Maharastra

Process Development and Basic Design Report for 1 Ton/Day of Furfural Alcohol and Furoic Acid from Furfural

The process for furfural alcohol and furoic acid was developed for M/s Srikusuma Harinadha Agro furan Ltd, Eluru.

Process knowhow for Dibromoethane

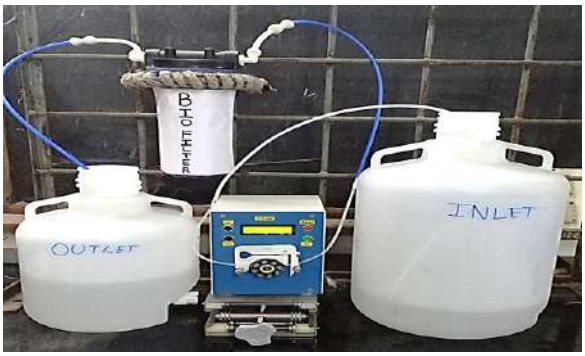
Continuous non catalytic thermal process was developed and demonstrated to M/s Intech Organics Ltd, Gurugoan.

Preparation of Polymer-Grade Vinylidene Fluoride

Process equipment design and scale-up studies to produce 5 kg batch of VDF.

Engineered Biochar from non-edible de-oiled seed cakes/stubble wastes was developed for used for removal of targeted herbicides/ pesticides from agricultural wastewaters and subsequent soil remediation

As a part of this project a modular unit was developed for the decontamination of pesticidal waste stream at a capacity of 5 L/h.



Modular biochar unit for the decontamination of pesticidal wastewater

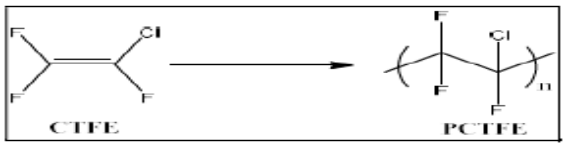
Development of Process Know-How for Industrial Chemicals

Objective: To develop process know-how for synthesis & purification of chemicals such as

Polychloro trifluoro ethylene, Hydroxypropyl Methyl Cellulose.

Summary of Execution: Development of process know-how is carried out in collaboration with other Departments in IICT (PFM, FAC Departments), as an initiative under industry sponsored projects.

PCTFE is a fluorine rich engineering thermoplastic with outstanding physical and mechanical properties. Its non-flammability, chemical resistance, near zero moisture absorption and excellent electrical properties make it a unique polymer, even within fluoro polymer family. Its ability to function in the temperature range of -2400C to 2000C makes it a specialty polymer. Present project was under taken to develop an economically viable, laboratory scale process for synthesis of a high performance grade PCTFE equivalent to Daikin's M400H.



Development of process for production of HPMC or Hypromellose, which has high market value, is sponsored by industry. These cellulose ether derivatives are very versatile and find application in number of industries such as, pharmaceutical, food, cosmetic and construction chemicals. To name a few, HPMC E5 is used in applications such as controlled or modified release formulations, while K100 LV is used as a soft gelatin capsule alternate to the animal based product used in gelatin capsules, K100 M used in construction industry. Project delivery plan includes the demonstration of 100 g per batch scale of HPMC to the industry.

Modelling and Simulation of Blending Unit Operation (Project Sponsored by Daiichi Sankyo Europe (DSE), Germany)

The main objective of this project is optimization of blending unit operation through numerical simulations in collaboration with DSE. Pharma ceutical industries have several unit operations involving solids, and blending is one of them. There are several challenges involved in such operations, and lack of insight into their operation leads to sub-optimal designs, causing several operational hurdles as well as off specification products resulting in huge losses. Therefore, modelling and simulation of such operations can provide some understanding leading to process improvements. However, modeling studies in this area are extremely limited and involve extensive computational effort. This project attempts to address the challenges in this area.

DEM Simulations on Tote Blender: Study of Operating Parameters

In this study, Discrete Element Method simulations have been performed to investigate the effect of operating parameters i.e. blender rotational speed (RPM) and fill level (%) on the mixing performance of a Gallay tote blender. The mixing performance of tote blender is characterized quantitatively using Lacey mixing index (*M*). The effect of rotational speed is studied at a fixed fill level of 40%, and it is observed that the performance of mixing increased with increase in rotational speed from 10-50RPM and then started decreasing at 60RPM. Further, the effect of fill level is studied at rotational speed of 50RPM, and it is observed that blending performance tends to increase with increase in fill level from 30-70%, and then it started dropping at 80% fill level. Thus, from the study of simulation experiments performed, the optimal parameters are 50rpmrotational speed with 70% fill level, resulting in a Lacey mixing index of 0.94. (*Proceedings ICACSE-2018*, **2018,** NIT, Tiruchirapalli, INDIA)

DEM Simulations on Tote Blender: Study of Particle Parameters

In the work, discrete element method (DEM) simulations are performed to study the effect of particle parameters i.e. particle size and cohesion energy density (CED) on mixing performance using a tote blender with top-bottom

filling with 70 (v/v)% fill level and blender rotational speed of 50 rpm. The effect of particle size is studied using bi-disperse particle system with smaller particle sizes ranging from 4-7mm and corresponding larger particle sizesranging from 8-14mm. Further, the effect of CED is studied for particles of sizes 6 and 12 mm by varying CED from 5 to 20 $x10^5$Ergs/cm^3. Quantitative analyses are performed using Lacey Mixing Index (LMI), which shows that the particles with smaller sizes resulted in better mixing performance with a LMI of 0.96 for (4mm & 8mm) particles. Further, particles having CED range (10-15)$x10^5$Ergs/cm^3resulted in improved mixing performance with of LMI of 0.98. (*Proceedings ICACSE-2018*, **2018**, NIT, Tiruchirapalli, INDIA)

Influence of Material Attributes and Process Conditions on Blending Performance of an Industrial Bin Blender: A DEM Study

Blending of granular materials is one of the important processing steps in chemical and allied industries. Variations in different operating parameters and granular properties play a vital role in influencing the blending efficiency of granular materials. Therefore, this study explores the impact of various material attributes and process conditions on the blending performance of a 50L industrial bin blender.

The geometry of blender consists of (1) a large cylinder with two baffles attached at the top lid at an angle of 45° with the vertical axis, (2) a conical hopper and (3) a small cylinder. The blender revolves around the horizontal axis at 3.5cm above the top lid. Bi-dispersed cohesive particles of diameter 6 and 12mm are considered. Discrete element method (DEM) simulations are performed using open source LIGGGHTS software. The Hertz and Mindlin & Deresiewicz theories are used to compute the contact forces between particles and between particle and wall, while the cohesion between particles and between particle and wall of blender are computed using simplified Johnson-Kendall-Roberts model.

The influence of four different parameters namely: fill level (% volume), blender speed (rpm), cohesion between particles expressed in terms of cohesion energy density, CED (ergs/cm^3), and composition of small particles (% weight) on the blending performance of bin blender is investigated in a step-wise manner. Firstly, parametric study is conducted with initial base case simulation parameters (and ranges of parameters) being fill level of 70% (60-80%), blender speed of 24rpm (12-36rpm), cohesion energy density of $20x10^5$ ergs/cm^3($10x10^5$-$30x10^5$ ergs/cm^3) and 20% composition of small particles (10-30%). The results indicate that the best blending performances are found at peripheral values of ranges considered (60% fill level, 36 rpm, $30x10^5$ ergs/cm^3 CED, 10% composition); therefore, another set of parametric study is performed with new base case parameters (and ranges of parameters) as 70% fill level (50 – 80%), revolution speed of 36rpm (24-48rpm), CED of $30x10^5$ ergs/cm^3 (10 - $35x10^5$ ergs/cm^3) and 20% composition of small particles (10-30%) with total 19 number of DEM simulations from both the sets. The performance measures, namely six-directional sampling mean Lacey mixing index (SDS-mLMI) and six-directional sampling mean relative standard deviation (SDS-mRSD) are used to evaluate the blending performance by dividing the whole particle mass into 800 number of samples with equal mass. SDS-mLMI and SDS-mRSD are computed after 150 seconds of blending time.

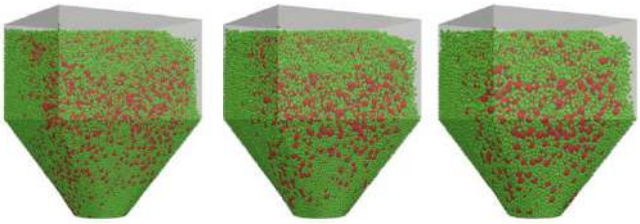
DEM simulations for both the sets revealed that the performance of blender goes through a maximum at 70% fill level and 36rpm. Higher fill level resulted in hindered particle transport due to smaller tumbling space available, whereas at low fill levels, blending is poor as the convection of particles is found to be less. At low blender speed, less diffusion is observed while at high speed, particles started centrifuging and becoming airborne with less convection. The performance of blender increased with increase in CED up to $25x10^5$ergs/cm^3 and showed stable

performance over a range (25 to 35x10^{5}ergs/ cm^3), beyond which lump formation is found to hinder blending. Further, the blending performance at 10% composition of small particles is slightly better than that at 30% composition. The optimum material attributes and process conditions resulting from this study are found to be: 70% fill level; blender speed of 36rpm; CED of 30x10^5 ergs/cm^3 and 10% composition of small particles. DEM simulation at the optimum parameters resulted in SDS-mLMI of 0.9960 and SDS-mRSD of 0.0302, illustrating the best blending performance. (*VI Intern. Conf. Particle-Based Methods (Particles-2019),* **2019,** Barcelona, Spain)

Full Factorial Design Based DEM Simulations for Blending of Cohesion-Less Bi-Disperse Spheres in A Tote Blender

In this study, Discrete Element Method (DEM) based simulations are carried out to understand the effect of three parameters, i.e. fill level, blender speed (rpm), and particle size on blending performance, considering a 14L Gallay tote blender reported by Sudah*et al.* (2005) as a case study. This blender consists of a top part with rectangular cross-section and a bottom hopper with axis of rotation passing through the center of blender inclined horizontally at 30°. Open source LIGGGHTS software is used to perform DEM simulations, where the contact forces between particles and between particles and wall are calculated based on Hertz and Mindlin & Deresiewicz theories.

Bi-disperse cohesion-less feed mixture with size ratio of 2 and composition of each component of 50% by weight is considered for all simulations. A 3-parameter, 3-level full factorial design is formulated resulting in total 27 simulation runs, and ranges of parameters are 70%-90% fill level, 45rpm-75rpm blender speed and 4mm-6mm smaller particle diameter. For each of these simulation runs, blending performance at 120sec is evaluated using SDS-mLMI and SDS-mRSD by dividing the total mixture into 600 samples of equal mass. From the simulation results, it is observed that irrespective of particle size, the SDS-mLMI at 120sec first increases with blender speed at all fill levels reaching a maximum, and then starts decreasing. To understand the dependency of SDS-mLMI and SDS-mSD on the three factors considered, multivariate linear regression analysis has been carried out to develop quadratic models with interactions. For each particle size, SDS-mLMI computed at the best operating parameters using regression model is compared with the corresponding SDS-mLMI obtained through DEM simulations, and it is observed that these values are matching reasonably well. For all the three sizes, 80% fill level and 60rpm is found to result in maximum SDS-mLMI and minimum SDS-mRSD. Further, the qualitative representation of blending performance of all the three sizes are illustrated in Figure below. Additional DEM simulations in the neighborhood of the best operating parameters are also carried out for validation of the regression model, and the LMI and RSD obtained are found to be reasonably close. The drop in SDS-mLMI at higher fill levels (>80%) can be attributed to the reduced free space for mixing. Rotation speed higher than 60 rpm is found to result in centrifugation. The present study is helpful in identifying the best operating conditions for blending of bi-disperse particles of different sizes. (*VI Intern. Conf. Particle-Based Methods (PARTICLES-2019),* **2019**, Barcelona, Spain)



(a) 4mm & 8mm (b) 5mm &10mm (c) 6mm &12mm
Blender for simulations with 80% fill level and 60rpm at 120seconds of blending time

Development of Process for Production of Choline Hydroxide/ Choline Etchant for Semi Conductor Laboratory (SCL), Mohali

Objective: To develop a suitable method for synthesis & purification of Choline hydroxide and provide a basis for scale up to productionize the Choline hydroxide for meeting SCL requirements, as an initiative under 'Make in India' move.

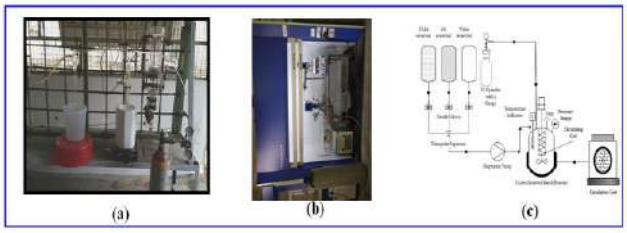
Summary of Project Execution:

This project was initiated with an objective to develop a suitable method for synthesis & purification of Choline hydroxide of 4 % concentration and provide a basis for scale up to productionize the Choline hydroxide for meeting SCL requirements. Based on the detailed literature study carried out (1st milestone), direct ethoxylation of TMA is adopted for the synthesis of Choline hydroxide. The ethoxylation is performed in batch mode, and trial runs were carried out to check the process feasibility, in 1L jacketed pressure reactor. Literature reported that higher concentrations of TMA most likely reduce the by-product (mono & di ethoxylated cholines) formation. Issues herein, with regard to handling of TMA and EO were resolved. At this stage, analysis of Choline hydroxide formation and unreacted TMA was carried out using LCMS ESI. This method of analysis gave an approximate analysis only. However, for initial feasibility studies, it proved to be useful. Procurement of reactor, milli-Q water unit and especially fume hood arrangement were time consuming.

Since, higher number of moles of TMA were being used, in order to remove TMA after reaction, some experiments were carried out in a 250 mL glass jacketed reactor, wherein, followed by the reaction, excess TMA was removed by nitrogen bubbling and mild heating. Based on literature as it was seen that heating of the product has the tendency to decompose choline, or even lead to by-product formation, optimization of mole ratio of EO to TMA was studied. This ratio was optimized to 1:1.1 (Reference E24; Time taken until this stage was 10 months). At this mole ratio, no unreacted TMA was detected through LCMS ESI, and hence the remaining experiments were conducted with this mole ratio.

As the experiments yielded 4 % concentration of choline hydroxide, it was thought desirable to carry out experiments for a higher concentration (10 %), in order to minimize added impurities at high dilutions. Thus, experiments were carried out in 1L pressure reactor to attain 10 % choline hydroxide. At this stage, colour change and composition change were observed, and hence stabilizer (paraformaldehyde) was used, for all subsequent experiments.

In parallel, efforts were on, to establish quantification of choline hydroxide accurately. LC-MS method was established. However, procurement of spares and addressing functional and operational issues took time. With this, even the previous experiment samples could be analyzed. Since product was being obtained consistently, in order to report established process conditions, we analyzed for presence of metal elements further to discussions with SCL and NCCCM. Here, we observed presence of metal elements. This also served as one of the factors of motivation for synthesizing higher concentration choline hydroxide, which can later be diluted to 4% as per requirement with zero ppb water. Thus higher concentrations of 20 %, 32 % and 40 % were explored and synthesized.



Experimental Set-up for Choline Etchant Preparation: (a) Condensation of ethylene oxide, (b) Reaction setup for synthesis and (c) Schematic of the Experimental setup

Design of an Efficient Sorption Enhanced Chemical Looping Reforming Process for Improved CO_2 Recovery (*Sponsored By DST*)

This project is sanctioned by DST which is aimed at enhancing the CO_2 capture and H_2/Syngas production, through improved design of Sorption

Enhanced Chemical Looping Reforming (SECLR) process that uses conventional methane as raw material. In this project, a novel, self-sustained, efficient process scheme has been proposed for the production of high purity hydrogen by integrating sorption enhanced steam methane reforming (SESMR) with chemical looping combustion (CLC) and by incorporating heat recovery steam generation (HRSG) as well as power generation sections. The integration between SESMR and CLC is proposed with the objectives of increasing H_2 productivity, reducing CO_2 emission while effectively conserving the process heat, which is achieved by coupling fuel reactor flue gases with reformer and air reactor outlet gases with regenerator.

Thermodynamic Analysis of Plant-Wide CLC-SESMR Scheme for H_2 Production: Studying the Effect of Oxygen Carrier Supports

Sorption enhanced steam methane reforming (SESMR) integrated with chemical looping combustion (CLC) is one of the most capable greener technologies that allows co-generation of H_2 from natural gas together with CO_2 capture. The performance of CLC mainly depends on the sustained reactivity, strength and durability of oxygen carriers (OCs). A suitable combination of active OCs with optimal inert composition is essential to meet the overall thermal demand of integrated CLC-SESMR process. The effect of inert OC supports on the performance of CLC-SESMR has been studied through thermo dynamic analysis based on steady-state plant wide models developed using ASPEN plus (*Aspen One 8.8 academic version*). Ni-based OCs are considered with two different support materials, SiC/Al_2O_3 and $MgAl_2O_4$ at different inert compositions ranging from 0 to 70% by weight. The sensitivity analysis results revealed that H_2 purity and CO_2 captured are directly proportional to the inert composition while H_2 yield is inversely proportional. The optimal inert compositions are found to be 30% and 40% by weight for the respective cases of SiC/Al_2O_3 and $MgAl_2O_4$. In both the cases, the overall performance of CLC-SESMR is found to be nearly same, i.e., with 97% overall methane conversion, 96% CO_2 captured, 98.3% H_2 purity, 2.24 H_2 yield, and 71.4% net plant efficiency. *(Intern. J. Hydrogen Energy*, **2019**, 44(5), 3250)

Long Term Measurement of Ozone, NOx and SO_2 at A Remote Site to Study the Emission Fluxes and Change in Their Concentrations *(Sponsored by ISRO)*

Surface Ozone (O_3) is one of the major greenhouse gases in the troposphere leading to atmospheric pollution as well as global warming. It is a secondary pollutant formed by the complex chemical reactions between oxygen (O_2), nitrogen oxides (NO_x), carbon monoxide (CO) and volatile organic compounds (VOC) in the presence of solar radiation. Unlike stratospheric O3, the tropospheric O_3 is highly reactive with strong oxidizing capacity causing adverse effects on materials, vegetation human and ecosystem. The current work is focused towards studying the correlations between O_3 and weather parameters and developing models to predict O_3 concentration using and multivariate linear regression (MLR) models and artificial neural networks (ANNs). Individual ANN models have been developed to predict the concentration of O_3 during day as well as night using the meteorological and other trace gases data. Further these results are compared with the results of 1st and 2nd order MLR models. The results demonstrate the efficacy of ANN in predicting O_3 levels in atmosphere as compared to regression models.

Yarn Dyeing Using Cavitation

Yarn dyeing is an important operation in textile and handloom industry. In handloom industry, dyeing process also involves high manual hours and direct manual exposure to hazardous chemicals. In the present study, a sustainable solution for yarn dyeing is proposed based on hydrodynamic cavitation to attain the target of uniform dyeing with deep dye penetration at ambient conditions and less processing

time. The unique physical and chemical changes taking place in the medium during the collapse of the cavitation bubbles that are the key factors held responsible for such a quick action and deep dye penetration under normal operating conditions. The lab scale studies were performed with cotton yarn obtained from local handloom park, Telangana. The yarn is subjected to dyeing within IICT hydrodynamic cavitation reactor that runs with a 0.5 KW motor for 10 min of operation and the results are compared with conventional technique i.e. dyeing in heating bath at temperature of 70°C that runs with 1 KW induction coil heater. The cotton yarn was tied with rubber straps and placed in the dye baths for 10 min. The observations revealed that the hydrodynamic cavitation technique imparted higher, deeper and uniform coloration when compared to heating technique. The frugal aspect of the innovation is that the power required for hydrodynamic cavitation is 50% lesser than the power required for heating. Moreover the dye penetration was uniform and even in the case hydrodynamic cavitation based dyeing process wherein heating based dyeing imparted no visible coloration on the yarn in 10 min. The uniform coloration of yarn through its thickness was also attained wherein the gap between the ties of the yarn is as less as one centimetre.

Hydrazine Hydrate Basic/Detailed Designs for M/s Gujarat Alkali Chemicals Ltd., Gujarat

Design Report for 10000 TPA of 80% Hydrazine Hydrate was submitted to GACL. The report was vetted and approved by GACL and their consultant LTHE. LTHE prepared the detailed engineering designs, specifications and drawings based on Basic Design Report of IICT for procurement and construction. After approval from IICT, commercial plant construction was begun and is in progress. It is expected to be ready for mechanical and process commissioning by December 2020. The Design Report and the drawings are well accepted by GACL and LTHE. The Department has again proven its competence and expertise in scale up and technology transfer from bench scale to commercial scale along with commercial plant design. Received FICCI Award 2017 and Golden Peacock Award 2020.

Basic Engineering Designs of PTBT and PTBBA

Vinati Organics Ltd, Mumbai approached IICT to provide Basic Engineering Designs for commercial plant to produce PTBT and PTBBA, based on pilot plant runs which were demonstrated successfully and the basic design report was submitted. Post-design work has already started at the site by the client. For this work, the IICT team was awarded **CSIR Technology Award for Physical Science including Engineering – 2018** for "Technology Transfer for Commercial Plants of 4000 MT per year of para-tert-butyltolune and 3000 MT per year of para-tert-butylbezoic acid".

Basic Engineering Designs of Para Tertiary Butyl Methyl Benzonate (PTBMB)

Basic Engineering Designs were carried out for esterification of para teritary butyl benzoic acid to PTBMB (Capacity enhanced from 6 TPD to 10 TPD). Pilot Plant runs were conducted and successfully demonstrated. The design report for the commercial plant was submitted. Post-design work has started at the site. The client is Vinati Organics Ltd, Mumbai.

Basic Engineering Designs of PMPAA Commercial Plant

Basic Engineering Design Report for commercial plant based on pilot plant runs has been submitted to the client Vinati Organics Ltd, Mumbai. Post-design work will be started by the client.

Basic Engineering Designs for Avobenzene Commercial Plant

Vinati Organics Ltd, Mumbai approached IICT for Basic Engineering Designs of commercial plant for the production of Avobenzene, based on pilot plant runs which were demonstrated successfully. The Process Flow Diagram has been prepared and is being discussed with the client.

Basic Engineering Designs of Benzaldehdye Commercial Plant

Vinati Organics Ltd, Mumbai approached IICT to provide Basic Engineering Designs for commercial plant for the production of Benzaldehyde, based on pilot plant runs. Pilot plant Detailed Engineering Report prepared and submitted to the client.

Basic Engineering Designs of Paracetamol Commercial Plant

Basic Engineering Design Report of commercial plant for Paracetamol is to be prepared for Bharat Chemicals Ltd, Mumbai. The commercial plant design is based on pilot plant runs which were demonstrated successfully. The Process Flow Diagram has been prepared and is being discussed with the client.

Facility Creation and Modernization of Pilot Plant

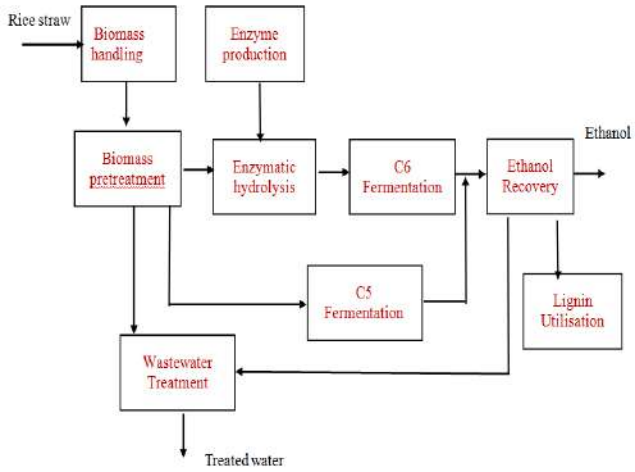
Under the budget head "Apparatus and Equipment" towards facility creation projects an amount of Rs 675 lakhs has been sanctioned from CSIR and three pilot plants (PP-I, PP-II and Hydrogenation) plants for renovation and modernization. The present modernized pilot plants are equipped to collect & generate data for commercial plant designs, be able to demonstrate the process to industrial clientele more effectively and help generate external cash flow. The probable clients are from drugs, pharmaceuticals, fine and speciality, pesticides, and this facility can be utilized for custom synthesis of high cost/low volume products for the processes developed for industrial clients. The technical services have been rendered to following industries:

- M/s PJS Pharma Ltd, Hyderabad.
- Lucas Technologies, Hyderabad
- ICRISAT, Hyderabad
- Covalent Laboratories Pvt. Ltd, Hyderabad

Technology Assessment and Integration of CSIR Lignocellulosic Ethanol Program/ Facilitating Technologies for 2 G Ethanol

Development of a 2G ethanol techno-economic model (an integrated technology for bioethanol production with absolute cost estimation for the ethanol from this process) which is to be achieved through selective integration of CSIR's existing process(es) and knowhow, after their validation at pilot scale and incorporating improvisations. Pretreatment is a key process step in 2G ethanol technology mainly associated with modification of the biomass material and making accessible to enzymatic saccharification which is mainly influenced by process steps of milling and pretreatment. The optimized process includes low temperature operation in atmospheric pressure, minimum chemical consumption. Presently, efforts are being put in to prepare value added products from rejected lignin, so that economically the cost of ethanol can be reduced. Several pretreatment processes though developed, all most of them involve high energy. A method developed by CSIR-IICT which is novel chemical treatment process operating at low temperature and atmospheric pressure was

used for pretreatment which retained more than 98% cellulose and hemicelluloses; and removes 80% of lignin. The pretreated water can be recycled 5-6 times and so obtained lignin rich water processed through membrane to retrieve 80% to recycle 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% saccarification within 16-20 hrs which depend on the substrate enzyme ratio. The above data was generated using rice straw as biomass. Based on the data generated, the process designing will be done in an integrated approach in collaboration with other CSIR laboratories information.



A schematic of the entire process of the PAN 2G ethanol program

Biomass pretreatment at different stages in a 10 L batch reactor

Design and Development of Wind Mill System for Underground Water Lifting

The Palle Srujana Organization approached CSIR-IICT to carry out the engineering designs for a water pump and gear train for the wind mill. The hydraulic pump is to draw the water and get the desired output of 5000 L/h for agricultural use. This project was taken up for societal benefit. An Engineering Design Report consisting of design calculations, mechanical fabrication drawings of gear box of windmill and plunger pump assembly was prepared and submitted. A CFD analysis was carried out and the report prepared.

The purpose of the study is to design and construct a wind mill that is able to provide water to rural villages of India. The overall design goals of this work are focused on affordability & simplicity of design to meet the farmers' desirable requirements.

Objective:

(1) Standardization of drive mechanism of windmill system

(2) The windmill pump design to meet the desired pump water discharge of 5000 liters/hr

(3) The design must be a low-cost model

Benefits: The wind is a natural and renewable resource that is freely available all over world. In present problem at coastal areas of Andhra Pradesh, India farmers are cultivating aquaculture. Aquaculture, also known as aqua farming, is the farming of fish, crustaceans, molluscs, aquatic plants, algae, and other organisms. Aquaculture involves cultivating freshwater and saltwater populations under controlled conditions, and can be contrasted with commercial fishing, which is the harvesting of wild fish.

The farmers of aquaculture are needed more water to cultivate aquaculture and also they need more amount of power to lift water from the ponds, well and underground etc.

Windmill is the best system to generate power for lifting water, which would save a lot on power costs for such aquaculture farmers.

Activities in Pilot Plant Complex (PPC)

The pilot plant complex supports in house R&D and Incubators in their activities. The in-house R&D pilot plants established includes Bio-Hydrogenation (10 M^3) pilot plant by BEEC division of IICT, a lemon grass field for lemon grass distillation. The incubates include M/s Maithri Aquatech Enterprises, M/s Khar Energy Optimisers besides M/s BHEL.

Maintenance Activities: As part of support to R&D activities, the maintenance water supply and maintenance of electrical power both grid supplied as well as stand-by power supply play a major part. New over head tanks of smaller capacities were installed and new pump sets (7.5 Hp and 10.0 Hp) were installed in place of defunct sets in order to provide trouble free water distribution. The electrical switch gear in the sub-station (2 x 500 kVA Transformers and 2000A LT Bus Bar, PCC &MCC Panels,) besides DG Sets (600 kVA and 165 kVA), street lighting etc., were periodically over hauled for safe power distribution.

The coal crushing unit, the coal conveyor, Boiler, Oxygen plant and DM plant which are auxiliary units of coal Gasifier, were condemned as these were non-functional for many years.

Lemon Grass Harvesting: It was proposed to harvest lemon grass for oil. An area of 1.5 acre is earmarked for the purpose. The area is cleaned off departmentally and in Co-ordination with CIMAP (sister laboratory under CSIR), the plantation was carried out by the garden section of IICT. Upkeep of the complex

New Pilot Plant Facilities

Agro Mission Project: The new plant structure plant comprises process development equipments like utoclave, Glass distillation column, SS Distillation column, tray dryer, agitated nutch filter, centrifuge, scrubbing system, vacuum pump, colling tower, chilling fluid circulator and the proposed budget including Erection and Commissioning of 11KV new Substation.

Distillation Unit: Under Aroma Mission, a distillation unit (500 kg) is indented from CSIR-IIIM, Jammu, CSIR sister Institute. The distillation unit with following specifications to be installed at IICT. SS Distillation tank (2400 lt), Condenser, Oil Separators, MS Chimney, Material unloading system, (Chain pulley block system with MS angle iron support structure), water tank with MS support structure, Portable Pump (Diesel engine) and other Accessories.

Activities at CSIR-IICT Main Campus

R&D Facilities:

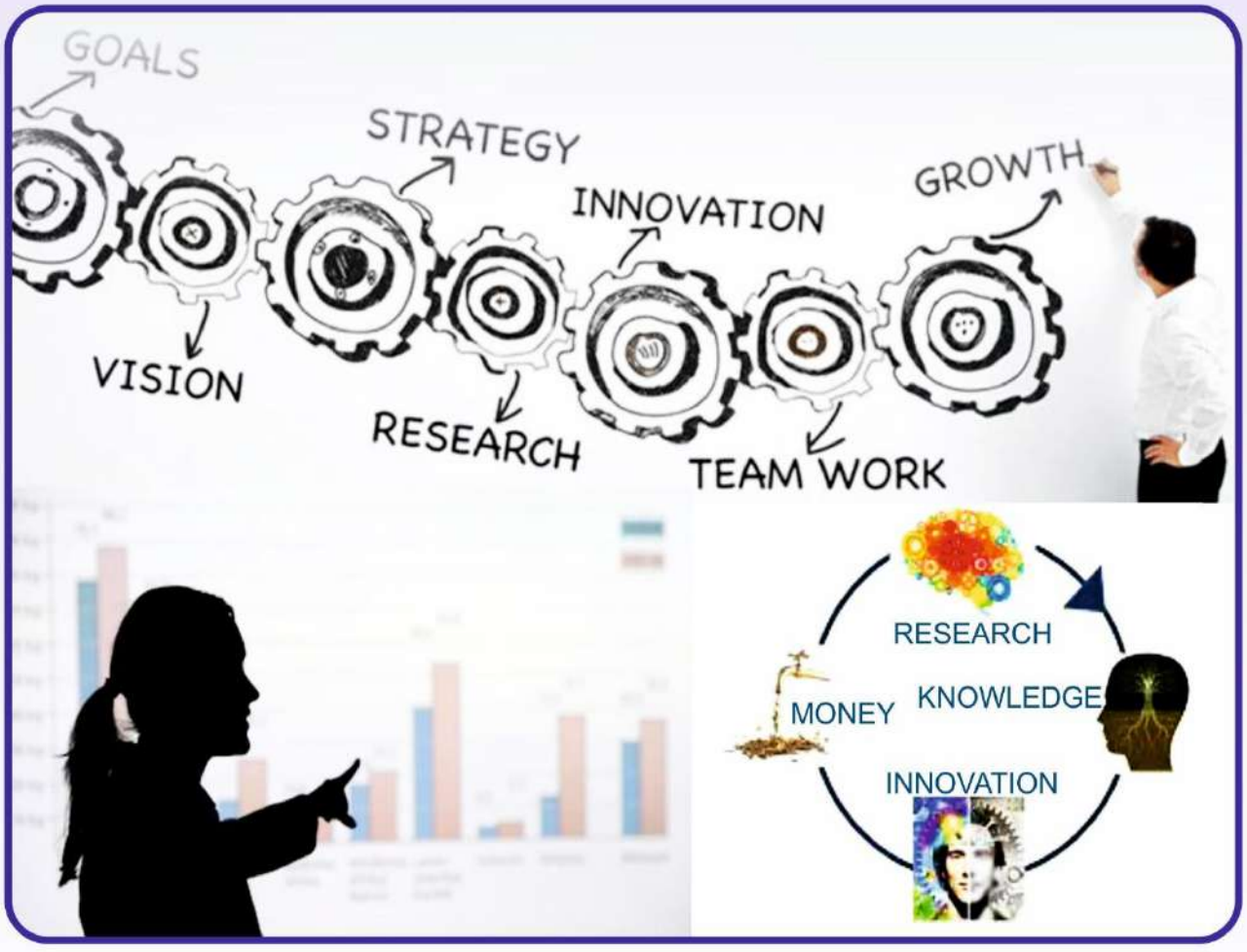
Bio mass gasification (2kg/h) unit: Under waste-to-energy initiatives, especially focusing on the agri waste, skid mounted bio-mass gasification unit comprising of gasification unit, hopper, gas liquid separation unit, quenching unit, steam generators with control circuit is installed at workshop.

As part of solar innovation one BLDC Pump driven by Solar Power was tested. This work includes making of Suitable pump to BLDC motor in the Machine shop and tested.

Maintenance Mechanical Work Shop (Machine Shop, Fabrication)

Periodic and the preventive maintenance of Electrical Switch Gear connected to shop floor machines, i.e., lathe machines, radial drilling, milling machines, slotting machines, shapping machines, hammering machines, automatic double column horizontal band saw machine, hydralic press, welding ding machines, air compressors and non-ibr boilers. Electrical Drives were installed at Prototype R&D area to test Palle Srujana projects and other activities which require to perform at different speeds of installed motors. As part of maintenance & repair of wide range of mechanical equipment and S.S. and M.S Fabrication works i.e modifications to storage vessels, Cover plates, Purifiers, Pumps, Frames, opening/Closing Valves for reactors/R&D equipment as per the requirements of scientists for easy and accurate sampling and also involved in making of M.S and Steel Trolley, Floor Mounted Cylinder Brackets, Cylinder Stands and other structure repair works on average 300 work order per year The shop floor supports R&D activities of entire Scientific fraternity and Institute in general. The Job Requisition Forms executed for the period is 1000 work order at an value of 10.0 lakhs.

BUSINESS DEVELOPMENT & RESEARCH MANAGEMENT



The Business Development and Research Management Division is the Institute-Industry-Societal Interaction Facilitation wing of CSIR-IICT. The Division aims to promote & propagate the expertise and capabilities of the Institute and enables offering research solutions that cater to industry and societal needs. The department is nodal for coordination, liaison and research management activities such as IP, ISTAD, RC meetings, CSIR funded projects and Skill development programs.

The following encompass the major activities of the Division:

- Business Development and Management
- Project coordination of CSIR funded projects
- Research Management Activities
- Entrepreneurial and Skill Development Programmes

ACTIVITIES

Business Development and Management:

Healthy Interaction between industry and academia provides the potential to lead scientists of CSIR to explore new and viable solutions that benefit the society. To harness this potential, the department creates seamless interaction platforms to identify areas of collaboration that match the business interests of the clients, while addressing issues that appeal the society at large. To this end, BDRM works closely with the research groups of CSIR-IICT and organize Industry Interactive Meets. This industry outreach program, aims to facilitate one-to-one interaction between industry and scientists of the Institute.

The core strengths of the institute are classified into three major sectors such as 1. Pharma and Agro chemicals 2. Catalysis and Fine chemicals and 3. Environmental and prospective industries are mapped against these sectors for building business. Connects with major associations like IDMA, BDMA 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 were organized biannually with panel discussions by experts on topics pertaining to current R & D issues and showcase the solutions that CSIR can offer. Participated in major exhibitions & events in the form of display of exhibits and lectures with clear objectives of capturing the interest of new clientele.

Business Management

BDRM activity is aimed to provide an interface between CSIR-IICT management, R&D departments and user agencies such as industries (National and Overseas), government departments, public sector organizations to offer R&D services like, technical, consultancy and technologies. The department undertakes multifarious activities to facilitate CSIR-IICT management achieve the above goal.

BDRM's charter is marketing of CSIR-IICT knowledge base and technical strengths to user agencies and prospective clients. Business Management activities play a key role in contributing to External Cash Flow (ECF) (Non Grant-in-Aid projects), by facilitating transfer of IP & technology development and providing S & T managerial services. The activity popularises the image of the institute and catalyses its performance.

The Major Activities that were undertaken in this Direction are:

- Projecting CSIR-IICT Capabilities and Expertise to Industrial Clients
- Attracting industry by planning and organizing industry meets for technology promotion, identifying industrial problems and to explore potential areas of collaboration.

- Prospective client's visits and exploring new research collaborations by projecting CSIR-IICT's R&D capabilities and expertise to them.
- Negotiating with Industrial Clients to Explore New Research Collaborations
- Coordination CSIR-IICT management, scientists and industrial clients to finalise the scientific framework of collaboration
- Pitching in with industries for identifying and finalizing new research collaborations.
- Arranging Non-Disclosure Agreements for exchange of information.
- Preparation of financial estimates of projects and liaison with 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 by coordination with clients and scientists.
- Obtaining necessary approvals from CSIR-IICT management, Management Council and CSIR HQ, wherever necessary
- Facilitating for realization of obligations and concerns of clients in the contracts
- Organise Project Monitoring and Evaluation meetings of all Industrial projects
- Regular follow up with clients and scientific teams to track the progress and activities of ongoing collaborations and facilitate smooth and timely completion of the projects.
- Raising Invoices and processing of 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

Project Management of CSIR funded projects:

BDRM plays an important role in handling administrative aspects of major projects like Mission Mode projects and Thematic projects such as Fast Track Translational (FTT), Focussed Basic Research (FBR), Nische Creating Projects (NCP) and Fast Track Commercial Projects (FCP) and other In-House sponsored projects etc. The department maintains the complete database of all the projects that includes fund sanction and receipts, expenditure, i.e., fund utilisation, deployment of temporary manpower, R&D achievements, progress reports etc. Also periodical project review meetings and project monitoring committee meetings (PMC) for performance evaluation and advice are organised with the committee of experts constituted for by the competent authority. In coordination with Theme Directorate, BDRM interfaces in providing information on various opportunities/ avenues available for R & D funding by CSIR-HQ from time to time. Processing of the new R & D proposals submitted by scientists as per the protocols of scrutiny by three-member committee and obtaining the necessary approvals and liaison with HQ is ably taken care by the department. Further, BDRM handles CAG/Internal Audit and the liaison/ Coordination of all ongoing projects of CSIR funded projects and In- house projects as well.

Table-1: Overview of CSIR-Funded projects during the financial year 2018-19 & 2019-20

Project Type	FY:2018-19 (INR in Lakhs)	FY:2019-20 (INR in Lakhs)
Mission Mode	2343.3	2328.8
Skill Development & JIGYASA	67.35	188.75
Thematic and Fast Track Translational	1345.2	1740.677
CSIR-HARIT	18.35	194.38

Entrepreneurial Programme with CSIR's labs S&T solutions:

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. Hence, on behalf of CSIR, BDRM, has conceived a new program entitled "**Be an Entrepreneur of Science and Technology - BEST**" in collaboration with NGO's, NRDC & CSIR HQ 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 subject them to grooming classes on the Technical and Business management aspects for commercial feasibility assessment, followed by mentoring the candidates for start-up and incubation with financial assistance from Bankers. Interested entrepreneurs were enrolled and were provided with the compendium of societal S & T interventions of all CSIR labs for helping them chose and classes were held to enlighten them on the offerings.

Training Programmes under CSIR Integrated Skill Initiative:

The skill India program at CSIR-IICT aims to create opportunities, space, scope for the development of the talents of the Indian youth and to develop more of those sectors which provide employment and entrepreneurship. The idea is to raise confidence, improve productivity, providing direction through a balanced growth in all the sectors so that all jobs should be given equal importance.

CSIR-IICT strongly believes that practical training cannot happen within closed doors. It is trying its best to bridge the gap between industry and academia. Today CSIR-IICT encourage innovation in ideas to support entrepreneurship, creating more platforms for knowledge sharing for the youth (on both technical and soft skills), encourage students to participate in skill competitions across the country/world and make a mark for themselves.

As part of CSIR-Integrated Skill initiative, job oriented Skill Development Training Programmes are designed in Chemical Sciences, Analytical Sciences, Biological and Mechanical Engineering Services. BDRM is nodal for planning, coordination and liaison of skill programs of the institute. Activities such as preparation of advertisement, brochures for promotion of the training programs, interfacing with course coordinator and the participants, certificates design and arrangements providing all administrative and managerial assistance for seamless conduct of the programs is done by the department. Organising the inaugural and valedictory ceremonies of the training programs and intermittent counselling to participants during their stay at the institute as and when required forms a regular part of the responsibilities.

Following are the Skill Development Training programmes being conducted by CSIR-IICT during the period.

Table – 2: SDP

Sl. No	Sponsoring industry/ Govt agency name	Name of the course	From date	End date	No. of candidates trained
1	Advertisement, CSIR-IICT	Certificate course in process plant drafting using Autocad	28-05-2018	22-06-2018	8
2	Advertisement, CSIR-IICT	Training Programme for M.Sc. (Chemistry) Students From North-Eastern States	01-09-2018	30-11-2018	37
3	OPCW, The Netherlands	Analytical Skill Development Course	03-12-2018	14-12-2018	19
4	Dr B V Raju College, Bhimavaram, AP	Basic Cheminformatics	21-01-2019	01-02-2019	27
5	Bhavan's College, Secunderabad	Basic Cheminformatics	18-02-2019	28-02-2019	30
6	Advertisement, CSIR-IICT	Refresher Course On "Processing And Analytical Methodologies Of Oils & Fats"	20-03-2019	22-03-2019	22
		Total			**143**

Details during 2018-19

Table – 3: SDP Details during 2019-20

Sl. No	Sponsoring industry/ Govt agency name	Name of the course	From Date	End Date	No. of candidates trained
01	CRCL, New Delhi	CRCL Batch I Group A Officers	22-04-2019	16-05-2019	20
02	Advertisement, CSIR-IICT	Process Plant Drafting using AutoCAD 2019	27-05-2019	21-06-2019	11
03	CRCL, New Delhi	CRCL Batch II Group B Officers	11-06-2019	12-07-2019	20
04	TSFCL, Telangana	Telangana State Forensic Science Laboratory	03-06-2019	06-06-2019	6
05	Ministry of Environment Forest & Climate Change (MoEF & CC), Govt. of India	Data Analysis	26-08-2019	11-10-2019	20
06	Advertisement, CSIR-IICT	Laboratory Animals in Biomedical Research (LABR)	05-09-2019	30-09-2019	5
07	CRCL, New Delhi	CRCL Batch III Group A Officers	19-082019	20-09-2019	20
08	Advertisement, CSIR-IICT	Orientation cum Training Programme to students of North Eastern States	03-09-2019	03-12-2019	51
09	CRCL, New Delhi	CRCL Batch IV Group B Officers	02-12-2019	27-12-2019	20
10	Advertisement, CSIR-IICT	Basic Cheminformatics	17-12-2019	27-12-2019	36
11	OPCW, The Netherlands	Analytical Skill Development Course	25-11-2019	06-12-2019	20
12	Advertisement, CSIR-IICT	Quality Control Chemist	06-01-2020	29-01-2020	8
13	Advertisement, CSIR-IICT	Lab Technician – Research & Development	06-01-2020	31-01-2020	2
14	Advertisement, CSIR-IICT	Basic Cheminformatics	17-02-2020	28-02-2020	33
Total					**272**

Research Management Activities:

- Processing of bilateral exchange agreements & visits, security/sensitivity and clearance of overseas projects proposals with CSIR Hqs for necessary approvals from MEA, DIPP, DG-CSIR
- Processing of foreign deputations of permanent staff, students and temporary staff To ISTAG committee of CSIR-IICT,
- Processing of Scientist G foreign deputation proposals to ISTAD, CSIR Headquarters and Director's proposals to MEA, MHA, and ISTAD-CSIR headquarters,
- Interaction with CSIR headquarters and other Govt. agencies related to R&D planning, overseas projects,
- Employment verification of temporary manpower,
- ISO Archives,
- Role mapping and national project mapping of employees and project mapping in ERP

The R&D achievement of the institute's reporting activity is done every monthly, quarterly and annually. The following reports are submitted to CSIR accordingly.

- Monthly R&D Achievement Reports.
- Quarterly & Annual Research Utilization Data.
- R&D achievements information for CSIR Annual Report.
- C-Data Intographics systems (C-DIS)

IPR Management and Licensing

One of the important roles of BDRM division is to judiciously manage the created IPs through the R&D

activities of the institute. The institute holds one of the highest IP portfolios among CSIR Laboraties. The major activites performed by the department in theis direction include :

- Coordination between IPU, inventors and attorneys to draft and timely responding of the staturory queries in the prosecution process of patents and other IPs.
- Coordination with CSIR-URDIP to avail various IP services as and when desired by our scientists and institute.
- Convening the IPR management committee meeting for considering new proposals of patents, renewal or lapsing of granted patents based on their utility.
- Providing the timely reply to CSIR queries, funding agencies queries, RTI and audit paras.

In addition, the department takes lead in promoting the IPs and attrat potential licencies. In the year 2017-19, a total of 91 patents got granted altogether in India and abroad and 14 patents got licensed. The licensing rate achieved by the departments is above 15%, which is way above to global average patent licensing ratio.

Processing the distribution of Premia/Royalty to the project staff involved in the completion of Sponsored / Consultancy projects as per quidelines.

COMPUTER CENTRE

The Computer Centre of IICT started in 1966 and is one of the oldest computer centres in CSIR Labs. It 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.

