CSIR-IICT

दैवार्षिक प्रतिवेदन
Biennial Report
2020-2022

CSIR
The Innovation Engine of India

सीएसआईआर - आईआईसीटी
CSIR - IICT
जीवन स्पर्शी
Touching Lives

सीएसआईआर – भारतीय रासायनिक प्रौद्योगिकी संस्थान
CSIR-INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY
(Council of Scientific & Industrial Research)
HYDERABAD - 500 007.
www.iict.res.in

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 the expertise in chemistry and chemical technology, the Institute provides solutions to challenges faced by Industry, Government Departments and Entrepreneurs through basic and applied research, and process development. The institute is internationally recognized for the contributions to chemistry research and is an ideal place for taking ideas to commercialization through state of the art research and development.

THE VISION

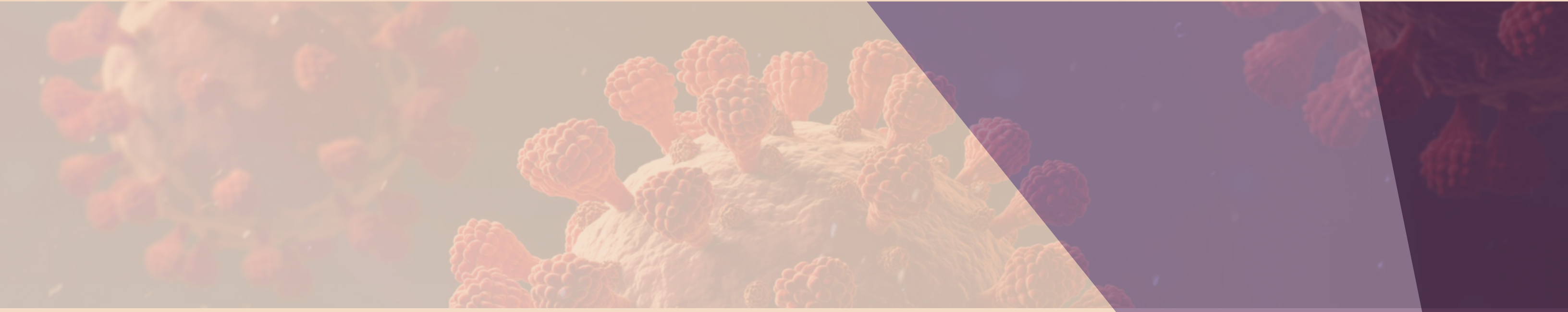
To serve society by creating an outstanding knowledge base in chemistry and chemical technology

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



Contents

प्रस्तावना

मुझे वर्ष 2020-2022 की अवधि की संस्थान की अनुसंधान एवं विकास गतिविधियों की द्विवार्षिक रिपोर्ट प्रस्तुत करते हुए प्रसन्नता हो रही है। इस अवधि के दौरान प्रमुख फोकस सार्स-सीओवी-2 वायरस के प्रभाव को सीमित करने के साधनों का विकास था। वैज्ञानिकों, कर्मचारियों और छात्रों ने स्थानीय रूप से उपलब्ध मुख्य प्रारंभिक सामग्री के साथ कम समय में फ़ेविपिरविर और रेमेडिसविर जैसी नई दवाओं के लिए नई प्रक्रियाओं को विकसित करने के लिए लगातार काम किया। विकसित प्रौद्योगिकी को उद्योग को स्थानांतरित कर दिया गया जिससे दवाओं की समय पर आपूर्ति हो सके। मुझे यह बताते हुए गर्व की अनुभूति हो रही है कि इस अवधि के दौरान हमें लगातार दो सीएसआईआर प्रौद्योगिकी पुरस्कार प्राप्त हुए। यूमिफेनोविर, बालोक्साविर और क्लोरोक्वीन/हाइड्रोक्सीक्लोरोक्वीन के लिए नए प्रक्रिया पद्धति की पहचान की गई। कोविड-19 के खिलाफ भारत का पहला स्वदेशी टीका कोवैक्सीन में एक सह-औषध के रूप में उपयोग किए जाने वाले टीएलआर 7/8 एगोनिस्ट मॉलिक्यूल (आईएमडीजी) के संश्लेषण के लिए प्रक्रिया प्रौद्योगिकी भारत बायोटेक इंटरनेशनल लिमिटेड (बीबीआईएल) को स्थानांतरित की गयी। संस्थान ने मनुष्यों और पशुओं के लिए स्वदेशी, किफायती स्वास्थ्य देखभाल के साधनों का समर्थन करने के लिए जैव चिकित्सा विज्ञान और टीकों के लिए अनूठा मंच प्रौद्योगिकी के विकास हेतु सहयोग के लिए एक मास्टर सहयोगात्मक करार किया।

किफायती, बहुस्तरीय, हाइड्रोफोबिक "साँस" फेस मास्क के लिए प्रौद्योगिकी विकसित की गई। हैंड सैनिटाइज़र तैयार किए गए और अग्रिम पंक्ति के कोविड योद्धाओं को वितरित किए गए, और हमारे वैज्ञानिकों ने संचार के विभिन्न तरीकों के माध्यम से वायरस के प्रसार को सीमित करने के लिए एहतियाती उपायों से आम जन को अवगत कराया। एजीआर तकनीक पर आधारित बोइनपल्ली बाजार प्रांगण में 10 टन/दिन के बायोगैस संयंत्र की सफलता की कहानी का माननीय प्रधान मंत्री श्री नरेंद्र मोदी जी ने अपने 'मन की बात' में उल्लेख किया। प्रक्रिया विकास और कृषि-रसायनों के विस्तार के लिए एक अत्याधुनिक सुविधा आचार्य पी सी रे किलो लैब राष्ट्र को समर्पित की गई, जो आत्मनिर्भर भारत की दिशा में एक कदम है।

हमने विजन इंडिया 2047 की मेजबानी की, जो एक अनूठा और अपनी तरह का पहला साइंस लीडर कॉन्क्लेव है, जिसने देश के विभिन्न शोध संस्थानों के 160 निदेशकों को आत्मनिर्भर भारत 2047 की दिशा में एक रोड मैप तैयार करने के लिए एक साथ लाया। कई शैक्षणिक संस्थानों और विश्वविद्यालयों के साथ सहयोगात्मक अनुसंधान के लिए समझौता ज्ञापन पर हस्ताक्षर किए गए। इस अवधि में संस्थान ने 72 प्रायोजित, 36 कंसल्टेंसी और 15 सहयोगी परियोजनाएं शुरू की।

मैं संस्थान के अनुसंधान परिषद और प्रबंधन परिषद के अध्यक्ष और सदस्यों को उनके बहुमूल्य मार्गदर्शन के लिए धन्यवाद देता हूँ।

(श्रीवारी चंद्रशेखर)

FOREWORD

I am pleased to present the Biennial Report of the Research and Development activities of the institute for the period 2020-2022. Major focus during the period was development of solutions to limit the effect of SARS-CoV-2 virus. Scientists, staff and students worked continuously to develop new processes for repurposed drugs such as Favipiravir and Remdesivir in a short period of time with locally available key starting materials. The technologies developed were transferred to industry ensuing timely delivery of the drugs. I am proud to state that two CSIR Technology Awards were received in consecutive years during this period. New process routes were identified for Umifenovir, Baloxavir and Chloroquine/Hydroxycloroquine. The process technology for the synthesis of TLR 7/8 agonist molecule (IMDG), used as an adjuvant in Covaxin, India's first indigenous vaccine against COVID-19 was transferred to Bharat Biotech International Ltd (BBIL). The institute entered into a Master Collaborative Agreement to collaborate on the development of novel platform technologies for Bio Therapeutics and vaccines to support the indigenous, affordable health care solutions for humans and animals.

The technology for affordable, multi-layered, hydrophobic "SaaNs" face masks was developed. Hand sanitizers were prepared and distributed to frontline COVID warriors, and our scientists through various modes of communication reached out to people on precautionary measures to limit the virus spread. The success story of a 10 ton/day biogas plant at Bowenpally market yard, based on AGR technology received a special mention from Honourable Prime Minister, Shri Narendra Modi Ji in Mann Ki Baat. Acharya P C Ray Kilo Lab, a state-of-the-art facility for process development and scale up of agro-chemicals was dedicated to the nation, another step towards Atma Nirbhar Bharat.

We hosted the Vision India 2047, a unique and first of its kind Science Leaders Conclave, that brought together 160 Directors of various Research institutions in the country to draw a road map towards Atma Nirbhar Bharat 2047. MoUs for collaborative research with several academic institutions and universities have been signed. The institute in the period undertook 72 sponsored, 36 consultancy and 15 collaborative projects.

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

(Srivari Chandrasekhar)

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Member Secretary

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Director
CSIR- IICT
Hyderabad

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Scientist,
CSIR-IICT

Dr S Prabhakar
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CSIR-IICT

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Chief Scientist,
CSIR-IICT

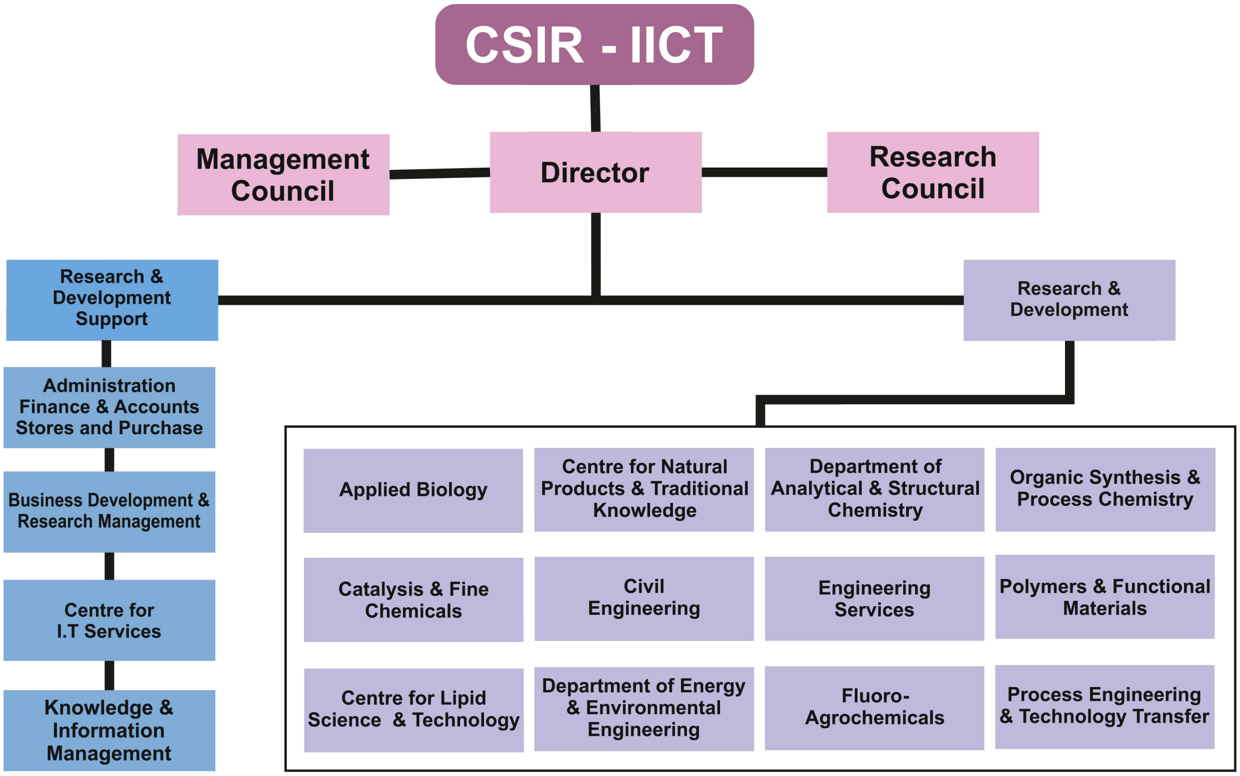
Dr. Anandavalli
Director, CSIR-SERC, Chennai

COFA / FA
CSIR-IICT, Hyderabad

Member-Secretary
COA/AO, CSIR-IICT

Research Council Meeting in Progress

ORGANISATIONAL STRUCTURE OF CSIR-IICT



RESEARCH ORIENTATION

FOCUSED RESEARCH AREAS

Adequate Clean Energy

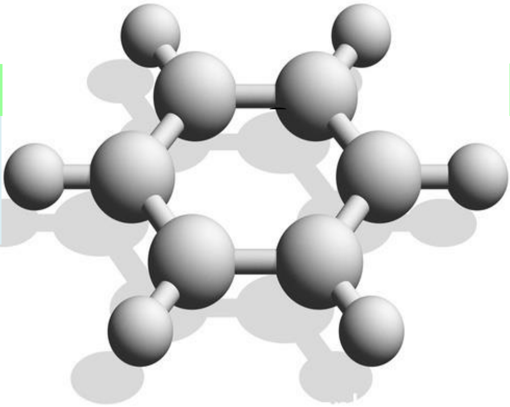
- Solar & Energy Materials
- Direct Coal Liquefaction
- Coal Gasification
- Carbon sequestration
- Biomass to energy
- Photobiological processes

Affordable Health Care

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

Environment

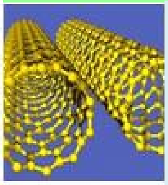
- Sustainable technologies
- Biohydrogen
- Waste utilization
- Biodigestors



Sustainable Chemistry

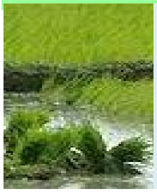
- Specialty Chemicals
- Fluorine Chemicals
- Membrane separations
- Biocatalysts
- Process Safety
- Process Intensification

Advanced Materials

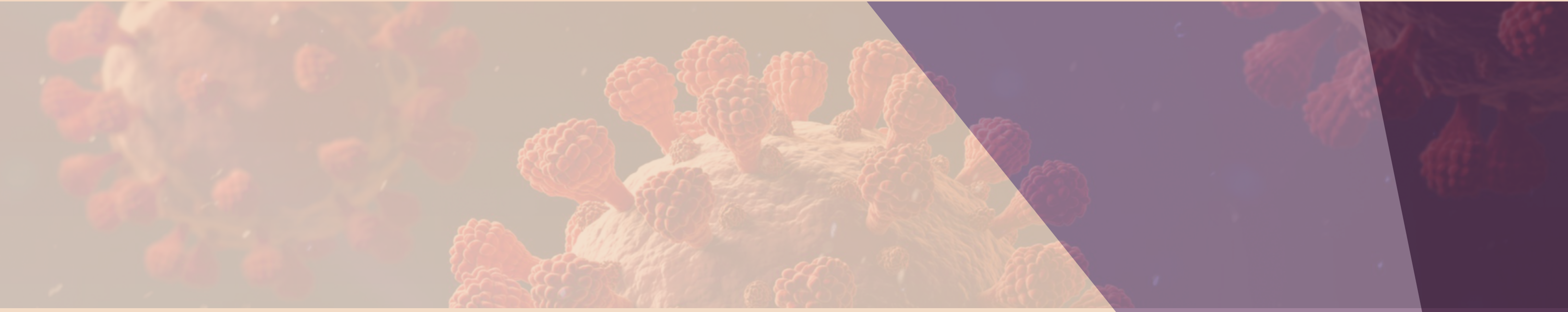


- Micro/nano materials for smart and intelligent coatings
- Stimuli responsive materials
- Graphene materials
- Photo functional materials

Agriculture, Food & Nutrition

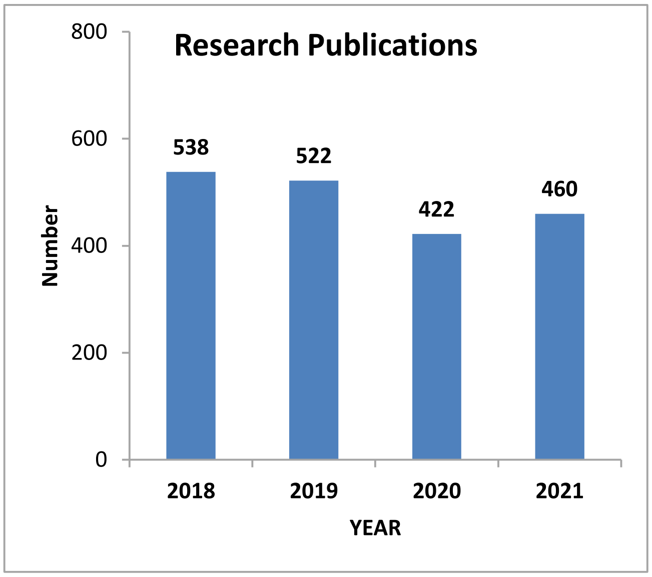


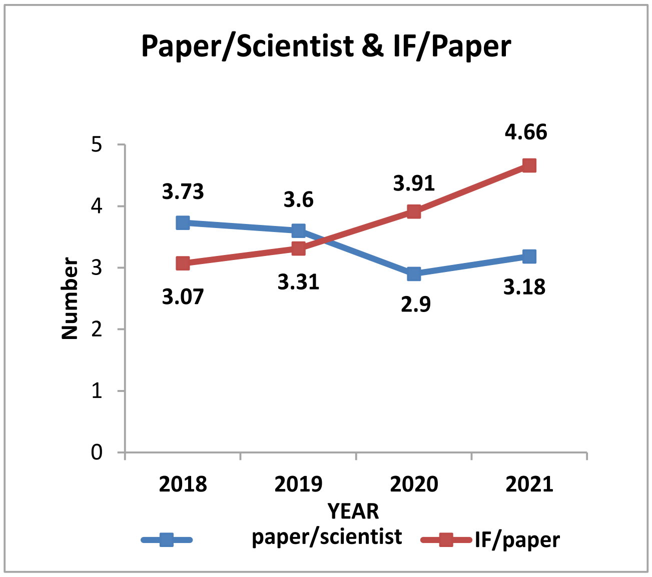
- Processes for edible non-edible oils
- Natural & synthetic Agrochemicals
- Plant volatiles
- Pheromone application

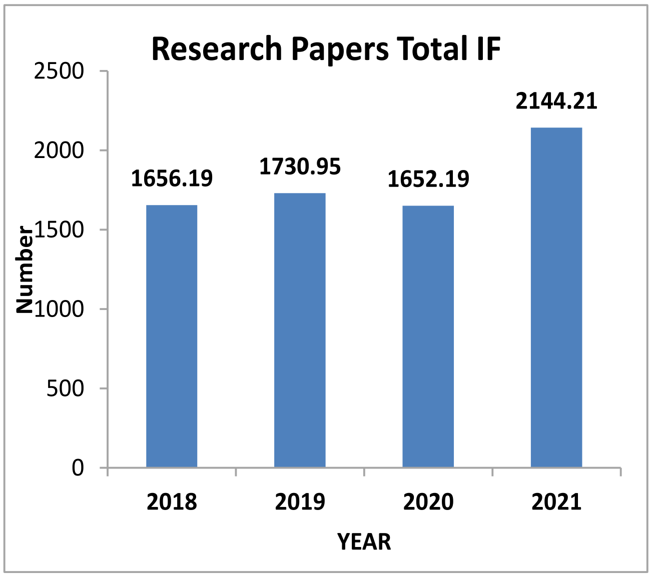


R & D
OUTPUTS

R & D OUTPUTS


Research Publications


Paper/Scientist & IF/Paper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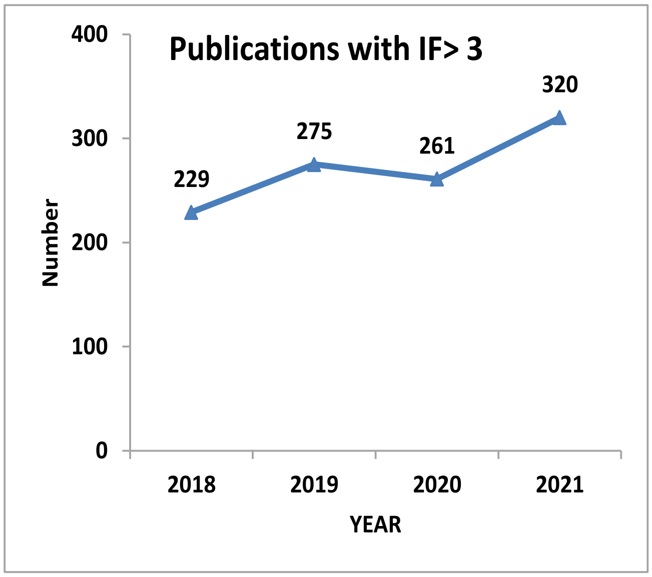
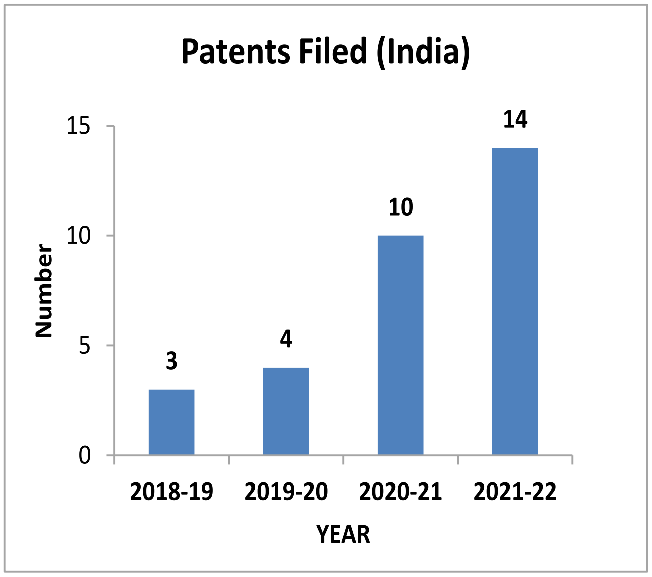

Publications with IF> 3

R & D OUTPUTS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5
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15
2018-19
2019-20
2020-21
2021-22
3
4
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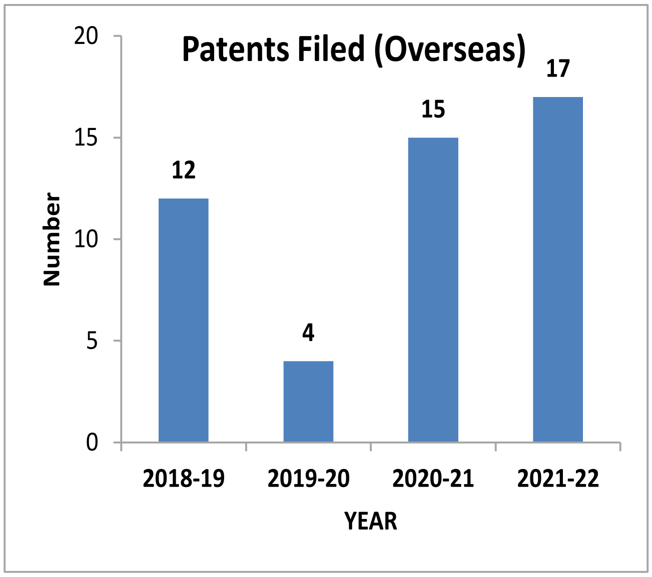
14


Patents Filed (Overseas)
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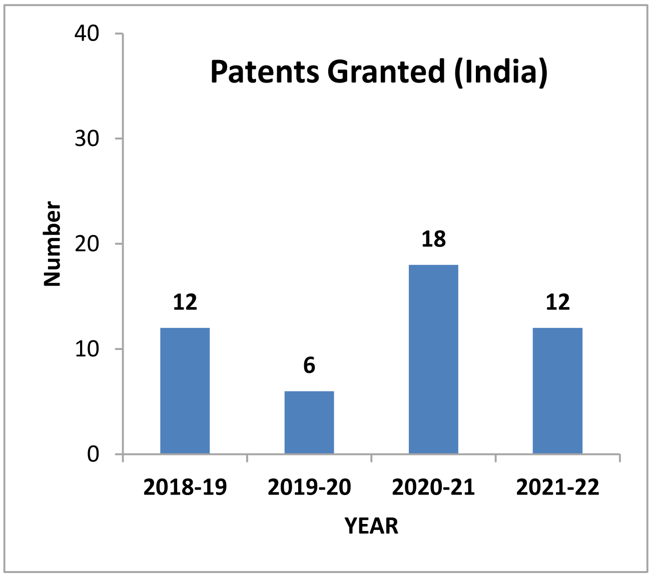
Patents Granted (India)
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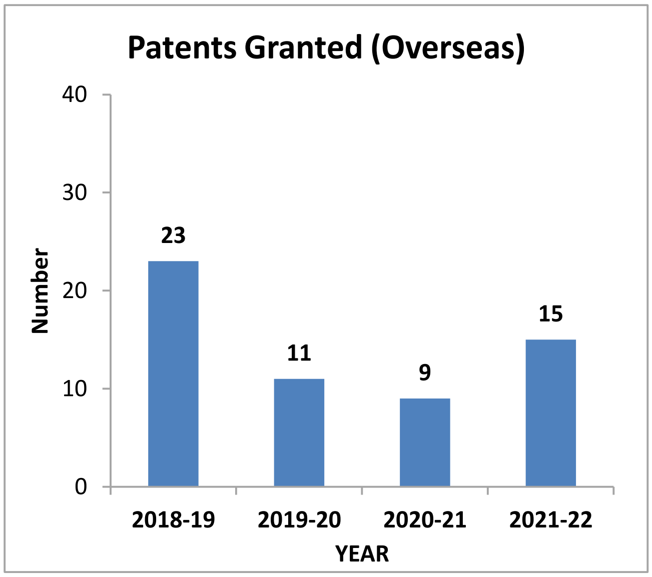
Patents Granted (Overseas)
Number
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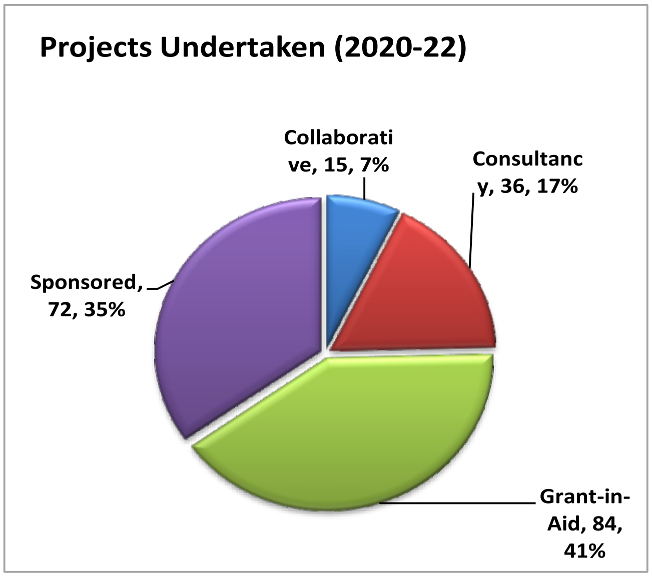
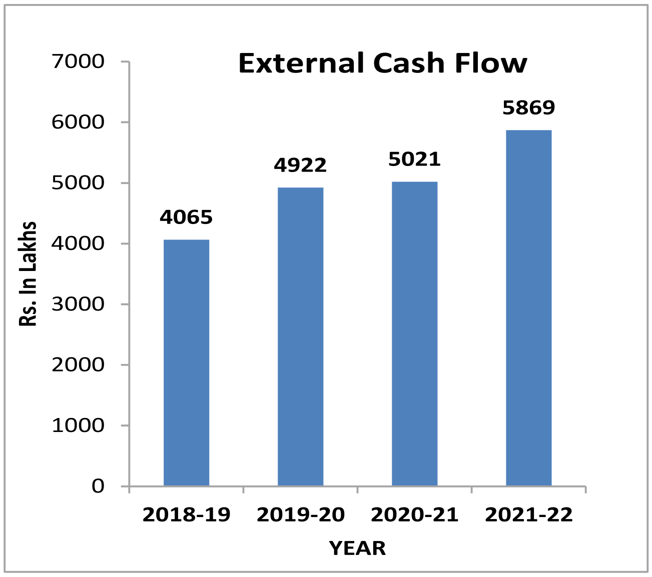
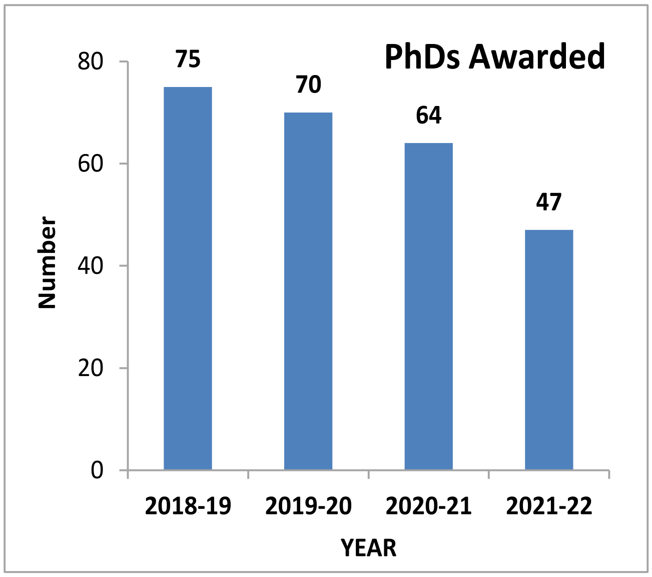
R & D OUTPUTS

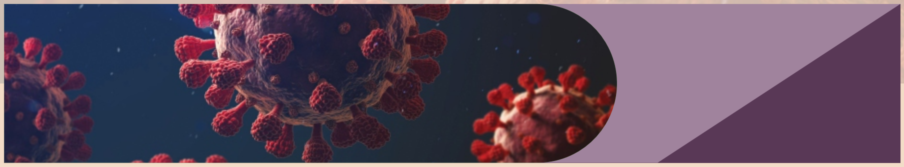




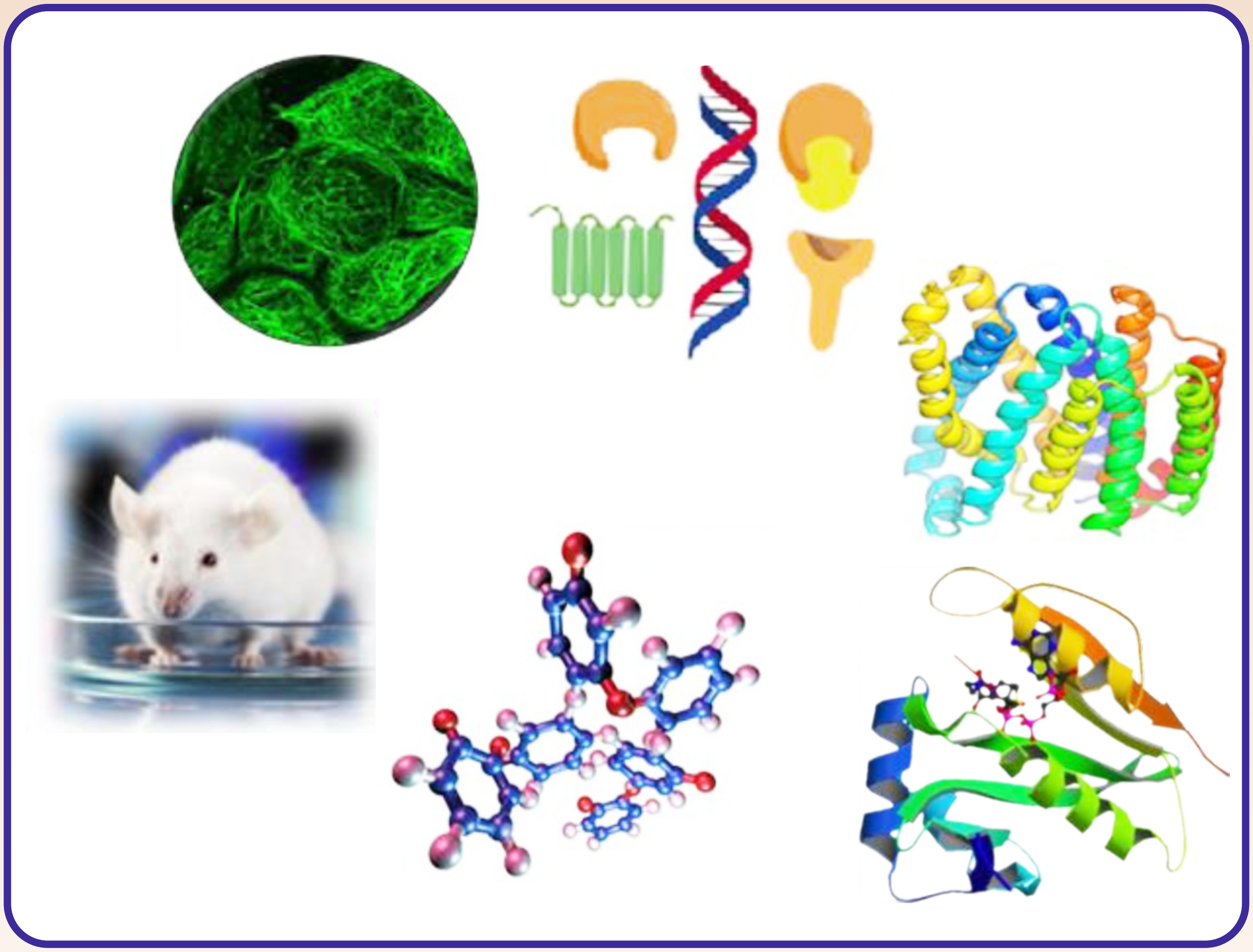
Human Resource Base		
	2020-21	2021-22
TOTAL STAFF		
***Total S & T Staff**	**479**	**467**
Scientist (Group-IV)	143	157
Technical (Group-III)	96	90
Technical (Group-II & I)	122	116
*** Total Administrative & Non-Technical**	118	104
*** Research Scholars/Assts.**		
NPDF/SPA etc...	16	34
SRF/JRF	64	76
Project Associate	39	138



R & D
PERFORMANCE



APPLIED BIOLOGY



APPLIED BIOLOGY

BASIC RESEARCH

Cancer Research

Methoxy-Enriched Cationic Stilbenes as Anticancer Therapeutics

A series of methoxylated stilbene-based cationic molecules have been developed. Through SAR study, a lead candidate has been identified that showed selective anticancer effect against cancer cells and exhibited unique self-associating property that allowed additional drug, withaferin to be encapsulated. These strategies allowed to add if not synergize anticancer activity through ROS generation, apoptosis and autophagy in cervical cancer cells (*Bioorg. Chem*.,**2020**, 98, 103719)

sp^3-Rich Glycyrrhetinic Acid Analogues using Late-Stage Functionalization as Potential Breast Tumor Regressing Agents

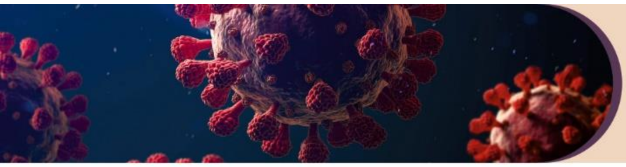
Late-stage functionalization (LSF) aids drug discovery efforts by introducing functional groups onto C-H bonds on pre-existing skeletons. We adopted the LSF strategy to synthesize analogues of the abundantly available triterpenoid, glycyrrhetinic acid (GA), by introducing aryl groups in the A-ring, expanding the Aring and selectively activating one methyl group of the gem-dimethyl groups. Intriguingly, two compounds were found to preferentially accumulate in the mitochondrial compartment of MDA-MB-231 breast cancer cells, to cause depolarization of mitochondrial membrane potential and to induce antiproliferative and anti-invasive effects through enhanced mitochondrial superoxide production with parallel depletion of GSH levels. Furthermore, intraperitoneal administration of these two compounds, in comparison with GA, greatly regressed breast tumor growth and metastasis in a SCID mouse model bearing labelled MDA-MB-231 cells. (*Chem. Med. Chem*.,**2020**, 15, 1826-1833)

Autophagy as an Alternate Therapeutic Option in Pancreatic Cancer

The autophagy modulation driven by the small molecule fluorinated thiazolidinol (FTZ), the underlying mechanism, and regulation of critical sentinels of oncogenic signaling in pancreatic cancer cells were examined. FTZ triggered autophagic cell death in pancreatic cancer cells, independent of apoptosis as evidenced by an increase in cytoplasmic vacuoles formation, autophagy flux, LC3-II expression, and p62 degradation was identified. The *in vivo* data revealed significant regression of tumors by FTZ in nude mice model. Overall, this study demonstrates that FTZ induces autophagic cell death in pancreatic cancer cells independent of apoptosis, which is accompanied by AMPK activation and suppression of critical sentinels of oncogenic signaling in pancreatic cancer cells. (*Chemico-Biol. Interactions*, **2021**, 343, 109433)

Quisinostat Mediated Autophagy is Associated with Differentiation in Neuroblastoma SK-N-SH Cells

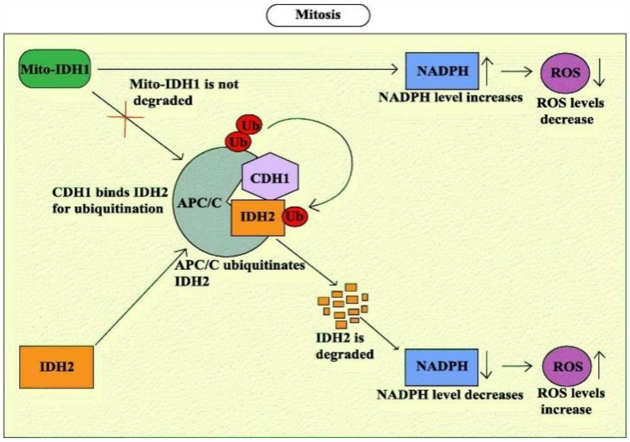
The response of NB cells to the second-generation histone deacetylase inhibitor (HDACi) JNJ-26481585(JNJ) and the lysosomotropic agent, Chloroquine (CQ) alone and upon JNJ/CQ treatment as a plausible therapeutic was explored. It was identified that while JNJ alone induced autophagy in NB cells, JNJ/CQ treatment decreased the viability and proliferation of NB cells *in vitro* by switching from autophagy to apoptosis. Further, it was found that autophagy inhibition by CQ pre-treatment led to the generation of ROS and a decrease in the mitochondrial membrane potential (MMP) that subsequently caused caspase-3-mediated apoptotic cell death in NB cells. It was observed that autophagy plays an important role in JNJ induced cell differentiation of SK-N-SH cells. It was demonstrated that autophagy is induced upon JNJ treatment and is



important for the neuronal differentiation of human SK-N-SH cells. (*Mol. Biol. Reports*, **2021**, 48, 4973–4979)

Mutant IDH2 Ubiquitination in Cancers

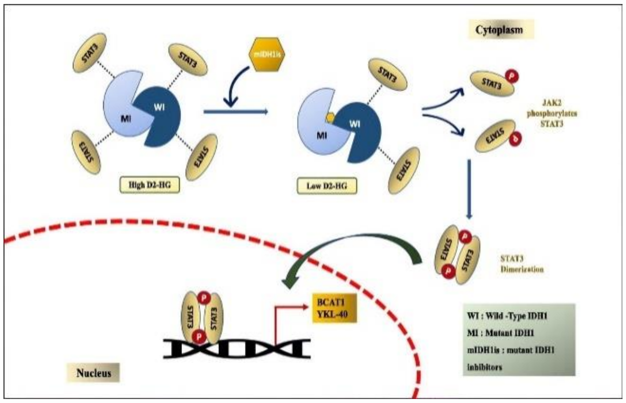
In a hypothesis, IDH2, a major NADPH-producing enzyme in mitochondria, was ubiquitinated for reactive oxygen species (ROS) to increase in mitosis. It was established that IDH2 is ubiquitinated in mitosis and on inhibiting anaphase-promoting complex/Cyclosome (APC/C) IDH2 was stabilized. It was observed that overexpressing APC/C coactivator CDH1 decreased IDH2, whereas depleting CDH1 decreased IDH2 ubiquitination. Overexpressing mitochondria-targeted-IDH1 decreased ROS by increasing NADPH in IDH2 ubiquitinated cells. APC/C CDH1 ubiquitinates IDH2, a major NADPH-producing enzyme in mitochondria contributing to ROS increase in mitosis. (*Cell Signal*, **2021,** 86, 110087)



APC/C CDH1 degrades mutant IDH2 in mitosis leading to ROS increase

Drug Resistance to Mutant IDH1 Inhibitors

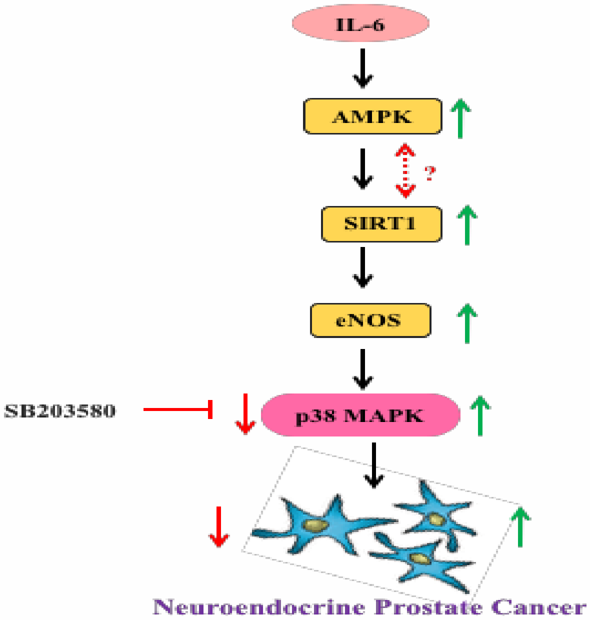
Allosteric mutant IDH1 inhibitors were used to treat mutant IDH1-expressing HT1080 cells, and examined for activation of oncogenes by assessing the levels of our read-outs: BCAT1 and YKL-40. It was found that mutant IDH1 inhibitors' treatments increased BCAT1 and YKL-40 levels in HT1080 cells. Upon examining the molecular mechanism of pSTAT3-Y705 activation in mutant IDH1 inhibitor-treated cells, it was found that mutant IDH1 strongly bound STAT3, but mutant IDH1 inhibitor treatment decreased mutant IDH1-STAT3 binding. Furthermore, it was observed that STAT3-knockdown and pharmacological inhibition of STAT3 attenuated the mutant IDH1 inhibitor-mediated increase in BCAT1 and YKL-40 levels, whereas STAT3 overexpression and Interleukin-6 (STAT3 activator) treatments increased BCAT1 and YKL-40 levels. The mutant IDH1 inhibitors activate the oncogenic transcription factor-STAT3 leading to an increase in BCAT1 and YKL-40 levels in mutant IDH1-expressing cells. (*Biochim. Biophys. Acta: Mol. Cell Res.*, **2021**, 1868, 119114)



Mutant IDH1 inhibitors activates STAT3 to increase BCAT1 and YKL40 in mutant IDH1 expressing cells

Neuroendocrine Prostate Cancer (NEPC)

The proteins and/or pathways involved in NED of LNCaP cells induced by IL-6 was investigated and charaterized their role in NED of PCa cells. Remarkably, IL-6 induces NED of LNCaP cells through activation of AMPK and SIRT1 and also both of these are co-regulated while playing a predominant role in NED of LNCaP cells. Pleiotropic effects of NO ultimately regulate p38MAPK in IL-6 induced NED. IL-6 induced AMPK-SIRT1 activation transfers its activation signals through p38MAPK for advancing NED of LNCaP cells. Moreover, inactivation of p38MAPK with specific inhibitor (SB203580) attenuated IL-6 induced NED of LNCaP cells. Therefore, IL-6 promotes NED of PCa cells *via* AMPK/SIRT1/p38MAPK signaling. Finally, targeting AMPK-SIRT1 or p38MAPK in androgen independent PC3 cells with neuroendocrine features reversed their neuroendocrine characteristics. (*Biochim. Biophys. Acta. Mol Cell Res*.,**2021,** 1868, 119085)



Model of IL-6 induced NED in PCa cells. IL-6 induces NED of PCa cells by activation of AMPK/SIRT1-NOsignaling that eventually transfers IL-6 activation signals through p38MAPK for advancing NED of PCa cells

Investigation on the Anticancer Activity of Symmetric and Unsymmetric Cyclic Sulfamides

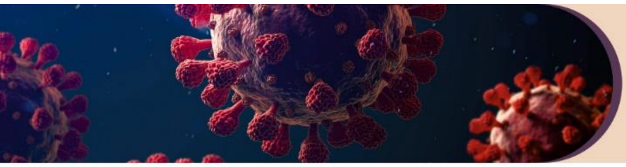
The study describes synthesis of 7- membered symmetric and asymmetric sulfamide compounds and their biological evaluation through the National Cancer Institute (NCI) panel of 60 human tumor cell lines (NCI-60) and the mechanism of action study. The results exhibited that many synthesized cyclic sulfamide compounds inhibited breast cancer (MDA-MB-468). The mechanism of action study of a representative compound 18 showed the inhibition of proliferation and apoptosis in A549 lung cancer cells. (*ACS Med Chem Lett*., **2021**,12, 202-210)

TWIST1-Mediated Transcriptional Activation of PDGFRβ in Breast Cancer Stem Cells Promotes Tumorigenesis and Metastasis

The present study reported that TWIST1, an EMT-TF, exhibits positive transcriptional regulation on the PDGFRβ promoter, thus identifying PDGFRβ as one of the downstream targets of EMT regulation in breast CSCs. Breast cancer cells overexpressing PDGFRβ exhibited a significant increase in physiological and molecular properties comparable to that of breast CSCs, while molecular silencing of PDGFRβ in breast CSCs perturbed these phenomena. Orthotopicxenograft transplantation of stable breast cancer cells and CSCs with PDGFRβ overexpression in nude mice led to a significant increase in tumorigenesis, and metastasis to the lung and liver. The study shows significant increase in human gene-specific PDGFRβ and CD44expression, and colocalization along with an expression of human-specific Alu sequences which were perturbed with stable silencing of PDGFRβ in breast CSCs. (*BBA Mol Basis of Dis*, **2021**, 1867, 166141)

Activation of CD44-Lipoprotein Lipase Axis in Breast Cancer Stem Cells Promotes tumorigenesis:

The study observed high CD44 expression in advanced-stage clinical breast tumor samples. CD44 activation in breast CSCs sorted from various triple-negative breast cancer (TNBC) cell lines induced proliferation, migration, invasion, and mammosphere formation that was reversed in presence of inhibitor, 4-methyl umbelliferone, or CD44 silencing. CD44 activation in breast CSCs induced Src,Akt, and nuclear translocation of pSTAT3. PCR arrays revealed differential expression of a metabolic gene, Lipoprotein lipase (LPL), and transcription factor, SNAI3. Differential transcriptional regulation of LPL by pSTAT3 and SNAI3 was confirmed by promoter-reporter and chromatin immunoprecipitation analysis. Orthotopicxenograft murine breast tumor model revealed high tumorigenicity of CD24-/CD44+-breast CSCs as compared with CD24+-breast cancer cells. Furthermore, stable breast CSCs-CD44 shRNA and/or intratumoral administration of Tetrahydrolipstatin (LPL inhibitor) abrogated tumor progression and neoangiogenesis. (*BBA Mol Basis of Dis*, **2021**, 1867, 166228)



SNAI1-Mediated Transcriptional Regulation of Epithelial-to-Mesenchymal Transition Genes in Breast Cancer Stem Cells

In-silico analysis of microarray data from luminal, Her2+, and TNBC cell lines was performed and identified 15 relatively unexplored EMT-related differentially expressed genes (DEGs) along with the markedly high expression of EMT-transcription factor (EMT-TF), SNAI1. Interestingly, stable overexpression of SNAI1 in MCF-7 induced the expression of DEGs along with increased migration, invasion, and in vitro tumorigenesis that was comparable to TNBCs. Next, stable SNAI1 overexpression led to increased expression of DEGs that was reverted with SNAI1 silencing in both breast cancer cells and CSCs sorted from various TNBC cell lines. The SNAI1-mediated activation of breast CSC phenotypes was perturbed by inhibition of downstream target, MMPs using Ilomastat. The molecular investigation for the gene regulatory framework in the present study identified MMPs, as a downstream effector in the SNAI1-mediated EMT regulation. (*Cell Signal,* **2021**, 87, 110151)

Multiple Myeloma: Multiple myeloma (MM) is a malignant neoplasm of B-cells characterized by the uncontrolled proliferation of plasma cells in the bone marrow. Despite the advancements in MM treatment, it has a poor prognosis with a median survival of 3-5 years. CD38 has been one of the key therapeutic targets for MM, due to its high expression in MM cells. Therefore, novel compounds targeting CD38 with low toxicity are warranted for improved MM therapy. Biochanin A (BCA) is an isoflavone reported to exhibit anticancer activity against a wide range of solid cancers but has not been tested against MM. Here we report for the first time that BCA has a strong anticancer activity against MM cell-lines compared to LND. BCA treatment induced apoptosis in MM cells and showed reduced cytokine levels. In-addition, BCA significantly reduced the CD38 population and cancer stem-cell markers in dose dependent manner. Consistently, we observed BCA treatment significantly reduced the stemness markers and invasion capability of cells. Mechanistic characterization revealed that BCA anti-cancer activities are exerted by modulating the NF-κB and MAPK signalling pathways. Overall, this study enlightens the application of BCA as a novel treatment modality for multiple myeloma with superior efficacy and reduced toxicity.

Oral Cancer: This project mainly focused on establishing the drug resistance cell lines, and isolation of primary cancer cell lines/organoid cultures to re-capitulate in-vivo conditions using oral cancer tissue organoid/sphere system (OCTO/S) for a prediction of lead molecule (against drug resistance cancer) success in oral cancer clinical trials. In this study we have generated 4 drug resistance cell lines, using SCC09 and Cal-27 oral cancer cell lines and two primary derived cell lines were also generated. Taken together, these studies helped us to develop an in-vitro model to screen novel drugs against drug-resistant cancers. Screening for flavonoid based anti-cancer agents using primary organoids and drug resistant cell line derived sphere system definitely give us proper results to precede further. Primary organoids represent an excellent preclinical model for human tumors, establishing PDX models will be a better tool, combining, this study promoting the translation research from basic cancer research to clinical practice.

Cardiovascular Research

Cloning and *in vivo* Metabolizing Activity Study of CYP3A4 on Amiodarone Drug Residues

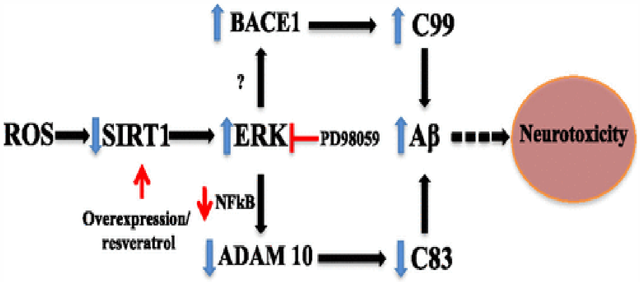
A possible probiotic and therapeutic option: The study intended to improve the activity of CYP3A4 *in silico*, and develop a recombinant *Saccharomyces cerevisiae* strain with probiotic and therapeutic properties overexpressing CYP3A4 for elimination or degradation of the left-over drug residues of amiodarone, which cause harmful effects in human beings. *Saccharomyces cerevisiae* strain was successfully utilized for expressing *in silico* improved human Cytochrome P4503A4. The *in vitro* and *in vivo* studies performed using recombinant probiotic yeast revealed the degradation of leftover drug residues of amiodarone. Further, recovery of organ damage was observed, as evident from the histopathological studies of the animal model indicating the plausible therapeutic and probiotic potential of the recombinant *S. cerevisiae* strain overexpressing the improved CYP3A4. (*Biomed. Pharmacother*., 2020, 127, 110128 – 1101137)

Neurobiology Research

Natural Product, Embelin, Confers Protection Against MPTP-Induced Dysfunction in Mitochondrial Bioenergetics and Biogenesis - Implications for Parkinson's Disease

Mitochondrial dysfunction, reduced complex-I and PGC1α levels were found to correlate with the pathology of Parkinson's disease (PD). The studies indicate that embelin protects from MPP+ -induced oxidative stress and apoptosis in a time and dose-dependent manner in N27 dopaminergic cells. Cells treated with embelin exhibited increased levels of pAMPK, SIRT1 and PGC1α leading to enhanced mitochondrial biogenesis. Though treatment of cells with MPP+ also increased pAMPK levels, but, SIRT1 and PGC1α levels decreased substantially. The mitochondrial uncoupling effects of embelin leading to increased NAD/NADH levels followed by enhanced SIRT1, PGC1α and mitochondrial biogenesis were found to confer embelin mediated protection as treatment of cells with SIRT1 inhibitor or siRNA nullified this effect. Embelin (10 mg/kg) also conferred protection *in vivo* in MPTP mouse model of PD, wherein, MPTP-induced loss of TH staining reduced striatal dopamine and markers of mitochondrial biogenesis pathway were averted by embelin. (*Biochim Biophys Acta Bioenerg*., **2020**, 1861, 148157 – 148170)

Extracellular-Signal-Regulated Kinase Inhibition Switches App Processing from β- to α-Secretase Under Oxidative Stress: Modulation of ADAM10 by SIRT1/NF-κB Signalling: It was demonstrated that pharmacological inhibition of mitogen-activated protein kinase/extracellular-signal-regulated kinase (MAPK/ERK) by mitogen-activated protein kinase kinase-1 (MEK-1) inhibitor (PD98059) restored the expression of a disintegrin and metalloproteinase 10 (ADAM10) with a concomitant decrease in β-site APP cleavage enzyme 1 (BACE1) under oxidative stress. Silent mating-type information regulation 2 homologue 1 (SIRT1) activation by resveratrol also mitigated alterations in secretase levels through MAPK/ERK signalling. Intracerebroventricular (ICV) administration of streptozotocin in rats showed amyloidogenic processing of APP and altered the SIRT1/ERK axis in the hippocampus. Bioinformatics analysis revealed the presence of putative nuclear factor kappa B (NF-κB) binding sites in the ADAM10 promoter region. Treatment of cortical neurons with the NF-κB inhibitor (Bay 11-7082) mitigated the transcriptional upregulation of ADAM10 by PD98059. (*ACS Chemical Neurosci*, **2021**, 12, 4175-4186)

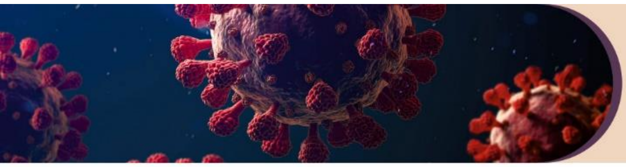


Scheme representing the plausible role of ERK-MAP kinase in regulating the generation of amyloid beta peptide

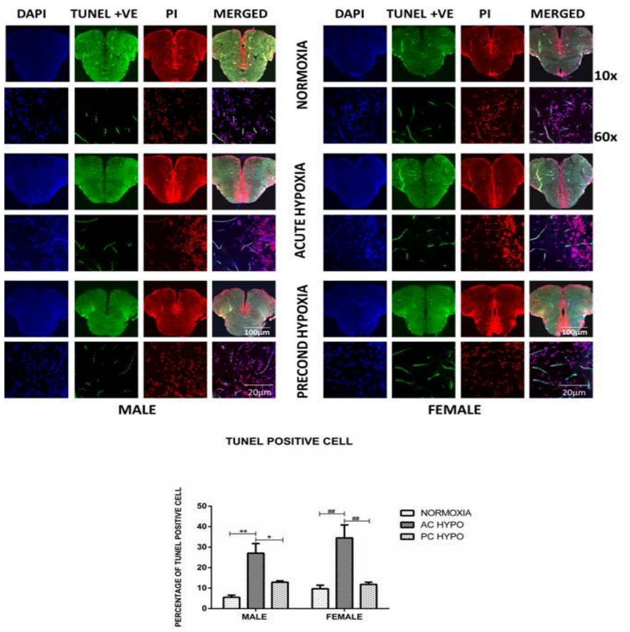
Neuropsychiatric and Neurologic Disorders

The use of a cost-effective neuro disease vertebrate model (zebra fish) including sex difference for better understanding of the disease mechanism and in identifying new drugs is reported.

Hypoxia leads to debilitating disease in infants via birth asphyxia and cerebral palsy, whereas in adults via heart attack and stroke. A natural protective phenomenon termed 'hypoxic preconditioning' (PH) occurs when prior exposures to hypoxia eventually result in robust hypoxia resistance. Accordingly, a novel model of hypoxic preconditioning in adult



zebrafish to mimic the tolerance of mini stroke(s) in human before any major stroke event was developed. The data indicate female zebra fish brains are more protected against the severity of acute hypoxia when exposed to the hypoxic preconditioning indicating differential signalling across the sexes (*Mol Neurobiol*.,**2020** 57, 5177-5192)



Sex-specific analysis of DNA damage protection in preconditioning hypoxia. TUNEL representative confocal images of zebrafish brain sections. Upper panel images in each group (× 10, bar = 100 µm), lower panel images in each group (× 60, bar = 20 µm) (a). Bar graph indicates percentage of TUNEL-positive cells (b), n = 15. p< 0.0001, *AHM/AHF vs NM/NF and #PHM/PHF vs NM/NF

Epigenetic regulators of the JMJD2/KDM4 family of lysine demethylases, in particular JMJD2D, appear to be critical mediators of the chronic stress effects on the neurogenesis in the chronic stress-induced depression mouse model. This study might help in strategizing the therapeutic approach to treat disorders like anxiety and depression. (*Brain Sci.*, **2020**, 10, 833)

Antidepressant potential of vorinostat (VOR) against chronic social defeat stress (CSDS) in mice was explored. Development of resilience vs. defeat to CSDS was found to be associated with the differential nuclear levels of GR, HDAC3 and HDAC6 in the hippocampus. (*Psychoneuroendocrinology*, **2021**,124, 105083 – 105093)

Changes in hippocampal gene expression in the phenytoin-resistant pentylenetetrazol (PTZ)-kindled mouse model of epilepsy was studied. Micro array data showed differential expression of genes involved in cholesterol biosynthesis in phenytoin-resistant and sensitive mice (*Neuromolecular Med*., **2021**, 23, 485-490)

Using a chronic unpredictable stress (CUS) paradigm, the characterization of an array of mood disorder phenotypes in adult zebra fish was achieved to evaluate the predictive validity of the model. Proteomic approach showed molecules that regulate neural progenitor cell proliferation or neurogenesis are crucially involved in chronic stress-induced mood disorders by affecting the circuitry which controls emotion and reward. (*PharmacolBiochemBehav*.,**2021**, 204,173170 - 173183).

The study aimed to find the effects of glucosamine in a recently developed, clinical condition mimicking mouse model of internal cerebral artery occlusion. The cumulative results confirming neuro protective, antineuro inflammatory, and proneurogenic effects of glucosamine enhance drug repurposing potential of glucosamine in cerebral ischemia. (*NeuroMolecular Med*., **2021,** 27)

Additionally, we also contributed for the studies in developing treatment strategies for limb ischemia since it is a severe type of peripheral artery disease occurs due to an inadequate supply of blood to limb extremities using limb ischemic model. Our data showed that theses treatment could ameliorate ischemia in rats at a faster rate by promoting therapeutic angiogenesis to the ischemic sites and offers an option of nanomedicine in limb ischemia as an alternative approach (Biomed Mater., **2021,** 16, 1-13). We have also reported for the first time that pro-angiogenic nanomaterials like zinc oxide nanoflowers (ZONF) exhibit neuritogenic activity and thereby improved neurobehavior and enhanced synaptic plasticity of neurons in cerebral ischemia rat model (Bioconjugate Chem. **2020**, 31(3):895-906).

Similarly, we also contributed in evaluating the efficacy of two more nanoparticles; PEGylated platinum nanoparticles for the treatment of melanoma [Mater SciEng C Mater Biol Appl. 2020, 108:110375] and Silver Prussian Blue Analogue Nanoparticles for Multifunctional Applications (ACS Biomater. Sci. Eng. **2020**, 6, 690−704).

Stem Cells and Regenerative Medicine

Cxcr6-based Mesenchymal Stem Cell Gene Therapy Potentiates Skin Regeneration in Murine Diabetic Wounds

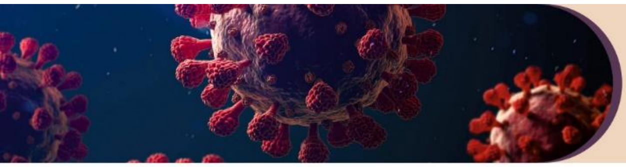
An increased expression of chemokine ligand, CXCL16 in the wound bed and its cognate receptor, CXCR6 on murine bone marrow-derived Mesenchymal stem cells (MSCs) suggested a putative therapeutic relevance of exogenous MSC transplantation therapy. Intravenous transplantation of allogenic stable MSCs with CXCR6 gene therapy potentiated skin tissue regeneration by increased recruitment, engraftment (A) as well as neovascularization (B), and re-epithelialization (C) at the wound site in excisional splinting wounds of type I and II diabetic mice. This study suggests that activation of the CXCL16-CXCR6 axis in bioengineered MSCs with CXCR6 overexpression provides a promising therapeutic approach for the treatment of diabetic wounds. (*Mol. Ther.*, ***2020***, 28, 1314-1326)

Programmed Endothelial Cell Transplantation Potentiates Neovascularization-Mediated Diabetic Wound Tissue Regeneration

To enrich the endothelial progenitor cell (EPC) repertoire from non-endothelial precursors, abundantly available mesenchymal stromal cells (MSCs) were reprogrammed into induced-endothelial cells (iECs). The study identified cell signaling molecular targets by meta-analysis of microarray datasets. BMP-2 induction leads to the expression of inhibitory Smad6/7-dependent negative transcriptional regulation of ID1, rendering the latter's reduced binding to TWIST1 during trans-differentiation of WJ-MSC into iEC. An increased or decreased co-localization of GFP with KDR/SFRP4 and CD31 in the regenerated diabetic wound bed with TWIST1 overexpression or silencing (piLenti-TWIST1-shRNA-GFP), respectively further confirmed improved neovascularization. (*Diabetes*, **2020**, 69, 1232-1247)

Infectious Diseases

Antioxidant and Biological Activities of Novel Structured Monoacylglycerol Derivatives with Phenolic Acids. Phenolic lipids are a diversified group of compounds derived from phenolic compounds grafted on to lipid moiety especially acyl glycerols or fatty acids. Phenolic lipids consist of both phenolic and lipidic natures making them amphiphilic molecules with diverse physico-chemical properties. Novel structured monoacylglycerol (MAG)-based phenolic lipids are synthesized from11-bromoundecanoic acid, phenolic acids, and solketal. Selected phenolic acids namely 4-hydroxy benzoic, vanillic, syringic, cinnamic, p-coumaric, sinapic, 4-fluorocinnamic, 4-hydroxyphenyl acetic acid, 3-(4-hydroxyphenyl) propanoic and dihydrocaffeic acids are employed for the synthesis of ten novel MAG-based phenolic lipids. The synthesized phenolic lipids are characterized by FT-IR, NMR, and mass spectra analysis. All the compounds were evaluated for antioxidant, antimicrobial, and cytotoxic activities. MAG derivative 8g of sinapic acid exhibited excellent antioxidant activity in both DPPH assay and inhibition of lipid oxidation assay. MAG derivative 8f bearing p-coumaric acid showed good antimicrobial activity against both Gram-positive and Gram-negative bacterial strains with a minimum inhibitory concentration (MIC) value of 6.25 μmmL−1. All the synthesized compounds were found to exhibit cytotoxicity against B16,



DU145, and CHO cell lines, while sinapic and p-coumaric acid derivatives exhibited better activities compared to other derivatives. (Eur. J. Lipid Sci. Technol. **2021**, 123, 2100055).

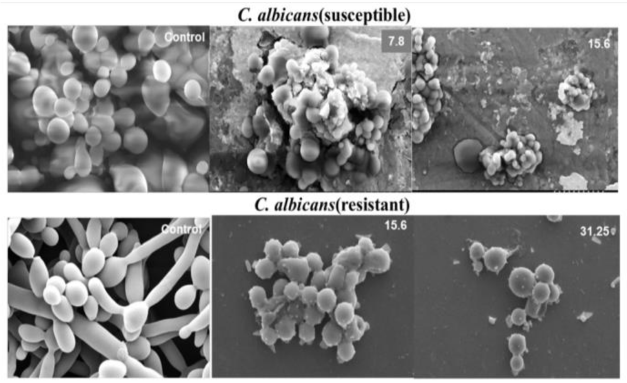
3- Arylsubstituted imidazo[1,2- a] pyridines as antituberculosis agents: Tuberculosis (TB) is a widespread chronic deadly infectious disease caused by the bacillus Mycobacterium tuberculosis (Mtb) which was identified by Robert Koch in 1882. TB predominantly affects the lungs, resulting in cough, fever, and weight loss, and it can be spread from one person to another, especially in immunocompromised persons like those co-infected with HIV. About over 30% of people with HIV are co-infected with Mtb and are approximately 30 times more likely to develop active TB. According to the global TB report of the World Health Organization (WHO), an estimated 10 million people fell ill due to TB worldwide and an estimated 1.2 million deaths occurred due to TB in the HIV- negative population in the year 2019. Most of the TB cases were reported from South-East Asia (44%), where India alone contributed 26% of cases in 2019. This indicates the need for new TB therapeutics with either a new mechanism of action or that can reduce the treatment time. In this line, Novel inhibitors are needed to tackle tuberculosis. Herein, we report the 3- arylsubstituted imidazo[1,2- a]pyridines as potent antituberculosis agents. A small library of 3- aryl- substituted imidazo[1,2- a]pyridines was synthesized using direct arylation, followed by nitro reduction and finally Pd- catalyzed C−N coupling reactions. The compounds thus obtained were evaluated against Mycobacterium tuberculosis H37Rv. Compound 26 was identified as an anti-tuberculosis lead with a minimum inhibitory concentration of 2.3 μg/ml against M. tuberculosis H37Rv. This compound showed a selectivity index of 35. The docking of 26 in the active site of the M. tuberculosis cytochrome bc1 complex cytochrome b subunit (Mtb QcrB) revealed key π–π interactions of compound 26 with the Tyr389 and Trp312 residues of Mtb QcrB. (Arch Pharm. **2021**; e2000419).

Antibacterial drug design

Using quantum chemistry-based cheminformatics and molecular dynamics, pharmacokinetic profiles of spirobenzimidazoquinazolines derivatives were evaluated. Quantum chemo-informatics based predicted activity for the synthesized compounds were concomitant with biological evaluation of broad spectrum antibacterial activity. Biological evaluation revealed that inhibition of biofilm formation was due to their potential antibacterial activity. The novel spirobenzimidazoquinazolines have the potential to be alternatives to aminocoumarins and classical quinazolines upon detailed target specific biological studies. (*Biomed Pharmacother*.,**2021,** 134, 111132 - 111145).

Anti-mycotic agents

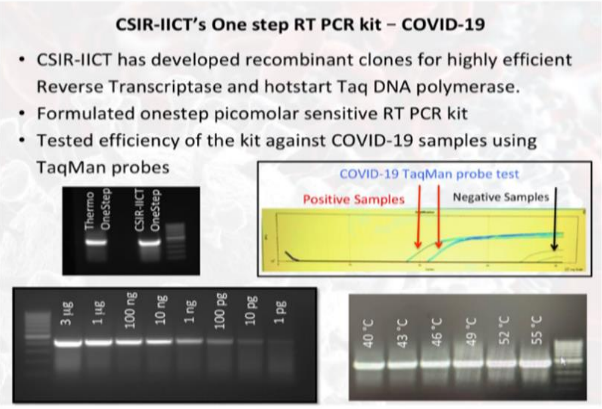
Active compounds responsible for anti-mycotic activities were identified from marine isolated *Neobacillus drentensis*, purified and characterized using biophysical techniques. Bioactivity of the cyclic peptides against azole resistant and susceptible *Candida* strains were examined for growth and biofilm formation. Novel Extracellular exopolymeric cyclic peptides (CLPs) exhibited promising tensio-active properties and antifungal efficacy against azole resistant and susceptible *Candida albicans*. It was observed that the CLPs repressed the *Candida albicans* growth and multiplication by inhibiting the biofilm formation and disruption of branching filamentous hyphae. CLPs have been found to arrest the *C. albicans* cell cycle by a block at G1-S transition followed by apoptotic cell death. (*Bioorg Chem.*,**2021,** 115,105180)



Micrographs showing cell morphology devoid of hyphalorganisation in (susceptible) *C. albicans*, and cells were observed to be shrunken in (resistant) *C.albicans* upon CLPs treatment

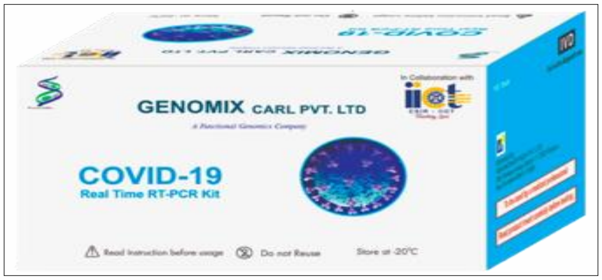
Mitigation of COVID-19: RT-PCR Kit, Drug Target Preparation and Screening, Application of Phytopharmaceutical to ARDS and lung fibrosis

RT-PCR: COVID-19 gave very little choice and time for mankind to fight against it. House arrest was the only option for billions of people across the globe. There was limited knowledge in terms of diagnosis and treatment. Due the global lockdown, supply of enzymes for RT-PCR was limited. Our lab took the challenge in developing RT-PCR diagnostic method. Several enzymes required for the assay were prepared and developed the RT-PCR kit was developed during the lockdown using patient samples



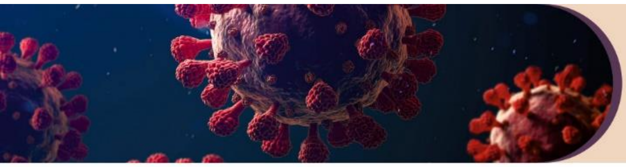
CSIR-IICT's One step RT PCR kit – COVID-19

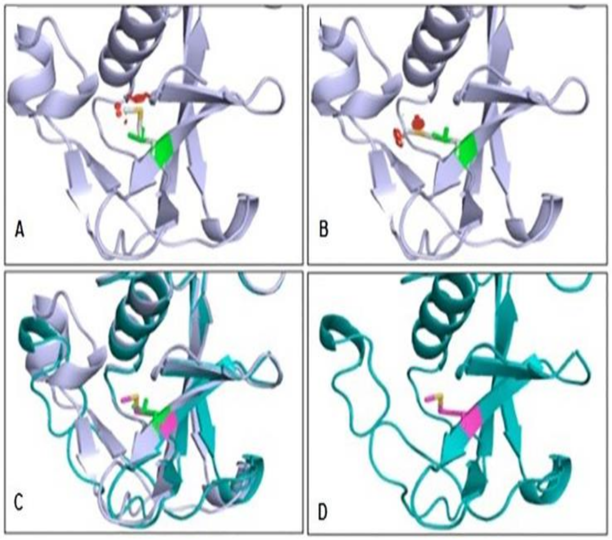
- CSIR-IICT has developed recombinant clones for highly efficient Reverse Transcriptase and hotstart Taq DNA polymerase.
- Formulated onestep picomolar sensitive RT PCR kit
- Tested efficiency of the kit against COVID-19 samples using TaqMan probes



RT-PCR COVID diagnostic kit developed with enzymes developed at CSIR-IICT. Technology is transferred to Genomix Carl Pvt. Ltd

COVID-19 Studies: Mortality due to COVID-19 caused by SARS-CoV-2 infection varies among populations and strains. Functional relevance of genetic variations in human Angiotensin-converting enzyme 2 (ACE2) and Transmembrane serine protease 2 (TMPRSS2), genes that are crucial host factors for viral entry, were investigated. About 510 patients who tested positive for COVID-19 were examined for their DNA. Associations between variants in ACE2 and TMPRSS2 with disease severity were identified through whole exome sequencing and targeted genotyping. Molecular dynamic simulations (MDS) were performed to explore functional relevance of the variants. Cleavage of spike glycoprotein by wild and variant TMPRSS2 was determined in HEK293T cells. Deleterious variant in TMPRSS2 (rs12329760, G > A, p. V160M, identified was responsible for disease severity. Studies using molecular dynamics revealed decreased stability of TMPRSS2 160 M variant. Spike glycoprotein cleavage by TMPRSS2 reduced ~2·4-fold in cells expressing 160 M variant. These studies demonstrate association of TMPRSS2 variant rs12329760 with decreased disease severity in COVID-19 patients from India (*Meta Gene.*,**2021,** 29, 100930 - 100938).



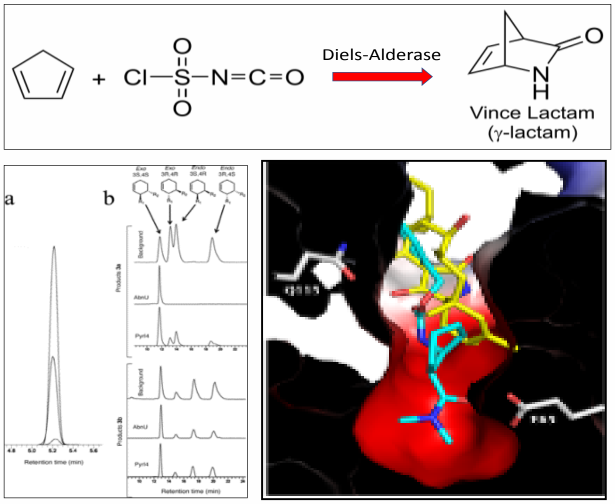


Molecular dynamics and simulation analysis of WT and V160M mutant TMPRSS2. Cartoon representation showing the N-terminal domain TMPRSS2 (A)Wild-Type TMPRSS2, (B) V160M mutant TMPRSS2 and (C and D) Superimposing of Wild-Type and V160M structures. The position of amino-acidValine and Methionineare shown in pink sticksand change in the TMPRSS2 secondary structure is noticeable

Structural Biology

Exo-Selective Intermolecular Diels–Alder Reaction by PyrI4 and AbnU on Non-Natural Substrates

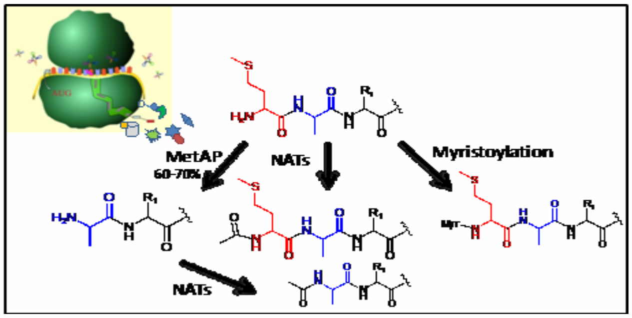
Two natural enzymes, PyrI4 and AbnU performing stereospecific intermolecular DAr on non-natural substrates. AbnU catalyses a single exo-stereoisomer by 32-fold higher than the background. PyrI4 catalyses the same stereoisomer (15-fold higher) as a major component (>50%). Structural, biochemical and fluorescence studies indicate that the dienophile enters first into the β-barrel of the enzymes followed by the 1,3-diene, yielding a stereospecific product. However, if some critical interactions are disrupted to increase the catalytic efficiency, stereoselectivity is compromised. Since it is established that natural enzymes can carry out intermolecular DAr on non-natural substrates, several hundreds of Diels-Alderases available in nature could be explored. (*Nature Commun. Chem.*, **2021**, 4, 113 – 122)



Characterization of intermolecular Diels-Alderase reaction by AbnU and PyrI4

Targeting the Ribosome Associated *M. tuberculosis* Proteins

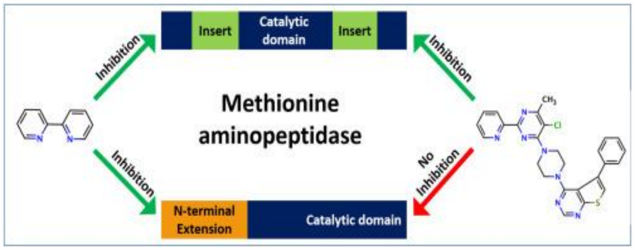
Specific focus has been on understanding the structure function relationship of *M. tuberculosis* proteins such as methionine aminopeptidase (MetAP), N-acetyl transferases (NATs) and peptide deformylase (PDF) that associate with the ribosome at the exit tunnel. Each of these enzymes is a validated as drug target. The challenge is developing selective inhibitors against microbial enzymes without affecting the human counterparts



Schematic diagram of the co-translational modifications such as methionine deformylation, methionine removal, N-terminal acetylation and myristoylation that occurs at the ribosome exit tunnel

Methionine Aminopeptidases

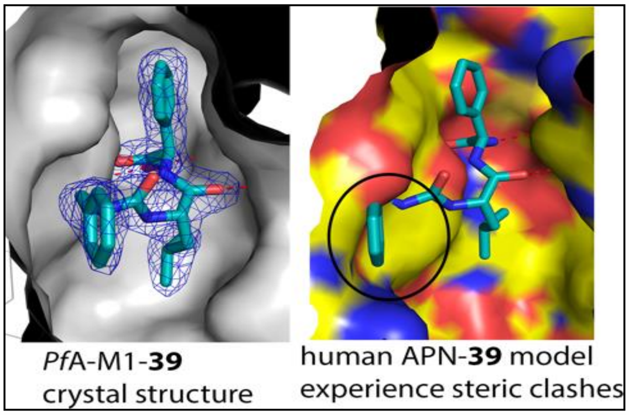
Several protein sequences and structures are analysed to identify the fine differences between microbial and human enzyme. Designed, synthesized (some in collaboration) and discovered several molecules that specifically target bacterial enzymes and not the human counterpart. (*Bioorg. Chem.*, **2021**, 115, 105185; *Eur. J. Med. Chem.*, **2021**, 209, 1; *Int J BiolMacromol.*,**2020**, 15, 1373)



Schematic representation of domain architecture of methionine aminopeptidases from different microbes

Discovery of a PfA-M1 Selective Inhibitor Over the Mammalian Counterpart as Antimalarial Agent

The design is to extend the binding of molecules beyond S1′ pocket of the enzyme to achieve specificity. Most of the 40 compounds described in this study display inhibition at sub-micromolar range against the recombinant *Pf*A-M1 with negligible cytotoxicity on human cell lines and strong inhibition of the malarial parasite growth. However, the selectivity index between the malarial and mammalian M1 aminopeptidases for all these compounds is less except for compound **39**, which inhibits the parasite enzyme by more than 160-fold. Crystal structures of *Pf*A-M1 at atomic resolution in complex with at least nine different compounds including compound **39** establish the structural basis for the observed inhibition. Binding of molecule **39** extends beyond the S2′ pocket where differences between the malarial and mammalian enzymes are apparent. (*Chinese Chem. Lett.*, **2021**, 33, 2550; *Int J BiolMacromol.*, **2020**, 15, 1373)



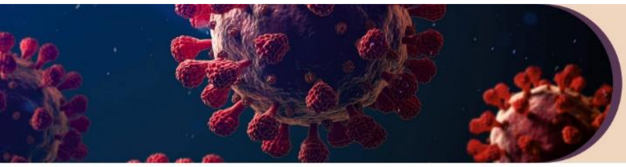
Left panel: X-ray crystal structure of the malarial M1 aminopeptidase in complex with the lead compound 39. Right panel: Alignment of M1-aminopeptidase complex over the human enzyme structure

Drug Delivery and Nanomedicine Research

As a new drug delivery strategy against cancer, CD13-receptor targeting NGRKC16-lipopeptide-associated liposomal withaferin delivery system for effectively killing CD13-receptor expressing pancreatic cancer and angiogenic endothelial cells has been developed. (*J. Drug Del. Sc. Tech.,* **2020**, 58, 101798 - 101802)

Continuing with glucocorticoid receptor targeting strategy, a self-assembling lipid-based hydrocortisone derivative has been developed. This is used as a multi-modal nanotherapeutics delivering itself as an anticancer drug, a separate small molecule drug, docetaxel cargo and also an anticancer gene to act additively toward efficient colon cancer reduction in orthotopic mouse model. (*Mol. Pharm.*, **2021**, 18(3), 1208-1228)

A carbon nanosphere (CSP)-based delivery system that could dually target sigma receptor (SR)-expressing glioma tumor-associated macrophages and tumor epithelial cells in the brain was developed. CSP, with its intrinsic property to glide through blood brain barrier (BBB) was modified for selective targeting to glioma lesions. Using a special cationic haloperidol-CSP nano conjugate, *in situ* glioma tumor regression with increased survivability of mice was accomplished**.** (*India Patent Appl. No*. 202111015505)



A functional and Self-Assembling Octyl-Phosphonium-Tagged Esculetin as an Effective siRNA Delivery Agent

A self-assembling octyl-TPP tagged esculetin (Mito-Esc) as a functional and novel small molecule siRNA delivery vector was documented. Mito-Esc was found to induce dose-and time-dependent cell death in MDA-MB-231 breast cancer cells, while preserving the viability of MCF-10A (normal mammary epithelial) cells. Mito-Esc, a delocalized cation, presumably enters more into cancer cells due to higher hyperpolarized mitochondrial membrane potential and destabilizes the mitochondrial integrity. The siRNA delivery property of Mito-Esc was proved by confocal microscopy using a fluorescently labeled Cy-5 siRNA. Wherein, only the 6,7 dihydroxy substitution but not the methoxy substitution or octyl TPP facilitated the intracellular delivery of siRNA. Overall, it was identified Mito-Esc as a novel small molecule siRNA delivery vector apart from inducing selective cancer cell death on its own, and efficient delivery of siRNAs intracellularly without the need of any excipient. (*Chem. Comm.*, **2021**, 57, 12329-12332).

Pharmacology and Toxicology

Toxicity evaluation of Ayurvedicherbo-metallic preparations: Therapeutic drugs formulated by combining various heavy metals with herbal ingredients are known as Herbo-metallic (HM) preparations. Different metals and herbs are used in these preparations hence their safety is a major concern. Lack of toxicological data on Ayurvedic drugs makes it difficult to determine if there is a risk associated with these drugs. Thus, there is an urgent need to develop rapid, accurate and efficient testing strategies to assess their health effects on humans. Therefore, the detailed scientific study of safety and efficacy of various ayurvedic formulations is the need of the hour. Arshokuthara Rasa (AR) Ekangaveer Rasa (ER) Chandramrit Rasa (CR) and Nityanand Rasa (NR) are ayurvedic HM formulations prepared using mercury, sulphur, iron, mica and several herbal ingredients. After acute and sub-chronic (90 days) of dosing the albino wistar rats with drugs Arshakuthar Rasa, Ekangaveer Rasa, Chandramrit Rasa (CR) and Nityanand Rasa (NR) the blood and vital organs were used to conduct the haematological, biochemical, genotoxicity and histopathological studies. Biochemical parameters such as Alanine aminotransferase (ALT/GPT), Aspartate aminotransferase (AST/GOT), Acetyl cholinesterase (AChE) assay in blood plasma and brain, Glutathione S-transferase (GSH- Superoxide dismutase (SOD) assay, Glutathione Reductase assay, Reduced Glutathione (GSH) assay, Glutathione peroxidase (GPX) assay, Catalase assay, Malondialdehyde (MDA) assay, estimation in serum, acute and sub-chronic dosed rats with drugs have been completed. Genotoxicity A) Chromosomal aberration assay B) Comet assay C) Biodistribution, Gene expression and histopathology studies, Micronucleus assay (Blood and Bone Marrow) in acute and sub-chronic dosed rats with drugs Arshakuthar Rasa, Chandramrit Rasa (CR) and Nityanand Rasa (NR) has been studied. The results from these studies will be useful in predicting the possible toxic hazards that may arise from the usage of these drugs.

Toxicological assessment of micro and nano plastics in water stored in polyethylene terephlate (PET) bottles using plant and animal models: PET is the most widely used material for bottling water. Due to its characteristics of resistance to chemicals, low gas and water vapour permeability, strength and impact-resistance, low weight, colourlessness and transparency and easy recycling procedures, PET has emerged as a good alternative to glass. Despite these properties, bottles made of PET may contaminate water with the material's components due to temperature and storage condition. Several reports suggest that phthalates may leach from PET bottles into the water as they are used in the manufacturing process. Phthalates are Phthalates are associated with increased adiposity and insulin resistance, and other adverse effects on the human reproductive system. Infants and children are especially vulnerable to the toxic effects of phthalates Lack of toxicological data on the chemical compounds released from the Indian bottled water (MP, NPs and their additives) makes it difficult to determine if there is a risk associated with these plastics. The use of bottled water in the world has increased in recent years, with an increment of 91% in seven years. Similarly, the Indian bottled water industry has also seen strong growth in past few years as people turn to packaged water in the absence of clean potable water. Thus there is an urgent need to develop rapid, accurate and efficient testing strategies to assess health effects of these particles on humans. Hence, we investigated whether these MP and NPs and their additives can leach into the bottled water during the bottling process, storage and temperature conditions causing toxicity in plant and animal models with a special focus on environmental and health risk assessment on humans.

Ecotoxicity Study of 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 was determined for 48 hrs in daphnia and for 96 h in Zebrafish.

Biological Evaluation of Natural Product Derived Small Molecules Against Cancer

The interdisciplinary study involved synthesis of the novel noscapine analogues with different functional groups appended at 9th position of natural noscapine. The anticancer activity of these compounds was investigated using various human cancer cell lines such as HeLa (cervical cancer), DU-145 (prostate cancer), MCF-7 (breast cancer) and IMR-32 (neuroblastoma). Further the mechanism of effective molecules was uncovered in detail, by understanding its impact on cell cycle progression, microtubule dynamics and apoptosis. (*ChemistrySelect,* **2020**, 5, 2972 –2980; *Drug. Dev. Res.*, **2021**, 1–10)

Bioactivity of Isomeric Corniculotides Derived from Cannonball Mangrove

Cannonball mangrove, *Xylocarpus granatum Koening* (Meliaceae), is widely distributed in Southeast Asia along the coastlines of the Indian Ocean. In the search for structurally and biologically significant secondary metabolites from the Indian mangrove flora, this interdisciplinary study reported three more isomeric corniculatolides, named corniculatolide B, isocorniculatolide B, and corniculatolide C, as rare metabolites along with the known macrolidesandfriedelin from the stems of the Xylocarpusgranatum and evaluation of the AGH inhibitory and cytotoxicity of the isolated compounds. (*Nat. Prod. Res.*, **2021**, 1-7)

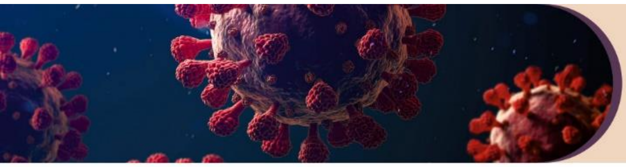
APPLIED RESEARCH

Climate-Based Malaria Forecasting System for Vishakhapatnam District of Andhra Pradesh, India

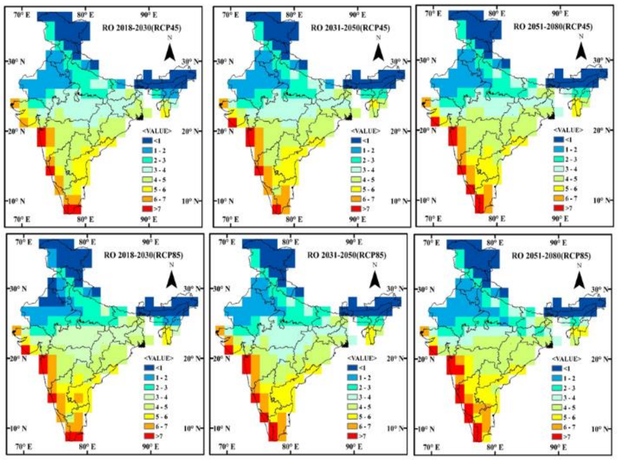
The study exploited multi-step polynomial regression and seasonal autoregressive integrated moving average (SARIMA) models to forecast malaria cases in Vishakhapatnam. The polynomial model predicted malaria cases with high predictive power. Moreover, mean temperature, rainfall and Normalized Difference Vegetation Index build a significant impact on malaria cases. The best fit model was SARIMA (1, 1, 2) (2, 1, 1)12 which was used for forecasting monthly malaria incidence for the period - January 2015 to December 2016. The performance accuracy of both models are similar, however, the lowest Akaike information criterion score was observed by the polynomial model, and this approach can be helpful for forecasting malaria incidence to implement effective control measures in advance for combating malaria in India. (*J. Parasit. Dis.,***2020**, 44, 497-510)

Dengue Situation in India: Suitability and Transmission Potential Model for Present and Projected Climate Change Scenarios

A climate driven dengue model was developed that predicted areas vulnerable for dengue transmission under present and future climate change scenarios in India. The study also projected the dengue

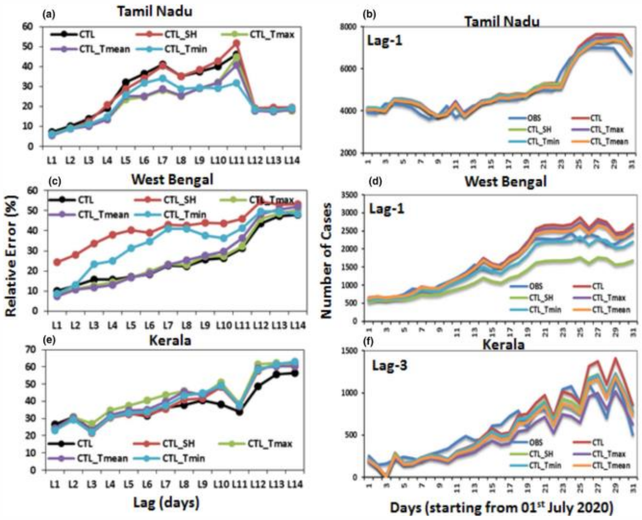


distribution risk map using representative concentration pathways (RCP4.5 and RCP8.5) in India in 2018–2030 (forthcoming period), 2031–2050 (intermediate period) and 2051–2080 (long period). Dengue cases assessed in India from 1998 to 2018 found that the transmission is gradually increasing year over year. Both RCP4.5 and RCP8.5 scenarios revealed that dengue outbreaks might occur at larger volume in Southern, Eastern, and Central regions of India. These results help in suggesting appropriate control measures to limit the spread. Also, a proper plan is required to mitigate greenhouse gas emissions to reduce the epidemic potential of dengue in India. (*Science of The Total Environment*, **2020**, 739, 140336 - 140342)



Risk maps represents the future dengue transmission in India

Prediction of COVID-19 cases using the weather integrated deep learning approach: Advanced and accurate forecasting of COVID-19 cases plays a crucial role in planning and supplying resources effectively. **Artificial Intelligence (AI) techniques** have proved their capability in time series forecasting non-linear problems. In this study, the relationship between weather factor and COVID-19 cases was assessed, and also developed a forecasting model using long short-term memory (LSTM), a deep learning model. The study found that the specific humidity has a strong positive correlation, whereas there is a negative correlation with maximum temperature, and a positive correlation with minimum temperature was observed in various geographic locations of India. The weather data and COVID-19 confirmed case data (1 April to 30 June 2020) were used to optimize univariate and multivariate LSTM time series forecast models. The optimized models were utilized to forecast the daily COVID-19 cases for the period 1 July 2020 to 31 July 2020 with 1 to 14 days of lead time (Figure-3). The results showed that the univariate LSTM model was reasonably good for the short-term (1-day lead) forecast of COVID-19 cases (relative error <20%). Moreover, the multivariate LSTM model improved the medium-range forecast skill (1–7 days lead) after including the weather factors. The study observed that the specific humidity played a crucial role in improving the forecast skill majorly in the West and northwest region of India. Similarly, the temperature played a significant role in model enhancement in the Southern and Eastern regions of India. (*Transboundary Emerging Diseases*, **2021**)



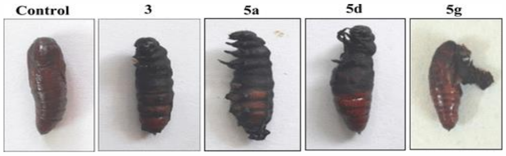
Skill (Average relative error) of univariate (CTL) and multivariate (CTL_SH, CTL_Tmax, CTL_Tmin, CTL_Tmean) LSTM models during the test period (1 July to 31 July 2020) for the states of Tamil Nadu, West Bengal, and Kerala

Machine Learning for Systematic Optimization of Reverse Phase High Performance Liquid Chromatography Method to Analyze Drugs

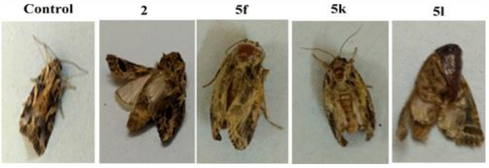
Objectives of current investigation are: To find the wavelength of maximum absorbance (λmax) for combined cyclosporin A and etodolac solution followed by selection of mobile phase suitable for RP-HPLC method; to define analytical target profile and critical analytical attributes (CAAs) for analytical quality by design; to screen critical method parameters with help of full factorial design followed by optimization with face-centered central composite design (CCD) approach-driven artificial neural network (ANN)-linked with the Levenberg–Marquardt (LM) algorithm for finding the RP-HPLC conditions; to perform validation of analytical procedures (trueness, linearity, precision, robustness, specificity and sensitivity) using combined drug solution; and to determine drug entrapment efficiency value in dual drug-loaded nanocapsules/ emulsions, percentage recovery value in human plasma spiked with two drugs and solution state stability analysis at different stress conditions for substantiating the double-stage systematically optimized RP-HPLC method conditions. The artificial neural network (ANN) topology (3:10:4) indicating the input, hidden and output layers were generated by taking the 20 trials produced from the face-centered CCD model. The optimized RP-HPLC method can be applied to analyze two drugs concurrently in different formulations, human plasma and solution state stability checking. (*AAPS PharmSciTech.*, **2021,** 22, 155)

Antifeedant activity of Limonoids from Fruits of Trichiliaconnaroides: UPLC-MSE guided isolation of CHCl3 extract from the fruits of Trichilia connaroides yielded two new mexicanolidetype limonoids trichanolide F (1) and trichanolide G (2) along with a known compound carapanolide U (3). The structures of the limonoids were characterized by extensive spectroscopic analysis (MS, IR, 2D NMR). These limonoids (1−3) were evaluated for their antifeedancy against Spodoptera litura F. To further explore and draw the meaningful structure activity relationship studies, secophragmalin-type limonoids, namely, secotrichagmalin B, C (4, 5) and semisynthetic derivatives (5a−5l) were also screened for antifeedancy. The results revealed that trichanolide F (1) displayed highest antifeedant index (AFI) and caused larval mortality at 24 h. Derivative 5b caused larval toxicity (Fig-4), whereas 3, 5a, 5d, and 5g lead to pupal mortality (Fig-5) and 2, 5f, 5k, and 5l caused adult deformities (Fig-6). Overall, the study provided new insights into the antifeedant potential of isolated and chemically modified limonoids from T. connaroides for the control of spodopteran pests.

Representative abnormal larvae pictures of 1 and 5b against S. litura larvae after 24 h of treatment



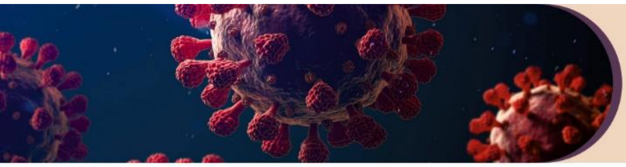
Representative malformed pupae pictures of 3, 5a, 5d, and 5g against S. litura.



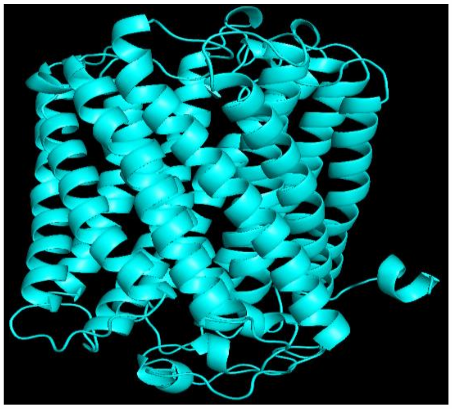
Representative deformed adult pictures of 2, 5f, 5k, and 5l against S. litura.

In silico Structural Characterization of Cytochrome C oxidase Subunit 1: A Transmembrane Protein from *Aedes aegypti*

The study proposed a series of computational techniques such as homology modelling, molecular simulation, and molecular docking to explore structural features and binding mechanism of Cytochrome c oxidase subunit I (COX1) protein with known inhibitors. The three-dimensional structure of mitochondrial transmembrane protein COX1 was built using homology modelling based on high-resolution crystal structures of *Bostaurus*. Known inhibitors such as carbon monoxide (CO) and nitric oxide (NO) inhibit their active binding sites of



mitochondrial COX1 and the inhibitors were docked into the active site of attained model. A structure-based virtual screening was performed on the basis of the active site inhibition with best scoring hits. (*J Vector Borne Dis,***2021**, 58, 106-114)



Three-dimensional structure of Cytochrome C oxidase Subunit 1 protein model of *Aedes aegypti*

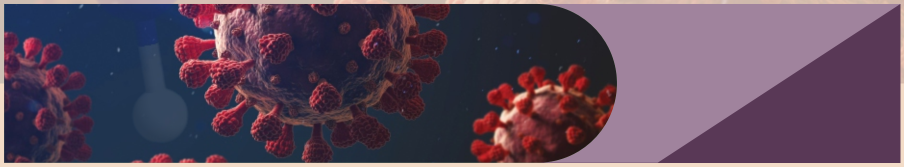
Pulmonary Research

Dehydrozingerone Ameliorates Lipopolysaccharide Induced Acute Respiratory Distress Syndrome by Inhibiting Cytokine Storm, Oxidative Stress *via* Modulating MAPK/NF-κB Pathway

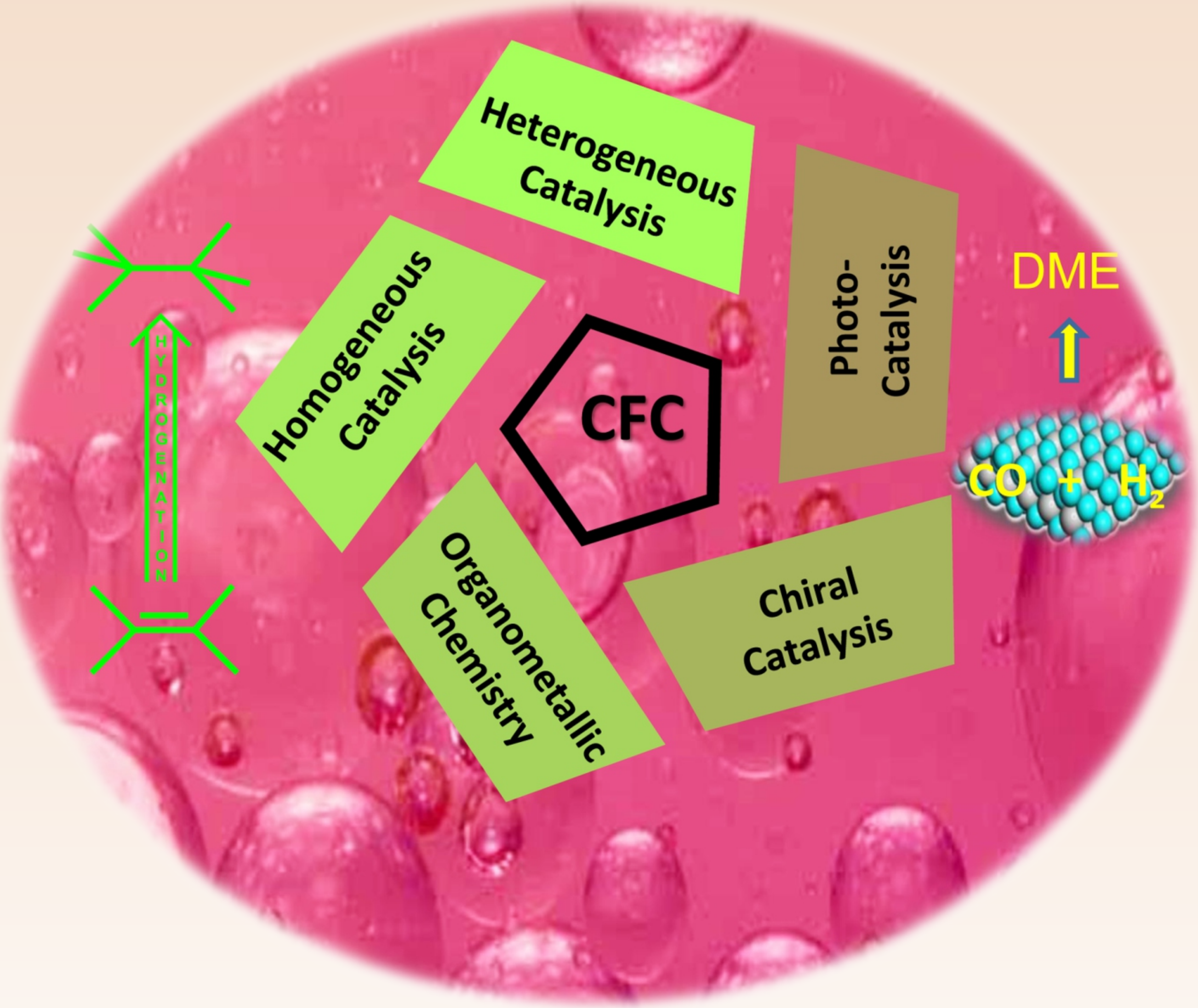
During COVID-19 pandemic, *in vitro* and *in vivo* models to screen drugs against LPS induced lung injury and cytokine expressions in *in vivo* and ARDS and Cytokine storm in *in vivo* were established. A few molecules were screened, and one which showed tremendous cytokine inhibition efficiency was selected. DHZ is a phenolic compound derived from ginger (*Zingiberofficinale)* rhizomes previously shown to possess anti-inflammatory and antioxidant activities. *In vivo* analysis showed that DHZ treatment significantly ($p < 0.001$) mitigated the LPS induced ARDS pathophysiology. LPS stimulated neutrophil-mediated events, apoptosis, alveolar wall thickening and alveolar inflammation were profoundly reduced by DHZ treatment in a rat model. (*Phytomedicine.***2021,** 92, 153729 - 153743)

mRNA platform development: The current study focuses on creating a model platform for mRNA vaccines by designing, synthesis and delivery of various mRNA vaccines with high specificity and superior selectivity with negligible or no allergic reactions. To develop mRNA platform technology, the study emphasized on the generation of mRNA vaccines against (i) human diseases (to start with SARS-CoV2) and (ii) later other infectious diseases. Currently, the mRNA platform technology developed is being, validated in *in vitro* and *in vivo*.

Nitric-oxide toxicity studies: Various reports suggest that, nitric oxide (NO) or its derivatives shown multiple benefits against viral infections. This could be due to inhibition of Interferon (IFN) mediated activation of macrophages. Considering these effects, it was hypothesized that, NO may show therapeutic effects on SARS-CoV-2 infection. Toxicity effects of Nitric Oxide Releasing Solution (NORS) indicated that, the prepared NORS are free from toxic effects as per acute study.



CATALYSIS AND FINE CHEMICALS



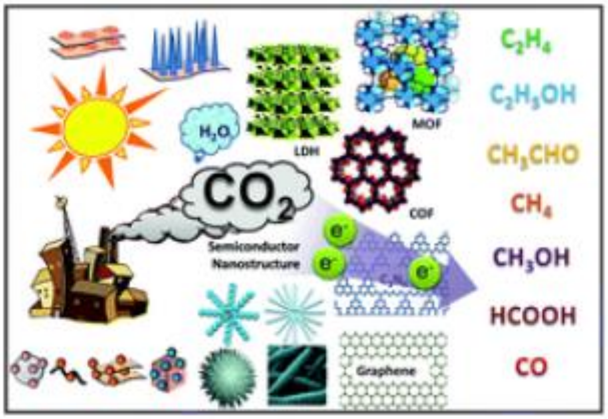
CATALYSIS & FINE CHEMICALS

BASIC RESEARCH

An Efficient Hydrogenation Catalytic Model Hosted in a Stable Hyper-Crosslinked Porous-Organic Polymer: From Fatty Acid to Bio-Based Alkane Diesel Synthesis

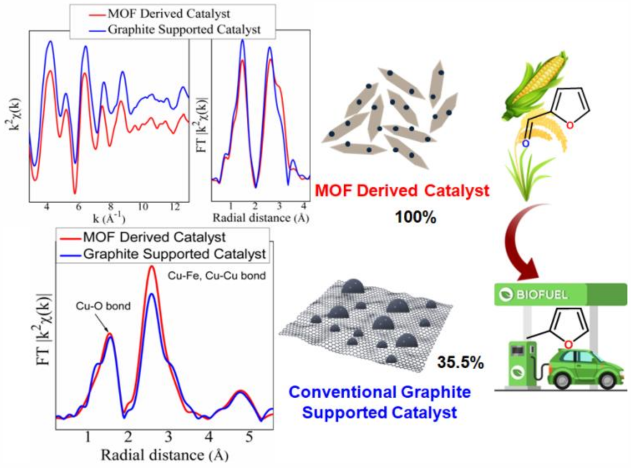
A cost-effective synthesis strategy for a new microporous hyper crosslinked POP through $FeCl_3$ assisted Friedel–Crafts alkylation reaction, followed by fabrication of Pd^0 NPs (2–3 nm) using a solid gas phase hydrogenation route to deliver a novel catalytic system is studied. This catalyst (Pd@PPN) exhibits versatile catalytic performance for different types of vegetable oils including palm oil, soybean oil, sunflower oil and rapeseed oil to furnish long chain diesel range alkanes. The catalyst shows high stability during five runs of recycling without leaching of Pd. On this catalyst, up to 90% conversion with 83% selectivity of C17-alkane has been achieved for stearic acid. (*Green Chemistry*, **2020**, *22*, 2049-2068)

Integrated Nano-Architectured Photocatalysts for Photochemical CO_2 Reduction This work primarily explored the basic principles of tailor-made nanostructured composite photocatalysts and how nano-structuring influences photochemical performance. Specifically, the study has summarized the recent developments related to integrated nanostructured materials for photocatalytic CO_2 reduction, mainly in the following five categories: carbon-based nano-architectures, metal–organic frameworks, covalent-organic frameworks, conjugated porous polymers, and layered double hydroxide-based inorganic hybrids. Besides, the technical aspects of nanostructure-enhanced catalytic performance in photochemical CO_2 reduction, some future research trends and promising strategies are addressed. (*Nanoscale*, **2020**, *12*, 23301-23332)



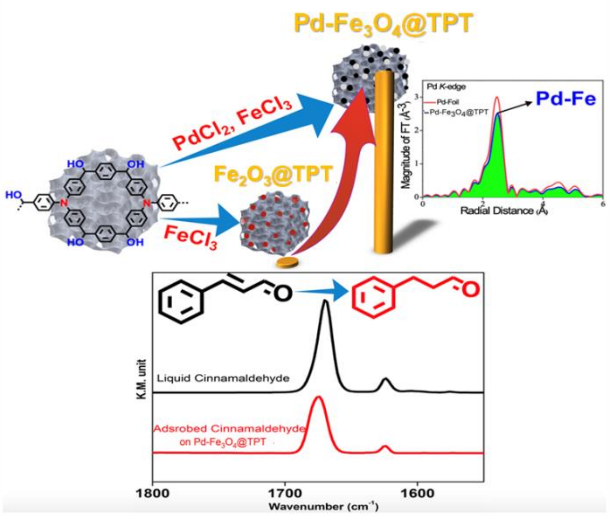
Leveraging $Cu/CuFe_2O_4$-Catalyzed Biomass-Derived Furfural Hydrodeoxygenation: A Nanoscale Metal–Organic-Framework Template Is the Prime Key

Non-noble metal-based metal/mixed metal oxide supported on carbon employing a metal–organic framework as a sacrificial template is demonstrated for the first time in the selective hydrodeoxygenation (HDO) of biomass-derived furfural (FFR) to 2-methyl furan (MF). The catalyst (referred to as $Cu/CuFe_2O_4$@C-A) exhibited extraordinary catalytic proficiency (100% selectivity toward MF) compared with the conventional $Cu/CuFe_2O_4$@C-B catalyst. The presence of more Lewis/weak acidic sites in this catalyst was beneficial for the hydrogenolysis step in HDO reaction. The adsorption of H_2 was stronger on the $Cu/CuFe_2O_4$@C-A than that over the conventional $Cu/CuFe_2O_4$@C-B catalyst. This work has great implication in developing a highly stable catalyst for the selective upgradation of biomass without deactivation of metal sites in extended catalytic cycles. (*ACS Appl. Mater. Interfaces*, **2020**, *12*, 21682−21700)



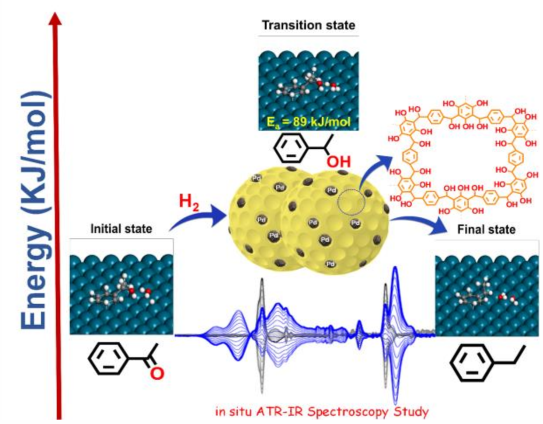
Porous-Organic-Polymer-Triggered Advancement of Sustainable Magnetic Efficient Catalyst for Chemoselective Hydrogenation of Cinnamaldehyde

In this study, a cost-effective, facile and metal & template-free strategy for the successful synthesis of hydroxyl enriched POP (denoted as TPT) was adopted. An integrated catalyst, Pd-Fe_3O_4@TPT, has been developed for the liquid phase selective hydrogenation cinnamaldehyde (CAL). Pd-Fe_3O_4@TPT exhibited excellent catalytic performance, providing 100% selectivity towards hydro cinnamaldehyde (HCAL) under mild reaction conditions, whereas Fe_2O_3@TPT appeared inert. Compared with the conventional catalytic systems, the newly designed catalyst was superior in many aspects, owing to the rigid nature of TPT-POP, which prevents aggregation and leaching of the metal nanoparticles. The study provides new inspirations for designing easily realizable, low-cost, and high-performance catalysts for sustainable chemistry *via* effective surface/interface engineering. (*ChemCatChem*, **2020,** *12*, 3687-3704)



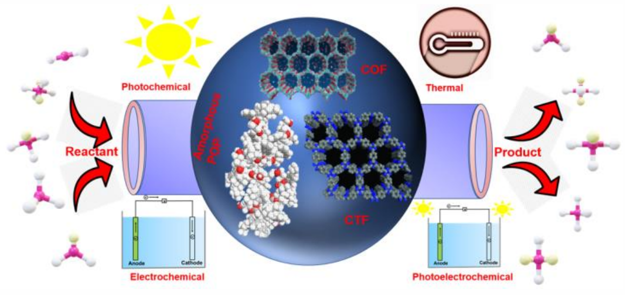
Realizing Catalytic Acetophenone Hydrodeoxygenation with Palladium-Equipped Porous Organic Polymers

The properties and catalytic activity of a template-free-constructed, hydroxy (−OH) group-enriched porous organic polymer (Ph-POP) bearing functional Pd nanoparticles (Pd-NPs) by one-pot condensation of phloroglucinol (1,3,5-trihydroxybenzene) and terephthalaldehyde followed by solid-phase reduction with H_2 was studied. The encapsulated Pd-NPs rested within well-defined POP nanocages and remained undisturbed from aggregation and leaching. This polymer hybrid nanocage Pd@Ph-POP is found to enable efficient liquid-phase hydrodeoxygenation (HDO) of acetophenone (AP) with high selectivity (99%) of ethylbenzene (EB) and better activity than its Pd@Al_2O_3 counterpart. All of the hydrogenation routes, including direct hydrogenation by surface hydrogen, hydrogen transfer, and the keto–enol pathway, are evaluated, providing insights into the experimental observations. (*ACS Appl. Mater. Interfaces*, **2020**, *12*, 50550 – 50565)



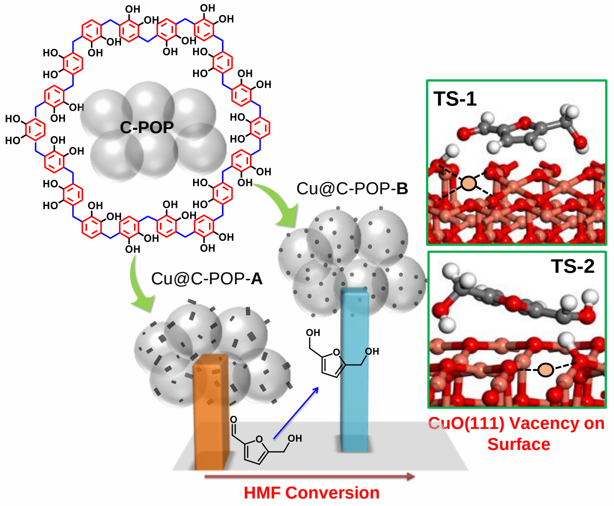
Presenting Porous–Organic–Polymers as Next Generation Invigorating Materials for Nanoreactors

This work provides an overview of existing research relating to diverse POP synthetic approaches (COFs, CTFs, and some amorphous POPs), the possible modification of the functionality of POPs, and their exciting application as next-generation nanoreactors. These POPs offer the potential for either metal-free or metalated polymer catalysts allowing photocatalytic CO_2 reduction to solar-fuel, biofuel upgrades, the conversion of waste cooking oil to bio-oil, and clean H_2 production from water, addressing many scientific and technological challenges and providing new opportunities for various specific topics in catalysis. (*Chem. Commun.*, **2021**, *57*, 8550-8567)



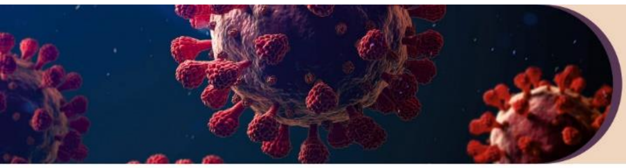
Navigating Copper-Atom-Pair Structural Effect inside a Porous Organic Polymer Cavity for Selective Hydrogenation of Biomass Derived 5-Hydroxymethylfurfural

Catalytic systems for 5-HMF hydrogenation with stable and balanced Cu^{0} and Cu^{x+} active surface species inside the nanocage of a catechol-based porous organic polymer (POP) endowed with large surface areas, impressive stabilities, and spatial restriction inhibiting nanoparticle aggregation were built. Batch reactor screening identified that a superior catalytic performance (DHMF selectivity of 98%) has been achieved with our newly designed Cu@C-POP at 150°C temperature and 20 bar H_2 pressure, which was also higher than that of other reported copper catalysts. The substantially boosted activity is induced by the presence of the bulk CuO_x phase and atomically dispersed Cu species incorporating isolated Cu ions, which are further confirmed through the positive binding energy shift of Cu $2p_{3/2}$ XPS spectra (~0.4 eV). The presence of Cu metal vacancies stabilized the reaction intermediates formed during 5-HMF hydrogenation and decreased the hydrogenation barriers, resulting in an enhanced catalytic activity of the Cu@C-POP-B catalyst. (*ACS Sustainable Chem. Eng*. **2021**, *9*, 2136–2151)

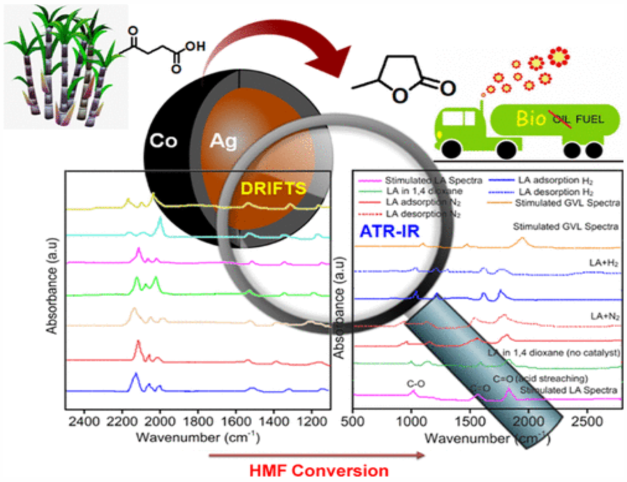


Looking into More Eyes Combining *in situ* Spectroscopy in Catalytic Biofuel Upgradation with Composition-Graded Ag–Co Core–Shell Nanoalloys

Silver–cobalt core–shell nanoalloy based catalysts through a simple wet impregnation method for selective conversion of LA to GVL have been sequentially synthesized. The highest catalytic proficiency had been achieved over a composition-

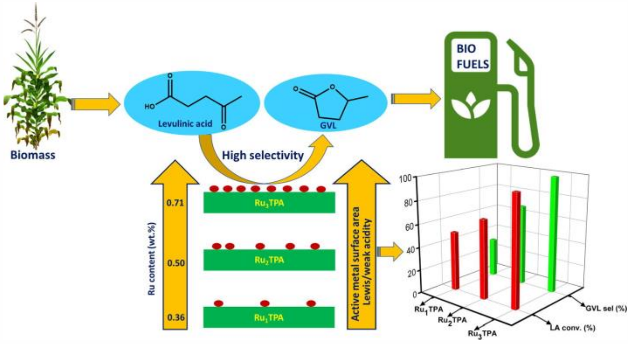


graded optimized catalyst, named 5Ag–15Co, under comparatively moderate reaction conditions (150°C, 1 MPa H_2 pressure). This finding also was emphasized by H_2 chemisorption analysis, which revealed the presence of the highest active metal surface area in the 5Ag–15Co catalyst. The detailed kinetic analysis revealed that the 5Ag–15Co catalyst had the lowest activation energy (41.34 kJ) among its counterparts, which accelerated the reaction rate. (*ACS Sustainable Chem. Eng*. **2021**, 9, 3750 – 3767)



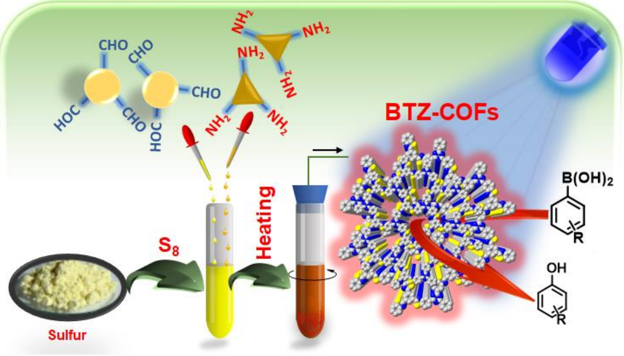
One-Pot Conversion of Levulinic Acid into γ-Valerolactone over a Stable Ru Tungstophosphoric Acid Catalyst

In this work ruthenium exchanged tungstophosphoric acid (TPA) catalysts with different ruthenium loading (Ru_xTPA (x = 1,2,3)) were studied for conversion of levulinic acid (LA) into γ-valerolactone (GVL) (a potential fuel/fuel additive). Under the conditions used (130°C, 1.0 MPa H_2, 2 h in 1,4 dioxane solvent) one of the prepared catalysts achieved excellent conversion and selectivity to GVL. This catalyst also compared favorably to Ru/C catalysts that have been previously studied in terms of rate of production of GVL per gram Ru. The best performing Ru3TPA catalyst was found to be highly recyclable with only a slight decrease in selectivity of GVL (from 100% to 98.3%) being observed after five cycles of testing. (*Fuel*, **2021,** *289*, 119900)



Benzothiazole-Linked Metal-free Covalent Organic Framework Nanostructures for Visible-Light-Driven Photocatalytic Conversion of Phenylboronic Acids to Phenols

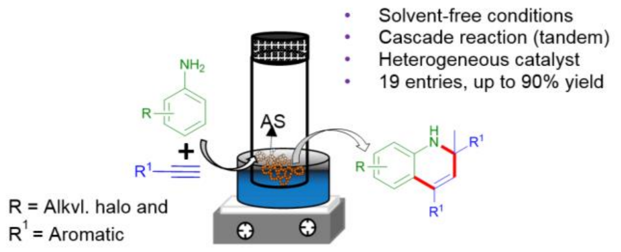
This study describes two benzothiazole-linked covalent organic framework nanostructures (BTZ-BCA-COF and BTZ-TPA-COF), which have been prepared *via* a highly efficient one-pot, multicomponent transition-metal-free C−H functionalization and oxidative annulation synthetic strategy and employing elemental sulfur as one of the key components. These COFs exhibit light-harvesting capacity as a photosensitizer for visible-light-assisted "carbon−boron" bond cleavage with a high functional group tolerance of the substrates. Our contribution sheds light on exploration of elemental sulfur to extended π-conjugation network-based photocatalysts, followed by instigating their structural uniqueness photocatalytic activity relationship. (*ACS Appl. Nano Mater*., **2021**, 4, 11732-11742)



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 a one-step synthesis of substituted dihydroquinolines *via* hydroarylation/hydroamination cascade reaction in a solvent-free conditions have 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 demonstrated with a variety of aromatic amines and alkynes. The catalytic protocol, utilizing simple starting materials and a heterogeneous catalyst in a clean reaction environment, makes as an alternative and economically viable route to a wide range of the 1,2-dihydroquinoline derivatives. (*Cat. Commun.*, **2020,** 135, 105888)



K10 Montmorillonite Catalyzed C-C Bond Formation of Aromatic Secondary Alcohols and Alkynes: A Green and Convenient Approach to β-aryl Ketones under Solvent-free Conditions

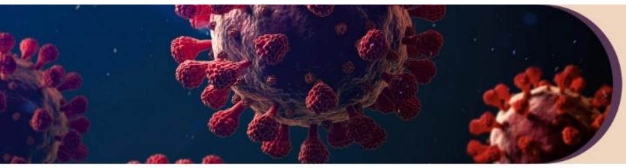
The synthesis of β-aryl ketones from aromatic alkynes and secondary alcohols catalyzed by heterogeneous K10 montmorillonite via C-C bond formation has been developed. This approach proceeds under solvent free conditions without any usage of further additives and immobilizations. This process is sustainable and exhibiting good compatibility among a range of various aromatic alkynes and secondary alcohols affording moderate to excellent yields. The presence of unique layered structure as well as strong acidic sites in the K10 montmorillonite might be responsible for the formation of β-aryl ketones. The efficacy and viability of the present catalytic system was demonstrated with gram scale experiments. (*Sus. Chem. Pharm.***,** **2020,** 15, 100227 - 100234)

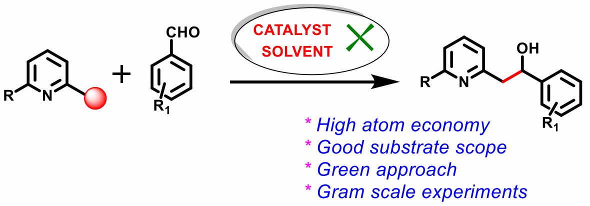
Metal-free Catalytic Esterification of Aryl Alkyl Ketones with Alcohols via Free-radical Mediated C(sp^3)-H Bond Oxygenation

A novel metal-free catalytic one-pot approach has been developed for the esterification of aralkyl ketones with alcohols under open-air atmospheric conditions. The inexpensive iodide/oxone reagent system allowed the cascade C(sp^3)-H bond oxygenation, selective C-C bond cleavage and esterification through the both radical and ionic pathways in a stepwise manner in one-pot. This mild, convenient and economically viable catalytic method tolerates the various functional groups to provide the corresponding alkyl benzoates in up to 98% yields with up to 99% selectivity. (*Asian J. Org. Chem.*, **2021**, 10, 594 - 601)

An Atom-Economical Addition of Methyl Aza-arenes with Aromatic Aldehydes *via* Benzylic C(sp^3)–H Bond Functionalization under Solvent- and Catalyst-free Conditions