VISION:

To establish a secure, reliable and high quality Information Technology infrastructure to facilitate the scientists and research students in carrying out their Research & Development activities

MISSION:

- To provide IT technical support and services
- To educate all staff and research scholars on effective utilization of IT infrastructure and services
- To provide effective technology support audio/ video, multimedia and web based applications
- To facilitate the institute with data storage, digital security and integrity of electronic data
- To develop, enhance and manage the digital network for providing seamless high speed connectivity among all information resources.
- To promote paperless operations
- To provide effective, timely, reliable and secure IT services in 24X7 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

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.
- SOPHOS UTM 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

Data Center

CORE COMPETENCIES:

- Security Management (UTM in High Availability, Servers, Clients)
- Windows/Linux Server Administration
- Virtualization
- Database management: RDBMS: Oracle/MSSQL/ MY-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/MY-SQL
- System: LDAP/DHCP/DNS/WINS/Samba
- Network – Firewall/NFS/NIS/SSL/SSH/ VPN
- Web Server: Apache/IIS

SOFTWARE DEVELOPMENT:

The Computer Centre is undertaking applications software development in the areas of scientific importance to institutional research programs as well as internal requirements. Additionally, it provides scientific inputs based on computer aided techniques to ongoing R&D Projects. Some of the application software developed for various internal departments depending upon their requirement viz.

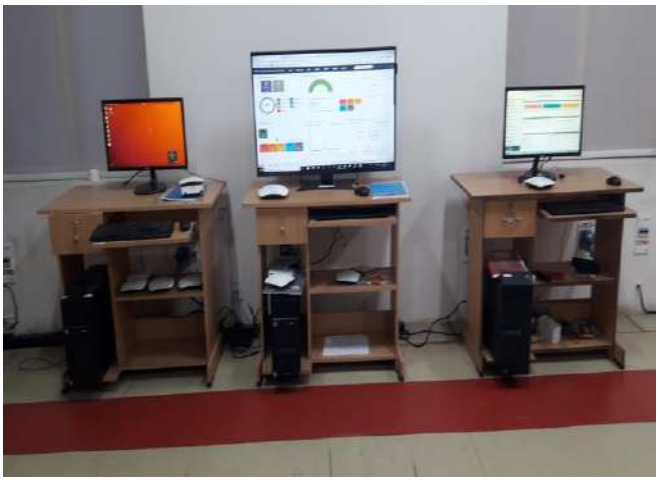
- Application for distribution of project monies (Honorarium and Royalty)
- Application for the Security Visitor's Pass System at main gate of IICT.
- Application for the Dispensary Pathological services for generating various pathological reports.
- Web portal for publicity of Analytical Facilities and Services available in IICT
- Web portal for accepting online applications for various skill initiative programmes organised in IICT
- Web portal for accepting online application for recruitment of various permanent positions in IICT
- Web portal for publicity of forth coming seminars
- Web portal for research career opportunities
- CCNET: An Intranet web portal for the various maintenance modules/ software installations/ software patches/ general instructions etc.

Support	Ongoing software projects
• Molbank IT support • Research Instruments IT support • NEERI Zonal lab IT support • MPDS: Molecular Modelling • Bio-Envis • Computational Chemistry • Biometric & Surveillance • Software support for Admin Groups	• Implementation of e-Notebook, Chem-Draw Professional software • GIGW Compliant website • Analytical facilities Portal • Online Recruitment Portal • Continuous Network vulnerability assessment

SCIENCE INDIA PORTAL:

Vijnana Bharathi is a non-profit organization with a mission to popularize swadeshi science in India and promote modern sciences that are adapted to national needs. Vijnana Bharati and CSIR have entered into an MOU with an objective to popularize Science in India among student community. As part of the

MOU, IICT computer centre hosted the Science India Portal (url: http://scienceindia.in)



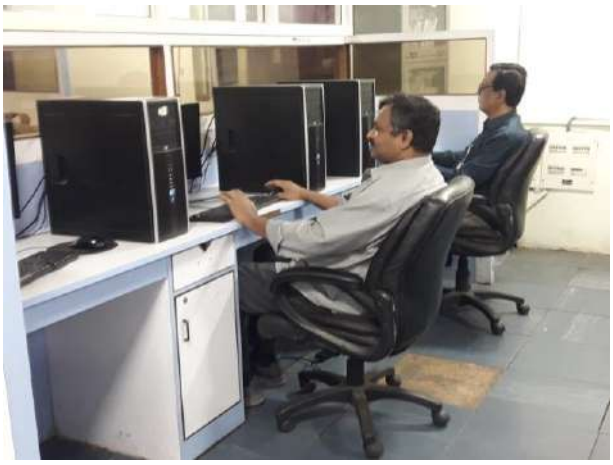
Network Operations Center (NOC)

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.

- Multimedia services
  - Video Conference / Skype/ OHP/ Public Address System for seminars, workshops, conferences, high level meetings etc
- User Services
  - Desktop/laptop troubleshooting services
  - Configuration of access to network services
  - Print/File services sharing across workgroup
  - Virus patches downloading/applying to PC
  - Operating System installation/ upgradation/ Hard Disk Error fixing
  - Managing user e-mail accounts
  - Personal folder management for user email accounts
  - Providing service like HTTP, FTP, TELNET etc to Power Users
  - All the client modules of Scientific Software implementation
  - Application Software Installation and User training

Multimedia Support services – VC/ Skype / OHP



Troubleshooting and service center

KNOWLEDGE & INFORMATION MANAGEMENT

Department of Knowledge & Information Management

The primary responsibility of DKIM is to ensure the smooth functioning of research activities of the institute by providing reliable and secure information which will be effective and transparent to assist the management in promotion, dissemination and exchange of knowledge. The Institute is engaged in a wide spectrum of R & D in both basic sciences and industry related work. Therefore, in the interest of the Institute's growth and to ensure better recognition and visibility a new **Department of Knowledge & Information Management (DKIM)** was created on February 1st, 2018.

DKIM is also associated with Human Resource Development and management which include facilitating temporary and permanent staff in projects and other research work. New Project Proposals are forwarded for funding to various agencies under the Grant-in-Aid (GAP) schemes. Processing and monitoring of temporary manpower requisitions and their induction are checked and facilitated the requests of the respective principal investigators. Apart from these activities DKIM plays an important role in MANAGING organizational responsibilities such as:

- Information Management
- Project Management
- HR Management
- Events Management
- Press and Media related activities
- Social Media

Information Management:

Library is a combined facility for two National Laboratories, CSIR-IICT and CSIR-CCMB It has internationally acclaimed reference collections in frontier areas of chemical, engineering and life sciences, thus playing a vital role in acquisition, organization, and dissemination of knowledge. It has an impressive collection both print and electronic resources, including books, journals, technical reports, standards, patents, theses and other materials. It has adequate infrastructure to meet the requirements of its users. The main thrust of the library continues to be the improvement of the quality services and facilities, achieving higher degrees 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 important journals. The total print collections are more than one Lakh in number. The Library subscribes to National and International journals both in print and electronic formats. Besides 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 houses a complete collection of Chemical Abstracts from the year of its inception i.e. 1907 This collection is now available online from January 2012.The Library's computer infrastructure has been upgraded and user rooms have been created to facilitate the usage of CD-Rom databases and browsing of E-Resources. Online databases and E-Journals are made available at their desktops. The CD-Rom/E databases include Chemical Abstracts, Indian and ASTM Digital Library, Collection of Annual Reports, and 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 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 any single source for scientific information in journal and patent literature from around the world. Moreover, unlimited access has been provided for this database to all the scientific staff of IICT.

Chemical Abstracts (Web Edition): Chemical Abstracts include 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 the same is available on CD's. January 2012 CA is also 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 with a view to support chemists in their daily search with focus and relevant information in chemistry by providers of Crossfire platform. Now crossfire has been migrated to Reaxys, an advanced platform over Crossfire.

Web of Science: The Web of Science provided through CSIR consortium enables seamless access to 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, users 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 met by 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 in addition to print journals of IICT, scientists have access to multiple journals at their desktops.

Library Home Page: Library Home page http://libdoc has also been designed and maintained by this division, serving as one-point access to all the above mentioned E-Resources. Its features have been enhanced by updating utilities from time to time.

Digital Repository of IICT (DRI): DRI is a digital archive of the research output of institute scientists. It is a mechanism for making research more widely available to researchers. This knowledge base consists of journal articles, technical reports, presentation/lectures, preprints, theses, images etc,. One can browse the documents referring to author, division, subject and date. Both simple as well as advanced search facilities have been provided here. Publications from the year 1947onwards and bibliographic details of Ph.D thesis from the year 1945 onwards are also available. The software that was chosen from amongst the landscape of software platforms for building DRI is ***Dspace*** (Dspace 1.5) with Java, Apache Ant, Maven, Postgre SQL and Apache Tomcat on Linux OS. This Software has the facility to upload preprints by the scientists themselves in to DRI.

Activities: Scientometric analysis of IICT research publications: Information on the bibliographical details along with the Impact factors of the research papers of IICT are regularly communicated to the management and NISCAIR of CSIR in calculating the research output of the Institute thereby 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.

Services: CSIR-IICT provides a range of Library and Information services like Circulation service, Inter-Library Loan service, Newspaper Clipping service, Photocopying service and Referencing service.

Services to Industry & Outside Agencies: It is to be noted that DKIM provides library utilization facilities to Industry and other Agencies on membership basis. Apart from Internal users, these facilities have also been extended to research scholars from Govt. Universities registered for Ph.D for free and to the corporate sector through the paid membership of the library.

Project Management & HR Management:

DKIM inform all scientists about various calls for new proposals from various National and International funding agencies. The details of the calls are circulated among the scientific staff and the department facilitates timely submission of the proposals. Subsequently, GAP proposal are processed by verifying and preparing all the documents, providing data on plagiarism check, internal committee report, endorsement, authorization and certificates etc., required for submission. This is based on the guidelines of the Institute and the approval of the competent authority

These proposals are forwarded for financial support to various Central and State government funding agencies like CSIR, DST, SERB, DBT, ICMR, BRNS, FSSAI, BIRAC, MNRE, IOCL, CSIR-TWAS, MOCF, etc, under various categories and schemes. All the information related to the proposals is updated on "RMANET", an internal database. DKIM also maintain all the related documents of sanctioned, ongoing and completed GAP projects.

Allotment of GAP Project No.s to the sanctioned projects is another activity of this division. Once the GAP number is allotted, it is informed to the PI Finance and Purchase department for smooth running of the project. This department helps Finance and Accounts department in Preparation of utilization certificates / statement of expenditure, replying to audit queries GAP projects, forwarding UCs and SEs to the funding agencies, uploading scanned copies of UCs and SEs in PFMS, and update information in One CSIR.

DKIM is processing and coordinates with the administration / Pl for manpower requirements of GAP Projects. This department also handles all queries related to deputation of Ph.D Students/Project assistants to attend Conference / Workshop under GAP Projects in coordination with the PI. SRF applications are processed for Ph.D and Research Associate programs. Temporary manpower is requisitioned and their induction is assisted from time to time. Various fellowship applications, National and International (CSIR-TWAS, Ramanujan, Ramalingaswamy Re-Entry fellowships, Short term international visit programs, CSIR-NPDF, DST Inspire, ICMR etc.) are also processed by this department as per the norms.

Certificates are designed and issued to students who complete their PhDs and Project (JRF, SRF, RA, NPDF, TWAS, Ramanujan, Ramalingaswamy and Inspire, etc).

Drafting of Agreements/ MOU's/MOAs for Academic and Joint Collaborations

The visibility of an institute is immensely enhanced by collaborations with other academic and research institutes and also with national and international universities of repute. CSIR-IICT always encourages these initiatives that are under scientists. The DKIM assists scientists in drafting and executing Inter-institutional and inter-disciplinary joint collaboration agreements

between CSIR-IICT and other National Universities and research institutions.

Events Management:

Organizing Institutional Science Events: Another important activity of the department is organizing various scientific events in the institute throughout the calendar year. Seminars, Conferences, Symposia's (National and International), Guest Lectures and Retirement events are either organized by the department or assistance are provided to the organizing. Correspondence with Chief Guest regarding lecture invitation, raising sanction order, approvals from competent authority, printing of invitation cards & posting them to retirees, Universities, CSIR Head quarters, Directors of other CSIR institutes and also other eminent personalities are taken care by this department including arrangement of logistics. Besides, the department involves itself in guiding visitors from Schools, Colleges, Organizations and Training Centers like ASCI and ni-msme, VIPs and VVIPs as well as visitors coming from abroad.

The following National events are also organized on the designated dates.

1. Feb.28th National Science Day
2. March 8th International Women's Day
3. May 11th National Technology Day
4. June 5th World Environment Day
5. August 5th CSIR-IICT Foundation Day
6. Sept. 26th CSIR Foundation Day
7. Organization of common farewell function for retirees on monthly basis

During this period, DKIM was actively involved in many functions organized in connection with **"Platinum Jubilee Year Celebrations",** CSIR-IICT's 75th year of service to the nation.

Awards Information:

The scientists of CSIR-IICT receive many Awards, Honors and Accolades throughout the year. On the occasion of awards announcement congratulatory notes are prepared to acknowledge the staff and students' recognition and honor. In case of very prestigious awards, press notes are issued for publicizing to the common people.

This department also plays key role in the selection and announcing the IICT annual appreciation awards and rewards for the staff members and also the annual CSIR awards to wards of the staff members.

Documentations:

Documentation is one of the most important activities of DKIM and it played very significant role in the preparation of various documents during this period.

75years Platinum Jubilee Celebrations Souvenir: In this souvenir, historical data was collected since the inception of RRL till date. A record of the glorious past of RRL to IICT was compiled in the form of pictures and literature depicting the landmark achievements over a period of 75 years.

CSIR-IICT Brochure: A colorful, glossy brochure was prepared with pictures of the Institute and the various Instruments housed in it with persuasive notes attracting the attention of the potential clients with a view to boost the transfer of technology and knowhow.

Designing and Compiling of Annual Diary: This department takes the responsibility to design the diary of every year and compile the data on the institute, details of the staff members, mission and vision of the institute and all important and

necessary information including contact numbers and mail IDs. Branding & Promotional Activities: DKIM also take active role in preparing posters, brochures, handouts, periodicals, biennial reports, face book, twitter exhibits.

Press related Activities:

Branding and publicity of CSIR-IICT is a major function of DKIM. The responsibility of projecting correct image of the institute and its scientists is of paramount importance. Besides, the public are informed about the work of our institute through various media platforms. The efforts of this department in this direction are:

Press Invites: For any event such as symposia, Foundation Day celebrations and major interaction with scientists and industry, it is required to publicize the programme. The first step in this direction is drafting a press invite to request the media to visit our institute to cover the programme. The press invites also serves as an event alert that is published in various newspapers. Through this the common public and other interested people are alerted about the impending event.

Interaction with Media: The media is invited to our campus to cover important events. Through such interactions, our work and events are prominently highlighted on various media platforms. The public gains knowledge about the work initiated in our institute. It helps to bridge the gap between scientists and common people. Press conferences are arranged to brief the media about significant achievements of the individual scientists/institute. Our Director and concerned scientists interact with the media and disseminate information about their work.

Press Releases, Content Generation: A press release details important points of the events held in our institute and it is shared to media houses for publication. There are two kinds of press releases – one is an after-event release, and the other is an announcement of awards, achievements of individual scientists and signing of MoUs and other related events of the institute. The after-event press release ensures that the information about the programme reaches various media houses even if their reporter was not present at the event. The release also serves as background information for most reporters to pen their article on the event.

Many scientists receive awards and distinction for their work in various scientific platforms. Such important news is conveyed through press releases for publication in various newspapers and other social media platforms.

Coordination with Print & Digital Media: Sufficient coordination is ensured between the institute and media personnel. This ensures that our institute is projected correctly public platforms, and gains publicity for the work of our scientists through special write ups. In many instances, special articles are prepared on achievements of our scientists and this is shared with the media for publication. Increased coordination with media personnel ensures that the articles are published without any hinderance.

Coordination with Vigyan Prasar (DST): Another important step towards communication by the Institute is coordinating with Vigyan Prasar to disseminate work of the institute to reach to a wider audience. Work with Vigyan Prasar involves sending all our press invitations to the central team. This is to alert the central team about the programme schedules to take place. At a later stage the central team is briefed about the event through press releases.

Apart from the above mentioned tasks, KIM also carries out several such assignments as entrusted by the Institute from time to time.

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 2020**,** 774 students were enrolled as Ph.D students and the 145 scientists of CSIR-IICT, Hyderabad are extending their services as faculty members to the AcSIR Academy in the disciplines of Chemical, Biological and Engineering Science

AcSIR FUNCTIONARIES:

Dr. S. Chandrasekhar	**Member, AcSIR Senate**
Dr. Ramanuj Narayan	Associate Dean, Chemical Sciences (from October 2014) Associate Dean, Biological Sciences (from February 2020)
Dr. Ch. Raji Reddy	AcSIR Coordinator, CSIR-IICT (from February 2016)

To streamline the activities of AcSIR the following committees, have been constituted .

ACADEMIC COUNCIL

S. No	Name	Designation	Committee
1	Dr. K. Rajender Reddy	Sr. Principal Scientist	Chairman
2	Dr. Ch. Raji Reddy	Sr. Principal Scientist	AcSIR Coordinator/Member
3	Dr. Galla V. Karunakar	Principal Scientist	Member
4	Dr. Rati Ranjan Nayak	Senior Scientist	Member
5	Dr. P. Aruna	Principal Scientist	Member
6	Dr. Rajkumar Banerjee	Sr. Principal Scientist	Member
7	Dr. C. Sumana	Sr. Principal Scientist	Member
8	Dr. Pratyay Basak	Principal Scientist	Member
9	Dr. Jagadeesh Babu Nanubolu	Senior Scientist	Member

COMMITTEES FOR CARRYING OUT ACSIR ACTIVITIES

1) Thesis Supervision Committee:

S. No	Name	Committee
1	Dr. K. Rajender Reddy	Co-Chairman
2	Dr. Anthony Addlagatta	Co-Chairman
3	Dr. Rajkumar Banerjee	Member
4	Dr. Chittaranjan Patra	Member
5	Dr. R.S. Prakasham	Member
6	Dr. K. Yamuna Rani	Member
7	Dr. S. Suresh	Member
8	Dr. A. Venugopal	Member
9	Dr. M. Mohana Krishna Reddy	Member

2) Societal Program Committee (CSIR-800 Project):

S. No	Name	Committee
1	Dr. Sunil Misra	Convener
2	Dr. S. Sridhar	Member
3	Dr. S. Venkata Mohan	Member
4	Dr. A. Gangagni Rao	Member
5	Dr. B.V. Subba Reddy	Member
6	Dr. P. Aruna	Member
7	Dr. K. Nagaiah	Member

3) Project Proposal/Review Committee:

S. No	Name	Committee
1	Dr. K. Srinivas	Chairman
2	Dr. Sanjit Kanjilal	Co-Chairman
3	Dr. Surya Prakash Singh	Member
4	Dr. Haridas B. Rode	Member
5	Dr. Amitava Das	Member
6	Dr. Nishant Jain	Member
7	Dr. H. S. Simha	Member
8	Shri. Jayant Kumar	Member

4) Course Curriculum Committee:

S. No	Name	Committee
1	Dr. S. V. Manorama	Chairperson
2	Dr. Shasi Vardhan Kalivendi	Co-chairperson
3	Dr. K. Yamuna Rani	Co-Chairperson
4	Dr. Subhash Ghosh	Member
5	Dr. Rohit Kumar Rana	Member
6	Dr. Ch. Ramakishan Rao	Member
6	Dr. S. Venkata Mohan	Member
8	Dr. C. Sumana	Member

5) Examination Committee:

S. No	Name	Designation	Committee
1	Dr. K. Rajender Reddy	Principal Scientist	Chairman
2	Dr. MSL Karuna	Senior Scientist	Member
3	Dr. Rajesh Chandra	Senior Scientist	Member
4	Dr. B. Nagendra Babu	Senior Scientist	Member

COURSES OFFERED IN ALL DISCIPLINES

S. No	Course Code	Course Name
1.	BIO-IICT-1-0004	Research Methodology
2.	BIO-IICT-1-0001	Biostatistics
3.	BIO-IICT-1-0002	Computation/bioinformatics
4.	BIO-IICT-1-0003	Basic Chemistry
5.	BIO-IICT-2-2901	Biotechniques & Instrumentation
6.	BIO-IICT-2-2902	Chemical Biology
7.	BIO-IICT-3-2901	Seminar course
8.	BIO-IICT-3-2905	Disease Mechanisms
9.	BIO-IICT-3-2907	Protein Science And Structural Based Drug Design And Development
10.	CHE-IICT-1-2901	Research Methodology
11.	CHE-IICT-1-2902	Analytical Tools and Instrumentation
12.	CHE-IICT-2-2902	Advanced Organic Chemistry
13.	CHE-IICT-2-2905	Advanced Catalysis
14.	CHE-IICT-2-2909	Green chemistry
15.	CHE-IICT- 3-2902/3-2903	Total Synthesis/ Asymmetric Synthesis
16.	CHE-IICT-3-2922	Homogeneous Catalysis /Catalysis for organic synthesis

17.	CHE-IICT-3-2921	Process Chemistry
18.	CHE-IICT-2-2913	Medicinal Chemistry
19.	ENG-IICT- 1-2951	Research Methodology 2-0-0-2
20.	ENG-IICT-2-2901	Numerical methods and Process Modeling
21.	ENG-IICT- 2-2902	Advanced Separation Processes
22.	ENG-IICT- 2-2906	Advanced Process Optimization
23.	ENG-IICT- 2-2907	Membrane Technology
24.	ENG-IICT- 3-2905	Software Applications in Chemical Engineering Problem Solving

AcSIR STUDENT INFORMATION

Discipline	August 2018	January 2019	August 2019	January 2020	Total
Chemical Sciences	37	22	27	36	**122**
Biological Sciences	16	08	16	08	**48**
Engineering Sciences	14	02	05	04	**25**
Total	**67**	**32**	**48**	**48**	**195**

NUMBER OF STUDENTS COMPLETED THEIR PRE-VIVA

Discipline	Pre-Viva
Chemical Sciences	45
Biological Sciences	12
Engineering Sciences	04
Total	**61**

NUMBER OF STUDENTS SUBMITTED Ph.D. THESIS (2018-20) AND AWARDED

Discipline	Thesis Submitted	PhD Awarded
Chemical Sciences	46	104
Biological Sciences	15	33
Engineering Sciences	04	08
Total	**65**	**145**

As a part of the AcSIR activity, a campus placement for the students was organized. Chemveda life Sciences, a prominent Hyderabad contract research organization conducted interviews for the CSIR-IICT students on 25th April, 2019.

To promote the science among the college students and as a part of the AcSIR students activities, a poster day was conducted on 20th February, 2020 by the students of CSIR-IICT. Several college students have been invited and the response was very good and a total of 400 students from 11 different colleges were attended and interacted with the student's community.

Samyukth (student fest) took place on February 27-28, 2020 at CSIR-IICT, Hyderabad. It involved scientific lectures and cultural activities performed by students. In association with National Science day, Shri P. Raghavendra Rao Secretary, Ministry of Chemicals & Fertilizers, and Prof. Rajender S. Sangwan, Director - AcSIR addressed the gathering. Highlighted the importance and application of science to society.

Promoting Science in Schools: To Promote Science in School we have visited Zilla Parishad High School (ZPHS), Nampally, Nalgonda District on September 19, 2019. During this visit faculty delivered lectures on the importance of Science and the IICT research scholars demonstrated live experiments to the school children's. Plantation, Lecture, Live experiments followed by Quiz for students have been conducted at School.

Societal Program : As a part of Societal Program, we have visited to ZPHS Vennampally, Saidapur, Karimnagar District, Telangana State on March 06, 2020 along staff members and students. As a part of this Science Inspiration Program we have presented a few demo experiments to showcase some of the achievements of CSIR and to inspire them towards science as their career.

Plantation of Saplings: Plantation program was carried at school premises. Scientist's, AcSIR Staff/ students and ZPHS School Staff and students were participated.

Lecture: A motivating lecture was delivered by Dr. Ch. Raji Reddy, highlighting about the "Life without Chemistry", which was highly appreciated by all the students and staff of the school.

Science Exhibition: Live demonstrations of experiments were carried out by IICT research Scholars to explain students and staff the current research activities being carried out at IICT, Hyderabad

HUMAN RESOURCE DEVELOPMENT

STAFF LIST (AS ON 31/03/2020)

DIRECTOR

Dr. S. Chandra Sekhar

CHIEF SCIENTIST

Dr. D. Shailaja
Dr. R.S. Prakasham
Dr. K. Yamuna Rani
Dr. K. Nagaiah
Sri. G.A. Raju
Dr. T. Shekharam
Dr. Sunkara V. Manorama
Dr. S. Raghavan
Dr. B. Jagadeesh
Dr. A. Seshu Kumar
Dr. A. Gangagni Rao
Dr. B.V. Subba Reddy
Dr. N. V. Satyanarayana

SENIOR PRINCIPAL SCIENTIST

Dr. P. Srihari
Dr. Ch. Raji Reddy
Dr. Shasi Vardhan Kalivendi
Dr. Anthony Addlagatta
Dr. Ramanuj Narayan
Dr. H.M. Sampath Kumar
Dr. A.V. Sesha Sainath
Dr. Ch. Ramakishan Rao
Dr. Debendra Kumar Mohapatra
Sri. P. Vijayanand
Dr. T. Venkateshwar Rao
Dr. Mohana Krishna Reddy Mudiam
Dr. Prathama S. Mainkar
Dr. Manika Pal Bhadra
Dr. K.V. Padmaja
Dr. L. Giribabu
Dr. Rohit Kumar Rana
Dr. B. Sreedhar
Dr. Subhash Ghosh
Dr. M. Chandrasekharam
Dr. Rajiv Trivedi
Dr. N. Narender
Dr. A. Venugopal
Dr. K. Rajender Reddy
Dr. N. Lingaiah
Dr. Rajkumar Banerjee
Dr. C. Sumana
Dr. G. Sarala Devi
Dr. S. Palaniappan
Dr. M. Sridhar
Dr. Pradosh P. Chakrabarti
Dr. Ashok Kumar Tiwari
Dr. Sistla Ramakrishna
Dr. A. Manjula
Dr. S. Prabhakar
Dr. Ghousia Begum
Dr. K.N. Prasanna Rani
Dr. S. Venkata Mohan
Dr. S. Rama Mohan
Dr. B. Satyavathi
Sri. S. Anand Kumar
Dr. S. Sridhar
Dr. K. Srinivas
Dr. B.L.A. Prabhavathi Devi
Sri. D.V.R. Murty
Dr. H. S. Simha
Sri. U. Ashutosh
Dr. D. Vijaya Kumar
Dr. Malothu Ramulu
Dr. T. Prathap Kumar
Dr. Pravin R. Likhar
Dr. D. Subhas Bose
Dr. B. China Raju
Dr. Lingaiah Nagarapu
Dr. A. Krishnaiah

PRINCIPAL SCIENTIST

Dr. A. Venkat Narsaiah
Dr. S. Indu Kumari
Dr. U.V.R. Vijaya Sarathi
Dr. Sutapa Ghosh
Dr. Sunil Misra
Dr. P. Mangala Gowri
Sri. G. Naga Srinivas
Dr. Ravindra Motiram Kumbhare
Dr. Prakriti Ranjan Bangal
Dr. M.S.L. Karuna
Dr. P. Aruna
Dr. B. Sridhar
Dr. A.V. Subrahmanya Sarma
Dr. Y. Soujanya
Dr. Sanjit Kanjilal
Dr. S. Sreelatha
Dr. Ujjwal Pal
Dr. Haridas B. Rode
Dr. Bathula Surendar Reddy
Dr. Sumana Chakravarty
Dr. Thota Jagadeshwar Reddy
Dr. Maddi Sridhar Reddy
Dr. Chittaranjan Patra
Dr. Rajesh Chandra

Dr. Srigiridhar Kotamraju
Dr. Pratyay Basak
Dr. Nivedita Sahu
Dr. Shankarachar M. Sutar
Dr. Amitava Das
Dr. Surya Prakash Singh
Dr. Galla V. Karunakar
Dr. Sidhanath Vishwanath Bhosale
Dr. J. Vatsala Rani
Sri. M. Naveen
Dr. G. Sudhakar
Dr. K. Suresh Babu
Dr. Saibal Das
Dr. P. Anand
Dr. Pavuluri Srinivasu
Dr. Sreepriya Vedantam

SENIOR SCIENTIST

Dr. Vasundhara Mutta
Dr. S. Nishant Jain
Dr. T. Anjana Devi
Sri. S. Chandra Sekhar
Dr. M. Srinivasa Rao
Dr. Surisetti Suresh
Dr. Ramesh Ummanni
Dr. Ram Chandra Reddy Jala
Dr. Rati Ranjan Nayak
Dr. Rambabu Chegondi
Dr. Kaki Shiva Shanker
Sri. P. Anil Kumar
Dr. Bathini Nagendra Babu
Dr. Jagadeesh Babu Nanubolu
Sri. Samuel L. Ralte

SCIENTIST

Sri. Jayant Kumar
Ms. Alka Kumari
Dr. Reddi Kamesh
Dr. Vineet Aniya
Ms. Pavani Vadthya
Dr. Siddhartha Moulik
Dr. John Mondal
Dr. G. Jithender Reddy
Dr. Sudhakar Manikrao Bansod
Dr. K. Muralidharan
Dr. Maqsood Ahmed
Dr. Andugulapati Sai Balagi
Dr. Sanjib Kr Paul
Dr. Praveen Kumar Reddy Adiyala
Dr. Ashok Kumar Pandey
Dr. Sri Rama Murthy Akondi
Dr. Punna Nagender
Dr. Abhishek Santra
Dr. Abhijit Hazarika
Dr. V. Ramalingam
Dr. T. Kumaraguru
Dr. Linga Banoth
Dr. L. Ravithej Singh

MEDICAL OFFICER (I)

Dr. Varsha Rajkumar Ohatker

MEDICAL OFFICER

Dr. Balthu Narender Kumar

PRINCIPAL TECHNICAL OFFICER

Sri. C. Sudhakar
Dr. G. Baskar Rajan
Dr. Gurrala Sheelu
Dr. Hafeez-ur-Rehman
Dr. K. Bhuvaneswari
Dr. K. Venkatram Reddy
Sri. Damodar Joshi
Dr. B.S. Sastry
Sri. T. Nageswara Rao
Dr. Sara Khalid
Dr. T. Venugopal Raju
Sri. K. Sriram
Sri. K. Gopi Krishna
Sri. G. Ranga Rao
Sri. G. Vijayamurthy
Sri. P. Krishna Murthy
Dr. Shobha Rajendra Pathak
Sri. A. Radhakrishna

SR. SUPERINTENDING ENGINEER

Sri. Ch. Srinivas
Sri. P. Narayana Rao

SR. TECHNICAL OFFICER (3)

Sri. S. Hemantha Kumar
Sri. A. Vishnu Vardhan
Dr. P. Ravinder Goud
Dr. M. Syamala
Sri. T. Mahesh Babu
Sri. B. Ashok Kumar
Dr. Ch. Ramesh
Sri. M. Sridhar Kumar
Sri. K. Shiva Kumar
Dr. L. Satyanarayana
Dr. B. Renuka
Dr. J. Laxmikanth Rao
Sri. A. Ramakrishna Reddy

Dr. K. Sugnana Sunder
Dr. B. Rajashaker
Sri. K. Saravanan
Sri. Sunil Kumar
Sri. S. Srikamal
Sri. Arsid Niranjan
Sri. B.V. Devendra Rao
Ms. M. Preethi

SR. TECHNICAL OFFICER (2)

Ms. L. Kiranmayi
Dr. V. Naveen Kumar
Sri. K.S. Srinivas
Dr. C. Krishnaveni
Sri. Prasenjit Das
Sri. G. Radha Krishna Murthy
Dr. K. Rekha
Sri. Kinnera Kiran
Sri. I. Ravi Kiran
Dr. D. Krishna Rao

Assistant Executive Engineer [Gr.III(4)]

Sri. D. Satish Kumar
Sri. Mirza Mohd. Habeeb

SR. TECHNICAL OFFICER (1)

Sri. K. Narsingh
Dr. A. Kiran Kumar
Sri. P.V.S.S. Srinivas
Dr. Kuncha Madhusudana
Dr. M.G. Bhagya Lakshmi
Ms. N. Manjula
Dr. S. Anubala
Dr. T. Ravinder
Sri. P. Sivanarayanan
Sri. R. Boopathy
Dr. C.N. Rohitha
Sri. L. Yugender Raju
Sri. P.N.S. Raghu Narayana
Sri. Chavali Siva Ranjith
Dr. Rathod Aravind Kumar
Sri. C. Chandrasekhar
Dr. B. Anjaneyulu
Sri. B. Vijaya Thomas
Dr. V. Lakshma Nayak

TECHNICAL OFFICER

Sri. Jeevan Prakash Pandey
Sri. T. Chand Kumar
Sri. T. Rama Linga Murthy
Sri. G. Siva Satish
Sri. Y. Kanaka Raju
Sri. Thirupathi Azmeera
Sri. K. Chandra Shekar
Sri. G. Sukumar
Ms. B. Supriya
Sri. L. Srinivas
Sri. G. Balakrishna
Sri. N. Rasheed Khan
Sri. E. Anjaneyulu
Sri. D.V.N.S. Ramachandra
Sri. Malavath Ratanlal
Sri. G. Sai Krishna
Sri. D. Venkateswara Rao
Sri. T. Nagendra Prasad
Ms. Baby Sowjanya Uyyala
Dr. Subhash Pawar
Sri. T. Sandeep Kumar
Sri. Appala Naidu Chokkapu
Sri. Chandrashekar Pendem

TECHNICAL ASSISTANT

Sri. Amit Kumar Rajak

SR. TECHNICIAN (3)

Sri. J.V.S.N. Murthy
Sri. T. Srinivasan
Dr. M. Shyam Sunder
Sri. P.V. Ravi
Sri. J. Sri Rama Murthy
Sri. T. Ramesh Babu
Sri. M. Utham Kumar
Sri. B.D. Sanjay
Ms. Ch. Swarna Latha
Ms. Amtul Zehra
Dr. V. Swapna
Dr. D.B. Rohini Kumar
Dr. K.V.S. Rama Krishna
Dr. B. Srinivas
Dr. V.V. Swarajya Lakshmi
Dr. S. Shailaja
Dr. M. Rama Krishna
Dr. K. Vijaya Kumar
Ms. Y. Swarna Latha
Sri. G. Veeraiah

SR. TECHNICIAN (2)

Sri. P.V. Sai Babu
Sri. N. Jai Prakash
Ms. S. Sumathi Reddy
Sri. M. Venkateswara Rao
Sri. Syed Ather Mehdi
Sri. D. Lingam
Sri. Babu
Sri. Abdul Mannan
Sri. N. Anjaiah

Sri. M. Madan Kumar/Sambaiah
Dr. K. Madhusudhan Rao
Ms. Mercy Joseph
Sri. S.B. Abbas Naqvi
Sri. T. Krishna Reddy
Ms. L. Vijaya Mary
Sri. P. Ramulu
Sri. N. Ramesh
Sri. Achal Singh
Sri. K. Venkatnarayana
Ms. Ch. Jagadeswari
Sri. K. Ramulu
Sri. M. Pulya Naik
Sri. K.S.S.Ch. Prasad
Sri. Farhath Hussain

SR. TECHNICIAN (1)

Sri. S. Bhupal
Sri. N. Narsing Rao
Sri. B. Satyanarayana
Sri. Aziz Pasha
Sri. S. Meharban Singh
Sri. N. Subba Rao
Sri. Chegondi Srinivasa Rao

TECHNICIAN (2)

Sri. T. Naresh Kumar
Sri. N. Amaralingeswara Rao
Sri. Murali Chikalametla
Sri. Sambhu Sankar Badatya
Sri. K. Venkatesh
Sri. Sanjeev Kumar Pradhan
Sri. R. Mahender
Sri. Y. Suresh
Sri. B. John Ramesh
Sri. Khaja Mansoor Ahmed
Sri. Mohammad Rafiq Basha
Sri. S. Salaiah
Sri. G. Raja Shekar Rao
Sri. K. Soori Babu
Sri. B. Sudarsana Rao
Sri. M. Munendra Kumar
Sri. M. Mahender
Sri. Hari Krishna Reddy

TECHNICIAN (1)

Sri. Md. Shabuddin
Sri. Ganji Ashok
Sri. Jarupula Shankar

LAB. ASSISTANT

Sri. K.M. Eashwar Rao
Sri. P. Ramulu
Sri. Mushtaq Ahmed
Sri. R. Satyanarayana Raju
Sri. J. Venkatesh
Sri. Ghulam Taher
Sri. Mohd. Khaja Moinuddin
Sri. M.A. Odud
Sri. Syed Fareed Ahmed
Sri. Aleemullah Khan
Sri. Mohd. Jaffar
Sri. J. Dasharatha
Sri. M. Ramulu/M. Chandraiah
Sri. K. Satyanarayana
Sri. Mirza Zahed Hussain
Sri. Mohd. Yousuf/Ismail Khan
Sri. D. Jaikishan/Nagaiah
Sri. G. Ashok/Mankaiah
Sri. Mohd. Maqbool
Sri. Jimmigari Mallesh
Sri. D. Gopala Krishna
Sri. D. Narsing Rao
Sri. M. Madan
Sri. D. Shiva Ramudu
Ms. Asghari Banu
Sri. G. Sai Ganesh
Sri. Mohammed Ahmed
Sri. C. Gnaneshwar
Sri. K. Ramesh
Sri. Razzak Ali/Sadiq Ali
Sri. Mir Mumtaz Ali
Sri. K. Omprakash
Sri. G. Damodar

LAB. ATTENDANT (1)

Ms. B. Durga Bai
Ms. T. Padma

CONTROLLER OF ADMINISTRATION

Ms. Sailaja Maddaly
Sri. Binod Dubey

CONTROLLER OF FINANCE & ACCOUNTS

Ms. M.P. Geetha

CONTROLLER OF STORES & PURCHASE

Sri. Uma Sankar Das

FINANCE & ACCOUNTS OFFICER

Ms. T. Manoja Prasad

STORES & PURCHASE OFFICER

Sri. Vijay Kumar Mahto
Dr. Bandi Srinivas

SR. HINDI OFFICER

Dr. S. Naseema

HINDI OFFICER

Sri. N. Satyanarayana

SECTION OFFICER (G)

Sri. Venkateswarlu Gadde

SECTION OFFICER (F&A)

Dr. D.S. Sujatha

SECTION OFFICER (S & P)

Sri. G. Ravi Rajlingam

PRIVATE SECRETARY

Ms. N. Sanjeeva Rani

Ms. Y. Sujatha

Ms. N.N.S.S.V.B.T. Sundari

Ms. M. Vanisree

Sri. P. Sailendra Rao

SENIOR STENO (ACP)

Ms. Y. Madhavi

Ms. M. Saroja

SENIOR STENO

Ms. E. Harathi Jawahar

Sri. Y. Murali Krishna

Ms. M. Saritha Kumari

Ms. V. Jaishi Rani

Sri. R.R. Yadu Krishna

Sri. N.K. Naveen Kumar

Ms. N. Lakshmi Sunitha

Ms. D. Shamantha

Sri. S. Revathi Kumar

Ms. K.L. Kavitha

Sri. Gattem Sainadh

Sri. Balaram Musunuri

JUNIOR STENO

Sri. Dumpati Saikumar

Sri. Kethavathu Kumar

Ms. Tayyaba Unnisa

Sri. Praful Paswan

Ms. Gosula Divya Bharathi

Ms. Pulagam Akhila

ASST. SECTION OFFICER (GEN)

Sri. G. Srikanth

Sri. S. Praveen Raju

Sri. G. Ravi Kiran

Sri. N. Anand

Sri. Vincent Thomas

Sri. P. Shankar

Ms. G. Uma Maheshwari

Sri. A. Venkateswara Rao

Ms. B. Koteshwari

Ms. Shaik Husn Afroze

Ms. S. Sai Bhavani

SR. SECRETARIAL ASSISTANT (GEN)

Ms. J. Saraswathi

Ms. Sunita Devi

Sri. A. Shiv Shankar

Sri. Vellala Srinivas Karthik

Sri. Kalagatha Panidhar

Sri. Ulasala Jaya Prakash

SR. SECRETARIAL ASSISTANT (F&A)

Sri. T. Madhava Subrahmanya Kumar

Sri. Rakesh Doure

Sri. Thommandrula Suneel Kumar

SR. SECRETARIAL ASSISTANT (S&P)

Sri. Duduku Madhusudhan

Sri. G.L.S. Prasad

ASST. SECTION OFFICER (F&A)

Ms. Kalaimathi R. Anbarasu

Ms. J. Latha

Sri. Syed Shhujayat Hussain

Ms. C. Annapurna

Sri. Muhammad Zafar Ahmad

Sri. K. Sudhakar

ASST. SECTION OFFICER (S&P)

Sri. Parki Ratan Raj

Sri. C. Nataraju

Sri. V. Ganesh

Sri. S. Krishnaiah

Sri. M. Naga Raju

SECURITY OFFICER

Sri. Dharmarao Kaspa

SR. SECURITY ASSISTANT

Sri. P. Sudersen

STAFF CAR DRIVER

Sri. B. Muralikrishna
Sri. B. Siddaramulu
Sri. P. Nageswara Rao
Sri. P. Venkatesham

ASSISTANT HALWAI

Sri. E. Krishna

COUPON CLERK

Sri. M. Parushaiah

COUNTER CLERK

Ms. M. Swarna Latha

COOK(CANTEEN)

Sri. M. Mohan Rao

BEARER (CANTEEN) (ACP)

Sri. K. Satyanarayana
Sri. M. Dasrath
Sri. V. Narender

BEARER (GH) (ACP)

Sri. Shaik Jahangir

WASHBOY/DISH CLEANER (ACP)

Sri. M. Balaiah

SWEEPER (CANTEEN)

Ms. C. Nagamani

TRAINEE

Sri. K. Rajasekhar

MULTI-TASKING STAFF

Ms. V. Sumathi
Sri. D. Rajesh
Sri. E. Arun Kumar
Sri. B. Mahender Kumar
Ms. D. Anuradha

FARRASH GR. B (ACP)

Sri. A. Sathyanarayana

FARRASH GR. B

Sri. Shaik Ismail/Afzal

FARRASH (ACP)

Sri. S. Chittaiah

FARRASH

Ms. A. Shashikala
Sri. Abdul Rehman
Sri. P. Nagabhushanam
Sri. M. Venkatesh
Sri. Mohd. Khadir
Sri. Masood Ali
Sri. N. Narsimha
Sri. G. Kumar
Sri. A. Babul
Sri. S. Srinivas
Sri. T. Mallesh
Sri. R. Narasing Rao
Sri. D. Shanker
Sri. B. Satyanarayana
Sri. M. Yadaiah
Sri. A. Satyanarayana
Sri. C. Vishwanath
Sri. A. Ramesh
Sri. C. Krishna
Sri. A. Chandra Mohan
Ms. K.C. Yesupadamma
Ms. J. Laxmi
Ms. M. Padma
Sri. D. Meghanath
Ms. P. Prabhavathi Nair

SAFAIWALA (ACP)

Sri. B. Ramulu/Sarvaiah
Ms. P. Renuka/P.N. Kumar
Ms. M. Devamma

PEON

Sri. Sri Pandari

ANNEXURE

CONFERENCES/SEMINARS WORKSHOPS ORGANZED

- A Two-day program on "IPR Awareness cum Interactive Session and Workshop". **April 23-24, 2018**
- A Two day National Seminar on "Emerging Trends in Analytical Sciences-2018 (ETAS-2018)" organized by Indian Society of Analytical Scientists (ISAS) Hyderabad Chapter along with CSIR-IICT. **July 30-31, 2018**
- Indo-US workshop on "Safeguarding Dual-Use Chemicals: The Application of Vulnerability Assessment Tools and Risk-Based Security Enhancements" at two different locations of Punjab University and GITAM University. **July, 2018**
- Conference on "Sustainable Chemistry on Health, Environment and Materials (SuCHEM 2018)" inaugurated by Dr. R. A. Mashelkar and Dr. T. Ramasami. **August 06, 2018**
- One Day Hindi Workshop on "Writing skills in Hindi in day to day work and Hindi grammar in the daily work". **August 27, 2018**
- XIV J-NOST Conference for Research Scholars was organized at CSIR-IICT. **November 28 - December 01, 2018**
- A joint RMIT (Australia) –AcSIR (India) Workshop was inaugurated at CSIR-Indian Institute of Chemical Technology, Hyderabad for the benefit of Scientists and Research Scholars of CSIR-IICT, CCMB and NGRI. **December 05-07, 2018**
- A one day program on "IPR Awareness cum Interactive Session and Workshop" organized by CSIR-IICT. **March 06, 2019**
- Hindi Workshop on official language rules and orders organized by CSIR-IICT. **March 20, 2019**
- A Workshop-cum-Interactive Session on Plagiarism conducted by M/s. Turnitin. **March 29, 2019**
- One-Day workshop on "Indo-UK Consortium-Global Challenge Research Fund Meeting" organized by CSIR-IICT. **April 10, 2019**
- National Seminar on "Emerging Trends in Analytical Sciences-2019 (ETAS-2019)" organized by Indian Society of Analytical Scientists (ISAS) Hyderabad Chapter along with CSIR-IICT. **June 21, 2019**
- A half day Platinum Jubilee Conference on "Organic Synthesis and Process Chemistry" was organized by CSIR-IICT. **June 25, 2019**
- A seminar on "Translational Research Trends in Process Engineering TRTPE-2019". **June 29, 2019**
- Indo-US Workshop on "Strengthening Supply Chain Security in the Pharmaceutical and Contract Chemical Synthesis Industries" at two different locations of Ahmedabad and Hyderabad. **July, 2019**
- A three day CSIR-Inter Institutional Student Conference on "Sustainable Chemistry for Health, Environment and Materials (SuCHEM YUVA 2019)" was inaugurated by Dr. Shekhar C. Mande, Director General, CSIR through video conference at CSIR-IICT. **July 24, 2019**
- One day seminar on "Beyond Valorization of Sustainable Knowledge in Oleochemicals" jointly organised by OTAI (SZ) & CSIR-IICT. **September 20, 2019**
- One day workshop on "Sustainable Societies and Humanity through AI & ML" (SSOHAM-19) organised by Vijnana Bharati (VIBHA) in association with CSIR-IICT. **October 18, 2019**
- The 8th Annual Conference of International Chemical Biology Society (ICBS) on "Navigating Translational Discoveries" was inaugurated by the Chief Guest, Dr. Shekhar C. Mande, Director

General, CSIR and Secretary DSIR at the auditorium of CSIR-IICT. **November 02, 2019**

- Workshop on "Prevention of Sexual Harassment of Women at Workplace" organized by CSIR-IICT and Rachakonda Security Council (RKSC). **March 06, 2020**

Release of Souvenir at SuCHEM-2018 by Dr. R. A. Mashelkar and Dr. T. Ramasami.

Inaugural session of RMIT (Australia) –AcSIR (India) Workshop

Release of Souvenir during the inaugural session of ICBS by the Chief Guest, Dr. Shekhar C. Mande.

A Lecture by Shri.Mahesh M Bhagwat, IPS.