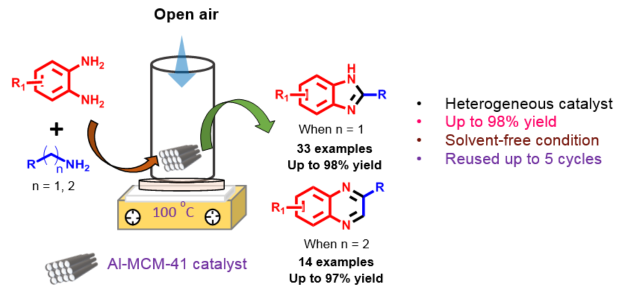
A convenient practical approach for the synthesis of 2-(pyridin-2-yl) ethanols by direct benzylic addition of aza-arenes and aldehydes under catalyst- and solvent-free conditions has been developed. This reaction was metal-free, green and carried out in facile operative environment without using any hazardous transition metal catalysts or any other coupling reagents. Different aromatic aldehydes and aza-arenes were monitored and the yields of products resulted from moderate to excellent. We have accomplished several aza-arene derivatives under neat conditions through high atom economical pathway. To evaluate the preparative potentiality of this process, gram scale reactions were performed up to 10 g scale. (*Beilstein J. Org. Chem.*, **2020**, 16, 3093 – 3103)





A Heterogeneous Catalytic Strategy for Facile Production of Benzimidazoles and Quinoxalines from Primary Amines using Al-MCM-41 Catalyst

A straightforward heterogonous catalytic (Al-MCM-41) approach to synthesize nitrogen heterocycle moieties from primary amines under solvent-free conditions has been developed. The Al-MCM-41 catalyst was prepared using a hydrothermal method and characterized by various analytical techniques. The catalytic methodology probability and limitations were presented with various substrates. The catalytic method grants an attractive route to a wide variety of benzimidazole and quinoxaline moieties with good to excellent yields. The gram scale and reusability (up to five cycles) capability of the Al-MCM-41 catalyst would greatly benefit industrial applications. (*Green Chemistry*, **2021**, 23, 9439 - 9446)

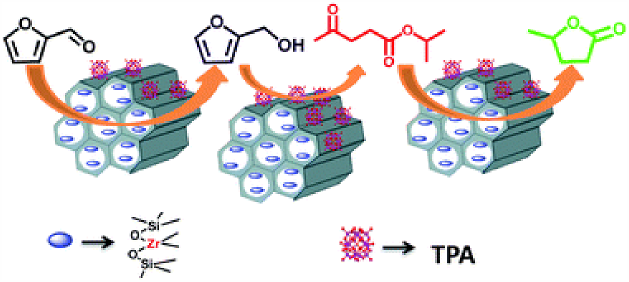


Biomass to Chemicals: Preparation of Fuel/fuel Additives

Biomass derived platform chemicals like carbohydrates, 5-hydroxyul methyl furfural (5-HMF) and furfural are converted to different value-added chemicals. A series of modified heteropoly acid catalysts are designed and used to prepare these chemicals by different processes like hydrolysis, esterification, etherification, catalytic transfer hydrogenation etc. Palladium exchanged vanadium incorporated supported heteropoly molybdate catalysts were developed for selective hydrogenation of furfural to yield Tetrahydrofurfuryl alcohol (THFAL). (*Sus. Energy & Fuels*, **2020**, 4 , 4768-4779)

One Pot Conversion of Furfural to γ-Valerolactone by Transfer Hydrogenation

One pot conversion of furfural to γ-valerolactone by transfer hydrogenation has been achieved over bifunctional mesoporous silica catalysts containing Zr and tungstophosphoric acid. The catalyst with ZrO_2 present inside the SBA-15 pores and TPA dispersed on the support showed the highest activity. The transfer hydrogenation activity depends on the interaction of the hydrogenating alcohol and the acid–base properties of the catalyst which are directed by the location of ZrO_2 or TPA in the support. (*Sustain. Energy & Fuels*, **2020**, *4*, 3428-3437; *Fuel*, **2020**, *1289*, 119900; *Sustain. Energy & Fuels*, **2021**, **5**, 3719 – 3728)



CO_2 Capture and Utilization

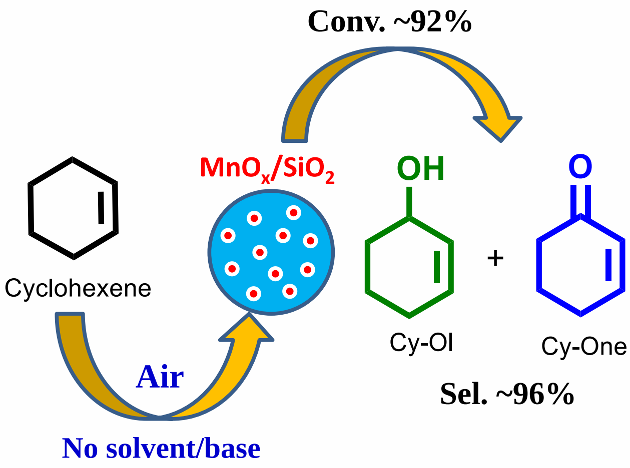
Waste biomass used for the preparation of biochar-based adsorbents for CO_2 capture at ambient conditions. The adsorbents were prepared by treating with acid, base and neutral condition. The acid treated adsorbents showed high adsorption activity. These carbon adsorbents also exhibited recyclability without any change in its adsorption capacity. (*Appl. Surf. Sci.*, **2020**, 530, 147226 - 147233)

Hydrogen Rich Syngas Production by Bi-Reforming of Methane with CO_2

Ni supported on mixed oxide catalysts are developed for the reforming of CO_2 with methane to yield synthesis gas. The activity of the catalysts depended on the mole ratio of mixed oxides and Ni content on the support. These are stable catalytic systems with more than 500 h stability. **(***Cat. Today***, 2020,** 356, 597-603)

Highly Dispersed MnO_x Nanoparticles on Shape-Controlled SiO_2 Spheres for Ecofriendly Selective Allylic Oxidation of Cyclohexene

This work reports the synthesis of a novel size- and shape-controlled catalyst, consisting of highly dispersed MnO_x nanoparticles (average particle size of 4.5 nm) on shape-controlled SiO_2 nanospheres (250–300 nm) for selective cyclohexene oxidation using air as the oxidant under solvent- and base-free conditions. The MnO_x/SiO_2 catalyst exhibited an excellent cyclohexene conversion (~ 92%) with a high selectivity (~ 96%) to the allylic products (2-cyclohexene-ol and 2-cyclohexene-one) under mild conditions, outperforming various SiO_2 supported CoO_x, FeO_x, and CuO_x catalysts. The study indicated the excellent stability of shape-controlled metal nanocatalysts in organic synthesis under economically viable and mild conditions. (*Cat. Lett.*, **2020,** 150, 3023 – 3035)

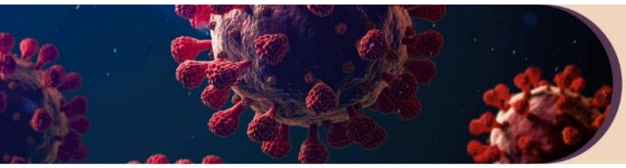


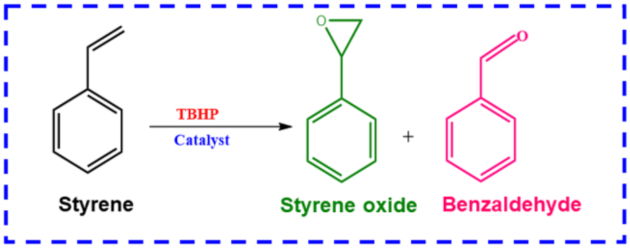
Solvent-Free Production of Glycerol Carbonate from Bioglycerol with Urea Over Nanostructured Promoted SnO_2 Catalysts

Nanostructured MoO_3 and WO_3 promoted SnO_2 solid acid catalysts were explored for the production of glycerol carbonate *via* carbonylation of bioglycerol with urea. The investigated reference SnO_2 and promoted catalysts were synthesized by fusion and wet-impregnation methods, respectively. Integration of SnO_2 with MoO_3 and WO_3 promoters leads to remarkable structural, textural, and acidic properties. A high quantity of acidic sites were observed over the MoO_3/SnO_2 catalyst followed by WO_3/SnO_2 and pure SnO_2, which played a key role in the carbonylation of bio glycerol with urea. The MoO_3/SnO_2 catalyst exhibited a high conversion and selectivity towards glycerol carbonate. This catalyst also exhibited remarkable stability with no significant loss of activity in the recycling experiments. (*Cat. Lett.*, **2020,** 150, 3626–3641)

Mesoporous Ce–Zr Mixed Oxides for Selective Oxidation of Styrene in Liquid Phase

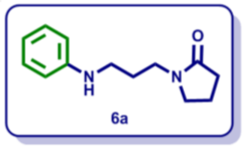
This work reports the synthesis of mesoporous Ce1-*x*-Zr*x*O2-δ (*x* = 0.5 and 0.8) mixed oxides with distinct Ce/Zr mole ratio by inverse micelle template method and their catalytic exploration for epoxidation of styrene in isopropanol solvent using TBHP as the oxidant. Among various catalysts investigated, the Ce0.8Zr0.2O2 combination catalyst exhibited best catalytic activity with ~ 98% conversion and ~ 90% selectivity to styrene epoxide. Catalytic efficiency was significantly improved with the increase of Ce and decrease of Zr content in the Ce–Zr mixed oxides. Reusability of the highly active Ce0.8Zr0.2O2 mixed oxide catalyst was also demonstrated. (*Appl. Petrochem. Res.***, 2020,**10, 67 - 76)





Ullmann Coupling Reaction of Bicyclic Amidines DBU/DBN with Aryl Halides: A Pathway to the Synthesis of γ-Caprolactam Derivatives

A selective mild approach to Ullmann amination of aryl halides to synthesize N-alkylated derivatives of γ-caprolactam. The synthetic route involves an *in situ* ring- opening of 1,8-diazabicyclo[5.4.0]undec-8-ene (DBU) followed by concurrent arylation with aryl halides in the presence of copper iodide as a catalyst under ligand-free conditions. This method provides a new entry to a wide variety of γ-caprolactam derivatives in a single synthetic sequence. Similarly, other bicyclic amidines such as 1,5-diazabicyclo-[4.3.0]non-5-ene (DBN), and 1,5,7 triazabicyclo [4.4.0] dec-5-ene (TBD) also showed good to very high reactivity. (*ChemistrySelect,* **2021,** 6, 5 - 8)



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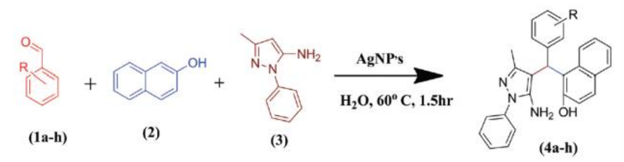
Bacterial Biosynthesis of Nanosilver: A Green Catalyst for Synthesis of (Amino Pyrazolo)-(Phenyl)Methyl Naphth-2-ol Derivatives and their Antimicrobial Potential

In the present study, heterogeneous silver nanoparticles, produced from isolated strain *Streptomyces sp*. RAB 10, 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 aqueous media. Some of the advantages of the multi-component one-pot protocol used in the study include shorter reaction time, good yield and ease of recoverability and reuse of the silver nanoparticles as catalysts. One of the important features of this methodology is the synthesis of a novel product with two reactive functional groups (hydroxy and free amine), which opens up avenues for the synthesis of a new array of compounds. The biosynthesized AgNPs as well as the naphthalene-2-derivatives exhibited moderate to good anti-microbial activity. (*New J. Chem.*, **2020**, 44, 13046 - 13061)



(η⁶-Arene) Ruthenium(II) Complexes with Ferrocene-Tethered Salicylaldimine Ligands: Synthesis, Characterization and Anti-Cancer Properties

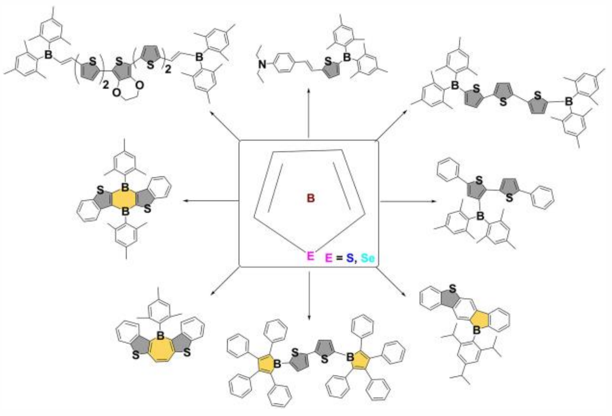
A series of ruthenium(II) complexes derived from ferrocenyl salicylaldimine ligands, coordinated in a chelating mode through the deprotonated phenolic oxygen atom and the imine nitrogen, were synthesized. The heterobimetallic Ru-Fe complexes were evaluated for *in vitro* anti-cancer activity against human liver cancer (HepG2) and human cervical cancer (HeLa) cell lines and showed better activities compared to the ferrocenyl salicylaldimine ligands. Among the heterobimetallic complexes, two compounds showed enhanced cytotoxicity against HeLa cancer cells (IC50 value of 9.34 mM compared to 31.32 mM for cisplatin), and HepG2 cancer cells (IC50 value of 15.74 mM compared to 27.95 mM for cisplatin), respectively. Mechanistic studies indicated the active compound induced cell cycle arrest in the S phase. Further it resulted in increased ROS generation and loss of mitochondrial membrane potential in HepG2 cells. (*Polyhedron,* **2020**, 192, 114829)

Bioactive Isatin (Oxime)-Triazole-Thiazolidinedione Ferrocene Molecular Conjugates: Design, Synthesis and Antimicrobial Activities

Molecular conjugates often combine the inherent properties of the individual components and exhibit a different characteristic feature. Introduction of an organometallic moiety can indeed augment the overall effect. This work narrates the synthesis of ferrocene appended isatin -2,4-thiazolidinedione molecular hybrid linked via a triazole moiety. Isatin and 2,4-thiazolidinedione were linked via a triazole unit formed by a simple copper catalysed alkyne-azide 1,3-dipolar cycloaddition reaction. Antimicrobial activity against some selected gram-positive and gram-negative strains, examined for the compounds revealed similar antimicrobial activity for all tested microbes and similar pattern to that of standard antibiotics. (*Journal of Organometallic Chemistry,* **2021**, 937, 121716 -121725)

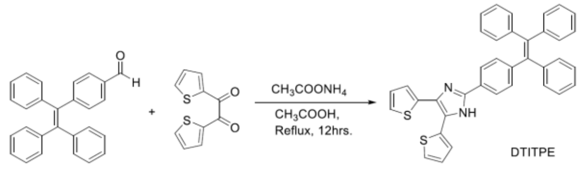
π-Conjugated Materials Derived from Boron-Chalcogenophene Combination. A Brief Description of Synthetic Routes and Optoelectronic Applications

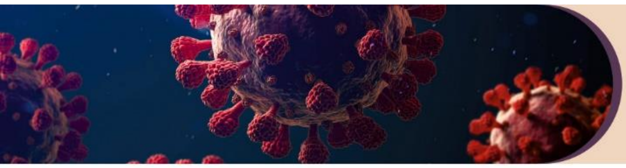
This review describes the categories, synthetic routes and optoelectronic applications of a range of boron-chalcogenophene conjugates. Conjugation and linking of different types of tri- and tetracoordinated boron moieties with chalcogenophenes have remained an important strategy for constructing a range of functional materials. Tin-boron and silicon-boron exchange protocols have been efficiently adapted to access these boron-chalcogenophenes. The chemical and electronic properties of such boron-chalcogenophene conjugates are directly influenced by the strong Lewis acid character of trivalent boranes which can further alter the intra- and intermolecular Lewis acid-base interactions. Apart from the synthetic protocols, recent advances in the application of these boron-chalcogenophene conjugates towards analyte sensing, organic electronics, molecular switches and several other aspects are discussed. (*Chem. Rec.* **2021**, 21, 1–34)



Tetraphenylethylene-Substituted Bis(thienyl)imidazole (DTITPE), an Efficient Molecular Sensor for Detection and Quantification of Fluoride Ions

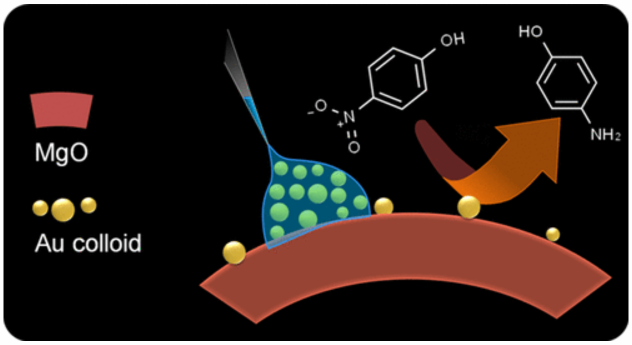
Fluoride ion plays a pivotal role in a range of biological and chemical applications however excessive exposure can cause severe kidney and gastric problems. A simple and selective molecular sensor, 4,5-di(thien-2-yl)-2-(4-(1,2,2-triphenylvinyl)-phenyl)-1H-imidazole, DTITPE, has been synthesized for the detection of fluoride ions, with detection limits of 1.37 x 10^{-7} M and 2.67 x 10^{-13} M, determined by UV-vis, and fluorescence spectroscopy, respectively. The variation in the optical properties of the molecular sensor in the presence of fluoride ions was explained by an intermolecular charge transfer (ICT) process between the bis(thienyl) and tetraphenylethylene (TPE) moieties upon the formation of a N-H—F hydrogen bond of the imidazole proton. Test strips coated with the molecular sensor can detect fluoride ions in THF, undergoing a color change from white to yellow, which can be observed with the naked eye, showcasing their potential real-world application. (*Chemosensors,* **2021**, 9, 285 – 299)





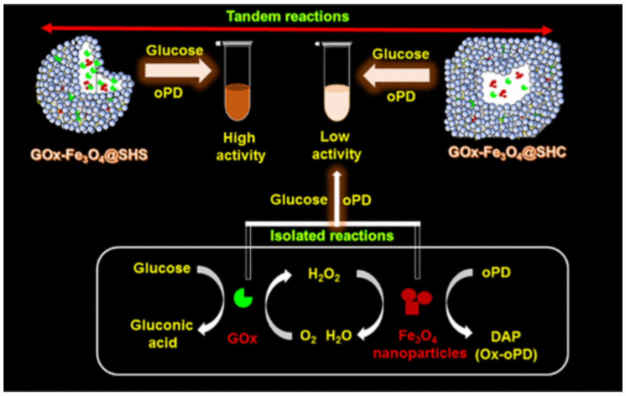
Influencing the Electron Density of Nanosized Au Colloids *via* Immobilization on MgO to Stimulate Surface Reaction Activities

Heterogenization of colloidal gold on MgO is demonstrated to facilitate its catalytic surface reactivity to obtain high activity. The immobilization of pre-synthesized colloidal Au on MgO leads to well-dispersed nanosized Au on MgO with an enhancement in the electron density of Au. The Au/MgO catalyst has a surface rate constant of $\sim 1.39 \times 10^{-3}$ mol m^{-2} s^{-1}, which is significantly higher than those reported for other catalysts. While it validates the higher catalytic activity with a TOF of 9456 h^{-1} observed for Au/MgO, the increased adsorption constant for 4-nitrophenol on Au/MgO further reflects the efficacy of MgO as the support. Thus the method not only allows effective heterogenization of the Au nanoparticles keeping the catalyst stable under the reaction conditions and being reused several times, but also renders a capability in reduction of other nitro group-containing substrates. (*Langmuir,* **2020,** 36, 14203–14213)



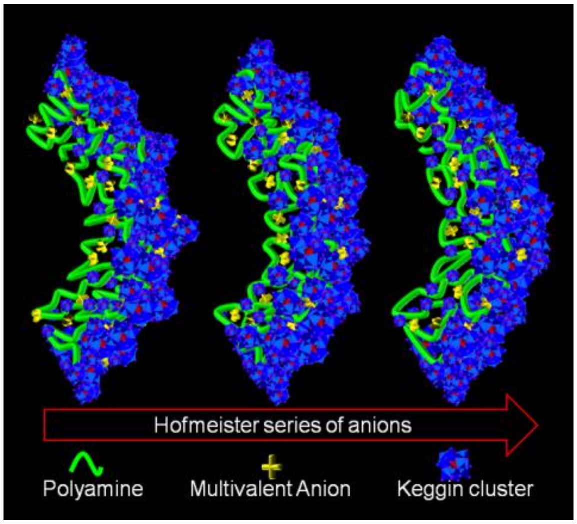
Spatial Confinement of Enzyme and Nanozyme in Silica-Based Hollow Microreactors

A strategy for encasing enzymes and nanozymes in microreactors with spatial confinement with improved selectivity and activity is demonstrated by utilizing glucose oxidase (GOx) and poly(ethylenimine)-conjugated magnetite nanoparticles (Fe_3O_4−PEI) as nanozyme. The microreactors are prepared by polyallylamine hydrochloride (PAH)-mediated silica nanoparticle assembly on $CaCO_3$ particles as a removable core. By tuning both shape and phase (vaterite/calcite and pure calcite) of $CaCO_3$, it allows construction of GOx and Fe_3O_4−PEI encapsulated silica hollow microspheres and microcubes. The confined GOx in the microreactors is able to catalyze oxidation of glucose to gluconic acid and hydrogen peroxide (H_2O_2), followed by the activation of H_2O_2 by Fe_3O_4-PEI for the oxidation of the chromogenic substrate *o*-phenylenediamine (oPD) to 2,3- diaminophenazine. The hollow microspheres result in activity 14 times higher than that of the hollow microcubes. The evaluation of kinetic parameters indicates a fivefold increase in the catalytic constant (kcat) of Fe_3O_4−PEI confined in hollow microspheres. (*ACS Appl. Mater. Interfaces,* **2020,** 12, 45476 - 45484)



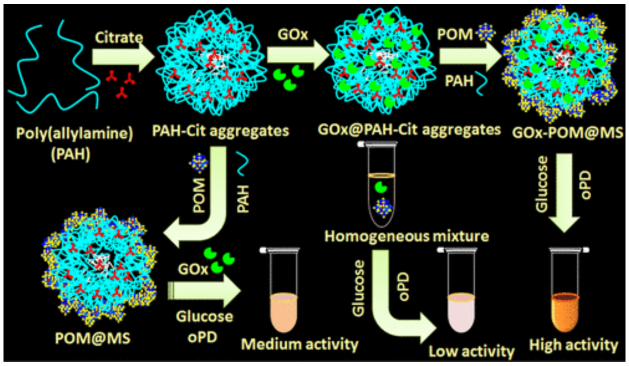
Tunable Surface Wrinkling by a Bio-Inspired Polyamine Anion Coacervation Process that Mediates Assembly of Polyoxometalate Nanoclusters

A bio-inspired method is developed to render controlled wrinkling surface patterns on supramolecular architectures assembled from polyoxometalate (POM) clusters. It involves a polyamine-multivalent anion interaction generating positively charged coacervates, which while dictating the assembly of POM into spherical structures further facilitate an interesting surface morphogenesis with wrinkling patterns. As the polyamine-anion interaction becomes stronger, the wrinkles turn denser with lesser depth, which eventually undergoes post-buckling to engender a complex surface pattern. Interestingly, the order of influence exerted by different anions on the morphology follows the Hofmeister series. (*Angew. Chem. Int. Ed.*, **2020**, *59*, 8160 - 8165)



A Bioinspired Assembly to Simultaneously Heterogenize Polyoxometalates as Nanozymes and Encapsulate Enzymes in a Microstructure

A polyamine-mediated bioinspired strategy to assemble polyoxometalate (POM) [phosphotungstic acid (PTA)/ phosphomolybdic acid (PMA)] nanoclusters and glucose oxidase (GOx) generating microsphere structures under very mild reaction conditions is demonstrated. The enzyme assay shows that the activity of GOx is totally preserved during the assembly process, and the enzyme loading is slightly improved with the increase in the pH of the medium. Importantly, the confinement and proximity of GOx and POM in the microspheres not only play a crucial role in defining the peroxidase-like activity of POM but also endow high selectivity (by virtue of GOx) in detecting glucose at physiological pH conditions. Thus, the microsphere assembly, while enabling effective heterogenization of the POM as a nanozyme, simultaneously addresses the issues related to high cost and instability associated with natural peroxidases.

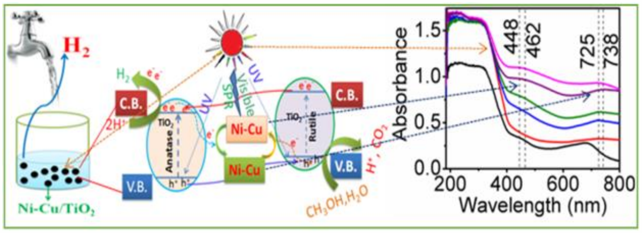


(*ACS Sustainable Chem. Eng.*, **2021**, *9*, 15819 -15829)

Hydrogen Production by Photocatalytic H_2O Splitting

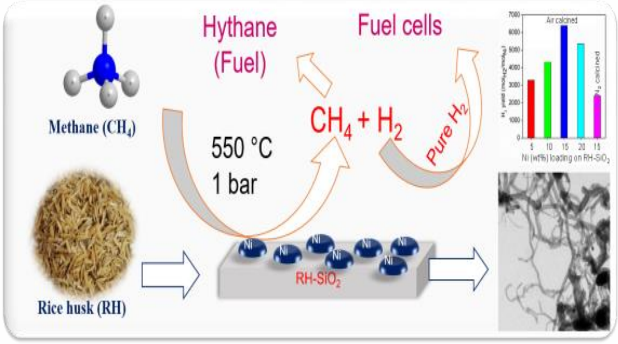
Improved H_2 Yields over Cu-Ni-TiO_2 under Solar Light Irradiation: Behaviour of Alloy Nano Particles on Photocatalytic H_2O Splitting

Bimetallic catalysts exhibit improved catalytic performance when compared with their monometallic catalysts. Among the base metals loaded TiO_2, the surface plasmonic resonance (SPR) effect of Ni and/or Cu based bimetallic photocatalysts have attracted much attention, since they represent a class of favorable photocatalysts which are playing a vital role. The present study has identified the bimetallic Cu-Ni alloy nanoparticles decorated on TiO_2 exhibited remarkably improved visible light photo catalytic activity (fourfold) when compared to their monometallic counterparts in H_2O splitting. The superior performance of Cu-Ni alloy particles was attributed to surface plasmon behavior of the Cu-Ni/TiO_2 photocatalyst. (*Appl. Catal. B: Environmental*, **2021**, *299*,120654 – 120665)



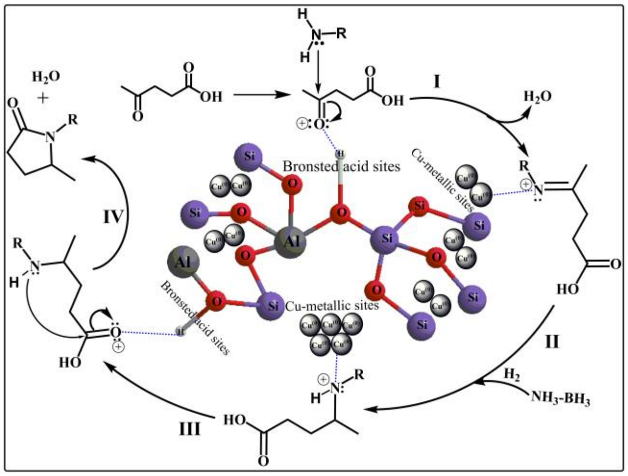
Hydrogen Production by Catalytic Cracking of CH_4 (CMC)

A wide variety of support materials such as SiO_2, TiO_2, MgO, Al_2O_3, ZrO_2 and zeolites were explored for Ni to enhance the longevity of the catalyst in CMC. The process of silica extraction from rice husk ash can be a feasible alternative to commercial silica precursors. Silica derived from rice husk (RH) was synthesized and examined for CH_4 cracking for the CO or/and CO_2 free H_2 production. The Ni supported on RH SiO_2 (calcined in air) showed higher catalytic performance than the RH-carbon–silica obtained in N_2 flow. The difference in catalytic activities of Ni supported on SiO_2-RH both air and N_2 calcined samples and the H_2 yields reported earlier over Ni supported on commercial SiO_2 were rationalized. (*J. Energy Inst.*, ***2021***, 99, 73-81)



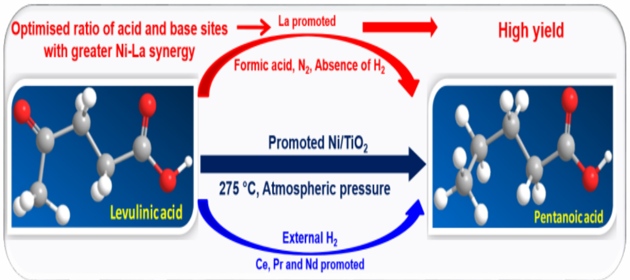
Chemoselective Synthesis of Pyrrolidones by Hydrogenation of Levulinic Acid (LA)

$Cu^{(0)}$/H-ZSM-5 was identified as a chemoselective catalyst in the reductive amination of levulinic acid for the synthesis of pyrrolidones at ambient pressure and in aqueous media. The chemoselective nature of Cu was explained by carbonyl interaction with surface Brønsted acid sites deduced by pyridine and acetone adsorbed *in situ* infrared (IR) spectroscopic studies in conjunction with N_2O titration. A strong polarization of band at 1685 cm^{-1} and an increase in its intensity with a decrease in Si/Al ratio of the H-ZSM-5 was found to be a key factor in the reductive amination activity. (*Appl. Catal. B: Environmental*, **2021**, 292, 120177)



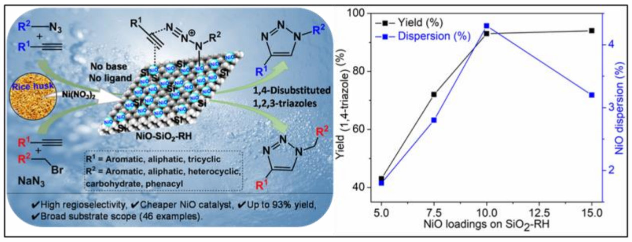
Hydrogenation of Levulinic Acid to γ-Valerolactone and Valeric Acid

Titania supported Ni catalyst modified by different lanthanides (La, Ce, Pr and Nd) were evaluated for the one-step conversion of levulinic acid (LA) to valeric acid (VA) using formic acid as a hydrogen source. Among these the La modified Ni/TiO_2 demonstrated better VA yields with an optimum LA to VA mole ratio 1:3. Presence of weak Lewis and strong basic sites present on the Ni-La/TiO_2 surface was the reason for higher VA selectivity. A combination of metallic Ni with surface acid-base sites were responsible for the formation of VA in single step. Using aqueous γ-valerolactone 99% selectivity towards VA was achieved. A plausible reaction mechanism has been proposed based on the kinetic data obtained at moderate temperatures and ambient pressures. (*ChemCatChem*, **2020**, *12*, 1; *Cat. Today*, **2021**, 375, 112)



Catalysis for Fine Chemical Synthesis

Renewable SiO_2 as support for NiO catalyst for regioselective synthesis of 1,4-disubstituted 1,2,3-triazoles from azide-alkyne cycloaddition in aqueous media. (*New J. Chem.*, **2020**, *44*, 5972 - 5979)

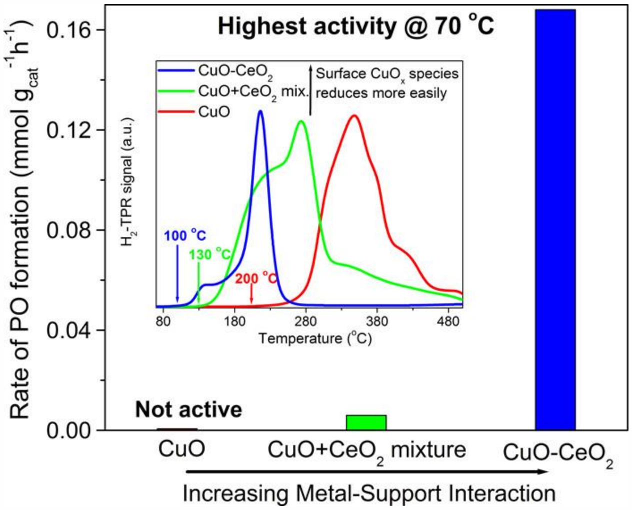


Ultra-Low-Temperature CO Oxidation Activity of Octahedral Site Cobalt Species in Co_3O_4 Based Catalysts: Unravelling the Origin of Unique Catalytic Property

In this study, three model spinel catalysts including $MnCo_2O_4$, $MnFe_2O_4$, and $CoCr_2O_4$ have been chosen to understand the unusual catalytic activity. Low-temperature CO oxidation activity decreases in the following order: $MnCo_2O_4 \gg MnFe_2O_4 > CoCr_2O_4$. It indicates that the Co^{2+} species in a tetrahedral site (in $CoCr_2O_4$) remains inactive for low-temperature catalytic activity, while Co^{3+} in an octahedral site (in $MnCo_2O_4$) is active in Co_3O_4 based catalysts. The intensity of the redox peak for CO oxidation involving a Co^{3+}/Co^{2+} couple in $MnCo_2O_4$ indicates a highly favourable reaction, while a nonresponsive behaviour of Co species is observed in $CoCr_2O_4$. (*J. Phys. Chem.C*, **2019**, *123*, 19557–19571)

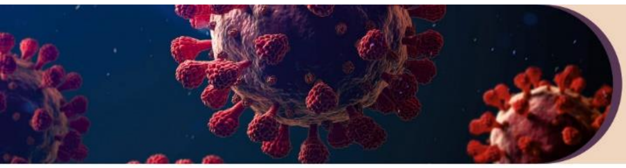
Low-Temperature Propylene Epoxidation Activity of $CuO-CeO_2$ Catalyst with CO + O_2: Role of Metal−Support Interaction on Reducibility and Catalytic Property of CuO_x Species

The propylene epoxidation activity of solution combustion synthesized Cu/CeO_2 catalysts with the CO + O_2 mixture at low temperatures (50−100 °C) peaking at ~80 °C was studied. The highest PO yield was obtained with 20−25% Cu loading in CeO_2. In contrast, the reaction over the catalyst containing nonreducible support such as Cu/SiO_2 occurred above 170 °C. The highest activity relates to the optimum presence of CuO along with $Ce_{1-x}Cu_xO_{2-\delta}$. The reducibility of the Cu species in two phases was significantly shifted toward lower temperatures. The substituted Cu^{2+} was reduced first, and then, the bulk CuO reduction was initiated. It is proposed that substituted Cu^{2+} along with Ce^{4+} is reduced easily, and then, Ce^{3+} promotes the reduction of the interfacial CuO phase that might donate active oxygen species for epoxidation reaction. (*J. Phys. Chem. C*, **2020**, *124*, 14131-14146)

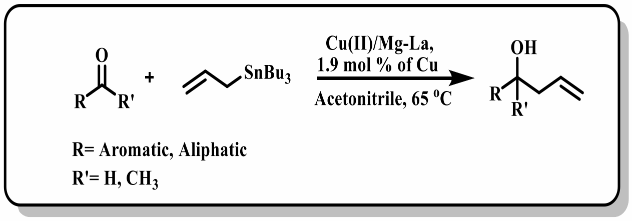


Copper-Impregnated Magnesium-Lanthanum Mixed Oxide: A Reusable Heterogeneous Catalyst for Allylation of Aldehydes and Ketones

Copper-impregnated magnesium-lanthanum mixed oxide [Cu(II)/Mg- La] was used as catalyst in synthesis of homoallylic alcohols from aldehydes and ketones using allyltributylstannane as the allylating source. The present protocol provides a great application potential for the synthesis of corresponding allyl alcohols with excellent yields and selectivity. The catalyst exhibits broad functional group compatibility with a variety of substituted aldehydes and ketones to furnish the desired products in high yields under heterogeneous conditions. Importantly, the heterogeneous catalyst could be recovered from the reaction mixture by



centrifugation and used up to three cycles. (*Adv. Synth. Catal.*, **2020**, *362*, 1176 – 1183)



APPLIED RESEARCH

Process Development for *p*-Methoxy Acetophenone from Anisole

p-Methoxy acetophenone (PMAP) is widely used as a fragrance, and a flavoring in food. It is also used as a pharmaceutical intermediate (for PMPAA preparation). Catalytic acylation of anisole under continuous mode with exclusive selectivity towards PMAP with high conversion has been developed.

Dicyanadiamide (DCDA)

The calcium carbide to calcium cyanamide route is world-wide accepted for the commercial production of DCDA. Calcium cyanamide is the key starting material for the production of dicyandiamide and it is not manufactured in India. An efficient process for DCDA was developed using three steps: Nitrogenation of Calcium Carbide; Hydrolysis of Calcium Cyanide and dimerization of cyanamide to DCDA, under MAKE IN INDIA flagship program.

Validation of the Heterogenous Catalyst Developed for Oxidation of Mesitylene to Produce 3,5 Dimethyl Benzoic Acid (DMBA)

Due to the disadvantages of homogeneous catalyst and process involved, a heterogeneous catalyst for the oxidation of mesitylene using O_2 as an oxidant to dimethyl benzoic acid has been developed.

Preparation of *o*-Chlorobenzonitrile by Ammoxidation of *o*-Chloro Toluene

The synthesis of aromatic nitriles particularly *o*-chloro benzonitrile is an important chemical widely used in pharma industry. A continuous catalytic process for its synthesis has been developed. The process was successfully demonstrated and transferred to industries (Indian Patent Application No: 0040NF2020).

Synthesis of 5-Chloro Indanone

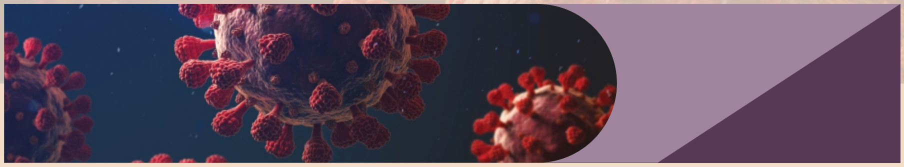
The catalytic process for synthesis of 5-Chloro Indanone from 3-Chloro-1-(4-chlorophenyl)-1-Propanone by vapour phase reaction using Zeolites as Catalysts was developed. The process involved regeneration of the catalysts, which was demonstrated.

Recovery of Hydrocarbons from Oil Sludge to Reduce Environmental Impact

Petroleum industries generate huge quantities of oil sludge containing hydrocarbons (PHCs), water, heavy metals, and solid particles. Variety of oily sludge treatment methods exist but, due to the recalcitrant nature of oily sludge, few technologies can reach a compromised balance between environmental benefits and treatment costs. Possibilities oil recovery from ONGC oil sludge was studied and achieved around 85% (without water) oil recovery using thermal cracking and distillation. The recovered oil obtained from thermal cracking is in the distillation range of 100-250 °C.

Exploratory Studies on Catalytic Process for the Preparation of Propylene Carbonate using Propylene Oxide and Carbon Dioxide

Propylene carbonate production is one of the carbon dioxide sequestration methods, which is considered as an important research area of green chemistry & catalytic chemistry. Carbon dioxide is the least expensive feedstock with lowest reactivity, and can be transformed into more reactive compounds such as urea and cyclic carbonates. Here propylene oxide and carbon dioxide at certain pressure and temperature directly reacted in presence of catalyst to give propylene carbonate. The established process using industrially known homogeneous catalysts and other parameters was demonstrated.



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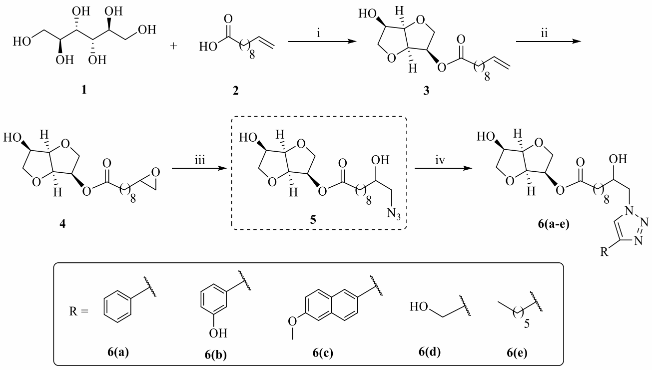
BASIC RESEARCH

Isomannide Monoundecenoate-based 1,2,3-Triazoles: Design, Synthesis, and *in vitro* Bioactive Evaluation: A new series of isomannide monoundecenoate-based 1,2,3-triazole analogs 6(a-e) were synthesized and screened against antibacterial and antifungal activities. Some of the products possessed highly selective inhibition towards Gram-positive bacterial strains, *Bacillus subtilis* and *Staphylococcus aureus* with MIC value of 3.9 µg/mL. Further, they also exhibited antifungal activity against the tested panel of *Candida* strains with MIC value of 3.9 µg/mL. These were evaluated for their *in vitro* cytotoxic activities against A549, MCF7, DU145 and HeLa cancer cell lines. One analog displayed good cytotoxic activity towards all tested human cancer cell lines without any significant effects on normal cell line (HUVEC). (*J. Heterocycl. Chem.*, **2020**, 57, 4312-4321)



Synthesis of isomannide monoundecenoate-based 1,2,3-triazoles

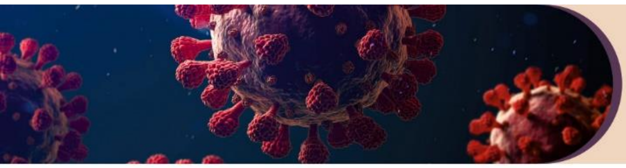
The Kinetics of the Esterification of Free Fatty Acids in Jatropha Oil using Glycerol based Solid Acid Catalyst: The work presents the kinetics of the esterification of Free Fatty Acids (FFA) in jatropha oil with methanol (Alc) using glycerol based solid acid catalyst (SAC). Based on the experimental results a second order kinetic model is proposed. The temperature influence on the rate of the reaction, Arrhenius constants and activation energies were evaluated. The reaction heat and energy of activation for the reaction were found to be 10.315 kcal/mol and 11.38 kcal/mol respectively. (*Eur. J. Sust. Devl. Res.*, **2020**, 4, em0116)

Synthesis of Ricinoleate Anion Based Ionic Liquids and their Application as Green Lubricating Oil Additives

Ricinoleate anion based ionic liquids (ILs) were synthesized from four different nitrogen containing cationic counterparts. Tribological performance of synthesized ILs were evaluated using four ball tribo tester by blending with two lubricant base oils namely epoxy 2-ethylhexyl esters of karanja fatty acids (EKE) and dioctyl sebacate (DOS). Anti-wear behavior was explored by varying different factors. It was found that the synthesized ILs in base oil significantly reduced the wear scar diameter for all the tested applied load (40 to 80 kg) and rotation speed (1200 rpm to 1742 rpm). Further, the load carrying capacity of base oil was improved by 25-43% at 1.25 wt% of IL dosage. The imidazolium cation containing IL outperform tribological performance among all the ILs being studied. The morphology of worn surface after the wear tests and deposition of elementals on the worn surface lubricated with neat base oil and IL blended base oil was studied. (*J. Saudi. Chem. Soc.*, **2020,** 24,742 - 753)

Synthesis and Tribological Investigation of 4-Vinyl Guaiacol–based Thioether Derivatives as Multifunctional Additives and their Interactions with the Tribo Surface using Quantum Chemical Calculations

Novel 4-vinyl guaiacol based thioether derivatives were synthesized in a three-step reaction procedure by thiol-ene coupling as the key step. It was found that the synthesized products exhibited superior antioxidant performance compared to butylated hydroxytoluene (BHT). All the three synthesized additives have improved tribological properties of the base oil 2-ethylhexyl esters of karanja fatty acids (EKE) and dioctyl sebacate (DOS). Dithio derivative at 0.75 wt% reduced the wear scar diameter by 36%



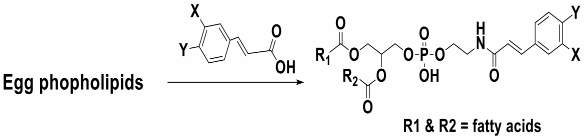
and at 1 wt% improved the weld point by 33% of base oil EKE. Surface and elemental analysis result suggests that in the tribochemical process the synthesized thioether derivatives decompose and form an effective tribofilms on interacting surfaces. X-ray Photoelectron Spectroscopy (XPS) of the surface lubricated with base oil containing DMFD was evidence for the formation of tribofilm with FeS, $FeSO_4$ and Fe_2O_3. Overall the dithio derivative is more effective as antiwear, extreme pressure and antioxidant bio lubricant additive than other thioether derivatives. (*J. Saudi. Chem. Soc.*, **2020,** 24, 942)

Synthesis of Fatty Alcohol based Sterically Hindered Esters as Potential Antioxidants for Bioadditives

Four hindered phenolic esters were prepared by esterification of 3-(3,5-Di-tert-butyl-hydroxyphenyl)propionic acid and fatty alcohols. The synthesized esters were studied for their antioxidant properties and thermal stability. Differential scanning calorimetry (DSC) and Rancimat studies were conducted to explore the effect of synthesized compounds on oxidation stability of base oil. The results from both the studies were correlated well. Thermo gravimetric analysis indicates that all the esters have significantly high thermal stability. Among all the prepared compounds myristyl alcohol ester showed better antioxidant properties whereas, stearyl alcohol ester exhibited higher thermal stability. The synthesized antioxidants can be potential bio additives for lubricant formulations. *(Pet. Chem.*, **2020**, 60, 1309 - 1316)

Synthesis, Characterization & Evaluation of Structured Phospholipids

Synthesis of new N-phenoyl phosphatidylethanolamine derivatives was carried out by the modification of natural egg phosphatidylethanolamine (PE) with various phenolic acids. The products were evaluated for their preliminary *in vitro* antioxidant and cytotoxic activities. The compounds N-4-hydroxy-3-methoxy cinnamoyl PE, N-4-hydroxy-3,5-dimethoxy cinnamoyl PE and N-(3,4)-di hydroxy cinnamoyl PE exhibited excellent radical scavenging activity with EC50 values of 9.7, 1.5 and 2.7 µg/mL, respectively which were lower than the standard BHT and α-tocopherols. The synthesized compounds exhibited moderate to very good anticancer activity against four cancer cell lines such as HeLa, B16-F10, SKOV3 and MCF-7 using doxorubicin as a positive control. (*SN Applied Sci.*, **2020**, 2, 1229 – 1239)



Synthesis of structured phospholipids

Synthesis, Cytotoxic Evaluation of Novel 2-((1H-Indol-3-yl) Methyl)-5-Alkyl-1,3,4- Oxadiazole and 2-Alkyl-5-(3,4,5-Trimethoxyphenyl)-1,3,4-Oxadiazole Derivatives

A series of novel 2-((1H-indol-3-yl) methyl)-5-alkyl-1,3,4-oxadiazoles and 2-alkyl-5-(3,4,5-trimethoxyphenyl)-1,3,4-oxadiazole analogues have been synthesized and evaluated for their cytotoxicity against A549, MCF-7 and HeLa cell lines. Almost all the tested compounds reveal cytotoxicity against all the cell lines, especially 2-((1H-indol-3-yl) methyl)-5-alkyl-1,3,4-oxadiazoles based compounds which display potent inhibitory activity with IC50 values ranging between 8.26 to 11.36 µM. (*Indian J. Chem.*, **2020**, 59B, 465-473)

Synthesis and Antimicrobial Evaluation of Novel Alkylated Piperazine-based Fluoroquinolone Carboxylate Derivatives

Alkylated quinolone-piperazine analogues, ethyl 1-ethyl-6-fluoro-7-(4- hexylpiperazin-1-yl)-4-oxo-1,4-dihydroquinoline-3-carboxylate and derivatives were synthesized and studied for antimicrobial activity. Hexyl analog exhibited potent antimicrobial activity against *Staphylococcus aureus* MTCC 96, *Bacillus subtilis* MTCC 121, *Micrococcus luteus* MTCC 2470 (MIC value 1.9µg/mL). Heptyl analogue and nonyl analogue showed significant activity with MIC value 3.9µg/mL. In the case of antifungal screening, some compounds showed significant antifungal activity against *Candida albicans* MTCC 3017 with MIC value ranged from 3.9 to 7.8µg/mL. Butyl analogue shows potent minimum bactericidal concentration activity with MIC value 3.9µg/mL against the tested strains. (*Indian J. Chem.*, **2020**, 59B, 474-484)

A Comparative Study on Some Lesser Known Tree Borne Oilseed-based Biodiesel Feedstocks of Indian Origin

Feasibility of biodiesel production from *Melia dubia* seed kernel oil, *Butea parviflora*, *Knema attenuata* seed oils were investigated and compared with *Swietenia mahagoni* biodiesel. All the fatty acid methyl esters were within the range of European Specification (≥96.5%). The oxidative stabilities of biodiesels were found to be within the range of ASTM specification (3 h minimum). Even though, *butea* (5.05) exhibits slightly higher viscosity compared to *knema* (4.6 cSt) their viscosity profiles are comparable to that of sunflower (4.52), soybean (4.2), rapeseed (4.4) biodiesels. Cloud points and pour points of all the biodiesels were within the range of ASTM specification (−3 to 12) and (−15 to 10°C), respectively. The flash points were also within the range of EN specifications (≥ 120°C) and are lower compared to that of soybean (171°C), sunflower (177°C) and rapeseed (170°C) biodiesels. (*J. Lipid Sci.Technol.*, **2020**, 52, 11-22)

Optimization of the Enzymatic Pre-Treatment Process for Mustard Oilseeds using Response Surface Methodology

The effect of an enzymatic pre-treatment process for the extraction of oil from black mustard seeds (*Brassica nigra*) using viscozyme, the reaction parameters such as temperature, buffer-to-seed ratio and enzyme concentration were considered as determinant factors in the central composite design. The effects of enzyme concentration (5–12%), temperature (40–55 °C), pH (5.0–6.0), and reaction time (1–7 h) on the free oil liberated were studied. Residual oil was collected by subjecting the treated meal to soxhlet extraction for 4 h. An enzyme dose of 7.5% (w/w), pH 5.0, 50 °C, and 5 h with constant shaking at 450 rpm were found to be optimal conditions. Centrifuging the mixture at 7000 rpm for 30 min separated the oil with a recovery of 71–73.1%. (*Grasas Y Aceites*, **2020**, 71, e351)

Selective Extraction of Polar Lipids of Mango Kernel using Supercritical Carbon Dioxide (SCe-CO₂) Extraction: Process Optimization of Extract Yield/Phosphorous Content and Economic Evaluation

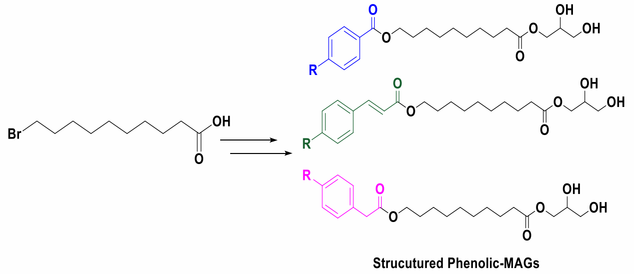
Supercritical carbon-dioxide is employed for the selective extraction of polar lipids from the lipid matrix in mango kernel for the first time. The process parameters affecting the extraction such as pressure, temperature and flow rate are ranged in the intervals of 30-50 MPa, 40-60 ^{o}C and 10-30 gmin^{-1}, respectively. Optimisation using Box Behnken design obtained the highest yield of 3.38% at 40^{o}C, 50 MPa and 30gmin^{-1}. The phosphorous content was evaluated to understand the behaviour of polar lipids extraction at higher pressures. (*Chemosphere,* **2020**, 260, 127639 - 127649)

Tribological Properties of 10-Undecenoic Acid-Derived Schiff Base Lubricant Additives

Four Schiff bases were synthesized by condensation of methyl 11-(2-aminoethylthio) undecanoate with various aromatic aldehydes and evaluated for their tribological and antioxidant performances in bio-lubricant base oil, namely epoxy 2-ethyl hexyl esters of karanja fatty acids. The Schiff bases act as good anti-wear and extreme pressure additives. A significant reduction in wear scar diameter was observed at a very low concentration (0.6 wt%), whereas, at 1 wt% concentration, weld point enhancement observed from 160 to 230 kg. Quantum chemical calculations based on density functional theory for the interactions of Schiff bases with surfaces correlated with experimental wear data. Overall, the dimethoxy-substituted phenyl ring containing Schiff base was more effective in enhancing the anti-wear and extreme pressure performance of base oil, whereas dihydroxy-substituted phenyl ring containing Schiff base exhibited good antioxidant property. (*Arab. J. Sci. Eng.*, **2021**, 46, 5593 - 5603)

Studies on Novel Structured Monoacylglycerol Derivatives with Phenolic Acids

Novel structured monoacylglycerol (MAG)-based phenolic lipids were synthesized from 11-bromoundecanoic acid, phenolic acids, and solketal. Selected phenolic acids were employed for synthesis of ten novel MAG-based phenolic lipids. All the compounds were evaluated for antioxidant, antimicrobial, and cytotoxic activities. MAG derivative comprising sinapic acid exhibited excellent antioxidant activity in both DPPH assay and inhibition of lipid oxidation assay. MAG derivative bearing *p*-coumaric acid showed good antimicrobial activity against both gram-positive and gram-negative bacterial strains with a minimum inhibitory concentration value of 6.25 μmmL^{-1}. All the synthesized compounds were found to exhibit cytotoxicity against studied cell lines, where sinapic and *p*-coumaric acid derivatives exhibit better activities compared to other derivatives. (*Eur. J. Lipid Sci. Technol.*,**2021**, 123, 2100055)



Synthesis of structured monoacylglycerol derivatives with phenolic acidsphospholipids

Isolation and Characterization of Seed Oils

The seeds of Red sanders (*Pterocarpus santalinus*) collected from the forest of southern region of India (Andhra Pradesh state) were analyzed for oil content along with physico-chemical properties. The seed kernel was found to contain 16.8% oil which was analyzed for various physico-chemical parameters. The prominent fatty acid was found to be linoleic acid (45.8 %) followed by oleic (17.5 %), palmitic (14.2 %) and stearic (8.1%) acids respectively. Neutral lipids were the dominant lipid fraction (98.4%) in the oil with linoleic as the most abundant fatty acid. (*J. Lipid Sci. Technol.*, **2021**, 53, 15-21)

Detection and Quantification of Palmolein and Palm Kernel Oil Added as Adulterant in Coconut Oil based on Triacylglycerol Profile

A HPLC method has been developed to detect and quantify the degree of adulteration of coconut oil with palmolein and palm kernel oil based on triglyceride structure. The normalized area percentage of trilaurin (LaLaLa; ECN36) among the three major TAG molecular species (ECN34, 36 and 38) of coconut oil was chosen as detection index for quantifying degree of adulteration of coconut oil with palm kernel oil. While the area ratio of POP: LaLaLa (dipalmitoyl-mono-olein : trilaurin) was chosen as detection index for quantifying adulteration of coconut oil with palmolein. The RP-HPLC based method is effective with a 2-4% minimum detection limit of adulterant oils and 78-98% detection accuracy depending on the degree of adulteration and types of oil. (*J. Food Sci. Technol.*, **2021**, 58, 4420-4428)

Extraction of γ-Oryzanol from De-Fatted Rice Bran using Supercritical Carbon Dioxide SCE-CO_2: Process Optimization of Extract Yield, Scale-Up and Economic Analysis

Supercritical carbon dioxide (SC-CO_2) extraction, an alternative to flammable, toxic, non-ecological solvent extraction was carried out in this study to extract γ-oryzanol, a potent bioactive ingredient, from defatted rice bran. The response surface methodology was applied on the handling parameters such as temperature, pressure and CO_2 flow rate. Extraction of γ-oryzanol is investigated at low pressures, such as 15, 20 and 25 MPa. The highest (optimum) yield of γ-oryzanol was 36000 mg.kg^{-1} at 10 w/w% of ethanol as co-solvent and the corresponding temperature, pressure and CO_2 flow rate were 48.9 ^{o}C, 23.9 MPa and 29.8 g.min^{-1}, respectively. The return of investment of the plant processing 3,000 tonnes of rice bran per year accounts for a net present value almost double the investment cost having a payback period of around 5 years. (*Process Saf. Environ. Prot.*, **2021**, 148, 179-188)

APPLIED RESEARCH

Process Development for the Enrichment of Phosphatidylcholine (PC) upto 90 & 95% from Sunflower and Soya Lecithin Powders

The study was to develop a process to enrich PC to >95% from soya lecithin powder and PC>90% from sunflower lecithin powder. Soya and sunflower lecithin powders containing 20-25% supplied by the client was subjected to a two step process namely, preparation of ethanol solubles and column purification of ethanol solubles. Soya and sunflower lecithin powders when subjected to ethanol fractionation resulted in the enrichment of PC to 65-70%. Enriched PC was purified on a column to obtain pure PC with 92-95% purity and about 50% yield. About 25 g of pure soya and sunflower PC with the required specifications were supplied to the industry for evaluation.

Contributions Towards COVID-19: Preparation of Phospholipid Excipients

Indian Pharma companies are procuring >70% of phospholipid-based excipients with huge cost from Lipoid (HSPC and DSPG). With the advent of Black Fungus problem in COVID-19 patients in India and growing demand for safe AmB Liposomal and m-RNA vaccine formulations, the institute initiated the process for development of the required phospholipid excipients and other lipid excipients used in various formulations of the drug with locally available ingredients. The institute prepared the following phospholipid-based excipients from natural soya/sunflower lecithinemploying chemo-enzymatic methodologiesduring this period.

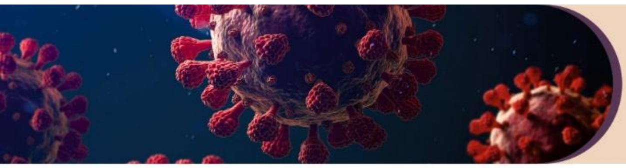
- Soya Lecithin Powder (**PC**, ~20-25%)
- Soya & Sunflower Lecithin (**PC**, ~60-70%)
- Soya & Sunflower Phosphatidylcholine (**SPC, ≥95%**)
- Soya Phosphatidylethanolamine (**SPE**, ≥95%)
- Hydrogenated Soya Phosphatidylcholine (**HSPC**, ≥98%)
- Glycerophosphocholine (**GPC**, ≥98%)
- 1,2-Distearoylphosphatidylcholine **(DSPC**, ≥98%)
- Soya Phosphatidylglycerol **(SPG/SPG Na+)**
- 1,2-Distearoylphosphatidylglycerol **(DSPG/ DSPG Na+)**

Development of Processes for the Preparation of Rice Bran Lecithin from Crude Rice Bran Gums

The project was to develop processes for preparation of refined rice bran lecithin from crude rice bran gums, to prepare PC-enriched lecithin (30 & 50% PC enriched lecithin) and modified lecithin-acetylated lecithin 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. When powdered lecithin was homogenized using ethanol at 65-70^{o}C, PC enrichment was achieved up to 50%. Acetylated rice bran lecithin with 100% purity was obtained by taking acetic anhydride, TEA, and hexane for a time period of 6 h. While under enzymatic method complete acetylation of rice bran lecithin was obtained by taking vinyl acetate and Novozyme 435, stirred at 60-65 ^{o}C for 20 h. The above processes have been optimized at lab scale and are ready for demonstration.

Preparation of Edible Oil Blends of Palmolein and Palm Stearin with Indigenous Edible Oils for Cooking and Trans-Free Solid Fat Formulation Applications

The work aims at preparing edible oil blends of Palmolein and Palm Stearin with indigenous edible oils for use in cooking and *trans*-free solid fat formulation applications. Different blends of Palmolein and Super Olein with indigenous oils and also with Olive oil were prepared in order to obtain an edible oil blend with balanced fatty acid ratios of SFA:MUFA:PUFA. The shortlisted Palmolein/Super Olein blends were interesterified using 1,3-specific



lipase TLIM at higher scale. In another activity, preparation of *trans*-free solid fats employing Palm Stearin and selected edible oils were carried out. Rice Bran based IE product was found to exhibit higher oxidative stability due to the presence of antioxidant γ-oryzanol. Blending sunflower and soybean oils with Palmolein helps to increase the oxidation stability for frying applications.

Exploratory Study on Dimerization of Unsaturated Fatty Acids and Characterization of Products

The process optimization studies were carried out at 500 g/scale for conversion of low cost by-product (fatty acid mixture rich in C-18 fatty acids) to high cost oleochemical, dimer acids. Process for the synthesis of dimer acid based polymeric products involves clay-catalyzed thermal polymerization of fatty acids mixture through Diels-Alder (4+2) cycloaddition reactions. The process was up-scaled at 2 kg/batch.

Polyol Esters of Medium Chain Fatty Acids

A new class of oleochemical-based polyol esters are prepared by esterification of different polyols having 5-6 carbon atoms and 2-4 hydroxyl groups with 10-undecenoic acid or/and undecanoic acid with a hydroxyl value of ≤ 1.0 mg KOH/g. The resulting esters were characterized for lubricant properties. The properties indicate their potential as promising lubricant base stocks for automotive lubricants, metal working oil, hydraulic oil and other industrial applications. (*Brazil Patent No.* PI 0915051-0, **2021**)

Orientation-Cum-Training Program for M.Sc. (Chemistry) Students from North-Eastern States

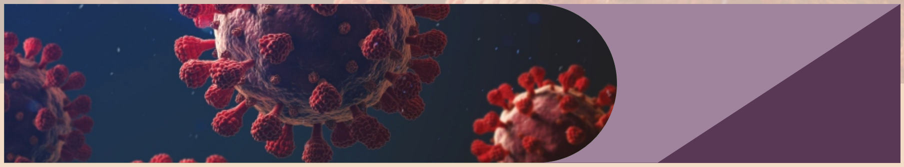
The institute is conducting three months long orientation-cum-training program every year for the students from North Eastern states of India to support the “Samarth Bharat” or “Skill India” program of the Government of India. The program was planned to encourage the students from this part of our country to choose a career in chemistry. This program was initiated on September 1, 2016. This program is now supported by M/s Cipla Foundation. The training was given to the students in hybrid mode. At the later stage, the students were called at IICT for on-campus training. The latest research trends in interdisciplinary sciences and the importance of state of the art analytical techniques were showcased through lectures and demonstrations. Special care was taken for improving communication skills and writing reports and also for knowledge on history of science. The students had the opportunities to meet distinguished scientists and visitors during their stay in the campus.

Participants with Shri G Kishan Reddy, Honourable Minister of Tourism, Culture and Development of North Eastern Region of India, Government of India; Dr S Chandrasekhar, Secretary, Department of Science and Technology; Dr Rajesh S Gokhale, Secretary, Department of Biotechnology; Dr Sekhar C Mande, Secretary Department of Scientific and Industrial Research and Director General, CSIR, Dr VM Tiwari, Director, CSIR-IICT, and Senior Scientists

Anal Food Skill Program

A Skill Development Program, AnalFoodSkill for BSc, Food Science students of the University College for Women, OU, was conducted in a hybrid mode with online lectures during 21st to 23rd March, 2022, and offline demonstrations during 28th March to 1st April, 2022. The program was focused on the analytical techniques related to food industries. Both the presentations and hands on training were conducted. Twenty one students underwent training on various analytical techniques used in the oils and fats, detection of contaminants and pesticides in food, analysis of inorganic elements employing AAS and ICPOES, membrane purification of water and characterization of various components employing HPTLC. The valedictory program was graced by Dr AS Prasad – Sponsorer of the AnalFoodSkill program, Director, NCC Group of Companies and Patil Rail Infrastructure Pvt Ltd. Certificates were issued to the students who successfully underwent the training.

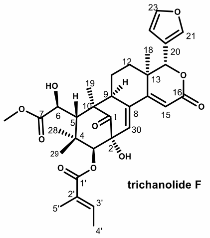
Food Science students of University College for Women, OU, Hyderabad with Dr AS Prasad (Program Sponsorer), Dr Shailaja (CSR Nodal Scientist), Dr MSL Karuna (Course coordinator) and Faculty



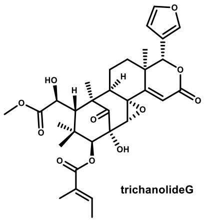
CENTRE FOR NATURAL PRODUCTS AND TRADITIONAL KNOWLEDGE

CENTRE FOR NATURAL PRODUCTS & TRADITIONAL KNOWLEDGE

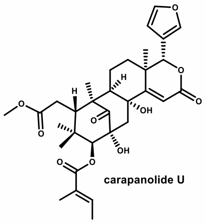
UPLC-MS^{E}Guided Isolation of New Antifeedant Limonoids from Fruits of *Trichiliaconnaroides*



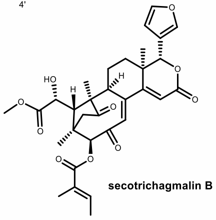
trichanolide F



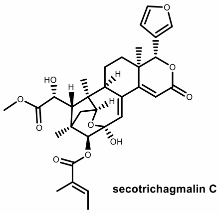
trichanolideG



carapanolide U



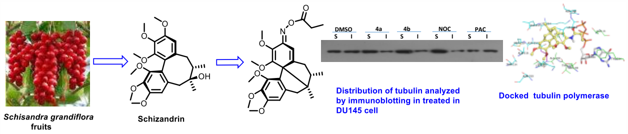
secotrichagmalin B



secotrichagmalin C

UPLC-MS^E guided isolation of $CHCl_3$ extract from the fruits of *Trichiliaconnaroides* yielded two new mexicanolide-type limonoidstrichanolide F and trichanolide G along with a known compound carapanolide U. These limonoids were evaluated for their anti-feedancy against *Spodoptera litura* F. Secophragmalin-type limonoids namely secotrichagmalin B, C and semi-synthetic derivatives were also screened for anti-feedancy. The results revealed that trichanolide F displayed highest antifeedant index (AFI) and caused larval mortality at 24 h. Overall, the study provided new insights into the antifeedant potential of isolated and chemically modified limonoids from *T. connaroides* for the control of spodopteranpests. (*J. Agric. Food Chem.*, **2020**, 68, 6826-6834)

Synthesis and Biological Evaluation of Schizandrin Derivatives as Tubulin Polymerization Inhibitors

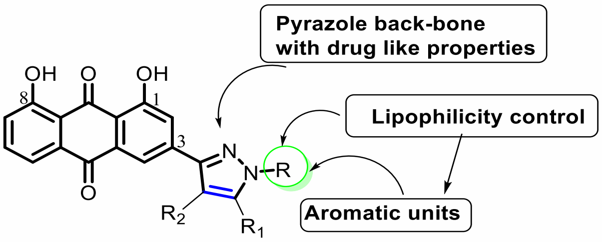


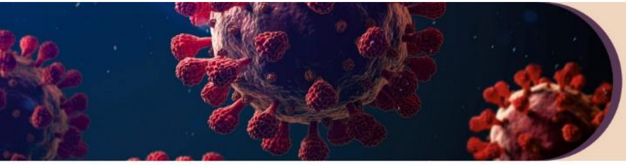
A series of oxime ester-derivatives were prepared by utilizing the schizandrin, a major compound isolated from *Schisandra grandiflora,* which is deployed in different traditional system of medicine. The *in vitro* anti-proliferative activities of the compounds were assessed against a selected panel of human cancer cell lines (A549, RKO P3, DU145 and Hela) and normal cell line (HEK293). Several of these derivatives were found more potent in comparison to parent compound, schizandrin. (*Bioorg.Med.Chem.Lett*., **2020**, 30, 127354 - 127360)

Bombax ceiba (Linn.) Calyxes Ameliorate Methylglyoxal-Induced Oxidative Stress *via* Modulation of RAGE Expression: Identification of Active Phytometabolites by GC-MS Analysis

Effect of aqueous methanol extract of *Bombax ceiba* L. Calyxes (BCCE) on MG induced protein glycation and oxidative stress, followed by the identification of phytometabolites present in the calyxes using gas chromatography-mass spectrometry (GC-MS) were studied. The observed beneficial effect might be attributed to the presence of these compounds in *B. Ceiba* calyxes. This is the first report presenting the antioxidant and anti-glycation activities of *B. ceiba* calyxes and GC-MS analysis of active phytometabolites. These observations show that *B. Ceiba* calyxes may become a potent and promising functional food to manage/control the development of diabetic complications. (*Food & Function,* **2020**, 11, 5486)

Design, Synthesis, Modelling Studies and Biological Evaluation of Pyrazole-linked Aloe emodin Derivatives as Potential Anti-Cancer Agents

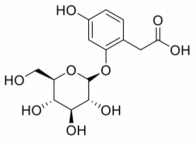




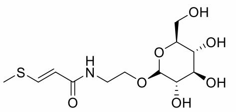
A series of aloe-emodin derivatives were synthesized and assessed potentials against cancer cell lines of different origin. Several of the derivatives were more active than the aloe-emodin and particularly, two derivatives manifested potent activity with IC$_{50}$ of 1.32 & 1.65 µM and 0.98 & 2.67 µM against MDA-MB-231 and MCF-7 cells, respectively. Moreover, these derivatives induce early and late apoptosis as well as arrest the cell cycle at G2/M phase in MDA-MB-231 cells. In conclusion, the aloe-emodin derivatives could be a potential drug for better treatment of breast cancer.(*RSC Med. Chem.*, **2021**, 12, 791-796)

Investigation of Cytotoxic Constituents from Seed Pulp of *Entada phaseoloides* and Metabolite Profiling using UPLC-QTOF-MS^{E}

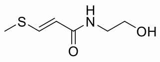
The present study summarizes the isolation and identification of bio-compounds from *n*-butanol extract and the demonstration of UPLC-QTOF-MS/MS analysis for the characterization of compounds in complex crude extracts. This is the first systematic study in structural characterization on complex saponins and other metabolites from crude extract of *E. phaseoloides* using UPLC-ESI-QTOF-MSE. (*J.AOAC Internat.*,**2021**, 104, 827-835)



PHASEOLOIDIN(**1**)



Entadamide A-β-D-glucopyranoside

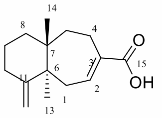


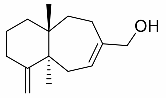
ENTADAMIDE A(**3**)

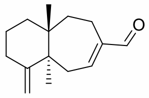
Phytometabolomic Analysis of Boiled Rhizome of *Nymphaea nouchali* (Burm.f.) and Evaluation of Antihyperglycemic and Antioxidant Activities

Phytometabolomic analysis of *Nymphaea nouchali* (Burm. F.) boiled rhizome was carried out and evaluated for antihyperglycemic and antioxidative stress potentials. Metabolomic analysis revealed the presence of multiple antidiabetic and antioxidant compounds. Boiled rhizome powder exhibited potent antihyperglycemic activity against sugar-induced postprandial hyperglycemia in rats. It also prevented hyperglycemia-induced hemoglobin and insulin glycation. It displayed antioxidative stress potential in assuaging H$_2$O$_2$ induced erythrocyte hemolysis and antioxidant activity by inhibiting membrane lipid peroxidation. Boiled rhizome was also found to preserve the loss of cellular antioxidants under H$_2$O$_2$ induced oxidative stress and disturbances caused to mitochondrial membrane potential. (*Food Chem.*, **2021**, 342, 128313)

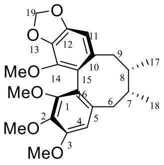
Bio-Active Constituents from *Schisandra grandiflora:* Isolation, Semi-Synthesis and Evaluation of their Anticancer Activities



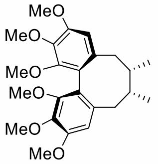




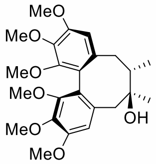
Widdaranal A



Gomisin N



(+) deoxyschiszandrin

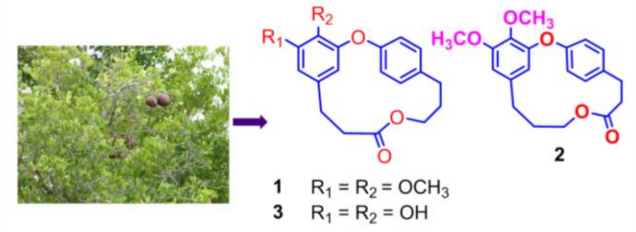


schiszandrin

Bio-activity directed investigation of *Schisandra grandiflora* led to the isolation of two new widdarane-sesquiterpenes. Further, a series of derivatives from a major compound, gomosin N were prepared by ring-opening of methylenedioxy group using Pb(OAc)$_4$ followed by esterification with different acids. The isolates and derivatives were screened for their potentials against cancer cell lines. Two derivatives were manifested promising activity than gomisin N (3) against MCF-7 and MIA PaCa cell lines. (*Phytochem. Lett.*, **2021**, 45, 184-189)

α-Glucosidase Inhibitory Isomeric Corniculatolides from the Stems of the Indian Mangrove Plant, *Xylocarpus granatum*

Three new isomeric corniculatolides with an unusual caffrane and isocorniculane framework, and five known metabolites were isolated from the chloroform extract of the stems of *Xylocarpus* *granatum*. The structure of the new metabolites were deduced as corniculatolide B, isocorniculatolide B, and corniculatolide C. The isolated compounds were evaluated for *in vitro* cytotoxicity and α-glucosidase (*Saccharomyces cerevisiae*) inhibitory potential. corniculatolide C possessed α-glucosidase inhibitory activity with an IC_{50} value of 24.8 µM, whereas these rare macrolides showed no effect on the mammalian cancer cell lines MIAPaCa-2, DU145, MCF-7, and HTC-116. (*J. Nat. Prod.*, **2020**, *83*, 1, 20-25)

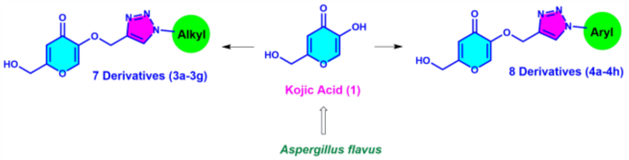


New *n*-Nonadecanoyl-β-sitosterol and other Constituents from the Stem-bark of *Anacardium occidentale*

A new steroidal ester bearing *n*-nonadecanoyl moiety 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 and the structures of the known compounds were identified as gallic acid and tanacetene. These compounds were evaluated for cytotoxicity against human cancer cell lines A549, SCOV3 and rat normal cell line NRK49f. (*Nat. Prod. Res.*, **2021**, *35*, 1357-1363)

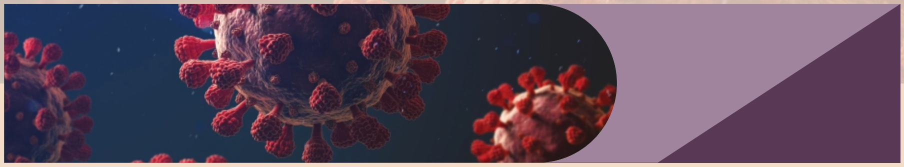
Click Linker: Efficient and High Yielding Synthesis of a New Family of Kojic Acid Congeners as Cytotoxic Agents

Highly efficient methodology was developed for the construction of functionalized Kojic acid involving Click linker via 1,3-dipolar cycloaddition and their cytotoxicity against MCF-7, MIAPaCa-2 and DU145 mammalian cell lines were evaluated. Substitution at C-2 of kojic acid as well as C-5 of 1,2,3-triazole motif played a major role in the activity profile. Kojic acid 1,2,3-triazole analogue containing an alkyl chain (n=6) exhibited two fold potent activity than the parent compound, kojic acid against MCF-7 and MIA PaCa-2 cell lines. It induced apoptosis in these cell lines via ID1/PARP1 mediated pathway. (*Nat. Prod. Res.* **2021**, 1-7)

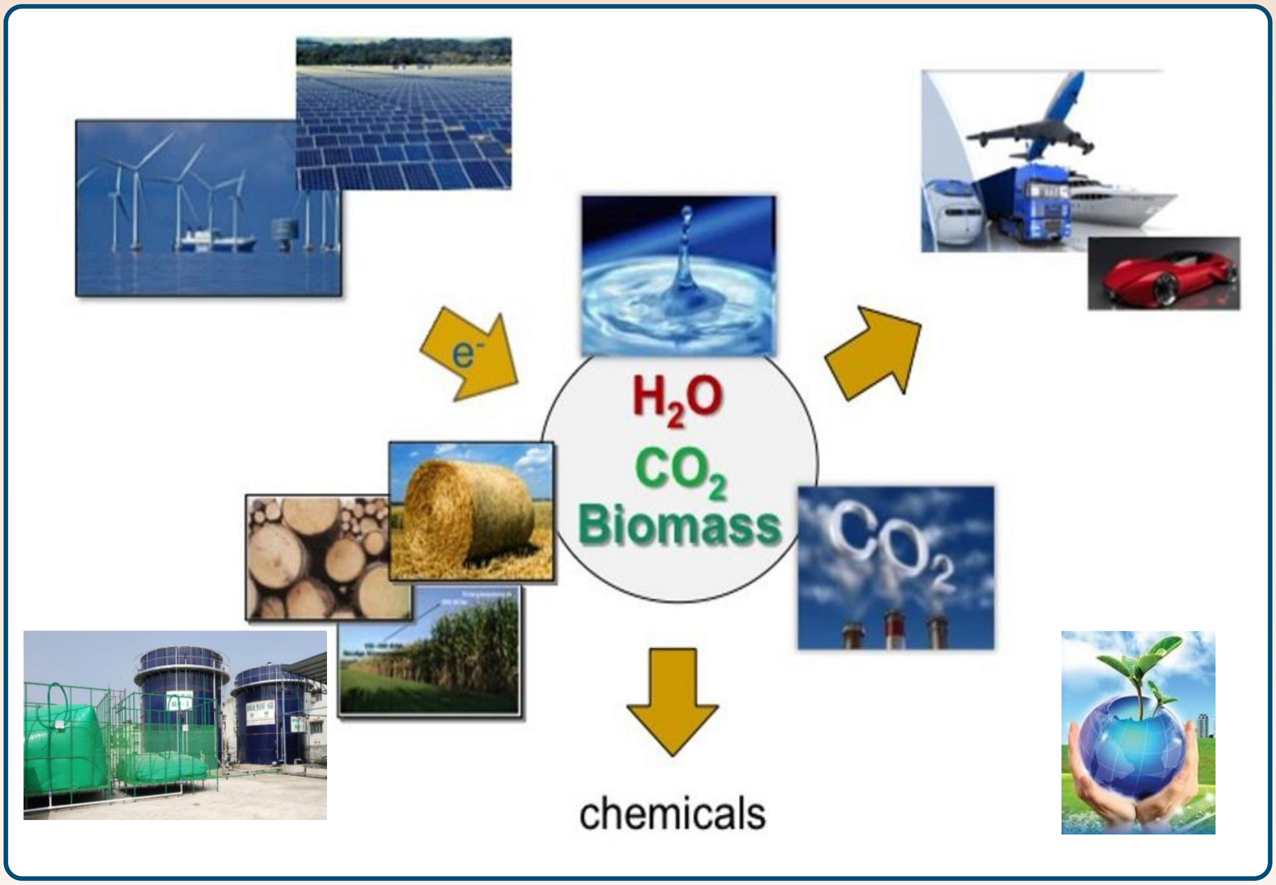


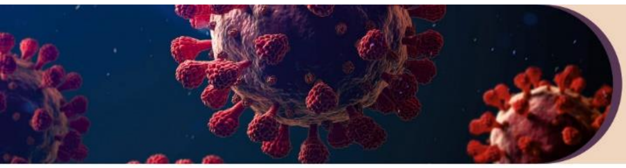
Design and Synthesis of New Isoxazole and Phenyl Acetylene Analogues of Arjunolic Acid as Potent Tyrosinase and Alpha Glucosidase Inhibitors

A series of new phenyl acetylene and isoxazole analogues of arjunolic acid were designed, synthesized and evaluated for tyrosinase and *alpha* glucosidase inhibitory potential. The analogues exhibited stronger inhibitory activity than the standard drug or parent compound. One of the compounds displayed the most potent tyrosinase inhibitory action with IC_{50} (14.3 ± 7.6) of about three folds more than the standard drug, kojic acid (41.5 ± 1.0). Another compound **(**14.5 ± 0.15) possessed the potent *alpha* glucosidase inhibitory action with IC_{50} value comparable to that of standard, acarbose (10.4 ± 0.06). (*Nat. Prod. Res.*, **2021**, 1-6)



DEPARTMENT OF ENERGY & ENVIRONMENTAL ENGINEERING





DEPARTMENT OF ENERGY AND ENVIRONMENTAL ENGINEERING

BASIC RESEARCH

Solid-State Anaerobic Co-Digestion of Food Waste and Cardboard in a Pilot-Scale Auto-Fed Continuous Stirred Tank Reactor System

This study evaluated the performance of a pilot-scale auto-fed continuous stirred tank reactor (CSTR) system for the solid-state anaerobic co-digestion (ACoD) of acetic acid rich food waste (FW) and cardboard (CB). This study concludes that exposing the CB to acetic acid-rich FW assisted the disintegration and depolymerization of CB without any pre-treatment step. The outcomes of this study provide new insight into the potential of implementing decentralized AD units for the treatment of FW and CB at source, which not only diverts waste from landfills but creates a revenue model through bioenergy generation and digestate sales. (*J. Clean. Prod.*, **2021**, 289, 125775 – 125786)

Anaerobic Co-Digestion of Ultrasound Pre-Treated Food Waste and Cardboard in Different Mixing Ratios

The impact of acetic acid assisted ultrasound pre-treatment of food waste (FW) and cardboard (CB) to overcome the barriers of substrate characteristics is investigated. Results revealed that the biogas yield obtained from ultrasound pre-treated samples regardless of mixing ratio was higher at a F/I ratio of 1:2 compared to 1:1. Ultrasound pre-treatment for 45 min was adequate for FW:CB of 100:0 and 80:20 while it was 60 min for 60:40 and 50:50 for increased sCOD between 37 % - 53 %. The CB mixing ratio is inversely related to SE while directly related to sCOD. Overall, during ACoD of FW and CB, the FW:CB of 80:20 gave a higher biogas yield of 471 mL/g VS_{added} followed by 60:40 and 50:50. (*Biochem. Engg. J.*, **2021**,166, 107853 – 107864)

Improved Biomethanation of Horse Manure Through Acid-Thermal Pretreatment and Supplementation of Iron Nanoparticles Under Mesophilic and Thermophilic Conditions

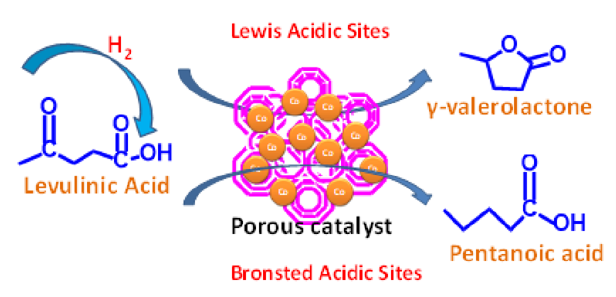
This study aimed to investigate the impact of dilute acid-thermal pretreatment of horse manure (HM) on the characteristic changes followed by biomethanation of untreated (control) and pretreated HM using iron oxide (Fe_3O_4) nanoparticles (NPs)as additives at concentrations of 20 mg/L, 40 mg/L and 60 mg/L at mesophilic (35 ± 2 °C) and thermophilic (55 ± 2 °C) temperature conditions. Results disclosed that the maximum methane yield of 0.16 L/g COD reduced and 0.175 L/g COD reduced was achieved under mesophilic and thermophilic conditions from pretreated HM with an addition of 40 mg/L of Fe_3O_4 NPs with a COD reduction of 68%and 56 %, respectively, whereas it was 0.14 L/g COD reduced and0.15 L/g COD reduced with an addition of 60 mg/L of Fe_3O_4 NPs with corresponding COD reduction of 58 % and 62.5 %, respectively, from untreated HM. (*Biomass Convers. Biorefin.*, **2020,** 1-14)

Optimization of Feed and Extractant Concentration for the Liquid–Liquid Extraction of Volatile Fatty Acids (VFA)from Synthetic Solution and Landfill Leachate (LL)

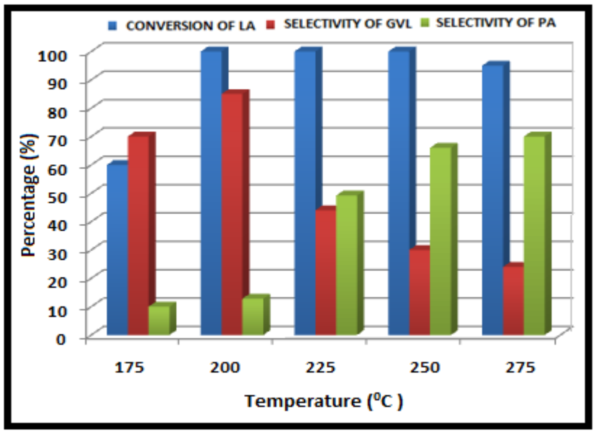
Liquid–Liquid Extraction of VFA from LL as well as synthetic solution (SS) whose concentration varied from 0.2 to 1 mol/L was investigated. The impact of extractant and feed VFA concentration on extraction efficiency (EE) and loading ratio (z) with the help of statistical analysis and process optimization using response surface methodology is presented. The optimal extractant concentration for TOA and TBP was found to be 37.8% and 39.09% at a feed concentration of 0.67 mol/L and 0.81 mol/L for SS respectively to achieve maximum EE of 91% while it was 29.3% and 36.2% at 0.2 mol/L for LL to achieve EE of 52% and 57% correspondingly. (*J. Ind. Eng. Chem.*, **2020,** 90, 190–202)

Biomass Derived Efficient Conversion of Levulinic Acid for Sustainable Production of γ-Valerolactone

Hydrogenation of biomass based levulinic acid at atmospheric pressure conditions using robust cobalt supported on porous heterogeneous catalyst has been studied at 200 °C in a continuous process. The present study is intended to develop noble-metal free, cost-effective, simple and continuous process for the deployment at larger scale production of γ-valerolactone. The proposed green and robust catalytic system will provide valuable insight to develop a sustainable approach for value-addition to biomass resources. (*J. Hazard. Mater.* **2021**,405, 123335)

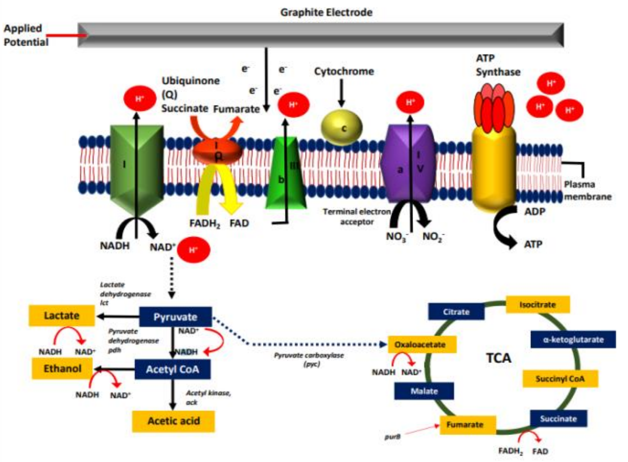


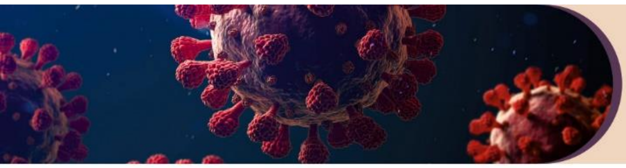
Schematic representation of catalytic continuous process and study of effect of temperature on sustainable production of γ-valerolactone.

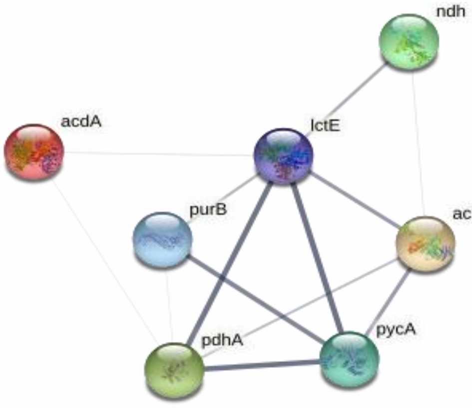


Metabolic Flux in Electro Fermentation System-Gene Expression *vs* Product Formation

The work demonstrated the role of poised (negative/positive) potential (0.2/0.4/0.6/0.8 V vs Ag/AgCl at anode) in electro-fermentation system (EF) to understand the metabolic flux of *Bacillus subtilis* with pyruvate as a carbon source. The relative expression of genes encoding pyruvate dehydrogenase (*pdhA*), lactate dehydrogenase (*lctE*), acetate kinase (*ackA*), pyruvate carboxylase (*pycA*), adenylosuccinatelyase (*purB*), acyl CoA dehydrogenase (*acdA*) and NADH dehydrogenase (ndh) allowed evaluation of metabolic changes in correlation to product formation and bio-electrochemical analysis. *lctE* gene encoding the lactate was found as core gene for pyruvate metabolism that regulates and controls the expression of other associated genes. (*Bioresour. Technol.*, **2021**, 342, 125854 – 125864)



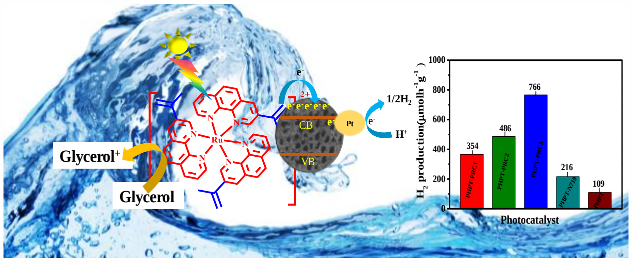




Metabolic flux of *Bacillus subtilis* under Poised Potential in Electro fermentation system

Rational Design of Ru-Phenanthroline Complex Sensitized TiO_2Photocatalyst for Efficient Hydrogen Production

The introduction of propenyl group in Ru-Phen complex shows enhanced light response (350-550 nm) with increased charge transfer behaviour and show substantial fluorescence at 590-700 nm with lifetime 77-127 ns. The PHPT-PRC3 composites possess superior hydrogen production activity of 3066 $\mu mol g^{-1}_{cat}$ and turnover number 123 after 4 h of light irradiation in an aqueous glycerol solution (pH 7) compare to without sensitizer (PHPT) and N719 sensitized PHPT (N719-PHPT) under similar experimental condition. The experimental observations corroborated with computational calculations supporting efficient charge separation and enhanced regeneration of oxidized dye. (*Renew. Energ.*, **2020,** 159, 1 - 9)



Plausible mechanistic hydrogengeneration approach of PHPT-PRC3 composite

Hot Injection-Induced Synthesis of ZnCdS–rGO/MoS_2Heterostructures for Efficient Hydrogen Production and CO_2Photoreduction

A highly efficient hybrid ZnCdS–rGO/MoS_2heterostructure is successfully synthesized through a hot injection method and control loading of rGO/MoS_2. The synergism provides an unprecedently high H_2-generation rate of 193.4 mmol H_2 g^{-1} h^{-1} from water under full arc solar radiation and MeOH production (5.26 mmol g^{-1} h^{-1}, AQY of 14.6% at k = 420, 20 nm) from CO_2 reduction. This work emphasizes a facile strategy to prepare noble metal-free high-performance materials for practical photocatalysis applications. (*Chem. Commun.*, **2021**, **57**, 8660 - 8663)

Technoeconomic Investigation of Amine-Grafted Zeolites and their Kinetics for CO_2 Capture

A series of amine-modified zeolites and their CO_2 capture efficiencies were reported. The amine impregnated molecular zeolite compounds were investigated for CO_2 adsorption capacity. The adsorption capacity for CO_2 adsorption was improved with amine loading up to a certain concentration over 13X-DETA-40, showing an adsorption capacity of 1.054 mmol of CO_2 per gram of zeolite in a very short length of time. The result was especially promising in terms of the initial adsorption capacity of zeolite, which adsorbed approximately 0.8 mmol/g zeolite within the first two minutes of experimentation. A technoeconomic study was conducted for the solid amine zeolites to understand the investment per ton of CO_2 adsorbed. (*ACS Omega.*, **2021**, 6, 6153 – 6162)

APPLIED RESEARCH

Development of Anaerobic Digester System for Generation of Enriched Methane from FoodWaste

The proposed strategies are high pressure anaerobic digestion (mono and co-digestion), dry anaerobic digestion, dark fermentation for biohydrogen production, addition of materials (nanoparticles, micronutrients of nanoparticles, conductive materials, carbon sources etc.,), development of hydrogen producing cultures, development of microbial cultures that are suitable for the conversion of CO_2 and H_2 to CH_4. One of the major findings of this project is the generation of biogas with 79 % methane using sodium acetate as substrate, while the dark fermentation of starch resulted in the generation of gas with 76 % hydrogen within 7 days.

Development of Biomethanation Process for Generation of Biogas and Biomanure from Lignocellulosic Biomass

The project is to understand the biogas generation potential of lignocellulosic biomass (rice straw/wheat straw, maize stalk etc.) and to develop a laboratory scale novel anaerobic reactor (20 kg/day) for the generation of biogas from untreated and pretreated lignocellulosic biomass and its validation at pilot scale

Reactor operated with Lignocellulosic biomass

High Rate Biomethanation of Market and Vegetable Waste

Five biogas plants based on Anaerobic Gas lift Reactor Technology are approved for installation in the vegetable market yards at Gudimalkapur (5 TPD), Gaddiannaram (5TPD), Kukatpally (500 kg/day), Erragadda (500 kg/day) and Baatasingaaram (500 kg/day) operated by Department of Agriculture Marketing (DAM), Govt. of Telangana. While 3 plants at Kukatpally, Erragadda and Batasingaram are functional, 4th plant is under installation at Gudimalkapur (5 TPD).

Solid State Anaerobic Digestion (AD) of Poultry Litter: Biogas Generation and Microbial Diversity Study

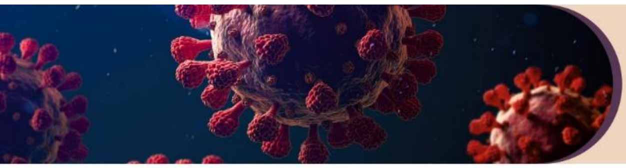
Investigation of the solid-state anaerobic digestion of poultry litter and to understand its microbial population in AD process. Poultry litter at different solids concentration was operated in anaerobic bioreactor for 45 days by operating critical parameters and measuring pH, ammonia, H_2S, methane, nitrates, nitrites, sulfates, sulphites, volatile fatty acids, alkalinity and biogas. Microbial studies-gene sequencing studies are performed to understand the microbial community in reactors.

Microbial Ecology of Anaerobic Gas-Lift Reactor (AGR) to Develop Efficient Microbial Consortia for Enhanced Production of Biogas (Methane)

A unique anaerobic gas lift reactor (AGR) technology for the production of biogas and bio manure from a variety of organic wastes was developed. The composition of CH_4 produced from AD is normally 50–75 percent, while that of CO_2 is about 25–50 percent. The broad aim of the study is to understand the microbial community behavior with respect to various substrates. To achieve optimal biogas production with increased methane content, suitable conditions must be set to preserve the balance of all microorganisms.

Understanding the Substrate Mediated Microbial Community Shift Within the Anaerobic Ecosystems *via* 16s Metagenomic Studies

This study elucidates the change in community structure of the consortia in AD process with respect to substrate complexity. Mixed microbial



consortium is used as the seed culture for the four different substrates to understand their biomethanation potential. Anaerobic batch experiments for all the four substrates namely rice straw, bagasse, press mud and vegetable waste resulted in the maximum methane yield of 0.38 L CH$_4$/(g VS added), 0.35 L CH$_4$/(g VS added), 0.35 L CH$_4$/(g VS added), and 0.34 L CH$_4$/(g VS added). Major bacterial phyla of the initial inoculum like Bacteroidetes, Firmicutes has decreased and the variable change can be observed in other microbial phyla from reactor to reactor treating different substrates. (*Bioresour. Technol. Rep.*, **2021**, 15, 100793 - 100801)

Methane Production Potential of High-Strength Landfill Leachate at Mesophilic and Thermophilic Temperature

The aim of this study was to investigate the biomethane potential (BMP) of a high-strength landfill leachate (LL)with low pH (5.0), high solids concentration (16%), and high organic matter (170 g/L of COD; 55 g/L of VFA) with ammonia nitrogen (17 g/L). The kinetic study revealed a fourfold reduction of lag phase in thermophilic compared to mesophilic reactors. There exists an inverse correlation between initial organic loadings (IOL) and organic matter removal efficiency. About 80% COD reduction was obtained at mesophilic temperature and 90% at thermophilic temperature, at an IOL of 42.5g/L and21 g/L of COD. (*Sci. Total Environ.*, **2020**, 715, 136658 - 136671)

Solid State Anaerobic Co-Digestion of Food Waste and Sewage Sludge

The aim of this study is to identify the optimum mixing ratio of food waste (FW) and Sewage sludge (SS) for co-digestion at mesophilic and thermophilic conditions and investigate the impact of the same on microbial diversity and methane yield. The consequent dynamic evaluation of microbial community structure was done by metagenomic analysis. It was learnt from the results that higher methane yield and VS reduction could be obtained when the FW and SS mixed in the ratio of 3: 1 in mesophilic and 2:1 in thermophilic. However, VS reduction and methane yield was 76% and 0.35 L CH$_4$/(g VS reduced) respectively at mesophilic temperature whereas it was 88 % and 0.42 L CH$_4$/(g VS reduced) at thermophilic temperature. (*Sci. Total Environ.*, **2021**, 793, 148586 - 148598)

Solid State Anaerobic Digestion of Sugarcane Bagasse at Different Solid Concentrations The main aim of this study was to determine the potential cellulose degrading bacteria in order to enhance the AD of sugarcane bagasse. In order to explore the effect of bioaugmentation on biogas generation and methane yield, experiments were conducted at 25%, 30%, 40% and 50% solid concentration of bagasse at optimized feed to inoculum (F/M) ratio and the enriched consortia was added to the reactors. An increase of 20-22% was observed in bioaugmented bagasse compared to non-bioaugmented (control). Metagenomic studies revealed the abundant bacterial phyla total microbial communities of both the reactors and also it showed that 90% of the Archaeal microorganisms found were affiliated to *Methanosaeta*, a strict acetoclastic methanogens. (*Bioresour. Technol.*, **2021**, 340, 125675)

Real Time Troubleshooting Strategies to Overcome Inhibition and Instability Issues in Food Waste Based Anaerobic Digesters

Food waste-based biogas plant of capacity 250 kg/day for implementation, incubation and micro-aeration strategy and its impact on the overall plant performance has been investigated. Results illustrate that incubation followed by aeration of the feed slurry maintains marginal difference in pH but a vast difference involatile fatty acid (VFA) concentration. The performance of the pilot biogas plant is that within a span of one year about 26,230 (26.23 ton) kg of food waste is treated which resulted in the generation of 3,376 m^3 of biogas. On an average, about 2.19 tons of food waste is treated per month which resulted in the generation of 281 m^3 of biogas for the replacement of about 114 kg of LPG per month.

High Rate Biomethanation of Market Vegetable Waste: Demonstration at Source and Real Time Strategies for Performance Enhancement

The demonstration plant installed at the Bowenpally vegetable market yard is serving as role model to all the vegetable market yards in India to install such biogas plants for the conversion of organic waste to bioenergy and recover nutrients in the form of organic fertilizer. The Bowenpally biogas plant with a net plant efficiency of 78 % resulted in the generation of 35 m^3 of biogas per ton on an average with 60-62 % CH_4. With n a span of 2 years a total of 4346 tons of vegetable is treated which resulted in the biogas generation of 1,54,833 m^3 (90,116 kWh of electricity).

Surveillance of SARS-CoV-2 Spread Using Wastewater Infrastructure

Sewage-based surveillance can be used as holistic approach to understand the spread of the infection SARS-CoV-2 pandemic within a community. Wastewater-based epidemiology (WBE) can measure the extent of infection in a community, with the added benefit of detecting individuals who haven't been tested, asymptomatic, mild symptomatic, pre- symptomatic and symptomatic. The transmission of SARS-CoV-2 in Hyderabad was investigated analysing the viral genome in sewage samples obtained from all major sewage treatment plants (STPs). Samples were collected with safety procedures between the 8th of July and 6th of August, 2020.The isolated RNA samples were tested for presence of SARS-CoV-2 RNA using FDA approved Fosun COVID-19 RT-PCR Detection Kit; targeting the envelope protein coding gene (E-gene; ROX labelled), nucleocapsid gene (N-gene; JOE labelled) and open reading frame1ab (ORF1ab; FAM labelled) of SARS-CoV-2. Based on the E gene C_T, viral gene copies per litre and viral particle shedding per individual and the total numbers of individuals exposed to SARS-CoV-2 were estimated. Inlet samples of STPs were positive for SARS-CoV- 2, while the outlets were negative, which signifies, standard sewage treatment methods are efficient in eliminating the SARS-CoV-2 viral particles. (*Sci. Total Environ.*, **2021**, 768, 144704 - 144711)

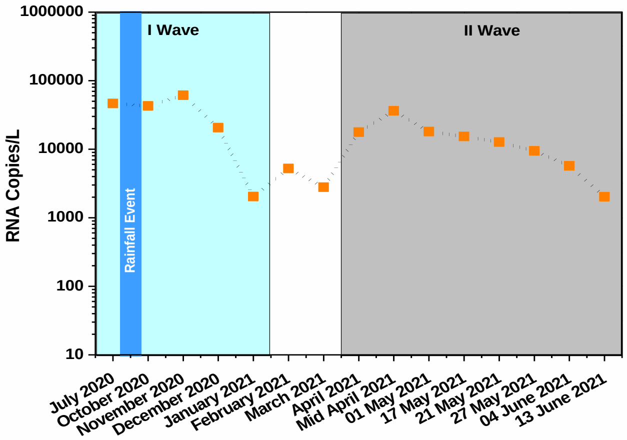
Methodological Approach for Wastewater Based Epidemiological (WBE) Studies

Experiments were performed to establish a methodological approach for conducting WBE studies in the framework of selecting of surveillance sites, standardizing sampling policy, designing sampling protocols to improve sensitivity, adopting safety protocol, and interpreting the data. Grab samples were collected for every hour from 5 am to 4 am (day-2). SARS-CoV-2 RNA was detected in all collected samples with temporal variation in the viral load. Data from hourly sampling indicated a peak in the viral RNA during the morning hours (6–9 am) when all the domestic activities are predominant. The daily sampling and processing revealed the dynamic nature of infection spread among the population. Overall, this study establishes a structured protocol for performing WBE studies to achieve measurable and reliable detection of viral load in wastewater. Moreover, this framework can be used to monitor several other clinically relevant diseases. (*Environ. Technol. Innov.*, **2021**, 23, 101696)

Long Term Surveillance of SARS-CoV-2 -Infection Dynamics

Long-term epidemiological surveillance was undertaken to assess the spread of SARS-CoV-2 (July 2020 to August 2021) in a selected community by longitudinal sampling. The study area represented the community with ~2.5 lakhs population covering Tarnaka, HMT Nagar, Lalaguda and Nacharam as part of Greater Hyderabad, Telangana, India. A consistent viral load was observed during the months from July 2020 to

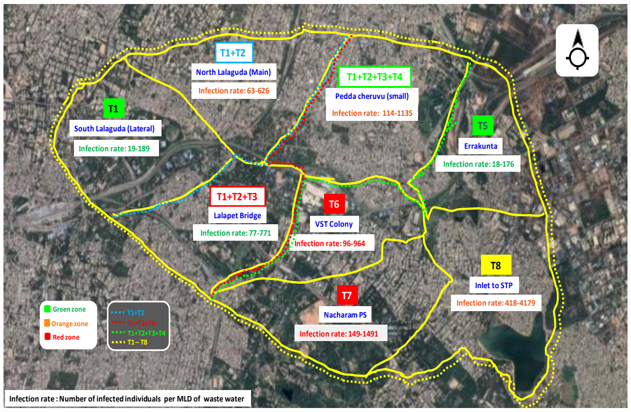
November 2020, suggesting persistence and spread of the viral infection among the community, followed by decrease in subsequent two months (December 2020 and January 2021). A marginal increase was observed during February 2021, hinting the onset of the second wave (from March 2021) that reached to peak in April 2021. This study evidences that, Wastewater Based Epidemiological study promotes inspection with simultaneous disease detection, in addition to an advance warning signal to anticipate outbreaks, with respect to the community/zones under study, to tackle, prepare for and manage the pandemic. (Int. J. Env. Res. Pub. Health, **2023**, 19(5): 2697)



RNA copies calculated based on linear fit equation of E-gene of samples collected (depicting 1st and 2nd Wave)

Community Zoning Based on Infection for Effective Management

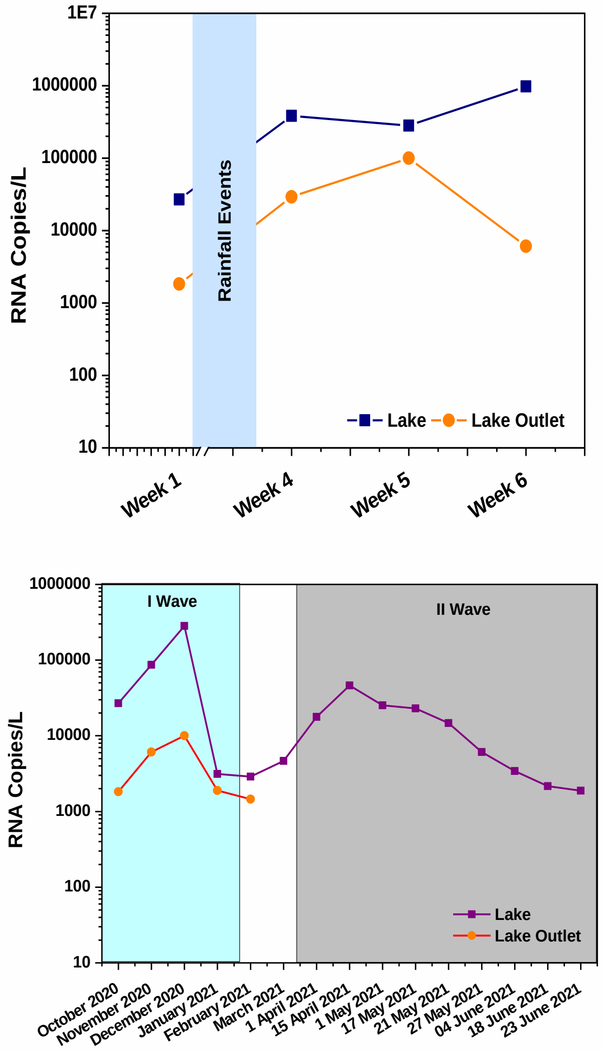
Longitudinal sampling provides the opportunity to zone the selected area based on the severity of the viral infection and spread. Four major lateral sampling points denotes the different distinct zones (T1: Zone I; T5: Zone II; T6: Zone III and T7: Zone IV) whereas the rest of the sampling points were at main drain that represents the extended zones area to the Zone I (T2: Extended Zone I; T3: Second Extended Zone I; and T4: Third Extended Zone I). At last, the terminal sampling point (T8) represents the entire study area. Weekly monitoring at each point over the period of five weeks assisted to study the spread of the viral genome spread among the communities. (Int. J. Env. Res. Pub. Health, 2022, 19 (5), 2697).



Zoning of the studied community based on the severity of infection (Courtesy: Google Map)

Temporal Surveillance of SARS-CoV-2 in Water Bodies-Early Signal of Second Wave Onset

Urban, peri-urban (PL) and rural lakes (RL) in and around Hyderabad were monitored for SARS-CoV-2 virus. Three lakes in the urban zones of Hyderabad viz., Nacharam Lake, Hussain Sagar lake and Nizam Talab lake were chosen for the study. Edulabad lake (PL) and Potharaju lake (RL) were sampled as referral lakes under peri-urban and rural areas. High viral load was observed during the peaks of Wave I and Wave II. The SARS-CoV-2 genes were not detected in peri-urban and rural lakes, whereas in urban lakes it was detected and results directly correlates with direct functional attributes from domestic activity. The outcome of the study showed that the urban water streams linked with domestic discharge function as a proxy in virus infection. Further implementation WBE on regular basis in water bodies/wastewater will help to understand the outbreak and spread of virus in the community. (Current Sci, **2022**, 123, 8, 987 – 994).



RNA copies of weekly and monthly samples calculated based on linear fit equation of E-gene of samples collected (depicting 1st and 2nd Wave)

Surveillance of SARS-CoV-2 in Andhra Pradesh State

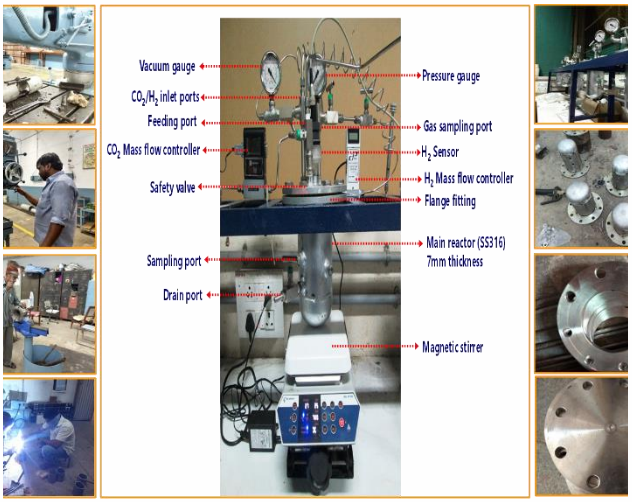
Wastewater Based Epidemiological (WBE) studies were conducted for entire Andhra Pradesh (A.P) state to monitor the prevailing infection of SARS-CoV-2. Sewage samples were collected STPs of major cities (Visakhapatnam, Vijayawada, and Kurnool) smaller cities (Rajahmundry [East Godavari] and Narasaraopeta [Guntur]) and towns (Pulivendala [YSR Kadapa], Tadipatri and Puttaparthi [Anantapur]) during 26th October to 16th November 2020. The infection rate of 30.8 Person/MLD, 21.3 Person/MLD and 5.6 Person/MLD was observed in major cities like Visakhapatnam, Vijayawada, Kurnool and Anantapur; confirmed cases in these cities, correlated well with the infected individuals obtained from sewage data. Finally, on the basis of district wise sewage generation, the capacity for total Andhra Pradesh was extrapolated (11,000 MLD) which showed 3,38,724 infected individuals with an active phase of infection to be 84,681 that accounts for an infection rate of 30.8 Person/MLD.

Decentralized Effluent Treatment Plant (ETP) for Combined Domestic and Dye Wastewater from Traditional Handloom/Weaving Village

The dyeing process, topography, and drainage pattern and wastewater parameters of Siripuram village (TS) was studied for 9 months. Aerial Drone (PHANTOM 4 RTK UAV) survey was performed for topographical survey to study the drainage lines, elevations, slopes and flow-pattern of the combined wastewater. Laboratory studies were performed with the real field effluents consisting textile dye wash water and domestic wastewater with hybrid process that helps to remove dye molecules and associated chemicals more effectively with self-induced oxidation. Based on the laboratory studies, a decentralize ETP plant (0.5 MLD) was designed to showcase a model ETP that bears low cost and easy to operate portfolio and can be implemented in a decentralized manner for traditional textile units operating in remote villages with a community-based approach.

Gas Fermentation for CO_2 Sequestration

Custom designed and fabricated gas fermentation (GF) systems were evaluated to optimize the headspace pressure, pH (6.5, 7.5, and 8.5), fermentation time, and substrate concentration by employing enriched homo-acetogenic chemo-lithoautotrophs in non-genetic approach. This low-cost designed gas fermenter demonstrated good conversion of inorganic carbon to short chain fatty acids. Maximum volatile fatty acid (VFA) yield of 3.7 g/L was observed at alkaline pH (8.5) under 2 bar pressure at carbon load of 10 g/L, 96 h. Gas fermentation strategy can function in decentralized way to address the carbon emissions to certain extent. (*Bioresour. Technol..,* **2022**, 126937)



Custom designed and fabricated Gas fermentation systems at CSIR-IICT

Microbial Electro-Catalyzed Conversion of CO_2 to Value-Added Products

Carbon cloth (CC), stainless steel mesh (SS) and combination of CC and SS were studied as cathode (3.5 × 1.5 cm) in novel membrane-less single-chambered Microbial electrosynthesis systems (MESs). Combined electrodes showed higher CO_2 conversion to VFA (1.4 g/L) with CO_2 sequestration (59%) followed by CC and SS. Electro-kinetic study also depicted the biocathode efficacy towards enhanced electrotrophy with confined electron losses by regulating electron flux in the system. Hybrid biocathode showed relatively higher reductive capabilities with lower electron losses that drive towards enhanced fatty acid synthesis. *(Bioresour. Technol*., **2021,** 320, 124272)

Green Hydrogen and H-CNG production from Biogenic Waste

An integration of acidogenesis (dark-fermentation) and methanogenesis for H-CNG production from food waste in two stages of operation was studied. The regulatory influence of biocatalyst and redox environment on anaerobic fermentation was evaluated through a rapid protocol in the context of biogas up-gradation with reference to H_2, CH_4 and H-CNG as major markers. Production of H_2 and H-CNG at varying organic loads (OL) of food waste was evaluated. Acidogenic reactor operated with FW at 40 g COD/L showed the higher cumulative H_2 production while 50 g COD/L showed higher CH_4 production. The acidogenic phase played a major role converting FW to green H_2 along with co-production of short (C_2-C_5) and medium-chain (Caproic acid, 1.16 g/L) fatty acids. (*Int. J. Hydrog. Energy.,* **2021**, 46, 18832 - 18843; *Bioresour. Technol*., **2021**, 340, 125643)

Bio-succinic acid (Bio-SA) production

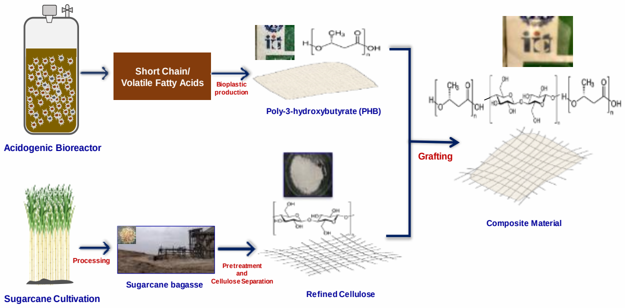
Isolated *Citrobacter amalonaticus* (NCIM 5782) was studied for bio-succinic acid (Bio-SA) production through fermentation and electro-fermentation processes. Integrated biorefinery approach was designed to utilize bio-H_2 and CO_2 generated during acidogenesis process for the production of bio-succinic acid (SA) along with polyhydroxyalkanoates as co-product. Bio-H_2 functions as an electron donor for the formation of reduced end product, SA. Bio-electrochemical synthesis offers a promising solution to transform organic and inorganic carbon to high-value added products using microorganisms under a constant applied potential. *Citrobacter amalonaticus* in presence of applied potential (AP; -0.7 to -0.9 V (vs. Ag/AgCl)) yielded SA production of 14.4 g/L at - 0.8 V. Absence of CO_2 resulted in the formation of higher acetic acid (6.34 gL-1) and lactic acid (6.13 gL-1), revealing a direct dependency. *(J. Chem. Eng.,* **2021,** 128377)

Production of Polyhydroxybutyrate (PHB)

Isolated bacterial strain *Providencia sp.* depicted dual production of polyhydroxybutyrate (PHB) and extracellular polymeric substances (EPS), respectively. The polymer production process was optimised by varying process parameters such as carbon load (20, 30 and 40 g/L) and pH (6, 7, 8) for enhancing PHB and EPS productivity. Maximum yield of both PHB (2.62 g/L) and EPS (3.92 g/L) was observed with carbon load of 30 g/L at pH 7. In addition to bacteria, microalgae *Chlorella sorokiniana* (SVMIICT8) was also evaluated for the synthesis of PHB under biphasic nutritional mode of cultivation. The PHB extraction procedure was modified and the extract was compared with the analytical grade PHB (Sigma-Aldrich Cat.: 36,350-2) as a reference. The maximal yield of 29.5 % of PHB from 0.94 gm L^{-1} of algal biomass was procured. The influence of biphasic cultivation on photochemical yield and electron transport rate was investigated using chlorophyll a fast kinetics that depicted the influence of Acetyl CoA activity over metabolic pathways. (*Bioresour. Technol.*, **2021**, 341, 125735; *Bioresour. Technol.*, 2022, 354, 127135)

Composite Grafting with Polyhydroxybutyrate and α-Cellulose

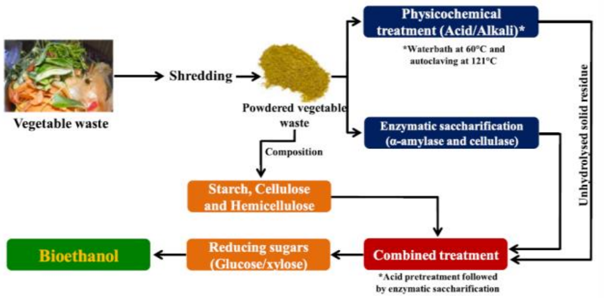
The study focuses on enhancing the properties and processability of PHB composites, obtained from grafting of waste-derived polyhydroxybutyrate (PHB) and bagasse cellulose (α-cellulose), making them an attractive and cost-effective biobased option that can decouple the usage of fossil-based plastics to a certain extent. Additional value from this process was further achieved by incorporating the concept of biorefinery, wherein acidogenic fermentation effluents were used for the production of PHA, which enabled the re-entry of products (VFA) to the production cycle, thus achieving circularity. (*Chemosphere*, **2021**, 279, 130563 – 130573)



Graphical Representation of Polyhydroxybutyrate production from dark-fermentative effluent and composite grafting with bagasse

Refining Vegetable Waste to Renewable Sugars for Ethanol Production

Potential of various vegetable wastes, such as composite vegetable waste (CVW), potato waste (PW), sweet potato waste (SPW), and yam waste (YW), as alternatives for producing renewable sugars and ethanol was examined. The sugars obtained were valorized into bio-ethanol through fermentation using *S. cerevisiae* by optimizing the pH and temperature. The highest ethanol yield of 251.85 mg/g was obtained from SPW at 35°C followed by YW (240.98 mg/g), PW (235.4 mg/g) and CVW (125.6 mg/g) at pH 5.0. (*Bioresour. Technol.*, **2021**, 340, 125650)



Refining of vegetable waste to renewable sugars for ethanol production

Coupling of Thermophilic Anaerobe and Mesophilic Micro-Aerobe for Bioethanol Production

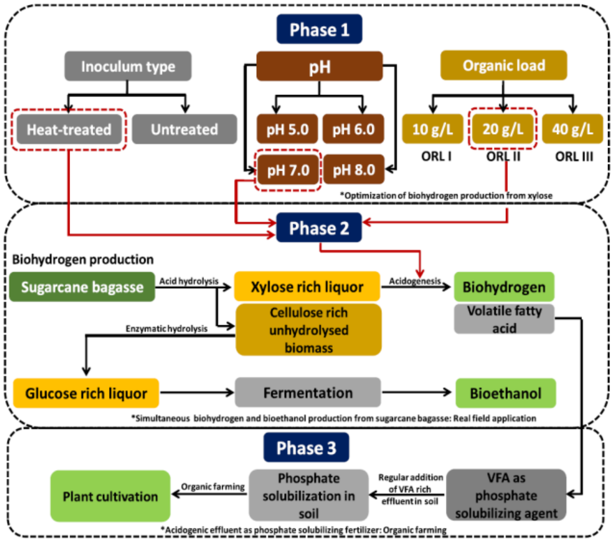
Sequential bio-processing (CBP_{SeqE}-II) driven by novel microbial pairing resulted in maximum ethanol of 0.26 g ethanol/g 0.5% NaOH treated BMSW (36.90 ± 0.10 g/L ethanol). This study substantiates efficacy of CBP_{SeqE}-II biosystem in sustainable bioethanol production in a single reactor without laborious steps. Thus suggesting, the applicability of sequential bioprocessing for higher carbon and energy recovery from CSPBMSW enabling sustainable waste valorization. (*Bioresour. Technol.*, **2020**, 308, 123260 - 123272)

Agri-Biomass Based Biorefinery to Create Circular Bio-economy

An integrated biorefinery system (IBS) was developed to valorize Agri-biomass (rice straw, sugarcane bagasse and wheat straw) into valuable products (cellulose, lignin, hemicellulose and reducing sugars). In IBS, a low-cost and sequential recovery strategy was followed with low input of chemicals and energy with zero-liquid discharge (ZLD). Lab scale process for 1 kg/batch feedstock was developed and demonstrated. Life cycle analysis (LCA) displayed value addition to the Agri-biomass sector; manifesting additional socio-economic benefit to the farming as it can facilitate employment to farmers in the off-season. Additionally, this sustainable agri-based bioeconomy strategy decarbonizes the agricultural production by reducing crop residue burning. Lignocellulosic biorefineries supports 'Chemurgy' that accounts for low-carbon processes/products, facilitating additional revenue to the agri-based sector. (*Green Sustain. Chem.*, **2021**, 27, 100392)

Green Hydrogen and Bioethanol Production from Sugarcane Bagasse (SCB) Hydrolysate with Circular Biorefinery Design

Feasibility of bio-H_2 production was initially evaluated with pure xylose and further validated with real field feedstock (SCB). Acid pre-treatment of SCB with 2% H_2SO_4 (v/v) yielded xylose rich hydrolysate (21.8 g xylose/100 g SCB), which was subjected to dark fermentation for bio-H_2 and VFA production. The un-hydrolyzed biomass recovered after acid hydrolysis of SCB was further subjected to simultaneous saccharification and fermentation (SSF) for bioethanol production. Utilization of segregated streams of SCB for bio- H_2 and bio-ethanol production with integrated organic farming in a closed loop and net-zero waste approach is established. (*Chem. Eng.*, **2021**, 425, 130386)



Representation of Green Hydrogen and Bioethanol production from Segregated Sugarcane Bagasse Hydrolysate

Bio-Crude and Low-Carbon Fuels Production - Hydrothermal Liquefaction (HTL) of *Scenedesmus sp Biomass*

Catalytic hydrothermal treatment of dried microalgae biomass (DAB) of *Scenedesmus* sp. SVMIICT1 for bio-crude was studied. The results depicted that H_2 atmosphere and catalyst loading improved the bio-oil with higher heating value and yields by hydro-deoxygenation. Aliphatic/aromatic hydrocarbons were predominantly observed in the bio-oil followed by carboxylic acids, furan derivatives, indanone derivatives, ketones, and substituted benzenes. The aqueous fraction was valorized through dark fermentation to produce the Bio-H_2 and Bio-CH_4, wherein maximum biogas yields were observed in NaOH catalyzed HTL. Thus, the integrated anaerobic digestion with HTL could maximize the energy and nutrient recovery with profitable by products in the biorefinery format. (Sustain. Energy Fuels, **2022**, 6, 1499-1511).

Duckweed Biorefinery- Dairy Wastewater Treatment with Microbial Protein Production

The work intends to evaluate the duckweed growth in an integrated biorefinery approach, firstly by utilizing dairy wastewater (DWW) as a substrate for biomass production, nutrient recovery, and valorization of value-added products. Secondly, duckweed hydrolysate (DWH) rich in carbon (C) and nitrogen (N) was evaluated as a nutrient media towards microbial protein (MP) production. The duckweed biomass offers multiple benefits including nutritional supplement in food/feed for livestock and poultry industries along with concurrent wastewater treatment and serving as potential feedstock in biorefinery. (Bioresour. Technol., **2022**, 126499)

Bioelectrocatalytic Reduction of Tellurium Oxyanions Towards Cathodic Recovery

A novel double-chambered BES coupled with biotic-anode and abiotic-cathode for Te^{+4} removal facilitating recovery of elemental tellurium (cathode) along with wastewater treatment (anode). The BES was operated at varied tellurite oxyanion (TeO_3^{2-};Te^{4+}) concentrations as cathodic terminal electron acceptor (CEA) at cathode to evaluate its regulatory influence on anodic electrogenic/enzymatic/ metabolic activity in correspondence to the ORR rates. Bioelectrochemical analysis supported the concentration-dependent Te^0 recovery with the influence of CEA variations in terms of proportional increase in biocatalytic currents and resulting in higher Te^{+4}reductions at cathode. (ACS EST Water, **2022**, 2, 1, 40-57)

Biotechnological Process for the Simultaneous Removal of Ammoniacal Nitrogen and COD from Industrial Wastewater

A sequential biological process for the “Simultaneous removal of Ammoniacal nitrogen and oxidizable Carbon from the industrial wastewaters (Bio-SAC)” was developed. The impact of bacterial cultures (aerobic, anoxic, and anaerobic) on the removal of ammoniacal nitrogen and COD from wastewaters using sequential 4 step biological process (BioSAC) in laboratory scale experiments were investigated and demonstrated at pilot scale. A skid mount pilot scale reactor was commissioned. In addition to the laboratory scale experiments, about 60 L of anaerobic, anoxic and aerobic cultures were developed for the operation of the pilot plant.