DISTINGUISHED LECTURES

Telangana Academy of Sciences (TAS) organized Darshan Endowment Lecture and Vepachedu Gopalkishan Rao Endowment Lecture at IICT. **April 28, 2018**

- A.V. Rama Rao Technology Award Lecture on "Search for opportunities in epigenetics and epigenomics for prevention and treatment" by Prof.V.M.Katoch NASI-ICMR Chair, Rajasthan University of Health Sciences (RUHS), Jaipur. **May 11, 2018**
- A Lecture on " Path of Success: "Practicing the Golden Rule" by Prof. Arun Tiwari . **June 22, 2018**
- A Plenary Lecture on "R&D for affordable Health Care-Opportunity for India" by Prof. T Ramasami. **August 06, 2018**
- The Foundation Day Lecture by Dr. Ella Krishna CMD, Bharat Biotech Ltd. **September 26, 2018**
- CSIR-IICT Platinum Jubilee Series Lecture on "Tailor-making Lipids for Human Nutirtion" by Prof. Xuebing Xu, Director and General Manager of Wilmar Global R&D Center, Shanghai, China. **October 24, 2018**
- A Lecture on "Chemistry and Physics: Synthesis and Vectorization of Compounds towards Tumors" by Prof. Janine Cossy, Professor of Chemistry, ESPCI Paris Tech, France (As a Part of Platinum Jubilee Lecture Series). **December 17, 2018**
- A Lecture on "Ethics in Research and Publishing" by Prof. S. Chandrasekaran, IISc, Bangalore. (As part of year long Platinum Jubilee Celebrations) **February 18, 2019**
- A Lecture by Mr. Krishnamurthy Venkataramanan, former, CEO and Managing Director, L&T and Chairman, L & T Hydrocarbon, Engineering Limited. (To commemorate the Raman's effect, National science day celebrations) **February 28, 2019**
- Platinum Jubilee Lecture on "Bridges between experiment and theory on catalytic functions" by Prof. Seiji Mori, Institute of Quantum Beam Science, Ibaraki University. **March 12, 2019**
- A Lecture on "Ayurvedic Plants - Natural Antioxidants as a new discovery" by Dr. K. Nagaiah, Chief Scientist, Natural Products and Traditional Knowledge Center. **March 21, 2019**
- A.V. Rama Rao Technology Award Lecture on "From Manned fighters to unmanned aircraft--The journey" by Dr. Kota Harinarayana,SERB Distinguished fellow, honorary advisor CSIR-NAL and Chairman General Aeronautics pvt ltd. Bangalore. **May 10, 2019**
- The Platinum Jubilee Lecture on "Introduction to the Modern Periodic Table" by Prof. C. N. R. Rao. **August 05, 2019**
- A Lecture on "Ethics in Science Education, Research and Governance" by Prof. Ashok Kumar Singhvi, Raja Ramanna Fellow, Physical Research Laboratory, Ahmedabad. **August 19, 2019**
- A Lecture on "Integrity- A way of life" by Padma Shri Dr. T. Hanuman Chowdary. (As part of Vigilance Awareness Week-2019) **November 01, 2019**
- Four Technical Lectures by Prof. Garry Rumbles, NREL-US, Prof. Akhila Kumar Sahoo, HCU-Hyderabad, Prof. Dave Hiddleton, University of Warwick-UK and Prof. Andrei Udin, University of Toranto, Canada in the eve of "RSC Road show 2019" at CSIR-IICT. **November 08, 2019**
- A Lecture on "Strategies and Tactics for the Rapid Synthesis of Molecular Complexity" by Prof. Scott Snyder, University of Chicago. **December 12, 2019**

TRAINING PROGRAMMES ORGANIZED

- An Orientation Program on "Hands on Training of Advanced Pharma and Biotechnology". **April 02, 2018 & May 15, 2018**
- Third edition of Orientation cum Training Program for M. Sc. Chemistry students of North-Eastern states and Karnataka. **September 01, 2018 - November 30, 2018**
- Training Course on "Analytical Skills Development" for international participants. **December 03-14, 2018 & November 25-December 06, 2019**
- A Skill Development Training Program on "Basic Cheminformatics" under CSIR Integrated Skill Initiative Program. **January 21, 2019 & February 18, 2019**
- A Refresher Course on "Processing and Analytical Methodologies of Oils & Fats". **March 20-22, 2019**
- Training Course on "Chromatographic and Spectroscopic Methods of Analysis" to CRCL officers. **April 22-May 16, 2019 & June 11-July 12, 2019 & December 02-27, 2019 & March 02 - April 03, 2020**
- A one day Awareness Training Program on "ISO 9001:2015". **April 29, 2019**
- A Unique Certificate Course in "Process Plant Drafting Using AutoCAD" conducted under CSIR Integrated Skill Development Program. **May 27-June 21, 2019**
- A One Week Training Course on "GC/MS Applications to Forensic Sciences" to the staff of TSFSL, Hyderabad. **June 2019**
- A Certificate Course on "Data Analysis (CCDA-2019)" under CSIR Integrated Skill Initiative Program. **August 26-October 11, 2019**
- Fourth edition of Orientation cum Training Program for M. Sc. Chemistry students from eight North-Eastern states, Chhattisgarh and Orissa. **September 01-November 19, 2019**
- A Certificate Course on "Laboratory Animals in Biomedical Research (LABR)" under CSIR Integrated Skill Initiative Program. **September 05-30, 2019**
- A Skill Development Certificate Course on "Basic Cheminformatics" under CSIR Integrated Skill Initiative Program. **December 16-27, 2019 & February 17-28, 2020**

Training Course for CRCL officers

Orientation cum Training Program for M. Sc. Chemistry students from eight North-Eastern states, Chhattisgarh and Orissa.

Snapshots of Skill Development Programmes (**2018 -2020**)

OTHER EVENTS ORGANIZED

- Organized American Chemical Society's flagship outreach program "ACS on Campus" at CSIR-IICT. **February 07, 2019**
- Celebrated Bharat Ratna Dr. B.R. Ambedkar's 127th birthday. **April 14, 2018**
- Swachhta Pakhwada activities were initiated in CSIR-IICT with Swachhta Pledge administered by Director, CSIR-IICT. **May 1-15, 2018**
- Organized World Environment day -A Green theater has been inaugurated by Dr. S. Chandrasekhar, Director, CSIR-IICT. **June 05, 2018**
- Conducted Yoga classes at IICT Staff Club (June 18-20) and celebrated International Yoga Day. **June 21, 2018**
- Science Fair on "Beat Plastic Pollution" jointly organized by Royal Society of Chemistry (London) – India Deccan Local Section, IICT Research Foundation (IRF), CSIR-IICT, White Board Ventures and Science India Portal at CSIR-IICT. **July 21, 2018**
- Two day 63rd Open Research Council Meeting of CSIR-IICT was held under the Chairmanship of Prof. G. R. Desiraju. **July 26-27, 2018**
- The Opening Ceremony of CSIR-IICT Platinum Jubilee Celebrations was held with the chief guest of Shri M. Venkaiah Naidu, The Hon'ble Vice President of India. **August 05, 2018**
- Celebrated 72nd Independence Day. **August 15, 2018**
- Initiated PINK BOLLWORM minimization program by CSIR-IICT in association with Department of Agriculture, Telangana State to protect 25000 acres of cotton crop in Telangana. **August 30, 2018**
- Organized "Hindi Mah and Hindi Day Celebrations". **August 14- September 14, 2018**
- Celebrated 76th CSIR Foundation Day at CSIR-IICT with the Chief Guest of Dr. Ella Krishna CMD, Bharat Biotech Ltd. **September 26, 2018**
- Pledge taken at various departments of IICT by Staff, Research Scholars and School students as part of Vigilance Awareness Week-2018. **October 29, 2018**
- Organized "Walkathon" as part of Vigilance Awareness Week-2018. **October 30, 2018**
- Organized 50th Shanti Swarup Bhatnagar Memorial tournament –Zonal III at CSIR-IICT, Hyderabad, jointly organized by CSIR-IICT and CSIR-Sports Promotion Board, New Delhi. **December 19-23, 2018**
- Organized an Industry interactive meet in the premises of Gujarat Chamber of Commerce & Industry (GCCI), Ahmedabad by CSIR-IICT. **January 03, 2019**
- Conducted a program to celebrate "150 Years of Periodic Table" in CSIR-IICT with the chief guest of Dr. Bipul Saha. **February 01, 2019**
- Took out a candle rally in memory of the CRPF Jawans who martyred in Pulwama attack in Jammu & Kashmir. **February 15, 2019**
- Celebrated student fest "SAMYUKTH-2019"at CSIR-IICT. **April 04-05, 2019**
- Held One day 64th Open RC meeting of CSIR-IICT. **May 03, 2019**
- Inaugurated "Dr. A. V. Rama Rao Kilo Lab Facility" by Dr. Shekhar C Mande, secretary DSIR and Director General CSIR at CSIR-IICT. **May 17, 2019**
- Conducted Two-Day Yoga practice session at IICT Staff Club. **June 19-20, 2019** & International Yoga Day. **June 21, 2019**
- Dr. Harsh Vardhan, Vice President CSIR, Hon'ble Union Minister for Health and Family Welfare, Science & Technology and Earth Sciences, laid the foundation stone for "Scale-

up facility for Agrochemicals" at CGP complex of CSIR-IICT. **July 20, 2019**

- Flaged off The first consignment of pheromone lures and traps for Mahbubnagar, Gadwal and Kamareddy districts by Dr S. Chandrasekhar, Director, IICT- as part of Fall Army Worm [FAW] Minimization Program in Maize and corn cultivation using insect sex pheromone lures. **July 22, 2019**
- Launched a door delivery Analytical Services for Bulk Drug, Pharma and Chemical Industries in the city by Dr. S. Chandrasekhar, Director CSIR-IICT at Bulk Drug Manufacturers Association office, Sanat Nagar, Industrial Estate, Hyderabad. **July 22, 2019**
- Celebrated 73rd Independence Day. **August 15, 2019**
- Organized The Director's Cup T20 Cricket Tournament by CSIR-IICT staff club. **September 13-15, 2019**
- Celebrated 77th CSIR Foundation Day at CSIR-IICT. **September 26, 2019**
- Organized "RSC Road show-2019" at CSIR-IICT in association with The Royal Society of Chemistry. **November 08, 2019**
- Conducted Poster Day as part of Annual Student Fest, SAMYUKTH-2020 by the students of CSIR-IICT in association with AcSIR. **February 20, 2020**
- Celebrated The National Science Day with the Chief Guest of Shri P. Raghavendra Rao, Secretary, Department of Chemicals and Petro Chemicals, Ministry of Chemicals and Fertilizers, Govt. of India. **February 28, 2020**
- Celebrated International Women's Day. **March 08, 2020**

Inaugural Ceremony of CSIR-IICT Platinum Jubilee Celebrations by Chief Guest Shri M. Venkaiah Naidu, The Hon'ble Vice President of India.

Inauguration of “Dr. A. V. Rama Rao Kilo Lab Facility” by Dr. Shekhar C Mande, secretary DSIR and Director General CSIR.

Foundation stone for “Scale-up facility for Agrochemicals” laid by Dr. Harsh Vardhan, Vice President CSIR, Hon'ble Union Minister for HFW, S&T and ES.

Shri P. Raghavendra Rao IAS, secretary, department of Chemicals and Petrochemicals, Ministry of Chemicals & Fertilizers, GOI as Chief Guest on 28th February, National Science Day Celebrations-2020

AWARDS AND HONORS

2018-2019

Name of the Awardee (s)	Prize/Award/Honor
Dr. T Prathap Kumar; Dr. B Satyavathi; Dr. Pravin Likhar; Dr. M Lakshmi Kantam; Dr. S Sridhar; Mr. K Ravindranath; Mr. S Anand Kumar; Dr. M Ramulu; Dr. Y V L Ravikumar; Mr. K Vijay Murty; Dr. Niveditha Sahu; Dr. Pavani Vadtya; Dr. Siddhartha Moulik; Dr. Madhumala Madupathi; Mr. Chandrasekhar; Ms. Bukke Vani	CSIR Technology Award-2018
Dr. S Chandrasekhar	2018 VASVIK Award
Dr P. Anand	Distinguished Scientist Award from Venus International Foundation", Chennai (2018)
Dr.Chitta Ranjan Patra	Editorial Board Member of Biomedical Materials Journal (IOP Publisher)
Dr. A Gangagni Rao	Fellow of AP Academy of Sciences
Dr. John Mondal	NASI-Young Scientist Platinum Jubilee Award
Dr. KV Padmaja	Dr S D Tirumala Rao Memorial Award
Dr. Ch. Raji Reddy	CRSI-Bronze Medal
Dr. Ramakrishna Sistla	Dr S B Pandey Oration award by Southern Regional Indian Pharmacology Society Conference
Dr. Sanjit Kanjilal	FSSAI - AFST(I) AWARD, International Food Convention (IFCoN 2018)
Dr. Siddhartha Moulik	Associate Fellow of Telangana Academy of Sciences (2018)
Dr. S Sridhar	Winner of 8th CIPET National Award 2018; Talented Industrial Biotechnologist Award; IIChE's NOCIL Award 2018
Dr. P. Srihari	CDRI Award-2018
Mrs. Jampala Annie Modestra, CSIR-SRF	AU-CBT Excellence Award
Ms.Komal Kaushik, UGC-SRF	"First in Oral Presentation" 5th International Conference on Angiogenesis: Targeted Anti-Angiogenesis therapy"; "Runner up - I of the Young Scientist Award" by Dr. K V Rao Scientific Society

Mr. A. Naresh Kumar, CSIR-SRF	WILEY Biotechnology Journal Sponsored Best Poster Award
Mr. S.M Rajesh Kotcherlakota, CSIR-SRF	Dr. KV Rao Research Award
Dr. Sai Prathima Parvathaneni, SRA	Fulbright-Nehru Postdoctoral Research Fellowship for 2018-2019.
Ms. Sameena	Young Scientist Award for the year 2018 by the Telangana Academy of Sciences.
Ms. Shikha Dahiya, CSIR- SRF	"AU-CBT Excellence Award 2018"

IICT Team receiving CSIR Technology Award-2018

Dr. Raji Reddy receiving CRSI-Bronze Medal

Dr. S. Sridhar receiving CIPET National Award-2018

AWARDS AND HONORS

2019-2020

Name of the Awardee (s)	Prize/Award/Honor
Dr. S. Chandrasekhar	AstraZeneca Oration Endowment Award
EEFF & PETT	1st, 2nd, 3rd & Consolation Prizes at the All India seminar on "Recent developments in technological options for resource recovery in chemical process Industry"
Dr. G Ganesh Kumar	"Talented Industrial Biotechnologist Award"
Dr. A Gangagni Rao	"Bharat Ratna Sir Mokshagundam Visvesvaraya Award" by Telangana State Centre on the occasion of 52nd Engineers Day Celebrations; Fellow award of The Biotech Research Society, India (BRSI)
Dr. L. Giribabu	Fellow of AP Academy of Sciences
Dr. Jagadeesh	Fellow of the Telangana Academy of Sciences (FTAS)
Dr. John Mondal	CSIR Young Scientist Award
Dr. Mohan Krishna Reddy Mudiam	Fellow of the Telangana Academy of Sciences (FTAS)
Dr. Nivedita Sahu	Second Prize in Poster Presentation, India International Sea Weed Expo and Summit 2019
Dr. Pavani Vadthya	"Associate Fellow of the Telangana Academy of Sciences (FTAS)"
Dr. Ram Chandra Reddy Jala	"S. D. Tirumala Rao Memorial Award" by OTAI
Dr. Sanjib Kr. Paul	National IPR Olympiad
Dr. Siddhartha Moulik	Sisir Kumar Mitra Memorial Award -2019 & IIChE NRC Award-2019 from Indian Institute of Chemical Engineers
Dr. K. Shiva Shanker	"Dr.Husain Zaheer Memorial Award" by OTAI
Dr. S. Sridhar	STEM Impact Award; Herdillia Award for Excellence in Basic Research in Chemical Engineering; HPCL New Generation Ideation Award 2019
Dr. S. Sridhar (Project Leader) and his Membrane Team Dr. M. Madhumala, Bukke Vani, D. Vaishnavi, T. Nagamani, F. Dileep Kumar and Karishma Mishra	Aqua Foundation's Excellence Award-2019 from Aqua foundation, New Delhi
Dr. K. Yamuna Rani	Fellow of the Telangana Academy of Sciences (FTAS); Life Fellow of Indian Institute of Chemical Engineers

Mr. Ajay Anand, SRF	Best Oral Presentation award received in International Conference on "Nutraceuticals and Chronic Diseases" INCD 2019
Dr. Althuri Avanthi, CSIR-Nehru Science PDF	"Associate Fellow of the Telangana Academy of Sciences (A FTAS)"
Miss. Bukke Vani	Best Oral Presentation on "Hydrology and Watershed Management"; "Best Presentation Award", National Conference on "Advanced Bharathi Institute of Technology (CBIT)
Mr. Chandra Shekar, SRF	Best Research Scholar Award, Telangana State Centre on the occasion of 52nd Engineers Day Celebrations
Mr. K Harishanker and Mrs K. Amulya	Best Poster Award from Environmental Science and Technology Journal, American Chemical Society Publications
Miss. Karishma Mishra	Best Poster Presentation, Current Promishing Advances in Nano Chemistry and Technology (CPANCT - 2019)"
Dr. Omprakash Sarkar	" Young Scientist of the Telangana Academy of Sciences (FTAS)"
Mr. M. V. Rohit	Best Poster Award
Dr. Seelam Prasanthkumar, DST-Inspire Faculty	"Associate Fellow of the Telangana Academy of Sciences (A FTAS)"
Miss. Sowmya Parakala	Best Poster Presentation, "Indo-German Joint Scientific Workshop on Membrane for Water and Energy"
Ms. Sulogna Chatterjee	Second prize for "Poster Presentation"
Mrs.Thummalapalli Nagamani	Best Oral Presentation, "Current Promising Advances in Nano Chemistry and Technology (CPANCT - 2019)"

Dr. A. Gangagni Rao received Bharath Ratna Sir Mokshagundam Visvesvaraya Award

Dr. John Mondal receiving CSIR Young Scientist Award

New Contracts Signed/ Assignments Undertaken 2018-19

Consultancy/ Collaborative/ Sponsored

Title of the Project	Sponsor/ Collaborator
Advisory consultancy in the area of chemistry	M/s. Kemio Solutions Pvt. Ltd., Bangalore
Advisory consultancy in the area of solid state forms of chemical compounds	M/s. UPL Ltd., Mumbai
Advisory consultancy in the area of trouble shooting in chemistry	M/s. Intonation Research Laboratories Pvt. Ltd., Hyderabad
Collaboration in R&D activities related to API's	M/s. Zunachem Pvt. Ltd., R.R. Dist.
Collaboration in R&D activities related to pharmaceuticals	M/s. Chandravadan Organics Pvt. Ltd., Maharasthra
Collaboration in setting up and operation of pilot scale water bottling facility	M/s. Auroma Clean Energy India Pvt. Ltd., Hyderabad
Collaboration in technology on development of indigenous atmospheric water generation machines	M/s. Maitri Aquatech Pvt Ltd., Hyderabad
Collaboration on R&D activities related to medicinal chemistry and Intermediate synthesis	M/s. NSJ Prayog Life Sciences Pvt. Ltd., Medak, Telangana (S)
Consultancy on analysis of samples using solid state NMR	Dr. Reddy's Labs, Hyderabad
Design of biofilter for odur control	M/s. Fleming Labs Ltd., Hyderabad
Design of biological processes for treatment of sewage	M/s. Nyrmala Bio-Engineering Solutions Pvt. Ltd., Hyderabad
Development of Cost effective route for SRC060	M/s. Eisai Pharmaceuticals India Pvt. Ltd., Visakhapatnam
Development of liquid electrolyte for rechargeable Al-Ion battery	M/s. Insmart Systems., Hyderabad
Development of technology for electroorganic continuos flow reactor	M/s. Amar Equipments Pvt. Ltd., Mumbai
Development of technology for Liquid-Liquid micro separator	M/s. Amar Equipments Pvt. Ltd., Mumbai
Development of technology for Manual Back pressure regulator	M/s. Amar Equipments Pvt. Ltd., Mumbai

Title of the Project	Sponsor/ Collaborator
Establishment of water analysis and purification laboratory at DBIT	M/s. Don Bosco Institute of Technology, Mumbai
Evaluation report on treatment efficiency of Biocleaner system	M/s. Nyrmala Bio-Engineering Solutions Pvt. Ltd., Hyderabad
Improving the Enantioselectivity of M-240	M/s. ADAMA India Pvt. Hyderabad
Impurity profile of agrochemical Bifenithron Technical	M/s. India Insecticides (India) Ltd., Mumbai
Installation of Biogas plant (500kg/day) at Agriculture market committee, Kurnool	M/s.Agriculture Market Committee, Kurnool
License of knowhow in indigenous atmospheric water generation machines	M/s. Maitri Aquatech Pvt Ltd., Hyderabad
Licensing of patents (1) Method of treatment of gastric ulcers and uclers induced by Aspirin (US Patent No. 7855200) (2) Intestinal alpha-glucosidase inhibitors process for isolation and use there of EP1986670	M/s. Sami Labs, Bangalore
Licensing of Patents on Anticancer Therapeutics Drug Resistant and Aggressive cancer	M/s. NanoDev Therapeutics LLC, Minnesota, USA
Membrane technology for produce of packaged drinking water	M/s. HPCL, Bangalore
Modular high rate bio digesters	M/s. Lars Enviro Pvt. Ltd., Hyderabad
Process development for preparation of superabsorbent polymer(SAP)	M/s. HPCL, Bangalore
Process development for the production of Dibromethane	M/s. Intech Organics Ltd., Gurugram, Harayana
Providing Oligonucleotide facility	M/s. Bio Artis Life Sciences Pvt. Ltd., Hyderabad
Report on characterization of challenged and referral coal samples of SECL mines	M/s. South Eastern Coalfields Ltd., Bilaspur, Chattisgarh
Report on testing biodegradability of primary amine in effluent samples	M/s. Indian Rare Earths Ltd., Orissa
Scale up studies for process validation and data generation for pilot plant sizing	M/s. PJS Pharma Pvt. Ltd., Hyderabad
Solid state NMR analysis of samples	M/s. Biocon Ltd., Bangalore

Title of the Project	Sponsor/ Collaborator
Supercritical carbondioxide extraction studies of pupal oil	M/s. Aspartika Biotech Pvt. Ltd., Bangalore
Synthesis of floatation reagents and process development for large scale synthesis	M/s. Tata Steel Ltd., Mumbai
Technology for purified drinking water	M/s. PH Seven Aqua Ltd., Hyderabad
Technology transfer of water purifying technology	M/s. Auroma Clean Energy India Pvt. Ltd., Hyderabad

Grant-in-Aid

Title of the Project	Sponsor
A convergent and chiral auxiliary based approach for the total synthesis of callyspongiolide A	SERB, New Delhi
Assessment of uremic toxins in patients with different stages of chronic kidney disease	MERIT, Telangana
Bio-prospecting of some indigenous medicinal plants of NE region of India with special reference to anti-inflammatory properties	DBT, New Delhi
BIOREVIEW: Biorefining value from industrial waste	DBT, New Delhi
Carbo and heterometallation of alkynes towards selective synthesis of alkenyl scaffolds	SERB, New Delhi
Centre for Technological Excellence in Water Purification (CTEWP)	DST, New Delhi
Computer aided catalyst design, synthesis and validation for methanol production	DST, New Delhi
DBT-JRF	DBT-BCIL, New Delhi
Design and development of molecular anchored nano-zeolite adsorbents for CO_2 capture from fossil fuel power plants	DST, New Delhi
Design and synthesis of 3-fluoro oxindole derivatives and evaluation of their anti-cancer activity	SERB, New Delhi
Design, Fabrication and Characterization of MOF-derived heterostructured-based photoactive-device for green hydrogen generation	DAE-BRNS, Mumbai
Design, synthesis and biological studies of pyrrole containing marine natural products and analogues	MoES, New Delhi

Title of the Project	Sponsor
Design, synthesis and molecular docking studies of benzoxepine based heterocyclic compounds and their biological, photo physical properties	SERB, New Delhi
Development of a process for 2,3,3,3-Tetrafluoropropene (HFO-1234yf)	DST, New Delhi
Development of catalysts for direct production of lower olefins from syngas	CHT, New Delhi
Development of efficient microwave based clean coal technologies for grinding, dewatering and desulphurization of coals using lab scale studies	DST, New Delhi
Development of new strategies to access the 3,4-fused indoles: Application to the synthesis of 3,4-fused indole alkaloids and their derivatives	DST, New Delhi
Development of nitrilase enzyme based bioreactor in production of chiral intermediates for pharma industries	DST, New Delhi
Development of oxindole based fluorescent, cell imager and its folate derivative as anti-cancer agents	SERB, New Delhi
Development of process for synthesis of hexafluoro-1, 3-butadiene (CAS 685-63-2) & purification to semiconductor grade	Semi-Conductor Laboratory(ISRO), Mohali
Development of tandem copper catalyzed arylation-cyclization strategies: Synthesis of biologically active compounds	SERB, New Delhi
Development of ultrapure chemical viz. methonol, hydrogen peroxide & Iso-propyl alcohol for semiconductor applications from commercially available grades by purification through advanced separation techniques	Semi-Conductor Laboratory(ISRO), Mohali
Development of ultrapure chemicals viz. TMAH, NH_4OH and TEOS for semiconductor applications from commercially available grades by purification through advance separation techniques	Semi-Conductor Laboratory(ISRO), Mohali
Development of ultrapure mineral acids viz. H_2SO_4, Hcl, H_3PO_4 and HNO_3 for seminconductor applications from commercially available grades by purification through advanced separation techniques	Semi-Conductor Laboratory(ISRO), Mohali
Exploiting interference as tool to enhance fault-tolerant feature of WSNs	DST, New Delhi
Glucocorticoid Receptor-Assisted Drug Sensitization (GRADS) in colorectal cancer therapy: Nano-therapeutic strategy towards repurposing of anti-cancer drugs	SERB, New Delhi
High mobility single crystals for n-Channel organic field-effect transistors	DST, New Delhi

Title of the Project	Sponsor
Hit to lead optimization of novel triazine analogues as potential autophagy modulators for the prevention of cancer	DBT, New Delhi
ICMR Fellowship	ICMR, New Delhi.
Identification and validation of small molecules modulators of CRISPR/cas9-based Homology Directed Repair (HDR) and Non-Homologous End Joining (NHEJ)	DBT, New Delhi
Impact of radiation based fragmentation of alpha glucans and their application potential	DAE-BRNS, Mumbai
Innovative algae platform for industrial wastewater valorization	DBT, New Delhi
INSPIRE Faculty Award	DST, New Delhi
INSPIRE Fellowship	DST, New Delhi
Magnetocaloric properties of manganite based magnetic materials	SERB, New Delhi
National Post-Doctoral Fellowship	SERB, New Delhi
Novel heterocyclic scaffolds for type II diabetes through targeting sodium-glucose co-transporter 2 (SGLT2) inhibition cascade: Synthesis and evaluation	SERB, New Delhi
Pathological role of peripheral insulin resistance in Alzheimers disease	DBT, New Delhi
Preparation of edible oil blends of palmolein and palm stearin with indigenous edible oils for cooking and trans-free solid fat formulation applications	Malaysian Palm Oil Board, Malaysia
Probing the effect of a modified graphene oxide surfactant on synthesis and material properties of fluoro acrylate amulsion as super-hydrophobic coatings	DST, New Delhi
Process know-how for 1-iodo-2,2,2-trifluoroethane 1-chloro-2,2,2-trifluoroethane (HCFC-133a)	CFEES (DRDO), New Delhi
Ramanujan Fellowship Award	SERB, New Delhi
Role of altered DDAH1 expression in prostate cancer progression and its molecular regulation promoting cancer metastasis	SERB, New Delhi
Self-fluorescent cell permeable glucose derived carbon nanospheres as a brain targeting vehicle: Implications in drug delivery and imaging	DBT, New Delhi

Title of the Project	Sponsor
Self-sustained design of photo-biorefinery for the closed loop production of fuels and chemicals	DBT, New Delhi
Stabilization of heteropolyacid clusters to design heterogeneous catalysis for selective oxidation of alcohols	SERB, New Delhi
Stereoselective desymmetrization of meso-cyclohexadienones for the rapid construction of highly functionalized natural product-like scaffolds	SERB, New Delhi
Substituted π-Allyl and allene nucleophiles: Total synthesis driven preparation of highly substituted dihydro and tetrahydropyran rings	SERB, New Delhi
Synthesis of diketopiperazine-based marine alaoids towards evaluation of anticancer activity: 18-Oxotryprostati A& 6-methoxyspirotryprostatin B and their analogues	MoES, New Delhi
Synthesis of heterocyclic molecules using vinyl azides as handy synthons	DST, New Delhi
To uncover the epigenetic mechanisms in etiopathology of schizophrenia with particular reference to hyperhomocystenemia and sex disparity	DST, New Delhi
Understanding role of the mTOR pathway in response to glucose and acetate in Glioblastoma: A functional genomics and proteomics approach	SERB, New Delhi
Understanding the link between xenobiotic exposure and the onset/progression of type 2 diabetes using drosophila as a model	Dept. of Health Research, Ministry of Health and Family Welfare, New Delhi

TECHNOLOGIES DEVELOPED AND TRANSFERRED

Name of the Technology	Client
Development of process knowhow for Na-TCP	M/s. PMFAI, Mumbai
Membrane technology for produce of packaged drinking water	M/s. HPCL, Bangalore
Modular high rate bio digesters	M/s. Lars Enviro 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
Synthesis of Polychloro-trifluoroethylene (PCTFE) from Chlorotrifluoroethylene (CTFE)”	Gujarat Flurochemicals Ltd, Gujarat

Name of the Technology	Client
Synthesis of Polychloro-trifluoroethylene (PCTFE) from Chlorotrifluoroethylene (CTFE)"	M/s. Gujarat Fluorochemicals Products (I) Pvt. Ltd., Gujarat
Technology for electroorganic continuous flow reactor	M/s. Amar Equipment's Pvt. Ltd., Mumbai
Technology for Liquid-Liquid micro separator	M/s. Amar Equipments Pvt. Ltd., Mumbai
Technology for Manual Back pressure regulator	M/s. Amar Equipments Pvt. Ltd., Mumbai
Technology for Production of Ultrapure Water for Biomedical and Biochemical Applications	Althion Tech Innovations Pvt Ltd
Technology for purified drinking water	M/s. PH Seven Aqua Ltd., Hyderabad
Technology transfer of water purifying technology	M/s. Auroma Clean Energy India Pvt. Ltd., Hyderabad
Transformation of water hyacinth to scalable nutrient rich organic fertiliser	M/s. Khar Energy Optimusers, 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

CSIR FUNDED PROJECTS UNDERTAKEN

Mission Mode Projects

Sl. No	Title
1	Crop protection chemicals
2	CSD-Catalysis for Sustainable Development
3	Food and Consumer Safety Solutions(Focus)
4	INPROTICS-Pharma and Agro

Skill Development and JIGYASA Projects

Sl. No	Title
1	JYGYASA
2	Skill Development

Thematic and Fast Track Translational Projects

Sl. No	Title
1	Catalytic conversion of linear of alkyl benzene raffinate to be utilized for jet rocket fuel.
2	Chronic Respiratory Disease Innovation & Solution Programme
3	Development of Engineered Biochar from non-edible de-oiled seed cakes/stubble wastes for the removal of targeted herbicides/pesticides from agricultural wastewaters and subsequent soil remediation.
4	Development of hybrid flocculants at 100 g scale for selective adsorption of low grade iron ore slimes and fines to recover iron ore more that 80% (HYBFLOC)
5	Enzymatic Process for the preparation of API intermediates
6	Facility Creation & Modernization of existing pilot plants
7	Indigenous enzymes for vegetable and rice bran oil degumming
8	Mimicking Muscles: Electro active polymers for Bionics(NCP)
9	Non-destructive depth profiling and identification of debonding defects across polymer interfacial layer by using portable single-sided NMR.
10	Process development of vinylidene fluoride (VDF) and chloro trifluoro ethylene (CTFE) their polymerisation processes
11	Scale up of materials for Dye Sensitized Solar Cells and Organic Photovoltaics
12	Sustainable production of edible oils from Microalgae
13	Vegetable oil-based Gels as trans free fat (Oleo gel)
14	Waste and Biomass to Value Added Products

HARIT Projects

Sl. No	Title
1	Reduced Emission Fire Works (HARIT)

CSIR-IICT and M/s. HPCL, Bangalore sign an agreement for Membrane Technology for Produce of Packaged Drinking Water

New Contracts Signed/ Assignments Undertaken 2019-20

Consultancy/ Collaborative/ Sponsored

Title of the Project	Sponsor/ Collaborator
A Laboratory scale process (100g/batch) for preparation of HPMC polymer	Godavari Biorefineries Ltd, Mumbai
A synergistic formulation useful as insect control agent and a process for the preparation thereof	Joish Agri Sciences (OPC) Pvt Ltd, Anantapur, Andhra Pradesh
Bioefficacy studies on VECTRAX and SPLAT-Bac formulations (April 2019-June 2020)	ATGC Biotech, Hyderabad
Carrying out vapour phase reaction in vapour phase catalytic facility	Aarti Industries Limited, Mumbai
Collaboration in R&D activities in the area of APIs	Uquifa India Private Limited, Hyderabad
Collaboration in R&D activities in the area of semio chemicals	Russell Integrated Pest Management private Ltd, Secunderabad
Collaboration in R&D activities related to development of electrostatic discharge products (July 2019 - July 2020)	SVS Pani Products, Hyderabad
Collaboration in R&D activities related to new processes / products	Bulk Drugs Manufacturers Association (India)
Collaboration in R&D activities related to semiochemicals (May 2019 - May 2020)	ATGC Biotech Private Ltd, Hyderabad

Title of the Project	Sponsor/ Collaborator
Collabortaive work on sustainable Energy (April 1, 2019 - Dec 31, 2019)	BHEL, Hyderabad
Design of Small scale anaerobic digester (IICT: Bio-Home) for decentralized applications for bio waste up to 150 kg/Day (July 2019 - Sep 2019)	KHAR Energy Optimisers, Hyderabad
Development of a scaleable cation transfer membrane for alkaline water cell	Micro Engineers, Ghaziabad, U.P.
Development of biomethanation process for palm oil empty fruit bunches and palm oil mill waste	Global environmental services Pvt ltd., Hyderabad
Development of biomethanation process from bagasse and spent wash	Spectrum Renewable Energy Private Limited, Hyderabad
Development of Process for Carboxymethyl Hydroxypropyl Guar Gum (CMHPG)	Chimique (India) Ltd, Haryana
Development of Process for extruded Nutrafood for management of 1) metabolic disorders, and 2) anaemia and malnutrition	Ameya Life , Hyderabad
Development of process knowhow for synthesis of Favipiravir, Remdesivir and Baloxavir	Cipla Ltd, Mumbai
Development of processes for preparation of rice bran lecithin from crude rice bran gums	AP Organics Litd, Punjab
Evaluation of nano-formulations for the molecules	InvAscent Advisory Pvt. Limited, Hyderabad
Exploratory studies on process development of 5,8-dimethoxy-[1,2,4]triazolo[1,5-c]pyrimidin-2-amine (DTPA)	Bhagiradha Chemicals, Hyderabad
Exploratory studies on Process Development of Trichlopyr-2-butoxyethylester	AIMCO Pesticides Pvt ltd, Mumbai
Insect Pheromone Lures to control the Pink Boll Worm in cotton fields (Aug 2019 - Jan 2020)	UPL Limited, Mumbai
Licensing of Patents on mitrochondria-targeted esculetin (Mito-Esc)	Sun Pharmaceutical Industries Ltd
Polymorphic study of BD-364 compound and investigation of its crystalline state in COSMOS formualtion	UPL Limited, Mumbai
Process development and BDR for 1 ton/day of Furfural alcohol and by-product 2 Furioc Acid from Furfural (June 2019 - Dec 2019)	Sri Kusuma Harnadha Agro Fural Ltd, West Godavari, A.P.
Process development for the enrichment of Phosphatidylcholine (PC) up to 90 & 95% from Sunflower and Soya lecithin powders	BGP Healthcare Private Limited, Gujarat

Title of the Project	Sponsor/ Collaborator
Process Development of Saflufenacil	AIMCO Pesticides Pvt ltd, Mumbai
Process improvement of pheromone molecules	ATGC Biotech Private Limited
Providing advisory consultancy for kinetic resolution of racemic BPRL - 102	Bioxera Pharma Research LLP, Pune
Providing advisory consultancy in conducting due diligence and techno-economic evaluations of tenders for setting up 15TPD of bio-methanation plants for treating wet waste in Corporation of the City of Panjim (CCP)	The Energy and Resources Institute, TERI, Bangalore
Providing advisory consultancy in the area of solid state forms of chemical compounds	UPL Limited, Mumbai
Providing advisory consultancy on revival of dormant food waste based biogas plant at Guwahati installed by Xeon Waste Managers	Xeon Waste Managers L.L.P, Pune
Recovery of hydrocarbons from oil sludge to reduce environmental impact	Sar Chandra Environ Solutions Pvt. Ltd., Kakinada
Synthesis of API Impurities (May 2019 - May 2020)	Sun Pharmaceutical Industries Ltd, Vadodara, Gujarat
Synthetic methodologies for pheromone for pink boll worm	NSJ Prayog Life Sciences Pvt Ltd, Medak
To develop a hybrid coating on steel strip for ready to paint (Feb 2020 - Feb 2022)	Tata Steel Limited, Jamshedpur

Grant-in-Aid

Title of the Project	Sponsor
2D transition metal layered double hydroxides: A cost-effective catalyst for hydrogen production by (photo) electrochemical water splitting	DST, New Delhi
ASEAN-Indian Research & Training Fellowship (AIRTF)	FICCI, New Delhi
ASEAN-Indian Research & Training Fellowship (AIRTF)	FICCI, New Delhi
Biotechnological process for the simultaneous removal of ammoniacal nitrogen and COD from industrial wastewater	DST, New Delhi
Catalytic sequential C-H activation for the generation of triazole-fused heterocyclic compounds	SERB, New Delhi
Design and investigation of new multicomponent crystalline forms of nonsteroidal antiandrogen drugs	DST, New Delhi
Development a public health informatics platform in India for a systems view of health and diseases	DST, New Delhi

Title of the Project	Sponsor
Development of candidate RL348 for methicillin and vancomycin-resistant staphyolcoccus aureus	DBT, New Delhi
Development of processes fir high import value fluorinated drug and agro intermediates	SERB, New Delhi
Development of processes for preparation of rice bran lecithin from crude rice bran gums	BIRAC, New Delhi
Drug discovery against malarial M1 and M17 class aminopeptidases: Structural, biochemical and medicinal chemistry approach	SERB, New Delhi
DST-IIT Delhi energy storage platform on batteries	DST, New Delhi
Establishing the oral cancer tissue organoid/sphere (OCTO S) system to envisage the sequence of events in drug resistant tumors: An armamentarium of drug discovery	SERB, New Delhi
Establishment of GLP compliant analytical facility at CSIR-IICT to augment biosimilars characterizations in India	BIRAC, New Delhi
Functional n-conjugated peptide based hybrid molecules: Emerging soft materials for optoelectronic applications	SERB, New Delhi
High rate biomethanation of market and vegetable waste-Telangana	DBT, New Delhi
ICMR Fellowship	ICMR, New Delhi.
Identification and validation of small molecules targeting prohibition in papillary thyroid cancer	MHFW, New Delhi
INSPIRE Fellowship	DST, New Delhi
Integrated information system to interpret, integrate and mitigation of cardio metabolic health care in North East tribes of Assam and Mizoram	ICMR, New Delhi.
Intensified continuous crystallizer for APIs: Design and development	SERB, New Delhi
Mechanisms of tumor dormancy and chemotherapy resistance in breast cancer: Implications for metastasis prevention	DBT, New Delhi
Model based design, synthesis and evaluation of Combined Sorbent Catalyst Materials (CSCM) for CO2 capture	DST, New Delhi
Network for scientific cooperation for food safety and applied nutrition	Food Safety and Standards Authority of India, New Delhi
Phycoremediation of wastewater for bioenergy carbon capture and storage	DST, New Delhi.
Plasma metabolomic profiling to identify metabolic biomarkers for early detection of prediabetes associated with pancreatogenic diabetes (Type3cDM)	SERB/AHF, New Delhi

Title of the Project	Sponsor
Polymer electrolyte integrated all-solid li-ion rechargeble batteries demonstrating operational feasibility	SERB, New Delhi
Protein phase separation: New drug target space for neurological disorders	DBT, New Delhi
Ramanujan Fellowship Award	SERB, New Delhi
Repositioning fluoxetine and salmeterol for treatment of dengue infections-Pre-clinical development and proof-of-concept studies	DBT, New Delhi
Research Training Fellowship-Development Countries Scientist (RTF-DCS)	FICCI, New Delhi
Targeting specifically breast tumor cells by developing potent derivative of tubulin binding anticancer agent, noscapine and conjugating it with folic acid	ICMR, New Delhi.
Unlocking therapeutic potential of some Indian flora and fauna	MoES, New Delhi
X-ray diffraction patterns of mixed-valent manganites	ICDD, USA

TECHNOLOGIES DEVELOPED AND TRANSFERRED

Name of the Technology	Client
Design of Small scale anaerobic digester for decentralized applications for Biowaste upto 150 kg/day	Khar Energy Optimisers, Hyderabad
Development of Biomethanation process from bagasse and spent wash	Spectrum Renewable Enerygy Pvt. Ltd., Kolhapur. (MH).
Development of Process for extruded Nutrafood for management of 1) metabolic disorders, and 2) anaemia and malnutrition	Ameya Life , Hyderabad
Process development and Basic Design Report for 1 ton/day of Furfural alcohol and by-product 2 Furioc Acid from Furfural	Sri Kusuma Harnadha Agro Fural Ltd., West Godavari, A.P.
Process development for the production of Dibromethane	M/s. Intech Organics Ltd., Gurugram, Harayana
Selective catalytic hydroxylation of benzene with molecular oxygen	M/s. Sabic Research & Technology Pvt. Ltd., UAE
Synthetic methodologies for pheromone for pink boll worm	NSJ Prayog Life Sciences Pvt Ltd, Medak

CSIR FUNDED PROJECTS UNDERTAKEN

Mission Mode Projects

Sl. No	Title
1	Crop protection chemicals
2	CSD-Catalysis for Sustainable Development
3	Food and Consumer Safety Solutions(Focus)
4.	INPROTICS-Pharma and Agro

Skill Development and JYGYASA Projects

Sl. No	Title
1	JYGYASA
2	Skill Development

Thematic and Fast track Translational Projects

Sl. No	Title
1	Accelerated Wound Healing by Bone marrow Stem Cells delivered using PEG-PU porous Polymer Scaffolds Grafted with KGF- and/or VEGF- Mimetic Peptides (GFART)
2	Autologous Transplantation of Transgenetically modified Hepatic Progenitor Cells expressing therapeutic genes- mediated Liver Regeneration (PROMPT)
3	Catalytic conversion of linear of alkyl benzene raffinate to be utilized for jet rocket fuel .
4	Chronic Respiratory Disease Innovation & Solution Programme
5	Development of Engineered Biochar from non-edible de-oiled seed cakes/stubble wastes for the removal of targeted herbicides/pesticides from agricultural wastewaters and subsequent soil remediation.
6	Development of hybrid flocculants at 100 g scale for selective adsorption of low grade iron ore slimes and fines to recover iron ore more that 80% (HYBFLOC)
7	Enzymatic Process for the preparation of API intermediates
8	Indigenous enzymes for vegetable and rice bran oil degumming
9	Mimicking Muscles: Electro active polymers for Bionics(NCP)
10	Non-destructive depth profiling and identification of debonding defects across polymer interfacial layer by using portable single-sided NMR.

Sl. No	Title
11	Pre-IND mission for undertaking validation studies of advance drug leads and filling the gaps for filling Investigational New Drugs (INDs)
12	Process development of vinylidene fluoride (VDF) and chloro trifluoro ethylene (CTFE) their polymerisation processes
13	Scale up of materials for Dye Sensitized Solar Cells and Organic Photovoltaics
14	Sustainable production of edible oils from Microalgae
15	Technology assessment and integration of CSIR's lignocellulosic etahnol programs/facilitating technologies for a feasible 2G ethanol technology(CSIR2GE)
16	Vegetable oil-based Gels as trans free fat (Oleo gel)
17	Waste and Biomass to Value Added Products
18	Water Treatment Technologies for portable water

HARIT Projects

Sl. No	Title
1	Pheromone Application Technology (PAT) : Pest management in Aspirational districts of Telangana state
2	Role of socioeconomic factors on malaria transmission in Arunachal Pradesh
3	Samadhankendra
4	Technologies and products for reduced emission Fire-Works (CSIR-HARIT)

CSIR-IICT and Sun Pharma sign an agreement for out licensing of patents on multiple therapeutic indications

PATENTS FILED IN INDIA & OVERSEAS

- A continuous flow Micro-total process system for preparation of CELECOXIB and Analogs thereof **Application No.** 201911004015 Dt: 01/02/2019 (India)
- A dewaxing aid for petroleum refining **Application No.** PCT/IN2018/05040 Dt: 26/06/2018 (PCT)
- A Process for the preparation of Nicotine **Application No.** 16/068464 Dt: 06/07/2018 (US); **Application No.** 17707968.8 Dt: 02/08/2018 (EP)
- An improved process for production of hydrazine hydrate **Application No.** 16/335225 Dt: 20/03/2019 (US)
- An improved process for the production of racemic lipoic acid **Application No.** 201811016688 Dt: 03/05/2018 (India)
- Gold nanoparticles based new formulations for the delivery of drugs and nucleic acids for HER2+cancer therapy **Application No.** 16/344519 Dt: 24/04/2019 (US)
- Indole(sulfomyl) N-hydroxy benzamide derivatives as selective HDAC inhibitors **Application No.** PCT/IN2018/050514 Dt: 06/08/2018 (PCT)
- Indole-Ynone mediated Benzoannulation process for preparation of carbazoles-carbazomycin A, Calothrixin B and staurosporinone thereof **Application No.** 201911012434 Dt: 29/03/2019 (India)
- Micro-electrolysis reactor for ultra fast, oxidant free, C-C coupling reaction and synthesis of Daclatasvir thereof **Application No.** 201911017478 Dt: 02/05/2019 (India)
- Nimbolide derivatives as Anticancer agents and preparation thereof **Application No.** 16/172045 Dt: 26/10/2018 (US)
- Novel polymeric biosurfactant preparations produced by newly isolated strains of microbacterium SP. strain BS-2 and Brevibacillus SP. Strain BS-207 and uses thereof **Application No.** 19150824.1 Dt: 08/01/2019 (EPA)
- Novel Saponin based vaccine adjuvant system **Application No.** 201811042595 Dt: 13/11/2018 (India)
- Ployaniline based supercapacitor **Application No.** 201811030628 Dt: 16/08/2018 (India)
- Process for the preparation of Tapentadol and Analogs thereof **Application No.** 201911012128 Dt: 28/03/2019 (India)
- Process for the preparation of zafirlukast and analogs thereof **Application No.** PCT/IN2018/050513 Dt: 06/08/2018 (PCT)
- Spirooxindole compounds as GSK3Â¿ inhibitors and process for preparation thereof **Application No.** 16/492,359 Dt: 09/09/2019 (US)
- Synthesis and Biological Evaluation of (E)-4-(4-Acrylamidophenoxy)-N-Methylpicolinamide Conjugates as Potential Anticancer Agents. **Application No.** 16/071105 Dt: 19/07/2018 (US); **Application No.** 17707967.0Dt: 02/08/2018 (EP)
- Synthesis and Biological Evaluation of 4Â¿-Amidotriazole linked Podophyllotoxin derivatives as Potential Anticancer Agents **Application No.** 16/084162 Dt: 11/09/2018 (US); **Application No.** 17725781.3 Dt: 11/10/2018 (EP)
- Synthesis of N-((1-pheny1-9H-pyrido[3,4-b]indo1-3-y1)methy1)cinnamamides as potential Anticancer Agents **Application No.** 16/071687 Dt: 20/07/2018 (US); **Application No.** 17714569.5 Dt: 23/07/2018 (EP)

PATENTS GRANTED IN INDIA & OVERSEAS

- 1,2,3 - Triazole tethered carbohydrate di and tri- lipidated cysteine conjugates useful as novel vaccine adjuvants and methods for the preparation there of **Granted No. 9969763 Dt: 15/05/2018 (US)**
- 3-Arylethynyl substituted quinazolinone compounds useful as potential anticancer agents **Granted No.300011 Dt: 16/08/2018 (India)**
- A highly enantioselective epoxide hydrolase from achromobacter **Granted No. 2748303 Dt: 03/10/2018 (EP, G Britain, France Germany)**
- A Process for the Preparation of Polyaniline **Granted No. 307163 Dt: 12/02/2019 (India)**
- A synergistic nanobioformulation useful as insect controlling agent and a method of its formulation **Granted No. 295354 Dt: 02/04/2018 (India)**
- Amidobenzothiazole analogues useful as potential anticancer agents and process for the preparation thereof **Granted No. 303610 Dt: 28/11/2018 (India)**
- An Improved method for the synthesis of silver hexacyanoferrate nanoparticles (prussian blue analogue) and its potential biomedical applications **Granted No. 10231996 Dt: 19/03/2019 (US)**
- Anaerobic gas lift reactor (AGR) for the treatment of organic solid waste. **Granted No. 307102 Dt: 11/02/2019 (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 **Granted No. 2895149 Dt: 24/04/2019 (Europe, G Britain, France, Germany)**
- Benzothiazole hybrids useful as potential anticancer agents and process for the preparation thereof **Granted No. 308121 Dt: 26/02/2019 (India)**
- Biological evaluation of 4-aza-2,3-didehydropodophyllotoxin analogues possessing potent antitumour activity **Granted No. 304893 Dt: 24/12/2018 (India)**
- Cationic lipid formulations for regressing established tumor **Granted No. 9944676 Dt: 17/04/2018 (US)**
- Chalcone linked pyrrolo[2,1-C][1,4] benzodiazepine hybrids as potential anticancer agents and process for the preparation thereof **Granted No. 302219 Dt: 15/10/2018 (India)**
- Diaryl ether linked pyrrolo[2,1-c][1,4]benzodiazepine hybrids as potential anticancer agents and process for the preparation thereof **Granted No. 305759 Dt: 16/01/2019 (India)**
- Isoxazole/isoxazoline / combretastatin linked dihydroquinazolinone hybrids a potential anticancer agents and process for the preparation thereof **Granted No. 300026 Dt: 16/08/2018 (India)**
- Methods for Inhabiting Tumor growth through RNA-Interference using liposomally associated CDC20siRNA **Granted No. 10227589 Dt: 12/03/2019 (US)**
- N-((3,4,5 - Trimethoxystyryl)aryl) cinnam amide derivatives as potential anticancer agents **Granted No. 3183230Dt: 24/10/2018 (EP, Britain, France, Germany)**
- Novel integrin binding RGD-Lipopeptides with gene transfer activities **Granted No. 300638 Dt: 31/08/2018 (India)**

- Novel polymeric biosurfactant preparations produced by newly isolated strains of microbacterium SP. strain BS-2 and Brevibacillus SP.Strain BS-207 and uses thereof **Granted No. 10106627Dt: 23/10/2018 (US); Granted No. 2947153 Dt: 09/01/2019 (EP, France, Germany, GB)**
- Phenyl nitrofurfuryl linked piperidino-oxadiazolone conjugates as antitubercular agents and process for the preparation there of **Granted No. 2511240 Dt: 13/06/2018 (Britain)**
- Process for Preparing 3-Substituted-3-Hydroxy Oxindole Derivatives **Granted No. 310615 Dt: 30/03/2019 (India)**
- Process for Synthesis of novel Mannose-Receptor selective lysinylated cationic amphiphile for invivo delivery of DNA Vaccines. **Granted No. 6360074 Dt: 29/06/2018 (Japan)**
- Process for the Preparation of highly efficient and stabilized copper (0) nanoparticles for Heck-, Suzuki-, Sonogashira-, and Stille- type coupling of Chloroarenes **Granted No. 305937 Dt: 19/01/2019 (India)**
- Progesterone-cationic lipid hybrid as anticancer agent and the process of synthesis thereof **Granted No. 10100079 Dt: 16/10/2018 (US)**
- Pyrazole linked benzimidazole conjugates as potential cancer agents **Granted No. 9951049 Dt: 24/04/2018 (US)**
- Pyrrolo[2,1-c][1,4] benzodiazepine linked imidazo[1,5-a]pyridine conjugates as potential antitumour agents and process for the preparation thereof **Granted No. 296587 Dt: 07/05/2018 (India)**
- Pyrrolo[2,1-c][1,4]naphthodiazepine linked substituted piperazine conjugates as potential antitumour agents and process for the preparation thereof **Granted No. 298164 Dt: 27/06/2018 (India)**
- Synthesis and biological evaluation of 3-(4-ethynyl phenyl) pyrido-pyrimidinone compounds as potential anticancer agents **Granted No. 2532627 Dt: 03/04/2019 (Britain); Granted No. 6333380 Dt: 11/05/2018 (Japan)**
- Synthesis and biological evaluation of mitochondria - targeted esculetin for its anti-atherosclerotic and age delaying effects **Granted No. 9963476 Dt: 08/05/2018 (US)**
- Synthesis and biological evaluation of pyrazolochalcone derivatives as potential anticancer agents **Granted No. 3039013 Dt: 12/09/2018 (Britain, France, EP, Germany); Granted No. 6338667Dt: 18/05/2018 (Japan)**
- Synthesis and in vitro anticancer activity of new pyrrolo[2,1-C][1,4] benzodiazepine derivatives with dithiocarbomate side chains and process for the preparation thereof **Granted No. 300470 Dt: 29/08/2018 (India)**
- Synthesis of highly efficient nano-structured photo-catalysts for hydrogen production under solar light irradiation. **Granted No. 302246 Dt: 16/10/2018 (India)**
- Synthesis of new benzothiazole derivatives as potential anti-tubercular agents **Granted No. 297106 Dt: 25/05/2018 (India); Granted No. 9949970 Dt: 24/04/2018 (US)**

PUBLICATIONS-2018

- Controlled photo-flow oxidative reaction (UV-FOR) platform for ultra-fast phthalide and API synthesis, **Green Chemistry, 4584-4590, 20(20) 2018**
- Axially substituted phosphorous(V) corrole with polycyclic aromatic hydrocarbons: syntheses, X-ray structures, and photoinduced energy and electron transfer studies, **New Journal of Chemistry, 8230-8240, 42(10) 2018**
- Synthesis of new 1,2-dideoxy C-linked carbo-beta-amino acids and alpha/beta-peptides with 11/9-helix, helix-turn and helix-turn-helix structures, **Tetrahedron, 6095-6106, 74(42) 2018**
- A simple approach to design chitosan functionalized Fe3O4 nanoparticles for pH responsive delivery of doxorubicin for cancer therapy, **Journal of Magnetism and Magnetic Materials, 199-207, 448(SI) 2018**
- Ir(iii)-catalyzed C-H/N-H functionalization of sulfoximines for the synthesis of 1,2-benzothiazines at room temperature, **Chemical Communications, 6288-6291, 54(49) 2018**
- Antimicrobial and anticancer potential of low molecular weight polypeptides extracted and characterized from leaves of Azadirachta indica, **International Journal of Biological Macromolecules, 906-921, 114, 2018**
- NaN3/NH4Cl-Promoted Aza-Cyclization: A Convenient Route for Bio-Active Diverse Isoindolinone Derivatives, **ChemistrySelect, 11950-11956, 3(42) 2018**
- Surface morphology of chlorine and castor oil-based polyurethane-urea coatings, **Polymer Bulletin, 5269-5285, 75(11) 2018**
- Synthesis and biological evaluation of Schizandrin derivatives as potential anti-cancer agents, **European Journal of Medicinal Chemistry, 182-192, 149, 2018**
- Quantitative determination of acidic hydrolysis products of Chemical Weapons Convention related chemicals from aqueous and soil samples using ion-pair solid-phase extraction and in situ butylation, **Journal of Separation Science, 689-696, 41(3) 2018**
- Administration of Roasted Barley and Roasted Horse Gram Powders Pacified Chronic Sucrose-induced Dysglycemia and Dyslipidemia in Rats and Exerted In Vitro Potent Antioxidative Stress Effect, **Pharmacognosy Magazine, 578-S590, 14(59) 2018**
- Synthesis and studies on gelation ability of phenol based maleate amphiphile and its application in nutraceutical release, **Colloids and Surfaces A: Physicochemical and Engineering Aspects, 310-317, 537, 2018**
- Translation of lignocellulosic waste to mesoporous solid acid catalyst and its efficacy in esterification of volatile fatty acid, **Microporous and Mesoporous Materials, 198-207, 264, 2018**
- Synthetic studies toward the marine metabolite prorocentin-4: synthesis of the C1-C23 fragment, **Organic & Biomolecular Chemistry, 4191-4194, 16(22) 2018**
- 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, **Bioresource Technology, 273-280, 253, 2018**
- Synthesis, single crystal X-ray, spectroscopic (FT-IR, UV–vis, fluorescence, 1H &13C NMR), computational (DFT/B3LYP) studies of some imidazole based picrates, **Journal of Molecular Structure, 277-285, 1158, 2018**
- Zika outbreak aftermath: status, progress, concerns and new insights, **Future Virology, 539-556, 13(8) 2018**
- **Editorial Material:** Computer Aided Drug Designing For Combating Diseases (Part 1), **Current Topics in Medicinal Chemistry, 1029-1030, 18(13) 2018**
- **Editorial Material:** Computer Aided Drug Design for Combating Diseases (Part-III), **Current Topics in Medicinal Chemistry, 2741-2742, 18(32) 2018**
- **Editorial Material:** Computer Aided Drug Design for Combating Diseases (Part-II), **Current Topics in Medicinal Chemistry, 2631-2632, 18(31) 2018**

- Investigations on anticorrosive, thermal, and mechanical properties of conducting polyurethanes with tetraaniline pendent groups, **Polymers for Advanced Technologies, 1620-1631, 29(6) 2018**
- Aniline-nonamer segmented polyurea: A facile electrocatalyst for detection of ascorbic acid, **Journal of Applied Polymer Science, Article Number: 46630, 135(37) 2018**
- 1,2,3-Triazole-fused spirochromenes as potential anti-tubercular agents: synthesis and biological evaluation, **RSC Advances, 16997-17007, 8(30) 2018**
- Formic acid assisted hydrogenation of levulinic acid to gamma-valerolactone over ordered mesoporous Cu/ Fe_2O_3 catalyst prepared by hard template method, **Journal of Chemical Sciences, Article Number: UNSP 16, 130(2) 2018**
- Nanoparticles for pest control: current status and future perspectives, **Journal of Pest Science, 1-15, 91(1) 2018**
- Stereoselective synthesis of 5'-hydroxyzearalenone, **Tetrahedron Letters, 3547-3549, 59(39) 2018**
- Palladium (II) Acetate/Base-Catalyzed Intermolecular Coupling of Imidazo[1,2-a]pyridine Esters with Aryl Halides, **Chemistry Select, 5639-5643, 3(20) 2018**
- Metal-free cross-dehydrogenative coupling approach for C-H bond functionalization of 2-phenyl pyridine derivatives in water, **Heteroatom Chemistry, Article Number: e21423, 29(3) 2018**
- One-step selective synthesis of 2-chlorobenzonitrile from 2-chlorotoluene via ammoxidation, **New Journal of Chemistry, 1892-1901, 42(3) 2018**
- Recent Advances in Halide-Based Perovskite Crystals and Their Optoelectronic Applications, **Crystal Growth & Design, 2645-2664, 18(4) 2018**
- Solvent-Assisted Tuning of the Size and Shape of CsPbBr3 Nanocrystals via Redispersion Process at Ambient Condition, **Langmuir, 15507-15516, 34(50) 2018**
- SIRT-3 Modulation by Resveratrol Improves Mitochondrial Oxidative Phosphorylation in Diabetic Heart through Deacetylation of TFAM, **Cells, Article Number: 235, 7(12) 2018**
- Synthesis and biological evaluation of imidazo[2,1-b]thiazole-benzimidazole conjugates as microtubule-targeting agents, **Bioorganic Chemistry, 515-526, 77, 2018**
- Study of forced degradation behaviour of cobicistat and atazanavir using LC/ESI/QTOF/MS; a combination of in-sourced and collision-induced dissociation for evaluation of the fragmentation patterns of degradation products, **New Journal of Chemistry, 19113-19128, 42(23) 2018**
- Characterization of forced degradation products of canagliflozine by liquid chromatography/quadrupole time-of-flight tandem mass spectrometry and in silico toxicity predictions, **Rapid Communications in Mass Spectrometry, 212-220, 32(3) 2018**
- First report on the pharmacokinetic profile of nimbolide, a novel anticancer agent in oral and intravenous administrated rats by LC/MS method, **Journal of Chromatography B-Analytical Technologies in the Biomedical and Life Sciences, 191-198, 1092, 2018**
- LC/QTOF/MS/MS characterization, molecular docking and in silico toxicity prediction studies on degradation products of anagliptin, **Journal of Pharmaceutical and Biomedical Analysis, 92-99, 159, 2018**
- Recent trends in electrochemical biosensors of superoxide dismutases, **Biosensors & Bioelectronics, 89-99, 116, 2018**
- Nanostructured Fused Pyrrole Thin Films: Encoding Nano "Bits" with Temporary Remanence, **Advanced Electronic Materials, Article Number: 1700626, 4(8) 2018**
- Studies on Synthesis of Novel Pyrido[2,3-d] pyrimidine Derivatives and Their Anticancer Activity, **Journal of Heterocyclic Chemistry, 2538-2544, 55(11) 2018**
- An aqueous medium-controlled stereospecific oxidative iodination of alkynes: efficient access to (E)-diiodoalkene derivatives, **New Journal of Chemistry, 17879-17883, 42(22) 2018**
- Design, Synthesis, and in vitro antitubercular activity of 1,2,3-triazolyl-dihydroquinoline derivatives, **Chemical Biology & Drug Design, 1315-1323, 92(1) 2018**

- A novel templates of piperazinyl-1,2-dihydroquinoline-3-carboxylates: Synthesis, anti-microbial evaluation and molecular docking studies, **Bioorganic & Medicinal Chemistry Letters, 1166-1170, 28(7) 2018**
- siRNA Delivery Using a Cationic-Lipid-Based Highly Selective Human DNA Ligase I Inhibitor, **ACS Applied Materials & Interfaces, 1616-1622, 10(2) 2018**
- Designing Microreactors Resembling Cellular Microenvironment via Polyamine-Mediated Nano particle-Assembly for Tuning Glucose Oxidase Kinetics, **Bioconjugate Chemistry, 2586-2593, 29(8) 2018**
- Evaluation of single and two stage anaerobic digestion of landfill leachate: Effect of pH and initial organic loading rate on volatile fatty acid (VFA) and biogas production, **Bioresource Technology, 364-373, 251, 2018**
- Direct Oxytosylation of 8-Amidoquinolines by Koser's Reagent: An Efficient Strategy for 5-Substituted 8-Amidoquinolines, **Synthesis-Stuttgart, 4089-4096, 50(20) 2018**
- Pd(II)/PhI(OAc)(2) promoted direct cross coupling of glucals with aromatic acids, **Carbohydrate Research, 1-3, 461, 2018**
- Potential anticancer activity of biogenic silver nanoparticles using leaf extract of Rhynchosia suaveolens: an insight into the mechanism, **Artificial Cells Nanomedicine and Biotechnology, S104-S114, 46(Supplement:1) 2018**
- Cardinal Epigenetic Role of non-coding Regulatory RNAs in Circadian Rhythm, **Molecular Neurobiology, 3564-3576, 55(4) 2018**
- Synthesis of new 2-(5-(4-alkyl-4H-dithieno[3,2-b:2 ',3 '-d]pyrrol-2-yl)thiophen-2-yl)methylene)malononitrile: Dopant free hole transporting materials for perovskite solar cells with high power conversion efficiency, **Solar Energy, 130-138, 174, 2018**
- Femtosecond, broadband nonlinear optical studies of a zinc porphyrin and zinc phthalocyanine, **Optics and Laser Technology, 418-425, 108, 2018**
- Chitosan-Thiobarbituric Acid: A Superadsorbent for Mercury, **ACS Omega, 13183-13194, 3(10) 2018**
- Studies towards the Total Synthesis of Aspergillide-B, **ChemistrySelect, 3391-3393, 3(12) 2018**
- An expeditious protocol for synthesis of Baylis-Hillman derived piperazine derivatives and evaluation of their AChE inhibition, **Research on Chemical Intermediates, 553-565, 44(1) 2018**
- Imidazopyridine linked triazoles as tubulin inhibitors, effectively triggering apoptosis in lung cancer cell line, **Bioorganic Chemistry, 714-720, 80, 2018**
- Synthesis and Cytotoxicity Evaluation of Novel Tricyclic Dihydropyrazolo [4,3-f] [1,2,3]triazolo Diazepines, **Letters in Drug Design & Discovery, 1020-1025, 15(10) 2018**
- 'AIE plus ESIPT' assisted photorelease: fluorescent organic nanoparticles for dual anticancer drug delivery with real-time monitoring ability, **Chemical Communications, 168-171, 54(2) 2018**
- 1,2,3-Triazole Tagged 3H-Pyrano[2,3-d]pyrimidine-6-carboxylate Derivatives: Synthesis, in Vitro Cytotoxicity, Molecular Docking and DNA Interaction Studies, **Chemistry & Biodiversity, Article Number: e18000101, 15(6) 2018**
- Synthesis of some novel orcinol based coumarin triazole hybrids with capabilities to inhibit RANKL-induced osteoclastogenesis through NF-kappa B signaling pathway, **Bioorganic Chemistry, 94-102, 78, 2018**
- Incorporation of graphene-Mn3O4 core into polyaniline shell: supercapacitor electrode material, **Ionics, 1467-1474, 24(5) 2018**
- Design and synthesis of ternary composite of polyaniline-sulfonated graphene oxide-TiO2 nanorods: a highly stable electrode material for supercapacitor, **Journal of Solid State Electrochemistry, 129-139, 22(1) 2018**
- Polyhydroxy-N-alkyl-2-pyrrolidinones as a new class of glycolipid analogues with immune modulation potential, **Journal of Carbohydrate Chemistry, 30-43, 37(1) 2018**

- What Has Come out from Phytomedicines and Herbal Edibles for the Treatment of Cancer?, **ChemMedChem, 1854-1872, 13(18) 2018**
- An Efficient Cr-TUD-1 Catalyst for Oxidative Dehydrogenation of Propane to Propylene with CO2 as Soft Oxidant, **Catalysis Letters, 576-585, 148(2) 2018**
- Pd/SBA-15 Catalysts for Hydrogenation of Furfuryl Alcohol to Tetrahydrofurfuryl Alcohol, **ChemistrySelect, 9946-9952, 3(34) 2018**
- Continuous Synthesis of Fuel Additives Alkyl Levulinates via Alcoholysis of Furfuryl Alcohol over Silica Supported Metal Oxides, **Catalysis Letters, 1731-1738, 148(6) 2018**
- Studies towards the total synthesis of Phostriecin, **Tetrahedron Letters, 454-456, 59(5) 2018**
- Effect of food to vegetable waste ratio on acidogenesis and methanogenesis during two-stage integration, **Bioresource Technology, 256-263, 254, 2018**
- Synthesis and Anticancer Evaluation of 1,2,4-Oxadiazole Linked Imidazothiadiazole Derivatives, **Russian Journal of General Chemistry, 1020-1024, 88(5) 2018**
- Liquid chromatography/electrospray ionization tandem mass spectrometry study of repaglinide and its forced degradation products, **Rapid Communications in Mass Spectrometry, 1181-1190, 32(15) 2018**
- Stereoselective Total Synthesis of (6S)-5,6-Dihydro-6-[(2R)-2-hydroxy-6-phenylhexyl]-2H-pyran-2-one from L-Malic Acid, **Natural Product Communications, 867-868, 13(7) 2018**
- Stereoselective Construction of Spiro-Indolenine Frameworks through a Prins/Friedel-Crafts Cyclization Cascade Reaction, **European Journal of Organic Chemistry, 1693-1698, 14, 2018**
- Microbial lipid production by Cryptococcus curvatus from vegetable waste hydrolysate, **Bioresource Technology, 284-289, 254, 2018**
- Alcaftadine: Selective Separation and Characterization of Degradation Products by LC-QTOF-MS/MS, **Chromatographia, 631-638, 81(4) 2018**
- In vitro and in vivo metabolic investigation of the Palbociclib by UHPLC-Q-TOF/MS/MS and in silico toxicity studies of its metabolites, **Journal of Pharmaceutical and Biomedical Analysis, 59-74, 157, 2018**
- Stereoselective Total Synthesis of 1,4-Dideoxy-1,4-imino-L-ribitol by an Intramolecular Ring Opening of Epoxide with a Tethered Amide, **Natural Product Communications, 1011-1012, 13(8) 2018**
- Three-component synthesis of amidomethylarenes and -heteroarenes over H beta zeolite under solvent-free conditions, **Catalysis Communications, 20-25, 105, 2018**
- Novel Amphiphilic G-Quadruplex Binding Synthetic Derivative of TMPyP4 and Its Effect on Cancer Cell Proliferation and Apoptosis Induction, **Biochemistry, 6514-6527, 57(46) 2018**
- Comparative study of cyto- and genotoxic potential with mechanistic insights of tungsten oxide nano- and microparticles in lung carcinoma cells, **Journal of Applied Toxicology, 896-913, 38(6) 2018**
- Synthesis and biological evaluation of triazole and isoxazole-tagged benzothiazole/benzoxazole derivatives as potent cytotoxic agents, **New Journal of Chemistry, 15546-15551, 42(19) 2018**
- Contemporary progress in the synthesis and reactions of 2-aminobenzothiazole: a review, **New Journal of Chemistry, 776-797, 42(2) 2018**
- Cu(i)-Catalyzed amidation/imidation of N-arylglycine ester derivatives via C-N coupling under mild conditions, **Organic Chemistry Frontiers, 788-792, 5(5) 2018**
- Food waste biorefinery: Sustainable strategy for circular bioeconomy, **Bioresource Technology, 2-12, 248(Part A) 2018**
- Direct Decomposition of NOX over TiO2 Supported Transition Metal Oxides at Low Temperatures, **Industrial & Engineering Chemistry Research, 16615-16621, 57(49) 2018**
- Our phytochemical research on Jatropha species, **Arkivoc, 114-133, SI(Part:1) 2018**

- Synthesis and biological activities of nicotinaldehyde based azlactones, **Indian Journal of Chemistry Section B-Organic Chemistry including Medicinal Chemistry, 98-107, 57(1) 2018**
- A Selective Three-Component, One-Pot Approach for the Synthesis of 1,2-Dihydroquinazolines and Quinazolines, **Chemistry Select, 9388-9392, 3(32) 2018**
- Anti-proliferative, structure-activity relationship of pyridinylchalcones and chromanones, **Medicinal Chemistry Research, 80-94, 27(1) 2018**
- Ceria-zirconia mixed oxides: Synthetic methods and applications, **Catalysis Reviews-Science and Engineering, 177-277, 60(2) 2018**
- Nutritionally enriched 1,3-diacylglycerol-rich oil: Low calorie fat with hypolipidemic effects in rats, **Food Chemistry, 210-216, 248, 2018**
- Recent Advances in Copper Intercalators as Anticancer Agents, **Journal of Fluorescence, 1195-1205, 28(5) 2018**
- Studies on gas sensing behavior of ZnNb2O6 nano composite towards hydrogen, **Materials Today Communications, 30-35, 15, 2018**
- Proposal of degradation pathway with toxicity prediction for hydrolytic and photolytic degradation products of timolol, **Journal of Pharmaceutical and Biomedical Analysis, 7-15, 154, 2018**
- One-dimensional hollow metal-complex as catalytic electrode for dye-sensitized solar cells, **Solar Energy, 502-507, 174, 2018**
- Mice With Partial Deletion of Y-Heterochromatin Exhibits Stress Vulnerability, **Frontiers in Behavioral Neuroscience, Article Number: 215, 12, 2018**
- Low Oxidative Stress-Mediated Proliferation Via JNK-FOXO3a-Catalase Signaling in Transplanted Adult Stem Cells Promotes Wound Tissue Regeneration, **Antioxidants & Redox Signaling, 1047-1065, 28(11) 2018**
- Synthesis of novel tetrazole containing hybrid ciprofloxacin and pipemidic acid analogues and preliminary biological evaluation of their antibacterial and antiproliferative activity, **Molecular Diversity, 83-93, 22(1) 2018**
- Computational Study of Enantioselectivity in the Asymmetric Allylation of Aldehydes with Chiral Pt(II) Phosphinite Complexes, **Journal of Organic Chemistry, 13911-13921, 83(22) 2018**
- 3D-2D lattice dimensionality, optical Eg and PL energy variations due to organic variant in two [ZnCl4]2- based hybrid materials, **Materials Chemistry and Physics, 98-104, 207, 2018**
- Platform Study on the Development of a Nondetoxified Rice Straw Hydrolysate to Its Application in Lipid Production from Mortierella alpina, **ACS Sustainable Chemistry & Engineering, 1225-1234, 6(1) 2018**
- Effect of Boiling and roasting on lipid quality, proximate composition, and mineral content of walnut seeds (Tetracarpidium conophorum) produced and commercialized in Kumba, South-West Region Cameroon, **Food Science & Nutrition, 417-423, 6(2) 2018**
- Effects of natural antioxidants extracted from Cameroonian ginger roots on the oxidative stability of refined palm olein, **European Food Research and Technology, 1015-1025, 244(6) 2018**
- Iodine promoted dual oxidative C(sp(3))-H amination of 2-methyl-3-arylquinazolin-4(3H)-ones: a facile route to 1,4-diarylimidazo[1,5-a]quinazolin-5(4H)-ones, **Organic & Biomolecular Chemistry, 1720-1727, 16(10) 2018**
- pH-Dependent self-assembly of water-soluble sulfonate-tetraphenylethylene with aggregation-induced emission, **Supramolecular Chemistry, 1-8, 30(1) 2018**
- Synthesis of Novel Thiophene-Chalcone Derivatives as Anticancer- and Apoptosis-Inducing Agents, **ChemistrySelect, 6859-6864, 3(24) 2018**
- Biochemical alterations induced by nickel oxide nanoparticles in female Wistar albino rats after acute oral exposure, **Biomarkers, 33-43, 23(1) 2018**

- BrOnsted acid promoted intramolecular cyclization of O-alkynyl benzoic acids: Concise total synthesis of exserolide F, **Synthetic Communications, 2403-2408, 48(18) 2018**
- Tetraphenylethylene-Based AIE-Active Probes for Sensing Applications, **ACS Applied Materials & Interfaces, 12189-12216, 10(15) 2018**
- Spermine-directed supramolecular self-assembly of water-soluble AIE-active tetraphenylethylene: nanobelt, nanosheet, globular and nanotubular structures, **New Journal of Chemistry, 15379-15386, 42(18) 2018**
- Interleukin-6 induced overexpression of valosin-containing protein (VCP)/p97 is associated with androgen-independent prostate cancer (AIPC) progression, **Journal of Cellular Physiology, 7148-7164, 233(10) 2018**
- Recovery of levulinic acid by reactive extraction using tri-n-octylamine in methyl isobutyl ketone: Equilibrium and thermodynamic studies and optimization using Taguchi multivariate approach, **Separation and Purification Technology, 314-324, 197, 2018**
- Synthesis and biological evaluation of 1-amino isochromans from 2-bromoethyl benzaldehyde and amines in acid medium, **Bioorganic & Medicinal Chemistry Letters, 196-201, 28(2) 2018**
- Vapor phase esterification of levulinic acid catalyzed by gamma-Al2O3 supported molybdenum phosphate catalysts, **Molecular Catalysis, 192-199, 451(SI) 2018**
- Effect of counterion on the properties of anionic waterborne polyurethane dispersions developed from cottonseed oil based polyol, **Journal of Polymer Research, Article Number: 186, 25(8) 2018**
- Stereoselective Synthesis of Northern Fragment of Eribulin Mesylate from D-Mannose, **Synthesis-Stuttgart, 1901-1906, 50(9) 2018**
- Synthesis of 2,3-dihydroquinazolin-4(1H)-ones from anthranilamide and ketones over H zeolite in aqueous media, **Synthetic Communications, 2866-2876, 48(22) 2018**
- A protecting-group-free synthesis of arbusculone, andirolactone, pinnatolide, ipomolactone, cyclocapitelline and isocyclocapitelline, **Tetrahedron Letters, 4172-4175, 59(47) 2018**
- Polyaniline-beta-Cyclodextrin-Graphene Nanocomposite for Energy Storage Application: Efficiency Enhancement through Radical Cation Stabilization, **Journal of the Electrochemical Society, A2549-A2556, 165(11) 2018**
- Excitation-dependent electron exchange energy and electron transfer dynamics in a series of covalently tethered N,N-bis(4-tert-butylbiphenyl-4-yl)aniline - [C-60] fullerene dyads via varying -conjugated spacers, **Physical Chemistry Chemical Physics, 21352-21367, 20(33) 2018**
- Stereoselective total synthesis and structural revision of the diacetylenic diol natural products strongylodiols H and I, **Beilstein Journal of Organic Chemistry, 2313-2320, 14, 2018**
- Synthesis and Characterization of Thiophene-Endcapped 3,7-Diphenyl Dipyrrolo[2,3-b:2,3-e]pyrazine-2,6(1H,5H)-diones as Non-Fullerene Acceptor Materials for Organic Solar Cells, **Asian Journal of Organic Chemistry, 2105-2112, 7(10) 2018**
- Oestrogen receptor-mediated liposomal drug delivery for treating melanoma, **Journal of Drug Targeting, 481-493, 26(5-6) 2018**
- L-Cysteine-Conjugated Ruthenium Hydrous Oxide Nanomaterials with Anticancer Active Application, **Langmuir, 1447-1456, 34(4) 2018**
- Stereoselective Total Synthesis of the Non-Contiguous Polyketide Natural Product (-)-Dolabriferol, **European Journal of Organic Chemistry, 1230-1240, (10) 2018**
- Molecular property diagnostic suite for diabetes mellitus (MPDSDM): An integrated web portal for drug discovery and drug repurposing, **Journal of Biomedical Informatics, 114-125, 85, 2018**
- High Affinity Neutral Bodipy Fluorophores for Mitochondria! Tracking, **ACS Medicinal Chemistry Letters, 618-622, 9(7) 2018**
- Study on Liposomal Encapsulation of New Bodipy Sensitizers for Photodynamic Therapy, **ACS Medicinal Chemistry Letters, 323-327, 9(4) 2018**

- Identification of novel beta-lactams and pyrrolidinone derivatives as selective Histamine-3 receptor (H3R) modulators as possible anti-obesity agents, **European Journal of Medicinal Chemistry, 148-159, 152, 2018**
- Synthesis and Liquid Crystalline Properties of Unsymmetrically Substituted Naphthalenediimides with a Polar Headgroup: Effect of Amide Hydrogen Bonding and Alkyl Chain Length, **ChemistryOpen, 61-67, 7(1) 2018**
- Synthetic Strategy toward the Pentacyclic Core of Melodinus Alkaloids, **Journal of Organic Chemistry, 2244-2249, 83(4) 2018**
- Rhodium-Catalyzed Highly Regio- and Enantioselective Reductive Cyclization of Alkyne-Tethered Cyclohexadienones, **ACS Catalysis, 1440-1447, 8(2) 2018**
- Design, Synthesis, In Vitro Evaluation and Docking Studies of Pyrazole-Thiazole Hybrids as Antimicrobial and Antibiofilm Agents, **ChemistrySelect, 8270-8276, 3(28) 2018**
- Total synthesis of cytotoxic pyranone B, **Synthetic Communications, 3133-3138, 48(24) 2018**
- Metformin treatment prevents SREBP2-mediated cholesterol uptake and improves lipid homeostasis during oxidative stress-induced atherosclerosis, **Free Radical Biology and Medicine, 85-97, 118, 2018**
- Supramolecular Chiral Helical Ribbons of Tetraphenylethylene-Appended Naphthalenediimide Controlled by Solvent and Induced by l- and d-Alanine Spacers, **Chemistry-An Asian Journal, 3947-3953, 13(24) 2018**
- Nano-Manufacturing Supramolecular Structures of Bio-Inspired Naphthalene Diimide Bolaamphiphile via Solvophobic Controlled Self-Assembly, **ChemistrySelect, 1460-1465, 3(5) 2018**
- Dynamic multistimuli-responsive reversible chiral transformation in supramolecular helices, **Scientific Reports, Article Number: 11220, 8, 2018**
- Syntheses of 2-Aroyl Benzofurans through Cascade Annulation on Arynes, **Journal of Organic Chemistry, 3325-3332, 83(6) 2018**
- Au-CGKRK Nanoconjugates for Combating Cancer through T-Cell-Driven Therapeutic RNA Interference, **ACS Omega, 8663-8676, 3(8) 2018**
- Designing Two-Dimensional Nanosheets for Improving Drug Delivery to Fucose-Receptor-Overexpressing Cancer Cells, **ChemMedChem, 2644-2652, 13(24) 2018**
- Synthesis and Industrial Catalytic Applications of Binary and Ternary Molybdenum Nitrides: A Review, **Catalysis Surveys from Asia, 166-180, 22(3) 2018**
- Role of the Feed Gas on the Selective Catalytic Dehydrogenation of Benzyl Alcohol over Cu/Hydrotalcite Catalyst, **ChemistrySelect, 8277-8284, 3(28) 2018**
- High performance polyurethane dispersion synthesized from plant oil renewable resources: A challenge in the green materials, **Polymer Degradation and Stability, 122-132, 150, 2018**
- Promotional Effect of Cu and Influence of Surface Ni-Cu Alloy for Enhanced H-2 Yields from CH4 Decomposition over Cu-Modified Ni Supported on MCM-41 Catalyst, **Energy & Fuels, 4008-4015, 32(3) 2018**
- Ammonolysis of (5S)-N-(tert-butoxycarbonyl)-5-(methoxycarbony1)-2-pyrroline with immobilized Candida antarctica lipase B (CAL B) in a packed bed reactor, **Process Biochemistry, 109-114, 65, 2018**
- Tuning Y-zeolite based catalyst with copper for enhanced activity and selectivity in vapor phase hydrogenolysis of glycerol to 1,2-propanediol, **Applied Catalysis A: General, 308-319, 550, 2018**
- Pyrene tethered imidazole derivative for the qualitative and quantitative detection of mercury present in various matrices, **Sensors and Actuators B: Chemical, 528-534, 256, 2018**
- The use of databases, data mining and immune informatics in vaccinology: where are we?, **Expert Opinion on Drug Discovery, 117-130, 13(2) 2018**

- Multiobjective optimization and experimental validation for batch cooling crystallization of citric acid anhydrate, **Computers & Chemical Engineering, 292-303, 112, 2018**
- PhI(OAc)(2)/NaX-mediated halogenation providing access to valuable synthons 3-haloindole derivatives, **New Journal of Chemistry, 18889-18893, 42(23) 2018**
- Synthesis of gamma-Valerolactone from Levulinic Acid and Formic Acid over Mg-Al Hydrotalcite Like Compound, **Chemistry Select, 6186-6194, 3(22) 2018**
- "Cell adhesion resistant, UV curable, polymer zinc oxide nanocomposite materials for intraocular lens application", **Polymers for Advanced Technologies, 1234-1241, 29(4) 2018**
- Polymer electrolyte integrated dye sensitized solar cells endow enhanced stability: Photoanode thickness and light intensity on cell performance, **Solar Energy, 159-166, 169, 2018**
- The performance enhancement of HTM-free ZnO nanowire-based perovskite solar cells via low-temperature TiCl4 treatment, **Solar Energy, 158-163, 170, 2018**
- Biofilm inhibition and anti-Candida activity of a cationic lipo-benzamide molecule with twin-nonyl chain, **Bioorganic & Medicinal Chemistry Letters, 1776-1780, 28(10) 2018**
- Recent Advances in the Development of Pharmaceutical Agents for Metabolic Disorders: A Computational Perspective, **Current Medicinal Chemistry, 5432-5463, 25(39) 2018**
- Determination of solubility, stability and degradation kinetics of morin hydrate in physiological solutions, **RSC Advances, 28836-28842, 8(50) 2018**
- I-2-Mediated Oxidative C-N and N-S Bond Formation in Water: A Metal-Free Synthesis of 4,5-Disubstituted/N-Fused 3-Amino-1,2,4-triazoles and 3-Substituted 5-Amino-1,2,4-thiadiazoles, **Journal of Organic Chemistry, 5715-5723, 83(10) 2018**
- Potential of the Bioinspired CaCO3 Microspheres Loaded with Tetracycline in Inducing Differential Cytotoxic Effects toward Noncancerous and Cancer Cells: A Cytogenetic Toxicity Assessment Using CHO Cells in Vitro, **Chemical Research in Toxicology, 629-636, 31(7) 2018**
- Synthesis of Polysubstituted Isoquinolines and Related Fused Pyridines from Alkenyl Boronic Esters via a Copper-Catalyzed Azidation/Aza-Wittig Condensation Sequence, **Journal of Organic Chemistry, 843-853, 83(2) 2018**
- Vapour phase selective hydrogenation of benzaldehyde to benzyl alcohol using Cu supported Mg-Al hydrotalicite catalyst, **Catalysis Communications, 73-77, 106, 2018**
- Synthesis, mechanistic and synergy studies of diarylidenecyclohexanone derivatives as new antiplasmodial pharmacophores, **Medicinal Chemistry Research, 2312-2324, 27(10) 2018**
- Highly Selective CO2 Gas Sensing Properties of CaO-BaTiO3 Heterostructures Effectuated through Discretely Created n-n Nanointerfaces, **ACS Sustainable Chemistry & Engineering, 4086-4097, 6(3) 2018**
- Stereoselective Access to the Core Structure of Macroline-Type Indole Alkaloids: Total Synthesis of Macroline and Alstomicine, **Organic Letters, 4782-4786, 20(16) 2018**
- Design of multifunctional peptide collaborated and docetaxel loaded lipid nanoparticles for antiglioma therapy, **European Journal of Pharmaceutics and Biopharmaceutics, 168-179, 132, 2018**
- Stereoselective total synthesis of paecilomycin E and F and its two congeners Cochliomycin C and 6-epi-Cochliomycin C, **Synthetic Communications, 1867-1875, 48(14) 2018**
- In Situ Generation of Cu-0 Supported on TiO2 Aerogel as a Catalyst for the Vapour Phase Hydrogenation of Nitrobenzene to Aniline, **Catalysis Letters, 2891-2900, 148(9) 2018**
- Real-time homonuclear broadband decoupled pure shift COSY, **Magnetic Resonance in Chemistry, 963-968, 56(10) 2018**

- Selective measurement of H-1-H-1 scalar couplings from crowded chemical shift regions: Combined pure shift and spin-echo modulation approach, **Magnetic Resonance in Chemistry, 941-946, 56(10) 2018**
- Isolation, Synthesis and AChE Inhibitory Potential of Some Novel Cinnamyl Esters of Taraxerol, the Major Metabolite of the Mangrove Bruguiera cylindrica, **Chemistry & Biodiversity, Article Number: e1800008, 15(4) 2018**
- Synthesis of Dihydrospiro Furo[2,3-c] pyrazoles Promoted by Hypervalent Iodine in Water, **Synlett, 1037-1042, 29(8) 2018**
- Regioselective synthesis of 2-carbonyl furans in a one pot three component reaction, **Tetrahedron Letters, 4168-4171, 59(47) 2018**
- Total Synthesis of Desmethyl Jahanyne and Its Lipo-Tetrapeptide Conjugates Derived from Parent Skeleton as BCL-2-Mediated Apoptosis-Inducing Agents, **ACS Omega, 63-75, 3(1) 2018**
- Benzyne Insertion onto beta-Keto Esters of Polycyclic Natural Products: Synthesis of Benzo Octacyclo Scaffolds, **Organic Letters, 7121-7124, 20(22) 2018**
- Epoxidation of styrene over MgO-rice derived carbon composite catalyst prepared by in situ transformation technique, **Indian Journal of Chemistry Section A-Inorganic Bio-Inorganic Physical Theoretical & Analytical Chemistry, 1106-1111, 57(8-9) 2018**
- Transition-Metal-Free Cyclization of Propargylic Alcohols with Aryne: Synthesis of 3-Benzofuranyl-2-oxindole and 3-Spirooxindole Benzofuran Derivatives, **Organic Letters, 3824-3828, 20(13) 2018**
- Polyaniline-grafted polyurethane coatings for corrosion protection of mild steel surfaces, **Journal of Applied Polymer Science, Article Number: 45806, 135(6) 2018**
- Metformin regulates mitochondrial biogenesis and senescence through AMPK mediated H3K79 methylation: Relevance in age-associated vascular dysfunction, **Biochimica Et Biophysica Acta-Molecular Basis of Disease, 1115-1128, 1864(4) 2018**
- Toward the synthesis of 1E-isomer of ent-hyptenolide, **Synthetic Communications, 2333-2338, 48(18) 2018**
- A green protocol for one pot synthesis of benzosuberone tethered thiadiazolopyrimidine-6-carboxylates using PEG-400 as potent anti-proliferative agents, **Tetrahedron Letters, 3015-3019, 59(31) 2018**
- 2,3-Dihydrofurans as Potential Cytotoxic and Antibacterial Agents: Tandem Knoevenagel-Michael Cyclization for the Synthesis of 2,3-Dihydrofurans by Using alpha-Tosyloxy Ketone Precursors, **Chemistry & Biodiversity, Article Number: e1800277, 15(11) 2018**
- Mitochondria-targeted esculetin inhibits PAI-1 levels by modulating STAT3 activation and miR-19b via SIRT3: Role in acute coronary artery syndrome, **Journal of Cellular Physiology, 214-225, 233(1) 2018**
- Carbonylative Suzuki-Miyaura Cross-Coupling Over Pd NPs/Rice-Husk Carbon-Silica Solid Catalyst: Effect Of 1,4-Dioxane Solvent, **ChemistrySelect, 7164-7169, 3(25) 2018**
- Design, synthesis and biological evaluation of 1, 4-dihydro indeno[1,2-c] pyrazole linked oxindole analogues as potential anticancer agents targeting tubulin and inducing p53 dependent apoptosis, **European Journal of Medicinal Chemistry, 104-115, 144, 2018**
- IBX/KI Promoted Synthesis of 2,5-Disubstituted 1,3,4-Oxadiazoles, **Letters in Organic Chemistry, 64-69, 15(1) 2018**
- Studies towards the synthesis of trocheliophorolides, **Tetrahedron Letters, 2157-2160, 59(22) 2018**
- Formal Synthesis of Angiopterlactone B via Enantioselective Reduction of Ketone with Daucus Carota Root, **ChemistrySelect, 1517-1520, 3(5) 2018**
- High-energy collision-induced dissociation of radiosensitizer anions: Nimorazole and metronidazole, **International Journal of Mass Spectrometry, 1-7, 431, 2018**
- Hierarchical porous organic polymer as an efficient metal-free catalyst for acetalization of carbonyl compounds with alcohols, **Molecular Catalysis, 43-50, 451(SI) 2018**