Skid mount pilot plant installed in CSIR-IICT

Scalable Process for Biosilica, Carbon and Lignin

Optimized nano-soft precipitation process for biomass waste using tailor made low cost approach was developed. The improved design process for production of nanoporousbiosilica and carbon from waste biomass is expected to reduce the construction and operating cost. Experiments with various 100 g, 500 g and 1 Kg of agricultural waste biomass such as rice straw, rice husk and ash were carried out under mild reaction conditions (60°C, 1 atm) and low of concentrations. Biomass materials are grounded by to get the size of less than 2 mm for the ease of nano-soft precipitation process. In addition, the cost-effective and sustainable path for porous carbon has been developed simultaneously.

Removal of NH_3 and H_2S from odour Causing Tannery Emissions Using Biological Filters

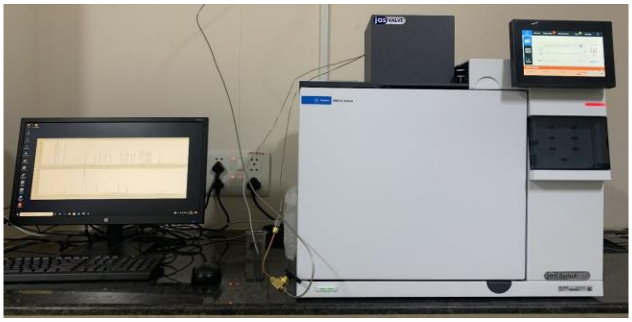
Pilot-scale studies were performed in a 2.7m^3 bio-filter with synthetic gas mixture containing hydrogen sulfide (H_2S) and ammonia (NH_3) to study the impact of bedding material and identification of various design parameters for scaleup. The removal efficacy of both NH_3 and H_2S was about 90–99% at an empty bed residence time of 55 seconds at an inlet concentration (NH_3 and H_2S) of 200 to 210 ppmV in 210 days. The microbial biodiversity analysis revealed the dominance of proteobacteria as well as Firmicutes and Acinetobacter. Removal efficiency of >99% in atannery since last three years was observed with a full-scale bio-filter (13.75m^3). (*J. Environ. Sci. Health* A, **2021**, 56, 625-634)

Long Term Measurement of Ozone, NO_x, $SO_2$and Total Solar Radiation at a Remote Site to Study the Emission Fluxes and Change in their Concentration

Monitoring of surface level air pollutants (O_3, NO_X ($NO+NO_2$), CO, SO_2, and VOC's) inclusive of meteorological parameters (Temperature, Relative Humidity and Wind Speed) at an urban site, (TIFR-NBF, Hyderabad, India;17.47ºN, 78.58ºE, and an altitude of 536m MSL) was studied during the entire year for different seasons. Results disclosed that the seasonal variations of air pollutants in Hyderabad are mainly influenced by meteorological conditions and other NMHC's present in the atmosphere. (*Environ. Processes,* **2021**, 8, 959-972; *Model. Earth Syst. Environ.,* **2020**, 6, 1981-1989)

Development of Efficient Microwave based Clean Coal Technologies: Grinding, Dewatering and Desulfurisation of Coals

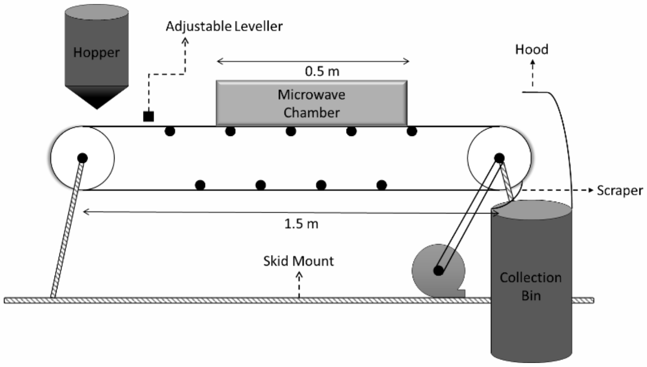
A single-step direct production of syn-olefins to increase per pass syngas conversion and reduce the cost of olefins production was developed. State-of-art facilities for Syngas conversion process has been created to evaluate various catalyst recipes at 4CC vol. Catalyst screening studies were conducted in dual high pressure fixed bead reactor unit over 30 nos catalyst recipes. Among these, two formulations Synol-1 & Synol-2(Oxide-Zeolite) emerged as most permissive catalysts for direct production of lower olefins.



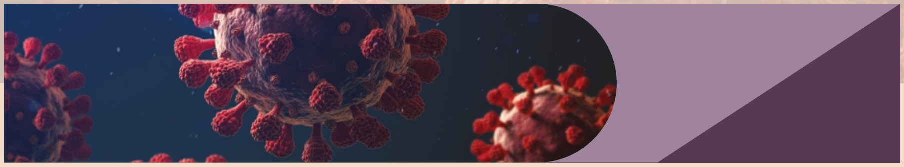
Dual high pressure fixed reactor unit with on-line refinery gas analyser

Development of Efficient Microwave Based Clean Coal Technologies for Grinding, Dewatering and Desulphurization of Coals using Lab Scale Studies

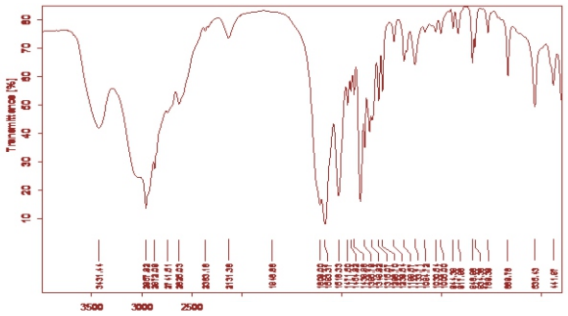
A microwave pre-treatment process to reduce the moisture of coals was undertaken. The process can reduce the moisture by 8-10% in 10-15% moisture containing coal within 1-3mins treatment time as opposed to 24-48 h taken in convection drying method. By enhancing the quality of coals, the net requirement of coals per unit energy would be reduced and thereby reducing carbon footprint. The microwave pre-treatment can be used to reduce moisture and increase gross calorific value, enhance grind ability and desulphurize Indian coals. The process is solely dependent on temperature of coal sample that is being treated.

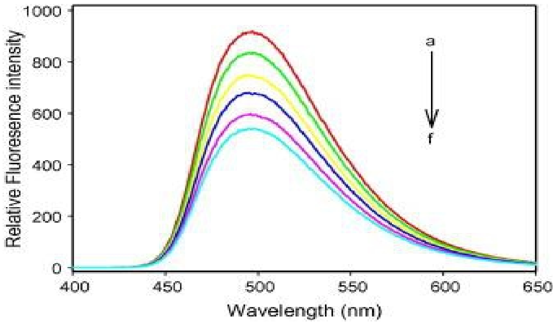


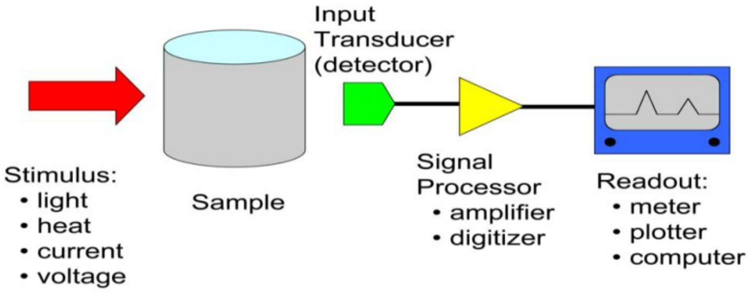
Conveyor belt microwave assembly (CMA)

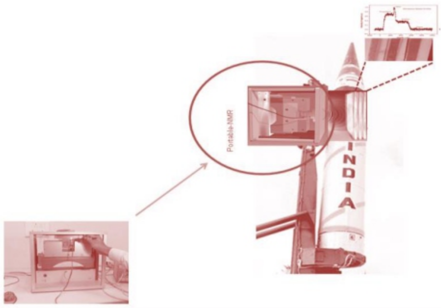


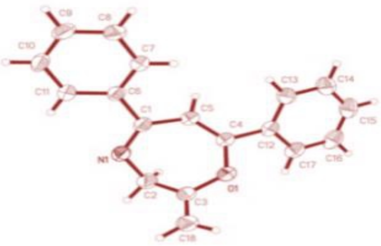
DEPARTMENT OF ANALYTICAL & STRUCTURAL CHEMISTRY









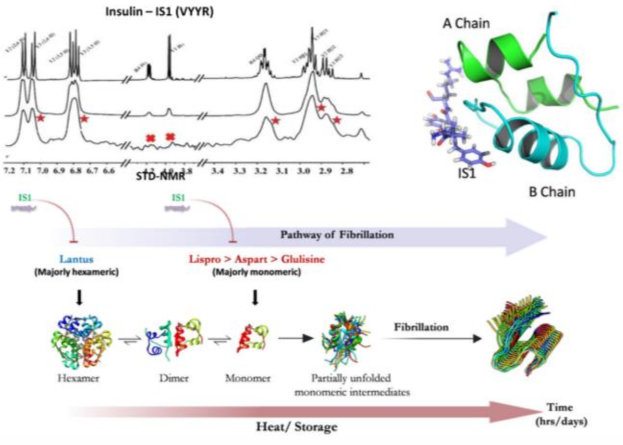


DEPARTMENT OF ANALYTICAL & STRUCTURAL CHEMISTRY

BASIC RESEARCH

Prion Derived Tetrapeptide Stabilizes Thermolabile Insulin *via* Conformational Trapping

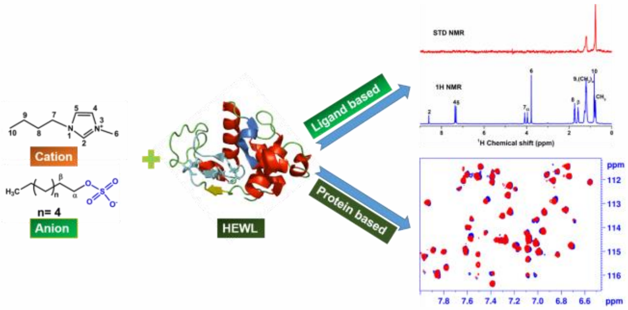
In search of cross amyloid inhibitors, prion-derived tetrapeptide library screening reveals a consensus V(X)YR motif for potential inhibition of insulin fibrillation. A tetrapeptide VYYR, iso-sequential to the β2-strand of prion effectively suppresses heat and storage-induced insulin fibrillation and maintains insulin in a thermostable bioactive form conferring adequate glycaemic control in mouse models of diabetes and impedes insulin amyloidoma formation. Besides elucidating the critical insulin-IS1 interaction (R4 of IS1 to the N24 insulin B-chain) by NMR spectroscopy, it was further demonstrated non-canonical dimer-mediated conformational trapping mechanism for insulin stabilization. In this study, structural characterization and preclinical validation introduce a novel class of tetrapeptide towards developing thermostable therapeutically relevant insulin formulation. (*iScience*, **2021**, 24, 102573 – 102586)



Stable complex of Insulin-Insulock(IS1) structure

NMR Investigations on Binding and Dynamics of Imidazolium-Based Ionic Liquids with HEWL

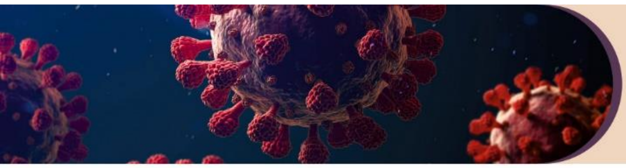
In the present work, interactions of ILs, namely, 1-butyl 3-methylimidazolium methyl sulfate (IL1), 1-butyl 3-methylimidazolium octyl sulfate (IL2) and 1-butyl 3-methylimidazolium chloride (IL3) with hen egg white lysozyme (HEWL) protein were investigated using solution-state nuclear magnetic resonance (NMR) spectroscopy. Among the ILs investigated, IL2 experiences significant interaction relative to those of IL1 and IL3, as revealed by the combined R1SEL and R1NS analysis. CSP analyses of 1H-15N HSQC spectra of aqueous P-IL mixtures enabled to identify the potential binding sites of ILs with HEWL. Whereas, 15N longitudinal (R1) and transverse (R2) spin-relaxation rates and 15N{1H} heteronuclear nuclear Overhauser effect (hetNOE) data subjected to the model free analyses for IL2 yielded the rotational correlation times and order parameters of various residues of HEWL. (*Phys. Chem. Chem. Phys.*, **2020**, 22, 23824-23836)



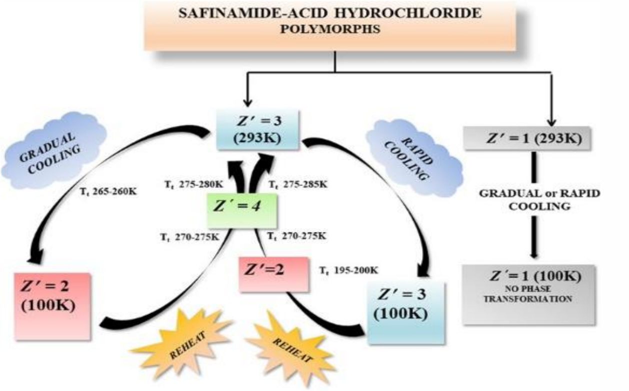
NMR based protocols for Protein-Ionic liquid interaction studies

Conformational Polymorphism in Safinamide Acid Hydrochloride and Observation of a Temperature-Dependent Reversible Single-Crystal to Single-Crystal Phase Transformation

Two concomitant polymorphs of safinamide acid hydrochloride were obtained in an attempt to prepare the O-protonated amide salt of safinamide from ethanolic HCl solution. The structural similarities in Z′ = 3, Z′ = 2, and Z′ = 4, the conformational variations, and the role of weak C−H···F and C−H···O intermolecular forces (which were able to form and break during the temperature modulation) without disturbance of the strong hydrogen-bonded network of N−H···Cl and O−H···Cl were identified as some of the key factors responsible for phase transitions in a single-crystal to



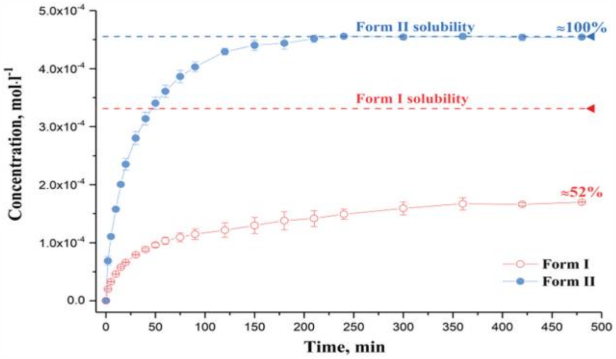
single-crystal fashion. (*Cryst. Growth Des.*, **2020**, 21, 133 – 148)



Temperature-dependent phase transition behavior of the Z′ = 3 polymorph of safinamide acid hydrochloride in a single-crystal to single-crystal fashion

Polymorphic forms of antiandrogenic drug nilutamide: Structural and thermodynamic aspects

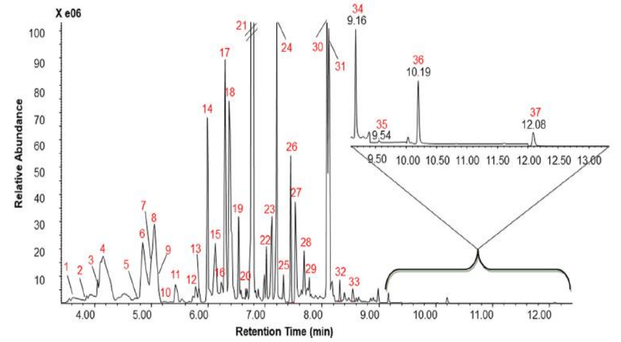
Two novel polymorphic forms of nilutamide were developed and characterized. The physicochemical properties and relative stability of the commercial Form I and newly obtained Form II were comprehensively investigated. The dissolution studies revealed that Form II demonstrates a higher solubility and an increased dissolution rate compared with Form I, which makes this polymorph a promising alternative to the commercial solid form of the drug. (Phys. Chem. Chem. Phys., **2021**, 23, 9695-9708)



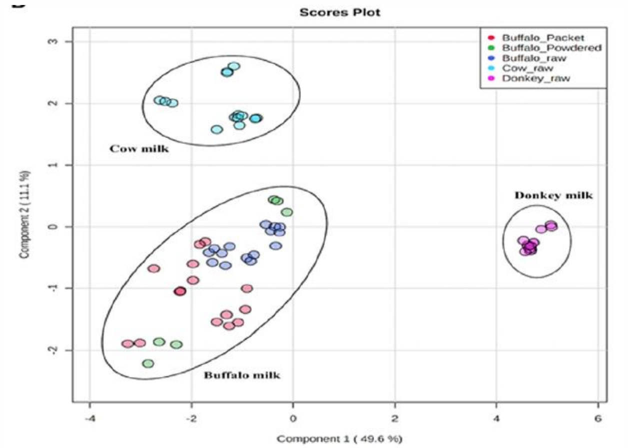
Dissolution profiles of Form I and Form II of nilutamide at pH 6.8 and 37.0°C

Targeted Screening Low-Molecular Weight Metabolites in Different Milk Samples by GC/MS

A rapid and straightforward single-phase extraction was developed followed by ECF derivatisation for the analyses of low molecular weight compounds such as amino acids, non-amino acids, and citric acid cycle metabolites in milk samples. The demonstrated method required less than one hour for screening 44 bioactive compounds. The sample preparation methods were separately optimised to measure the total (free and bound) and free amino acids in the milk sample. A simple ACN-based extraction enabled the holistic metabolic view of milk samples with minimal sample manipulation. A typical GC/MS SIM method with 13.37 min of run time was optimised, which was substantially (2-5x) more sensitive and faster. A GC/MS (SIM) method was then applied to different animal milk samples (i.e., buffalo, bovine, and donkey) and processed milk samples (i.e., pasteurised and dried), essential and nonessential amino acid content was found to be high in donkey milk. (*Inter. Diary J.*, **2021**, 105045 – 105057)

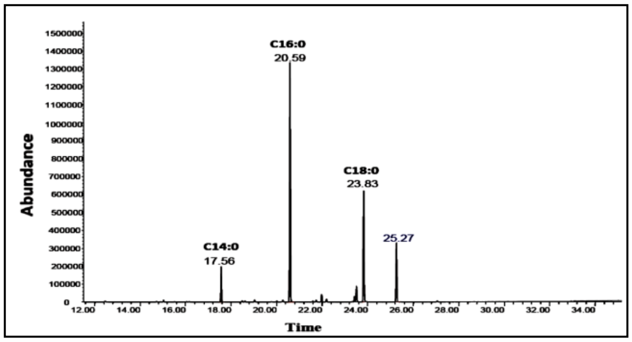


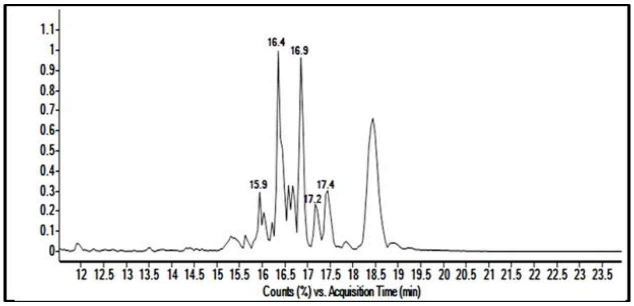
(Top) GC/MS chromatogram of buffalo milk
(Bottom) The PCA of 17 amino acids from different milk samples



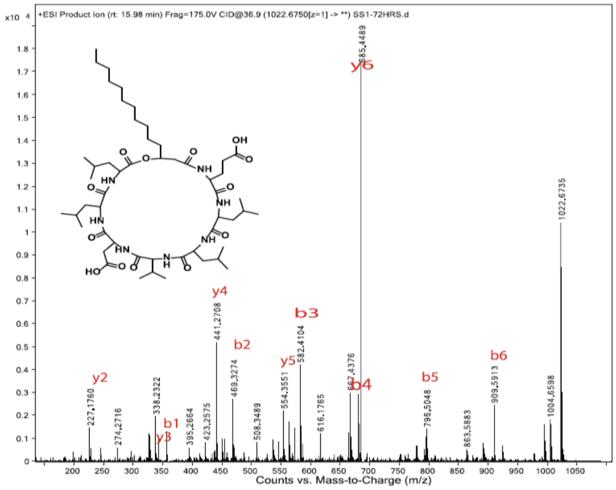
Identification and Characterization of Novel Agntifungal Cyclic Peptides from *Neobacillus drentensis*

A new exopolymeric biosurfactant cluster, composed of five lipoheptapeptides was isolated and characterized from a marine bacterium, *Neobacillus drentensis*. The cluster is composed of three new isoforms with completely different amino acid sequence and rest two were found to be identical to the natural standard surfactin. CLPs showed potential antifungal activity against azole susceptible and resistant *C. albicans*. Additionally, the CLPs disrupted the mature biofilms and biofilm formation of *C. albicans*. Altogether cyclic lipopeptide biosurfactant induced apoptosis in both susceptible and resistant strains, with remarkable morphological changes may lead to the development of marine lipopeptides. Our study suggests the use of cyclic lipopeptide exopolymeric biosurfactant to be more efficient against azole susceptible and resistant *Candida albicans* strains compared to the standard and other combinatorial formulations (*Bioorg. Chem.*, **2021**, 115, 105180 – 105190





GC/MS total ion chromatogram of the fatty acid methyl esters identified in CLP isomers (bottom) LC/MS total ion chromatogram of CLP isomers were performed using HPLC equipped with mass spectrometry as mentioned in the methods

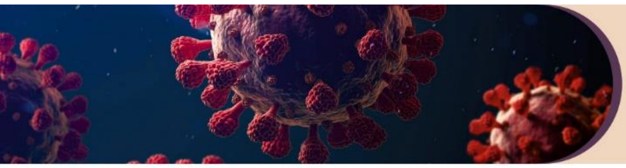


C14-Glu-Leu/Ile-Leu/Ile-Val-Asp-Leu/Ile-Leu/Ile

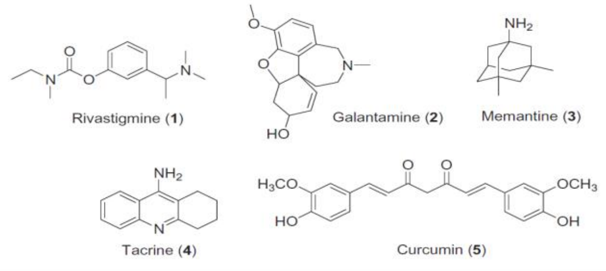
LC-ESI-MS/MS of cyclic lipopeptide isolated from AKLSR2 eluted at 15.98 min (m/z 1022.67)

Gas Phase Basicities and Proton Affinities of Alzheimer's Disease (AD) Drugs by Kinetic Method

The study explores the measurement of gas-phase thermochemical properties such as GB and PA of four commercially available drugs, namely, rivastigmine, galantamine, memantine, and tacrine, for AD and curcumin. The extended kinetic method is employed for this purpose using positive ESI-MS/MS technique. All the studied drugs have estimated GB and PA values in the high basic regions and this could be due to the presence of basic nitrogen atom (amino group), except in curcumin. The PA value of rivastigmine stood first in the order and the least was curcumin. The basicity of these compounds (either solution/gas-phase) may be one of the reasons



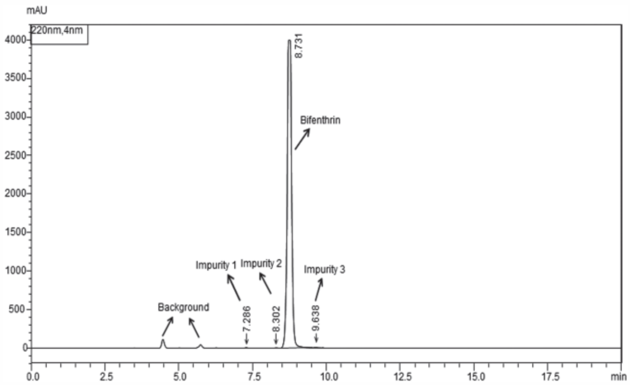
behind their pharmacological activity in the treatment of AD. (*Eur. J. Mass Spectrom.***2020**, 26, 388-399)

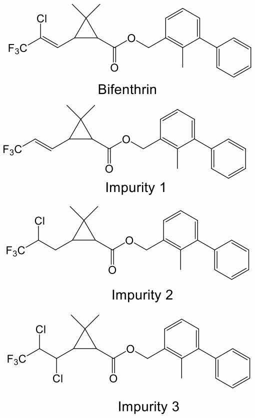


Chemical structures of the studied drugs

Identification and Characterization of Impurities in an Insecticide, Bifenthrin Technical

The impurities of bifenthrin were successfully studied by HPLC and GC/MS. Three impurities ranging from 0.175%–0.541% were detected by the HPLC-DAD method. The LC/MS analysis of bifenthrin and the prep-HPLC enriched fractions of impurities did not provide any mass signals due to failure in ionization under ESI or APCI conditions. The GC/MS analyses under EI and CI conditions, however, offered valuable molecular weight and structural information by which the structures of all the impurities could be elucidated. The EI mass spectra of bifenthrin and three impurities showed molecular ion and structure indicative fragments with additional isotopic pattern information for the presence/absence of chlorine atoms. (*J. Mass Spectrom*. **2020**, 55, e4605)

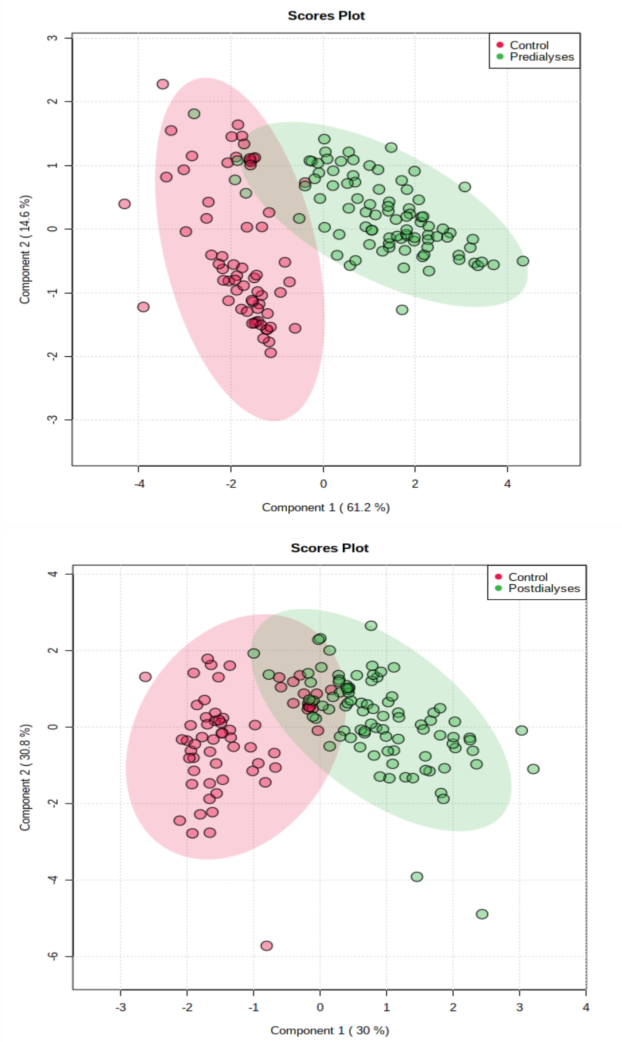




(Top) The GC/MS chromatogram of bifenthrin (showing 3 impurities) and (Bottom) characterized structures

Estimation of Arginine Metabolites in Plasma of Hemodialysis Patients

In the present study, arginine and methylated arginines were quantitatively measured in the plasma of pre-hemodialysis (PRE-HD), post-hemodialysis (POST-HD) and healthy control (HC) groups using the LC-MS/MS (SRM) technique. Different statistical analyses showed the distinctive differences in targeted metabolite concentration levels among the PRE-HD, POST-HD and HC groups. Among the measured metabolites, SDMA concentrations were significantly increased in HD patients compared with the HC group. Whereas, the other metabolites were altered slightly in HD patients and HC group samples. After the dialysis process (POST-HD), the dialytic clearances of these targeted metabolites were between 40-60-% except MMA and it showed the dialytic clearance is 28%. The higher accumulation of SDMA in HD patients can be used for CVD risk predictor as it reduces the HDL cholesterol. Besides this, SDMA/ADMA ratio (SAR) value is higher in HD patients when compared with the HC group.



PLS-DA score plots using SDMA, ADMA, MMA, HARG, CIT and ARG concentrations in PRE-HD group and HC group (Top) in POST-HD and HC group (Bottom). In this figure green colour represents PRE-HD group (n=90) and red colour represents the HC group (n=65)

Identification of Metabolites in Artificial Ripening of Fruits

The studies include the following.

i) SEC-MS/MS determination of amino acids from mango fruits and application of the method for studying amino acid perturbations due to post harvest ripening (*LWT - Food Sci. Tech.*, **2021**, 138, 110680)

ii) GC-MS based targeted metabolomics approach for studying the variations of phenolic metabolites in artificially ripened banana fruits (*LWT - Food Sci. Tech.*, **2020**, 130, 109622)

iii) Quantitative determination of targeted and untargeted pesticide residues in coconut milk by liquid chromatography –Atmospheric pressure chemical ionization –high energy collisional dissociation tandem high-resolution mass spectrometry (*J. Chromatogr. A* **2021**, 1659, 462649)

iv) Determination of 2-chloroethylphosphonic acid and its intermediate vinylphosphonic acid from artificially ripened sapota fruit by modified dispersive solid-phase extraction cleanup and gas chromatography/mass spectrometry analysis (*Rapid Commun. Mass Spectrom.*, **2020**, 34 e8907)

v) Gas chromatography–mass spectrometric determination of organic acids in fruit juices by multi-walled carbon nanotube– based ion-pair dispersive solid-phase extraction and *in situ* butylation (*Rapid Commun. Mass Spectrom*., **2021**, 35, e9165)

vi) Identification of calcium carbide-ripened sapota (*Achras sapota*) fruit by headspace SPME-GC-MS (Food additives & contaminants: part A, **2020**, 37, 1601).

2-Cyano-3-(2-thienyl) Acrylic Acid as a New MALDI Matrix for the Analysis of a Broad Spectrum of Analytes

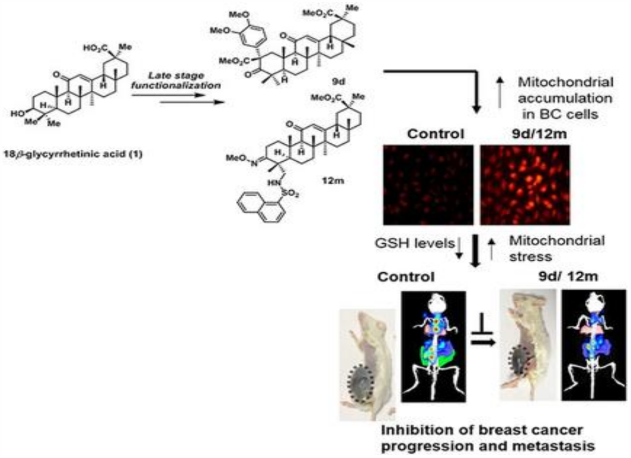
A low-cost synthetic 2-cyano-3-(2-thienyl)acrylic acid (CTA) is developed as a new MALDI matrix for the analysis of various classes of compounds such as lipids (e.g., fatty acids), peptides, proteins, saccharides, natural products (i.e., iridoids), PEGs, and organometallics in the positive-ion mode. The difficulty in the analysis of high molecular mass PEGs was overcome by using CTA as matrix even at low concentrations. The mass spectra of all of the studied analytes with CTA showed high signal-to-noise (S/N) ratios and spectral resolutions. However, in the case of peptide analysis with CTA, the resulting mass spectra are found to be similar to that of the well-established HCCA matrix. The CTA works as a proton/cation or electron-transfer matrix and can be used as a common matrix for the analysis of majority classes of analytes instead of using a specific matrix for particular class of analytes. (*J. Am. Soc. Mass Spectrom.*, **2021**, 32, 387 - 393).

Identification and Characterization of Degradation Products of Remdesivir using Liquid Chromatography/Mass Spectrometry

The drug remdesivir (RDV) was stressed under acidic, basic and neutral hydrolysis, oxidation, photolysis, and thermal conditions according to the International Council for Harmonisation (ICH) prescribed guidelines Q1A (R2). A total of nine degradation products were formed under acidic (DP1-DP5), basic (DP5-DP8) and neutral (DP5) hydrolysis, and oxidation (DP9) stress conditions, whereas the drug was found to be stable under thermal and photolytic stress conditions. The structures of the degradation products were elucidated by using a simple and rapid ultra-high-performance liquid chromatography coupled to electrospray interface with quadrupole time-of-flight tandem mass spectrometer (UPLC/ESI-Q-TOF-MS/MS) method (*New J. Chem.*, **2021**, 45, 7217 - 7224).

Identification and Characterization of Degradation Products of Indacaterol using Liquid Chromatography/Mass Spectrometry

Indacaterol (IND), 5-[2-[(5,6-Diethyl-2,3-dihydro-1H-inden-2-yl) amino] -1-hydroxyethyl] -8-hydroxyquinolin-2(1H)-one, is an active pharmaceutical ingredient (API) which is used to treat chronic obstructive pulmonary disease (COPD). Stressed degradation of the drug was performed under hydrolytic (alkaline, acidic and neutral), photolytic, oxidative and thermal conditions. Identification and characterization of IND and its forced degradation products (DPs) were demonstrated by using LC-HRMS and MS/MS method. A total of three DPs (DP1-DP3) were identified and characterized. The IND was found to be stable under photolytic, oxidative and thermal conditions, whereas it produced three DPs in acidic, basic and neutral hydrolytic stress conditions (*Eur J Mass Spectrom*, **2020**, 26, 425)

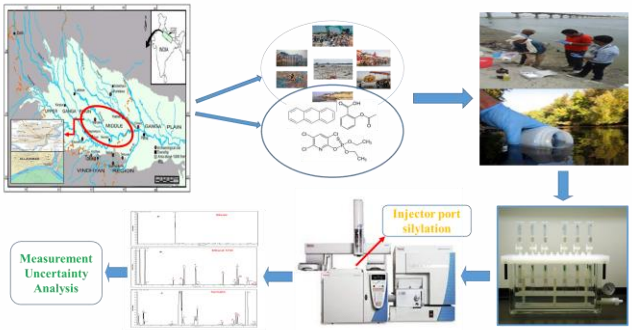


Development of an Analytical Method for the Quantitative Determination of Multi-Class Nutrients in Different Food Matrices by Solid-Phase Extraction and Liquid Chromatography tandem Mass Spectrometry

A simple and rapid analytical method based on solid-phase extraction (SPE) followed by liquid chromatography-tandem mass spectrometry (LC-MS/MS) with the aid of design of experiments (DOE) approach was developed and validated for simultaneous determination of multi-class nutrients (water- and fat-soluble vitamins and flavonoids) in various food matrices (vegetables, fruits, and cereals). The SPE-LC-MS/MS method was validated in terms of limit of detection (1.29-29.17 ng/g), linearity range (25-1000 ng/g), coefficient of determination (0.993-0.999) and recovery (72.53-104.24%) for multi-class nutrients in different food samples. Inter-and intra-day precision were evaluated and found to be within acceptable range. (*Food Chemistry*, **2021**, 341, 128173)

Estimation of Measurement Uncertainty for the Quantitative Analysis of Pharmaceutical Residues in River Water Using Solid-Phase Extraction Coupled with Injector Port Silylation-Gas Chromatography-Tandem Mass Spectrometry

The present study aims to estimate MU of an analytical method used for analyzing the pharmaceutical residues in river water by using solid-phase extraction (SPE) followed by auto injector port silylation coupled with gas chromatography-tandem mass spectrometry (IPS-GC-MS/MS) system. The calibration curves of all pharmaceutical residues showed dynamic linearity in the concentration range of 10–2000 ng/L with coefficient of determination (R2) ranging between 0.985 and 0.999. The limit of detection, limit of quantification, and recovery were found to be in the range of 2.52–7.31 ng/L, 8.33–24.12 ng/L and 81.82–114.14%, respectively. The method robustness was found within acceptation limit (<15% RSD) for system suitability. The expanded uncertainty was estimated in the range of 1.28–32.96% for the SPE method. Precision and recovery were identified as major uncertainty sources of SPE-IPS-GC-MS/MS method for the analysis of pharmaceutical residues in river water (*Microchem. J.*, **2020**, 159, 105560)



Graphical view of estimation of pharmaceutical residues in river water by SPE-IPS-GC-MS/MS with MU estimation

Development of a Multiclass Method to Quantify Phthalates, Pharmaceuticals, and Personal Care Products in River Water using Ultra-High Performance Liquid Chromatography Coupled with Quadrupole Hybrid Orbitrap Mass Spectrometry

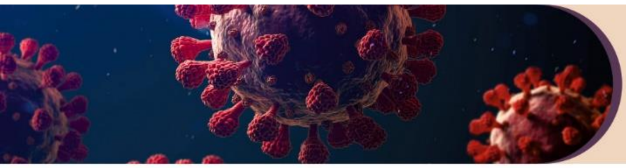
The organic micro pollutants were extracted from river water by solid-phase extraction (SPE) using hydrophilic-lipophilic balance sorbent and analyzed using an ultra-high performance liquid chromatograph (UHPLC) equipped with C18 stationary phase for chromatographic separation. The targeted mass experiments were conducted in a Q-Orbitrap-MS system in positive and negative electrospray ionization mode. The method performance was evaluated by analyzing real samples collected from River Ganga, and the concentrations of 21 analytes were found to be in the range of 0.76-9.49 ng/L for pharmaceuticals, 1.49–8.67 ng/L for phthalates, and 0.9-7.58 ng/L for personal care products (*Anal. Sci. Adv.*, **2021**, 2, 373 - 386)

Using Bio-Analytical Tools to Detect and Track Organic Micro Pollutants in River Ganga Near Two Major Cities

A panel of *in vitro* bioanalytical tools were employed to quantify estrogenic, androgenic, progestogenic, glucocorticoid and peroxisome proliferator-like activity in water extracts collected from two Indian cities in the river Ganga Basin. Cytotoxicity of the water extracts in a human-derived cell line and the potential to cause oxidative stress in a fish cell line were also investigated. High levels of activity for all endpoints in samples directly receiving urban drain discharge and low levels at sites upstream from drain discharges were found. Estrogenicity was detected at levels equivalent to 10 ng/L 17β-estradiol, representing a high likelihood of biomarker effects in fish. Sites located downstream from drain discharges exhibited low to intermediate activity in all assays. (*J. Hazard. Mater.*,**2021**, 404, 124135)

Quantitative Determination of Phenolic Antioxidants (PA) in Fruit Juices by GCMS/MS after QuEChERS Extraction Using Injector Port Silylation

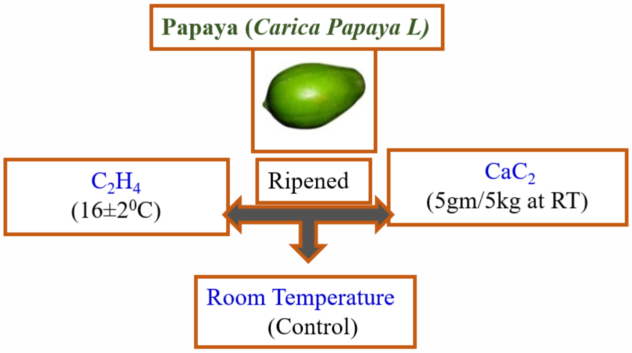
This study is focussed to develop and validate an analytical method for the quantitative determination of 11 PAs in packed fruit juices by QuEChERS method followed by injector port silylation-gas chromatography-tandem mass spectrometry (IPS-GC-MS/MS). The developed method was found to be linear in the concentration range of 100-1000 ng/L with a coefficient of determination (R2) ranged between 0.996-0.999. The limit of detection and limit



of quantification were found to be in the range of 8.14-25.45 ng/L and 27.13-84.85 ng/L, respectively. The per cent recoveries of 11 PAs in fruit juice were found to be in the range of 73.2-119.9%. (*Microchem. J.*, **2021**, 160, 105705)

Understanding the Metabolic Perturbations in *Carica papaya* Linn. Using Gas Chromatography-Mass Spectrometry Based Metabolomics

The metabolic perturbations in *Carica papaya* Linn. (papaya), which has been ripened either by the ripening practice (room temperature process as control) and/or ripening agents (calcium carbide and ethylene) using gas chromatography-mass spectrometry (GC-MS) based metabolomics were studied. The partial least squares-discriminant analysis revealed significant alternations in 13 metabolites mainly sugars, amino acids, fatty acids, and organic acids as well as disturbances in five metabolic pathways due to different ripening practice/agents. The individual comparison of calcium carbide with control and ethylene with control found 13 and 11 metabolites, respectively, which are common to the PLS-DA of three ripening groups. The GC-MS–based metabolomics has been able to predict the metabolic perturbations in papaya resulting from the ripening practice/agents. (*Anal. Sci. Adv.*, **2020**, 1, 183 – 193)



Graphical view of MS based metabolomics to understand the perturbations in papaya due to different ripening agents/practices

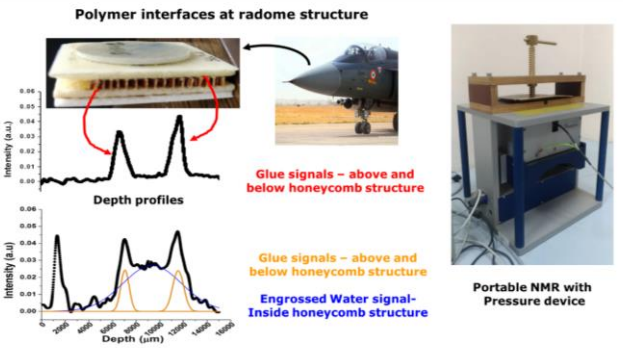
Micronutrients and Phytochemicals Content in Various Rice (*Oryza Sativa*Linn.) Micronutrient and phytochemical contents in different rice (*Oryza sativa* Linn.) samples available in market were analysed. Effect of aqueous-ethanol extract of each type of rice was evaluated against intestinal α-glucosidase to examine extract's influence on carbohydrate digestion. Brown-rice presented highest (54%) α-glucosidase inhibition followed by parboiled-rice (52%), idly-rice (48%), hand-pounded rice (42%), dosa-rice (40%) and basmati-rice (39%). Polished white sona-masoori rice presented least enzyme inhibitory (31%) activity. Presence of higher α-glucosidase inhibitory activity was regarded as slow digesting rice that would impart lesser postprandial glycemic excursion. Brown and parboiled-rice presented highest ABTS$^+$ radical scavenging (74%) activity whereas; idly-rice displayed highest DPPH scavenging (50%) activity. Higher polyphenol and niacin contents in rice were found significantly ($p<0.0001$ and $p<0.01$ respectively) correlated with enzyme inhibitory activity. Higher polyphenol content was found responsible for enhanced free-radicals scavenging activity. (*Indian J. Tradit. Knowl.*, **2020**, 19, 821 – 831)

APPLIED RESEARCH

Non-Destructive Depth Profiling and Identification of Debonding Defects across Polymer Interfacial Layers by Using Portable Single-Sided NMR

A portable single-sided NMR approach was developed for spatially resolved layer-by-layer characterization of polymer films/adhesive layers/coatings of unconventionally large dimensions and correlated the results with those obtained from high-resolution solid-state NMR.

In this method we also established the interplay of micro structural changes and polymer chain dynamics under high pressures and its impact on the quality of the adhesives used in strategic applications.



Characterization of water entrapped in polymer interfaces of random structure using portable single-side NMR device

Characterization and Validation Studies of BD-364 Polymorphs F-I, F-II and Monohydrate through Powder X-Ray Diffraction (PXRD) and Differential Scanning Calorimetry (DSC) Analyses

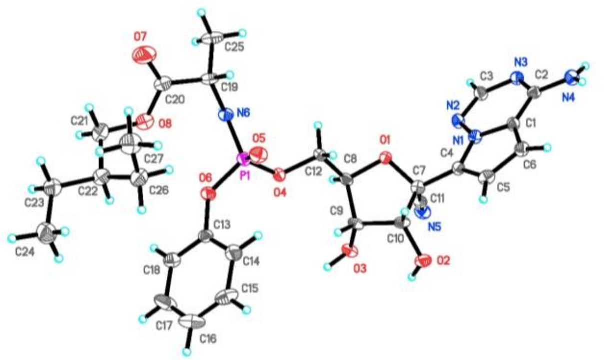
PXRD and DSC techniques were used for characterization of BD-364 polymorphs F-I and F-II and monohydrate. Both techniques provided comparable LOD of F-II in F-I material (0.7% by PXRD and 0.5% by DSC) and comparable LOQ values (2% by PXRD and 1.5% by DSC). Quantification of monohydrate in F-I sample could not be conducted by DSC technique as it was known to undergo phase transformation to F-I upon dehydration. By PXRD technique, the LOD and LOQ were achieved from 0.5% and 1.75%, respectively, for monohydrate in F-I.

Powder X-ray Diffraction (PXRD) Study of ZS9 Samples for Pore Size Determination

A lot of activities are going on the zirconium cyclosilicate (ZS-9) for first-in-class therapy for hyperkalemia with improved capacity, selectivity, and speed for entrapping K+ when compared to currently available options. One important characterization is to determine its pore size.

Crystal Structure Determination of Remdesivir, Anti-COVID Drug

Remdesivir (Veklury) was the first drug approved by the FDA for treating the SARS-CoV-2 virus. The client approached us to develop the single crystal and also wants know the chirality of the molecule through single crystal X-ray diffraction studies. The remdesivir molecule contains six chiral centres and their absolute configuration was confirmed by unambiguous refinement of the absolute structure parameter.



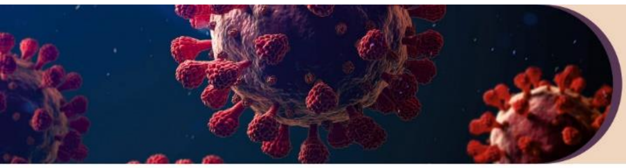
Crystal structure of Remdesivir

Analytical Services to In-House Projects

NMR Centre of Department of Analytical & Structural Chemistry, 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 enhances sensitivity. During pandemic (2020 and 2021), NMR centre provided 24/7 emergency support to all COVID centric projects.

Bruker AVANCE III 700 MHz

Bruker AVANCE NEO 600 MHz



Bruker AVANCE III HD 500 MHz

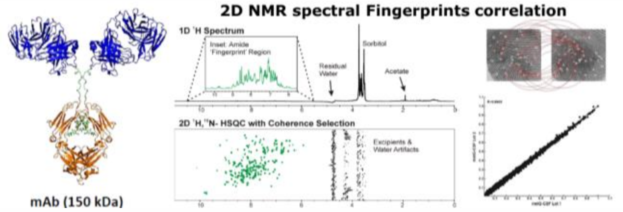
Value Added Services for Pharmaceutical Industries

By virtue of its technical strength and scientific expertise, the NMR centre is the best choice for many pharmaceutical industries and academic institutes in the country for high quality analytical services. The centre extensively provides these services with regulatory ambience. 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 with no observations.

The Centre for X-ray Crystallography is well-known for its expertise in powder and single-crystal X-ray diffraction analyses and infrastructure. These activities are helping various pharmaceutical and agrochemical industries in India.

Establishment of GLP Compliant Analytical Facility to Augment Biosimilars Characterizations in India

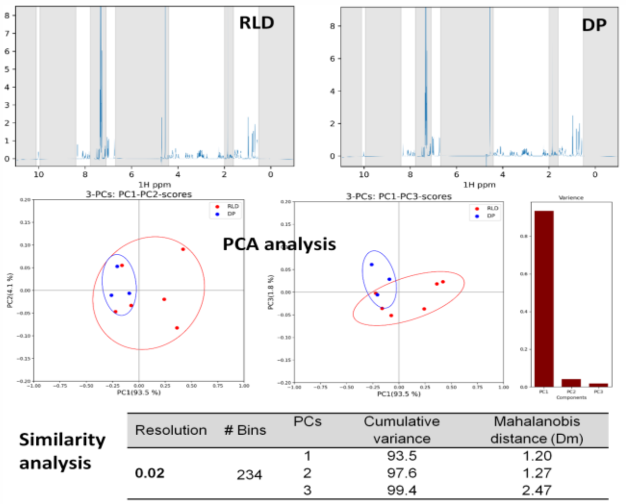
The GLP compliant analytical facility for biosimilars characterizations is first of its kind facility and extensively helps enhance the research on biosimilars product development in India. We design new ‘quick to use’ analytical approaches for biosimilars characterizations. We also generate skilled manpower to work in biosimilars industry. With this setup, CSIR-IICT is a one stop centre to develop/adopt analytical strategies for biosimilars characterization for regulatory submissions and the facility can act as a referral laboratory in biosimilars characterization.



2D NMR based fingerprinting protocols for characterization of biosimilars in formulation

In-house NMR Protocols for Higher Order Structure Similarity Assessment of Biopharmaceuticals

High-resolution NMR spectroscopy is versatile, non-invasive, chemically and structurally specific analytical technique that can provide atomic-level information for the evaluation of HOS of biosimilars. In-house NMR methods and analysis protocols were developed for HOS similarity assessment using one and two-dimensional (1D and 2D) NMR experiments complemented with chemometric methods like multivariate analysis and similarity distance measurements. NMR methods were optimized to overcome challenges posed by low drug concentrations, low natural abundance and high formulation excipients which are physiologically relevant. High throughput Python based statistical analysis protocols were built for unbiased and high throughput HOS analysis. These protocols are routinely used for industrial sample analysis, which are aimed for regulatory drug approvals. The similarity parameter, called Mahalanobis distance (Dm) value should be less than or equal to 3.3 is acceptable value established by FDA for the biosimilar to meet the requirement.



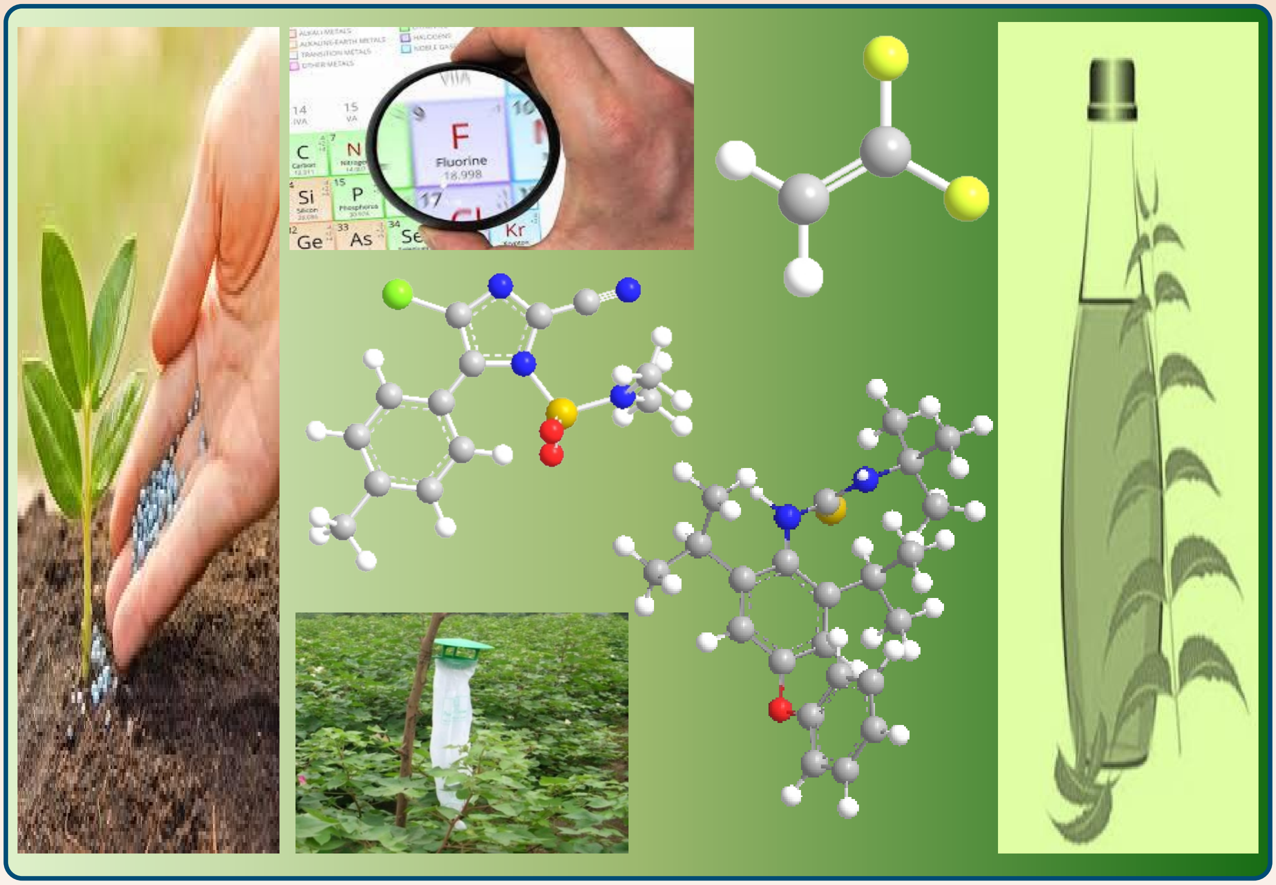
	Resolution	# Bins	PCs	Cumulative variance	Mahalanobis distance (Dm)
Similarity analysis	0.02	234	1	93.5	1.20
			2	97.6	1.27
			3	99.4	2.47

NMR protocols for HOS similarity analysis of biosimilars(DP) with reference product (RLD)

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

AnalyticCSIR is a new initiative to share analytical and research facilities in various CSIR-laboratories across the country. Our institute designed and developed the AnalytiCSIR Web portal. This initiative facilitates academic, industrial and other researchers to utilize sophisticated scientific equipment, which is on par with global standards. The portal provides an easy online access for researchers to locate and order online their desired analytical service at the nearest CSIR lab. Presently, 1453 equipments are listed on the portal that offers 1994 different tests. Each year about 1.5 lakh internal and about 30,000 external services are rendered.

FLUORO AND AGROCHEMICALS

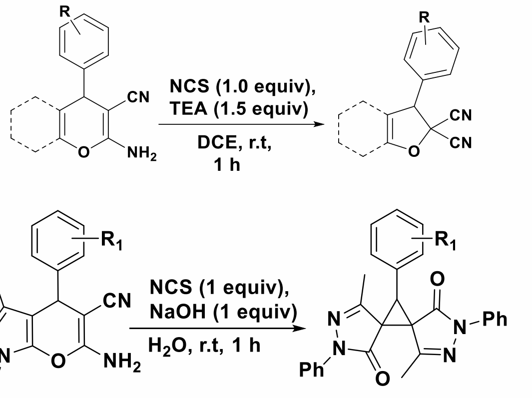


FLUORO-AGROCHEMICALS

BASIC RESEARCH

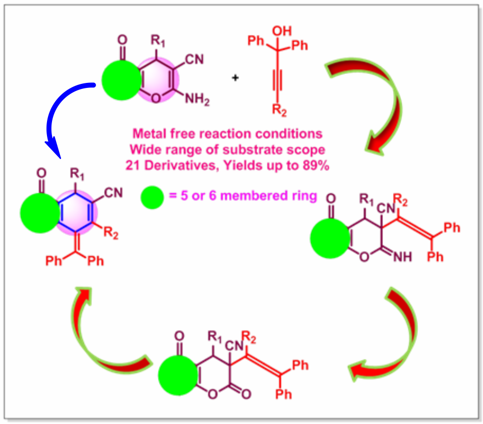
Base-Promoted Synthetic Transformation of 4*H*-Chromenes into Dihydrobenzofurans and Bispyrazolospirocyclopropanes via Intramolecular Cyclization

A novel protocol is accomplished for transformation of 2-amino-7,7-dimethyl-5-*oxo*-4-phenyl-5,6,7,8-tetrahydro-4*H*-chromene-3-carbonitrile into dihydrobenzofuran-2,2-dicarbonitriles by reacting with *N*-chlorosuccinimide in presence of base at ambient temperature. On the other hand, same reaction with 6-amino-3-methyl-1,4-diphenyl-1,4-dihydropyrano[2,3-*c*]pyrazole-5-carbonitrile and NCS, surprisingly lead to formation of bispyra zolospirocyclopropanes.. *(ChemistrySelect*, **2021**, 6, 37, 9867-9872



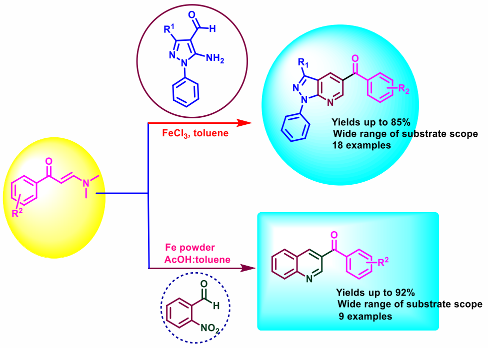
Acid Promoted Cascade Reaction of 4*H*-Chromenes: Access to Hexahydronapthalenes *via* Decarboxylative Intramolecular Cyclization

Acid promoted cascade reaction of 4*H*-chromenes with propargylic alcohol has been described. The reaction proceeds through Meyer-Schuster type of rearrangement of propargylic alcohol and reaction of 4*H*-chromene with *in situ* generated allene followed by decarboxylative intramolecular cyclization leading to hexahydronapthalene scaffolds with good to excellent yield.. (*ChemistrySelect*, **2021**,6,5, 983-986)



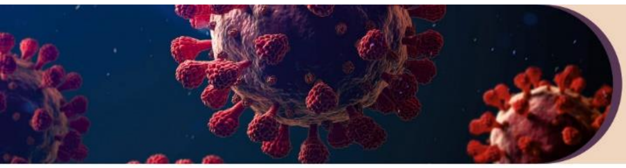
Iron(III)Chloride Induced Synthesis of Pyrazolopyridines & Quinolines

A simple and straightforward protocol has been accomplished for synthesis of pyrazolo[3,4-*b*]pyridines by reacting 5-amino-1-phenyl-3-(trifluoromethyl)-1*H*-pyrazole-4-carbaldehyde and β-enaminoketones promoted by Iron(III)chloride. This protocol also produced quinolines when *o*-nitrobenzaldehydes and β-enaminoketones were reacted. (*Synth. Commun.*,**2020**, 50, 23, 3642–3651)

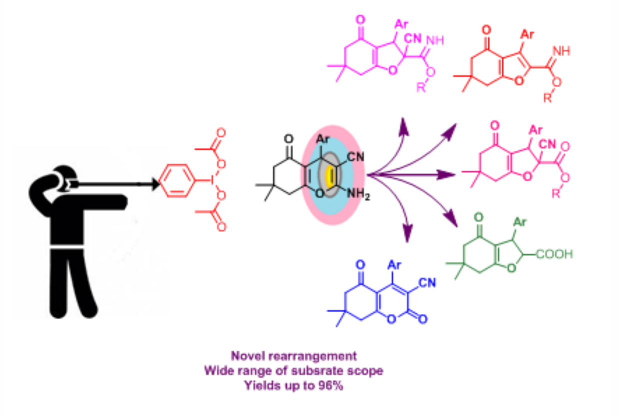


Hypervalent Iodine Promoted Transformation of 4*H*-Chromenes into Dihydrofurans and 2*H*-Chromenes

A novel protocol for synthetic transformation of 4*H*-chromenes into dihydrofurans and 2*H*-chromenes promoted by hypervalent iodine has been accomplished, in a one pot reaction, at ambient temperature. Dihydrofurans are exclusively formed



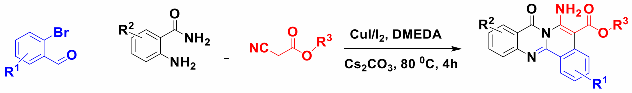
under basic reaction condition, whereas, 2*H*-chromenes are the products under acidic condition. (*Synth. Commun.*, **2020**, 50, 21, 3264-3275)



Novel rearrangement
Wide range of subsrate scope
Yields up to 96%

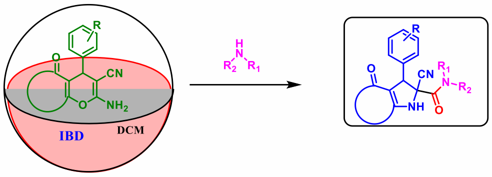
CuI/I$_2$-Catalyzed Concise Synthesis of Substituted 6-Aminoisoquinazolino-Quinazoline Carboxylates from Anthranilamide

A one pot sequential addition protocol for synthesis of polycyclic quinazolines with *β*-amino acid motifs has been achieved starting from anthranilamide. Initial *in situ* formation of 2-(2-bromophenyl)quinazolin-4(3*H*)-one followed by addition of alkyl cyanoacetates, catalyzed by copper (I) salts, gives the target compound in good to excellent yields. The expedient and facile cascade protocol involves nucleophilic α-arylation, intramolecular cycloamidation of nitriles followed by 1,3-hydrogen shift allowing direct access to 6-amino-8-oxo-8*H*-isoquinolino[1,2-*b*]quinazoline-5-carboxylates. *ChemistrySelect,* **2020**, *5*, 11685–11689)



Synthesis of Dihydropyrrole Derivatives by Oxidative Functionalization of 2-amino-4*H*-Chromenes using Hypervalent Iodine Reagents

An efficient simple, metal free, one pot protocol for the synthesis of dihydropyrrole derivatives has been achieved *via* sequential addition of iodobenzenediacetate and secondary amine to 2-amino-4*H*- pyran derivatives. The one-pot protocol proceeds *via* tandem oxidative functionalization, rearrangement and ring contraction providing an entirely new strategy for the construction of the dihydropyrrole skeleton. (*Synlett,* **2021**,*32*, 1109–1116)

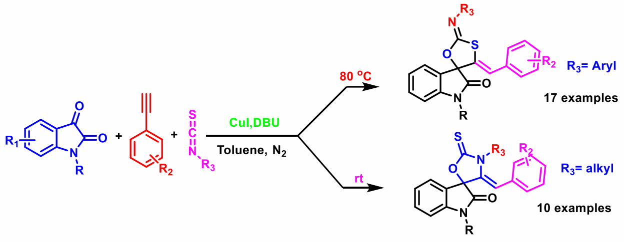


Crop Protection Chemicals: Future Pathways and Opportunities

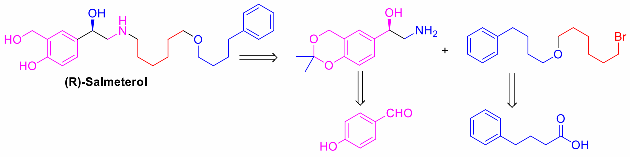
Buffeted by various forces the crop protection chemical industry is at the cross roads and faces daunting challenges. At the same time the challenges are opening up novel opportunities ranging from foraying into new chemistries creating environmentally benign products, shifting to bio-products and /or hybrids, integrated pest management to altering company structures involving mergers and acquisitions, etc. (*Chemical Industry Digest,* August **2021**, 46-50)

Multicomponent Domino Approaches for the Synthesis of Spirooxazolidine-2-thiones and Spirooxothiolane-2-imines

In a DBU mediated reaction, isatin, phenyl acetylenes, and aryl isothiocyanates undergo hydrothiolation whereas aliphatic isothiocyanates undergo hydroamination. In the presence of a strong base, NaOH for instance, isothiocyanates are exclusively hydrothiolated. This domino approach proceeding by the addition and 5-*exo* dig cyclization *via* hydroamination/ hydrothiolation, involves consecutive C-C, C-O, C-S/C-N bond formations. Further an attempt has been made to understand the reactivity pattern *via* DFT level of theory calculations. (*Eur. J. Org.Chem*., **2021**, 5348-5358)

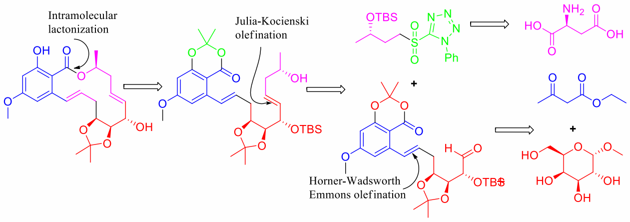


Enantioselective Synthesis of Bronchodilating Agent (*R*)-Salmeterol



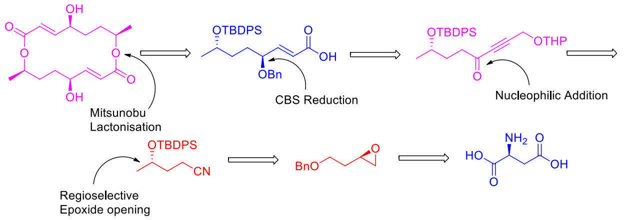
The key precursor, chiral *a*-amino alcohol synthesized, from 4-hydroxybenzaldehyde, which on phenolic Aldol with formaldehyde gave, 4-hydroxy-3(hydroxymethyl)benzaldehyde. Acetonide protection, followed by Wittig afforded, 2,2-dimethyl-6-vinyl-4*H*-benzo[*d*][1,3] dioxine,which on reaction with AD-mix-*β*, gave chiral diol, followed by selective protection and azide formation. Subsequent reduction of azide gave chiral amino alcohol. The second fragment is synthesized from phenylbutanoic acid, which on reduction gave 4-phenylbutan-1-ol. Thus obtained primary alcohol on coupling with 1,6-dibromohexane resulted, {4[(6-bromohexyl)oxy]butyl} benzene. The key fragments on coupling, followed by acetonide deprotection gave the target molecule, (*R*)-Salmeterol. *(Ind. J. Chem. B*.,**2021**, 60B, 1347)

Stereoselective Synthesis of Resorcylic Acid Lactone Cochliomycin B.