- High-Performance Microwave Synthesized Mesoporous TS-1 Zeolite for Catalytic Oxidation of Cyclic Olefins, **Industrial & Engineering Chemistry Research, 3567-3574, 57(10) 2018**
- Synthesis and Preliminary Antiproliferative Activity of Novel 4-Substituted Phenylsulfonyl Piperazines with Tetrazole Moiety, **Indian Journal of Pharmaceutical Sciences, 930-939, 80(5) 2018**
- Selective hydrogenation of biomass-derived ethyl levulinate to gamma-valerolactone over supported Co catalysts in continuous process at atmospheric pressure, **Journal of Industrial and Engineering Chemistry, 227-235, 61, 2018**
- Mesoporous silica supported cobalt catalysts for gas phase hydrogenation of nitrobenzene: role of pore structure on stable catalytic performance, **New Journal of Chemistry, 15714-15725, 42(19) 2018**
- Capsaicin, the pungent principle of peppers, ameliorates alcohol-induced acute liver injury in mice via modulation of matrix metalloproteinases, **Canadian Journal of Physiology and Pharmacology, 419-427, 96(4) 2018**
- Synthesis of Hydrocinnamaldehyde via Vapor Phase Dehydrogenation of Hydrocinnamyl alcohol over Rice-Derived MgO-Supported Copper Catalysts, **Chemistry Select, 3079-3086, 3(11) 2018**
- Alkoxylation Followed by Iodination of Oxindole with Alcohols Mediated by Hypervalent Iodine Reagent in the Presence of Iodine, **European Journal of Organic Chemistry, 4556-4564, (33) 2018**
- Nanomedicine for Cancer Therapy Using Autophagy: An Overview, **Current Topics in Medicinal Chemistry, 2599-2613, 18(30) 2018**
- Enantioselective total synthesis of beta-zearalenol from (s)-propylene oxide, **Synthetic Communications, 747-752, 48(7) 2018**
- Catalyst-free synthesis of pyrazole-aniline linked coumarin derivatives and their antimicrobial evaluation, **Journal of Saudi Chemical Society, 665-677, 22(6) 2018**
- Design, synthesis and biological evaluation of new beta-carboline-bisindole compounds as DNA binding, photocleavage agents and topoisomerase I inhibitors, **European Journal of Medicinal Chemistry, 1563-1577, 143, 2018**
- Shining light on panchromatic ruthenium sensitizers towards dye-sensitized photocatalytic hydrogen evolution, **International Journal of Hydrogen Energy, 6963-6976, 43(14) 2018**
- Kinetics of dye regeneration in liquid electrolyte unveils efficiency of 10.5% in dye-sensitized solar cells, **Journal of Materials Chemistry C, 11444-11456, 6(42) 2018**
- Substituent-Induced Deformed Ni-Porphyrin as an Electrocatalyst for the Electrochemical Conversion of Water into Dioxygen, **European Journal of Inorganic Chemistry, 1549-1555, 14, 2018**
- Lewis acidity induced heteropoly tungustate catalysts for the synthesis of 5-ethoxymethyl furfural from fructose and 5-hydroxymethylfurfural, **Molecular Catalysis, 108-115, 448, 2018**
- Stacking of microbial fuel cells with continuous mode operation for higher bioelectrogenic activity, **Bioresource Technology, 210-216, 257, 2018**
- Defatted algal biomass as feedstock for short chain carboxylic acids and biohydrogen production in the biorefinery format, **Bioresource Technology, 408-416, 269, 2018**
- Acidogenic valorization of vegetable waste for short chain carboxylic acids and biohydrogen production: Influence of pretreatment and pH, **Journal of Cleaner Production, 1055-1066, 203, 2018**
- Synthesis of Novel 2-Thioxothiazolidin-4-one and Thiazolidine-2, 4-dione Derivatives as Potential Anticancer Agents, **Natural Product Communications, 589-591, 13(5) 2018**
- Synthesis of Sex Pheromones of the Citrus Leafminer (CLM) (Phyllocnistis citrella), **Natural Product Communications, 599-602, 13(5) 2018**

- Photochemical Oxidative Coupling of 2-Naphthols using a Hybrid Reduced Graphene Oxide/Manganese Dioxide Nanocomposite under Visible-Light Irradiation, **ChemCat Chem, 1844-1852, 10(8) 2018**
- Ternary rGO/InVO4/Fe2O3 Z-Scheme Heterostructured Photocatalyst for CO2 Reduction under Visible Light Irradiation, **ACS Sustainable Chemistry & Engineering, 8201-8211, 6(7) 2018**
- Unprecedented synthesis of 1,2,3-triazolocinnolinone via Sonogashira coupling and intramolecular cyclization, **Organic & Biomolecular Chemistry, 4840-4848, 16(26) 2018**
- Targeting of EGFR, VEGFR2, and Akt by Engineered Dual Drug Encapsulated Mesoporous Silica-Gold Nanoclusters Sensitizes Tamoxifen-Resistant Breast Cancer, **Molecular Pharmaceutics, 2698-2713, 15(7) 2018**
- Studies on hydroquinone based maleate bolaamphiphile organogels and their drug formulations, **Soft Materials, 108-116, 16(2) 2018**
- Lasiosan, a new exopolysaccharide from Lasiodiplodia sp strain B2 (MTCC 6000): Structural characterization and biological evaluation, **Process Biochemistry, 162-169, 72, 2018**
- Synthesis of novel hetero ring fused pyridine derivatives; Their anticancer activity, CoMFA and CoMSIA studies, **Bioorganic & Medicinal Chemistry Letters, 2328-2337, 28(13) 2018**
- A nickel-catalyzed anti-carbometallative cyclization of alkyne-azides with organoboronic acids: synthesis of 2,3-diarylquinolines, **Chemical Communications, 759-762, 54(7) 2018**
- Studies towards the Synthesis of Portentol, **Chemistry Select, 11316-11319, 3(40) 2018**
- Rapid identification of limonoids from Cipadessa baccifera and Xylocarpus granatum using ESI-Q-ToF-MS/MS and their structure-fragmentation study, **Journal of Pharmaceutical and Biomedical Analysis, 224-233, 152, 2018**
- UPLC-MS/MS quantitative analysis and structural fragmentation study of five Parmotrema lichens from the Eastern Ghats, **Journal of Pharmaceutical and Biomedical Analysis, 45-57, 156, 2018**
- Synthesis of Novel Pyrido[2 ',3 ':3,4]Pyrazolo[1,5-alpha]Quinazoline Derivatives, Their Biological Evaluation and Molecular Modelling Studies, **ChemistrySelect, 7813-7821, 3(27) 2018**
- Synthesis of enamino-2-oxindoles via conjugate addition between alpha-azido ketones and 3-alkenyl oxindoles: Cytotoxicity evaluation and apoptosis inducing studies, **Bioorganic & Medicinal Chemistry Letters, 3564-3573, 28(22) 2018**
- TBAI/TBHP mediated oxidative cross coupling of ketones with phenols and carboxylic acids: Direct access to benzofurans, **Tetrahedron Letters, 33-37, 59(1) 2018**
- Influence of Acetylation/Deacetylation on Aggregation-Induced Emission, Chirality and Self-Assembly Behavior of beta-D-Glucopyranoside-Tethered Naphthalene Diimide Amphiphiles, **ChemistrySelect, 9393-9401, 3(32) 2018**
- Structural, spectral, theoretical and anticancer studies on new co-crystal of the drug 5-fluorouracil, **Journal of Molecular Structure, 951-958, 1173, 2018**
- Catalyst and Sensitizer-Free Visible-Light-Induced C(sp(2))-H Chalcogenation of Arenes/ Heteroarenes with Dichalcogenides, **Asian Journal of Organic Chemistry, 1689-1697,7(8) 2018**
- A comprehensive study on equilibrium and kinetics of morpholine extraction from aqueous stream with CA in toluene: Experimental evaluation, extraction model and parametric optimization employing desirability function, **Chemical Engineering Research & Design, 243-254, 133, 2018**
- Fullerene derivatives: A review on perovskite solar cells, **Materials Express, 389-406, 8(5) 2018**
- Aurora kinase B siRNA-loaded lactoferrin nanoparticles potentiate the efficacy of temozolomide in treating glioblastoma, **Nanomedicine, 2579-2596, 13(20) 2018**

- Design and Synthesis of New Etodolac-Pyridazinones as Potent Anticancer Agents Using Pb(OAc)(4) to Assist N-N Bond Formation, **ChemistrySelect, 5050-5054, 3(18) 2018**

- A Concise and Stereoselective Total Synthesis of Pestalotioprolide C Using Ring-Closing Metathesis, **Synthesis-Stuttgart, 1152-1158, 50(5) 2018**

- Design, Synthesis and Antibactertal Evaluation of Compounds Based on New Benzoxepine-oxime-1 2,3-triazole Hybrid, **Mini-Reviews in Medicinal Chemistry, 803-809, 18(9) 2018**

- CLC-Pred: A freely available web-service for in silico prediction of human cell line cytotoxicity for drug-like compounds, **PLoS One, Article Number: e0191838, 13(1) 2018**

- Conformation of flexibly linked triterpene dimers by using RDC-enhanced NMR spectroscopy, **Journal of Molecular Structure, 26-30, 1162, 2018**

- Fabrication of Pd/CuFe2O4 hybrid nanowires: a heterogeneous catalyst for Heck couplings, **New Journal of Chemistry, 1646-1654, 42(3) 2018**

- Kinetics and optimization studies using Response Surface Methodology in biodiesel production using heterogeneous catalyst, **Chemical Engineering Research & Design, 129-139, 135, 2018**

- Novel organophosphorus aminopyrimidines as unique structural DNA-targeting membrane active inhibitors towards drug-resistant methicillin-resistant Staphylococcus aureus, **MedChemComm, 1529-1537, 9(9) 2018**

- Novel aminopyrimidinyl benzimidazoles as potentially antimicrobial agents: Design, synthesis and biological evaluation, **European Journal of Medicinal Chemistry, 66-84, 143, 2018**

- An alternative stereoselective synthesis of (-)-1-tetrahydropyrenophorol, **Arkivoc, 112-119, (Part:3) 2018**

- Molecular interaction of novel benzothiazolyl triazolium analogues with calf thymus DNA and HSA-their biological investigation as potent antimicrobial agents, **European Journal of Medicinal Chemistry, 228-247, 150, 2018**

- Azoalkyl ether imidazo[2,1-b]benzothiazoles as potentially antimicrobial agents with novel structural skeleton, **Bioorganic & Medicinal Chemistry Letters, 2426-2431, 28(14) 2018**

- Facile redbrick clay as splendid catalyst for selective dehydration of alcohols, **Research on Chemical Intermediates, 7619-7639, 44(12) 2018**

- Vapor phase selective tetrahydrofuran production from dehydration of biomass derived 1,4-butanediol using ecofriendly red brick catalyst, **Catalysis Communications, 38-41, 110, 2018**

- Synthesis and In Vitro Anticancer Activity of Novel 1,3,4-Oxadiazole-Linked 1,2,3-Triazole/Isoxazole Hybrids, **Journal of Heterocyclic Chemistry, 863-870, 55(4) 2018**

- Synthesis of novel 1,3-thiazole-triazole and 1,3-thiazole-isoxazole hybrids, **Indian Journal of Chemistry Section B-Organic Chemistry including Medicinal Chemistry, 811-815, 57(6) 2018**

- Membrane contactor aided catalyst recycle and organic acid recovery from aqueous solutions using porous hydrophobic polyvinylidene fluoride barriers, **Journal of Cleaner Production, 923-936, 199, 2018**

- Synthesis of Bi(hetero)aryls via Sequential Oxidation and Decarboxylation of Benzylamines in a Batch/Fully Automated Continuous Flow Process, **European Journal of Organic Chemistry, 2831-2835, (22) 2018**

- Silver-Catalyzed Arylation of (Hetero)arenes via Oxidative Benzylic C-C Bond Cleavage of Benzyl Alcohols/ Benzaldehyde, **ChemistrySelect, 12336-12340, 3(43) 2018**

- A lipid-based cell penetrating nano-assembly for RNAi-mediated anti-angiogenic cancer therapy, **Chemical Communications, 1489-1492, 54(12) 2018**

- Synthesis of new spiro pyrrole/pyrrolizine/thiazole derivatives via (3+2) cycloaddition reactions, **New Journal of Chemistry, 13819-13827, 42(16) 2018**

- Exploring the potential of iron to replace ruthenium in photosensitizers: a computational study, **Journal of Molecular Modeling, Article Number: 341, 24(12) 2018**
- Roccellatol, a new -orcinol based metabolite from the lichen Roccella montagnei, **Natural Product Research, 268-274, 32(3) 2018**
- Stereoselective synthesis of the lichen metabolite, (+) montagnetol and its congeners as antimicrobial agents, **Synthetic Communications, 2992-2999, 48(23) 2018**
- Nanostructured Nickel/Silica Catalysts for Continuous Flow Conversion of Levulinic Acid to gamma-Valerolactone, **ACS Omega, 16839-16849, 3(12) 2018**
- Tandem Synthesis of 3,4-Disubstituted Pyrroles from Aldehydes, 1,3-Diketones and TosMIC Under Metal-Free Conditions, **ChemistrySelect, 2730-2733, 3(10) 2018**
- 5-Bromo-1-(4-chlorobenzyl-1H-indole-2-carboxamides as new potent antibacterial agents, **Heterocyclic Communications, 327-332, 24(6) 2018**
- Allium cepa root tip assay in assessment of toxicity o magnesium oxide nanoparticles and microparticles, **Journal of Environmental Sciences, 125-137, 66, 2018**
- Genotoxicity, biochemical, and biodistribution studies of magnesium oxide nano and microparticles in albino wistar rats after 28-day repeated oral exposure, **Environmental Toxicology, 396-410, 33(4) 2018**
- Synthesis of medium-sized aryl-fused nitrogenous heterocycles via sequential aryne aza-Claisen rearrangement/ring-closing metathesis, **Organic & Biomolecular Chemistry, 2134-2142, 16(12) 2018**
- Molecular iodine-catalysed oxidative CO-C(alkyl) bond cleavage of aryl/heteroaryl alkyl ketones: an efficient strategy to access fused polyheterocycles, **New Journal of Chemistry, 15820-15829, 42(19) 2018**
- A stereoselective approach for the total synthesis of (5R,7R,9R)-7,9-dihydroxy-5-decanolide, **Tetrahedron Letters, 2893-2895, 59(30) 2018**
- Discovery, Structural and Biochemical Studies of a rare Glu/Asp Specific M1 Class Aminopeptidase from Legionella pneumophila, **International Journal of Biological Macromolecules, 1111-1118, 120(Part: A) 2018**
- Impact of rotamer diversity on the self-assembly of nearly isostructural molecular semiconductors, **Journal of Materials Chemistry A, 383-394, 6(2) 2018**
- Epigenetic regulation of miR-200 as the potential strategy for the therapy against triple-negative breast cancer, **Gene, 248-258, 641, 2018**
- Cellular crosstalk mediated by platelet-derived growth factor BB and transforming growth factor beta during hepatic injury activates hepatic stellate cells, **Canadian Journal of Physiology and Pharmacology, 728-741, 96(8) 2018**
- Ferulic acid protects lipopolysaccharide-induced acute kidney injury by suppressing inflammatory events and upregulating antioxidant defenses in Balb/c mice, **Biomedicine & Pharmacotherapy, 304–315, 100, 2018**
- Supplementation of oat (Avena sativa L.) extract abates alcohol-induced acute liver injury in a mouse model, **Nutrition Research, 80-92, 54, 2018**
- Comparative Evaluation of Synthetic Routes and Antibacterial/Antifungal Properties of Zn-Al Layered Double Hydroxides Containing Benzoate Anion, **Environmental Engineering Science, 247-260, 35(3) 2018**
- Identification of diluent degradation products in radiolyzed PUREX solvent, **Solvent Extraction and Ion Exchange, 54-65, 36(1) 2018**
- Synthesis of the Polyoxygenated Cyclohexanoid Core of Bioactive Glycosides Xylosmin and Flacourtosides E and F, **Journal of Organic Chemistry, 10573-10579, 83(17) 2018**
- Total synthesis of epoxyquinone meroterpenoid natural product biscognienyne B, **Tetrahedron Letters, 4036-4038, 59(45) 2018**
- Ruthenium Nanoparticle-Decorated Porous Organic Network for Direct Hydrodeoxygenation of n Long-Chain Fatty Acids to Alkanes, **ACS Sustainable Chemistry & Engineering, 1610-1619, 6(2) 2018**

- Two way controls of apoptotic regulators consign DmArgonaute-1 a better clasp on it, **PLoS One, Article Number: e0190548, 13(1) 2018**
- Proton Triggered Colorimetric and Fluorescence Response of a Novel Quinoxaline Compromising a Donor-Acceptor System, **Sensors, Article Number: 3433, 18(10) 2018**
- Enrichment of hydrazine from aqueous solutions by vacuum membrane distillation through microporous polystyrene membranes of enhanced hydrophobicity, **Separation and Purification Technology, 159-167, 203, 2018**
- Chitosan-polytetrafluoroethylene composite membranes for separation of methanol and toluene by pervaporation, **Carbohydrate Polymers, 28-38, 193, 2018**
- Unveiling the Reversibility of Crystalline-Amorphous Nanostructures via Sonication-Induced Protonation, **Journal of Physical Chemistry C, 10255-10260, 122(18) 2018**
- Photobleaching of Triphenylamine-Phthalocyanine Entails Mixed Valence-State Triggered Self-Assembled Nanospheres, **Journal of Physical Chemistry C, 19946-19952, 122(34) 2018**
- Superior catalytic performance of a CoOx/Sn-CeO2 hybrid material for catalytic diesel soot oxidation, **New Journal of Chemistry, 14149-14156, 42(17) 2018**
- Noble metal-free CeO2-based mixed oxides for CO and soot oxidation, **Catalysis Today, 227-235, 309, 2018**
- New (3-(1H-benzo[d]imidazol-2-yl))/(3-(3H-imidazo [4,5-b]pyridin-2-yl))-(1H-indol-5-yl)(3,4,5-trimethoxy phenyl) methanone conjugates as tubulin polymerization inhibitors, **MedChemComm, 275-281, 9(2) 2018**
- Temperature-dependent conformational dynamics of cytochrome c: Implications in apoptosis, **Journal of Molecular Graphics & Modelling, 140-148, 79, 2018**
- Formal synthesis of Pellasoren - A, **Tetrahedron Letters, 4209-4212, 59(48) 2018**
- Alpha-Tocopherol-based cationic amphiphiles with a novel pH sensitive hybrid linker for gene delivery, **Organic & Biomolecular Chemistry, 2932-2946, 16(16) 2018**
- 1,2,3-triazole tethered Indole-3-glyoxamide derivatives as multiple inhibitors of 5-LOX, COX-2 & tubulin: Their anti-proliferative & anti-inflammatory activity, **Bioorganic Chemistry, 1-20, 81, 2018**
- Liquid phase hydrogenation of furfural using 2-propanol over, **Journal of Chemical Sciences, Article Number: UNSP 66, 130(6) 2018**
- Selective vapour phase dehydrogenation of biomass-derived 1,4-butanediol to gamma butyrolactone over Cu/ZrO2 catalysts: influence of La2O3 promotor, **Research on Chemical Intermediates, 5817-5831, 44(10) 2018**
- Product Selectivity as a Function of ZrO2 Phase in Cu/ZrO2 Catalysts in the Conversion of Cyclohexanol, **Catalysis Letters, 3042-3050, 148(10) 2018**
- First Stereoselective Total Synthesis of Tumonoic Acid A and its Derivatives, **SynOpen, 251-255, (2) 2018**
- CuI/TBHP: A versatile reagent system for the synthesis of 5-iodomethyl-2-aryl-4,5-dihydrooxazoles from N-allylarylamides, **Synthetic Communications, 1001-1007, 48(9) 2018**
- Synthesis of Phthalimides: A New Entry via TBAI-Catalyzed Intramolecular Cyclization of 2-(Hydroxymethyl) benzamides, **SynOpen, 145-149, (2) 2018**
- Delayed fluorescence based phenanthroimidazoles as OLED emitters having electron transporting properties, **Indian Journal of Chemistry Section B-Organic Chemistry including Medicinal Chemistry, 229-240, 57(2) 2018**
- Metabolic phasing of anoxic-PDBR for high rate treatment of azo dye wastewater, **Journal of Hazardous Materials, 49-58, 343, 2018**
- Supported liquid extraction and LC-MS-MS determination of iloperidone and olanzapine in rat plasma: Application to a pharmacokinetic study, **Journal of Chromatographic Science, 879-887, 56(10) 2018**
- **News Item:** Chemical Research Society of India Awards 2018, **Angewandte Chemie-International Edition, 2029-2030, 57(8) 2018**

- First stereoselective total synthesis of an anti-fouling agent, C-2-symmetric natural macrolide trichobotryside A, **Arkivoc, 495-508, (Part:7) 2018**
- Synthesis of imidazo-thiadiazole linked indolinone conjugates and evaluated their microtubule network disrupting and apoptosis inducing ability, **Bioorganic Chemistry, 420-436, 76, 2018**
- Studies towards the Synthesis of Lepranthin, **ChemistrySelect, 1024-1026, 3(4) 2018**
- Iodine-mediated new strategy for the synthesis of 2,5-disubstituted oxazoles from methyl ketones and TosMIC, **Synthetic Communications, 1986-1993, 48(15) 2018**
- Temperature Controlled Evolution of Silver Polypods from Biomass Encapsulated Nano-Droplets, **Journal of Nanoscience and Nanotechnology, 394-400, 18(1) 2018**
- An efficient and selective benzylic oxidation of tetralin to 1-tetralone on Cu (II) immobilized gamma-Fe2O3@SBA-15 magnetic nanocatalyst in green water medium without base or additives, **Molecular Catalysis, 74-84, 453, 2018**
- Biogenesis of silver nanoparticles using leaf extract of Indigofera hirsuta L. and their potential biomedical applications (3-in-1 system), **Artificial Cells Nanomedicine and Biotechnology, S1138-S1148, 46(Supplement:1) 2018**
- Applied resistance for power generation and energy distribution in microbial fuel cells with rationale for maximum power point, **Chemical Engineering Journal, 267-274, 335, 2018**
- LC-MS/MS Determination of Antihypertension Drugs in Rat Plasma and Urine: Applications to Pharmacokinetics, **Chromatographia, 1551-1557, 81(11) 2018**
- Insulin receptor knockdown blocks filarial parasite development and alters egg production in the southern house mosquito, Culex quinquefasciatus, **PLoS Neglected Tropical Diseases, Article Number: e0006413, 12(4) 2018**
- Amphiphilic comb-like polymer-modified graphene oxide and its nanocomposite with polystyrene via emulsion polymerization, **Colloid and Polymer Science, 133-144, 296 (1) 2018**
- Tandem Aza Michael Addition-Vinylogous Nitroaldol Condensation: Construction of Highly Substituted N-Fused 3-Nitropyrazolopyridines, **Journal of Organic Chemistry, 6454-6465, 83(12) 2018**
- Synthesis and biological evaluation of 12-, 13-, 14-membered macrolides and open chain 2,6-trans-disubstituted dihydropyran analogues for aspergillides, **Tetrahedron Letters, 2570-2576, 59(26) 2018**
- Constrained dynamics of the sole tryptophan in the third intracellular loop of the serotonin(1A) receptor, **Biophysical Chemistry, 34-41, 240, 2018**
- Wavelength-Selective Fluorescence of a Model Transmembrane Peptide: Constrained Dynamics of Interfacial Tryptophan Anchors, **Journal of Fluorescence, 1317-1323, 28(6) 2018**
- Effect of Phospholipid Headgroup Charge on the Structure and Dynamics of Water at the Membrane Interface: A Terahertz Spectroscopic Study, **Journal of Physical Chemistry B, 5066-5074, 122(19) 2018**
- Synthesis of Asthma Drug Zafirlukast (Accolate) Using Intramolecular Oxidative Coupling via sp(3) C-H Bond Activation, **ACS Omega, 4289-4294, 3(4) 2018**
- Antibacterial, in vitro antitumor activity and structural studies of rhodium and iridium complexes featuring the two positional isomers of pyridine carbaldehyde picolinic hydrazone ligand, **Arabian Journal of Chemistry, 714-728, 11(5) 2018**
- Design and synthesis of (Z/E)-2-phenyl/H-3-styryl-2H-chromene derivatives as antimicrotubule agents, **Journal of Chemical Sciences, Article Number: UNSP 127, 130(9) 2018**
- **Letter:** Naturally occurring chrysophanol as matrix-assisted laser desorption ionization matrix for the analysis of a broad spectrum of analytes, **Rapid Communications in Mass Spectrometry, 451-456, 32(5) 2018**

- **Editorial Material:** Preface-1st International Conference on Bioresource Technology for Bioenergy, Bioproducts & Environmental Sustainability (BIORESTEC), **Renewable Energy, 677-677, 129(Special Issue: SI) 2018**
- Promotion of unsupported nickel catalyst using iron for CO2 methanation, **International Journal of Hydrogen Energy, 4987-5000, 43(10) 2018**
- Magnesia-ceria mixed oxide catalysts for the selective transesterification of glycerol to glycerol carbonate, **Molecular Catalysis, 135-142, 451(SI) 2018**
- Regioselective Chlorination of Aryl C-H bonds with Hypervalent Iodine(III) Reagent 1-Chloro-1,2-benziodoxol-3-one, **Asian Journal of Organic Chemistry, 324-327, 7(2) 2018**
- Regulating BMI1 expression via miRNAs promote Mesenchymal to Epithelial Transition (MET) and sensitizes breast cancer cell to chemotherapeutic drug, **PLoS One, Article Number: e0190245, 13(2) 2018**
- One pot, three component 1,3 dipolar cycloaddition: Regio and diastereoselective synthesis of spiropyrrolidinyl indenoquinoxaline derivatives, **Tetrahedron Letters, 2688-2694, 59(27) 2018**
- Insight of aroma in brown rice through chemical assessment of 2-Acetyl-1-pyrroline (2AP) in aromatic germplasm of India, **Cereal Chemistry, 679-688, 95(5) 2018**
- Vapor Phase Selective Production of Ethyl Lactate over ZrO2-SiO2 Catalysts Using Lactic Acid and Ethanol, **ChemistrySelect, 10843-10848, 3(39) 2018**
- Unraveling the structural properties and reactivity trends of Cu-Ni bimetallic nanoalloy catalysts for biomass-derived levulinic acid hydrogenation, **Sustainable Energy & Fuels, 1516-1529, 2(7) 2018**
- Suzuki-Miyaura cross-coupling for efficient synthesis of aryl-substituted & ITN&IT-heteroarenes catalyzed by recyclable&IT N&IT-phenylpiperazine-Palladium (II) complex, **Inorganica Chimica Acta, 227-232, 477, 2018**
- Copper(I) Halide for Regioselective Ortho-Halogenation of Directed Arenes, **Catalysis Letters, 1067-1072, 148(4) 2018**
- Phanindrudu, Mandalaparthi; Wakade, Sandip Balasaheb; Tiwari, Dipak Kumar; Likhar, Pravin R; Tiwari, Dharmendra Kumar; Transition-Metal-Free Approach for the Synthesis of 4-Aryl-quinolines from Alkynes and Anilines, **Journal of Organic Chemistry, 9137-9143, 83(16) 2018**
- Nitrogen rich hyperbranched polyurethane-carbon nanohorn composite: Implications on the development of multifunctional coatings, **Polymer Composites, E772-E779, 39(Supplement 2) 2018**
- An Efficient Direct Access to Carbamates from Alcohols and TosMIC Mediated by Iodine in DMSO, **Synlett, 2039-2042, 29(15) 2018**
- Bismuth oxide cocatalyst and copper oxide sensitizer in Cu2O/TiO2/Bi2O3 ternary photocatalyst for efficient hydrogen production under solar light irradiation, **Ceramics International, 11783-11791, 44(10) 2018**
- Water-PEG-400 Mediated an Efficient One-Pot Eco-Friendly Synthesis of Functionalized Isoxazole Substituted Chromeno[2,3-b]pyridine-3-carboxylate Derivatives, **Chemistry Select, 7766-7770, 3(27) 2018**
- On the Structure of (R)-2-Methylheptyl Isonicotinate: Evidence for the Structural Solution from Total Synthesis, **Natural Product Communications, 335-338, 13(3) 2018**
- Biotransformation of Artemisinin to 14-Hydroxydeoxy artemisinin: C-14 Hydroxylation by Aspergillus flavus, **Journal of Agricultural and Food Chemistry, 10490-10495, 66(40) 2018**
- Potuganti, Gal Reddy; Indukuri, Divakar Reddy; Alla, Manjula; An Efficient One-Pot Multicomponent Synthesis of Tetracyclic Quinazolino[4,3-b] quinazolines by Sequential C-N Bond Formation and Copper-Mediated Aerobic Oxidative Cyclization, **Synlett, 1717-1722, 29(13) 2018**

- Copper-Catalyzed Domino Addition, Hydroamination, and Cyclization: A Multicomponent Approach to Spiro Oxazolidinone Derivatives, **Journal of Organic Chemistry, 15186-15194, 83(24) 2018**
- Cyclic lipopeptide biosurfactant from Bacillus tequilensis exhibits multifarious activity, **3 Biotech, Article Number: 261, 8(6) 2018**
- A synthetic study toward the core structure of (-)-apicularen A, **Organic & Biomolecular Chemistry, 8810-8818, 16(45) 2018**
- Novel menadione hybrids: Synthesis, anticancer activity, and cell-based studies, **Chemical Biology & Drug Design, 220-233, 91(1) 2018**
- Iron-Catalyzed Arene C-H Amidation Using Functionalized Hydroxyl Amines at Room Temperature, **ACS Catalysis, 8369-8375, 8(9) 2018**
- Glycogen synthase kinase-3 and its inhibitors: Potential target for various therapeutic conditions, **European Journal of Medicinal Chemistry, 843-858, 144, 2018**
- Synthesis of 8 ',11 '-dihydrospiro[cyclohexane-1,2 '-oxepino[2,3-h] chromen]-4 '(3 ' H)-ones with ring closing metathesis as a key step, **RSC Advances, 38673-38680, 8(67) 2018**
- Development of pyrrolo[2,1-c][1,4]benzodiazepine β-glucoside prodrugs for selective therapy of cancer, **Bioorganic Chemistry, 288-293, 76, 2018**
- Preparation of (1R,4S)-4-hydroxycyclopent-2-en-1-yl acetate via Novozym-435 (R) catalyzed desymmetrization of cis-3,5-Diacetoxy-1-cyclopentene, **Tetrahedron, 6673-6679, 74(46) 2018**
- Stereoselective carbon-carbon bond formation via 1,2-asymmetric induction by a beta-substituent in the reaction of alpha-chloro sulfides with organozinc reagents, **Indian Journal of Chemistry Section B-Organic Chemistry including Medicinal Chemistry, 327-339, 57(3) 2018**
- A short convergent synthesis of the [3.2.1] dioxabicyclo octane subunit of sorangicin A via regioselective epoxide opening, **Tetrahedron, 1071-1077, 74(10) 2018**
- Iodine mediated oxidative cross-coupling of unprotected anilines and heteroarylation of benzothiazoles with 2-methylquinoline, **Organic & Biomolecular Chemistry, 635-644, 16(4) 2018**
- Quantitative Analysis of Intermolecular Interactions in 3-Cyano-2-Pyridones: Evaluation through Single Crystal X-ray Diffraction and Density Functional Theory, **ChemistrySelect, 5864-5873, 3(21) 2018**
- Comb-like polymer-graphene nanocomposites with improved adhesion properties via surface-initiated atom transfer radical polymerization (SI-ATRP), **Journal of Applied Polymer Science, Article Number: 45885, 135(8) 2018**
- 3-Heterosubstituted Benzofurans from Hydroxyphenyl Propargyl Alcohols via ortho-Quinone Methide through a Metal-/Catalyst-Free Conjugate Addition/Oxy-Cyclization, **ACS Omega, 17155-17163, 3(12) 2018**
- Nickel Catalyzed syn-Selective Aryl Nickelation and Cyclization of Aldehyde/Enone-Tethered Terminal Alkynes with Arylboronic Acids, **Journal of Organic Chemistry, 15361-15371, 83(24) 2018**
- A One-pot Facile Construction of 1H-1,2,3-Triazolyl 1,2-Dihydropyridyl Derivatives and Evaluation of Bioactivity Profile, **ChemistrySelect, 13729-13735, 3(48) 2018**
- 8-Hydroxypyrene-1,3,6-trisulfonic acid trisodium salt (HPTS) based high fluorescent, pH stimuli waterborne polyurethane coatings, **Polymer, 157-165, 136, 2018**
- First total synthesis of Brevipolide N and total synthesis of Brevipolide M, **Tetrahedron Letters, 4213-4215, 59(48) 2018**
- Reversible Fluorescence Modulation in a Dyad Comprising Phenothiazine Derivative and Spiropyran, **Asian Journal of Organic Chemistry, 2254-2262, 7(11) 2018**
- Copper-Catalyzed Direct Oxidative alpha-Functionalization of Tetrahydroquinoline in Water under Mild Conditions, **Advanced Synthesis & Catalysis, 4080-4083, 360(21) 2018**

- Cu-Catalyzed Coupling of O-Acyl Oximes with Isatins: Domino Rearrangement Strategy for Direct Access to Quinoline-4-Carboxamides by C-N Bond Cleavage, **European Journal of Organic Chemistry, 2963-2971, 23, 2018**
- Mn(OAc)(3)*2H(2)O promoted addition of arylboronic acids to quinoxalin-2-ones, **Tetrahedron Letters, 628-631, 59(7) 2018**
- One-step synthesis of PEDOT-PSSauTiO(2) by peroxotitanium acid: a highly stable electrode for a supercapacitor, **Ionics, 1475-1485, 24(5) 2018**
- TiO2 Nanoparticle Catalyzed Rapid Synthesis of Spiroxindole-Pyrrolidine in Aqueous Medium and Evaluation of their Antimicrobial Properties, **ChemistrySelect, 9096-9101, 3(31) 2018**
- Asymmetric Synthetic Strategies of (R)-(-)-Baclofen: An Antispastic Drug, **Synthesis-Stuttgart, 211-226, 50(2) 2018**
- Stereoselective synthesis of the C3-C15 fragment of callyspongiolide, **Tetrahedron Letters, 3579-3582, 59(39) 2018**
- Solvent-Controlled, Tunable Domino Reaction of 3-Ylideneoxindoles with in Situ-Generated alpha-Aryldiazomethanes: A Facile Access to 3-Spirocyclopropyl-2-oxindole and Pyrazoloquinazolinone Scaffolds, **ACS Omega, 12349-12360, 3(10) 2018**
- Synergistic Gold and Copper Dual Catalysis for Intramolecular Glaser-Hay Coupling: Rapid Total Synthesis of Ivorenolide B, **European Journal of Organic Chemistry, 4376-4380, (32) 2018**
- Silver(i)-catalyzed sequential hydroamination and Prins type cyclization for the synthesis of fused benzo-delta-sultams, **Organic & Biomolecular Chemistry, 5163-5166, 16(28) 2018**
- **Proceedings Paper:** PEO based polymer composite with added acetamide, NaI/I-2 as gel polymer electrolyte for dye sensitized solar cell applications, **International Conference on Advances in Materials and Manufacturing Applications (IConAMMA-2017), Article Number: UNSP 012012, 310, 2018**
- Aggregation Behavior of pHLIP in Aqueous Solution at Low Concentrations: A Fluorescence Study, **Journal of Fluorescence, 967-973, 28(4) 2018**
- Selective allylic oxidation of cyclohexene over a novel nanostructured CeO2-Sm2O3/SiO2 catalyst, **Research on Chemical Intermediates, 6151-6168, 44(10) 2018**
- Ag-2[Fe(CN)(5)NO] Nanoparticles Exhibit Anti bacterial Activity and Wound Healing Properties, **ACS Biomaterials Science & Engineering, 3434-3449, 4(9) 2018**
- Synthesis and Optoelectrical Characterization of Novel Squaraine Dyes Derived from Benzothiophene and Benzofuran, **ACS Omega, 13919-13927, 3(10) 2018**
- Molecular Engineering and Structure-Related Properties of Squaraine Dyes Based on the Core and Wings Concept, **ACS Omega, 15416-15425, 3(11) 2018**
- **Proceedings Paper:** Porous zirconium phosphate solid acid catalysts with variable Zr/P ratio for gas phase glycerol dehydration to acrolein, **Materials Today-Proceedings, 25773-25781, 5(12) 2018**
- Total Synthesis of the Anticancer Marine Natural Product Mycalol, **European Journal of Organic Chemistry, 398-412, (3) 2018**
- Decarboxylative Coupling of Cyclic alpha-Amino Acid with Aldehyde and Kojic Acid: Direct Access to 2-Pyrrolidinyl and 2-Piperidinyl Kojic Acid Derivatives, **ChemistrySelect, 13110-13112, 3(46) 2018**
- Copper-Catalyzed Direct Amination of Aryl C-H Bonds with Alkylamines via Bidentate Chelation Assistance from 8-Aminoquinoline Motif at Room Temperature, **ChemistrySelect, 11148-11151, 3(40) 2018**
- An efficient non-fullerene acceptor based on central and peripheral naphthalene diimides, **Chemical Communications, 5062-5065, 54(40) 2018**
- One pot selective transformation of biomass derived chemicals towards alkyl levulinates over titanium exchanged heteropoly tungstate catalysts, **Catalysis Today, 269-275, 309, 2018**
- Synthesis and biological evaluation of novel flavone/triazole/benzimidazole hybrids and flavone/ isoxazole-annulated heterocycles as antip roliferative

and antimycobacterial agents, **Molecular Diversity, 803-814, 22(4) 2018**

- Novel actinomycin group compound from newly isolated Streptomyces sp RAB12: isolation, characterization, and evaluation of antimicrobial potential, **Applied Microbiology and Biotechnology, 1241-1250, 102(3) 2018**
- Copper-Catalyzed Domino C-C Bond Cleavage of 2,3-Unsubstituted Indoles/Indolines and Oxindoles via Oxidation and Directed Insertion of 2-Aminopyridines: Direct Access to Quinazolinediones, **Advanced Synthesis & Catalysis, 3009-3014, 360(16) 2018**
- Synthesis and Anti-proliferative Activity of 4H-Chromone Based Phenylhydrazones, Pyrazole carboxylates and Pyrazolylmethanones, **Acta Chimica Slovenica, 34-49, 65(1) 2018**
- Differential cationization of fatty acids with monovalent cations studied by electrospray ionization tandem mass spectrometry and a computational approach, **Rapid Communications in Mass Spectrometry, 1126-1134, 32(14) 2018**
- Rh(III)-Catalyzed Cascade Annulations To Access Isoindolo[2,1-b]isoquinolin-5(7H)-ones via C-H Activation: Synthesis of Rosettacin, **Organic Letters, 150-153, 20(1) 2018**
- Synthetic Studies toward (+/-)-Furanocembranoid 1: Construction of the Acyclic Carbon Framework, **ACS Omega, 15628-15634, 3(11) 2018**
- Cu(I)-Catalyzed Aminative Aza-Annulation of Enynyl Azide using N-Fluorobenzenesulfonimide: Synthesis of 5-Aminonicotinates, **Organic Letters, 3128-3131, 20(10) 2018**
- One-Pot Synthesis of Triazolo-Heterolignans: Biological Evaluation and Molecular Docking Studies as Tubulin Inhibitors, **Anti-Cancer Agents in Medicinal Chemistry, 1702-1710, 18(12) 2018**
- Synthesis and biological evaluation of longanlactone analogues as neurotrophic agents, **Bioorganic & Medicinal Chemistry Letters, 673-676, 28(4) 2018**
- Synthetic Access to Cyclopenta[a]inden-2(1H)-ones from Morita-Baylis-Hillman Products of 2-Alkynyl Benzaldehydes, **ACS Omega, 15734-15742, 3(11) 2018**
- Ru(II)-Catalyzed Oxidative Functionalization of Arylhydrazine-1,2-dicarboxylates with Internal Alkynes for the Synthesis of Enecarbamates, **ACS Omega, 9746-9753, 3(8) 2018**
- Total Synthesis of Cryptorigidifoliol K: Confirmation of Structure and Absolute Configuration, **Asian Journal of Organic Chemistry, 2504-2510, 7(12) 2018**
- Highly meta-selective halogenation of 2-phenylpyridine with a ruthenium(I) catalyst, **Organic Chemistry Frontiers, 1118-1123, 5(7) 2018**
- Propargylamine (secondary) as a building block in indole synthesis involving ultrasound assisted Pd/Cu-catalyzed coupling-cyclization method: Unexpected formation of (pyrazole)imine derivatives, **Tetrahedron Letters, 4587-4592, 59(52) 2018**
- Photoinduced energy transfer in carbazole-BODIPY dyads, **Physical Chemistry Chemical Physics, 27418-27428, 20(43) 2018**
- Simultaneous determination of fast and slow dynamics in molecules using extreme CPMG relaxation dispersion experiments, **Journal of Biomolecular NMR, 1-9, 70(1) 2018**
- Stereoselective Synthesis of C1-C7 and C6-C22 Fragments of Phostriecin, Goniothalamines, and Their Analogues, **European Journal of Organic Chemistry, 4389-4399, (32) 2018**
- Synthesis of beta(3)-amino acid and peptides from D-ribose, **Synthetic Communications, 1487-1493, 48(12) 2018**
- Dimethylarginine dimethylaminohydrolase-1 (DDAH1) is frequently upregulated in prostate cancer, and its overexpression conveys tumor growth and angiogenesis by metabolizing asymmetric dimethylarginine (ADMA), **Angiogenesis, 79-94, 21(1) 2018**
- Ru(II)-Catalyzed Hydroarylation of Maleimides with Cyclic N-SulfonylKetimines through ortho-C-H Bond Activation, **ChemistrySelect, 5062-5065, 3(18) 2018**
- Green Approach for the Domino Reduction/Reductive Amination of Nitroarenes and Chemoselective Reduction of Aldehydes Using Fe/aq. Citric

Acid/Montmorillonite K10, **ChemistrySelect, 13670-13674, 3(48) 2018**

- Metal-free One-pot Synthesis of 1,2,4-Triazolo[4,3-a]pyridines from 2-Hydrazinylpyridines, **Advanced Synthesis & Catalysis, 3069-3073, 360(16) 2018**
- Tandem Prins cyclization for the synthesis of 1,8-dioxa-3-azaspiro[4.5] dec-2-ene derivatives, **Tetrahedron Letters, 1084-1086, 59(12) 2018**
- Domino Oxidative Cyclization for the One-Pot Synthesis of Pyrrolo[1, 2-a]quinoxaline Derivatives, **ChemistrySelect, 9881-9884, 3(34) 2018**
- Medium-Chain Fatty Acids (MCFA) Production Through Anaerobic Fermentation Using Clostridium kluyveri: Effect of Ethanol and Acetate, **Applied Biochemistry and Biotechnology, 594-605, 185(3) 2018**
- Sustainable production of medium chain fatty acids (MCFA) with an enriched mixed bacterial culture: microbial characterization using molecular methods, **Sustainable Energy & Fuels, 372-380, 2(2) 2018**
- Photocatalytic Reforming of Biomass Derived Crude Glycerol in Water: A Sustainable Approach for Improved Hydrogen Generation Using Ni(OH)(2) Decorated TiO2 Nanotubes under Solar Light Irradiation, **ACS Sustainable Chemistry & Engineering, 3754-3764, 6(3) 2018**
- CuO Quantum Dots Decorated TiO2 Nanocomposite Photocatalyst for Stable Hydrogen Generation, **Industrial & Engineering Chemistry Research, 568-577, 57(2) 2018**
- Ru(II)-Catalyzed spirocyclization of aryl N-sulfonyl ketimines with aryl isocyanates through an aromatic C-H bond activation, **Organic & Biomolecular Chemistry, 2522-2526, 16(14) 2018**
- Emerging Role of Green Oxidant I-2/DMSO in Organic Synthesis, **Current Organic Synthesis, 815-838, 15(6) 2018**
- Fellutamide B Synthetic Path Intermediates with in Vitro Neuroactive Function Shows Mood-Elevating Effect in Stress-Induced Zebrafish Model, **ACS Omega, 10534-10544, 3(9) 2018**
- Metal-free, highly regioselective sulfonylation of NH-1,2,3-triazoles with sodium sulfinates and thiosulfonates, **Tetrahedron Letters, 2014-2017, 59(21) 2018**
- Asymmetric Reaction of p-Quinone Diimide: Organocatalyzed. Michael Addition of alpha-Cyanoacetates, **Organic Letters, 2572-2575, 20(9) 2018**
- Importance of Baylis-Hillman adducts in modern drug discovery, **Tetrahedron Letters, 2859-2875, 59(30) 2018**
- Comparative study of nano and bulk Fe3O4 induced oxidative stress in Wistar rats, **Biomarkers, 425-434, 23(5) 2018**
- 4 beta-amidotriazole linked podophyllotoxin congeners: DNA topoisomerase-II alpha inhibition and potential anticancer agents for prostate cancer, **European Journal of Medicinal Chemistry, 595-611, 144, 2018**
- An efficient synthesis of versatile synthon 3-chlorooxindoles with NaCl/oxone, **New Journal of Chemistry, 20152-20155, 42(24) 2018**
- DMAP catalysed vinylogous Rauhut-Currier reaction of allenoates with para-quinone methides, **Tetrahedron Letters, 2631-2635, 59(27) 2018**
- Quantum Yield and Fatty Acid Profile Variations With Nutritional Mode During Microalgae Cultivation, **Frontiers in Bioengineering and Biotechnology, Article Number: 111, 6, 2018**
- Gel-Emulsion Properties of Nontoxic Nicotinic Acid-Derived Glucose Sensor, **Industrial & Engineering Chemistry Research, 2847-2855, 57(8) 2018**
- Identification and characterization of reaction products of 5-hydroxytryptamine with methylglyoxal and glyoxal by liquid chromatography/tandem mass spectrometry, **Rapid Communications in Mass Spectrometry, 1529-1539, 32(17) 2018**
- An overview of experimental designs in HPLC method development and validation, **Journal of Pharmaceutical and Biomedical Analysis, 590-611, 147, 2018**

- Zeolitic Imidazolate Framework-Mediated Synthesis of Co_3O_4 Nanoparticles Encapsulated in N-Doped Graphitic Carbon as an Efficient Catalyst for Selective Oxidation of Hydrocarbons, **ACS Applied Nano Materials, 4836–4851, 1(9) 2018**
- Aminobenzosuberone Scaffold as a Modular Chemical Tool for the Inhibition of Therapeutically Relevant M1 Aminopeptidases, **Molecules, Article Number: 2607, 23(10) 2018**
- Palladium-Catalyzed Cross-Coupling of 1,3,4-Oxadiazoles and Styrenes: An Efficient Method to Synthesize 2-Alkenyl-1,3,4-Oxadiazoles, **Synlett, 71-74, 29(1) 2018**
- Unactivated sp3 C-H Functionalization by I-2/DMSO: An Efficient Method to Synthesize Isatins, **ChemistrySelect, 8019-8022, 3(28) 2018**
- Direct Access to Halogenated Fused Imidazo[1,5-a]N-heteroaromatics through Copper-Promoted Double Oxidative C-H Amination and Halogenation, **European Journal of Organic Chemistry, 3036-3047, 23, 2018**
- Solubility Measurement and Thermodynamic Modeling of Benzoic Acid in Monosolvents and Binary Mixtures, **Journal of Chemical and Engineering Data, 2028-2037, 63(6) 2018**
- Acetyl-d-glucopyranoside functionalized carbon nanotubes for the development of high performance ultrafiltration membranes, **Separation and Purification Technology, 134-143, 191, 2018**
- Recent advances on sources and industrial applications of lipases, **Biotechnology Progress, 5-28, 34(1) 2018**
- Mechanical, Dynamic Mechanical and Thermal Properties of Banana Fiber/Recycled High Density Polyethylene Biocomposites Filled with Flyash Cenospheres, **Journal of Polymers and the Environment, 200-213, 26(1) 2018**
- Synthesis of DNA interactive C3-trans-cinnamide linked beta-carboline conjugates as potential cytotoxic and DNA topoisomerase I inhibitors, **Bioorganic & Medicinal Chemistry, 4916-4929, 26(17) 2018**
- Synthesis of podophyllotoxin linked β-carboline congeners as potential anticancer agents and DNA topoisomerase II inhibitors, **European Journal of Medicinal Chemistry, 557-571, 144, 2018**
- C-H···Ni and C-H···π(chelate) interactions in nickel(II) complexes involving functionalized dithiocarbamates and triphenylphosphine, **Journal of Molecular Structure, 156–166, 1159, 2018**
- Stereoselective synthesis of C12-C21 common fragment of thermolides 1-5, **Tetrahedron Letters, 2828-2830, 59(29) 2018**
- Studies towards the Synthesis of Thermolide-6', **ChemistrySelect, 1000-1003, 3(4) 2018**
- Process optimization for the supercritical carbon dioxide (SC-CO2) extraction of wheat germ oil with respect to yield, and phosphorous and tocol contents using a Box Behnken design, **Grasas Y Aceites, Article Number: e259, 69(3) 2018**
- Studies on the Total Synthesis of Antibiotic Macrolactin S: A Conventional Approach for the Synthesis of the C1-C9 and C10-C24 Fragments, **Synthesis-Stuttgart, 663-675, 50(3) 2018**
- Impact of Glycolipid Hydrophobic Chain Length and Headgroup Size on Self-Assembly and Hydrophobic Guest Release, **Langmuir, 8875-8886, 34(30) 2018**
- Nonionic Glycolipids for Chromium Flotation- and Emulsion (W/O and O/W)-Based Bioactive Release, **Langmuir, 14347-14357, 34(47) 2018**
- Carbon dioxide assisted toluene side-chain alkylation with methanol over Cs-X zeolite catalyst, **Journal of Co_2 Utilization, 254-261, 26, 2018**
- Chiral Supramolecular Assemblies from an Achiral Naphthalene Diimide Bearing a Urea Moiety, **Chemistry-An Asian Journal, 3268-3273, 13(21) 2018**
- Dithiafulvenyl-Naphthalenediimide-based Small Molecules as efficient Non-Fullerene Electron-Transport Layer for Inverted Perovskite Solar Cells, **Asian Journal of Organic Chemistry, 2294-2301,7(11) 2018**

- Identification and structural characterization of in vivo metabolites of balofloxacin in rat plasma, urine and feces samples using Q-TOF/LC/ESI/MS/MS : In silico toxicity studies, **Journal of Pharmaceutical and Biomedical Analysis, 200-211, 159, 2018**
- Facile in-situ formation of rGO/ZnO nanocomposite: Photocatalytic remediation of organic pollutants under solar illumination, **Materials Chemistry and Physics, 218-228, 218, 2018**
- One-pot hydrothermal synthesis of TiO2/graphene nanocomposite with simultaneous nitrogen-doping for energy storage application, **Journal of Electroanalytical Chemistry, 208-216, 829, 2018**
- Synthesis, Anticancer Evaluation, and Molecular Docking Studies of Novel (4-Hydroxy-2-Thioxo-3,4-Dihydro-2H-[1,3]Thiazin-6-Yl)-Chromen-2-Ones via a Multicomponent Approach, **Journal of the Chinese Chemical Society, 810-821, 65(7) 2018**
- Total Synthesis of Callyspongiolide: An Anticancer Marine Natural Product, **ACS Omega, 16563-16575, 3(12) 2018**
- Stereo selective synthesis of C3-C12 fragment of iriomoteolide-1a, **Journal of Saudi Chemical Society, 165-172, 22(2) 2018**
- A pyrene formulation for fluorometric visualization of latent fingermarks, **Methods and Applications in Fluorescence, Article Number: 035004, 6(3) 2018**
- Latent fingermark development using a novel phenanthro imidazole derivative, **Journal of Photochemistry and Photobiology A: Chemistry, 253-260, 351, 2018**
- An indirect approach for encapsulation of chiral cobalt catalyst in microporous Zeolite-Y, **Microporous and Mesoporous Materials, 31-39, 272, 2018**
- Characterization and reactivity of vanadium oxide supported on TiO2-SiO2 mixed oxide support, **Molecular Catalysis, 228-237, 451(SI) 2018**
- 2,4-Thiazolidinedione as a Bioactive Linker for Ferrocenyl Sugar-Triazole Conjugates: Synthesis, Characterization and Biological Properties, **European Journal of Inorganic Chemistry, 1571-1580, 14, 2018**
- Facile synthesis, characterisation and anti-inflammatory activities of ferrocenyl ester derivatives of 4-arylidene-5-imidazolinones, **Applied Organometallic Chemistry, Article Number: e4021, 32(2) 2018**
- N-Arylation of ferrocenyl 2,4-thiazolidinedione conjugates via a copper-catalysed Chan-Lam cross coupling reaction with aryl boronic acids and their optoelectronic properties, **New Journal of Chemistry, 12587-12594, 42(15) 2018**
- MOF-Derived Bifunctional Iron Oxide and Iron Phosphide Nanoarchitecture Photoelectrode for Neutral Water Splitting, **ChemElectroChem, 2842-2849, 5(19) 2018**
- Cu-Pd bimetallic nanoalloy anchored on a N-rich porous organic polymer for high-performance hydrodeoxy genation of biomass-derived vanillin, **Catalysis Science & Technology, 2195-2210, 8(8) 2018**
- Ruthenium-bipyridine complex catalyzed C-H alkenylation of arylpyrazole derivatives, **Journal of Chemical Sciences, Article Number: UNSP 87, 130(7) 2018**
- Access to small molecule semiconductors via C-H activation for photovoltaic applications, **Chemical Communications, 7322-7325, 54(53) 2018**
- Chemical characterization of an Ayurvedic herbo-mineral preparation-Arogyavardhani Vati: A potential tool for quality assurance, **Indian Journal of Traditional Knowledge, 176-183, 17(1) 2018**
- Direct Aryl-Aryl Coupling without Pre-Functionalization Enabled by Excessive Oxidation of Two-Electron Ag(I)/Ag(III) Catalyst, **Advanced Synthesis & Catalysis, 2032-2042, 360(10) 2018**
- Fabrication of surfactant-stabilized nanosuspension of naringenin to surpass its poor physiochemical properties and low oral bioavailability, **PhytoMedicine, 48-54, 40, 2018**
- Metal- and Oxidant-Free Modular Approach To Access N-Alkoxy Oxindoles via Aryne Annulation, **Organic Letters, 4848-4853, 20(16) 2018**

- Nitromethane as a Carbanion Source for Domino Benzoannulation with Ynones: One-Pot Synthesis of Polyfunctional Naphthalenes and a Total Synthesis of Macarpine, **Angewandte Chemie-International Edition, 16847-16851, 57(51) 2018**
- EPR and optical investigation of ultraviolet-emitting Gd3Ga5O12 garnet, **Journal of Materials Science-Materials in Electronics, 944-951, 29(2) 2018**
- Costunolide induces micronuclei formation, chromosomal aberrations, cytostasis, and mitochondrial-mediated apoptosis in Chinese hamster ovary cells, **Cell Biology and Toxicology, 125-142, 34(2) 2018**
- Dehydrocostus lactone induces prominent apoptosis in kidney distal tubular epithelial cells and interstitial fibroblasts along with cell cycle arrest in ovarian epithelial cells, **Biomedicine & Pharmacotherapy, 956-969, 99, 2018**
- Zoledronic acid induces micronuclei formation, mitochondrial-mediated apoptosis and cytostasis in kidney cells, **Life Sciences, 305-314, 203, 2018**
- Design of Efficient Noble Metal Free Copper-Promoted Nickel-Ceria-Zirconia Nanocatalyst for Bio-Fuel Upgrading, **ChemistrySelect, 6174-6185, 3(22) 2018**
- Tandem Prins-type cyclization for the stereoselective construction of fused polycyclic ring systems, **Organic Chemistry Frontiers, 1320-1324, 5(8) 2018**
- Flexible, hard, and tough biobased polyurethane thermosets from renewable materials: glycerol and 10-undecenoic acid, **Journal of Coatings Technology and Research, 199-210, 15(1) 2018**
- Hypochlorite-Mediated Modulation of Photoinduced Electron Transfer in a Phenothiazine-Boron dipyrro methene Electron Donor-Acceptor Dyad: A Highly Water Soluble "Turn-On" Fluorescent Probe for Hypochlorite, **Chemistry-An Asian Journal, 1594-1608, 13(12) 2018**
- Mass spectral studies of N-oxides of chemical weapons convention-related aminoethanols by gas chromatography/mass spectrometry after silylation, **European Journal of Mass Spectrometry, 442-453, 24(6) 2018**
- Biopesticide treated double layered bags: novel method of application of botanicals for Sitophilus oryzae L. management in stored maize, **Maydica, Article Number: M3, 63(1) 2018**
- Thermoreversible gelation of poly(urethane acyl-semicarbazides) carrying cycloaliphatic moieties and studies on selective adsorption of dyes from wastewater, **European Polymer Journal, 90-101, 99, 2018**
- Electrofermentation of food waste - Regulating acidogenesis towards enhanced volatile fatty acids production, **Chemical Engineering Journal, 1709-1718, 334, 2018**
- A Bird's Eye view on process and engineering aspects of hydrogen storage, **Renewable & Sustainable Energy Reviews, 838-860, 91, 2018**
- An odyssey of process and engineering trends in forward osmosis, **Environmental Science-Water Research & Technology, 129-168, 4(2) 2018**
- Selective substitution of Ni by Ti in LaNiO3 perovskites: A parameter governing the oxy-carbon dioxide reforming of methane, **International Journal of Hydrogen Energy, 4136-4142, 43(8) 2018**
- Calcination Thermokinetics of Carbon Capture Using Coal Fly Ash Stabilized Sorbent, **Energy & Fuels, 3716-3725, 32(3) 2018**
- Synthesis, anticancer evaluation and molecular docking studies of bis(indolyl) triazinones, Nortopsentin analogs, **Chemical Papers, 1369-1378, 72(6) 2018**
- Synthesis of novel beta(2,2)-amino acid from D-mannose and attempted synthesis of peptides from the amino acid, **Journal of Carbohydrate Chemistry, 94-101, 37(2) 2018**
- Styryl Quinazolinones as Potential Inducers of Myeloid Differentiation via Upregulation of C/EBP alpha, **Molecules, Article Number: 1938, 23(8) 2018**
- A General Diastereoselective Strategy for Both cis- and trans-2,6-Disubstituted Tetrahydropyrans: Formal Total Synthesis of (+)-Muconin, **Organic Letters, 6910-6914, 20(21) 2018**

- Synthesis, characterisation, cellular uptake and cytotoxicity of functionalised magnetic ruthenium (II) polypyridine complex core-shell nanocomposite, **Journal of Photochemistry and Photobiology B: Biology, 270-276, 178, 2018**
- Oxone-mediated annulation of 2-aminobenzamides and 1,2-diaminobenzenes with sec-amines via imine-N-oxides: new syntheses of 2,3-dihydroquinazolin-4(1H)-ones and 1H-benzimidazoles, **New Journal of Chemistry, 3188-3191, 42(5) 2018**
- New method for the preparation of N-chloroamines by oxidative N-halogenation of amines using oxone-KCl, **Synthetic Communications, 699-704, 48(6) 2018**
- A Triphenylamine-Naphthalenediimide-Fullerene Triad : Synthesis, Photoinduced Charge Separation and Solution-Processable Bulk Heterojunction Solar Cells, **Asian Journal of Organic Chemistry, 220-226, 7(1) 2018**
- Complexes of DNA bases and Watson-Crick base pairs interaction with neutral silver Ag-n (n=8, 10, 12) clusters: a DFT and TDDFT study, **Journal of Biomolecular Structure & Dynamics, 1050-1062, 36(4) 2018**
- Theoretical studies of optoelectronic, magnetization and heat transport properties of conductive metal adatoms adsorbed on edge chlorinated nanographenes, **RSC Advances, 17723-17731, 8(32) 2018**
- Theoretical studies on the electronic and optoelectronic properties of [A.2 AP(w)/A*.2AP(WC)/C.2AP(w)/ C*.2AP(WC)/C.A(w)/C*.A(WC)]-Au-8 mismatch nucleobase complexes, **Molecular Physics, 263-272, 116(2) 2018**
- Total synthesis of patulolide A through ring closing metathesis, **Synthetic Communications, 496-499, 48(5) 2018**
- Stereocontrolled Total Synthesis of Nonenolide, **Journal of Natural Products, 1399-1404, 81(6) 2018**
- Synthesis of benzo[d]imidazo[2,1-b]thiazole-chalcone conjugates as microtubule targeting and apoptosis inducing agents, **Bioorganic Chemistry, 1-12, 76, 2018**
- An Efficient Synthesis and Bio Efficacy Confirmation of Female Sex Pheromone of the Rice Moth, Corcyra Cephalonica Stainton, **Journal of Rice Research, Article No: 196, 6(4) 2018**
- A fluorene-core-based electron acceptor for fullerene-free BHJ organic solar cells-towards power conversion efficiencies over 10%, **Chemical Communications, 4001-4004, 54(32) 2018**
- Biomimetic synthesis of gum acacia mediated Pd-ZnO and Pd-TiO2 – Promising nanocatalysts for selective hydrogenation of nitroarenes, **Materials Chemistry and Physics, 27-36, 204, 2018**
- Two New Cerioptins (A-B) from the Mangrove Ceriops tagal, **ChemistrySelect, 8926-8929, 3(31) 2018**
- Stereoselective Total Synthesis of (-)-6-epi-Hygrophorone B-14 and (-)-4-epi-Hygrophorone D-14, **ChemistrySelect, 9596-9599, 3(33) 2018**
- Iodine mediated pyrazolo-quinoline derivatives as potent anti-proliferative agents, **Bioorganic & Medicinal Chemistry Letters, 664-667, 28(4) 2018**
- Anti-proliferative activity, molecular modeling studies and interaction with calf thymus DNA of novel ciprofloxacin analogues, **Journal of Chemical Sciences, Article Number: UNSP 121, 130(9) 2018**
- Dibenzofuran, dibenzothiophene and N-methyl carbazole tethered 2-aminothiazoles and their cinnamamides as potent inhibitors of Mycobacterium tuberculosis, **Bioorganic & Medicinal Chemistry Letters, 1610-1614, 28(9) 2018**
- Mono substituted pyrenes as multifunctional materials for OLED: Analysis of the substituent effects on the charge transport properties using DFT methods, **Computational and Theoretical Chemistry, 48-56, 1138, 2018**
- Substrate-Directed C-H Functionalization of 2-Aryl Pyridines by Transition Metal Complexes, **ChemistrySelect, 47-70, 3(1) 2018**
- Selectfluor-Mediated Synthesis of Fluoro Spiro 3(2H)-Furanone Derivatives via Domino Fluorination-Defluorination, **European Journal of Organic Chemistry, 413-417, (3) 2018**

- Novel 1,2,3-Triazole-Functionalized 1,2-Benzothiazine 1,1-Dioxide Derivatives: Regioselective Synthesis, Biological Evaluation and Docking Studies, **ChemistrySelect, 2398-2403, 3(8) 2018**
- Benzodithiazole-Based Hole-Transporting Material for Efficient Perovskite Solar Cells, **Asian Journal of Organic Chemistry, 2497-2503, 7(12) 2018**
- Regioselective Ring Expansion of Isatins with In Situ Generated alpha-Aryldiazomethanes: Direct Access to Viridicatin Alkaloids, **Organic Letters, 3639-3642, 20(12) 2018**
- Facile synthesis of 2-aryl 5-hydroxy benzo[d]oxazoles and their in vitro anti-proliferative effects on various cancer cell lines, **Bioorganic & Medicinal Chemistry Letters, 3639-3647, 28(23-24) 2018**
- Solubility Measurement, Modeling, and Thermodynamic Functions for para-Methoxyphenylacetic Acid in Pure and Mixed Organic and Aqueous Systems, **Journal of Chemical and Engineering Data, 3369-3381, 63(9) 2018**
- Synthesis and cytotoxicity studies of newly designed benzyl-hydroquinone derivatives, **Medicinal Chemistry Research, 1050-1065, 27(4) 2018**
- Water mediated proton conductance in a hydrogen-bonded Ni(II)-bipyridine-glycoluril chloride self-assembled framework, **Crystengcomm, 1094-1100, 20(8) 2018**
- Optimization of the extraction of natural antioxidants from Coffea robusta leaves and evaluation of their ability to preserve palm olein from oxidation during accelerated storage, **Food Science & Nutrition, 1751-1761, 6(6) 2018**
- Polyphenol antioxidants from cocoa pods: Extraction optimization, effect of the optimized extract, and storage time on the stability of palm olein during thermoxidation, **Journal of Food Processing and Preservation, Article Number: e13592, 42(5) 2018**
- Antimicrobial activity of simplified mimics of celogentin C, **Tetrahedron, 1288-1293, 74(12) 2018**
- DBU-Mediated Efficient Synthesis of Diaryl Ethynes and Enynes from 1,1-Dibromoalkenes at Room Temperature, **European Journal of Organic Chemistry, 6280-6285, 45, 2018**
- Crosslinked enzyme aggregates (CLEA) of phytase with soymilk proteins, **Journal of Biotechnology, 67-69, 282, 2018**
- Hierarchical Porous TiO2 Embedded Unsymmetrical Zinc-Phthalocyanine Sensitizer for Visible-Light-Induced Photocatalytic H-2 Production, **Journal of Physical Chemistry C, 495-502, 122(1) 2018**
- **Editorial Material:** Sulforaphane salads, **Pharmacognosy Magazine, 3-3, 14(53) 2018**
- In vitro Assessment of Selected Benzoic Acid Derivatives as Anti-Inflammatory Compounds, **Journal of Scientific & Industrial Research, 330-336, 77(6) 2018**
- Hypervalent Iodine(III)-Mediated Solvent-Free, Regioselective Synthesis of 3,4-Disubstituted 5-Imino-1,2,4-thiadiazoles and 2-Aminobenzo[d]thiazoles, **Advanced Synthesis & Catalysis, 2806-2812, 360(15) 2018**
- Identification and characterization of stress degradation products of sumatriptan succinate by using LC/Q-TOF-ESI-MS/MS and NMR: Toxicity evaluation of degradation products, **Journal of Mass Spectrometry, 963-975, 53(10) 2018**
- Catalyst free synthesis of mono- and disubstituted pyrimidines from O-acyl oximes, **Tetrahedron Letters, 2430-2433, 59(25) 2018**
- Methyl triphenylphosphonium permanganate as a novel oxidant for aniline to polyaniline-manganese(II, IV) oxide: material for high performance pseudocapacitor, **Journal of Solid State Electrochemistry, 407-415, 22(2) 2018**
- Exploration of Conformations, Analysis of Protein and Biological Significance of Histidine Dimers, **Chemistry Select, 3070-3078, 3(11) 2018**

- Pharmacokinetic Study on Piplartine and Piperine after Oral Administration of Piper chaba Root by Liquid Chromatography-mass Spectrometry/mass Spectrometry, **Pharmacognosy Magazine, S161-S166, 14(55) 2018**
- In vitro apoptotic mechanism of a novel synthetic Quinazolinyl derivative: Induces caspase-dependent intrinsic pathway on THP-1, leukemia cell line, **Chemico-Biological Interactions, 117-127, 280, 2018**
- Multicomponent synthesis and anticancer activity studies of novel 6-(Trifluoromethyl)-1, 2, 3, 4-tetrahydropyrimidine-5-carboxylate derivatives, **Synthetic Communications, 2226-2231, 48(17) 2018**
- An alternative stereoselective total synthesis of Verbalactone, **Arkivoc, 50-57, (Part:7) 2018**
- Fabrication of highly efficient carbon coated exfoliated tungsten disulfide nanosheets core-shell nanostructure as a promising solar-light driven photocatalyst, **Materials Research Bulletin, 446-455, 107, 2018**
- Studies on synthesis of novel pyrido[2,3-d]pyrimidine derivatives, evaluation of their antimicrobial activity and molecular docking, **Bioorganic & Medicinal Chemistry Letters, 1670-1675, 28(9) 2018**
- Influence of Support for Ru and Water Role on Product Selectivity in the Vapor-Phase Hydrogenation of Levulinic Acid to gamma-Valerolactone: Investigation by Probe-Adsorbed Fourier Transform Infrared Spectroscopy, **Journal of Physical Chemistry C, 19670-19677, 122(34) 2018**
- Chitosan stabilized nasal emulsion delivery system for effective humoral and cellular response against recombinant tetravalent dengue antigen, **Carbohydrate Polymers, 129-138, 190, 2018**
- Synthesis and biological evaluation of 3,6-dialkyl substituted-[1,2,4]triazolo[3,4-b][1,3,4] thiadiazoles, **Journal of Chemical Sciences, Article Number: UNSP 23, 130(3) 2018**
- Towards the Total Synthesis of Schisandrene: Stereoselective Synthesis of the Dibenzocyclooctadiene Lignan Core, **Synlett, 908-911, 29(7) 2018**
- Waste derived bioeconomy in India: A perspective, **New Biotechnology, 60-69, 40(Part A) 2018**
- Low temperature microwave sintering of yttrium and samarium co-doped ceria solid electrolytes for IT-SOFCs, **Ionics, 1429-1438, 24(5) 2018**
- Transition (Mn, Fe) and rare earth (La, Pr) metal doped ceria solid solutions for high performance photocatalysis: Effect of metal doping on catalytic activity, **Research on Chemical Intermediates, 2523-2543, 44(4) 2018**
- An insight on the influence of surface Lewis acid sites for regioselective C-H bond C3-cyanation of indole using NH4I and DMF as combined cyanide source over Cu/SBA-15 catalyst, **Molecular Catalysis, 43-51, 445, 2018**
- Hydrodeoxygenation activity of W modified Ni/H-ZSM-5 catalyst for single step conversion of levulinic acid to pentanoic acid: An insight on the reaction mechanism and structure activity relationship, **Applied Catalysis A: General, 142-150, 550, 2018**
- Luminescent properties of green emitting Tb3+ doped Sr2ZnSi2O7 phosphors, **Optik, 1302-1307, 158, 2018**
- EPR and PL studies on UVB-emitting gadolinium-doped SrAl12O19 phosphors, **Optik, 1227-1233, 158, 2018**
- Synthesis and cytotoxic evaluation of undecenoic acid-based oxime esters, **Indian Journal of Chemistry Section B-Organic Chemistry including Medicinal Chemistry, 1015-1022, 57(8) 2018**
- Revisiting 1-chloro-1,2-benziodoxol-3-one: efficient ortho-chlorination of aryls under aqueous conditions, **New Journal of Chemistry, 8953-8959, 42(11) 2018**
- Design and operation of extractive distillation systems using different class of entrainers for the production of fuel grade tert-butyl Alcohol:A techno-economic assessment, **Energy, 1013-1025, 144, 2018**
- Identification of an Alternatively Spliced alpha-Synuclein Isoform That Generates a 41-Amino Acid N-Terminal Truncated Peptide, 41-syn: Role in Dopamine Homeostasis, **ACS Chemical Neuroscience, 2948-2958, 9(12) 2018**

- Investigation on the physicochemical properties of Ce0.8Eu0.1M0.1O2-delta (M = Zr, Hf, La, and Sm) solid solutions towards soot combustion, **New Journal of Chemistry, 5276-5283, 42(7) 2018**
- Reversible NIR fluorescent probes for Cu2+ ions detection and its living cell imaging, **Sensors and Actuators B: Chemical, 3235–3247, 255(Part 3) 2018**
- Synthesis of Co1-xZnxFe2O4 and Evaluation of Structural, Magnetic, Antimicrobial Properties of ZnFe2O4, Co0.6Zn0.4Fe2O4 by Citrate Gel Method, Calcined at 600 degrees C, **Russian Journal of Applied Chemistry, 1281-1290, 91(8) 2018**
- Synthesis, Characterization and Catalytic Dehydration of Glycerol to Acrolein Over Phosphotungstic Acid Supported Y-Zeolite Catalysts, **Catalysis Letters, 397-406, 148(1) 2018**
- Synthesis and Cytotoxicity Evaluation of Unusual Mixture Acid Acetate-protected Monogalacto syldiacylglycerols, **Indian Journal of Pharmaceutical Sciences, 1143-1150, 80(6) 2018**
- Synthesis and cytotoxic evaluation of cholesteryl 6-O-acyl-beta-D-galactopyranosides, **Indian Journal of Chemistry Section B-Organic Chemistry including Medicinal Chemistry, 91-97, 57(1) 2018**
- Design, synthesis, and cytotoxicity evaluation of threonine-based galactoceramide with aromatic groups and various fatty-acyl side chains, **Medicinal Chemistry Research, 285-307, 27(1) 2018**
- Potent ACE inhibitors from 5-hydroxy indanone derivatives, **Bioorganic Chemistry, 660-665, 77, 2018**
- Fabrication of diverse nano-architectures through the self-assembly of a naphthalene diimide derivative bearing four carbamates, **New Journal of Chemistry, 6785-6793, 42(9) 2018**
- Transient global cerebral ischemia differentially affects cortex, striatum and hippocampus in Bilateral Common Carotid Arterial occlusion (BCCAo) mouse model, **Journal of Chemical Neuroanatomy, 1-15, 92, 2018**
- Specific G-quadruplex ligands modulate the alternative splicing of Bcl-X, **Nucleic Acids Research, 886-896, 46(2) 2018**
- D-pi-A-pi-D Structured Diketopyrrolopyrrole-Based Electron Donors for Solution-Processed Organic Solar Cells, **ACS Omega, 13365-13373, 3(10) 2018**
- An Efficient Catalytic Approach for Epoxidation of Styrene over Activated Marble Powder, **ChemistrySelect, 8473-8478, 3(29) 2018**
- Ni/KIT-6 catalysts for hydrogenolysis of lignin-derived diphenyl ether, **Journal of Chemical Sciences, Article Number: UNSP 106, 130(8) 2018**
- Hepatoprotective Cocrystals and Salts of Riluzole: Prediction, Synthesis, Solid State Characterization, and Evaluation, **Crystal Growth & Design, 1047-1061, 18(2) 2018**
- Studies towards the Total Synthesis of Cruentaren B, **ChemistrySelect, 12210-12212, 3(43) 2018**
- Stereoselective Total Syntheses of Acutifolone A, Bisacutifolone A and B, Pinguisenol, and Isonaviculol, **ACS Omega, 636-647, 3(1) 2018**
- Characterization of acetylated histidine b(1)-ion structure: A competition between oxazolone and side chain imidazole moiety, **European Journal of Mass Spectrometry, 261-268, 24(3) 2018**
- Spirooxindole-fused pyrazolo pyridine derivatives: NiO-SiO2 catalyzed one-pot synthesis and antimicrobial activities, **Synthetic Communications, 255-266, 48(3) 2018**
- Organocatalytic Enantioselective Michael Addition of 3-Indolinone-2-Carboxylates to Maleimides, **European Journal of Organic Chemistry, 1364-1371, (11) 2018**
- Asymmetric Robinson Annulation of 3-Indolinone-2-carboxylates with Cyclohexenone: Access to Chiral Bridged Tricyclic Hydrocarbazoles, **Organic Letters, 4195-4199, 20(14) 2018**
- Oxidative Asymmetric Aza-Friedel-Crafts Alkylation of Indoles with 3-Indolinone-2-carboxylates Catalyzed by a BINOL Phosphoric Acid and Promoted by DDQ, **Chemistry-An Asian Journal, 1327-1334, 13(10) 2018**
- Characterization of degradation products of macitentan under various stress conditions using liquid chromatography/mass spectrometry, **Rapid Communications in Mass Spectrometry, 1075-1084, 32(13) 2018**

- Self-sustained photocatalytic power generation using eco-electrogenic engineered systems, **Bioresource Technology, 23-29, 260, 2018**
- Spatial variation of electrode position in bioelectro chemical treatment system: Design consideration for azo dye remediation, **Bioresource Technology, 374-383, 256, 2018**
- Novel carbazole-triazole conjugates as DNA-targeting membrane active potentiators against clinical isolated fungi, **European Journal of Medicinal Chemistry, 579-589, 155, 2018**

PUBLICATIONS-2019

- Integrated continuous flow/batch protocol for the photoreduction of ortho-methyl phenyl ketones using water as the hydrogen source, **Reaction Chemistry & Engineering, 812-817, 4(5) 2019**
- Antenna-like Ring Structures via Self-Assembly of Octaphosphonate Tetraphenyl Porphyrin with Nucleobases, **ACS Omega, 11408-11413, 4(7) 2019**
- Catalyst- and reagent-free 1,6-hydrophosphonylation of p-quinone methides: a practical approach for the synthesis of diarylmethyl phosphine oxides, **Organic & Biomolecular Chemistry, 7536-7546, 17(32) 2019**
- Evaluation of the in vivo genotoxicity of liposomal formulation for delivering anticancer estrogenic derivative (ESC8) in a mouse model, **Saudi Pharmaceutical Journal, 637-642, 27(5) 2019**
- Planar Antiaromatic Core-Modified 24 pi Hexaphyrin (1.0.1.0.1.0) and 32 pi Octaphyrin (1.0.1.0.1.0.1.0) Bearing Alternate Hybrid Diheterole Units, **Chemistry-A European Journal, 2859-2867,25(11) 2019**
- Thermodynamic analysis of plant-wide CLC-SESMR scheme for H-2 production: Studying the effect of oxygen carrier supports, **International Journal of Hydrogen Energy, 3250-3263, 44(5) 2019**
- Stevioside, a diterpenoid glycoside, shows anti-inflammatory property against Dextran Sulphate Sodium-induced ulcerative colitis in mice, **European Journal of Pharmacology, 192-201, 855, 2019**
- Single pot bioprocessing for ethanol production from biogenic municipal solid waste, **Bioresource Technology, 159-167, 283, 2019**
- The synthesis of 3-ethyl-5-methyl-2,6-diarylpiperidin-4-on-1-ium picrates and their spectral, XRD and theoretical studies, **New Journal of Chemistry, 11003-11014, 43(27) 2019**
- Residue-specific identification of phase separation hot spots of Alzheimer's-related protein tau, **Chemical Science, 6503-6507, 10(26) 2019**
- Fixation of CO2, electron donor and redox microenvironment regulate succinic acid production in Citrobacter amalonaticus, **Science of the Total Environment, Article Number: UNSP 133838, 695, 2019**
- Design and synthesis of novel 4-hydrazone functionalized/1,2,4-triazole fused pyrido[2,3-d]pyrimidine derivatives, their evaluation for antifungal activity and docking studies, **Medicinal Chemistry Research, 1509-1528, 28(9) 2019**
- Arora, Neelima; Banerjee, Amit Kumar; Dereplication in Natural Product Discovery, **Current Topics in Medicinal Chemistry, 101-102, 19(2) 2019**
- Synthesis of Biaryl Derivatives of Spirofurochromanone in Water and Their Anticancer Activity, **Russian Journal of General Chemistry, 2129-2135, 89(10) 2019**
- Novel pyrano [3,2-b]xanthen-7(2H)-ones: Synthesis, antimicrobial, antioxidant and molecular docking studies, **Journal of Molecular Structure, 215-228, 1177, 2019**
- A unified, RCM anchored approach to spiro[4.5]decane-based sesquiterpenoids: Collective synthesis of (+/-)-alpha & beta-vetispirenes, (+/-)-beta-vetivone, (+/-)-agarospirol and (+/-)-hinesol, **Tetrahedron Letters, 1570-1573, 60(24) 2019**
- The mitochondrial effects of embelin are independent of its MAP kinase regulation: Role of p53 in conferring selectivity towards cancer cells, **Mitochondrion, 158-163, 46, 2019**
- Vapour Phase Selective Hydrogenation of Furfural to Furfuryl Alcohol Over Cu-Cr-Zn Mixed Oxide Catalysts Prepared by Utilizing Gamma Radiation, **Catalysis Letters, 2758-2766, 149(10) 2019**
- Synthesis of N-alkylated Derivatives of epsilon-Caprolactams from Bicyclic Amidine DBU, **Asian Journal of Organic Chemistry, 103-106, 8(1) 2019**

- MA(2)CoBr(4): lead-free cobalt-based perovskite for electrochemical conversion of water to oxygen, **Chemical Communications, 6779-6782, 55(47) 2019**
- Ultra-Low-Temperature CO Oxidation Activity of Octahedral Site Cobalt Species in Co3O4 Based Catalysts: Unravelling the Origin of the Unique Catalytic Property, **Journal of Physical Chemistry C, 19557-19571, 123(32) 2019**
- Studies Towards the Stereoselective Total Synthesis of 7-O-methylnigrosporolide, **ChemistrySelect, 5531-5534, 4(19) 2019**
- Asymmetric total synthesis of antiviral agents (+)-sattazolin and (+)-sattabacin, **Arkivoc, 167-173, (Part: 6) 2019**
- A comprehensive study on rearrangement reactions in collision-induced dissociation mass spectrometric fragmentation of protonated diphenyl and phenyl pyridyl ethers, **Rapid Communications in Mass Spectrometry, 1440-1448, 33(18) 2019**
- Identification and structural characterization of hydrolytic degradation products of alvimopan by LC/QTOF/MS/MS and NMR studies, **Journal of Pharmaceutical and Biomedical Analysis, 399-409, 165, 2019**
- Temperature-Dependent Photoluminescence and Energy-Transfer Dynamics in Mn2+-Doped (C4H9NH3)(2)PbBr4 Two-Dimensional (2D) Layered Perovskite, **Journal of Physical Chemistry C, 4739-4748, 123(8) 2019**
- Discovery of a new class of type 1 methionine aminopeptidases that have relaxed substrate specificity, **International Journal of Biological Macromolecules, 523-529, 129, 2019**
- Synergistic Catalysis of Ag(I) and Organo-N-heterocyclic Carbenes: One-Pot Synthesis of New Anticancer Spirooxindole-1,4-dihydropyridines, **ChemistrySelect, 2562-2567, 4(9) 2019**
- Structural characterization and biological evaluation of Staphylosan (dimannooleate), a new glycolipid surfactant produced by a marine Staphylococcus saprophyticus SBPS-15, **Enzyme and Microbial Technology, 1-7, 120, 2019**
- Microwave-Assisted Rapid Regioselective One-Pot Synthesis of Novel 2-Oxothiazolidine Dicarboxylate, **Chemistry Select, 6697-6701, 4(22) 2019**
- Influence of silica architecture on the catalytic activity of immobilized glucose oxidase, **Bioinspired Biomimetic and Nanobiomaterials, 72-80, 8(1) 2019**
- Microwave-Assisted One-Pot [3+2] Cycloaddition of Azomethine Ylides and 3-Alkenyl Oxindoles: A Facile Approach to Pyrrolidine-Fused Bis-Spirooxindoles, **ChemistrySelect, 1727-1730, 4(5) 2019**
- Hydrogenation of levulinic acid to valeric acid over platinum-tungsten catalysts supported on gamma-Al2O3, **New Journal of Chemistry, 18003-18011, 43(46) 2019**
- The selectively regulated vapour phase dehydrogenation of 1,4-butanediol to gamma-butyrolactone employing a copper-based ceria catalyst, **New Journal of Chemistry, 11968-11983, 43(30) 2019**
- The Mukaiyama type aldol reaction for the synthesis of trans-2,6-disubstituted tetrahydropyrans: synthesis of diospongin A and B, **Organic & Biomolecular Chemistry, 9169-9181, 17(41) 2019**
- Optoelectronic, femtosecond nonlinear optical properties and excited state dynamics of a triphenyl imidazole induced phthalocyanine derivative, **RSC Advances, 36726-36741, 9(63) 2019**
- Synthesis, Optical, Electrochemical, DFT Studies, NLO Properties, and Ultrafast Excited State Dynamics of Carbazole-Induced Phthalocyanine Derivatives, **Journal of Physical Chemistry C, 11118-11133, 123(17) 2019**
- Description of a Novel Phosphodiesterase (PDE)-3 Inhibitor Protecting Mice From Ischemic Stroke Independent From Platelet Function, **Stroke, 478-486, 50(2) 2019**
- Unravel the surface active sites on Cu/MgLaO solid base catalyst by DRIFT spectroscopy and adsorption techniques for the synthesis of triazoles by click reaction, **Molecular Catalysis, Article Number: UNSP 110523, 476, 2019**

- Effect of Non-Ideal Mixing on Heat Transfer of non-Newtonian Liquids in a Mechanically Agitated Vessel, **International Journal of Chemical Reactor Engineering, Article Number: 20180015, 17(6) 2019**
- Bio-based castor oil organogels and investigations on their anion-tuning properties, **Colloid and Polymer Science, 1411-1421, 297(11-12) 2019**
- Polyethylene-Glycol-Based Thermoreversible Biscarbamate Hydrogels and Metallogels Synthesized through Non-Isocyanate Route, **ChemistrySelect, 11052-11060, 4(37) 2019**
- Development of biobased polyurethane-imides from maleinized cottonseed oil and castor oil, **Polymers for Advanced Technologies, 2742-2749, 30(11) 2019**
- Bioinspired First Stereoselective Total Synthesis of Spinosulfate B, **ChemistrySelect, 8911-8914, 4(31) 2019**
- Design of DNA-intercalators based copper(II) complexes, investigation of their potential anti-cancer activity and sub-chronic toxicity, **Materials Science & Engineering C-Materials for Biological Applications, Article Number: 110079, 105, 2019**
- Novel trisaccharide based phospholipids as immunomodulators, **International Immunopharma cology, Article Number: 105684, 74, 2019**
- Metal-free oxidative acylation/cyclization of N-methacryloyl-2-phenylbenzoimidazole with aryl aldehydes: an easy access to benzimidazo[2,1-a]isoquinolin-6(5H)-ones, **Organic & Biomolecular Chemistry, 9627-9630, 17(44) 2019**
- BOP1-a key player of ribosomal biogenesis, **Current Science, 422-433, 117(3) 2019**
- Cu-catalyzed direct ortho-chlorination/-oxygenation of aryls: Switching of oxidant, control the diversity of products, **Tetrahedron Letters, 115-119, 60(2) 2019**
- Uncatalyzed, on water oxygenative cleavage of inert C-N bond with concomitant 8,7-amino shift in 8-aminoquinoline derivatives, **Green Chemistry, 1735-1742, 21(7) 2019**
- Mutanase Enzyme from Paracoccus mutanolyticus RSP02: Characterization and Application as a Biocontrol Agent, **Indian Journal of Microbiology, 436-444, 59(4) 2019**
- Acute and subacute oral toxicity of copper oxide nanoparticles in female albino Wistar rats, **Journal of Applied Toxicology, 702-716, 39(5) 2019**
- Mesoporous carbon supported MgO for CO2 capture and separation of CO2/N-2, **Korean Journal of Chemical Engineering, 1482-1488, 36(9) 2019**
- Influence of the backbone structure of the donor material and device processing conditions on the photovoltaic properties of small molecular BHJSCs, **Solar Energy, 84-93, 186, 2019**
- Efficient resource valorization by co-digestion of food and vegetable waste using three stage integrated bioprocess, **Bioresource Technology, 373-380, 284, 2019**
- Coupling of CH3OH and CO2 with 2-cyanopyridine for enhanced yields of dimethyl carbonate over ZnO-CeO2 catalyst, **Journal of Chemical Sciences, Article Number: UNSP 86, 131(8) 2019**
- Stereoselective Synthesis of the C1-C22 Carbon Framework of (-)-Amphidinolide K, **Journal of Organic Chemistry, 9584-9602, 84(15) 2019**
- **Editorial:** The National Organic Symposium Trust-Shaping Organic Chemistry in India for Over 30 Years, **Angewandte Chemie-International Edition, 9294-9295, 58(28) 2019**
- Substrate-Controlled Aza-Ene/Prins Cyclization for the Synthesis of Dihydroquinoline and Oxocene Derivatives, **ChemistrySelect, 3620-3623, 4(12) 2019**
- Green Catalysis Preface, **Catalysis Today, 1-2, 324(Special Issue: SI) 2019**
- Waste Eggshells for the Decoration of Carbon Nanotubes and Graphene Nanosheets with Hydroxyapatite for Preparation of LLDPE Nanocomposites, **Journal of Polymers and the Environment, 2352-2359, 27(11) 2019**
- Isolation and structural characterization of degradation products of afatinib dimaleate by LC-Q-TOF/MS/MS and NMR: cytotoxicity evaluation of afatinib and isolated degradation products, **Journal of**

Pharmaceutical and Biomedical Analysis, 139-146, 166, 2019

- Organocatalytic Asymmetric Synthesis of Tetrahydrofuran and 1,2-Dihydrobenzofuran Scaffolds, **European Journal of Organic Chemistry, 6890-6910, 2019(41) 2019**
- Insights into the structure and tubulin-targeted anticancer potential of N-(3-bromobenzyl) noscapine, **Pharmacological Reports, 48-53, 71(1) 2019**
- Synthesis of 4,6-disubstituted pyrazolo[3,4-d]pyrimidine analogues: Cyclin-dependent kinase 2 (CDK2) inhibition, molecular docking and anticancer evaluation, **Journal of Molecular Structure, 538-551, 1176, 2019**
- Synthesis of non-symmetrical alkyl carbonates from alcohols and DMC over the nanocrystalline ZSM-5 zeolite, **Green Chemistry, 2938-2945, 21(11) 2019**
- Synthesis of internal olefins by direct coupling of alcohols and olefins over Mo beta zeolite, **Catalysis Communications, 114-118, 123, 2019**
- Synthesis of new multivalent metal ion functionalized mesoporous silica and studies of their enhanced antimicrobial and cytotoxicity activities, **Journal of Materials Chemistry B, 7235-7245, 7(45) 2019**
- Synthesis, characterization and cytotoxic investigations of novel bis(indole) analogues besides antimicrobial study, **Arabian Journal of Chemistry, 2721-2731, 12(8) 2019**
- Design, synthesis of novel N prenylated indole-3-carbazones and evaluation of in vitro cytotoxicity and 5-LOX inhibition activities, **Arabian Journal of Chemistry, 2328-2335, 12(8) 2019**
- Stereoselective synthesis of C3-C17 and C18-C34 subunits of bullatanocin utilizing alpha-chloro sulfide intermediates, **Tetrahedron Letters, Article Number: 151132, 60(41) 2019**
- Protonation of curcumin triggers sequential double cyclization in the gas-phase: An electrospray mass spectrometry and DFT study, **International Journal of Mass Spectrometry , 107-114, 438, 2019**
- Selective control of volatile fatty acids production from food waste by regulating biosystem buffering: A comprehensive study, **Chemical Engineering Journal, 787-801, 357, 2019**
- A Review of Low Temperature NH3-SCR for Removal of NOx, **Catalysts, Article Number: 349, 9(4) 2019**
- Revealing sex-specific molecular changes in hypoxia-ischemia induced neural damage and subsequent recovery using zebrafish model, **Neuroscience Letters, Article Number: 134492, 712, 2019**
- Tumor protein D52 (isoform 3) interacts with and promotes peroxidase activity of Peroxiredoxin 1 in prostate cancer cells implicated in cell growth and migration, **Biochimica Et Biophysica Acta-Molecular Cell Research, 1298-1309, 1866(8) 2019**
- Zoledronic acid induces cytogenetic toxicity in male germline cells of Swiss albino mice, **Drug and Chemical Toxicology, 371-377, 42(4) 2019**
- Effectiveness of Solvent Vapor Annealing over Thermal Annealing on the Photovoltaic Performance of Non-Fullerene Acceptor Based BHJ Solar Cells, **Scientific Reports, Article Number: 8529, 9, 2019**
- Application of an agro-industrial waste for the removal of As (III) in a counter-current multiphase fluidized bed, **International Journal of Environmental Science and Technology, 279-294, 16(1) 2019**
- Economic and environmental impact assessment of extractive distillation with renewable entrainers for reprocessing aqueous 2-Propanol, **Chemical Engineering and Processing-Process Intensification, Article Number: 107616, 143, 2019**
- In silico design, synthesis and activity of potential drug-like chrysin scaffoldd-erived selective EGFR inhibitors as anticancer agents, **Computational Biology and Chemistry, Article Number: UNSP 107156, 83, 2019**
- Changes in the photosynthetic apparatus and lipid droplet formation in Chlamydomonas reinhardtii under iron deficiency, **Photosynthesis Research, 253-266, 139(1-3) 2019**
- Synthesis, spectroscopic characterization, biological screening and in vitro cytotoxic studies of 4-methyl-3-thiosemicarbazone derived Schiff bases and their Co

(II), Ni (II), Cu (II) and Zn (II) complexes, **Applied Organometallic Chemistry, Article Number: e5154, 33(10) 2019**

- Optimization of process parameters for slow pyrolysis of neem press seed cake for liquid and char production, **Journal of Environmental Chemical Engineering, Article No:102905, 7(1) 2019**
- Asymmetric total synthesis of filamentous fungi related resorcylic acid lactones 7-epi-zeaenol and zeaenol, **Heterocyclic Communications, 78-84, 25(1) 2019**
- Metal Free Domino beta-Azidation/[3+2] Cycloaddition Reaction for the Synthesis of 1,2,3-Triazole-Fused Dihydrobenzoxazinones, **Journal of Organic Chemistry, 10546-10553, 84(16) 2019**
- Gram-Scale Solution-Phase Synthesis of Heptapeptide Side Chain of Teixobactin, **Synlett, 2268-2272, 30(20) 2019**
- Base catalysed diastereoselective Tamura cycloaddition of vinylidene indanediones, **Tetrahedron Letters, 1-4, 60(1) 2019**
- Enantioselective Desymmetrization of Prochiral Cyclopentene-1,3-iones Triggered by Remote C(sp(2))-N Bond Formation, **Journal of Organic Chemistry, 15735-15744, 84(23) 2019**
- In vitro genotoxicity assessment of nickel(II) oxide nanoparticles on lymphocytes of human peripheral blood, **Journal of Applied Toxicology, 955-965, 39(7) 2019**
- Repeated oral dose toxicity study of nickel oxide nanoparticles in Wistar rats: a histological and biochemical perspective, **Journal of Applied Toxicology, 1012-1029, 39(7) 2019**
- Influence of strong electron donating nature of phenothiazine on A(3)B- type porphyrin based dye sensitized solar cells, **Solar Energy, 620-627, 184, 2019**
- Intramolecular electron transfer in porphyrin-anthraquinone donor-acceptor systems with varying molecular bridges, **Journal of Porphyrins and Phthalocyanines, 628-638, 23(6) 2019**
- Functional π -conjugated tetrathiafulvalene decorated with benzothiadiazole organic sensitizers for dye sensitized solar cells, **New Journal of Chemistry, 8919-8929, 43(23) 2019**
- Enjamuri, Nagasuresh; Sarkar, Santu; Reddy, Benjaram M; Mondal, John; Design and Catalytic Application of Functional Porous Organic Polymers: Opportunities and Challenges, **Chemical Record, 1782-1792, 19(9) 2019**
- Total synthesis and stereochemical revision of relgro and 10 '-oxorelgro, **Organic & Biomolecular Chemistry, 5601-5614, 17(22) 2019**
- Understanding the interdependence of operating parameters in microbial electrosynthesis: a numerical investigation, **Physical Chemistry Chemical Physics, 10761-10772, 21(20) 2019**
- Phytochemical investigation and cytotoxic activity of hydro alcoholic fraction of Trianthema decandra, **Indian Journal of Biotechnology, 193-203, 18(3) 2019**
- Synthesis of novel derivatives of 7,8-dihydro-6H-imidazo[2,1-b][1,3]benzothiazol-5-one and their virus-inhibiting activity against influenza A virus, **Archiv Der Pharmazie, Article Number: e1800225, 352(2) 2019**
- Na3+x[CrxTi2-x(PO4)(3)] glass-ceramic electrolyte: ionic conductivity and structural correlations for different heat treating temperatures and time schedules, **Ionics, 4179-4188, 25(9) 2019**
- A carboxylic acid functionalized SBA-15 supported Pd nanocatalyst: an efficient catalyst for hydrogenation of nitrobenzene to aniline in water, **New Journal of Chemistry, 11871-11875, 43(30) 2019**
- Evaluating the metabolic perturbations in Mangifera indica (mango) ripened with various ripening agents/practices through gas chromatography - mass spectrometry based metabolomics, **Journal of Separation Science, 3086-3094, 42(19) 2019**
- A review on HCV inhibitors: Significance of non-structural polyproteins, **European Journal of Medicinal Chemistry, 576-601, 164, 2019**
- Unraveling structural insights of ribokinase from Leishmania donovani, **International Journal of Biological Macromolecules, 253-265, 136, 2019**
- Transition metal-free functionalized hydration of alkynes: one-pot synthesis of fluorinated beta-keto-

imidates using Selectfluor, **Organic & Biomolecular Chemistry, 4440-4445, 17(18) 2019**