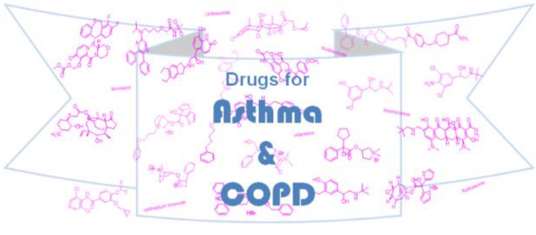
Synthesis started from, *D*-galactose, *L*-aspartic acid, orcinol and ethyl acetoacetate. The target molecule, obtained from precursor through intramolecular lactonization. The precursor in turn obtained *via* Julia-Kocienski olefination between aldehyde fragment and sulfone fragment. The sulfone fragment obtained from terminal epoxide, which in turn derived from *L*-aspartic acid. The aldehyde fragment containing *trans* double achieved from phosphonate and aldehyde by *E*-selective Horner-Wadsworth-Emmons olefination. Phosphonate of resorcylic acid core synthesized from ethyl orsellinate, which could be designed from ethyl acetoacetate. Aldehyde accessed from *D*-galactose. Thus this strategy derives C11´stereocenter from *L*-aspartic acid, whereas C4,C5´,C6´ stereocenters from *D*-galactose and resorcylic acid core from ethyl acetoacetate. *Tetrahedron Lett.*,**2021**, 82, 153410)

Stereoselective synthesis of C_2-Symmetric natural products Pyrenophorol and its derivatives.

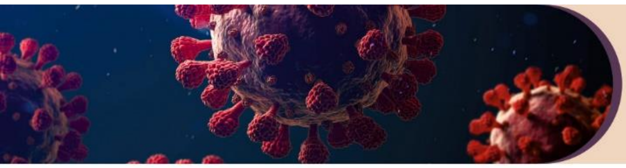


Synthesis started from monomer *via* deprotection of TBDPS ether followed by Mitsunobu macrolactonization using Gerlach procedure. The intermediate prepared from stereoselective reduction of keto group under CBS condition to obtained, nucleophilic addition of aldehyde. The intermediate obtained from regioselective epoxide opening, *in situ* protection of hydroxyl group followed by reductive cleavage of benzyl ethers and one carbon elongation using cyanation reaction. The intermediate epoxide prepared from diazotization, followed by epoxide formation using *L*-Aspartic acid. *(Prod. Res*., **2020,** 34, 15, 2173)

Synthetic approaches to FDA approved drugs for asthma and COPD from 1969 to 2020



Respiratory infections resulting from pulmonary inflammation are emerging as a leading cause of



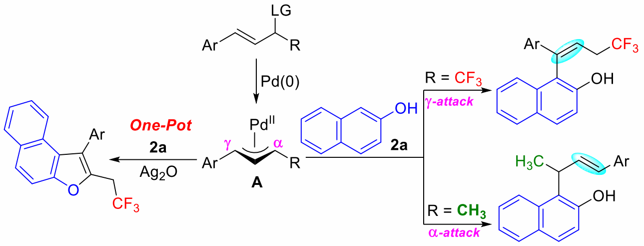
death worldwide. However, only twenty-seven new drugs were approved in the last five decades. In this review, we presented synthetic approaches for twenty-seven FDA-approved medications used to treat asthma and chronic obstructive pulmonary diseases (COPD), along with their mode of action. *(Bioorg. Med. Chem.,***2021**, 41, 116212)

Microwave-Assisted Efficient Synthesis of Pyrazole-Fibrate Derivatives as Stimulators of Glucose Uptake in Skeletal Muscle Cells

The design and synthesis of a series of pyrazolo[3,4-*d*]pyrimidinones containing fibrate side chains have been accomplished by utilizing the concept of molecular hybridization. All the synthesized compounds were evaluated for the glucose uptake stimulatory effect in L6 rat skeletal muscle cells. Four compounds were found to show significant stimulation of glucose uptake. Further these four compounds have been examined for their Glut4 translocation stimulatory effect in L6-Glut4myc myotubes. A Compound was found to exert maximum increase in GLUT4myc translocation. *(Bioorg. Med. Chem. Lett.,***2021**, 34, 127760)

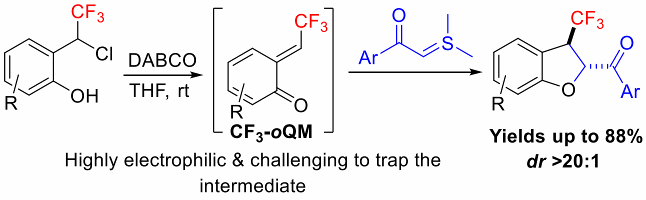
Palladium-Catalyzed ortho-Vinylation of β-Naphthols with α-TrifluoromethylAllylcarbonates: One-Pot Access to Naphtho[2,1-*b*]furans

Highly regio- and stereoselective palladium-catalyzed C_1-vinylation of *β*-naphthols has been reported for the first time using easily accessible CF_3-allyl carbonates. The present transformation is accomplished by a sequential decarboxylative allylation and double bond isomerization. The regioselective nucleophilic attack on the γ-carbon of CF_3-π-allyl Pd-intermediate is the key to furnish the (*Z*)-CF_3-vinylnaphthols in good yields. Conspicuously, the CH_3-π-allyl Pd-intermediate delivered the simple allylated product via an α-attack. Furthermore, we achieved a one-pot synthesis of trifluoromethyl substituted naphtho[2,1-*b*]furans in good yields through an uninterrupted *C*-vinylation/silver mediated radical cyclization reactions. It is noteworthy to mention that the present approach ensues in an eco-friendly solvent medium PEG-400. (*Org. Biomol. Chem*., **2021**, 19, 8241-8245)



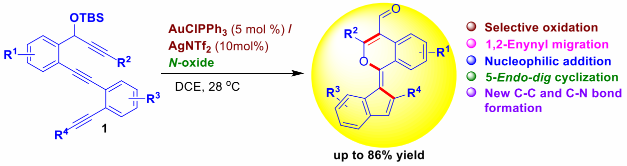
Diastereoselective Synthesis of CF_3-Dihydrobenzofurans by [4+1] Annulation of *in-situ* Generated CF_3-*o*-Quinone Methides and Sulfur Ylides

An efficient and highly diastereoselective synthesis of CF_3-dihydrobenzofurans by the reaction of *in-situ* generated CF_3-*o*QMs with sulphur ylides is disclosed. The generality of the present developed method is well studied with diverse substrates to access the corresponding products in excellent yields. The highly electrophilic and reactive CF_3-*o*QM is utilized first time for the annulation reaction. *(RSC Adv*., **2020**, 10, 38588)



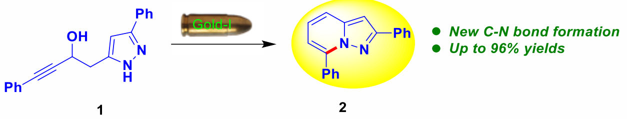
Gold-Catalyzed Synthesis of 1*H*-Isochromene-4-Carbaldehydes *via* Oxidative Cascade Cyclization

An efficient gold-catalyzed formation of indenylidene-derived 1*H*-isochromene-4-carbaldehydes from substituted 1,5,10-triyne-*O*-silanes was developed under mild reaction conditions. In this reaction gold- catalyzed selective oxidation, 1,2-migration, nucleophilc addition and then 5-*endo*-dig cyclization took place regioselectively. The indenylidene-derived isochromene-4-carbaldehydes were synthesized in moderate to very good yields *via* the formation of a new C-C and C-O bonds in one-pot. (*Org. Biomol. Chem*. **2021**, *19*, 3634-3643)



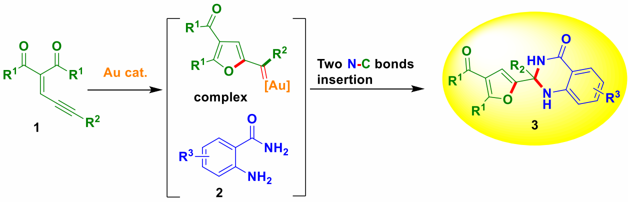
Gold-Catalyzed Synthesis of Pyrazolo[1,5-*a*] pyridines Regioselectively *via* 6-*endo-dig* Cyclization

An efficient gold-catalyzed synthesis of pyrazolo[1,5-*a*]pyridines have been developed from pyrazolo substituted propargyl alcohols *via* 6-*endo-dig* cyclization. In this intramolecular cyclization reaction a new C-N bond was formed regioselectively and good to excellent yields of pyrazolo[1,5-*a*]pyridines were obtained in one-pot. (*ChemistrySelect*, **2021**, *6*, 8791-8796)

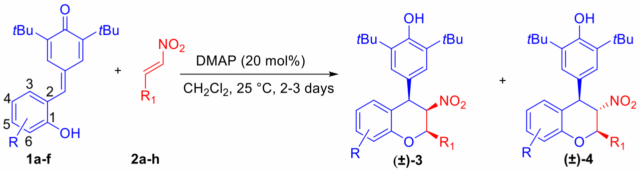


Gold (iii) Promoted Formation of Dihydroquinazolinones: Double X–H Activation by Gold

An efficient 2-furyl gold-carbene promoted synthetic method was developed for the formation of dihydroquinazolinones from enynones by dual insertion of anthranilamides. In this organic transformation a new C-O and two C-N bond formations occurred and dihydroquinazolinones were obtained with a quaternary centre in moderate to very good yields in one-pot synthesis. Nitrogen-containing heterocyclic molecules such as substituted quinazolinones were gained much attention due to their wide range of biological and pharamacological applications. (*RSC Advances*, **2020**, *10*, 35681-35691)



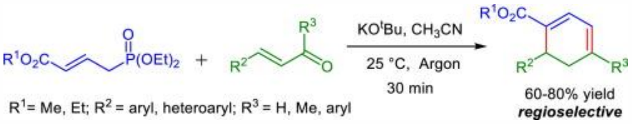
DMAP Catalyzed Addition-Cyclization Reaction Of 2-Hydroxyphenyl-*Para*-Quinone Methide with Nitroalkenes: Facile Entry into Highly Substituted Chromane Derivatives



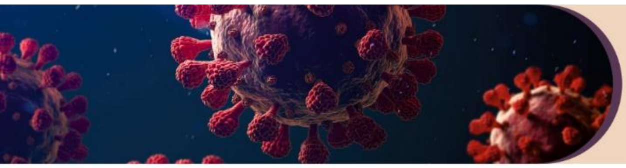
Yield 50 – 95 %; dr 60:40 to 90:10

The base catalyzed reaction of 2-hydroxyphenyl-*para*-quinone methide (*p*-QM) with nitroalkenes is reported. The DMAP catalyzed reaction afforded substituted chromane derivatives in excellent yields with moderate diastereoselectivity. The conversion of the initial products to other useful structures has also been achieved. (*Tetrahedron Lett.*,**2020,** *Volume 61, Issue 9, 151554*)

Regioselective synthesis of substituted cyclohexa-1,3-dienes via the base-mediated cyclisation of α,β-unsaturated carbonyl compounds and γ-phosphonylcrotonates



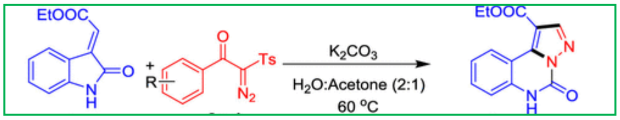
The base-mediated reaction of α,β-unsaturated carbonyl compounds and γ-phosphonylcrotonates under an argon atmosphere readily furnishes substituted cyclohexa-1,3-dienes. The cyclisation proceeds with complete regioselectivity to afford products that are readily amenable to further redox manipulations. The presented method allows the



rapid and regioselective syntheses of six-membered carbocycles at three different oxidation levels. (*Tetrahedron Lett*., **2020**, *Volume 61, Issue 39, 152380*)

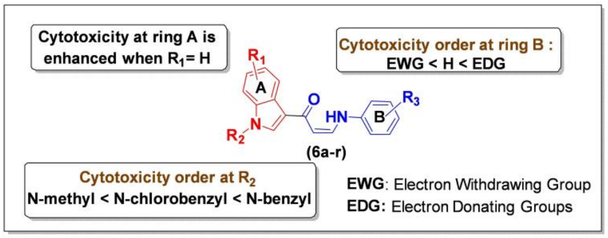
Regioselective Ring Expansion of 3-Ylideneoxindoles with Tosyldiazomethane (TsDAM): A Metal-Free and Greener Approach for the Synthesis of Pyrazolo-[1,5-c]quinazolines

An efficient, metal-free approach to access pyrazolo-[1,5- c]quinazolines with 3-ylideneoxindoles and tosyldiazomethane (TsDAM) under mild aqueous reaction conditions has been developed and the solvent involvement in the present reaction has also been explored for the first time. This greener approach involves 1,3-dipolar cycloaddition, regioselective ring expansion, followed by the elimination of tosyl group with aqueous base in a single operation, and the product can be isolated in high purity without column chromatographic separation. The method is also compatible with a large variety of functional groups, providing good to excellent yields in water, thus resulting in a decrease of environmental impact in the pharmaceutical industry. (*J. Org. Chem.,* **2020**, 85, 8, 5370–5378)



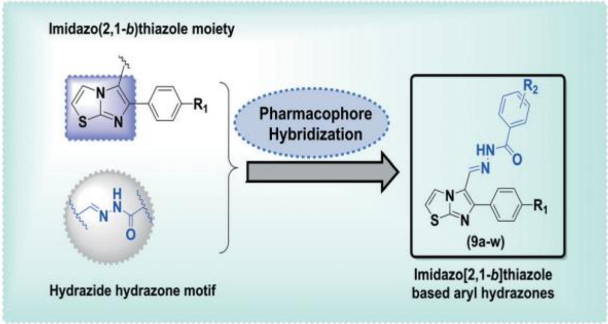
New Indolyl-Arylaminopropenone Conjugates: Synthesis, Cytotoxicity and Apoptotic Inducing Studies

A series of indolyl-arylaminopropenone Conjugates were prepared and evaluated for their antiproliferative potential against selected human cancer cell lines. Among them, two compounds demonstrated promising IC50 values of 2.3µM and 1.9µM against MCF-7 (human breast cancer) cell line. In addition, morphological studies indicated that these compounds were cytotoxic to MCF-7cell line and resulted in dose dependent decrease of viable cells. Moreover, the flow cytometric analysis of these potential compounds suggested that they caused cell cycle arrest at G0/G1 phase. Furthermore, Annexin V-FITC study revealed that they induce cell death by apoptosis. Molecular docking studies provided valuable insights about the binding interactions of these potential compounds with anti-apoptotic Bcl-2 protein. (*ChemistrySelect,* **2020,** Volume5, Issue 6, 2063-2069)



New imidazo[2,1-*b*]thiazole-based aryl hydrazones: unraveling their synthesis and antiproliferative and apoptosis-inducing potential

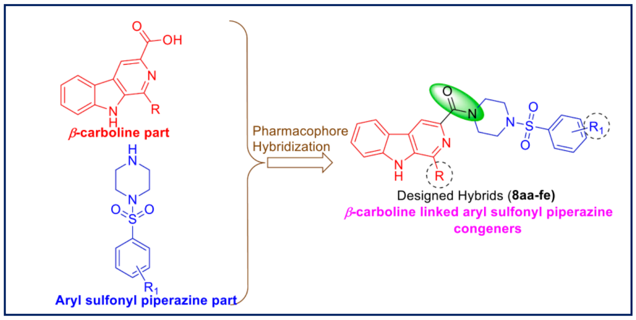
A series of imidazo[2,1-*b*]thiazole-based aryl hydrazones were synthesised and evaluated their anti-proliferative activity. Based on biology results, two of the compounds were found to be effective cytotoxic agents (*RSC Med.Chem.,* **2020**, 11, 1178-1184)



Design and synthesis of β-carboline linked arylsulfonyl piperazine derivatives: DNA topoisomerase II inhibition with DNA binding and apoptosis inducing ability

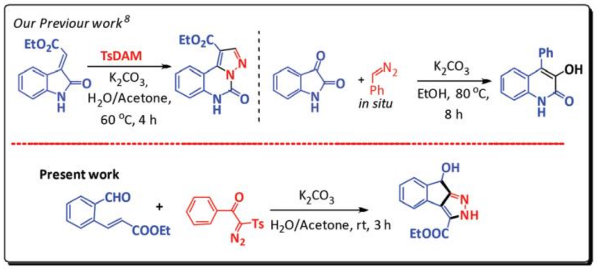
A series of new β-carboline linked aryl sulfonyl piperazine congeners have been synthesized by coupling various β-carboline acids with substituted aryl sulfonyl piperazines. Evaluation of their anticancer activity against a panel of human cancer cell lines such as colon (HT-29), breast (MDA-MB-

231), bone osteosarcoma (MG-63), brain (U87 MG), prostate (PC- 3) and normal monkey kidney (Vero) cell line has been done. Two compounds have shown most potent cytotoxicity with an IC50 values of 2.80 ± 0.10 µM and 0.59 ± 0.28 µM against MG-63 cell line. They were found to inhibit Topo II that is confirmed by specific Topo II inhibition assay. DNA binding studies, cell cycle analysis, Annexin V study indicate that these compounds have potential anticancer activity. *(Bioorg. Chem.*, **2020**,101, 103983)



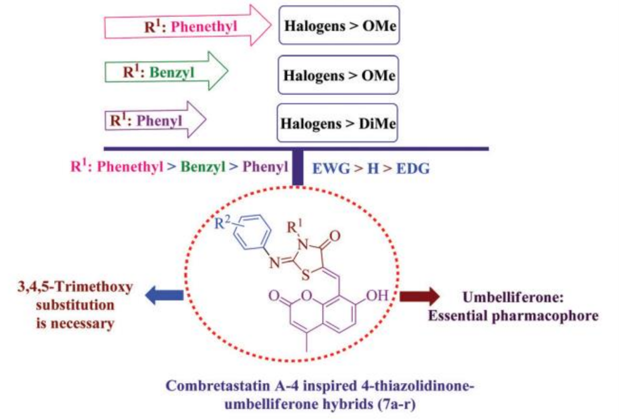
A facile and metal-free domino reaction of TsDAM and 2-alkenylarylaldehyde: An easy access to 8-hydroxy-2,8-dihydro indeno [2,1-*c*]pyrazoles

An efficient straightforward, metal free, domino approach was developed for the synthesis of various 8-hydroxy-2,8-dihydroindeno[2,1-*c]*pyrazoles *via* [3 + 2] cycloaddition of substituted alkenes and TsDAM (TosylDiAzoMethane). *(Org. Biomol. Chem.*, **2021**,19, 4118-4125)



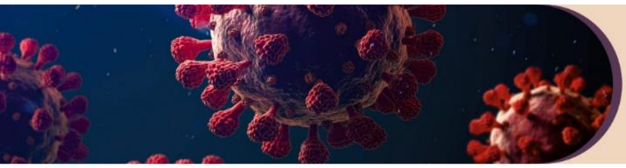
Targeting tubulin polymerization and DNA binding of 4-thiazolidinone–umbelliferone hybrids: synthesis and cytotoxicity

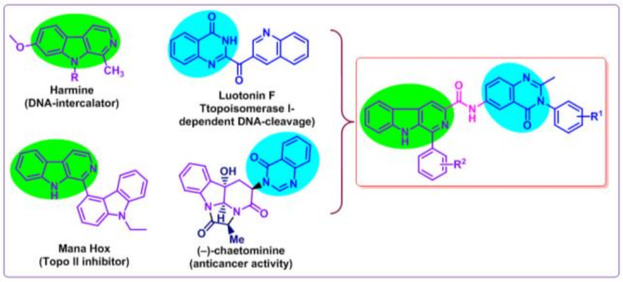
A novel class of 4-thiazolidinone–umbelliferone hybrids were developed. The anti-proliferative activities of the synthesized compounds were evaluated in human cancer cell lines (adherent and suspension) and are compared with a normal human cell line. Further, target based studies demonstrated the tubulin polymerization inhibition of one of the compounds at an IC50 value of 2.65±0.47 mM and also exhibited effective binding with CT-DNA. Molecular modeling studies demonstrated that the potential compound binds at the active site of tubulin. *(New J. Chem.*, **2021**,45, 18908-18923)



Design, Synthesis and Biological Evaluation of Hybrid C3-Quinazolinone linked β-carboline Conjugates as DNA Intercalative Topoisomerase I Inhibitors

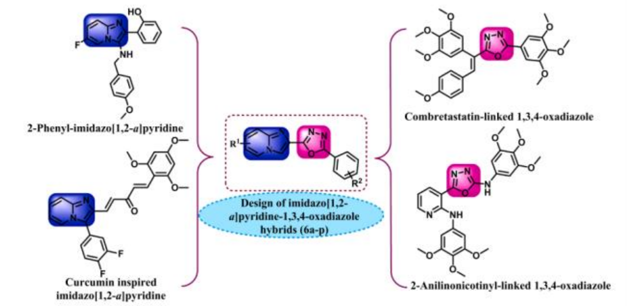
A series of new quinazolinone linked β-carboline conjugates as DNA intercalative topo I inhibitors were synthesized. These compounds displayed good cytotoxic activity, particularly in A549 cells as well as promising DNA binding affinity. The active compounds showed good correlation between their topo I inhibitory activity and cytotoxicity toward tested cancer cell lines. Investigation of the structure-activity relationship studies indicated that the electron donating and halogen groups present on both phenyl rings (R1 and R2) are important in enhancing both cytotoxic activity as well as enzyme inhibition. *(J Clin Pharm*, **2021**, 5(1): 1020)





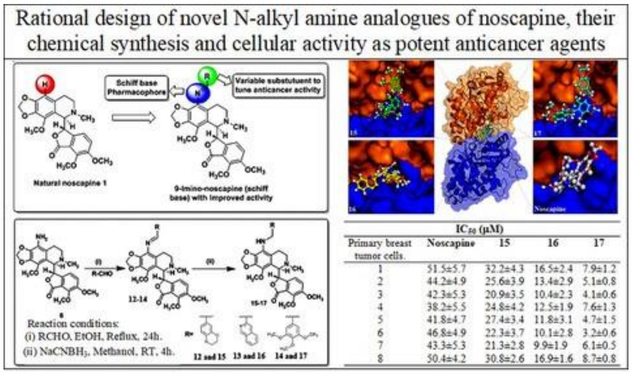
Synthesis and biological evaluation of novel imidazo[1,2-*a*] pyridine-oxadiazole hybrids as anti-proliferative agents: Study of microtubule polymerization inhibition and DNA binding

Successfully synthesized, characterized and evaluated a series of novel imidazo[1,2-*a*]pyridine-oxadiazole hybrids and studied their anti-cancer potential. Anti-proliferative activities of the synthesized compounds were evaluated in lung cancer (A549) and prostate cancer (PC-3, DU-145) cell lines using MTT assay. The cell cycle analysis disclosed that one of the compounds showed significant G2/M phase arrest in A549 cells. An immunohistochemistry assay on A549 cell lines showed significantly disrupted the microtubule organization. Target based studies demonstrated the tubulin polymerization inhibition at an IC_{50} value of 3.45 ± 0.51 μM and also exhibited effective binding with CT-DNA. The molecular modeling studies inferred that active compound binds at the active site of α/β-tubulin with prominent binding affinity. Physico-chemical and ADME/T properties examined were in the acceptable range. *(Bioorg Med Chem.,***2021** 43,116277)



9-Ethynyl noscapine induces G2/M arrest and apoptosis by disrupting tubulin polymerization in cervical cancer

Novel noscapine analogs with different functional groups appended at ninth position of natural noscapine have been synthesised. Biological studies demonstrated that 9-ethynyl noscapine decreased cell viability and colony formation in HeLa cells in a concentration dependent manner. test compound's effect on cell cycle progression, microtubule dynamics, and apoptosis were evaluated. Cell cycle and western blotting analysis revealed that 9-ethynyl noscapine treatment resulted in cell cycle arrest atG2/M and decreased CDK1 and cyclinB1 protein expression. 9-Ethynyl noscapine treatment leads to disruption in tubulin polymerization and induction of apoptosis by decreasing expression of bcl2, pro-caspase 3, and activation of cytochrome C. Taken together, our results indicate that 9-ethynyl noscapine effectively suppresses the growth of cervical cancer cells (HeLa) by disrupting tubulin polymerization, cell cycle progression leading to apoptosis. *(Chemical Biology & Drug Design,* **2021,*98(3)*, 445-465)**

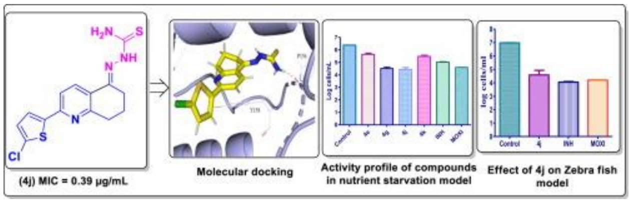

Rational design of novel N-alkyl amine analogues of noscapine, their chemical synthesis and cellular activity as potent anticancer agents

Reaction conditions:
(i) RCHO, EtOH, Reflux, 24h.
(ii) $NaCNBH_3$, Methanol, RT, 4h.

	IC_{50} (μM)			
Primary breast tumor cells.	Noscapine	15	16	17
1	51.5±5.7	32.2±4.3	16.5±2.4	7.9±1.2
2	44.2±4.9	25.6±3.9	13.4±2.9	5.1±0.8
3	42.3±5.3	20.9±3.5	10.4±2.3	4.1±0.6
4	38.2±5.5	24.8±4.2	12.5±1.9	7.6±1.3
5	41.8±4.7	27.4±3.4	11.8±3.1	4.7±1.5
6	46.8±4.9	22.3±3.7	10.1±2.8	3.2±0.6
7	43.3±5.3	21.3±2.8	9.9±1.9	6.1±0.5
8	50.4±4.2	30.8±2.6	16.9±1.6	8.7±0.8

Synthesis of a series of novel aryl tethered 7,8-dihydroquinolin-5(6*H*)-ylidenehydrazinecarbothioamides which showed *in vitro* and *in vivo* antimycobacterial activity against *Mycobacterium tuberculosis (Mtb)* H37Rv

The intermediates dihydro-6*H*-quinolin-5-ones were synthesized from β-enaminones, reacting with cyclochexane-1,3-dione/5,5-dimethylcyclohexane-1,3-dione and ammonium acetate using a modified Bohlmann-Rahtz reaction conditions. They were further reacted with thiosemicarbazide to give the respective hydrazine carbothioamides. Among the twenty-two compounds screened for *in vitro* antimycobacterialactivity against *Mycobacterium tuberculosis* H37Rv (ATCC27294), two compounds, exhibited the highest inhibition with an MIC of 0.39 µg/mL. The observed increase in potency provides a clear evidence that hydrazinecarbothioamide is a potential pharmacophore, collectively imparting synergistic effect in enhancing antitubercular activity of the dihydroquinolinone core. The *in vivo* (Zebra fish) antimycobacterial screening of the *in vitro* active molecules led to the identification of a hit compound, with significant activity in the *Mtb* nutrient starvation model (2.2-fold reduction). Docking studies showed a hydrogen bond with the P156 residue of the protein. (*Bioorg. Chem.*, **2020,** *96*, 103626)



(4j) MIC = 0.39 µg/mL

Molecular docking

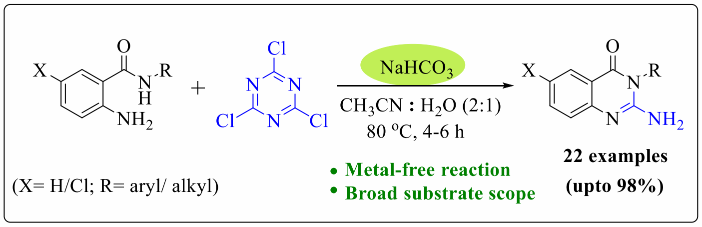
Activity profile of compounds in nutrient starvation model

Effect of 4j on Zebra fish model

Identification and characterization of impurities in an insecticide, Bifenthrin technical

The HPLC-DAD and GC/MS methods were successfully used for the identification and characterization of the impurities in an agrochemical insecticide, bifenthrin technical. Three impurities ranging from 0.175%–0.541% were detected by the HPLC-DAD method. The LC/MS technique with ESI or APCI source failed to detect the impurities detected by HPLC-DAD, due to lack of ionization in ESI or APCI. The three impurities were enriched by prep-HPLC, and then their structures were elucidated based on the GC/EIMS and CIMS data. The EI mass spectra of bifenthrin and its impurities displayed molecular ion and provided structure indicative fragment ions; the CIMS data further confirmed their molecular weight. The identity of the impurity 1 was further confirmed by the synthesis of the authentic sample followed by NMR and GC/MS data. (*J. Mass Spectrometry*, **2020,** 55, e4605**)**

Annulation of Cyanuric Chloride and 2-Aminobenzamides: A New Approach to 2-Amino-3-substituted Quinazolin-4(3H)-ones: A simple and efficient method for preparation of 2-amino-3-substituted quinazolin-4(3H)-ones by reaction of cyanuric chloridewith 2-amino N-substituted benzamides in acetonitrile-water (2:1)using sodium bicarbonate as a mild base is described. Using thismetal-free method, a variety of 2-amino-3-substituted quinazolin-4(3H)-ones were obtained in good to excellent yields. Here, bothorganic and inorganic bases were found to promote this reaction andthe best results were observed with sodium bicarbonate. This studyis the first observation of cyanuric chloride to act as a source forcreation of amine functionality in 2-amino-3-substitutedquinazolin-4(3H)-ones. (*Chemistry Select*, **2021**, 6, 896-901)



$NaHCO_3$

$CH_3CN : H_2O$ (2:1)

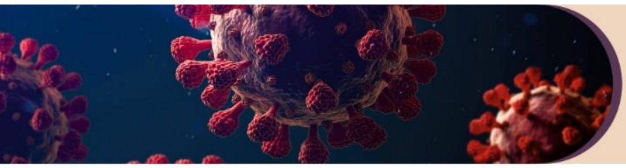
80 °C, 4-6 h

(X= H/Cl; R= aryl/ alkyl)

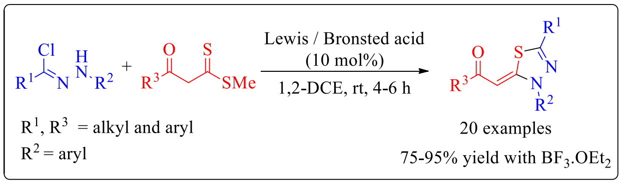
- **Metal-free reaction**
- **Broad substrate scope**

22 examples
(upto 98%)

A Study of [3+2] Cycloaddition Reaction of Hydrazonoyl Chloride and β-Oxodithioester Under Lewis Acid Catalysis: Stereoselective Synthesis of



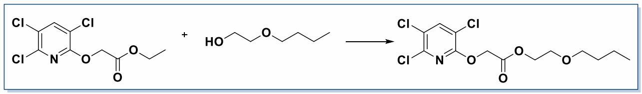
(Z)-1,3,4-Thiadiazol-2(3H)-Ylidenes: Hydrazonoyl chlorides underwent unprecedentedstereoselective [3+2] cycloaddition reaction with β-oxodithioestersand β-oxothioamides under Lewis acid catalysisproducing (Z)-1,3,4- thiadiazol-2(3H)-ylidenes in high yields. These products are obtained also with a base. Though sameproducts are obtained in both these conditions, theyinvolve different reaction mechanisms. In base mediatedreactions, 1,3-dipolar cycloaddition of a nitrilimine to C=S isoperative and in Lewis acid catalyzed reactions, β-oxodithioester/β-oxothioamide undergoes addition-cyclizationreactions with a hydrazonoyl chloride. (Asian J. Org. Chem., **2021**, 10, 1–5)



APPLIED RESEARCH

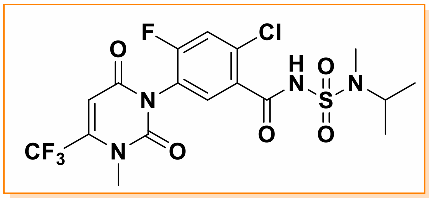
Process Demonstration of Trichlopyr-2-butoxyethylester (TBE)

Trichlopyr-2-butoxyethylester (TBE) is the butoxyethyl derivative of 3,5,6-Trichloro-2-pyridinyloxyacetic acid, a popular systemic foliar herbicide. Though the product is in use sincelong, very limited reports are available in literature on its preparation with economic viability. Studies were conducted and emerged with a highly efficient process technology by involving a very inexpensive & new catalyst that lead to the desired product in 93%yields with 98%purity. Thus, the developed process technology was successfully demonstrated to the industrial client.



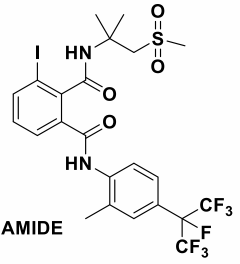
Process Development of Saflufenacil

Saflufenacil is an important herbicide belongs to the pyrimidinedione chemical class used to control annual broadleaf weeds in soybeans and corn. Presently, optimization & reproducibility studies are in final stage and process will be demonstrated soon



Process Development of Flubendiamide:

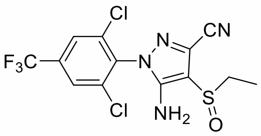
An economically viable route was devised starting from Pthalic anhydride, experimental studies were conducted, optimum parameters were established and the product was accomplished at the bench scale. Simultaneously, studies are also conducted and established feasible conditions to prepare key starting materials.



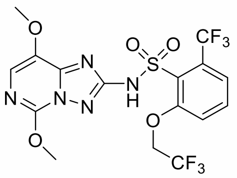
FLUBENDIAMIDE

Process Development of Ethiprole & Phenoxsulam:

Development of process for the two agrochemical products, Ethiprole and Phenoxsulam is being initiated.



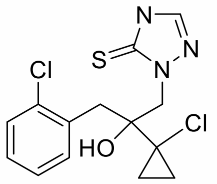
ETHIPROLE



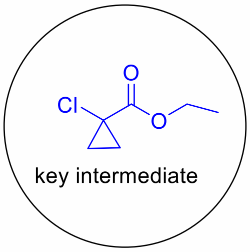
PHENOXSULAM

Process development of Prothioconazole:

A new process for prothioconazole with less expensive starting materials was proposed. The process involves improved coupling step with minimal side products and a possibility of asymmetric Corey – Chaykovsky reaction so that more active (*S*)-isomer can be produced, if necessary. Availability of in-house hydrazine hydrate technology is an added advantage, as it is one of the raw materials for the proposed project. Synthesis of the key starting material, methyl/ ethyl 1-chlorocyclopropane-1-carboxylate was carried out.



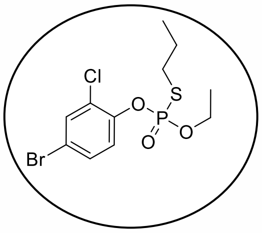
prothioconazole



key intermediate

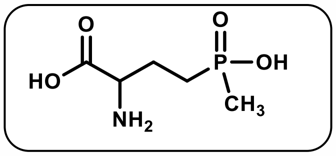
Transfer of Mercaptan free Profenofos synthesis technology

Profenofos is an important member of the OP class of insecticides and is considered as the safe alternative to Monocrotophos, which is being phased out in the country. There are commercial manufacturers in India but with a process generating ethyl mercaptan as a major obnoxious effluent. With a view to overcome the pollution problem and to provide better quality product, an innovative environmentally benign and cost effective technology was worked out in a shortest time avoiding mercaptan release at a lab scale. This approach for manufacture of profenfos involves 4 steps starting from 2-chlorophenol.



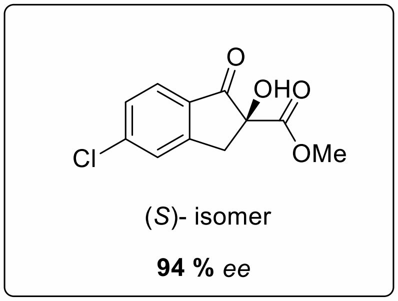
Development of Process for the Synthesis of Glufosinate

Glufosinate is a non-selective herbicide with contact and some systemic action. It is a safer herbicide originally developed by Bayer Crop Science. The original patent expired in 2018, thus opening the market for production. A viable manufacturing process of Glufosinate would make it sustainable. Development of an environmental-friendly and a non-cyanide route for Glufosinate is the aim of the project.



Towards the chiral synthesis of M-240: Enantioselective hydroxylation of 5-chloroindanone-2-carboxylate

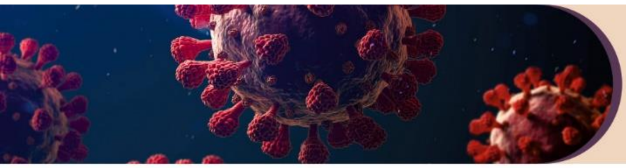
Indoxacarb, a highly useful insecticide is also marketed as a racemate, although the (*S*)- isomer is found to be the active enantiomer. The critical intermediate for the preparation of (*S*)-indoxacarb is the (*S*)-5-chloro-2-hydroxy-indanone-2-carboxylate, which is obtained by the hydroxylation of 5-chloroindanone-2-carboxylate. The enantioselective hydroxylation of 5-chloroindanone-2-carboxylate with up to 94 % enantiomeric excess has been successfully carried out and the laboratory scale process was demonstrated.

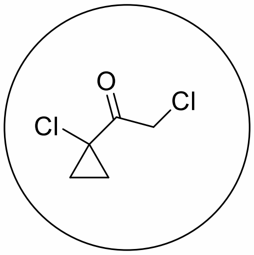


(*S*)- isomer

94 % *ee*

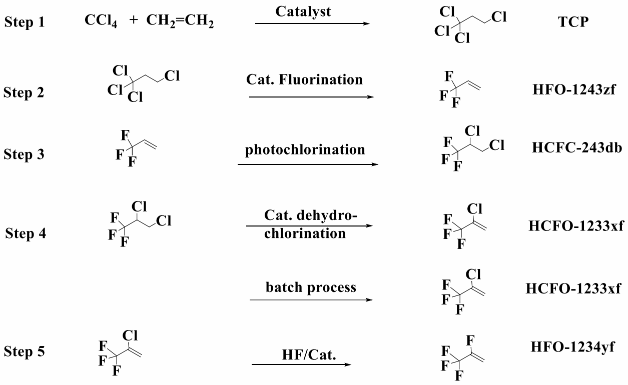
Process know-how for 2-chloro-1-(1-chlorocyclopropyl)ethan-1-one (a key starting material for prothioconazole)





A four step process for the industrial scale synthesis of 2-chloro-1-(1-chlorocyclopropyl)ethan-1-one, a key intermediate for production of block buster fungicide Prothioconazole, is undertaken.

Development of Process for New Generation Refrigerant HFO-1234yf: HFO-123yf (2,3,3,3-tetrafluoropropene) is an 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 sponsored this project and we developeda viable five-step process for this molecule starting from carbon tetrachloride and ethylene as shown below:



Development of Process for Hexafluoro-1,3-butadiene (HFBD): HFBD is a new generation plasma etching gas used in semiconductor industry. Unlike other commonly used etchants such as SF6, NF3, chlorine and tetrafluoromethane; HFBD is an environmentally non-corrosive, non-ozone depleting and environmentally safe etchant gas because of its very low atmospheric life. We successfully developed a scalable process for hexafluoro-1,3-butadiene under a project sponsored by Semiconductor Laboratory (SCL), Mohali and submitted 1.5 Kg of semiconductor grade (purity 99.9%) to SCL along with process report. This process was developed starting from chlorotrifluoroethylene in three steps.

Development of processes for benzotrifluorides from benzotrichloridesby reaction with anhydrous hydrogen fluoride: This project was sponsored by M/s Aarti Industries Ltd., and developed processes for benzotrifluoride, 2-chlorobenzotrifluoride from the corresponding benzotrichlorides.

Development of Process for 2-bromoheptafluoropropane: This project was sponsored by M/s Nichino India Pvt., Ltd., and a scalable process was developed from heptafluoropropane and demonstrated to sponsor at bench scale.

Popularization of Pheromone Application Technology (PAT): A Versatile Agro Practice for Pest Management:

Centre for Semiochemicals (CSC) is making concerted efforts to develop and bring PAT into practice for managing important crop (lepidopteran) pests. For the first time in India, PAT is introduced and is successfully demonstrated both as a monitoring/surveillance tool in Integrated Pest Management (IPM) and as an alternative to pesticides through mass trapping technique for the control of major pests of economically important field crops.

For the benefit of the small farm holders, village based demonstrations under farmers' participatory approach was proposed to create greater impact & awareness of PAT in the farming community of Telangana state for the management of the insect pests of vegetables & field crops.

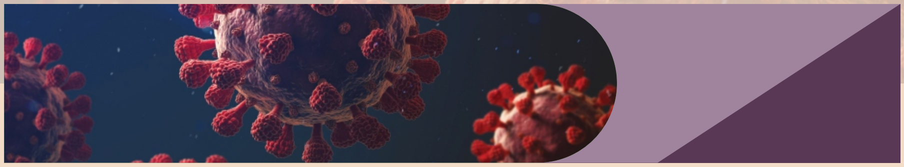
- Successfully developed indigenous methodologies for the synthesis of pheromone blends of all the project insect pests selected for PAT demonstration:

- Cost effective pheromone lures with indigenously synthesized pheromone blends were achieved.

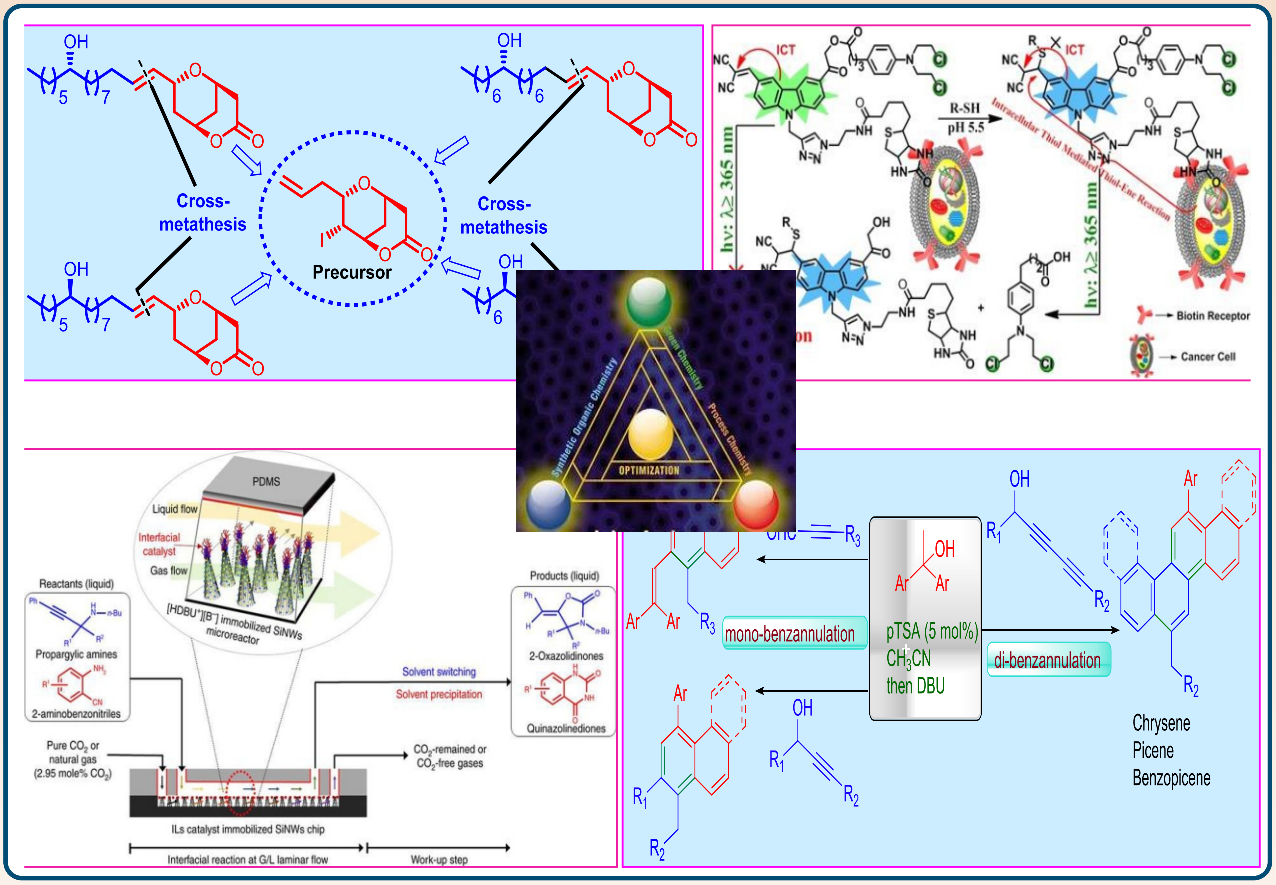
- CSIR-IICT under farmers' participatory approach successfully demonstrated PAT through mass trapping technique & controlled the devastating pests - Rice yellow stem borer; Brinjal shoot & fruit borer; Pink Bollworm on Cotton; Fruit fly on vegetables;Tomato/chilli pod borer; Tobacco caterpillar. The pest damage was effectively brought down in all the demonstrations resulting in increased yields.

- CSIR-IICT along with Departments of Agriculture of Telangana, Andhra Pradesh and Odisha states, and NRRI implemented pheromone technology in cotton, paddy, maize, sweet potato etc., during crop season 2020-21 and 2021-22.
- Also implemented the pheromone technology in aspirational districts of Telangana during the Kharif season 2020, for monitoring and mass trapping pink bollworm (PBW), which is a major damaging pest in Cotton, to the cover of 25000 acres in five mandals of Asifabad, Bhupalapally & Khammam districts under CSIR-HARIT program.
- CSIR-IICT-Hyderabad and NRRI-Cuttack worked on a project during 2021-22 that aims to reduce the usage of harmful pesticides through PAT for managing major insect pests in rice, maize, vegetables, oilseeds and fruit crops in an area of 1500 ha in different districts of Odisha. The program was launched in Dhenkanal district on October 22, 2021 through a workshop attended by senior officials.

The technology was popularized through training programs and field demonstrations in Parjang, Sogor, Hatipada, Saptasajia and Parvathiya villages in Dhenkanal district covering 400 ha. The technology benefited 500 farmers directly. Usage of pesticides reduced to 50-60% in cabbage, cauliflower, brinjal, tomato, cucurbits, groundnut, vegetables. PAT will be popularised in another 1500 ha in other districts of Odisha during the current year. The technology is receiving widespread appreciation and acceptance, as there is an increasing demand for lures. Also, entrepreneurs and many farmer producer organizations are expressing interest to promote PAT.



ORGANIC SYNTHESIS AND PROCESS CHEMISTRY

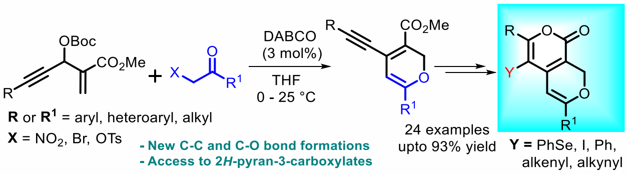


ORGANIC SYNTHESIS AND PROCESS CHEMISTRY

BASIC RESEARCH

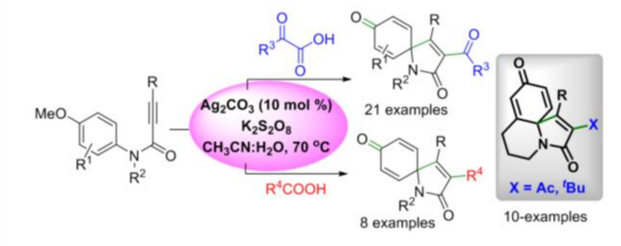
Oxa-[3+3] Annulation of MBH-Carbonates of Propiolaldehydes with α-Nitro/Bromo Ketones to Access 2*H*-pyrans

A novel alkyne-assisted annulation reaction of MBH-carbonates of propiolaldehydes α-nitro/bromo ketones is reported, providing a facile synthesis of substituted 2*H*-pyrans in good yields. This reaction divulges the inimitable reactivity of the MBH-carbonates of propiolaldehydes as C3-synthons wherein the alkyne functionality promoted the reaction without participating in the oxa-[3+3] annulation. The obtained products, having alkyne and ester functionalities, allowed further annulations to generate diverse pyrano[3,4-c]pyran-1-ones. (*Chem. Commun.*, **2020**, *56*, 7191-7194)



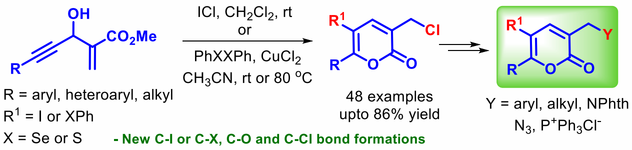
Ag-Catalyzed Oxidative *ipso*-Cyclization *via* Decarboxylative Acylation/Alkylation: Access to 3-Acyl/Alkyl-spiro[4.5]trienone

A strategy to functionalized spiro[4.5]trienones, by domino silver-catalyzed decarboxylative acylation or alkylation/ *ipso*-cyclization of *N*-arylpropiolamides with α-keto acids/alkyl carboxylic acids, is presented. This transformation offers a wide range of substituted 3-acyl/alkyl-spiro[4.5]trienones in high yields with a broad substrate scope. The approach was further extended to access fused tricyclic frameworks, 6,7-dihydro-3*H*-pyrrolo[2,1-j]quinoline-3,9(5*H*)-diones. The ease of operation, wide substrate scope, and readily accessible starting materials are the salient features to make the current method valuable. (*Org. Lett*. **2020**, *22*, 5342–5346)



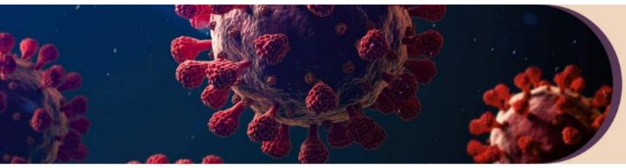
Iodo- and Chalcogenoannulation of Morita−Baylis−Hillman Alcohols of Propiolaldehydes: Entry to Functionalized 2-Pyrones

A unique method for synthesis of chloromethyl 2H-pyran-2-ones having additional iodo/seleno/sulfino groups, starting from MBH alcohols of propiolaldehydes has been developed. The reaction displays a broad substrate choice generating the products with handy substitutions. Moreover, the corresponding products provided a short and efficient access to structurally diverse hitherto known 2*H*pyran-2-one derivatives, which constitute a significant set of pharmaceutically related molecules. The ease of procedure, readily accessible starting materials, and generation of distinctive pyrones make this protocol convenient. (*Org. Lett*. **2021**, *23*, 4749−4753)

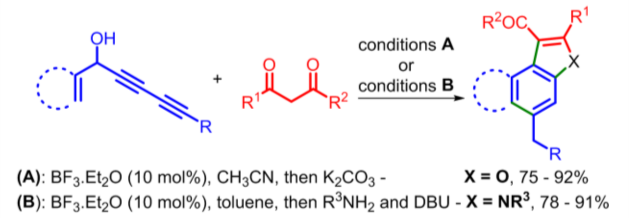


Domino Reaction of 2,4-Diyn-1-ols with 1,3-Dicarbonyl Compounds: Direct Access to Aryl/Heteroaryl-Fused Benzofurans and Indoles

A domino propargylation/furanylation (intramolecular exo-dig-cyclization)/benzannulation reaction of 2,4-diyn-1-ols with 1,3-dicarbonyl compounds has been developed for the first time. This provides a novel and effective method for the preparation of aryl/heteroaryl-fused benzofurans



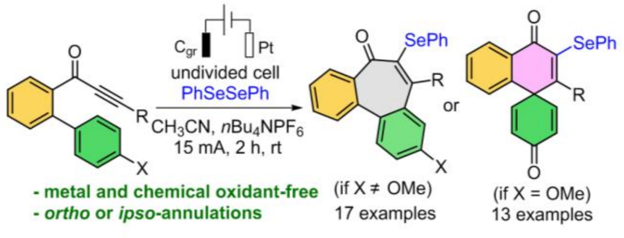
from easily accessible starting materials in a single step. The methodology was extended to pyrrolyl-benzannulation to obtain aryl/heteroarylfused indoles. Further, application of this approach in the synthesis of eustifoline D and dictyodendrin structural frameworks has been demonstrated. (*Org. Lett.* **2021**, *23*, 4882−4887)



(A): $BF_3.Et_2O$ (10 mol%), CH_3CN, then K_2CO_3 - **X = O**, 75 - 92%
(B): $BF_3.Et_2O$ (10 mol%), toluene, then R^3NH_2 and DBU - **X = NR^3**, 78 - 91%

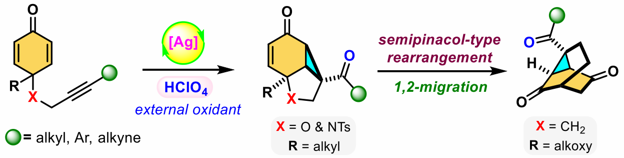
Electrochemical Selenylative Carbannulation of Biaryl Ynones to Seleno-Dibenzocycloheptenones/Spiro[5.5]Trienones

Electrooxidative-induced synthesis of structurally diverse seleno-dibenzocy clohepten-5-ones and seleno-spiro[5.5] trienones by selenylative carbannulation of biaryl ynones with diaryl diselenide has been developed. The switchable reactivity, intramolecular ortho-annulation or dearomative *ipso*-annulation, is directed by the substituent present on the ortho-aryl group of arylynone. The prominent features of this method include metal-free, external chemical oxidant-free conditions, and readily accessible substrates. (*J. Org. Chem.*, **2021**, *86*, 17071-17081)



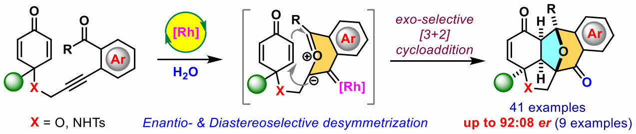
Silver(I)-Catalysed Oxidative Intramolecular Cyclopropanation: Access to Complex Tricyclo[3.3.1.0]nonanediones *via* Semipinacol-type Rearrangement

An unconventional Ag(I)-catalyzed intramolecular cyclopropanation of prochiral alkyne-tethered cyclohexadienones has been developed using simple perchloric acid as an external oxidant. The transformation involves the formation of a per-chloryloxy vinyl-silver species, which then proceeds through either intramolecular conjugate addition or α-oxo silver carbene pathway to yield cyclopropane fused tricyclic enones with high diastereoselectivity. In case of C-tethered cyclohexadi-enones, the reaction proceeds further *via* acid mediated semipinacol-type rearrangement to give complex and highly strained tricyclo[3.3.1.0]nonanediones. This cascade annulation has wide functional-group tolerance and broad substrate scope. Late-stage functionalization of estrone was also demonstrated with excellent diastereoselectivity. (*Org. Lett.* **2020**, *22*, 7019–7024)



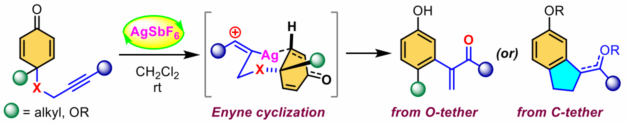
Rh(I)-Catalyzed Stereoselective Desymmetrization of Prochiral Cyclohexadienones *via* Highly *exo*-Selective Huisgen-Type [3+2] Cycloaddition

A Rh(I)-catalyzed highly stereoselective desymmetrization of 2-alkynylbenzaldehyde-tethered cyclohexadienones triggered by intramolecular Huisgen-type [3+2] cycloaddition has been developed. This method enables convergent construction of complex epoxy-bridged polycyclic ring systems with five contiguous stereocenters with excellent exo-selectivity and broad substrate scope. The highly atom-economical process involves 6-endo-dig cyclization of carbonyl oxygen onto the activated alkyne resulting in the highly reactive metal-benzopyrylium intermediate, which readily undergoes intramolecular [3+2] annulation/ hydration. Asymmetric induction is also achieved for the first time in Rh(I)-catalyzed 1,3-dipolar cycloaddition using an easily accessible chiral diene as the ligand. (*Chem. Sci.* **2021**, *12*, 1544-1550)



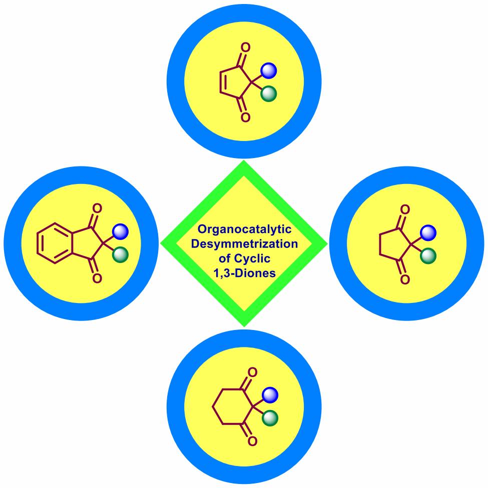
Silver(I)-Catalyzed Enyne Cyclization/ Aromatization of Alkyne-Tethered Cyclohexadienones to Access meta-Substituted Phenols

A highly regioselective silver(I)-catalyzed intramolecular annulation of alkyne-tethered cyclohexadienones to access meta-substituted phenols with enone functionality, which is difficult to synthesize from conventional methods reported. The reaction proceeds *via* intramolecular 1,6-enyne cyclization followed by aromatization and subsequent oxetene ring-rearrangement. This strategy has also been compatible with wide range of C-tethered cyclohexadienones to afford indanes in high yields. The unique functionality on products allows further transformations to expand the diversity. (*Org. Lett.*, **2021**, *23*, 317-323)



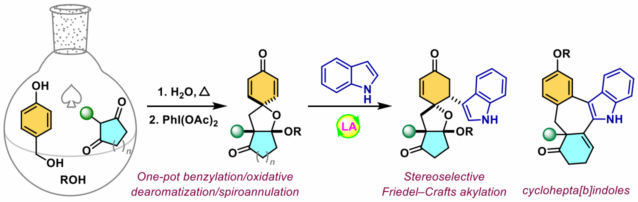
Organocatalytic Enantioselective Desymmetrization of Prochiral 2,2-Disubstituted Cyclic 1,3-Diones *(Invited Review to the Special Issue on Organocatalysis)*

Enantioselective desymmetrization of prochiral 1,3-cyclodiketones is the most convenient and highly desired transformation to access densely functionalized, enantiomerically enriched scaffolds with multiple chiral centers. In recent years, organocatalysis has made significant progress in this research area along with other traditional metal- or enzyme-catalyzed reactions. This mini-review provides an overview of the recent developments in the domain of organocatalytic enantioselective desymmetrization along with a brief discussion about future perspectives. (*Asian J. Org. Chem.*, **2021**, 10, 1267 – 1281)

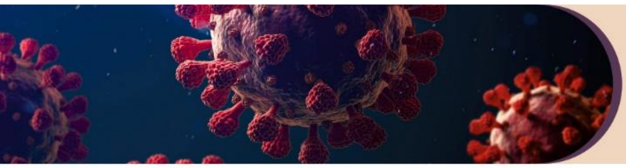


Design, Synthesis and Application of Spiro[4.5]cyclohexadienones *via* One-pot Sequential *p*-Hydroxybenzylation/Oxidative Dearomatization.