- A Diuranyl(VI) Complex and Its Application in Electrocatalytic and Photocatalytic Hydrogen Evolution from Neutral Aqueous Medium, **Inorganic Chemistry, 14410-14419, 58(21) 2019**
- Copper-catalyzed oxidative cleavage of Passerini and Ugi adducts in basic medium yielding alpha-ketoamides, **New Journal of Chemistry, 14459-14474, 43(36) 2019**
- Comparative study of vapour phase glycerol dehydration over different tungstated metal phosphate acid catalysts, **New Journal of Chemistry, 16860-16869, 43(43) 2019**
- Novel anisotropic ordered polymeric materials based on metallopolymer precursors as dye sensitized solar cells, **Chemical Engineering Journal, 1166-1175, 358, 2019**
- Solvent-Induced Self-Assembly of Naphthalenediimide Conjugated to Tetraphenylethene through D- and L-Alanine, **ChemistrySelect, 2626-2633, 4(9) 2019**
- Solvent directed self-assembly of naphthalenediimide-tryptophan-glutamate conjugates, **Indian Journal of Chemistry Section B-Organic Chemistry including Medicinal Chemistry, 200-208, 58(2) 2019**
- Synthesis and biological evaluation of novel 4,7-dihydroxycoumarin derivatives as anticancer agents, **Bioorganic & Medicinal Chemistry Letters, 1819-1824, 29(14) 2019**
- Electrochemical synthesis, single-crystal growth, physicochemical and dielectric studies of tetrabromobisphenol A, **Indian Journal of Physics, 349-359, 93(3) 2019**
- Mesoporous Aluminosilicates in the Synthesis of N-Heterocyclic Compounds, **Kinetics and Catalysis, 733-743, 60(6) 2019**
- Aluminosilicates with Different Porous Structures in the Synthesis of 2-Ethyl-3-Methylquinoline, **Petroleum Chemistry, 719-725, 59(7) 2019**
- A hierarchically zeolite Y for the N-heterocyclic compounds synthesis, **Journal of Saudi Chemical Society, 452-460, 23(4) 2019**
- Gold-catalyzed formation of aryl-fused pyrazolooxazepines via intramolecular regioselective 7-exo-dig cyclization, **Organic & Biomolecular Chemistry, 2809-2817, 17(10) 2019**
- In vivo targeting of DNA vaccines to dendritic cells using functionalized gold nanoparticles, **Biomaterials Science, 773-788, 7(3) 2019**
- Photo-sensitized oxy-thiocyanation of terminal alkynes/1,3-aryldienes and their one-pot conversion to 2-hydroxy 4-substituted aryl thiazoles, **Organic & Biomolecular Chemistry, 2232-2241, 17(8) 2019**
- Ni-Al-Ti Hydrotalcite Based Catalyst for the Selective Hydrogenation of Biomass-Derived Levulinic Acid to gamma-Valerolactone, **ChemistrySelect, 202-210, 4(1) 2019**
- Influence of surface Lewis acid sites for the selective hydrogenation of levulinic acid to gamma-valerolactone over Ni-Cu-Al mixed oxide catalyst, **Reaction Kinetics Mechanisms and Catalysis, 601-616, 127(2) 2019**
- Total syntheses of surinone B, alatanones A-B, and trineurone A, **Journal of Asian Natural Products Research, 262-269, 21(3) 2019**
- Asymmetric Total Synthesis of 16-Methyleicos-(4E)-en-1-yn-3-ol from the Marine Sponge Cribrochalina vasculum: Establishment of Absolute Configuration of Chiral Centers, **ChemistrySelect, 399-402, 4(1) 2019**
- Betulinic acid derivatives: a new class of alpha-glucosidase inhibitors and LPS-stimulated nitric oxide production inhibition on mouse macrophage RAW 264.7 cells, **Natural Product Research, 2618-2622, 33(18) 2019**
- IITZ-01, a novel potent lysosomotropic autophagy inhibitor, has single-agent antitumor efficacy in triple-negative breast cancer in vitro and in vivo, **Oncogene, 581-595, 38(4) 2019**
- A novel and stretchy polysaccharide tool for biomedical and nutritional applications, **International Journal of Biological Macromolecules, 852-863, 132, 2019**
- Role of the Fe oxidation states on the catalytic oxy-dehydrogenation of ethylbenzene using CO2 as a soft oxidant over FeOX/carbon-alumina, **Catalysis Communications, 1-4, 118, 2019**

- CH4 Cracking over the Cu-Ni/Al-MCM-41 Catalyst for the Simultaneous Production of H-2 and Highly Ordered Graphitic Carbon Nanofibers, **Energy & Fuels, 12656-12665, 33(12) 2019**
- Influence of flour type on physico-chemical characteristics during deep frying, **Journal of Food Science and Technology-Mysore, 3471-3480, 56(7) 2019**
- Isolation and antiproliferative activity of triterpenoids and fatty acids from the leaves and stem of Turraea vogelii Hook. f. ex benth, **Natural Product Research, 296-301, 33(2) 2019**
- One-Pot Allylation-Intramolecular Vinylogous Michael Addition-Isomerization Cascade of o-Hydroxy cinnamates and Congeners: Synthesis of Substituted Benzofuran Derivatives, **Organic Letters, 1823-1827, 21(6) 2019**
- Synthesis and mechanistic studies of diketo acids and their bioisosteres as potential antibacterial agents, **European Journal of Medicinal Chemistry, 67-82, 163, 2019**
- Self-sustainable azolla-biorefinery platform for valorization of biobased products with circular-cascading design, **Chemical Engineering Journal, 1042-1053, 373, 2019**
- Microalgae-biorefinery with cascading resource recovery design associated to dairy wastewater treatment, **Bioresource Technology, 424-429, 284, 2019**
- Preparation, Optimization, and Evaluation of Hyaluronic Acid-Based Hydrogel Loaded with Miconazole Self-Nanoemulsion for the Treatment of Oral Thrush, **AAPS Pharmscitech, Article Number: 297, 20(7) 2019**
- Alteration of benzo(a)pyrene biotransformation by resveratrol in Apc(Min/+) mouse model of colon carcinogenesis, **Investigational New Drugs, 238-251, 37(2) 2019**
- Hypervalent Iodine Mediated Efficient Solvent-Free Regioselective Halogenation and Thiocyanation of Fused N-Heterocycles, **Synlett, 1573-1579, 30(13) 2019**
- Synthesis of Combretastatin-A4 Carboxamidest that Mimic Sulfonyl Piperazines by a Molecular Hybridization Approach: in vitro Cytotoxicity Evaluation and Inhibition of Tubulin Polymerization, **ChemMedChem, 2052-2060, 14(24) 2019**
- Transition metal-free one-pot synthesis of substituted pyrroles by employing aza-Wittig reaction, **RSC Advances, 30659-30665, 9(53) 2019**
- Synthesis and in vitro cytotoxicity evaluation of beta-carboline-combretastatin carboxamides as apoptosis inducing agents: DNA intercalation and topoisomerase-II inhibition, **Bioorganic & Medicinal Chemistry, 3285-3298, 27(15) 2019**
- Diastereoselective Desymmetrization of p-Quinamines through Regioselective Ring Opening of Epoxides and Aziridines, **Organic Letters, 10115-10119, 21(24) 2019**
- Rh-Catalyzed diastereoselective desymmetrization of enone tethered-cyclohexadienones via tandem arylative cyclization, **Organic & Biomolecular Chemistry, 1937-1946, 17(7) 2019**
- **Book Chapter:** A Critical Analysis of Molecular Mechanisms Underlying Membrane Cholesterol Sensitivity of GPCRs, **Cholesterol Modulation of Protein Function: Sterol Specificity and Indirect Mechanisms, 21-52, 1115, 2019**
- Low-temperature elemental mercury removal over TiO2 nanorods-supported MnOx-FeOx-CrOx, **Catalysis Today, 174-182, 324(Special Issue:SI) 2019**
- Flower-like Mn3O4/CeO2 microspheres as an efficient catalyst for diesel soot and CO oxidation: Synergistic effects for enhanced catalytic performance, **Applied Surface Science, 209-221, 473, 2019**
- Designing of fatty acid-surfactant conjugate based nanomicelles of morin hydrate for simultaneously enhancing anticancer activity and oral bioavailability, **Colloids and Surfaces B-Biointerfaces, 202-211, 175, 2019**
- [HgCl4](2-)[C5H6N2Cl](2+) inorganic-organic hybrid material with structural and optical properties, **Results in Physics, Article Number: 102421, 14, 2019**

- I-2-Catalyzed oxidative synthesis of N,4-disubstituted quinazolines and quinazoline oxides, **Organic & Biomolecular Chemistry, 3714-3717, 17(15) 2019**
- Base-catalyzed synthesis of quinazolines in aqueous medium, **Tetrahedron Letters, Article Number: 151186, 60(44) 2019**
- Hydrothermal synthesis of novel Mn1/3Ni1/3Co1/ 3MoO4 on reduced graphene oxide with a high electrochemical performance for supercapacitors, **Journal of Alloys and Compounds, 900-912, 778, 2019**
- Uncovering Structural and Molecular Dynamics of ESAT-6:beta 2M Interaction: Asp53 of Human beta 2-Microglobulin Is Critical for the ESAT-6:beta 2M Complexation, **Journal of Immunology, 1918-1929, 203(7) 2019**
- One-pot, Multicomponent Cascade Reaction for the Synthesis of Various Aralkyl/alkylthio-3,5-dimethyl-1H-pyrazolyl-4H-1,2,4-triazol-4-amine and Their Docking Studies, **Journal of Heterocyclic Chemistry, 1012-1019, 56(3) 2019**
- Synthesis, characterization and evaluation of 1-monoacylglycerols of unsaturated fatty acids as potential bioactive lipids, **Grasas Y Aceites, Article Number: e325, 70(4) 2019**
- Synthesis, Molecular Docking and Biological Evaluation of 1-(benzo[d]thiazol-2-ylamino) (phenyl) methyl)naphthalen-2-ol Derivatives as Antiproliferative Agents, **Letters in Organic Chemistry, 837-845, 16(10) 2019**
- Oxyanion-Binding in a Bioinspired Nanoparticle-Assembled Hybrid Microsphere Structure: Effective Removal of Arsenate/Chromate From Water, **ACS Applied Nano Materials, 1525-1532, 2(3) 2019**
- Pd/Cu-catalyzed facile approach to stilbenes: A novel diversity of TosMIC as an aryl source, **Tetrahedron Letters, 1978-1981, 60(30) 2019**
- Gold-Catalyzed Synthesis of 6-Hydroxyindoles from Alkynylcyclohexadienones and Substituted Amines, **Journal of Organic Chemistry, 12228-12236, 84(18) 2019**
- Lag effect of climatic variables on dengue burden in India, **Epidemiology and Infection, Article Number: UNSP e170, 147, 2019**
- Temperature dependent transmission potential model for chikungunya in India, **Science of the Total Environment, 66-74, 647, 2019**
- An alternative total synthesis of diplodialide-B, **Synthetic Communications, 3324-3328, 49(23) 2019**
- Na2S-promoted reduction of azides in water: synthesis of pyrazolopyridines in one pot and evaluation of antimicrobial activity, **Organic & Biomolecular Chemistry, 3186-3194, 17(12) 2019**
- Efficient and green sulfamic acid catalyzed synthesis of new 1,2-dihydroquinazoline derivatives with antibacterial potential, **Arabian Journal of Chemistry, 3546-3554, 12(8) 2019**
- Recent Advances in Intramolecular Metal-Free Oxidative C-H Bond Aminations Using Hypervalent Iodine(III) Reagents, **European Journal of Organic Chemistry, 1687-1714, (8) 2019**
- Toward the synthesis of macrolide aspergillide D, **Synthetic Communications, 3191-3197, 49(22) 2019**
- Demagnetization field driven charge transport in a TiO2 based dye sensitized solar cell, **Solar Energy, 281-289, 187, 2019**
- Copper Catalyzed C-H Activation, **Chemical Record, 1302-1318, 19(7) 2019**
- Squalane-based emulsion vaccine delivery system: composition with murabutide activate Th1 response, **Pharmaceutical Development and Technology, 269-275, 24(3) 2019**
- Phenazine-1-carboxamide functionalized mesoporous silica nanoparticles as antimicrobial coatings on silicone urethral catheters, **Scientific Reports, Article Number: 6198, 9, 2019**
- Chumacin-1 and Chumacin-2 from Pseudomonas aeruginosa strain CGK-KS-1 as novel quorum sensing signaling inhibitors for biocontrol of bacterial blight of rice, **Microbiological Research, Article Number: 126301, 228, 2019**

- Synthesis of diarylidenecyclohexanone derivatives as potential anti-inflammatory leads against COX-2/mPGES1 and 5-LOX, **New Journal of Chemistry, 9012-9020, 43(23) 2019**
- Synthesis and biological evaluation of 2,4,5-trisubstituted thiazoles as antituberculosis agents effective against drug-resistant tuberculosis, **European Journal of Medicinal Chemistry, 315-328, 178, 2019**
- Studies towards the stereoselective total synthesis of Gliomasolide A, **Tetrahedron Letters, Article Number: 151169, 60(48) 2019**
- Studies towards the Synthesis of (+)-Lochnerine, **ChemistrySelect, 4203-4205, 4(14) 2019**
- Polyethylenimine-Modified Zeolite 13X for CO2 Capture: Adsorption and Kinetic Studies, **ACS Omega, 16441-16449, 4(15) 2019**
- Hybrid material of polyaniline incorporated industrial waste of fly ash to enhance the electrode performance of polyaniline in supercapacitor application, **Journal of Solid State Electrochemistry, 3231-3242, 23(12) 2019**
- Polyaniline salt catalyzed synthesis of hyperbranched polyester and its use as dopant in polyaniline salt for coating, fluorescence, and supercapacitor electrode, **Ionics, 191-202, 25(1) 2019**
- To promote aniline to polyaniline-glycopolymers for fluorescence, electro active material, and electrostatic discharge applications, **Journal of Applied Polymer Science, Article Number: 48043,136(41) 2019**
- Synthesis, structural, spectral, third order nonlinear optical and quantum chemical investigations on hydrogen bonded novel organic molecular adduct 4-(dimethylamino) benzaldehyde 4-nitrophenol for opto-electronic applications, **Journal of Molecular Structure, 352-365, 1178, 2019**
- Novel benzosuberone conjugates as potential anti-proliferative agents: Design, synthesis and molecular docking studies, **Journal of Molecular Structure, 355-362, 1180, 2019**
- A facile construction of oxygen heterocycles by the reaction of benzoxepine-4-carboxylates with dihaloalkanes and activated alkynes, **Organic & Biomolecular Chemistry, 6645-6653, 17(27) 2019**
- Palladium(II)-catalyzed synthesis of indenones through the cyclization of benzenecarbaldehydes with internal alkynes, **RSC Advances, 31162-31168, 9(53) 2019**
- A One-pot Multicomponent 'Click' Approach to the Synthesis of Novel Tamoxifen-triazole Conjugates using Nano Iron Oxide Catalyst and their Preliminary Antiproliferative Activity Studies, **Letters in Drug Design & Discovery, 846-860, 16(8) 2019**
- Estimation of boswellic acids in herbal formulations containing Boswellia serrata extract and comprehensive characterization of secondary metabolites using UPLC-Q-Tof-MSe, **Journal of Pharmaceutical Analysis, 414-422, 9(6) 2019**
- Hofmann rearrangement of primary carboxamides and cyclic imides using DCDMH and application to the synthesis of gabapentin and its potential peptide prodrugs, **Tetrahedron Letters, 552-556, 60(7) 2019**
- Cycloxygenase-2 inhibition potentiates trans-differentiation of Wharton's jelly-mesenchymal stromal cells into endothelial cells: Transplantation enhances neovascularization-mediated wound repair, **Cytotherapy, 260-273, 21(2) 2019**
- Endothelial progenitor cell therapy for chronic wound tissue regeneration, **Cytotherapy, 1137-1150, 21(11) 2019**
- An unusual synthesis of 3-(2-(arylamino)thiazol-4-yl)-2H-chromen-2-ones from ethyl 2-(chloromethyl)-2-hydroxy-2H-chromene-3-carboxylate via benzopyran ring opening, **Molecular Diversity, 443-452, 23(2) 2019**
- Simple diphenylamine based D-pi-A type sensitizers/co-sensitizers for DSSCs: a comprehensive study on the impact of anchoring groups, **Physical Chemistry Chemical Physics, 10603-10613, 21(20) 2019**
- One-Pot Synthesis and Biological Evaluation of Arylpropenone Aminochalcone Conjugates as Potential Apoptotic Inducers, **ChemistrySelect, 4672-4678, 4(16) 2019**

- Design, synthesis, in silico pharmacokinetics prediction and biological evaluation of 1,4-dihydroindeno[1,2-c]pyrazole chalcone as EGFR /Akt pathway inhibitors, **European Journal of Medicinal Chemistry, 636-648, 163, 2019**
- Synthesis of new bis-pyrazole linked hydrazides and their in vitro evaluation as antimicrobial and anti-biofilm agents: A mechanistic role on ergosterol biosynthesis inhibition in Candida albicans, **Chemical Biology & Drug Design, 1339-1351, 94(1) 2019**
- An overview on the synthetic and medicinal perspectives of indenopyrazoles, **European Journal of Medicinal Chemistry, 1-12, 178, 2019**
- miR-30 Family miRNAs Mediate the Effect of Chronic Social Defeat Stress on Hippocampal Neurogenesis in Mouse Depression Model, **Frontiers in Molecular Neuroscience, Article Number: 188, 12, 2019**
- Stenotrophomonas maltophilia Gd2: A potential and novel isolate for fibrinolytic enzyme production, **Saudi Journal of Biological Sciences, 1567-1575, 26(7) 2019**
- Effect of boiling and roasting on the physicochemical properties of Djansang seeds (Ricinodendron heudelotii), **Food Science & Nutrition, 3425-3434, 7(11) 2019**
- Applications of machine learning techniques to predict filariasis using socio-economic factors, **Epidemiology and Infection, Article Number: PII S0950268819001481, 147, 2019**
- Tribological studies of alpha-lipoic acid esters as effective environmentally friendly multifunctional lubricant additives, **Energy Sources Part A-Recovery Utilization and Environmental Effects, 700-712, 41(6) 2019**
- Measurement and correlation studies of phase equilibria and thermophysical properties of 4-tert-butylbenzaldehyde, **Journal of Molecular Liquids, 11-17, 280, 2019**
- Biosynthesized Gold Nanoparticles: In Vivo Study of Near-Infrared Fluorescence (NIR)-Based Bio-imaging and Cell Labeling Applications, **ACS Biomaterials Science & Engineering, 5439-5452, 5(10) 2019**
- Restoration of p53 Function in Ovarian Cancer Mediated by Gold Nanoparticle-Based EGFR Targeted Gene Delivery System, **ACS Biomaterials Science & Engineering, 3631-3644, 5(7) 2019**
- A New Series of EDOT Based Co-Sensitizers for Enhanced Efficiency of Cocktail DSSC: A Comparative Study of Two Different Anchoring Groups, **Molecules, Article Number: 3554, 24(19) 2019**
- Enhanced solar light-driven photocatalytic degradation of pollutants and hydrogen evolution over exfoliated hexagonal WS2 platelets, **Materials Research Bulletin, 246-254, 109, 2019**
- Tetrahydrothiopyran-4-one as Five-Carbon Source for Scalable Synthesis of (+/-)-Tapentadol, **Organic Process Research & Development, 1369-1373, 23(7) 2019**
- Synthesis of some novel orsellinates and lecanoric acid related depsides as alpha-glucosidase inhibitors, **Journal of Asian Natural Products Research, 1013-1027, 21(10) 2019**
- Solution processed aligned ZnO nanowires as anti-reflection and electron transport layer in organic dye-sensitized solar cells, **Optical Materials, Article Number: UNSP 109243, 95, 2019**
- Efficient near IR porphyrins containing a triphenylamine-substituted anthryl donating group for dye sensitized solar cells, **Journal of Materials Chemistry C, 13594-13605, 7(43) 2019**
- Krishna, K. Vamshi; Mohan, S. Venkata; Purification and Characterization of NDH-2 Protein and Elucidating Its Role in Extracellular Electron Transport and Bioelectrogenic Activity, **Frontiers in Microbiology, Article Number: 880, 10, 2019**
- Studies on wound healing potential of red pigment isolated from marine Bacterium Vibrio sp., **Saudi Journal of Biological Sciences, 723-729, 26(4) 2019**
- Copper-Catalyzed One-Pot Synthesis of Pyrrolo[1,2-a]quinoxaline Derivatives from 1-(2-Aminophenyl)-pyrroles and Aldehydes, **ChemistrySelect, 250-253, 4(1) 2019**

- Microbial electro-hydrolysis of sewage sludge for acidogenic production of biohydrogen and volatile fatty acids along with struvite, **Chemical Engineering Journal, 1264-1274, 374, 2019**
- Stereoselective Synthesis of the A,E-Ring Bicyclic Core of Calyciphylline B-Type Alkaloids, **Synlett, 2157-2160, 30(19) 2019**
- Phenoxy-Alkyl Maleates as Phase-Selective Organogelators for Gelation of Edible Oils, **European Journal of Lipid Science and Technology, Article Number: 1800364, 121(2) 2019**
- Supramolecular phenoxy-alkyl maleate-based hydrogels and their enzyme/pH-responsive curcumin release, **New Journal of Chemistry, 5559-5567, 43(14) 2019**
- Impact of Hybrid-polar Histone Deacetylase Inhibitor m-Carboxycinnamic Acid bis-Hydroxyamide on Human Pancreatic Adenocarcinoma Cells, **Anti-Cancer Agents in Medicinal Chemistry, 750-759, 19(6) 2019**
- Organocatalytic Enantioselective Mannich Reaction: Direct Access to Chiral beta-Aino Esters, **ACS Omega, 2168-2177, 4(1) 2019**
- Rh(III)-Catalyzed Intramolecular Oxidative Annulation of Propargyl Amino Phenyl Benzamides to Access Pyrido/ Isoquinolino Quinoxalinones, **Advanced Synthesis & Catalysis, 4825-4830, 361(20) 2019**
- Isophorone-boronate ester: A simple chemosensor for optical detection of fluoride anion, **Applied Organometallic Chemistry, Article Number: e4688, 33(1) 2019**
- Synthesis and biological evaluation of bergenin-1,2,3-triazole hybrids as novel class of anti-mitotic agents, **Bioorganic Chemistry, Article Number: UNSP 103161, 91, 2019**
- Cu(OAc)(2)-Promoted Thiolation and Selenylation of C(sp2)-H Bonds Using a 2-Amino Oxazole Directing Group, **Letters in Organic Chemistry, 110-116, 16(2) 2019**
- Integrated Microfluidic Photo-Flow Process (mu-PFP) for Direct Upconversion of Exhaust Gas to Value-Added Chemicals, **ACS Sustainable Chemistry & Engineering, 19605-19611, 7(24) 2019**
- A Metal-Free, Organo Lewis Acid Catalyzed Synthesis of Highly Substituted Oxazoles, **ChemistrySelect, 8973-8977, 4(31) 2019**
- Cationic Pd(IV)-Induced Highly Diastereoselective Arylative Cascade Cyclization of Allene-Tethered Cyclohexadienones Leading to Oxygenated Bicyclic Motifs, **Organic Letters, 6300-6304, 21(16) 2019**
- Parametric optimization and rate laws determination for the conversion of 4-tert-butylbenzoic acid to methyl 4-tert-butylbenzoate, **Indian Journal of Chemical Technology, 289-299, 26(4) 2019**
- Synthesis of Dihydropyridine Derivatives under Eco-friendly Approach and Investigation of Cytotoxic Activity, **Journal of Heterocyclic Chemistry, 1661-1666, 56(5) 2019**
- Tungstophosphoric acid supported on mesoporouus niobiumoxophosphate: an efficient solid acid catalyst for etherification of 5-hydroxymethylfurfural to 5-ethoxy methylfurfural, **Catalysis Today, 53-60, 325(Special Issue:SI) 2019**
- Metal free montmorillonite KSF clay catalyzed practical synthesis of benzoxazoles and benzothiazoles under aerobic conditions, **Synthetic Communications, 3335-3342, 49(23) 2019**
- A stereoselective synthesis of (R)-5-hydroxy-3-(4-methoxyphenethyl) cyclohex-2-enone, towards total synthesis of Prelunularin, **Tetrahedron Letters, Article Number: 151134, 60(41) 2019**
- Lade, Dhanaji M; Aher, Yogesh N; Pawar, Amit B; Cp*Ir(III)-Catalyzed C-H/O-H Functionalization of Salicylaldehydes for the Synthesis of Chromones at Room Temperature, **Journal of Organic Chemistry, 9188-9195, 84(14) 2019**
- Lakkakula, R; Roy, A; Mukkanti, K; Sridhar, G; Synthesis and Anticancer Activity of 1,2,3-Triazole Fused N-Arylpyrazole Derivatives, **Russian Journal of General Chemistry, 831-835, 89(4) 2019**
- Lakshmi, Dhana D; Rao, Srinivasa B; Lingaiah, N; Synthesis of dimethyl carbonate from methanol and urea over zinc-strontia mixed oxide catalysts, **Catalysis Communications, 1-4, 122, 2019**

- Lakshmireddy, V. M; Veera, Y. Naga; Reddy, T. J; Rao, V. J; Raju, B. China; A Green and Sustainable Approach for Selective Halogenation of Anilides, Benzanilides, Sulphonamides and Heterocycles(dagger), **Asian Journal of Organic Chemistry, 1380-1384, 8(8) 2019**
- Latha, M; Rani, J. Vatsala; WS2/Graphene Composite as Cathode for Rechargeable Aluminum-Dual Ion Battery, **Journal of the Electrochemical Society, Article Number: UNSP 070501, 167(1) 2019**
- Latha, S. Vani; Flower, G. Little; Reddy, M. Srinivasa; Raju, L. Yugandhar; Rao, C. V. Nageswara; Ratnakar, A; Thermo physical, optical and spectroscopic perspectives of molecular interactions in binary mixtures of Ethyl Lactate and Dimethyl Adipate at T=303.15-318.15 K and atmospheric pressure, **Physics and Chemistry of Liquids, 816-839, 57(6) 2019**
- Li, Zhen-Zhen; Tangadanchu, Vijai Kumar Reddy; Battini, Narsaiah; Bheemanaboina, Rammohan R. Yadav; Zang, Zhong-Lin; Zhang, Shao-Lin; Zhou, Cheng-He; Indole-nitroimidazole conjugates as efficient manipulators to decrease the genes expression of methicillin-resistant Staphylococcus aureus, **European Journal of Medicinal Chemistry, 723-735, 179, 2019**
- Formulation and evaluation of cyclodextrin complexes for improved anticancer activity of repurposed drug: Niclosamide, **Carbohydrate Polymers, 252-259, 212, 2019**
- Maadwar, Sasikala; Gana, Rajitha; Cytotoxic oxindole derivatives: in vitro EGFR inhibition, pharmacophore modeling, 3D-QSAR and molecular dynamics studies, **Journal of Receptors and Signal Transduction, 460-469, 39(5-6) 2019**
- Review on biological wastewater treatment and resources recovery: attached and suspended growth systems, **Water Science and Technology, 2013-2026, 80(11), 2019**
- Identification, synthesis and evaluation of CSF1R inhibitors using fragment based drug design, **Computational Biology and Chemistry, 374-383, 80, 2019**
- Design and Evaluation of PEGylated Liposomal Formulation of a Novel Multikinase Inhibitor for Enhanced Chemo sensitivity and Inhibition of Metastatic Pancreatic Ductal Adenocarcinoma, **Bioconjugate Chemistry, 2703-2713, 30(10) 2019**
- La2O3 promotional effect to Co3O4/gamma-Al2O3 catalyst in the oxidative dehydrogenation of ethylbenzene with CO2 as soft oxidant, **Journal of Saudi Chemical Society, 678-690, 23(6) 2019**
- Unique influence of rare earth (Pr, Nd, and Er) oxide surface acidic texture over CeO2/gamma-Al2O3 catalysts for selective production of styrene using CO2 flow, **Research on Chemical Intermediates, 2749-2770, 45(5) 2019**
- Advantage of Co Embedded gamma-Al2O3 Catalysts Over MgO and SiO2 Solid Oxides in the Selective Production of Styrene Monomer, **Catalysis Letters, 3238-3252, 149(11) 2019**
- Role of Cobalt Oxide-Based Catalysts for Styrene Production: A Review on Significance of Various Promoters, Calcination Temperature, Chemical Behavior of Support Materials and Synthesis Procedure, **Catalysis Surveys from Asia, 290-310, 23(4) 2019**
- Condensation of 4-chloro-2H-chromene-3-carbalde hydes and ethyl-3-aminocrotonates with p-TsOH: a facile approach for the synthesis of chromenyldihydro pyridines, **Synthetic Communications, 2538-2545, 49(19) 2019**
- Dimedone-Based Rigid Organic Scaffold for Organizing Symmetrical Helical Peptide Chains, **ChemistrySelect, 11518-11522, 4(39) 2019**
- Micro-electro-flow reactor (mu-EFR) system for ultra-fast arene synthesis and manufacture of daclatasvir, **Chemical Communications, 11852-11855, 55(79) 2019**
- Tandem Addition/Electrocyclization/Benzylation of Alkyl Aryl-1,3-dienes and Aromatic Aldehydes: Access to Highly Substituted Indenes, **Journal of Organic Chemistry, 7815-7828, 84(12) 2019**
- S-2 and mixed aggregate state emission of thiophene-BODIPY, **Journal of Photochemistry and Photobiology A-Chemistry, 147-152, 368, 2019**

- Impact of FRET between Molecular Aggregates and Quantum Dots, **Chemistry-An Asian Journal, 597-605, 14(4) 2019**
- Synthesis and evaluation of alpha-aminoacyl amides as antitubercular agents effective on drug resistant tuberculosis, **European Journal of Medicinal Chemistry, 665-677, 164, 2019**
- Novel 1,3,4-oxadiazoles as antitubercular agents with limited activity against drug-resistant tuberculosis, **Future Medicinal Chemistry, 499-510, 11(6) 2019**
- Multicomponent access to novel proline/cyclized cysteine tethered monastrol conjugates as potential anticancer agents, **Journal of Saudi Chemical Society, 503-513, 23(4) 2019**
- Total Synthesis and Structural Revision of Monocillin VII, **Organic Letters, 5952-5956, 21(15) 2019**
- Doxorubicin induces prostate cancer drug resistance by upregulation of ABCG4 through GSH depletion and CREB activation: Relevance of statins in chemosensitization, **Molecular Carcinogenesis, 1118-1133, 58(7) 2019**
- A Fast Isolation Method for Glycyrrhizic Acid, the Bioactive Marker of Glycyrrhiza glabra, and Its Quantitative Evaluation in Some Single and Multiherbal Formulations Using High-Performance Thin-Layer Chromatography, **JPC-Journal of Planar Chromatography-Modern TLC, 81-87, 32(2) 2019**
- Design, synthesis, anti-inflammatory, cytotoxic and cell based studies of some novel side chain analogues of myrrhanones A & B isolated from the gum resin of Commiphora mukul, **Bioorganic Chemistry, 306-323, 82, 2019**
- Isolation, Chemical Modification, and Anticancer Activity of Major Metabolites of the Lichen Parmotrema mesotropum, **Chemistry of Natural Compounds, 825-831, 55(5) 2019**
- Hydrogen Production from Water Splitting: Fabrication of ZnO Nanorod Decorated Cu NW Heterogeneous Hybrid Structures for Photocatalytic Applications, **Journal of Cluster Science, 449-457, 30(2) 2019**
- Magnesium-Graphene Composite Coated on SS Mesh as Cathode Material for Rechargeable Magnesium ion Battery, **Transactions of the Indian Institute of Metals, 2503-2510, 72(9) 2019**
- Synthesis of Substituted Cinnamido Linked Quinazolinone Congeners as Potential Anticancer Agents via Mitochondrial Dependent Intrinsic Apoptotic Pathway, **Anti-Cancer Agents in Medicinal Chemistry, 1935-1948, 19(16) 2019**
- A metal-free approach for the synthesis of amides/esters with pyridinium salts of phenacyl bromides via oxidative C-C bond cleavage, **Beilstein Journal of Organic Chemistry, 1864-1871, 15, 2019**
- High performance CO2 gas sensor based on noble metal functionalized semiconductor nanomaterials for health and environmental safety, **Materials Research Express, Article Number: 125041, 6(12) 2019**
- Iodine-mediated C-N and N-N bond formation: a facile one-pot synthetic approach to 1,2,3-triazoles under metal-free and azide-free conditions, **RSC Advances, 27021-27031, 9(46) 2019**
- Iodine-promoted one-pot synthesis of 1,3,4-oxadiazole scaffolds via sp(3) C-H functionalization of azaarenes, **New Journal of Chemistry, 15999-16006, 43(40) 2019**
- Glutathione S-transferase omega 1 inhibition activates JNK-mediated apoptotic response in breast cancer stem cells, **FEBS Journal, 2167-2192, 286(11) 2019**
- alpha-beta Unsaturated Acylsilanes as Surrogates of Acrolein for Morita-Baylis-Hillman Reactions, **European Journal of Organic Chemistry, 56-65, (1) 2019**
- 5-Chloro-2-thiophenyl-1,2,3-triazolylmethyldihydro quinolines as dual inhibitors of Mycobacterium tuberculosis and influenza virus: Synthesis and evaluation, **Bioorganic & Medicinal Chemistry Letters, 2664-2669, 29(18) 2019**
- Synthesis of novel morpholine, thiomorpholine and N-substituted piperazine coupled 2-(thiophen-2-yl) dihydro quinolines as potent inhibitors of Mycobacterium tuberculosis, **European Journal of Medicinal Chemistry, 171-178, 164, 2019**

- Synthesis and evaluation of novel substituted 1,2,3-triazolyldihydroquinolines as promising antitubercular agents, **Bioorganic & Medicinal Chemistry Letters, 529-533, 29(4) 2019**
- Molecular-Iodine-Promoted Synthesis of Dihydrobenzo furan-3,3-dicarbonitriles through a Novel Rearrangement, **Synlett, 293-298, 30(3) 2019**
- A rational design of a Pd-based catalyst with a metal-metal oxide interface influencing molecular oxygen in the aerobic oxidation of alcohols, **Green Chemistry, 2494-2503, 21(9) 2019**
- Shikimoyl-ligand decorated gold nanoparticles for use in ex vivo engineered dendritic cell based DNA vaccination, **Nanoscale, 7931-7943, 11(16) 2019**
- Neighboring Carbonyl Group Assisted Hydration of Unsymmetrical Aryl Alkynes Overriding Regular Selectivity, **European Journal of Organic Chemistry, 5787-5797, 2019(33) 2019**
- A lysosome-specific near-infrared fluorescent probe for in vitro cancer cell detection and non-invasive in vivo imaging, **Chemical Communications, 14182-14185, 55(94) 2019**
- Green synthesis of enantiopure quinoxaline alcohols using Daucus carota, **Chirality, 312-320, 31(4) 2019**
- Modestra, J. Annie; Mohan, S. Venkata; Capacitive biocathodes driving electrotrophy towards enhanced CO2 reduction for microbial electrosynthesis of fatty acids, **Bioresource Technology, Article Number: 122181, 294, 2019**
- **Editorial Material:** Special Issue On "Biotechnological Research and Innovation for Sustainable Development (BioSID 2019)" Preface, **Indian Journal of Experimental Biology, 783-783, 57(11) 2019**
- P-Stereogenic Phosphonates via Dynamic Kinetic Resolution: A Route towards Enantiopure Tertiary Phosphine Oxides, **European Journal of Organic Chemistry, 7836-7841, 2019(48) 2019**
- Photoinduced Fabrication of Cu/TiO2 Core-Shell Heterostructures Derived from Cu-MOF for Solar Hydrogen Generation: The Size of the Cu Nanoparticle Matters, **Journal of Physical Chemistry C, 26073-26081, 123(43) 2019**
- Ruthenium(iii)-bis(phenolato)bipyridine/TiO2 hybrids: unprecedented photocatalytic hydrogen evolution, **Dalton Transactions, 10070-10077, 48(27) 2019**
- Total synthesis of the proposed structure of xylarolide, **Tetrahedron Letters, Article Number: 150944, 60(34) 2019**
- Synthesis of Substituted Thioamides from gem-Dibromoalkenes and Sodiumsulfide, **European Journal of Organic Chemistry, 7159-7163, 2019(42) 2019**
- Stipulating Low Production Cost Solar Cells All Set to Retail horizontal ellipsis ...!, **Chemical Record, 661-674, 19(2-3) 2019**
- Voltage Stimulated Anion Binding of Metalloporphyrin-induced Crystalline 2D Nanoflakes, **Chemistry-An Asian Journal, 537-541, 14(4) 2019**
- Recent Advances on Stimuli-Responsive Smart Materials and their Applications, **ChemPlusChem, 1103-1121, 84(8) 2019**
- Ceria Promoted Cu-Ni/SiO2 Catalyst for Selective Hydrodeoxygenation of Vanillin, **ACS Omega, 4770-4778, 4(3) 2019**
- Studies towards the Synthesis of Aldgamycin - M, **ChemistrySelect, 3002-3005, 4(11) 2019**
- Alpha-Tocopherol-ascorbic acid hybrid antioxidant based cationic amphiphile for gene delivery: Design, synthesis and transfection, **Bioorganic Chemistry, 178-191, 82, 2019**
- Direct catalytic asymmetric method for the synthesis of tetrahydropyranopyrazoles through allene zwitterion chemistry, **Tetrahedron Letters, 703-706, 60(10) 2019**
- CO2 capture and adsorption kinetic study of amine-modified MIL-101 (Cr), **Chemical Engineering Research & Design, 241-248, 143, 2019**
- Enhancement of CO2 capture and separation of CO2/N-2 using post-synthetic modified MIL-100(Fe), **New Journal of Chemistry, 9725-9731, 43(24) 2019**

- Magnesium Aluminate Supported Cu Catalyst for Selective Transfer Hydrogenation of Biomass Derived Furfural to Furfuryl Alcohol with Formic Acid as Hydrogen Donor, **ChemistrySelect, 145-151, 4(1) 2019**
- A novel microbial fuel cell incorporated with polyvinylchloride/4A zeolite composite membrane for kitchen wastewater reclamation and power generation, **Materials Chemistry and Physics, 175-185, 224, 2019**
- **Synthesis** and biological evaluation of pyrazole linked benzothiazole-beta-naphthol derivatives as topoisomerase I inhibitors with DNA binding ability, **Bioorganic & Medicinal Chemistry, 708-720, 27(5) 2019**
- PhI(OAc)(2)-Mediated Regioselective Synthesis of 5-Guanidino-1,2,4-thiadiazoles and 1,2,4-Triazolo[1,5-a]pyridines via Oxidative N-S and N-N Bond Formation, **Synthesis-Stuttgart, 3600-3610, 51(19) 2019**
- Conversion of O-Propargyl beta-enones to 2-Allylidene 1,3-Diones and Furan Derivatives via [3,3]-Sigmatropic Rearrangement, **ChemistrySelect, 2053-2058, 4(7) 2019**
- Highly Efficient Benzo-Furan-Based Electron Acceptor Derived from One-Pot Synthesis for High-Performance Bulk Heterojunction Solar Cells, **ACS Applied Energy Materials, 1019-1025, 2(2) 2019**
- Copper-Catalyzed Glaser-Hey-Type Cross Coupling of 9-Ethynyl-alpha-Noscapine Leading to Unsymmetrical 1,3-Diynyl Noscapinoids, **Asian Journal of Organic Chemistry, 1495-1500, 8(8) 2019**
- Imidazo[2,1-b]thiazole-Coupled Natural Noscapine Derivatives as Anticancer Agents, **ACS Omega, 19382-19398, 4(21) 2019**
- Synthesis and Antiproliferative Activity of 9-Formyl and 9-Ethynyl Noscapines, **ChemistrySelect, 4092-4096, 4(14) 2019**
- Evolvement of nutraceutical onion plants engineered for resveratrol biosynthetic pathway, **Plant Cell Reports, 1127-1137, 38(9) 2019**
- Construction of Oxa-Bridged Tetracyclic Frameworks through a Prins Bicyclic Annulation, **European Journal of Organic Chemistry, 3567-3574, (22) 2019**
- Impact of A-D-A-Structured Dithienosilole- and Phenoxazine-Based Small Molecular Material for Bulk Heterojunction and Dopant-Free Perovskite Solar Cells, **Chemistry-A European Journal, 16320-16327, 25(71) 2019**
- Design, Synthesis, and Biological Evaluation of 2-(4-Aminophenyl) benzothiazole Analogues as Antiproliferative Agents, **Journal of Heterocyclic Chemistry, 520-532, 56(2) 2019**
- Engineered Nanoparticles for Effective Redox Signaling During Angiogenic and Antiangiogenic Therapy, **Antioxidants & Redox Signaling, 786-809, 30(5) 2019**
- Recent advances in inorganic nanomaterials for wound-healing applications, **Biomaterials Science, 2652-2674, 7(7) 2019**
- Convergent Stereoselective Synthesis of the C16-C37 Subunit of Sorangicin A, **Organic Letters, 7778-7781, 21(19) 2019**
- Measurement and Modeling of Solid-Liquid Equilibria of L-Glutamic Acid in Pure Solvents and Aqueous Binary Mixtures, **Journal of Chemical and Engineering Data, 1155-1165, 64(3) 2019**
- Design and synthesis of 4 beta-Acetamidobenzofuranone-podophyllotoxin hybrids and their anti-cancer evaluation, **Bioorganic & Medicinal Chemistry Letters, 2153-2156, 29(16) 2019**
- Extramembranous Regions in G Protein-Coupled Receptors: Cinderella in Receptor Biology?, **Journal of Membrane Biology, 483-497, 252(4-5) 2019**
- Direct ethanol condensation to diethyl acetal in the vapour phase at atmospheric pressure over CuNP/SBA-15 catalysts, **New Journal of Chemistry, 10003-10011, 43(25) 2019**
- ESI-MS/MS analysis of protonated N-methyl amino acids and their immonium ions, **Journal of Mass Spectrometry, 761-771, 54(9) 2019**
- Binding preference of nitroimidazolic radiosensitizers to nucleobases and nucleosides probed by electrospray ionization mass spectrometry and density functional theory, **Journal of Chemical Physics, Article Number: 014302, 150(1) 2019**

- Decomposition of protonated ronidazole studied by low-energy and high-energy collision-induced dissociation and density functional theory, **Journal of Chemical Physics, Article Number: 164306, 151(16) 2019**
- Comparative study of toxicological assessment of yttrium oxide nano- and microparticles in Wistar rats after 28 days of repeated oral administration, **Mutagenesis, 181-201, 34(2) 2019**
- Effective separation of methylene blue dye from aqueous solutions by integration of micellar enhanced ultrafiltration with vacuum membrane distillation, **Chemical Engineering Journal, Article Number: UNSP 122015, 375, 2019**
- Parameshwar, Matam; Rajesh, Manda; Balasubramanian, Sridhar; Reddy, Maddi Sridhar; Base Mediated Tandem Vinylogous Addition and Cyclization of gamma-Phosphonyl/Sulfonyl Crotonates and Ynones: Synthesis of Functionalized 2-Pyrones, **ACS Omega, 18846-18854, 4(20) 2019**
- Functionalized Rutile TiO2(110) as a Sorbent To Capture CO2 through Noncovalent Interactions: A Computational Investigation, **Journal of Physical Chemistry C, 3491-3504, 123(6) 2019**
- Graphene modified electrodes for bioelectricity generation in mediator-less microbial fuel cell, **Journal of Materials Science, 11604-11617, 54(17) 2019**
- First observation of microspherule from the infratrappean Gondwana sediments below Killari region of Deccan LIP, Maharashtra (India) and possible implications, **Geoscience Frontiers, 2281-2285, 10(6) 2019**
- Conversion of fructose into 5-hydroxymethylfurfural over mesoporous-ZrO2-phosphomolybdic acid nanocomposite catalysts, **Indian Journal of Chemistry Section A-Inorganic Bio-Inorganic Physical Theoretical & Analytical Chemistry, 313-320, 58(3) 2019**
- Zirconium Exchanged Phosphotungstic Acid Catalysts for Esterification of Levulinic Acid to Ethyl Levulinate, **Catalysis Letters, 2500-2507, 149(9) 2019**
- A Naphthalimide-Benzothiazole Conjugate as Colorimetric and Fluorescent Sensor for Selective Trinitrophenol Detection, **Chemosensors, Article Number: 38, 7(3) 2019**
- Merocyanine-Benzothiazole Chromophore-Based Sensor for Selective Picric Acid Detection, **ChemistrySelect, 10013-10020, 4(34) 2019**
- Total Synthesis of 5-Hydroxygoniothalamin, **Synthesis-Stuttgart, 780-786, 51(3) 2019**
- Role of group V elements on the hydrogenation activity of Ni/TiO2 catalyst for the vapour phase conversion of levulinic acid to gamma-valerolactone, **Catalysis Today, 68-72, 325(Special Issue: SI) 2019**
- Metal-organic-framework derived Co-Pd bond is preferred over Fe-Pd for reductive upgrading of furfural to tetrahydrofurfuryl alcohol, **Dalton Transactions, 8791-8802, 48(24) 2019**
- Esterification by Redox Dehydration Using Diselenides as Catalytic Organooxidants, **Journal of Organic Chemistry, 4954-4960, 84(9) 2019**
- Discovery of natural product ovalicin sensitive type 1 methionine aminopeptidases: molecular and structural basis, **Biochemical Journal, 991-1003, 476(Part:6) 2019**
- Design, synthesis, biological and in silico evaluation of coumarin-hydrazone derivatives as tubulin targeted antiproliferative agents, **Bioorganic Chemistry, Article Number: UNSP 103143, 91, 2019**
- Design, Synthesis and Pharmacological Evaluation of 4-Hydroxycoumarin Derivatives as Antiproliferative Agents, **ChemistrySelect, 10805-10809, 4(36) 2019**
- Iodine-Mediated Nucleophilic Direct Oxidative alpha-Acetoxylation and alpha-Alkoxylation of Ketones, **ChemistrySelect, 12333-12336, 4(42) 2019**
- Design, synthesis, molecular modelling, ADME prediction and antihyperglycemic evaluation of new pyrazole-triazolopyrimidine hybrids as potent alpha-glucosidase inhibitors, **Bioorganic Chemistry, Article Number: UNSP 103307, 93, 2019**

- Synthesis and biological evaluation of 1,2,4-oxadiazole linked 1,3,4-oxadiazole derivatives as tubulin binding agents, **Synthetic Communications, 1603-1612, 49(13) 2019**
- Bombesin receptors as potential targets for anticancer drug delivery and imaging, **International Journal of Biochemistry & Cell Biology, Article Number: UNSP 105567, 114, 2019**
- Achieving Enhanced Photocatalytic Activity of ZnO Supported on MWCNTs towards Degradation of Pollutants Under Visible Light, **Proceedings Paper: Materials Today-Proceedings, 419-426, 8(Part:1) 2019**
- The facile hydrothermal synthesis of CuO@ZnO heterojunction nanostructures for enhanced photocatalytic hydrogen evolution, **New Journal of Chemistry, 6794-6805, 43(17) 2019**
- Design and Synthesis of Novel Pyrimidine /Hexahydro quinazoline-Fused Pyrazolo[3,4-b] Pyridine Derivatives, Their Biological Evaluation and Docking Studies(#), **ChemistrySelect, 138-144, 4(1) 2019**
- Neighboring Carbonyl Group Assisted Oxyacetoxylation of Propargylic Carboxylates with Retention of Chirality under Metal Free Condition, **Advanced Synthesis & Catalysis, 3605-3611, 361(15) 2019**
- Synthesis and biological evaluation of 1-benzyl-N-(2-(phenylamino)pyridin-3-yl)-1H-1,2,3-triazole-4-carbox amides as antimitotic agents, **Bioorganic Chemistry, 535-548, 83, 2019**
- Transition-Metal-Free One-Pot Tandem Synthesis of 3-Ketoisoquinolines from Aldehydes and Phenacyl Azides, **Journal of Organic Chemistry, 12334-12343, 84(19) 2019**
- Experimental Studies of Dissimilar Metals Welded Joint by FSW, **Proceedings Paper: Materials Today-Proceedings, 3276-3285, 18(Part:7) 2019**
- A Cluster-based Approach for Minimizing Energy Consumption by Reducing Travel Time of Mobile Element in WSN, **International Journal of Computers Communications & Control, 691-709, 14(6) 2019**
- Anti-proliferative and anti-malarial activities of spiroisoxazoline analogues of artemisinin, **Archiv Der Pharmazie, Article Number: e1800192, 352(1) 2019**
- Promotional role of Ceria in CeO2/MgAl2O4 spinel catalysts in CO2 assisted selective oxidative dehydrogenation of ethylbenzene to styrene, **Journal of Industrial and Engineering Chemistry, 97-105, 79, 2019**
- Gold-carbene assisted formation of tetraarylmethane derivatives: double X-H activation by gold, **Organic & Biomolecular Chemistry, 4856-4864, 17(19) 2019**
- Bengamides display potent activity against drug-resistant Mycobacterium tuberculosis, **Scientific Reports, Article Number: 14396, 9, 2019**
- Efficient anti-tumor nano-lipoplexes with unsaturated or saturated lipid induce differential genotoxic effects in mice, **Nanotoxicology, 1161-1175, 13(9) 2019**
- Bombesin conjugated solid lipid nanoparticles for improved delivery of epigallocatechin gallate for breast cancer treatment, **Chemistry and Physics of Lipids, Article Number: UNSP 104770, 224(SI) 2019**
- Styryl quinazolinones and its ethynyl derivatives induce myeloid differentiation, **Bioorganic & Medicinal Chemistry Letters, 2286-2289, 29(16) 2019**
- Effect of Amphiphilic Polymer Modified Graphene Surfactant on the Thermal, Viscoelastic and Tensile Properties of Nitrile Latex Nanocomposites, **Journal of Macromolecular Science Part B-Physics, 489-504, 58(4) 2019**
- Synthesis and biological evaluation of phenyl-amino-pyrimidine and indole/oxindole conjugates as potential BCR-ABL inhibitors, **Medicinal Chemistry Research, 633-645, 28(5) 2019**
- Rahman, Mohammad Ataur; Reddy, N. Mallikarjuna; Yadav, Jhillu Singh; Progress towards the Synthesis of (-)-Ushikulide A: Synthesis of C1-C15 Aliphatic and C17-C31 Spiroketal Fragments by an Aldol Approach, **ChemistrySelect, 4726-4730, 4(16) 2019**
- Synthesis and biological evaluation of 1H-pyrrolo[2,3-d]pyrimidine-1,2,3-triazole derivatives as novel anti-

tubercular agents, **Bioorganic & Medicinal Chemistry Letters, 284-290, 29(2) 2019**

- Protective effect of galangin against dextran sulfate sodium (DSS)-induced ulcerative colitis in Balb/c mice, **Inflammation Research, 691-704, 68(8) 2019**
- Self-Assembled Uniform Silver Nanoparticles (SAAgNPs) and Their Supported MoO3 Nanocatalysts for Effective Degradation of Azo Dyes, **ChemistrySelect, 10770-10776, 4(36) 2019**
- Mesoporous silica-supported copper catalysts for dehydrogenation of biomass-derived 1,4-butanediol to gamma butyrolactone in a continuous process at atmospheric pressure, **Biomass Conversion and Biorefinery, 719-726, 9(4) 2019**
- Copper-Catalyzed Double Friedel-Crafts Alkylation of Tetrahydroquinolines Under Aqueous Conditions: Efficient Synthesis of gem-Diarylacetic Esters, **European Journal of Organic Chemistry, 742-745, (4) 2019**
- BINOL-phosphoric acid catalyzed asymmetric Mannich addition of beta-ketoesters to indolenines generated in situ by DDQ, **Tetrahedron, Article Number: 130620, 75(44) 2019**
- Cu doped ZIF Catalyzed Synthesis of Propargyl Amines with Quaternary Carbon Center Under Solvent Free Conditions, **ChemistrySelect, 9045-9049, 4(31) 2019**
- Simultaneous quantification of nimesulide, phenylpropanolamine, caffeine and chlorpheniramine in rat plasma by RP-HPLC/PDA method and application to pharmacokinetic studies in healthy rat subjects, **Arabian Journal of Chemistry, 2320-2327, 12(8) 2019**
- Synthesis and evaluation of a novel quinoline-triazole analogs for antitubercular properties via molecular hybridization approach, **Bioorganic & Medicinal Chemistry Letters, Article Number: UNSP 126671, 29(20) 2019**
- Regioselective ring expansion followed by H-shift of 3-ylidene oxindoles: a convenient synthesis of N-substituted/un-substituted pyrrolo[2,3-c] quinolines and marinoquinolines, **RSC Advances, 35068-35072, 9(60) 2019**
- Energy Transfer Dynamics of Highly Stable Fe3+ Doped CsPbCl3 Perovskite Nanocrystals with Dual-Color Emission, **Journal of Physical Chemistry C, 17026-17034, 123(27) 2019**
- Non-lethal nitrate supplementation enhances photosystem II efficiency in mixotrophic microalgae towards the synthesis of proteins and lipids, **Bioresource Technology, 373-377, 283, 2019**
- Exploring membrane permeability of Tomatidine to enhance lipid mediated nucleic acid transfections, **Biochimica Et Biophysica Acta-Biomembranes, 327-334, 1861(1) 2019**
- SO3Cu-Carbon: A Novel Heterogeneous Catalyst for the Synthesis of beta-Hydroxy 1,2,3-Triazoles by One Pot Cycloaddition Reaction, **ChemistrySelect, 10133-10142, 4(34) 2019**
- Copper-Catalyzed Oxidative C-H Bond Functionalization of N-Allylbenzamide for Regioselective C-N and C-O Bond Formation, **Chemistry-An Asian Journal, 1448-1451, 14(9) 2019**
- Copper-catalyzed oxidative C-H bond functionalization of N-allylbenzamide for C-N and C-C bond formation, **Tetrahedron Letters, 1437-1440, 60(21) 2019**
- Synthesis and Biological Evaluation of Benzothiazole-piperazine-sulfonamide Conjugates and Their Antibacterial and Antiacetyicho-linesterase Activity, **Letters in Organic Chemistry, 723-734, 16(9) 2019**
- Synthesis of Novel Benzamide- piperazine-sulfonamide Hybrids as Potential Anticancer Agents, **Croatica Chemica Acta, 393-402, 92(3) 2019**
- One pot selective conversion of furfural to gamma-valerolactone over zirconia containing heteropoly tungstate supported on beta-zeolite catalyst, **Molecular Catalysis, 52-59, 466, 2019**
- Effect of Local Anesthetics on the Organization and Dynamics of Hippocampal Membranes: A Fluorescence Approach, **Journal of Physical Chemistry B, 639-647, 123(3) 2019**
- Abundance of d-2-hydroxyglutarate in G2/M is determined by FOXM1 in mutant IDH1-expressing cells, **FEBS Letters, 2177-2193, 593(16) 2019**

- Ru(II)-catalyzed alpha-sulfonamidation of cyclic beta-ketoesters with sulfonyl azides, **Tetrahedron Letters, Article Number: 151083, 60(41) 2019**
- Design and synthesis of DNA-intercalative naphthalimide-benzothiazole/cinnamide derivatives: cytotoxicity evaluation and topoisomerase-II alpha inhibition, **MedChemComm, 72-79, 10(1) 2019**
- Arylcinnamido-propionone conjugates as tubulin polymerization inhibitors and apoptotic inducers, **Arabian Journal of Chemistry, 4740-4755, 12(8) 2019**
- A series of V-shaped small molecule non-fullerene electron acceptors for efficient bulk-heterojunction devices, **Dyes and Pigments, Article Number: UNSP 107677, 171, 2019**
- Triphenylamine-Merocyanine-Based D1-A1-pi-A2/A3-D2 Chromophore System: Synthesis, Optoelectronic, and Theoretical Studies, **International Journal of Molecular Sciences, Article Number: 1621, 20(7) 2019**
- Butterfly architecture of NIR Aza-BODIPY small molecules decorated with phenothiazine or phenoxazine, **Chemical Communications, 12535-12538, 55(83) 2019**
- Chiron approach to fully functionalized cyclohexane frame of (+)-Resiniferatoxin, **Tetrahedron Letters, Article Number: 151133, 60(41) 2019**
- Saliva and urine metabolic profiling reveals altered amino acid and energy metabolism in male farmers exposed to pesticides in Madhya Pradesh State, India, **Chemosphere, 636-644, 226, 2019**
- Glucose starvation-induced oxidative stress causes mitochondrial dysfunction and apoptosis via Prohibitin 1 upregulation in human breast cancer cells, **Free Radical Biology and Medicine, 428-441, 145, 2019**
- A Concise and Stereoselective Total Synthesis of Paecilomycin E, **Natural Product Communications, 131-133, 14(1) 2019**
- Preface, **Catalysis Today, 1-1, 325(Special Issue: SI) 2019**
- Metal-free propargylation/aza-annulation approach to substituted beta-carbolines and evaluation of their photophysical properties, **Organic & Biomolecular Chemistry, 9291-9304, 17(42) 2019**
- [4+2]-Annulation of MBH-Acetates of Acetylenic Aldehydes with Imidazoles/Benzimidazoles To Access Imidazo[1,2-a]pyridines/Benzimidazo[1,2-a]pyridines, **Journal of Organic Chemistry, 9169-9178, 84(14) 2019**
- Total synthesis of pandangolide 1 proposed structure*, **Synthetic Communications, 2709-2716, 49(20) 2019**
- Synthesis of the southern furan segment of furanocembranoids, **Synthetic Communications, 1153-1158, 49(9) 2019**
- Copper-Catalyzed Intramolecular Chalcogenoamination of Enynyl Azides: Synthesis of 5-Selenyl/Sulfenyl Nicotinates, **Organic Letters, 623-626, 21(3) 2019**
- A Facile Approach to 3,4-Oxepino-Fused Tricyclic Indoles from MBH-Acetates of Acetylenic Aldehydes via Successive Allylic Substitution/Intramolecular [3+2] Annulation (dagger), **Chemistry Select, 8229-8232, 4(28) 2019**
- Facile Strategy to Access the Indolo[2,3-a]quinolizidine Framework: Synthetic Study on Tangutorine, **Synthesis-Stuttgart, 3715-3722, 51(19) 2019**
- Synthesis, free radical scavenging and alpha-glucosidase inhibitory activities of 2H-chromenylphenyloxazolones, **Indian Journal of Chemistry Section B-Organic Chemistry including Medicinal Chemistry, 680-690, 58(6) 2019**
- Metallated Macrocyclic Derivatives as a Hole - Transporting Materials for Perovskite Solar Cells, **Chemical Record, 2157-2177, 19(10) 2019**
- Ambient stable, hydrophobic, electrically conductive porphyrin hole-extracting materials for printable perovskite solar cells, **Journal of Materials Chemistry C, 4702-4708, 7(16) 2019**
- Unsymmetrical phenanthro-imidazole/phenothiazine conjugates for optoelectronic applications, **Materials Letters, 384-387, 253, 2019**
- An efficient and green approach: One pot, multi component, reusable catalyzed synthesis of

pyranopyrazoles and investigation of biological assays, **Journal of Saudi Chemical Society, 263-273, 23(3) 2019**

- Total Synthesis of (3R, 4S)-4-Hydroxylasiodiplodin via Ring Closing Metathesis Protocol, **ChemistrySelect, 5345-5347, 4(18) 2019**
- Reddy, K. Nagarjuna; Chary, D. Yogananda; Sridhar, B; Reddy, B. V. Subba; Rh(III)-Catalyzed Tandem Bicyclization of 2-Arylimidazo[1,2-a]pyridines with Cyclic Enones for the Construction of Bridged Scaffolds, **Organic Letters, 8548-8552, 21(21) 2019**
- BINOL Phosphoric Acid-Catalyzed Asymmetric Mannich Reaction of Cyclic N-Acyl Ketimines with Cyclic Enones, **Chemistry-An Asian Journal, 2958-2965, 14(17) 2019**
- Novel Cellularly Active Inhibitor Regresses DDAH1 Induced Prostate Tumor Growth by Restraining Tumor Angiogenesis through Targeting DDAH1/ADMA/NOS Pathway, **ACS Combinatorial Science, 241-256, 21(4) 2019**
- First Stereoselective Total Synthesis of Anti-Inflammatory Metabolite Penicillinolide A, **Synthesis-Stuttgart, 1427-1434, 51(6) 2019**
- First stereoselective total synthesis of antibiotic macrolide Berkeleylactone F, **Tetrahedron Letters, 504-506, 60(6) 2019**
- Gem-Difluorination of Triazole Alkyl Functionalized Amino Pyrazoles by Selectfluor to Access 4,4-Difluoro-pyrazol-3-ones/Pyrazol-3-imines, **European Journal of Organic Chemistry, 2409-2413, (13) 2019**
- Synthesis of Highly Substituted Fluoro Chromenones in a "One-Pot Four-Component Strategy" Using NFSI as a Fluorinating Reagent, **ChemistrySelect, 13768-13771, 4(47) 2019**
- Selective Aerobic Oxidation of Vanillyl Alcohol to Vanillin Catalysed by Nanostructured Ce-Zr-O Solid Solutions, **Catalysis Letters, 533-543, 149(2) 2019**
- Robust Trajectory Tracking in a Reactive Batch Distillation Process using Multirate Nonlinear Internal Model Control, **Industrial & Engineering Chemistry Research, 11364-11381, 58(26) 2019**
- Crafting Carbazole-Based Vorinostat and Tubastatin-A-like Histone Deacetylase (HDAC) Inhibitors with Potent in Vitro and in Vivo Neuroactive Functions, **ACS Omega, 17279-17294, 4(17) 2019**
- Cs2CO3-Mediated Vicinal Thiosulfonylation of 1,1-Dibromo-1-Alkenes with Thiosulfonates: An Expedient Synthesis of (E)-1,2-Thiosulfonylethenes, **Advanced Synthesis & Catalysis, 1587-1591, 361(7) 2019**
- Comprehensive Analysis of Secondary Metabolites in Usnea longissima (Lichenized Ascomycetes, Parmeliaceae) Using UPLC-ESI-QTOF-MS/MS and Pro-Apoptotic Activity of Barbatic Acid, **Molecules, Article Number: 2270, 24(12) 2019**
- Potent and Selective Cytotoxic and Anti-inflammatory Gold(III) Compounds Containing Cyclometalated Phosphine Sulfide Ligands, **Chemistry-A European Journal, 14089-14100, 25(62) 2019**
- Carbonyl Compounds ' Journey to Amide Bond Formation, **Chemistry-An Asian Journal, 344-388, 14(3) 2019**
- Controlled Assembly of a Ternary-Component Photocatalyst: Illustrating the Importance of Interfacial-Integration of Ag-ZnO-rGO in Visible-Light-Induced Catalytic Activity, **ChemistrySelect, 5888-5896, 4(19) 2019**
- Pyrazolo-benzothiazole hybrids: Synthesis, anticancer properties and evaluation of antiangiogenic activity using in vitro VEGFR-2 kinase and in vivo transgenic zebrafish model, **European Journal of Medicinal Chemistry, Article Number: UNSP 111609, 182, 2019**
- Environmentally benign one-pot multicomponent synthesis of 1,4-dihydropyridine derivatives applying montmorillonite K10 as reusable catalyst, **Chemistry of Heterocyclic Compounds, 60-65, 55(1) 2019**
- Strategies towards the synthesis of anti-tuberculosis drugs, **Organic & Biomolecular Chemistry, 5428-5459, 17(22) 2019**
- Excited State Decay Dynamics in 3-Formyl-4-hydroxy Benzoic Acid: Understanding the Global Picture of an ESIPT-Driven Multiple-Emissive Species, **ChemistrySelect, 6702-6712, 4(22) 2019**

- Induction of apoptosis in lung carcinoma cells by antiproliferative cyclic lipopeptides from marine algicolous isolate Bacillus atrophaeus strain AKLSR1, **Process Biochemistry, 142-154, 79, 2019**
- Why Does the Photoluminescence Efficiency Depend on Excitation Energy in Case of a Quantum Dot? A Case Study of CdSe-Based Core/Alloy Shell/Shell Quantum Dots Employing Ultrafast Pump-Probe Spectroscopy and Single Particle Spectroscopy, **Journal of Physical Chemistry C, 6922-6933, 123(11) 2019**
- Chemical, isotopic and amino acid composition of Mukundpura CM2.0 (CM1) chondrite: Evidence of parent body aqueous alteration, **Geoscience Frontiers, 495-504, 10(2) 2019**
- Influence of Solid Solution Formation on the Activity of CeO2 Supported Ni-Cu Mixed Oxide Catalysts in Dry Reforming of Methane, **Catalysis Letters, 2597-2606, 149(9) 2019**
- Analysis of structural, optical and electrical properties of nano-particulate indium doped zinc oxide thin films, **Materials Research Express, Article Number: 1150a6, 6(11) 2019**
- NDI-based small molecules as electron transporting layers in solution-processed planar perovskite solar cells, **Journal of Solid State Chemistry, 51-57, 270, 2019**
- A facile greener synthesis, antimicrobial evaluation and molecular modelling of new 4-aryl-2-(3-(2-(trifluoromethyl) phenyl)-1,8-naphthyridin-2-yl) phthalazin-1(2H)-one derivatives, **Research on Chemical Intermediates, 2007-2022, 45(4) 2019**
- Oxidative coupling of carboxylic acids or benzaldehydes with DMF using hydrotalicite-derived oxide catalysts, **Applied Catalysis B-Environmental, 348-357, 240, 2019**
- One-Pot Synthesis of 3-Sulfenyl/Selenylimidazo[1,5-a]quinolines from 2-Methylquinolines, Aliphatic Amines/Amino Acids, and Dichalcogenides, **European Journal of Organic Chemistry, 6122-6131, 2019(35) 2019**
- Integration of Interfacial and Alloy Effects to Modulate Catalytic Performance of Metal-Organic-Framework-Derived Cu-Pd Nanocrystals toward Hydrogenolysis of 5-Hydroxymethylfurfural, **ACS Sustainable Chemistry & Engineering, 10349-10362, 7(12) 2019**
- Interface Engineering of Graphene-Supported Cu Nanoparticles Encapsulated by Mesoporous Silica for Size-Dependent Catalytic Oxidative Coupling of Aromatic Amines, **ACS Applied Materials & Interfaces, 11722-11735, 11(12) 2019**
- Highly Efficient Direct Synthesis of Scaffold 9a,10,12,12a-Tetrahydrobenzo[b] cyclopenta[f] pyrrolo [1,2-d][1,4] diazepinone by Using Active Phosho molybdic Acid, **Journal of Heterocyclic Chemistry, 1111-1116, 56(3) 2019**
- B(C6F5)(3) catalyzed synthesis of dihydropyrano[3,2-b]chromenediones under solvent-free conditions, **Synthetic Communications, 1143-1152, 49(9) 2019**
- Cyclic Extrusion of Recycled High Density Polyethylene/Banana Fiber/Fly Ash Cenosphere Biocomposites: Thermal and Mechanical Retention Properties, **International Polymer Processing, 47-58, 34(1) 2019**
- TMSOTf-Promoted Synthesis of 4-(2-Aryl or 2-Alkyl-3,6-dihydro-2H-pyran-4-yl)-1,2,3,6-tetrahydropyridine Derivatives, **ChemistrySelect, 3366-3368, 4(12) 2019**
- The base-free van Leusen reaction of cyclic imines on water: synthesis of N-fused imidazo 6,11-dihydro beta-carboline derivatives, **Organic & Biomolecular Chemistry, 5234-5238, 17(21) 2019**
- A systematic surface studies on the glycolipids to understand the surface adsorption behavior, **Colloids and Surfaces A-Physicochemical and Engineering Aspects, 226-236, 563, 2019**
- Synthesis of Benzo[d]imidazo[2,1-b]thiazole-Propenone Conjugates as Cytotoxic and Apoptotic Inducing Agents, **Anti-Cancer Agents in Medicinal Chemistry, 347-355, 19(3) 2019**
- Influences of Structural Modification of Naphthalene diimides with Benzothiazole on Organic Field-Effect Transistor and Non-Fullerene Perovskite Solar Cell Characteristics, **ACS Applied Materials & Interfaces, 44487-44500, 11(47) 2019**

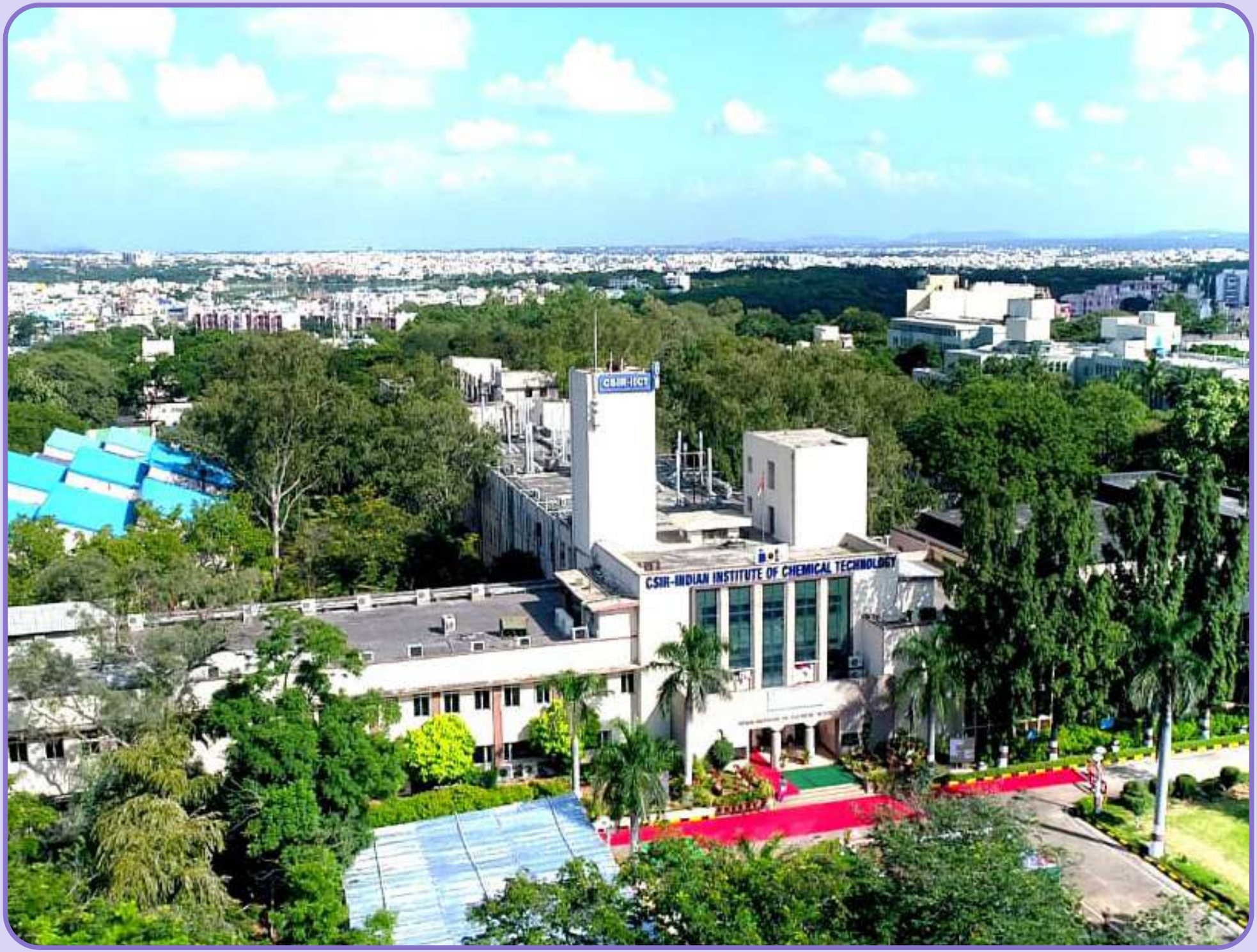
- Identification and structural characterization of the stress degradation products of omeprazole using Q-TOF-LC-ESI-MS/MS and NMR experiments: evaluation of the toxicity of the degradation products, **New Journal of Chemistry, 7294-7306, 43(19) 2019**
- Metal-Free, One-Pot Oxidative Triple Functionalization of Azaarenes with Methyl Arenes Mediated by Molecular Iodine/TBHP: Synthesis of N-Benzylated Iodo(iso) quinolinones, **Asian Journal of Organic Chemistry, 2162-2171, 8(11) 2019**
- Design, Synthesis and Biological Evaluation of Substituted (1-(4-chlorobenzyl)-1H-indol-3-yl) 1H-(1,2,3-triazol-4-yl) methanones as Antifungal Agents, **ChemistrySelect, 2258-2266, 4(8) 2019**
- Design, synthesis, and antimicrobial evaluation of 1,4-dihydroindeno[1,2-c]pyrazole tethered carbohydrazide hybrids: exploring their in silico ADMET, ergosterol inhibition and ROS inducing potential, **MedChemComm, 806-813, 10(5) 2019**
- Synthesis of new triazole fused imidazo[2,1-b]thiazole hybrids with emphasis on Staphylococcus aureus virulence factors, **Bioorganic & Medicinal Chemistry Letters, Article Number: UNSP 126621, 29(19) 2019**
- The search for the "next" euphoric non-fentanil novel synthetic opioids on the illicit drugs market: current status and horizon scanning, **Forensic Toxicology, 1-16, 37(1) 2019**
- Fixing Transient Iodine on Developed Latent Fingermarks, **Journal of Forensic Sciences, 1859-1866, 64(6) 2019**
- The deglycase activity of DJ-1 mitigates alpha-synuclein glycation and aggregation in dopaminergic cells: Role of oxidative stress mediated downregulation of DJ-1 in Parkinson's disease, **Free Radical Biology and Medicine, 28-37, 135, 2019**
- A multi-component reaction for the synthesis of pyrido [1,2-b] isoquinoline derivatives via the [3+2] cycloaddition reaction between alkynes and in situ generated isoquinolinium ylides, **Organic & Biomolecular Chemistry, 4121-4128, 17(16) 2019**
- Base-Catalyzed Tandem Cyclization: Diastereoselective Access to the 3,4-Dihydroisoquinolin-2(1H)-one Core, **Synthesis-Stuttgart, 1473-1481, 51(6) 2019**
- Acid-Catalyzed Four-Component Tandem Double Cyclization: Access to Dihydroindolizino[8,7-b]indoles, **ChemistrySelect, 8550-8553, 4(29) 2019**
- Porous Organic Polymer-Driven Evolution of High-Performance Cobalt Phosphide Hybrid Nanosheets as Vanillin Hydrodeoxygenation Catalyst, **ACS Applied Materials & Interfaces, 24140-24153, 11(27) 2019**
- Synthesis and anti-microbial activity of 2H-chromenylmethylene benzohydrazides, **Indian Journal of Chemistry Section B-Organic Chemistry including Medicinal Chemistry, 497-503, 58(4) 2019**
- Reactions in Water - A Greener Approach Using Ruthenium Catalysts, **Chemical Record, 1935-1951, 19(9) 2019**
- Discovery of certain benzyl/phenethyl thiazolidinone-indole hybrids as potential anti-proliferative agents: Synthesis, molecular modeling and tubulin polymerization inhibition study, **Bioorganic Chemistry, Article Number: UNSP 103188, 92, 2019**
- New Porous High Surface Area, TiO2 Anatase/SAPO-35 Mild Bronsted Acidic Nanocomposite: Synthesis, Characterization and Studies on it's Enhanced Photocatalytic Activity, **ChemistrySelect, 9135-9142, 4(31) 2019**
- **Proceedings Paper:** Molecular Weight Control in Semi Batch Copolymerization Reactor through Temperature Tracking: Evaluation of Control Strategies, **2019 Fifth Indian Control Conference (ICC), 213-218, 2019**
- Noble metal-free integrated UiO-66-PANI-Co3O4 catalyst for visible-light-induced H-2 production, **Chemical Communications, 14494-14497, 55(96) 2019**
- An innovative in situ method of creating hybrid dendrimer nano-assembly: An efficient next generation dendritic platform for drug delivery, **Nanomedicine-Nanotechnology Biology and Medicine, Article Number: 102043, 21, 2019**

- A General Carbazole Synthesis via Stitching of Indole-Ynones with Nitromethanes: Application to Total Synthesis of Carbazomycin A, Calothrixin B, and Staurosporinone, **Organic Letters, 3372-3376, 21(9) 2019**
- Benzannulation of arynes with dimethylacetonedi carboxylates via an insertion-fragmentation-Dieckman-aromatization cascade: Expeditious entry to naphthoresorcinols and binaphthoresorcinols, **Tetrahedron, 2923-2932, 75(21) 2019**
- Rhodamine functionalized mesoporous silica as a chemosensor for the efficient sensing of Al3+, Cr3+ and Fe3+ ions and their removal from aqueous media, **New Journal of Chemistry, 15563-15574, 43(39) 2019**
- Understanding the glucose tolerance of an archaeon beta-glucosidase from Thermococcus sp., **Carbohydrate Research, Article Number: UNSP 107835, 486, 2019**
- Energy level tuning of 'Z'-shaped small molecular non-fullerene electron acceptors based on a dipyrrolo[2,3-b:2',3'-e]pyrazine-2,6(1H,5H)-dione acceptor unit for organic photovoltaic applications: a joint experimental and DFT investigation on the effect of fluorination, **New Journal of Chemistry, 5173-5186, 43(13) 2019**
- The effects of carbonized Eucalyptus globulus leaves on castor seed oil based urethane coating system, **Progress in Organic Coatings, 42-48, 131, 2019**
- Secophragmalin-Type Limonoids from Trichilia connaroides: Isolation, Semisynthesis, and Their Cytotoxic Activities, **Journal of Natural Products, 2731-2743, 82(10) 2019**
- Multifunctional polyurethane coatings derived from phosphated cardanol and undecylenic acid based polyols, **Progress in Organic Coatings, 91-102, 134, 2019**
- Cink4T, a quinazolinone-based dual inhibitor of Cdk4 and tubulin polymerization, identified via ligand-based virtual screening, for efficient anticancer therapy, **European Journal of Medicinal Chemistry, 115-132, 165, 2019**
- **Review:** Developmental trends in CO2 methanation using various catalysts, **Catalysis Science & Technology, 4478-4504, 9(17) 2019**
- Synthesis, antiproliferative and apoptosis induction potential activities of novel bis(indolyl) hydrazide-hydrazone derivatives, **Bioorganic & Medicinal Chemistry, 1043-1055, 27(6) 2019**
- Oxidative sp(3) C-H Functionalization of Methyl Substituted Aza-Aromatics: An Easy Access to N-Fused Polyheterocycles, **European Journal of Organic Chemistry, 6800-6806, 2019(40) 2019**
- Iron-Catalyzed Minisci Type Acetylation of N-Heteroarenes Mediated by CH(OEt)(3)/TBHP, **European Journal of Organic Chemistry, 1815-1819, (8) 2019**
- Efficient Synthesis and Antimicrobial Activity of 2-Pyridyl-4-thiazolidinones from 2-Chloro Nicotinaldehydes, **Iranian Journal of Chemistry & Chemical Engineering-International English Edition, 97-105, 38(3) 2019**
- Raphanus sativus (Linn.) fresh juice priming moderates sucrose-induced postprandial glycemia as well as postprandial glycemic excursion in rats, **Indian Journal of Traditional Knowledge, 339-345, 18(2) 2019**
- An Integrated Continuous Flow Micro-Total Ultrafast Process System (mu-TUFPS) for the Synthesis of Celecoxib and Other Cyclooxygenase Inhibitors, **Organic Process Research & Development, 1892-1899, 23(9) 2019**
- Zinc Dependent Histone Deacetylase Inhibitors in Cancer Therapeutics: Recent Update, **Current Medicinal Chemistry, 7212-7280, 26(40) 2019**
- Synthesis of 2-anilinopyridyl linked benzothiazole hydrazones as apoptosis inducing cytotoxic agents, **New Journal of Chemistry, 7150-7161, 43(18) 2019**
- Synthesis and Anticancer Activity of Oxadiazole Incorporated Ellipticine Derivatives, **Russian Journal of General Chemistry, 505-510, 89(3) 2019**
- New indolo carbazole-based non-fullerene n-type semiconductors for organic solar cell applications, **Journal of Materials Chemistry C, 543-552, 7(3) 2019**

- Impact of end groups on the performance of non-fullerene acceptors for organic solar cell applications, **Journal of Materials Chemistry A, 22701-22729, 7(40) 2019**
- A gold-catalyzed facile intramolecular rearrangement and cyclization sequence for synthesis of 2,5-dihydrofurans, **Organic & Biomolecular Chemistry, 6015-6024, 17(24) 2019**
- Synthesis and biological evaluation of new bisindole-imidazopyridine hybrids as apoptosis inducers, **Bioorganic Chemistry, 484-494, 87, 2019**
- Ipomeolides A and B, Resin Glycosides from Ipomoea pes-caprae and Combination Therapy of Ipomeolide A with Doxorubicin, **Journal of Natural Products, 1292-1300, 82(5) 2019**
- g-C3N4-Mediated Synthesis of Cu2O To Obtain Porous Composites with Improved Visible Light Photocatalytic Degradation of Organic Dyes, **ACS Omega, 17301-17316, 4(17) 2019**
- A Facile One Pot Synthesis of Cu2O@TiO2: A Nanocomposite Catalyst for Enhanced Visible Light Driven Photocatalysis, **ChemistrySelect, 2249-2257, 4(8) 2019**
- Synthesis of alpha-Fluoroamides with a C-F Quaternary Stereogenic Center by Electrophilic Fluorination: One-Pot Four-Component Strategy, **European Journal of Organic Chemistry, 3654-3657, (22) 2019**
- Panchromatic sensitization of new terpyridine ligated thiocyanate-free Ru-complex, **Solar Energy, 305-311, 188, 2019**
- Synthesis, characterization and antimicrobial evaluation of ferrocene-oxime ether benzyl 1H-1,2,3-triazole hybrids, **New Journal of Chemistry, 8341-8351, 43(21) 2019**
- Intumescent Phosphorus and Triazole-Based Flame-Retardant Polyurethane Foams from Castor Oil, **ACS Omega, 1086-1094, 4(1) 2019**
- Stereoselective synthesis of marine macrolide Aspergillide D, **Arkivoc, 307-318, (Part:5) 2019**
- A 9.16% Power Conversion Efficiency Organic Solar Cell with a Porphyrin Conjugated Polymer Using a Nonfullerene Acceptor, **ACS Applied Materials & Interfaces, 28078-28087, 11(31) 2019**
- Controlled addition of Cu/Zn in hierarchical CuO/ZnO p-n heterojunction photocatalyst for high photoreduction of CO2 to MeOH, **Journal of Co2 Utilization, 207-214, 31, 2019**
- Ni-Doped CsPbBr3 Perovskite: Synthesis of Highly Stable Nanocubes, **Langmuir, 17150-17155, 35(52) 2019**
- One-pot regioselective synthesis of substituted pyrazoles and isoxazoles in PEG-400/water medium by Cu-free nano-Pd catalyzed sequential acyl Sonogashira coupling-intramolecular cyclization, **Catalysis Science & Technology, 6471-6481, 9(22) 2019**
- Studies on Epoxidised Castor Oil as Co-Plasticizer with Epoxidised Soyabean Oil for PVC Processing, **Journal of Renewable Materials, 775-785, 7(8) 2019**
- Stereoselective Desymmetrization of Cyclohexa dienone-Tethered Enones: Efficient Access to Highly Strained Polycyclic Indoles, **ACS Catalysis, 10012-10019, 9(11) 2019**
- Dianiline conjugated Schiff base molecule: Electrical and electrochemical properties, **Synthetic Metals, 240-247, 247, 2019**
- Synthesis of star shaped electroactive, LEB state aniline oligomer and its high performing Pt and Pt-Au nanocatalyst for MOR, **International Journal of Hydrogen Energy, 11066-11078, 44(21) 2019**
- DBU-Mediated Synthesis of Aryl Acetylenes or 1-Bromoethynylarenes from Aldehydes, **Advanced Synthesis & Catalysis, 611-616, 361(3) 2019**
- New dithienosilole- and dithienogermole- based BODIPY for solar cell applications, **New Journal of Chemistry, 8735-8740, 43(22) 2019**
- Tetrathiafulvalene Scaffold-Based Sensitizer on Hierarchical Porous TiO2: Efficient Light-Harvesting Material for Hydrogen Production, **Journal of Physical Chemistry C, 70-81, 123(1) 2019**

- **Letter:** Indian scientific research and Indian research journals, **Current Science, 173-173, 117(2) 2019**
- **Editorial Material:** The Antioxidant Paradox, **Pharmacognosy Magazine, 173-175, 15(64) 2019**
- In vitro and in vivo investigation of metabolic fate of riociguat by HPLC-Q-TOF/MS/MS and in silico evaluation of the metabolites by ADMET predictor (TM), **Journal of Pharmaceutical and Biomedical Analysis, 326-336, 164, 2019**
- New method of synthesis of hierarchical mordenite of high crystallinity and its application in hydroizomerization of benzene-n-heptane mixture, **Journal of Porous Materials, 995-1004, 26(4) 2019**
- Corticosteroids protect infected cells against mycobacterial killing in vitro, **Biochemical and Biophysical Research Communications, 117-121, 511(1) 2019**
- Mycobacterium tuberculosis virulence inhibitors discovered by Mycobacterium marinum high-throughput screening, **Scientific Reports, Article Number: 26, 9, 2019**
- Modulating the site-specific oral delivery of sorafenib using sugar-grafted nanoparticles for hepatocellular carcinoma treatment, **European Journal of Pharmaceutical Sciences, Article Number: UNSP 104978, 137, 2019**
- Gold- catalysed regioselective cascade cycloisomerisation reactions of aza- enediynes for the synthesis of substituted benzoisoquinoline derivatives, **Organic & Biomolecular Chemistry, 369-373, 17(2) 2019**
- High-performance supercapacitor coin cell: polyaniline and nitrogen, sulfur-doped activated carbon electrodes in aqueous electrolyte, **Journal of Solid State Electrochemistry, 295-306, 23(1) 2019**
- Polyaniline nanofibers and porous Ni[OH](2) sheets coated carbon fabric for high performance super capacitor, **Journal of Applied Polymer Science, Article Number: 48042, 136(41) 2019**
- 3-(2-(5-Amino-3-aryl-1H-pyrazol-1-yl) thiazol-4-yl)-2H-chromen-2-ones as Potential Anticancer Agents: Synthesis, Anticancer Activity Evaluation and Molecular Docking Studies, **ChemistrySelect, 4324-4330, 4(14) 2019**
- Ultrafiltration membrane assisted cost effective ionizer for production of therapeutic alkaline ionized water, **Journal of Water Process Engineering, Article Number: 100951, 32, 2019**
- Alpinoid c analog inhibits angiogenesis and induces apoptosis in COLO205 cell line, **Chemico-Biological Interactions, 1-10, 308, 2019**
- Synthesis and Cytotoxic Studies of Undecenoic Acid-based Schiff's Base Derivatives Bearing 1,2,4-Triazole Moiety, **Indian Journal of Pharmaceutical Sciences, 737-746, 81(4) 2019**
- Bimolecular photoinduced electron transfer between 7-methylbenzo [a] pyrene and aromatic amine donors in stationary and static regimes, **Journal of Photochemistry and Photobiology A-Chemistry, 212-223, 376, 2019**
- Excited-State Quenching of Porphyrins by Hydrogen-Bonded Phenol-Pyridine Pair: Evidence of Proton-Coupled Electron Transfer, **Journal of Physical Chemistry C, 23342-23351, 123(38) 2019**
- Design and synthesis of novel sulphamide tethered quinazolinone hybrids as potential antitumor agents, **Journal of Molecular Structure, 403-411, 1181, 2019**
- Total synthesis of (+/-)-galanthamine from GABA through regioselective aryne insertion, **Organic & Biomolecular Chemistry, 2192-2198, 17(8) 2019**
- An effective performance of F-Doped hexagonal boron nitride nanosheets as cathode material in magnesium battery, **Materials Chemistry and Physics, 356-361, 226, 2019**
- Electroanalytical characterization of F-doped MoS2 cathode material for rechargeable magnesium battery, **Functional Materials Letters, Article Number: 1950041, 12(3) 2019**

- Synthesis, cytotoxic evaluation of substituted cinnamic-based 1,2,4-triazolo thiadiazoles, **Indian Journal of Chemistry Section B-Organic Chemistry including Medicinal Chemistry, 475-481, 58(4) 2019**
- Construction of metal oxide decorated g-C3N4 materials with enhanced photocatalytic performance under visible light irradiation, **Journal of Chemical Sciences, Article Number: UNSP 13, 131(2) 2019**
- Magnetic and antimicrobial properties of cobalt-zinc ferrite nanoparticles synthesized by citrate-gel method, **International Journal of Applied Ceramic Technology, 1944-1953, 16(5) 2019**
- C- C coupling at a zeolite- supported Rh.I) complex. DFT search for the mechanism, **Catalysis Science & Technology, 2781-2793, 9(11) 2019**
- Supramolecular super-helix formation via self-assembly of naphthalene diimide functionalised with bile acid derivatives, **Scientific Reports, Article Number: 12825, 9, 2019**
- Synthesis of 3-keto-quinolines from enaminones, anilines and DMSO: Transition metal free one pot cascade, **Tetrahedron, 4024-4030, 75(30) 2019**
- An all-small-molecule organic solar cell derived from naphthalimide for solution-processed high-efficiency nonfullerene acceptors, **Journal of Materials Chemistry C, 709-717, 7(3) 2019**
- First Stereoselective Total Synthesis of (3S,7R)-De-O-methylbotryosphaeriodiplodin, **Natural Product Communications, 135-140, 14(1) 2019**
- 1,2,3-Triazole derivatives of 3-ferrocenylidene-2-oxindole: Synthesis, characterization, electrochemical and antimicrobial evaluation, **Applied Organometallic Chemistry, Article Number: e4817, 33(4) 2019**
- Cu-doped zeolitic imidazolate framework catalysed highly selective conversion of alkynes to -keto and vinyl sulfones using sodium sulfinates, **Journal of Chemical Sciences, Article Number: UNSP 8, 131(1) 2019**
- Synthesis of solandelactone F, constanolactone A and an advanced intermediate towards solandelactone E from a common synthetic intermediate, **Organic & Biomolecular Chemistry, 4572-4592, 17(18) 2019**
- Formal total synthesis of mandelalide A, **Journal of Chemical Sciences, Article Number: UNSP 25, 131(3) 2019**
- 2-Mercapto Benzthiazole Coupled Benzyl Triazoles as New COX-2 Inhibitors: Design, Synthesis, Biological Testing and Molecular Modeling Studies, **ChemistrySelect, 11081-11092, 4(37) 2019**
- Olefin metathesis of fatty acids and vegetable oils, **Journal of Chemical Sciences, Article Number: UNSP 39, 131(5) 2019**
- Modified conductive polyaniline-carbon nanotube composite electrodes for bioelectricity generation and waste remediation, **Bioresource Technology, 148-154, 284, 2019**
- Tri-phasic engineered wetland system for effective treatment of azo dye-based wastewater, **NPJ Clean Water, Article No:13, 2, 2019**


CSIR-IICT
CSIR-INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY

सी एस आई आर – भारतीय रासायनिक प्रौद्योगिकी संस्थान
CSIR-INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY

Ministry of Science & Technology, Govt. of India, Tarnaka, Hyderabad - 500 007, Ph : 040-27193719, 27193030

Compiled, Edited & Produced by : Department of Knowledge & Information Management on behalf of Director, CSIR-IICT

Assisted by the Biennial Report Committee

www.iict.res.in www.facebook.com/iictindia