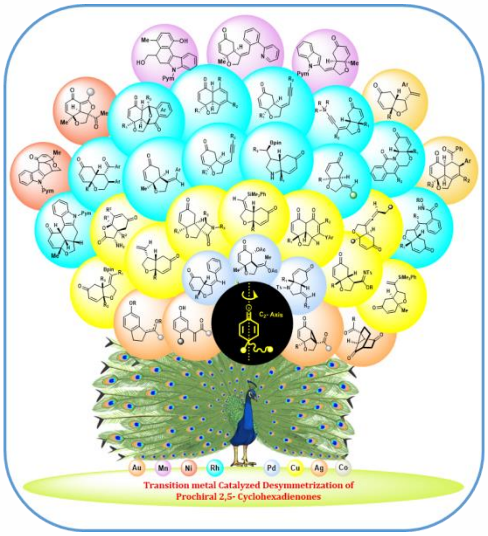
One-pot sequential p-hydroxybenzylation/oxidative dearomatization/spiroannulation has been designed for the efficient construction of tetrahydrofuran containing spiro-cyclohexadienones. This reaction proceeds through the p-hydroxybenzylation of 1,3-diketones with p-hydroxybenzyl alcohol *via* quinone methide formation followed by oxidative dearomatization/spiroannulation with suitable alcohol. The Friedel−Crafts alkylation of spiro[4.5]cyclohexadienones with indoles provided a broad array of highly diastereoselective C-3 alkylated spirocycles and cyclohepta[b]indoles depends on the ring size of fused cyclic ketones. (*Chem. Commun.*, **2021**, 57, 5574-5577)



Transition-Metal Catalyzed Stereoselective Desymmetrization of Prochiral Cyclohexadienones

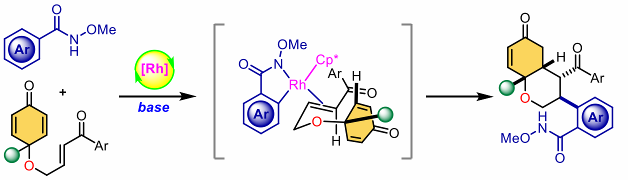


The development of transition-metal catalyzed enantioselective and diastereoselective transformations has contributed many advances in the field of synthetic organic chemistry. Particularly, stereoselective desymmetrization of prochiral cyclohexadienones represents a powerful strategy for accessing highly functionalized and stereochemically enriched scaffolds, which are often found in biologically active compounds and natural products. In recent years, several research groups including our group have made a significant progress on transition-metal catalyzed stereoselective desymmetrizations of 2,5-cyclohexadienones. In this account, we will provide an overview of the recent developments in this area employing Pd, Cu, Rh, Au, Ag, Ni, Co, and Mn-catalysts. (*Chem. Rec.*, **2021**, 21, 3689-3726)



Rh(III)-Catalyzed Diastereoselective Cascade Annulation of Enone-Tethered Cyclohexadienones *via* a C(sp2)−H Bond Activation

Herein, we report a highly diastereoselective arylative cyclization of enone-tethered cyclohexadienone *via* Rh(III)-catalyzed C−H activation of N-methoxybenzamides. This reaction proceeds through the formation of five-membered rhodacycle followed by bis-Michael cascade annulation to access functionalized bicyclic scaffolds with four contiguous stereocenters with broad substrate scope. These products have excellent functional handles, allowing the further synthetic transformation to increase the structural complexity. Furthermore, mechanistic studies of arylative cyclization and a gram-scale experiment are also presented. (*Chem. Commun.*, **2021**, *57*, 13598-13601)

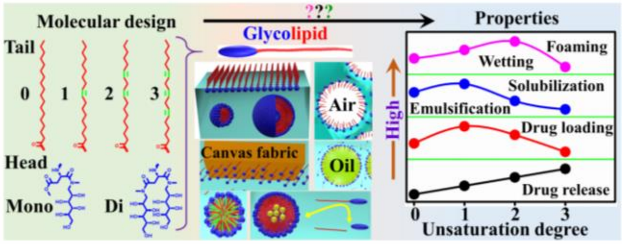


Supramolecular Glycolipid-based Gels

Glycolipids with variation in un-saturation of hydrophobic tail and polar headgroup size were designed and their gelation ability was studied. The encapsulation capacity and kinetic release behavior of hydrophobic/hydrophilic bioactives like curcumin/riboflavin from the hydrophobic/hydrophilic pockets of glycolipids hydro/organogels was examined. A typical function of the hydrogels of glycolipid is metal chelation and enzyme-triggered release behavior, enabled them as promising material for Cr, Cu removal from edible oils and controlled release of water soluble/insoluble bioactives. Further, C16 chain length glycolipid formed molecular hydrogel with injectable and thixotropic behaviors. Overall, glycolipid amphiphile designed by upholding proper hydrophilic-lipophilic balance can form multifunctional supramolecular hydrogel with excellent implementation in drug delivery system. (*Langmuir*, **2020**, 36, 3080−3088)

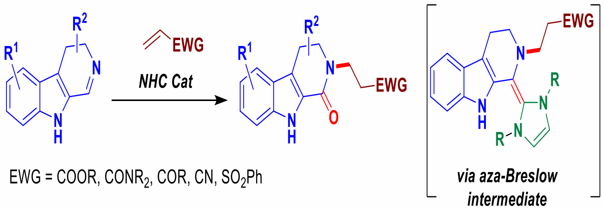
Synthetic Biosurfactant and their Self-Assembly

Bio-based glycolipids were synthesized to ascertain the structure–property relationship *via* changing unsaturation degree of hydrophobic chain and polar glucosidic moiety. Studies on encapsulation and enzymatic release of hydrophobic bioactive from glycolipid self-assemblies revealed them as nano-carriers. A mixture of two glycolipids at various hydrophobic chain lengths was prepared. Surface-active properties were employed at different mole fraction of short chain glycolipid (χ_{SGL}) to explore synergistic and antagonistic interactions between the hydrophobic chains of glycolipids. The mixed glycolipid system provided enhanced surface activity at air-water interface. (*Colloids Surf. A; Physicochem. Eng. Asp.*, **2020,** 601, 125008.



N-Heterocyclic Carbene (NHC)-Catalyzed Tandem Imine Umpolung–aza-Michael Addition–Oxidation of β-Carboline Cyclic Imines

An NHC catalyzed umpolung of β-carboline-based cyclic imines for their conversion to the corresponding N-substituted cyclic amideshas been disclosed. The key to the success of this transformation appears that NHC upon reaction with the imine concomitantly goes through the generation of aza-Breslow intermediate and aza-Michael addition followed by the oxidation with molecular oxygen to deliver the *N*-substituted amide products. The developed method has enabled to synthesize various biologically relevant β-carboline-1-one derivatives in good yields. (*Chem. Commun.*, **2020**, 56, 2803-2806)

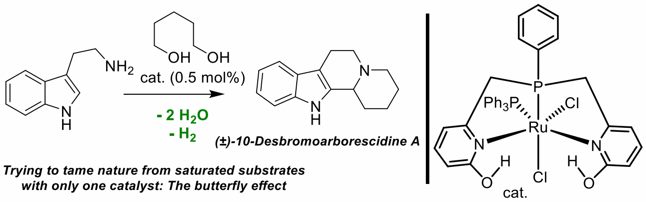


Substrate Controlled, Regioselective Carbopalladation for the One-pot Synthesis of C4-Substituted Tetrahydroisoquinoline Analogues

6-*Exo-trig* cyclization reaction through regioselective carbopalladation has been demonstrated with *N*-(2-halobenzyl)-*N*-allylamines to furnish the corresponding C4-substituted tetrahydroisoquinoline derivatives. The scope of the reaction is extended to the synthesis of C4-quaternary tetrahydroisoquinoline derivatives also. The nature of the substituent on the olefin moiety dictates the course of the carbopalladation sequence. Regioselective carbopalladation is substantiated by performing the reaction with unsymmetrical diallylated amine substrates. (*RSC Adv.*, **2020**, 10, 15794-15799)

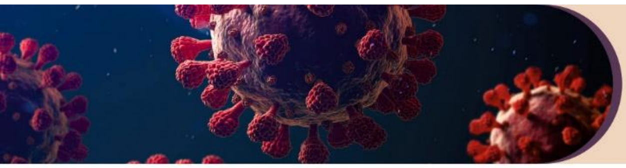
Direct Access to (±)-10-Desbromoarborescidine A from Tryptamine and Pentane-1,5-diol

A single step synthetic strategy for (±)10-desbromoarborescidine A is described. Starting from tryptamine and pentane-1,5-diol, this acceptorless dehydrogenative condensation process is efficiently catalyzed by a ruthenium complex featuring proton-responsive phosphine-pyridone ligand. (*Asian J. Org. Chem.*, **2020**, 9, 910-913)

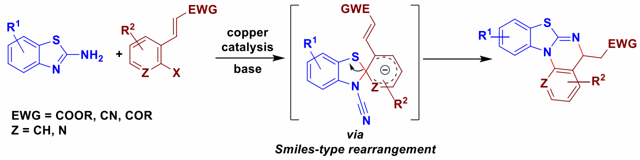


Tandem Copper-Catalyzed Regioselective *N*-Arylation–Aza-Michael Addition: Synthesis of Tetracyclic 5*H*-Benzothiazolo[3,2-*a*]quinazoline Derivatives

A copper-catalyzed tandem process integrating regioselective *N*-arylation, followed by aza-Michael addition, is disclosed using 2-aminobenzothiazoles and *ortho*-halo cinnamic acid congeners. This process generated diverse tetracyclic 5*H*-benzothiazolo[3,2-*a*]quinazoline derivatives in moderate to good yields. The present tandem reaction appears to proceed through concomitant ring opening of 2-aminobenzothiazole and *S*-arylation to give the *ortho*-cyanamide-substituted diaryl thioether intermediate. The thus generated intermediate likely undergoes an unprecedented Truce−Smiles-type rearrangement involving *S*- to *N*-aryl migration, followed by reformation of the thiazole ring and intramolecular

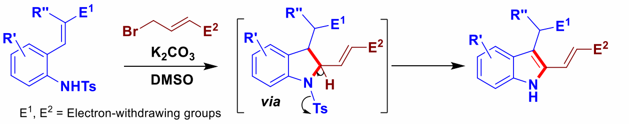


aza-Michael addition to furnish the title products. (*J. Org. Chem.*, **2020**, 85, 8780-8791)



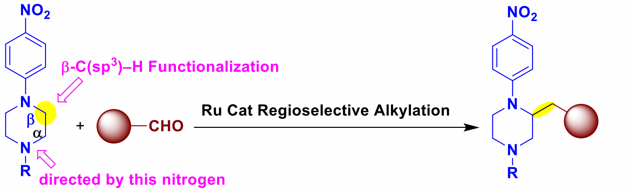
Design and Application of Intramolecular Vinylogous Michael Reaction for the Construction of 2-Alkenyl Indoles

A base-mediated transformation based on a designed intramolecular vinylogous Michael addition (intra-VMA) is presented to access 3-substituted 2-alkenyl indole derivatives. The reaction represents the first example of the intra-VMA for the construction of indoles. A one-pot *N*-allylation of *ortho*-tosylamidocinnamates/congeners with γ-bromocrotonates followed by intra-VMA has been described to provide access to a diverse range of 2-alkenyl indole derivatives in reasonable to high yields. (*Chem. Commun.*, **2021**, 57, 231-234)



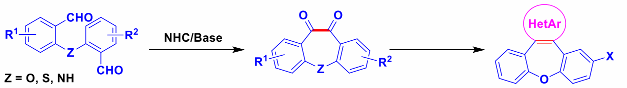
Ruthenium Catalyzed Regioselective β-C(sp³)–H Functionalization of *N*-Alkyl-*N'*-*p*-nitrophenyl Substituted Piperazines using Aldehydes as Alkylating Agents

A ruthenium-catalyzed regioselective β-C(sp³)–H bond functionalization on the piperazine core using aldehydes as alkylating agents has been disclosed. This transformation appears to go through the dehydrogenation of the piperazine to propagate to enamine *in situ*, followed by nucleophilic addition to the aldehyde and hydrogenation to result in the regioselective β-C(sp³)–H alkylation. A variety of aromatic, heteroaromatic, aliphatic aldehydes were employed for the C-3 alkylation of *N*-alkyl-*N′*-*p*-nitrophenyl substituted piperazines. (*Adv. Synth. Catal.*,**2021**, 363, 453–458)



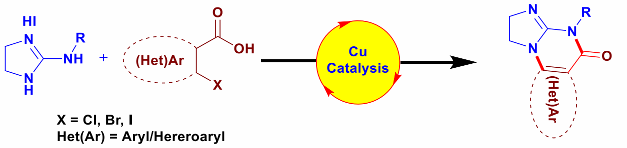
N-Heterocyclic Carbene (NHC)-Catalyzed Intramolecular Benzoin Condensation–Oxidation

NHC-Catalyzed intramolecular benzoin condensation–oxidation is developed for the expedient synthesis of diverse cyclic 1,2-diketones incorporated in dibenzo-fused seven-membered heterocycles in good to excellent yields, under ambient conditions. The presented carbene-catalyzed transformation appears to proceed through the benzoin intermediate followed by aerobic oxidation. (*Org. Biomol. Chem.*, **2021**, 19, 1488-1492)



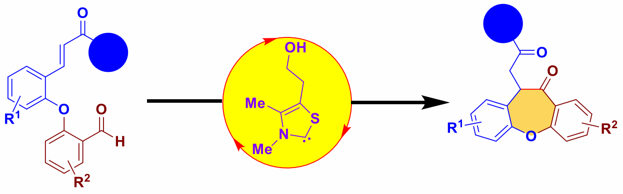
Tandem Copper Catalyzed Regioselective *N*-Arylation–Amidation: Synthesis of Angularly Fused Dihydroimidazoquinazolinones and the Anticancer Agent TIC10/ONC201

A copper-catalyzed tandem reaction of 2-aminoimidazolines and *ortho*-halo(hetero)aryl carboxylic acids that causes the regioselective formation of angularly fused tricyclic 1,2-dihydroimidazo[1,2-*a*]quinazolin-5(4*H*)-one derivatives has been reported. The reaction involved in the construction of the core six-membered pyrimidone moiety transpired *via* regioselective *N*-arylation–condensation. (*Org. Biomol. Chem.*, **2021**,19, 8497-8501)



N-Heterocyclic Carbene (NHC)-Catalyzed Intramolecular Stetter Reaction to Access Dibenzo-fused Seven-membered Heterocycles

An NHC-catalyzed transformation to access dibenzo-fused seven-membered heterocyclic compounds *via* intramolecular Stetter reaction under ambient conditions has been developed. A range of dibenzo[*b*,*f*]oxepine and dibenzo[*b*,*f*]thiepine derivatives have been generated in very good to excellent yields. The 1,4-dicarbonyl functionality of a representative derivative has undergone further heterocyclization *via* Paal-Knorr reaction. (*Asian J. Org. Chem.*, **2021**, 10, 1406–1409)

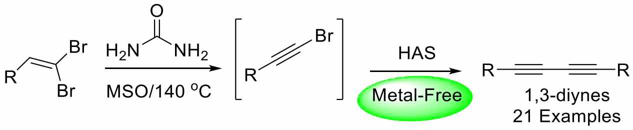


Copper-Mediated Synthesis of (*E*)-1-Azido and (*Z*)-1,2-Diazido Alkenes from 1-Alkene-1,2-diboronic Esters. A Direct Approach to Mono- and 1,2-di-(1,2,3-Triazolyl)-Alkenes and Fused bis-(1,2,3-Triazolo)-Pyrazines

A stereoselective and convenient route has been demonstrated to access (*Z*)-1,2-diazido alkenes from the corresponding 1,2-diboronic esters *via* a copper-mediated reaction with sodium azide. Alternately, the mono-functionalization was regioselectively carried out with trimethylsilylazide as azidation reactant. The in situ conversion of bis-azides to the corresponding bis-triazoles can bereadily achieved in the presence of copper sulfate and sodium ascorbate, while the modification of the catalytic system opened a new convenient route tobis-triazolo-pyrazines, a new class of fused heterocycles. (*J. Org. Chem.*, **2020**, 85, 15104 -15115)

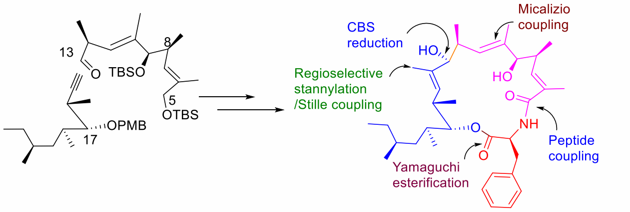
Urea-Promoted Metal-Free Homolytic Alkynyl Substitution (HAS): Metal-Free C-C Coupling of Alkynyl Bromides Formed *in situ* from 1,1-Dibromoalkenes

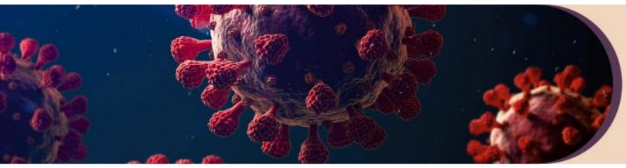
Herein, the unique method reports the efficacy of abundantly available urea for the generation of alkynyl radicals from 1-bromoalkynes under metal-free conditions. Urea as a sole reagent enabled the transformation of 1,1-dirbomoalkenes or 1-bromoalkynes to 1,3-diynes *via* Homolytic Alkynyl Substitution (HAS). Urea further showed efficiency in synthesizing disubstituted alkyne *via* Sonogashira type cross-coupling of 1,1-dibromalkene/1-bromoalkyne with aryl iodide. The Azobisisobutyronitrile (AIBN) trap detected the existence of short-lived alkynyl radical during the reaction. This method might be the first report with Homolytic Alkynyl Substitution under metal-free conditions, whereas Homolytic Aromatic Substitution is well reported. (*ChemistrySelect*, **2021**, 6, 2387-2393)



Total Synthesis of the Proposed Structure of Metacridamide B

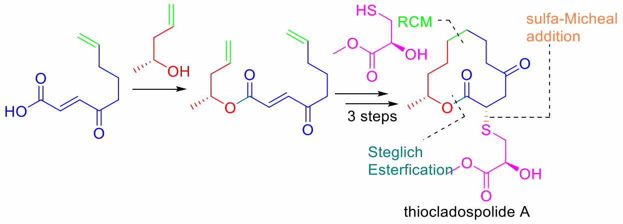
The first asymmetric total synthesis of the proposed structure of metacridamide B, a 17-membered macrolide with anticancer activity has been accomplished in a highly convergent and flexible manner. The key features of our synthesis involved hydroxyl directed ruthenium catalyzed alkyne functionalization, Stille coupling, asymmetric Corey-Bakshi-Shibata reduction, Micalizio coupling and Yamaguchi macrolactonization. Careful comparison of ^{1}H and ^{13}C NMR spectroscopic data confirmed that the natural metacridamide B had been erroneously represented as its C9-epimer. (*Tetrahedron Lett.*, **2021**, 82, 153374–153379)





First Total Synthesis of thiocladospolide A and its C2-epimer

The first total synthesis of recently isolated thiocladospolide A and its C2-epimer have been achieved in nine straightforward linear steps with 12% of overall yield. The key feature of the synthesis is the construction of the macrocyclic ring *via* late stage ring-closing metathesis reaction followed by alkene reduction. (*Synthesis*, **2021**, *54*, 683-688)



Stereoselective Synthesis of C19-C39 Fragment of Bastimolide A

The synthesis of C19-C39 fragment of antimalarial natural product Bastimolide A has been achieved *via* addition of functionalized C19-C26 alkyne fragment to the C27-C39 aldehyde fragment. Opening of terminal epoxide and Noyori asymmetric reduction were used as key steps in the synthesis. (*SynOpen*, **2021**, 5, 285-290)

Epoxy-Tethered Diels–Alder Reaction Toward the Tricyclic Core of Kalihinols

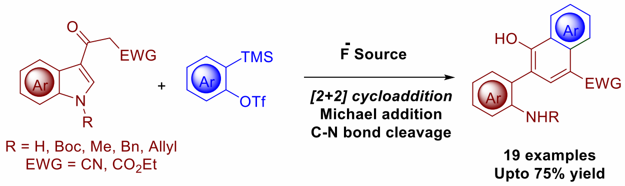
A chiral-template-driven intramolecular Diels–Alder reaction has been used to build the tricyclic core of kalihinols, a group of anti-malarial marine natural products. The key starting materials are commercially available nerol and sulcatone. (*Org. Lett.*, **2020**, 22, 3557–3560)

Diastereoselective Synthesis of CF$_3$-Dihydrobenzofurans by [4+1] Annulation of *insitu* - Generated CF$_3$-*o*-Quinone Methides and Sulfur Ylides

An efficient and highly diastereoselective synthesis of CF$_3$-dihydrobenzofurans by the reaction of *in situ*-generated CF$_3$-*o*QMs in the presence of a base with sulphur ylides is put forward. The generality of the present developed method was well studied with diverse substrates to access the corresponding products in excellent yields. The highly reactive CF$_3$-*o*QM has been utilized first time for the annulations reaction. **(*RSC Adv.*,2020, 10**, 38588-38591)

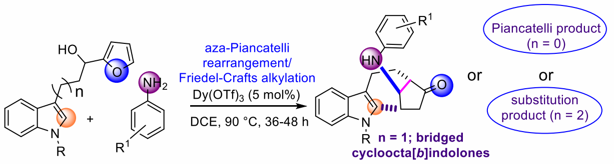
Synthesis of 2-Amino-2′-hydroxy-1,1′-biaryls *via* Cascade Benzannulation and C–N Bond Cleavage Sequence

A serendipitous synthesis of *N*-substituted 2-amino-2′-hydroxy-1,1′-biaryls through an aryne annulation with indolyl β-ketonitrile/ester in a cascade manner is demonstrated. The reaction sequence involves benzyne-mediated [2+2] Stoltz-type cycloaddition–cleavage and intramolecular Michael addition followed by C–N bond cleavage under transition-metal-free reaction conditions. Interestingly, while [4+2] Diels–Alder reaction is a possible pathway, no traces of the regioisomer was isolated. **(*Org. Lett.*, 2020, 22, 8224 – 8228)**



Cation Triggered Domino Aza-Piancatelli Rearrangement/Friedel–Crafts Alkylation of Indole-Tethered Furfuyl Alcohols to Access Cycloocta[b]indole Core of Alkaloids

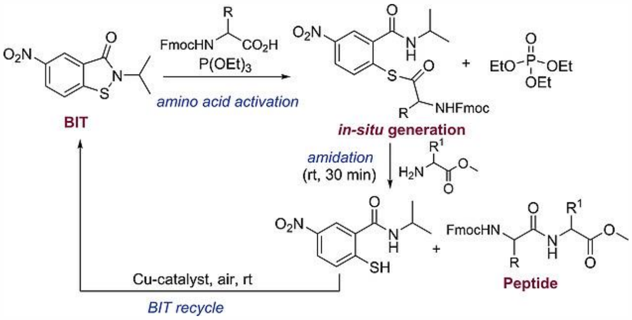
A domino approach to bridged cycloocta[b]indolone through a cascade of aza-Piancatelli rearrangement/Friedel–Crafts alkylation is developed. This transformation has been realized by reaction of an indole-tethered 2-furylcarbinol and substituted aniline in the presence of a Lewis acid to initiate aza-Piancatelli rearrangement followed by an in situ intramolecular Friedel–Crafts alkylation to access bridged tetracyclic frameworks in one pot. (***Org. Lett.*, 2020, 22,** 8555–8560)



Formation of complex skeleton in single step in short time
Three new bonds (C-N, two C-C bonds) in one-pot

Benzoisothiazolone (BIT): A Fast, Efficient, and Recyclable Redox Reagent for Solid Phase Peptide Synthesis

A fast and efficient coupling protocol for SPPS using benzoisothiazolone (BIT) under mild conditions with minimal waste was developed. BIT recycling is demonstrated on a gram scale reaction and amino acid consumption has been minimized irrespective of the peptide length. This coupling protocol has been successfully applied for the synthesis of side chain of recently discovered antibiotic, teixobactin. (*Eur. J. Org. Chem*., **2020**, 5358-5362)

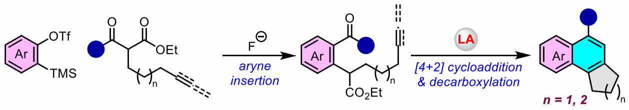


Diastereoselective Formal Synthesis of Polycyclic Meroterpenoid (±)-Cochlearol A

A formal synthesis of (±)-cochlearol A was accomplished. The synthesis features Suzuki coupling and Friedel–Crafts cyclization as a convergent strategy to the functionalized tetralone ring and an intramolecular construction of the C/D ring involving sequential epoxide formation/acetal formation. **(*J. Org. Chem.*, 2021, 86,** 5412-5416**)**

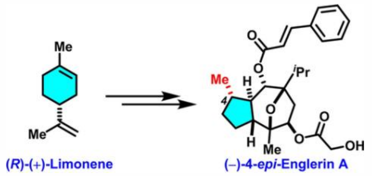
Aromaticity-Driven Access to Cycloalkyl-Fused Naphthalenes

An efficient synthesis of cycloalkyl-fused naphthalenes through the [4+2]-cycloaddtion/decarboxylative aromatization of alkyne-tethered aryne insertion adducts has been reported. These scaffolds were difficult to synthesize using conventional reactions. The reaction proceeds *via* the formation of a benzopyrylium intermediate followed by intramolecular [4+2] cycloaddition and a subsequent decarboxylation pathway. This method is also compatible with allene-tethered substrates to afford similar products. In addition, the one-pot synthesis of polysubstitutednaphthalenes *via* aryne insertion/benzannulation has also been developed in good yield. **(*Org. Lett.*, 2021, 23,** 4013–4017)



Total Synthesis of (−)-4-*epi*-Englerin A

(*R*)-(+)-Limonene has been used as chiral pool starting material towards the total synthesis of (−)-4-*epi*-englerin A. The key steps include Sharpless asymmetric dihydroxylation, aldol reaction, and transannular epoxide opening reaction. **(*Eur. J. Org. Chem.*, 2021,** 3190–3196)

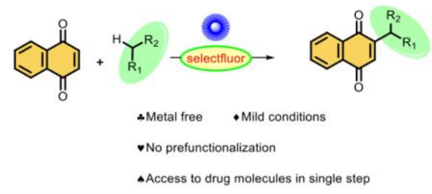


Scalable Synthesis of L-*allo*-Enduracididine: The Unusual Amino Acid Present in Teixobactin

A scalable synthesis of l-allo-enduracididine is achieved from commercially available (*S*)-glycidol in ten linear steps involving well-established synthetic transformations. The synthetic route is flexible and can be used to synthesize all four diastereomers by changing the stereochemistry of glycidol and Sharpless asymmetric dihydroxylation reagent. **(*Synlett*, 2021, 32,** 1465–1468**)**

Visible light-promoted Selectfluor-mediated quinone functionalization with Unactivated Csp^3-H components

A visible light-promoted metal-free cross-dehydrogenative-coupling (CDC) method for the alkylation of 1,4- naphthoquinones is reported using Selectfluor as a hydrogen atom transfer (HAT) agent. This protocol is suitable for a variety of 1,4-naphthoquinones and Csp3-H compounds and it facilitates the formation of pharmaceutically important quinone scaffolds under mild conditions. Using this methodology, the antimalarial drug, parvaquone, was synthesized in a single step. (*Arkivoc*., **2021**, part iii, 115-124)



♣Metal free ♦Mild conditions

♥No prefunctionalization

♠Access to drug molecules in single step

Intermolecular Trifluoromethyl-Alkenylation of Alkenes Enabled by Metal-Free Photoredox Catalysis

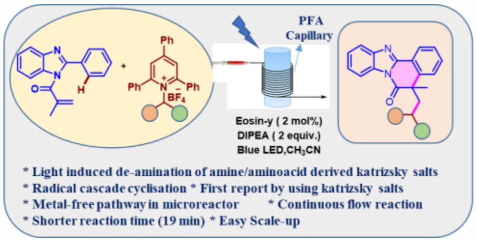
A three-component and redox-neutral trifluoromethylative alkenylation of unactivated alkenes with β-nitrostyrenes has been developed under visible-light. This metal-free protocol utilizes the easy to handle Langlois reagent (CF_3SO_2Na) as the CF_3 source and is suitable for various unactivated alkenes and β-nitrostyrenes, affording a series of trifluoromethylated aromatic alkenes under mild conditions in good to excellent yields. **(*Chem. Commun.*, 2021, 57,** 5582–5585**)**

Continuous-Flow Photo-Induced Decarboxylative Annulative Access to Fused Imidazole Derivatives *via* a Microreactor Containing Immobilized Ruthenium

Visible-light-driven continuous-flow decarboxylative annulation was achieved and used along with a microreactor containing immobilized ruthenium catalyst to construct valuable fused imidazole derivatives with high yields under an open atmosphere. Notably, this chemistry included the use of L-proline and α-azidochalcone as precursors of an α-amino radical and 2H-azirine *via* photo-induced decarboxylation and denitrogenation, respectively, to give the annulated imidazole derivatives as a result of the formation of two new C–N bonds. Moreover the novel, environmentally benign and efficient continuous-flow protocol was further improved by carrying out the reaction in a polydimethylsiloxane (PDMS) microreactor with immobilized Ru3+ under fluorescent or white LED light, enabling excellent yields (70–94%) at a reaction time (2 min) significantly shorter than that (16 h) of the batch protocol. (*Green Chem*., **2020**, 22, 1565-1571)

Visible-Light-Induced Deaminative Alkylation/Cyclization of Alkyl Amines with N-Methacryloyl-2-phenylbenzoimidazoles in Continuous-Flow Organo-Photocatalysis

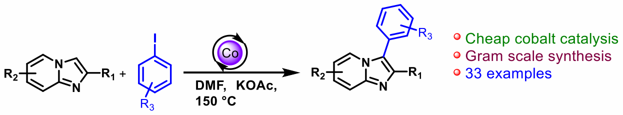
A metal-free visible-light-induced eosin-y-catalyzed deaminative strategy for the sequential alkylation/cyclization of N-methacryloyl-2-phenylbenzoimidazoles with alkyl amine-derived Katritzky salts, which provides an efficient avenue for the construction of various benzo[4,5]imidazo[2,1-a]isoquinolin-6(5H)-one derivatives is presented. Utilization of redox-active pyridinium salts from abundant and inexpensive primary amine feedstocks that were converted into alkyl radicals *via* C–N bond scission and subsequent alkylation/cyclization with N-methacryloyl-2-phenylbenzoimidazoles by the formation of two new C–C bonds are highlighted. A continuous-flow regime was carried out by utilizing a perfluoroalkoxy alkane tubing micro reactor under optimized reaction conditions with a blue light-emitting diode light source, enabling excellent yields and a shorter reaction time (19 min) versus the long reaction time (16 h) of the batch reaction. The reaction displays excellent functional group tolerance, easy operation, scalability, mild reaction conditions, and broad synthetic utility. (*J. Org. Chem.* **2021**, 86, 12908–12921)



* Light induced de-amination of amine/aminoacid derived katrizsky salts
* Radical cascade cyclisation * First report by using katrizsky salts
* Metal-free pathway in microreactor * Continuous flow reaction
* Shorter reaction time (19 min) * Easy Scale-up

Cobalt-Catalyzed Direct Arylation of *Imidazo[1,2-a]pyridine* with Aryl Iodides

The Co(II)Cl_2.6H_2O catalyzed C-H activation/direct arylation of imidazo[1,2-*a*]pyridine with aryl/heteroaryl iodide is reported. The cost effective, ligand and additive free protocol using KOAc successfully afforded 3-arylimidazo[1,2-*a*]pyridines in good yields. *Imidazo[1,2-a]pyridines* with electron withdrawing and electron donating substituents with various aryl iodides were well tolerated. The reaction was performed in a Screw-top V-Vial® to expedite the synthesis. The antibacterial 3-napthyl *imidazo[1,2-a]pyridine* was smoothly prepared using this protocol. (*Eur. J. Org. Chem*., **2020**, 1823-1827)

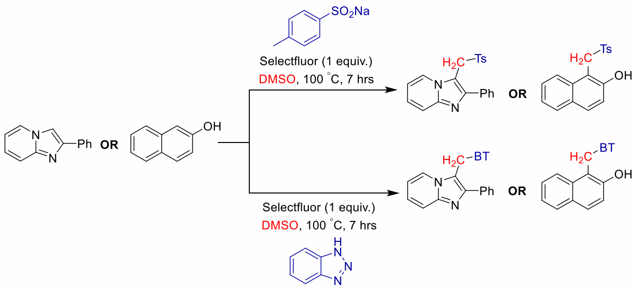


Difluorinative-Hydroxylation and C-3 Functionalization (Halogenation/SCN/NO) of Imidazopyridine using Selectfluor as Fluorine Source or Oxidant Respectively

An efficient route for the difluorinative-hydroxylation through dearomativedifunctionalization of imidazopyridine using Selectfluor as fluorine source was developed in an aqueous medium. The reaction proceeded through ionic followed by radical pathway. The method was successfully applied for a gram-scale production of 3,3-difluoro-2-(4-fluorophenyl)-2,3-dihydroimidazo[1,2-*a*]pyridin-2-ol. The Zolimidine drug successfully underwent difluorinative-hydroxylation in high yield. Interestingly, addition of the tetra-*n*-butyl ammonium halide or NaI or KSCN or $NaNO_2$ in the reaction provided oxidative functionalization of imidazopyridine wherein Selectfluor acted as an oxidant. The C-3 substituted (Cl, Br, I, SCN and NO) imidazo[1,2-*a*]pyridines were prepared in good yields. These two significant reactions provided wide functional group tolerance, metal/ base-free, and green approach. (*Tetrahedron Lett*., **2021**, 71, 153028 - 153032)

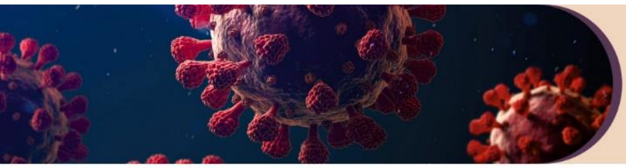
Methylene-Tethered Arylsulfonation and Benzotriazolation of Aryl/Heteroaryl C–H Bonds with DMSO as a One-Carbon Surrogate

The Selectfluor mediated approach towards the synthesis of methylene-tethered arylsulfonation and benzotriazolation of imidazopyridines has been described. The reaction involves imidazopyridine, arylsulfinate or benzotriazole and DMSO in the presence of Selectfluor where DMSO acts as one carbon synthon. The protocol has been extended to the methylene-tethered arylsulfonation and benzotriazolation of *β*-napthols. The mechanistic insights show that the intermediate 3-((methylthio)methyl)-2-phenylimidazo[1,2-*a*]pyridine is generated from imidazopyridine, DMSO and Selectfluor. The nucleophilic displacement by arylsulfinate salt or benzotriazole on intermediate afforded the product. (*J. Org. Chem*., **2021**, 86, 17684–17695)



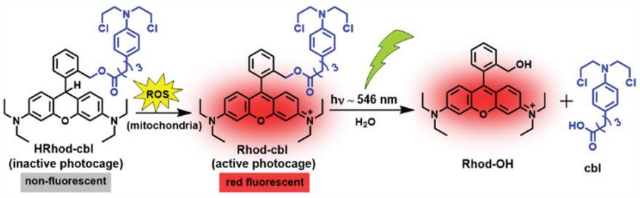
Improved Tumor-specific Therapeutic Strategy by Spatio-Temporal *in situ* Formation of Cu(II)-complex, Leading to Prompt Cell Apoptosis *via* Photoactivation of the Prodrug

The anti-tumor activity of Cu complexes is well established in cancer research. A biotin-tagged Cu-chelating prodrug that is activated by one-photon and two-photon irradiation for the target specific and spatio-temporally controlled *in situ* generation of a Cu complex was developed. In this way, the copper from a ‘‘cancer-promoting’’ agent to an anticancer agent was transformed. (*Chem. Commun*., **2020**, *56*, 4559 – 4562)



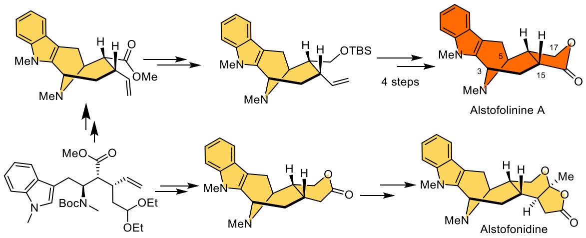
Mitochondria-Localized *in situ* Generation of Rhodamine Photocage with Fluorescence Turn-on Enabling Cancer Cell-Specific Drug Delivery Triggered by Green Light

A rhodamine dye based water soluble, mitochondria-indicating photocage was developed which gets activated in the mitochondria producing a fluorescent signal and on-demand releases the caged anticancer drug, chlorambucil, in the cancer cells selectively upon irradiation of green light. (Chem. Commun.,**2020**, *56*, 8412–8415)



Total Synthesis of Indole alkaloids

The total synthesis of indole alkaloids such as alstofolinine A is accomplished from an easily accessible tetracyclic core *via* TBS protected intermediate. This tetracyclic core bears all required stereocenters, along with suitable functional groups for necessary transformations facilitated in quick accessing of the target molecule alstofolinine A in minimal steps. The synthesis supports the absolute configuration of alstofolinine A. The pentacyclic core facilitated putative biosynthetic congener access, thereby allowing a rapid synthesis of alstofonidine from the proposed biosynthetic pathway. Interestingly, both tetracyclic and pentacyclic cores were accessed from a common intermediate developed in our laboratory. (*Asian J. Org. Chem.***2020**, *9*, 1172-1173; *Tetrahedron,* **2021**, *82*, 131930-131935)



A Unified Approach to the Salicylaldehyde Containing Polyketide Natural Products: Total Synthesis of ent-Pyriculol, ent-Epipyriculol, ent-Dihydropyriculol, ent-Epidihydropyriculol, Sordariol, Sordarial, 12-Methoxy Sordariol, and Agropyrenol

Many fungal metabolites are salicylaldehyde containing polyketide natural products and are often isolated from the fungus culture broth. These metabolites commonly exhibit phytotoxicity, however, some compounds exerted other biological activities including immunosuppressive activity. A unified synthetic strategy has been developed that provides easy access to ent-pyriculol, ent-epipyriculol, ent-dihydropyriculol, ent-epidihydropyriculol, sordariol, sordarial, 12-methoxy sordariol and agropyrenol. (*Tetrahedron,* **2020**, *76*, 131368-131380)

The Synthesis of Indeno[de]Isochromene Derivatives from Arylvinyl Epoxides and Carbonyl Compounds *via* Tandem Nazarov and Oxa-Pictet–Spengler Cyclizations

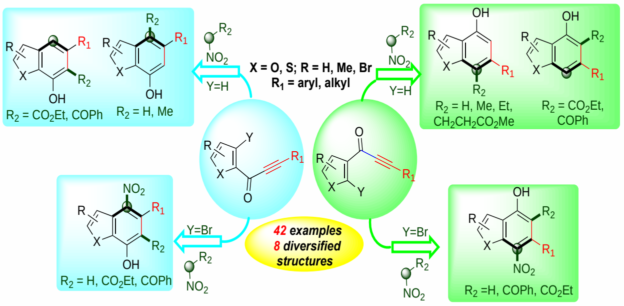
The reaction of arylvinyl alkoxides with chloro(aryl)carbenes would provide the corresponding arylvinyl epoxides that underwent Nazarov cyclization in a catalytic amount of scandium triflate, providing easy access to several highly substituted indenes, including some resveratrol-derived natural products. In addition, aryl vinyl epoxides and carbonyl compounds in the presence of a catalytic amount of $BF_3.OEt_2$ delivered indeno[de]isochromenes *via* tandem Nazarov and oxa-Pictet-Spengler cyclizations. This protocol is operationally simple and generates three bonds (two C-C and one C-O), thereby providing a structural skeleton of pharmaceutical interest and a natural product like polycyclic frameworks. (*Synlett*, **2021**, 32, 605–610; *New J. Chem.*,**2021**, 16248-16253)

Gram Scale Synthesis of Honokiol

The total synthesis of honokiol (1) has been accomplished in an efficient and convenient method that proceeds in six linear steps with 64% overall yield from commercially available starting materials. Our synthesis enables the access of pure honokiol in gram quantities, insuring its availability as a reference sample for future chemical and biological studies. (*Org. Prep. Proced. Int.*, **2021**, 54, 49-55)

Stitching Ynones with Nitromethanes: Domino Synthesis of Functionally Enriched Benzofurans and Benzothiophenes

A convenient one-pot benzannulation of regioisomeric 2- or 3-substituted furan and thiophene ynones with a range of nitromethanes has been discovered to directly access densely and diversely functionalized benzofurans and benzothiophenes. In this protocol, the nitro group in nitromethanes functions as recursive carbanion activator to setup tandem Michael addition-6π- electrocyclization, and its eventual sacrificial elimination facilitates aromatization and overall benzannulation. This benzannulation was also explored with furan/thiophene based o-halo ynones wherein a Michael addition-S$_N$Ar process operates and nitromethanes leave their imprint to deliver nitro substituted benzo-furans and -thiophenes. (*J. Org. Chem.*, **2021**, 86, 12093−12106)

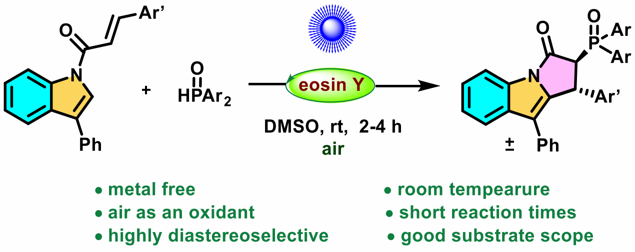


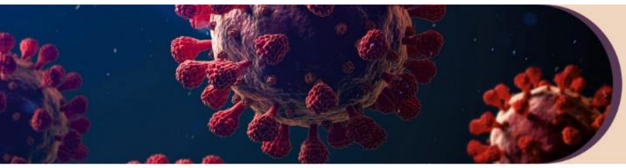
Bacterial Biosynthesis of Nanosilver: A Green Catalyst for the Synthesis of (Amino Pyrazolo)-(Phenyl)Methyl Naphth-2-Ol Derivatives and their Antimicrobial Potential

Heterogeneous reusable silver nanoparticles produced from isolated strain *Streptomyces sp*. RAB 10, 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 aqueous media. One of the important features of this methodology is the synthesis of a novel product with two reactive functional groups (hydroxy and free amine), which opens up avenues for the synthesis of a new array of compounds. The biosynthesised AgNPs as well as the naphthalene-2-derivatives exhibited moderate to good anti-microbial activity. (*New J. Chem.*, **2020**, 44, 13046-13061)

Visible-Light-Driven Metal-Free Aerobic Synthesis of Highly Diastereoselective Phosphinoylpyrroloindoles

A visible-light-driven metal-free carbon-phosphorus functionalization for the construction of 2-phosphinoyl-3*H*-pyrrolo[1,2,*a*]indoles is described. This mild tandem phosphinoylation/cyclization protocol utilizes air as a green oxidant and proceeds in a short span of time at room temperature with high functional group tolerance, excellent chemo- and diastereoselectivity. (*Org. Biomol. Chem.*, **2020**, 18, 1354–1358)





Visible-Light Promoted Photocatalyst and Additive-Free Intermolecular Trifluoromethyl-Thio(Seleno)cyanation of Alkenes

A visible-light promoted highly selective and efficient strategy for the trifluoromethyl-thiocyanation of alkenes under transition-metal, photocatalyst and additive-free conditions has been reported using stable and recyclable Umemoto reagent II as the CF_3 source and inexpensive ammonium thiocyanate as thiocyanating agent. This economical and environmentally benign protocol is suitable for styrenes, acrylates and unactivated alkenes and delivers various trifluoromethyl-thiocyanates in good to excellent yields. In addition, trifluoromethyl-selenocyanation of alkenes is also demonstrated for the first time using this protocol with potassium selenocyanate. (*Green Chem.*, **2020**, 22, 5589 - 5593)

Intermolecular Trifluoromethyl-Alkenylation of Alkenes Enabled by Metal-Free Photoredox Catalysis

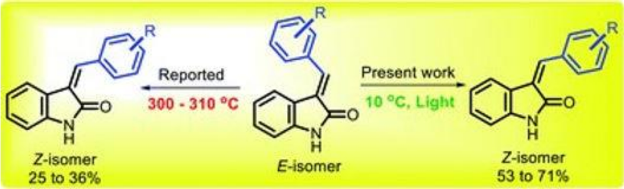
A three-component and redox-neutral trifluoromethylative alkenylation of unactivated alkenes with β-nitrostyrenes has been developed under visible-light. This metal-free protocol utilizes the easy-to-handle Langloi's reagent (CF_3SO_2Na) as the CF_3 source and is suitable for various unactivated alkenes and β-nitrostyrenes, affording a series of trifluoromethylated aromatic alkenes under mild conditions in good to excellent yields. (*Chem. Commun.*, **2021**, 57, 5582–5585)

Electricity-Induced Micro-Flow C–H/N–H Alkyne Annulation: AGreener Approach to Access Heteroaromatic Compounds

Fast access to structurally diverse hetero aromatic compounds is demonstrated in an integrated continuous-flow manner without employing any expensive oxidant. The process involves an electro-flow heating reactor that uses electricity as the green oxidant to promote the reaction, leading to a fast (2 min) annulation reaction for the synthesis of heteroaromatic compounds. (*React. Chem. Eng.*, **2021**,6, 1801-1805)

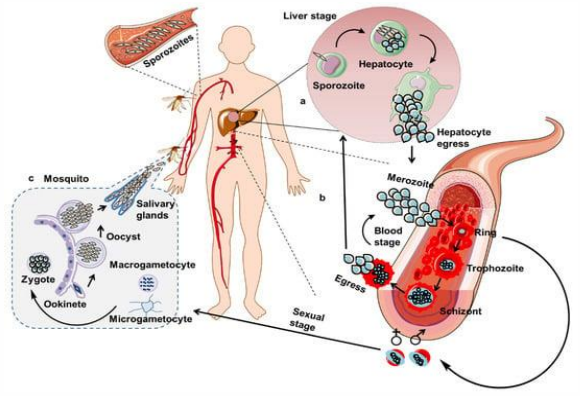
E-Z Isomerization of 3-benzylidene-indolin-2-ones Using a Microfluidic Photo-Reactor

A controlled *E–Z* isomeric motion of the functionalized 3-benzylidene-indolin-2-ones under various solvents, temperature, light sources, and most importantly effective enhancement of light irradiance in microfluidic photoreactor conditions is reported. Stabilization of the *E–Z* isomeric motion is failed in batch process, which might be due to the exponential decay of light intensity, variable irradiation, low mixing, low heat exchange, low photon flux etc. This photo-µ-flow light driven motion is further extended to the establishment of a photo stationary state under solar light irradiation. (*RSC Adv.*, **2020**, 10, 28630–28634)



Plasmodium falciparum Malaria Vaccines and Vaccine Adjuvants

Malaria, a parasite vector-borne disease, is a global health problem. *Plasmodium falciparum* has proven to be the deadliest among *Plasmodium* spp., which causes malaria in humans. The present article provides an overview of the current knowledge of anti-malarial immunity against *P. falciparum* and different options of vaccine candidates in development. A special emphasis has been made on the mechanism of action of clinically used vaccine adjuvants. (*Vaccines*, **2021**, 9, 2927 – 2970)



Artemisinin-Derived Dimers from a Chemical Perspective

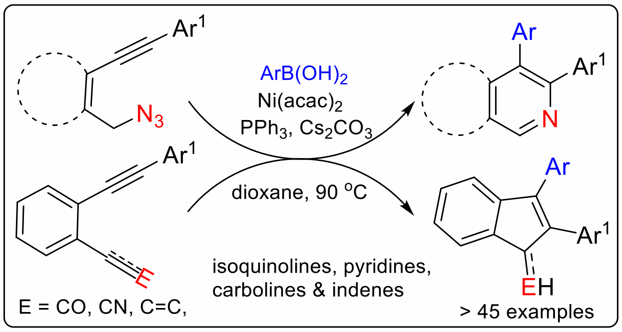
Considerable progress has been made with the rather recently developed dimer approach, which has already found applications in the development of new effective artemisinin-derived anti-malarial, anticancer, and antiviral agents. One observation common to these potential applications is the significant (i.e., much more than double) improvement in activity of artemisinin based dimers, which are not toxic to normal cells and have fewer or less harmful side effects, with respect to monomers against parasites, cancer cells and viruses. Due to the high potential of the dimerization concept, many new artemisinin-derived dimer compounds and their biological activities have been recently reported. In this review an overview of the synthesis of dimer drug candidates based on the clinically used drug artemisinin and its semisynthetic derivatives is given. Besides, the highlighting of biological activities of the selected dimers, the main focus is set on different synthetic approaches toward the dimers containing a broad variety of symmetric and non-symmetric linking moieties. (*Med. Res. Rev*., **2021**, 41, 2927-2970)

Structural Hybridization as a Facile Approach to New Drug Candidate

Strategies of drug-drug combinations have been adopted to generate hybrid conjugates of many clinically used drugs, designed to address inherent problems associated with drug candidates against various diseases including microbial infections, virus infections and cancer. Thus, the design of hybrids was aimed to achieve higher efficacy through possible multi-target interactions, selective delivery of the drug to the site of action with the aim to improve bioavailability, alleviate toxicity and circumvent drug resistances. In this review article, the progress made in recent years in the rapidly growing field of drug discovery, focusing on the rationality of the hybrid design with particular emphasis on the linker architecture, which plays a crucial role in the overall success of a hybrid drug, is summarized**.** (*Bioorg. Med. Chem. Lett.*, **2020**, 30, 12751-12765)

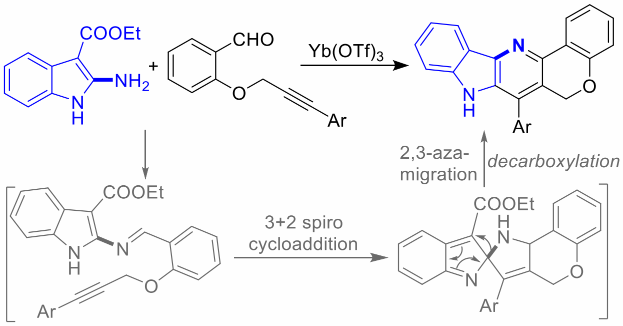
Ni-Catalyzed Electrophile Driven Regioselective Arylative Cyclization of *Ortho*-Functional Diaryl Acetylenes for Pyridine and Indene Derivatives

A regioselective carbonickelation followed by cyclization, an arylative cyclization, of ortho functional diaryl acetylenes is achieved apparently through an electrophile driven alkyne polarization. A series of selectively substituted diaryl isoquinoline, pyridine and indene derivatives are thus accessed from diarylacetylenes with azide, carbonyl and cyanide tethers. (*Org. Chem. Front*. **2020**, 7, 30–34)



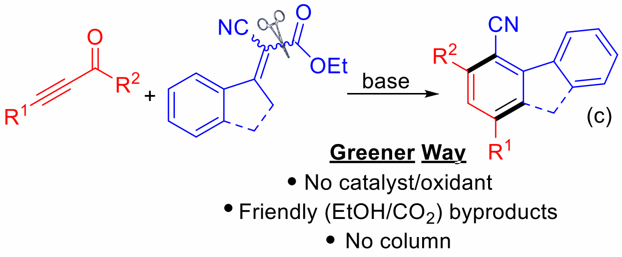
Lewis Acid Catalyzed Decarboxylative Annulation of 2-Aminoindole-3-Carboxylate with Ynals Involving [3+2] Spirocy-cloaddition and 2,3-Aza Migration

2-Aminoindole-3-carboxylates undergo a Lewis acid-catalyzed decarboxylative annulation with ynals to afford dihydrochromeno-fused δ-carbolines through a 2,3-aza migration, *via* a spirocyclic intermediate generated from an initial [3+2] spirocycloaddition. Brønsted acid interference changes the path from a [3+2] to a [4+2] addition. 2-Aminoindoles without an ester functional group at C3 underwent a different condensation, followed by hetero-Diels Alder reaction to generate chromeno-fused α-carbolines. (*Org. Lett.*, **2020**, 22, 1117-1123)



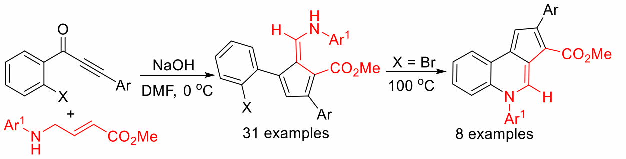
Base Mediated Benzannulation of α-CyanoCrotonates with Ynones: Facile Synthesis of Benzonitriles and Fluorenes

A strategic rapid approach for benzonitriles and cyanofluorenes *via* [3 + 3] benzannulation of readily available alkynones and α-cyanocrotonates, a protocol par excellence for aryl nitriles is demonstrated. This decarboxylative annulation is assisted solely by a base without the need of any catalyst. The only by-product is EtOH (and CO2) and the product is cleanly filtered off the contents after reaction at ambient temperature. (*Green. Chem.*,**2020**, 22, 2370-2374)



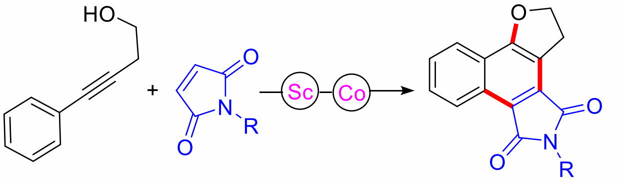
Base Mediated Cyclopentannulation of Ynones with Amino Croto-nates for Regio- & Stereoselective Synthesis of Pentafulvenes and Cyclopenta[c]quinolines

A regio- and stereoselective synthesis of unsymmetrically substituted pentafulvenes is reported *via* the condensation of readily available ynones and amino crotonates under very mild conditions. The mechanism of this 3+2 annulation involved a vinylogous Michael addition followed by an intramolecular enamine aldol condensation. Substrates with *o*-bromo tether further cyclized to pentannulatedhydroquinolines through an isomerization/S_NAr in the same reaction pot at the elevated temperature. (*J. Org. Chem.* **2020**, 85, 6970-6980)



A Sequential Activation of Alkyne & C-H Bonds for the Tandem Cyclization & Annulation of Alkynols and Maleimides through Cooperative Sc (III) and Cp* Free Co (II) Catalysis

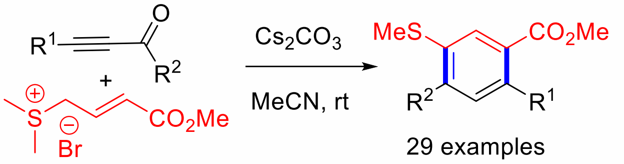
[4+2] oxidative Diels-Alder reaction of readily available alkynols with maleimide is achieved for the rapid access of pthalimide fused multicyclic compounds. The reaction is proposed to go through a sequence of $Sc(OTf)_3$ catalyzed electro-philic cyclization, ligand exchange with Cp*-free cobalt, C−H activation followed by maleimide insertion. (*Org. Lett.*, **2020**, 22, 5326-5330)



Regioselective Benzannulation of Allylic Sulfur Ylides with Ynones: A Rapid Access to Substituted Thioanisoles

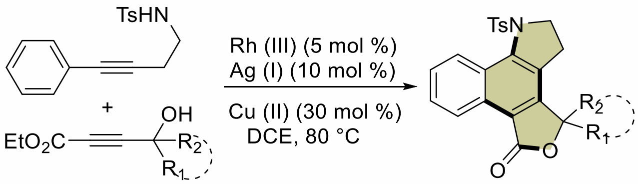
The efficiency and selectivity of annulation reactions are often difficult to control in the presence of multiple potential reactive centers, like in case of allylic sulfur ylides (ASY). A novel base mediated

[3+3] benzannulation of ASY and readily available alkynones that accomplishes the regioselective formation of multi substituted thioanisoles, highly sought after chemical scaffolds is described. A new reactivity pattern of ASY has been unearthed, where it acted as both 3C component and sulfur source in benzannulation. Use of handy base, operational simplicity and broad substrate scope are the additional salient features of the conversion. (*Chem. Commun.* **2020**, 56, 13457-13460)



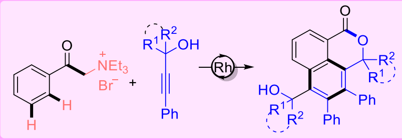
Harnessing Rhodium-Catalyzed C-H Activation: Regioselective Cascade Annulation for Fused Polyheterocyclics

In the realm of transition metal catalyzed arene functionalization, rhodium (III) catalysis is considered as exemplary due to its propensity to activate C-H bonds to obtain comprehensive molecular assembly. A new rhodium (III) catalyzed assembly of polyheterocyclic scaffolds *via* C-H activation and regioselective annulation of 4-arylbut-3-yn-1-amines with 4-hydroxy-2-alkynoates is demonstrated. Heterocyclization and trans-metallation prior to annulation is the key for initiation of this relay redox-neutral catalytic cascade. (*J. Org. Chem.* **2021**, *86*, 8069 – 8077)



Rhodium-Catalyzed Annulation of Phenacyl Ammonium Salts with Propargylic Alcohols *via* a Sequential dual C-H and a C-C bond Activation: Modular Entry to Diverse Isochromenones

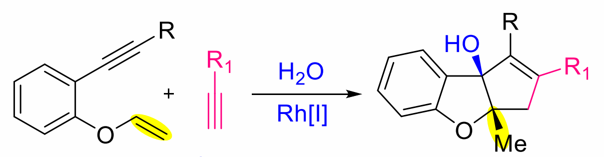
A dual (ortho/meta) C-H and a C-C activation of phenacyl ammonium salts (acylammonium as traceless directing group) towards annulation with propargylic alcohols to accomplish rapid access for novel isochromenones by means of rhodium catalysis from readily available starting materials is disclosed. This operationally simple protocol features broad substrate scope and wide functional group tolerance. Importantly, the protocol circumvented the need of any stoichiometric metal oxidants and proceeds under aerobic conditions. (*Org. Lett.*, **2021**, 23, 7888 – 7893)



dual C-H and a C-C activation
air as green oxidant
regioselectivity
novel fused isochromenones

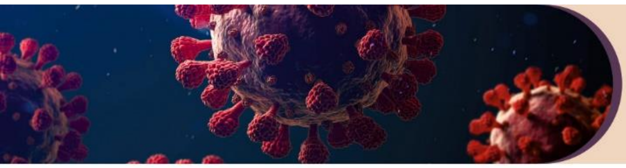
Diastereoselective [2+2+1] Hydrative Annulation of Phenol-Linked 1,6-Enynes with Acetylenes Through Rhodium Catalysis: A Rapid Access to Cyclopenta[b]benzofuranols

An unprecedented [2+2+1] hydrative annulation of 1,6-enynes with terminal alkynes is achieved using catalytic cationic Rh(I). Thus, a modular assembly of cyclopenta[b]benzofuranols with two consecutive quarternary stereocentres is achieved from readily available alkynes. The reaction is proposed to go through a sequence of 5-membered rhoda-cycle formation, regioselective acetylene insertion, 1,5 H-shift, substrate controlled stereoselective addition of water molecule followed by 1,2-rhodium migration gave contracted rhoda-cycle D and reductive elimination. Necessary control/labelling experiments were conducted to gain insight in to the mechanism. (*Chem. Eur. J.*, **2021**, 27, 17570-17575)



- stereo & regio-selective
- formation of two quarternary centers
- H_2O insertion & 100% atom economy

APPLIED RESEARCH



Oleogels and its Food Applications

Oleogel emulsions displayed good stability in terms of storage, particle size, and oil binding capacity (> 90 %). Formulated oleogel emulsions can act as promising alternative for mayonnaise. Further, rice bran/sunflower wax-based oleogels using eight refined food grade oils such as sunflower oil, mustard oil, soybean oil, sesame oil, groundnut oil, rice bran oil, palm oil, coconut oil were prepared. Sunflower wax oleogels unveiled rapid crystal formation with maximum oil binding capacity of 99.46 % in highly unsaturated sunflower oil with maximum PUFA content. Further, the applicability of this wax based oleogels as solid fat substitute in marketed butter products was also scrutinized. The lowest value of solid fat content (SFC) in oleogel was 0.20 % at 25 °C, resembling closely with the marketed butter products. Depending upon prerequisite, oleogel properties can be modulated by tuning wax type and oil unsaturation. This wax-based oleogel can be used as solid fat substitute in food products. (*J. Am. Oil Chem. Soc.*, **2021,** 98, 1189-1203; *ACS Food Sci. Technol.*, **2021,** 1, 152-164)

Formal Synthesis of Merck's Clinical Agent MK-7246 for the Treatment of Respiratory Diseases

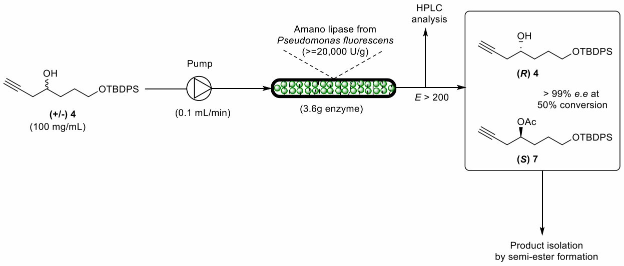
The methodology developed on the intramolecular vinylogous Michael addition was applied in the formal synthesis of an intermediate of Merck's clinical agent MK-7246, which is a potent and selective CRTH2 [chemo-attractant receptor expressed on T helper type 2 (Th2) cells] antagonist, for the treatment of respiratory diseases. The starting 2-alkenyl indole was subjected to palladium-catalyzed hydrogenation to effect the reduction of the *exo*-alkenyl moiety. The hydrogenated compound was treated with *t*-butyl bromoacetate to give the corresponding *N*-alkylated intermediate. The agent MK-7246 can formally be synthesized from the *N*-alkylated intermediate using the reported synthetic route. (*Chem. Commun.*, **2021**, 57, 231-234)

Total Synthesis of Anticancer Clinical Agent TIC10/ONC201

The total synthesis of the anticancer clinical agent TIC10/ONC201, a TRAIL inducer, in only three steps was accomplished applying tandem copper catalyzed strategies. The reaction of 2-aminoimidazoline and 4-chloronicotinic acid under copper catalyzed tandem N-arylation–amidation conditions produced the corresponding angular tricyclic fused heterocycle based on imidazoline-pyrimidine-pyridine derivative. The hydrogenation of the tricyclic heterocycle using PtO_2 catalyst enabled to obtain the corresponding tetrahydropyridine derivative in 92% of yield. Benzyl bromide was utilized to afford *N*-benzylation of the *NH* group of the tetrahydropyridine derivative to ultimately build the target molecule TIC10/ONC201. (*Org. Biomol. Chem.*, **2021**, 19, 8497 - 8501)

Chemoenzymatic Process for the Preparation of (S)-7-((*tert*-Butyldiphenylsilyl)oxy)hept-1-yn-4-ol in a Continuous Packed-Bed Reactor, a Key Intermediate for Eribulin Synthesis

A practical chemo-enzymatic process has been developed for the preparation of optically pure (S)-7-((tert-butyldiphenylsilyl)oxy)hept-1-yn-4-ol, (S)-4. This was prepared via enantioselective acylation of racemic homopropargylic alcohol (+/-)-4 catalyzed by Amano lipase from Pseudomonas fluorescens. The acylation reaction was studied in a packed bed reactor for the production of optically pure alcohol (S)-4 in a continuous mode. At substrate concentration of 100 mg/mL (272 mM) and flow rate of 0.1 mL/min, both the isomers are obtained in > 95% theoretical yield and >99 % e.e. at steady state in a packed reactor with 3.6 g enzyme. The advantage of this protocol is that the enzyme can be recycled many times. Finally, this was converted to (R)-tert-butyl((4-chloro-6-iodohept-6-en-1-yl)oxy)diphenylsilane, 3 which is key building block for the synthesis of C14-C19 intermediate of eribulin. (Org. Process Res. Dev., 2020, 24, 2657 – 2664)



sp^3-Rich Glycyrrhetinic Acid Analogues Using Late-Stage Functionalization as Potential Breast Tumor Regressing Agents

Late-stage functionalized analogues of glycyrrhetinic acid (GA) significantly induces antiproliferative and anti-invasive effects in triple negative breast cancer cells, selectively accumulated more in the mitochondrial compartment of cancer cells. GA analogues greatly regressed breast tumor growth and metastasis to various organs in a SCID mouse model. *(ChemMedChem.,* **2020**, 15, 1826-833)

A Perspective on Medicinal Chemistry Approaches Towards Adenomatous Polyposis coli and Wnt Signal-Based Colorectal Cancer Inhibitors

Colorectal cancer (CRC) is one of the major causes of carcinogenic mortality in numbers only after lung and breast cancers. The mutations in adenomatous polyposis coli (APC) gene leads to formation of colorectal polyps in the colonic region and which develop as a malignant tumour upon coalition with patient related risk factors. The protein-protein interaction (PPI) of APC with Asef (A Rac specific guanine nucleotide exchange factor) overwhelms the patient's conditions by rapidly spreading in the entire colorectal region. The current broad spectrum perspective is attempted to elaborate the sources of identification, development of selective APC inhibitors by targeting emopamil-binding protein (EBP) & dehydrocholesterol reductase-7 & 24 (DHCR-7 & 24); APC-Asef, β-catenin/APC, Wnt/β-catenin, β-catenin/TCF4 PPI inhibitors with other vital Wnt signal cellular proteins and APC/Pol-β interface of colorectal cancer. (*Eur. J. Med. Chem.,* **2021**, 212, 113149-113182**)**

In vitro and *in vivo* Studies Reveal α-Mangostin, a Xanthonoid from *Garcinia mangostana*, as a Promising Natural Antiviral Compound against Chikungunya Virus

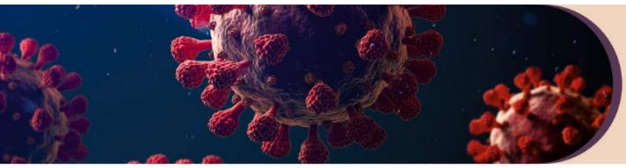
Chikungunya virus (CHIKV), a serious health problem in several tropical countries, is the causative agent of chikungunya fever. Approved antiviral therapies or vaccines for the treatment or prevention of CHIKV infections are not available. Diverse natural phenolic compounds have been shown to possess antiviral activities. The antiviral activity of α-Mangostin, a xanthanoid, against CHIKV infection was explored. (*Virol J.* **2021**, 18, 47-58)

An Experimental Toolbox for Structure-Based Hit Discovery for P. aeruginosa FabF, a Promising Target for Antibiotics

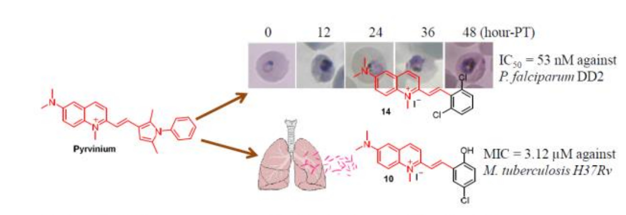
FabF (3-oxoacyl-[acyl-carrier-protein] synthase 2), which catalyses the rate limiting condensation reaction in the fatty acid synthesis II pathway, is an attractive target for new antibiotics. FabF from P. aeruginosa (PaFabF) as antibiotics against this pathogen was focused. An experimental toolbox consisting of binding assays using bio-layer interferometry (BLI) as well as saturation transfer difference (STD) and Water LOGSY NMR was set up in addition to robust conditions for structure determination. The suitability of the toolbox to support structure-based design of FabF inhibitors was demonstrated through the validation of hits obtained from virtual screening. Screening a library of almost five million compounds resulted in 6 compounds for which binding into the malonyl-binding site of FabF was shown. For one of the hits, the crystal structure in complex with PaFabF was determined. Based on the obtained binding mode, analogues were designed and synthesized, but affinity could not be improved. (*ChemMedChem.,***2021**, 16, 2715-2726)

Synthesis and Efficacy of Pyrvinium-Inspired Analogs Against Tuberculosis and Malaria Pathogens

The synthesis and evaluation of pyrvinium-based antimalarial and antitubercular compounds was reported. The pyrrole moiety was replaced with various aryl or heteroaryl substituents to generate



pyrvinium analogs. The profiling of these compounds against malaria parasite *P. falciparum* 3D7 revealed analogs with better antimalarial activity than pyrvinium pamoate. Two promising compounds showed IC_{50} of 23 nM and 60 nM against *P. falciparum* 3D7. These compounds were also effective against drug-resistant malaria parasite *P. falciparum* Dd2 with IC_{50} of 53 nM and 97 nM. The cytotoxicity against CHO-K1, HEK and NRK-49F cells revealed better selectivity index for these new analogs compared to pyrvinium. Additionally, this series of compounds showed activity against *M. tuberculosis* H37Rv. (*Bioorg. Med. Chem. Lett.*, **2020**, 30, 127037-127042)



The chemical modifications of pyrvinium, an anthelmintic drug, provided analogs effective against drug-resistant malaria parasite *P. falciparum* 3D7. Additionally, these analogues were effective against *M. tuberculosis* H37Rv.

Synthesis of Novel 4,5-dihydropyrrolo[1,2-*a*]quinoxalines, Pyrrolo[1,2-*a*]quinoxalin]-2-ones and their Antituberculosis and Anticancer Activity

A facile strategy was developed for the synthesis of biologically important 4,5-dihydropyrrolo[1,2-*a*]quinoxalines and pyrrolo[1,2-*a*]quinoxalin]-2-ones by treating 2-(1*H*-pyrrol-1-yl)anilines with imidazo[1,2-*a*]pyridine-3-carbaldehyde or isatin using amidosulfonic acid (NH_3SO_3) as a solid catalyst in water at room temperature. The protocol was extended to ninhydrin electrophile. The catalyst could be recycled for six times without loss of activity. The compounds were evaluated for their antituberculosis, anti-bacterial and anticancer activity. Important to note that two compounds demonstrated MIC of 6.25 µM against *M. tuberculosis* H37Rv. (*Arch. Pharm.*, **2020**, 353, e2000192)

Polymer Supported Cross-Linked Enzyme Aggregates (CLEAs) of Lipase B from *Candida antarctica*: An Efficient and Recyclable Biocatalyst for Reactions in Both Aqueous and Organic Media

Lipase B from *Candida antarctica* (CAL-B) was immobilized on epoxy-activated polymer support functionalized with polyethyleneimine (PEI) *via* preparation of enzyme aggregates by precipitation with polyethylene glycol (PEG 600). This involves adsorption of the aggregates on the functionalized polymer followed by cross-linking with glutaraldehyde. The apparent activity of the immobilized enzyme was found to be 750 TBU/g at optimum pH 7.5 and temperature 30 °C. The immobilization yield was 24%. The immobilized enzyme could be recycled (5 times) in both aqueous buffer and organic solvents. Further, the expensive polymer support was also recycled (5 times) after the immobilized enzyme lost its activity by washing with 1N HCl. (*Biocatal. Biotransformation*, **2021**, 40, 1-13)

3-Aryl Substituted Imidazo[1,2-*a*]pyridines as Antituberculosis Agents

The 3-aryl substituted imidazo[1,2-*a*]pyridines as potent antituberculosis agents were discovered. A small library of 3-aryl substituted imidazo[1,2-*a*]pyridines was synthesized using direct arylation followed by nitro reduction and finally Pd-catalyzed C−N coupling reactions. Thus obtained compounds were evaluated against *M. tuberculosis* H37Rv. The lead compound showed MIC of 2.3 µg/ml against *M. tuberculosis* H37Rv. This compound showed selectivity index of 35. The docking of lead compound in the active site of *Mycobacterium tuberculosis* cytochrome bc1 complex cytochrome b subunit (MtbQcrB) revealed key π-π interactions of compound with Tyr389 and Trp312 residues of MtbQcrB. (*Arch. Pharm.*, **2021,** 354, e2000419)

Integrated Multi-Step Continuous Flow Synthesis of Daclatasvir Without Intermediate Purification and Solvent Exchange

The fabrication of fully integrated flow-based manufacturing systems offers greener, and more economical approach. A compact manufacturing machine was developed for the synthesis of antiviral API Daclatasvir which is easily reconfigured, has a much-reduced footprint, and enables multi-step synthesis using innovative reaction chemistry and post-synthesis purification equipment. The developed integrated system enabled the ultra-fast production of DCV as its free base (within 28.2 min.) with a throughput of 11.8 g/day (equivalent to 200 doses of Daclinza, 60 mg tablets) in 98% HPLC purity. (*React. Chem. Eng.* **2020**, *5*, 2109–2114)

Characterization and Photoprotective Potentiality of Lime Dwelling Pseudomonas Mediated Melanin as Sunscreen Agent against UV-B Radiations

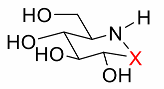
The present study focuses on production, structural characterization and evaluation of photo protective nature of melanin pigment derived from lime dwelling *Pseudomonas* sp. *in vitro* cytotoxicity and photo-protective effect of Pseudomonas derived melanin (Mel-P) against UV-B (Broad Band-BB) radiations were assessed on mouse fibroblasts NIH 3 T3 cell lines. A natural melanin obtained from Pseudomonas sp. contains 5, 6- dihydroxy indole 2-carboxyic acid (DHICA) as its basic constituent and possess typical properties of eumelanin. Mel-P has shown cell viability of 61.33 ± 6.58% at the concentration of 500 μg/mL proving its non-cytotoxic effect. Owing to its anti-oxidant property, melanin efficiently protected the mouse fibroblast cells from UV-B (BB) irradiation in a dose dependant manner demonstrating its potential as an active photoprotective agent. (*J. photochem. and photobiol. B, Biology*, **2021**, 216, 112126)

Novel 1,2,3-Triazole-Tethered Pam3CAG Conjugates as Potential TLR-2 Agonistic Vaccine Adjuvants

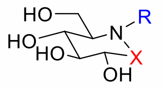
A focused library of water soluble 1,2,3-triazole tethered glycopeptide conjugates derived from variety of azido-monosaccharides and aliphatic azido-alcohols were synthesized through manipulation at the C-terminus of Pam3CAG and screened for their potential as TLR2 agonistic adjuvants against HBsAg antigen. *In vitro* ligand induced TLR2 signal activation was observed with all the analogues upon treatment with HEK blue TLR2 cell lines. Conjugate derived from ribose (6e), which exhibited pronounced HBsAg specific antibody (IgG) titer also shown enhanced CD8+ population indicating superior cell mediated immunity compared to standard adjuvant Pam3CSK4. Further, docking studies revealed ligand induced heterodimerization between TLR1 and 2. Overall, the result indicates the usefulness of novel conjugates as potential vaccine adjuvant. (*Bioorg. Chem.*, **2021**, 111, 104838)

Design, Synthesis, and Preliminary Immunopotentiating Activity of New Analogues of Nojirimycin

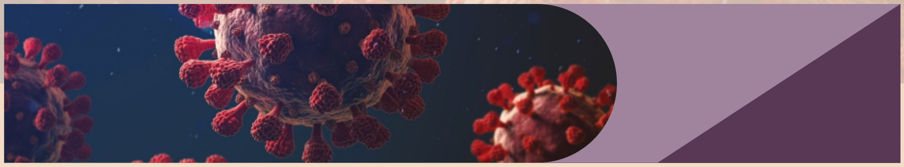
Three new classes of nojirimycin analogues viz. N-alkyl with C1-substituent (4-phenylbutyl), N-substituted 1-deoxynojirimycin and its congener δ-lactam, and a 4-phenylbutyl-β-C-glycoside were synthesized for immunological studies. The resulting diverse compound library exhibited proliferation of B Cells and T cells induced by LPS and Con A, respectively. A deoxynojirimycin-triazole conjugate of phytosphingosine analogue was superior in their responses and exhibited nitric oxide response equal to LPS. In comparison to findings on its congeners with immunosuppressive action, early immunological tests show that the novel nojirimycin analogues have immunopotentiating effect. (*Carbohydr. Res.*, **2021**, 511, 108479)



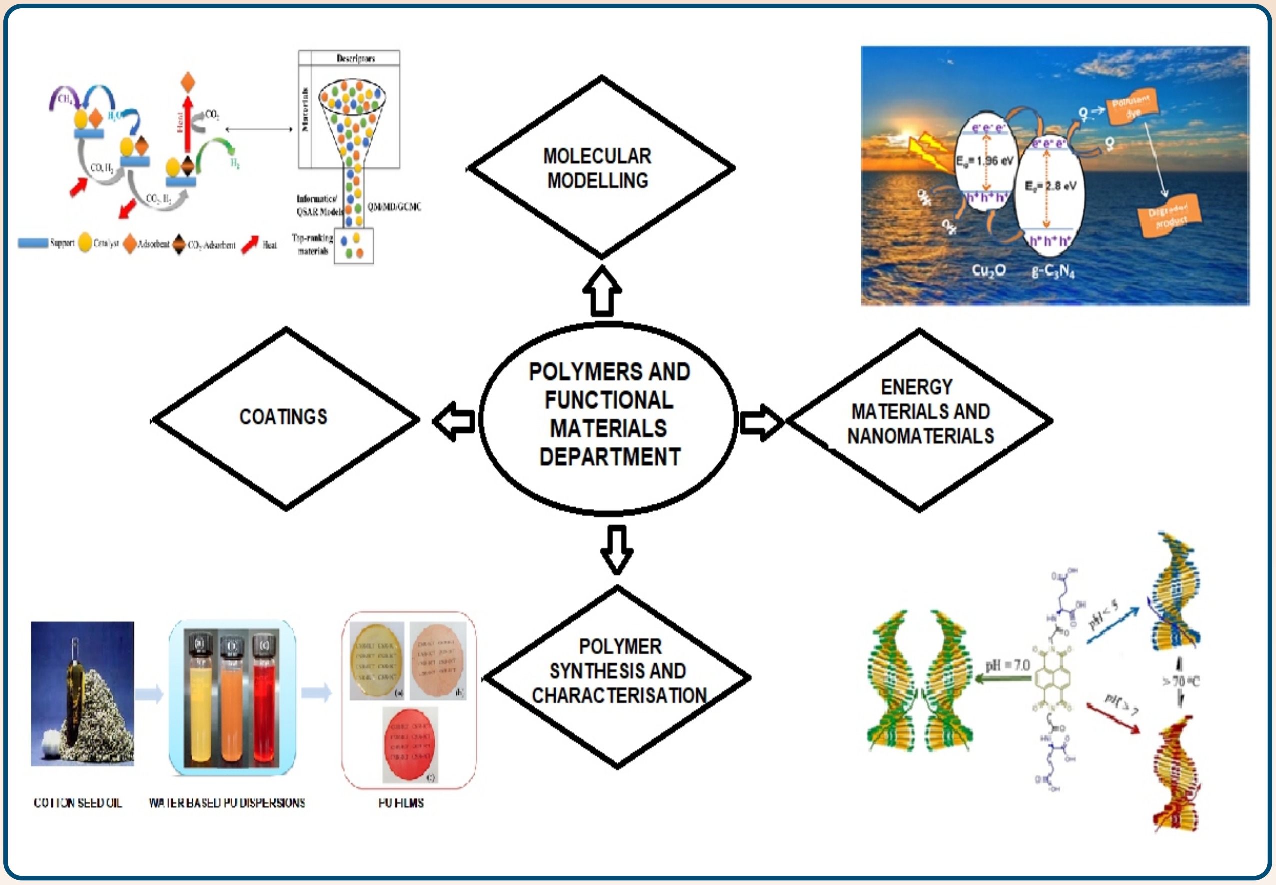
X = CH(OH) (Nojirimycin)
= CH_2 (1-Deoxynojirimycin)

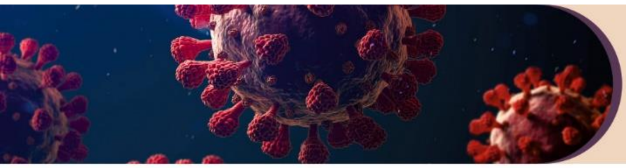


X = CH_2 (or) CO (or) $CH(CH_2)_4Ph$
R = Aliphatic chain variation



POLYMERS AND FUNCTIONAL MATERIALS



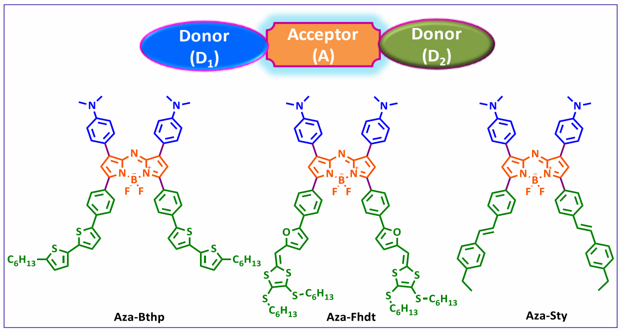


POLYMERS & FUNCTIONAL MATERIALS

BASIC RESEARCH

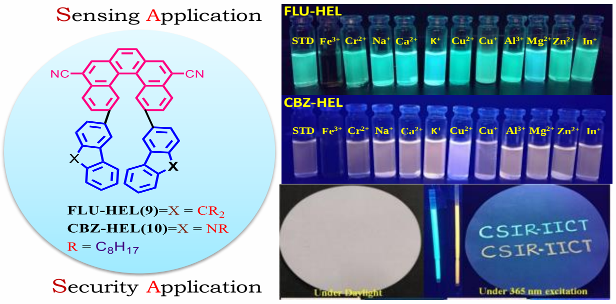
Panchromatic aza-Bodipy Based π-Conjugates

A series of three aza-Bodipy donor molecules namely Aza-Bthp, Aza-Sty, and Aza-Fhdt have been synthesized. The compounds exhibit panchromatic absorption spanning approximately 280–1000 nm in solution state and possess suitable energy levels for their usefulness as donors in organic solar cells. Under optimized conditions, using PC70BM as an acceptor, power conversion efficiencies (PCE %) of 2.44, 1.2, and 2.52 were afforded for Aza-Bthp, Aza-Fhdt, and Aza-Sty respectively. (*New J. Chem.* **2021**, 45, 7792-7798)



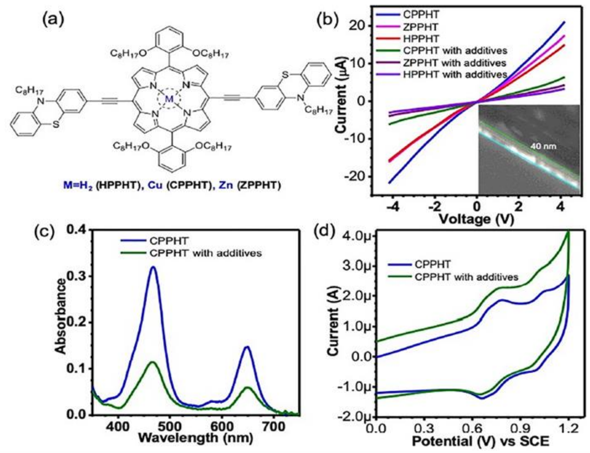
Blue-Red Emitting 2,12-Disubstituted [5] Helicenes for High Fluorescence Efficiency and Sensing Application

Photochemical synthesis of two new fluorene and carbazole-based 2,12-disubstituted helicenes namely **FLU-HEL** and **CBZ-HEL** respectively, was studied. The fluorescence quantum yield (Φ_f) = 27% and 30% and life time $\langle\tau_f\rangle$= 9.7 ns and 4.2 ns were observed for both helicenes, respectively. Also, both the helicene dyes have shown very good sensing properties towards Fe^{3+} transition metal ion than other transition metal ions. Feasibility of these compounds for security applications have ben explored. (*J. Photochem. Photobio. A: Chemistry* **2021**, 411, 113203)



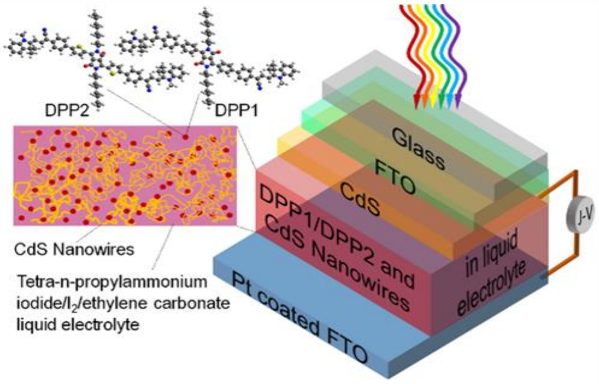
HTMs for Perovskite Solar Cells

A hydrophobic Donor-π-Donor concept based porphyrin HTMs in which phenothiazine as donor and porphyrin as π-spacer with free-based, Cu(II) and Zn(II) derivatives was designed. These HTMs showed device conversion efficiency of 13% with moisture resistivity.



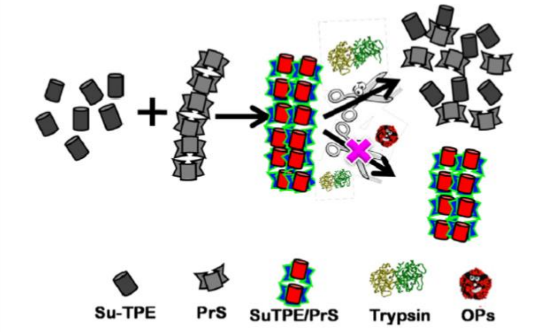
Aggregation Induced Emission (AIE) Materials Based on Diketopyrrolopyrrole Chromophore for CdS Nanowire Solar Cell Applications

Two diketopyrrolopyrrole (DPP) derivatives (DPP1 and DPP2) that are substituted with phenyl and thiophene moieties in between DPP core and merocyanine dyes, respectively, was developed. The introduction of thiophene ring subunit at core position endows DPP2 significantly alters the photophysical, electrochemical and aggregation induces enhanced emissive (AIEE) properties compared to those of DPP1.As a practical point of view, DPP1 and DPP2 as sensitizer on CdS nanowires for fabrication of dye sensitized solar cell (DSSCs) was successfully employed. The DSSC based on DPP2 (0.268%) dye yielded higher power conversion efficiency (PCE) as compared to DPP1 (0.195%) under standard illumination of Sunlight (AM 1.5 G, 100 mW/cm^2). (*Journal of Electroanalytical Chemistry*, **2021**, *895*, 115451)



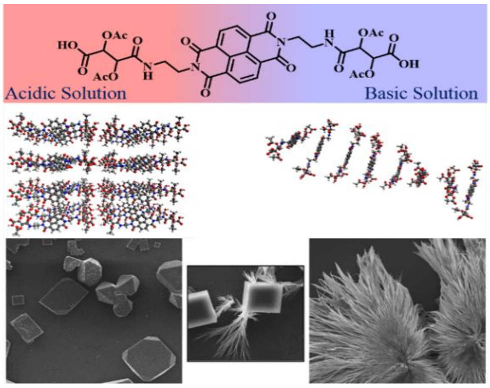
An Anionic Tetraphenyl Ethylene Based Simple and Rapid Fluorescent Probe for Detection of Trypsin and Paraoxon Methyl

An aggregation induced emission (AIE) based simple, sensitive, rapid and convenient sensing platform for detection of trypsin and organophosphorous pesticides was developed. The biosensor is composed of tetra-anionic sulphonyl derivative of tetraphenylethylene (Su-TPE) and cationic polyelectrolyte protamine (PrS), assembled by electrostatic interactions without any complex process of integration. The AIE phenomenon of free Su-TPE molecules, into PrS initiated aggregated supramolecular complex formation, has been supported by studying Su-TPE/PrS system under various environmental factors such as pH, temperature, ionic strength. After, establishing the AIE phenomenon of Su-TPE/PrS complex, the potential of the sensing platform, for trypsin detection, has been explored based on the principle of trypsin dependent PrS hydrolysis. The detection system is highly sensitive in the linear Trypsin concentration range of 0 - 0.016 μM with detection limit of 22.2 nM. (*Journal of Molecular Liquids*, **2021**,*333*, 115980)



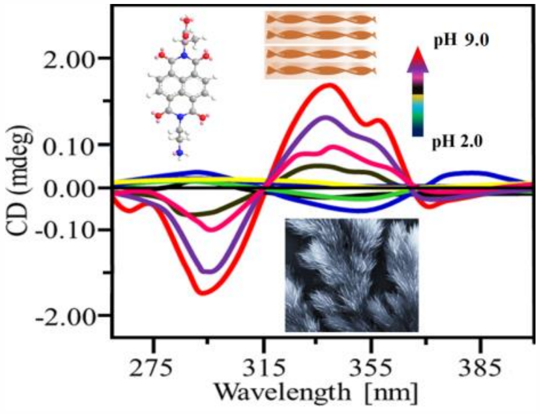
Characteristics of pH-Regulated Aggregation-Induced Enhanced Emission (AIEE) and Nanostructure Orchestrate *via* Self-Assembly of Naphthalene Diimide–Tartaric Acid Bolaamphiphile: role in cellular uptake

Tartaric acid (TA) appended naphthalene diimide (NDI) based bolaamphiphile (NDI-TA) was synthesized to investigate the effect of head group on the nanostructures fabricated by their self-assembly. The findings show that the chirality of NDI-TA is significantly impacted in the pH range 2 to 9. Importantly the NDI-TA bolaamphiphile showed remarkable selectivity and biocompatibility in binding to markers in MDA-MB 231 cancer cells compared to NDI alone even with its improved solubility. The cell morphology and uptake studies using confocal fluorescence microscopy exhibited blue to green fluorescence, a parameter that can be further explored for the efficient monitoring the inter-cellular pH levels and related cellular changes. (*New J. Chem.*, **2021**, *45*, 8775–8785)



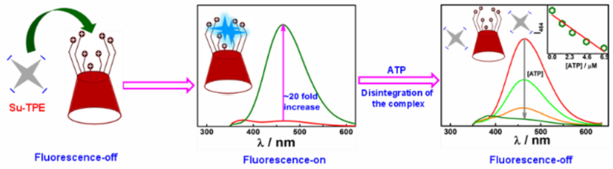
pH-Controlled Supramolecular Self-Assembly of Naphthalene Diimide Appended L-Alanine and Ethylenediamine Asymmetric Bolaamphiphile

Design, synthesis and characterization of novel (R)-2-(7-(2-aminoethyl)-1,3,6,8-tetraoxo-7,8-dihydrobenzo[lmn][3,8]phenanthrolin-2(1H,3H,6H)-yl)propanoic acid (**1**) bolaamphiphile, which combine naphthalene diimide (NDI) appended with L-alanine at one end of imide and ethylenediamine at other end. An L-alanine bearing NDI-based asymmetric bolaamphiphile self-assembled at various pH ranging from 2 to 10 forms a variety of supramolecular nanostructures. Experimental circular dichroism (CD) spectroscopy results inferred and revealed the induction of chirality into the supramolecular systems, which was shown to be pH dependent. (*Helv. Chim. Acta* **2021**, *104*, e2100011)



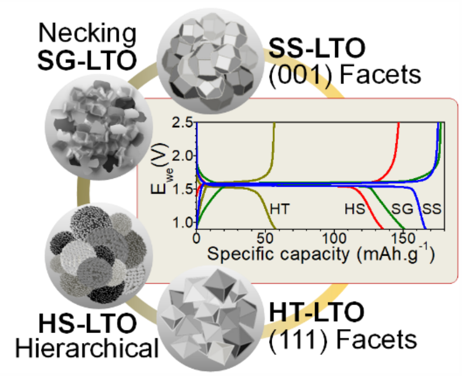
Host-Assisted Aggregation-Induced Emission of a Tetraphenylethylene Derivative and Its Responses Towards External Stimuli

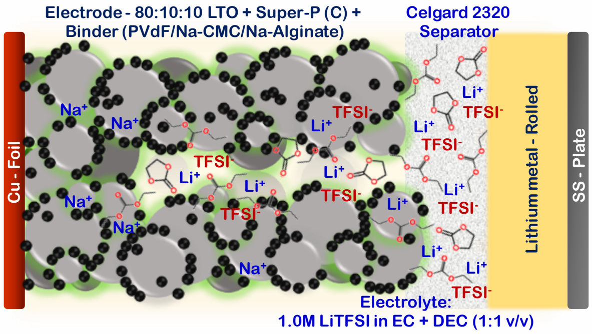
AIE of a polyanionicsulfonato-tetraphenylethylene (Su-TPE) derivative, achieved through non-covalent interaction assisted aggregation of the dye on its interaction with a multi-cationic amino-β-cyclodextrin (AβCD) derivative was studied. Studies indicate that AβCD induced aggregation of Su-TPE occurs mainly due to strong electrostatic interaction between Su-TPE and AβCD that causes significant charge neutralization for the polyanionic dye molecules supporting their stacking at the multi-cationic host portal. Job's plot studies suggest 2:1 dye to host stoichiometry for the complexes formed. The Su-TPE-AβCD system responds suitably to quantify the important bio-analyte, ATP, following a competitive binding strategy. (*J. Phys. Chem. B* **2021**, *125*, 11122−11133)



Polymer Electrolyte Integrated All-Solid State Li^+/Na^+-ion Rechargeable Batteries: Demonstrating Operational Feasibility

The polymer electrolytes are projected to address multiple issues related to device performance, factors such as relatively low ionic conductivity. The ability of polymer electrolytes to operate with highly reactive electrodes such as lithium over a wider temperature range without deterioration and electrolyte properties, the high interfacial electrode-electrolyte impedances are still major technological roadblocks. In recent years, a class of semi-Interpenetrating polymer networks as a promising system that supports fast ion conduction and appreciable electrochemical stability has been developed in our laboratory. The attempts also include probing the impact of nanostructuring the electrodes with controlled morphologies and role of alternate binders on the overall performance.

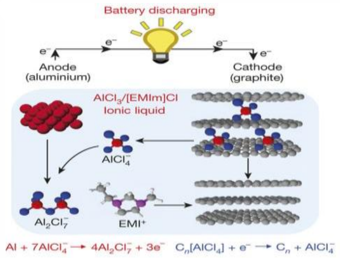


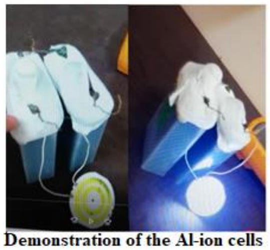


Rechargeable Al-ion battery

An aluminium based redox couple, which involves a three-electron transfer that occurs during the electrochemical charge/discharge reactions, provides a storage capacity that rivals that of the single-electron lithium-ion battery. Its relatively low atomic weight of 26.98 and trivalent state confer it a gram-equivalent weight of 8.99 and an electrochemical equivalence of 2.98 Ahg-1, as compared with 3.86 Ah g-1 for lithium. Because of its lower reactivity, easier handling, and greater safety, an Al-based battery may offer significant cost savings and safety improvements over Li ion batteries.

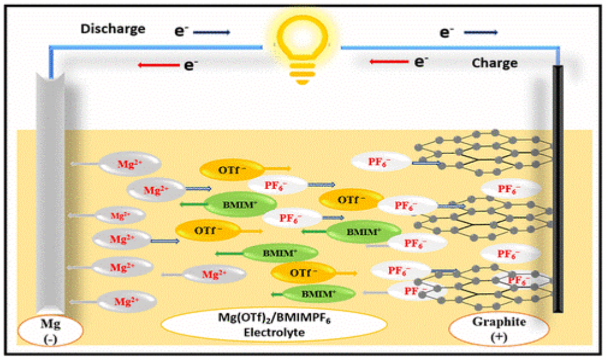
An aluminium based prismatic rechargeable battery with aluminium metal anode, graphite cathode and ionic liquid based electrolyte was developed and demonstrated.




Demonstration of the Al-ion cells

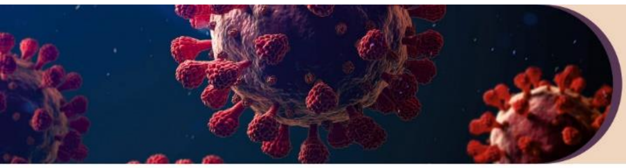
Phosphate-Based Electrolyte and Pristine Graphite Cathode for a High-Voltage Rechargeable Dual-Ion Magnesium Battery

The pristine graphite cathode and Mg anode magnesium dual-ion battery (MDIB) consists of a noncorrosive and nonvolatile electrolyte, i.e., 0.1 M magnesium trifluoromethanesulfonate (Mg(OTf)$_2$), in a 1-butyl-3-methyl-imidazolium hexafluorophosphate (BMIMPF6) ionic liquid. In the TGA analysis, the thermal stability of the electrolyte at Tonset 383 °C indicated its high stability. The electrolytes define a wide potential window until 4.65 V vs Mg/Mg^{2+} when measured on a Pt plate and were examined by the linear cyclic voltammograms (LSV) technique. The electrochemical analysis of the magnesium–graphite cell in the electrolyte showed defined sharp anodic and cathodic peaks that correlate the intercalation and deintercalation of PF6– anions through the graphite lamellar spaces in addition to the dissolution and deposition of Mg that occur at the negative electrode. The assessment of the charge–discharge analysis on the Mg–graphite cell showed a good capacity up to 51 mAh/g, retaining a 62% Coulombic efficiency that was sustained for >60 cycles. (*ACS Appl. Energy Mater.***2021**, 4, 5, 5165–5174).



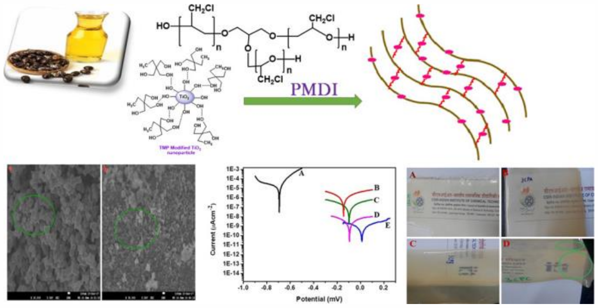
Antimicrobial polymers

Polyurethane cationomers carrying hydrophobic alkyl groups as counter ions to the quarternary ammonium moieties are well proven for their antimicrobial activity. In the present study, N-methyl diethanolamine has been used as a chain extender to introduce tertiary amino groups into the backbone which upon further quaternization with alkyl halides (of varying chain length viz, C6, C8, C10, C12 etc) give ionomeric PUs. The materials were found to be thermoplastic i.e. they could be melt processed under heat and pressure. All the compositions exhibited antibacterial properties by not allowing the organisms to grow over it till 48h.



Surface Modification of TiO_2 Nanoparticles with 1,1,1-Tris(hydroxymethyl)propane and its Coating Application Effects on Castor Seed Oil-PECH Blend Based Urethane Systems

Surface modification of peripheral hydroxyl groups of TiO2 with trimethylolpropane (TMP) was successfully carried out and characterized. This hybrid material (TiO_2-TMP) was added in percentages to a polyol blend of castor seed oil (a renewable resource and nontoxic material) and poly(epichlorohydrin)-triol (PECH-triol) {a cross-linker}. After ultrasonication of the polyol blend with TiO2-TMP, through a one-pot synthesis, the mixture was made to react with polymeric 4,4′-methylene diphenyl diisocyanate (PMDI) using 4-Methyl-2-pentanone as a reacting solvent. The doped composites showed improved coating properties, especially PU-TiO2-TMP (1.0 wt%), which possesses the highest percentage of TiO2-TMP nanoparticle. (*Prog. Org. Coat.*, **2021**, 161, 106469)

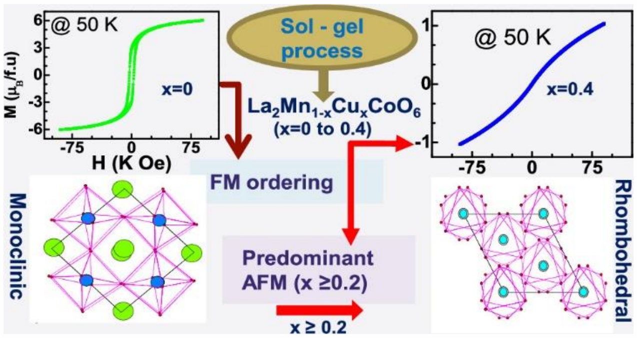


Hierarchical Nanostructures for Device Applications

Synthesizing semiconductor heterostructures (SHs) from viewpoints of improved band energetics in an optoelectronic device was demonstrated in Cao-ZnO systems. The formation of straddled (type II) band alignment in the CaO-ZnO hierarchical heterostructures and the valence and conduction band offsets in Ca-ZMS heterojunction were studied. The experimental and theoretical band alignment were correlated by XPS and UV-DRS analysis at the *n-n* nanointerfaces of CaO-ZnO heterostructure. The study of valence/conduction band offsets at the heterojunction and its correlation with potential barrier height is anticipated to provide supporting insights bound to enhance the quality of devices used in varied environmental applications. (*Materials Science and Engineering B*, **2021**, 265,115005)

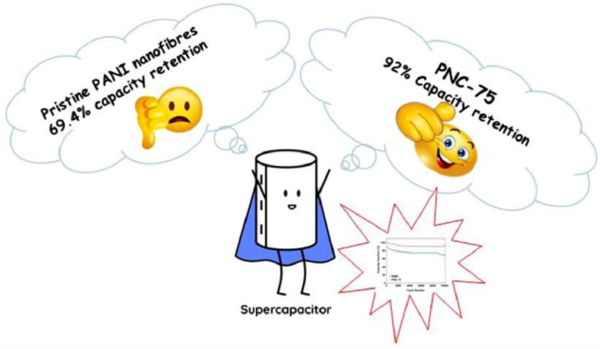
Double Perovskites Ln_2MnMO_6 (Ln: rare earth and M: transition metal) with Ferromagnetic Insulating Behaviour

The role of copper doping in double perovskite La_2MnCoO_6 is realized through the associated changes in structure, cation valence and magnetic state of the samples. Several antiferromagnetic (AFM) interactions are evolved at the expense of ferromagnetic (FM) interactions. The AFM interactions are developed at the expense of FM interactions which explain the observed magnetization in $La_2Mn_{1-x}Cu_xCoO_6$ ($0 \leq x \leq 0.4$). The results show that one can achieve the AFM state within the landscape of ternary cations of mixed valences which are fundamental ingredients of magnetic frustration due to randomness and competing interactions, though the frustration does not cease to exist completely. The study enriched the understanding of complex structural and magnetic behaviour of multivalent mixed cations-based perovskite oxides in the B-site. (*J. Phy. Chem. C*, **2021**,125, 5, 3088-3101)



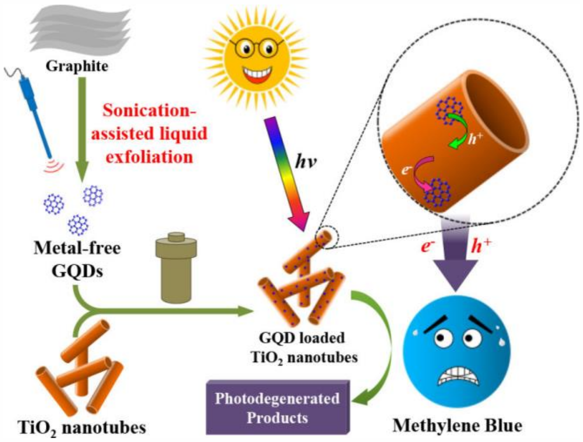
Development of PANI Based Ternary Nanocomposite with Enhanced Capacity Retention for High Performance Supercapacitor Application

Ternary nanocomposites using graphene, $CuCr_2O_4$ and polyaniline as potent electrode material is developed. A simple sonication-assisted mechanical mixing of pre-synthesized N-doped graphene, $CuCr_2O_4$ and polyaniline at varied proportions was carried out. The prepared composites have been analyzed by different characterization techniques to comprehend the successful formation of the composite. The electrochemical characterizations revealed that the nanocomposite shows the specific capacitance of 443.4 F g^{-1} at a current density of 1 A g^{-1} with excellent capacity retention of 92% even after 10,000 GCD cycles, thereby validating the fact that N-doped graphene and $CuCr_2O_4$ have enhanced the stability of pristine PANI.(*Electrochimica Acta* **2021**, 388, 138564)



Graphene Quantum Dots Decorated TiO_2 Nanostructures: Sustainable Approach for Photocatalytic Remediation of an Industrial Pollutant

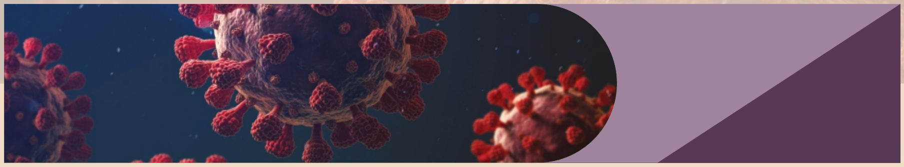
A novel metal-free graphene quantum dots/TiO_2 nanotube composite have been synthesized via facile hydrothermal technique for visible light assisted photocatalytic degradation of the industrial pollutant, methylene blue. The incorporation of only 2 wt% GQDs on TiO_2 nanotube effectively tunes the band gap of the composites which is capable of degrading 96.7 % of the dye within 120 min under visible light irradiation. (*ChemistrySelect*, **2021**, 6, 10957)



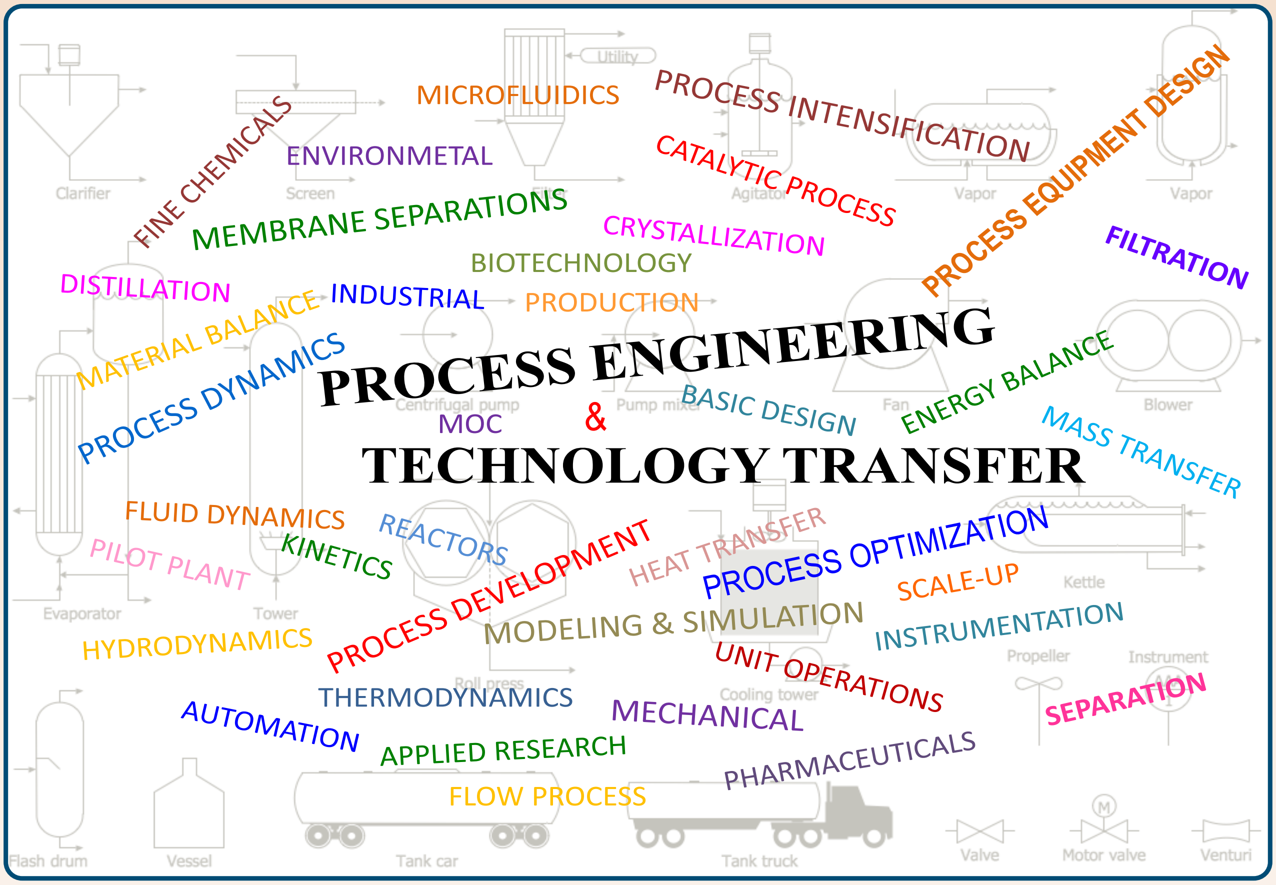
APPLIED RESEARCH

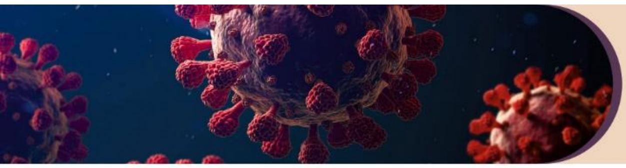
Centre of Excellence (CoE) on Polymer Coatings for Protective, Decorative & Strategic Applications

The CoE on Polymer Coatings has been conceptualized and designed to help and support the paint and related raw materials manufacturers specially the MSMEs and start up to act as a one stop facility to develop their product & processes including the testing, quality assurance and training facility. The focus will be on supporting them in the decorative and protective market segments where they have the major business. In addition, the CoE will support the strategic sectors for niche applications.



PROCESS ENGINEERING & TECHNOLOGY TRANSFER





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BASIC RESEARCH

Kinetic Modeling of Liquid Phase Esterification of Acetic Acid with *n*-Butanol using Heterogeneous poly(*o*- methylene *p*-toluene Sulfonic Acid) as Catalyst

Liquid phase esterification of acetic acid with *n*-butanol to *n*-butyl acetate is studied in the presence of a polymeric catalyst, that is, poly(*o*-methylene *p*-toluene sulfonic acid). Kinetic models are validated through additional experiments, and it is observed that the simple concentration based PH model is able to predict experimental data with least deviation compared to activity based PH, Eley Rideal (ER), and Langmuir Hinsel wood Hougen Watson (LHHW) models. The developed kinetic models are also tested using the Fisher Snedecor test (Ftest) and are found to be acceptable. By incorporating both modelling data and validation data, the overall absolute average deviations of different models are found to be: concentration based PH model 4.354%, activity based PH model 5.006%, ER I model 5.189%, ER II model 5.403%, ER III model 5.437%, and LHHW model 6.104%, illustrating the superiority of the simple concentration based PH model. (*Int. J. Chem. Kinet.*, **2020**, 54, 277-277)

Rational Design of High Power Density "Blue Energy Harvester" Pressure Retarded Osmosis (PRO) Membranes Using Artificial Intelligence-Based Modeling and Optimization

In this study, a data-driven approach has been adopted for designing optimum membranes as well as operating conditions. About 200 papers, from last decade, were extensively reviewed and 34 experimental research articles were shortlisted for possible data mining, to predict water flux (*WF*) and *PD*. Two artificial neural network (ANN) models were explored (i) Levenberg-Marquardt (*ANN-LM*), and (ii) Bayesian Regularization (*ANN-BR*) along with a combination of three different activation functions i.e., hyperbolic tangent sigmoid transfer function (*Tan-Sigmoid*), logarithmic sigmoid transfer function (*Log-Sigmoid*) in the input and output layers. Out of the six resulting combinations, the best performing combination was found to be *Tan-Sigmoid* activation function in both layers with *ANN-BR* model having an R^2 value of *0.97* for *WF* and *0.98* for *PD*. Membrane properties like the type of membrane, thickness, and water permeability coefficient were found to be the major contributing factors for the prediction of *WF* while for *PD*, operating conditions such as applied pressure were found to play the major contributing factor (10–16 %). Optimization results yield a maximum *WF* of 147 LMH and *PD* of 87 W/m^2. These results were compared with the solution diffusion (S-D) model. (*Energy Convers. Manag.*, **2021**, 253, 115160)

Iterative EKF as a Controller in Novel MPC Formulation: First Principles Model based IEKF-MPC for SISO Systems

A novel MPC control strategy, using first principles models and complete state information is formulated using iterative EKF as predictive controller. This is based on extension of iterative EKF control estimation concept to MPC, instead of solution of an optimization problem approach followed in conventional MPC. The performance of the proposed control strategy is evaluated through simulation case studies of SISO anaerobic digestion process and isothermal methyl methacrylate polymerization reactor with relative degree 1 and 2, respectively. The proposed strategy has shown superior performance over standard MPC in terms of faster response, set point tracking and disturbance rejection in both the case studies. The approach is found to be computationally efficient than the standard MPC. (*Comput. Chem. Eng.*, **2021**, 163, 107833)

Process Design, Modeling, Intensification, Simulation and Optimization Economic Assessment and Application of Bio-Composite Membrane in Microbial Fuel Cell

A novel cost-effective chicken feathers biochar (CFsBC) doped sulfonated polyethersulfone (SPES) proton exchange membrane was synthesized using solution casting and solvent evaporation method for microbial fuel cell application. The CFsBC was obtained through pyrolysis at different temperatures with an optimum yield at 550 °C. The addition of CFsBC to SPES leads to a reduction of 46% friction-free volume due to its increased packing density that ultimately disrupts the oxygen diffusion path. The low cost and high performance of BC membrane showed huge potential for its applicability in MFC operation for wastewater treatment. (*J. Environ. Chem. Eng.*, **2021,** 9, 106477)

Thermodynamic Measurements and Correlation of Properties for Tribromomethane

Experimental saturated vapor pressure data were measured using a Modified Swietoslawski-type ebulliometer and correlated with the Antoine, Clarke–Glew, and Wagner equations. A least root-mean-square deviation (RMSD) was obtained for the Antoine (0.667) and Wagner (0.796) equations while the group contribution and group interaction (GCGI) method by Nanoolal et al. showed an RMSD of 1.094. The estimated enthalpy of vaporization is found to be 46.87 $kJ \cdot mol^{-1}$ and 38.56 $kJ \cdot mol^{-1}$ at reference temperature (298.15 K) and normal boiling point (422.28 K), respectively. The critical properties and acentric factor are reported based on the GCGI method. Experimental density data are reported and are well correlated with the DIPPR 116 correlation with an RMSD of 0.00416. Joback's method predicted the densities well with a maximum absolute deviation (MAD) of 0.00548. (*J. Solution Chem.*,**2021**, 50,723-751)

Phase Equilibria and Thermo-Physical Properties of Dibromomethane: Measurement and Correlation Studies

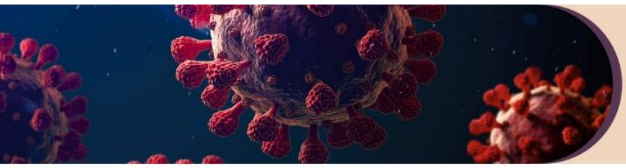
Halomethane (Dibromomethane) saturated vapor pressure was measured at the isobaric condition from 11.48–94.79 kPa using a Swietoslawski-type ebulliometer and well correlated with Antoine and Clark-Glew equations. The acentric factor-based Ambrose-Walton Corresponding states is found to be 0.339. Density is measured and correlated with a function of temperature (288.15–359.15 K). The critical parameters (based on different methods) with the Rackett equation were used to predict density and among them, Nannoolal parameters were able to predict the density with the lowest RAD of 0.05126×10^{-2}. (*J. Mol. Liq.*, **2020**, 306, 112917)

A Non-Edible Waste as a Potential Sorptive Media for Removal of Herbicide from Watershed

A non-edible waste, from biodiesel processing industry is being turned to 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. A multivariate optimization using central composite design was performed employing desirability function. (*J. Hazard.Mat.*, **2020**, 390, 121671)

Design of Oxygenated Microporous Adsorbent for Removal of 2,4,6-Trichlorophenol from Wastewater: Kinetics, Density Function Theory and Mechanism

An oxygenated rich functional biochar/adsorbent was prepared from a renewable source with its potential application for the adsorptive removal of 2,4,6-Tricholrophenol (TCP) from agricultural wastewater. The chemical oxidation showed an increase in single-bonded oxygen surface functional groups (OSFGs) in the moieties of phenolic and hydrolyzed products of lactones. The molecular dynamics simulation certifies the adsorption of TCP onto the adsorbent surface is through OSFGs present on the surface through chemisorption and the π–π interaction between aromatic rings. (*Int. J. Environ. Sci. Technol.*, **2021**, 1-18)



Optimization of Catalytic Hydrothermal Liquefaction Process Using Central Composite Design for Yield Improvement of Bio-Oil

Experiments were conducted with rice straw, glycerol and sodium carbonate as catalyst. The effect of temperature (220°C, 240°C, 260°C, 280°C), reaction time (15 min, 30 min, 45 min, 60 min), catalyst dosage (5wt%, 12.5wt %), biomass to water ratio (1:5, 1:10), glycerol to water ratio (0:10, 5:5) were done for evaluation of process performance in terms of yield and selectivity of bio-oil. Central composite design was further used to optimize the process variables and optimal operating conditions of 12.5 wt% of Na_2CO_3 at 260°C for 60 min at equal ratios of water and glycerol are established. The bio-oil on analysis revealed the constitution of ketones, alcohols, phenolics and aldehydes. (*Biomass Conv. Bioref,*. 2021)

Ultrapure Chemicals

Several experimental trials have been performed using a membrane process, resin treatment, and distillation techniques. For solvents, membrane process and distillation were tried. Membranes such as HPA-RO, polyether sulfone-based HFT, and HPA of 150, 250, and 300 Da MWCO were prepared and scaled up. Simple distillation of methanol and vacuum distillation of isopropanol and ethylene glycol showed considerable separation of metal ion impurities. In the case of alkalis, a combination of the above membranes and mixed bed resin (MBR) was attempted for the separation of metal ions being observed in the case of TMAH.

For acids, resins such as HCl resin HNO_3 resin, and H_3PO_4were used. However, vacuum distillation was found to be effective in the case of HCl for the separation of all four metal ions and to some extent half of the cationic impurities from H_3PO_4. (*J. Environ. Chem. Eng.*,**2021**, 9, 106125)

Development of a Mechanism for Fuel Cell Application

Synthetic polymeric aliphatic and aromatic membranes were prepared for the treatment of domestic wastewater. It showed high tensile strength, good resistance, and hydrolytic stability. A cost-effective and novel proton exchange membrane was prepared by blending proton–conductive SPPSU and PVDF blends. (*Renewable Energy*, **2020**, 146, 1262-1277; *Journal of Environmental Engineering*, **2020**, 146, 04020073-1-10)

Novel Membranes for Pervaporation; Hydrophilic Blend and Cross-Linked Membranes of Sodium Alginate and Polyvinylpyrrolidone

The membranes were prepared by mixing 6 % SA and1 % PVP in water at 300 rpm. Then, the membrane is cast on a glass petri dish and it is dried atroomtemperaturefor3days.The membrane is cross linkedwith0.1M$CaCl_2$ at room temperature for 24 h. These membranes can be used for the separation of acetone-water mixtures and other organic/water separations. Preparation of blend membranes of poly-vinyl-butyrate-CTFE copolymers: 4 % PVA was dissolved in dimethylformamide at 90-100 °C and 1% vinyl butyrate is added. After obtaining a homogenous solution the membrane was cast in hot conditions on a glass plate and then dried in an oven for 5-6 h at 40-50°C. The synthesized membrane was used for dehydration of ethylene glycol by pervaporation. (*Chem. Eng. J.*, 397, **2020,** 124050)

APPLIED RESEARCH

Integrated Membrane Bioreactor (IMBR) for Wastewater Treatment

Mixed microbial consortia: A mixed microbial consortium was isolated from a soil sample by serial dilution technique from 10 to 10^{-10} of the original concentration. The isolated mixed microbial culture from the soil sample effectively reduced the levels of pollutants and showed good efficiency in the degradation of pollutants as compared to single bacterial culture in the bioreactor process. The configuration is highly feasible for upscaling due to the easy availability of aerobic reactors of robust design as well as advanced versions of ultrafiltration and reverse osmosis membranes. (*Journal of Water*

Pollution & Purification Research, **2021,** 8, 31-36; *Journal of Industrial and Engineering Chemistry*, **2020**, *90*, 190-202; *Journal of Water Process Engineering*, **2020**, 37, 101436)

Treatment of UK Aromatic Multi-Effect Evaporator Effluent Using Reverse Osmosis

The study describes the treatment of multi-effect evaporator (MEE) condensate using the HPA HR RO membrane. The direct discharge of the wastewater into the ecosystem is a major concern for health issues because the water is contaminated by chemical and biological contaminants. Therefore, wastewater treatment depends on biodegradability, as a ratio of COD (Chemical Oxygen Demand), and total dissolved solids (TDS). This research deals with the treatment of wastewater through the HPA HR RO membrane at different pressures. (*Chem. Eng. J.*, **2021**, 412, 128598)

Environmental Management of Brine Discharge from Desalination Plants: A Zero Liquid Strategy of thermal Desalination Integrated with Crystallization

The current study is focused on the MLD (Minimum Liquid Discharge) and ZLD (Zero Liquid Discharge) options by integrating Crystallizer with MSF-OT (Multi-Stage Flash Once-through) consisting of 15 stages. The study considered different combinations of crystallizer with MSF-OT to achieve the maximum recovery of potable water and to study the thermal energy required by the system. Additionally, the thermal energy required for desalination of saline water was calculated for different salinities with MSF-OT. The results were compared with the minimum energy demand for desalination irrespective of the technologies and it was observed that there is an enormous gap between the numbers. Therefore, reducing the thermal energy is the challenging task which when overcome could be a better alternative to reverse osmosis membranes.

Design and Development of Hand-Operated Hollow Fiber Ultrafiltration Membrane Systems for Surface Water Treatment

A simple, inexpensive, novel high flux polymeric polyethersulfone ultrafiltration hand-operated membrane system that can run without electricity, is easy to operate, has high mobility, and is lightweight was developed. Designed and developed novel high flux polyethersulfone based hand operated hollow fiber membrane system for surface water treatment. The device produces potable water with a high flow rate of 700 LPH. A smart chlorine cartridge assembled in the system eliminates secondary contamination. The highly compact nature of the design enables its portability and easy installation in remote villages.

The developed membrane system is fully commercialized. (*Chemistry and Chemical Technology*, 14, **2020**, 239-250; *Applied Water Science,* **2020**, 230, **2020)**

Highly Compact and Inexpensive Membrane Electrolyzer for Production of Alkaline Ionized Water for Potable and Therapeutic Applications

Various membranes like Ultrafiltration 5, 50 kDa, and high flux nanofiltration membranes were synthesized using phase inversion and interfacial polymerization techniques respectively. An alkaline water ionizer with low-cost electrodes and highly selective indigenous polymeric HF-NF 300 AR membrane for producing 15-20 Lit/h of alkaline ionized water with a TDS of 250 – 350 ppm and pH of 8.5 to 10at 24 Vwas developed. The alkaline water produced from the ionizer applicable for drinking and biomedical purposes is cost effective.

Alkaline Ionized Water Electrolyzer

Design of a Mini Pilot Plant for Surface Water Purification Based on Ultrafiltration Hollow Fibers (100 LPH)

Hollow fibers prepared using Polysulfone (PSF) showed greater mechanical strength than Polyethersulfone (PES). The polyurethane-based resin was used for potting the ultrafine hollow fiber membrane modules instead of epoxy resin. The developed modules were evaluated with DM water for leaks and permeation. High-depth PTFE molds were fabricated and used to increase the sealing capacity. The model has uniflow membranes that have high flux and no reject outlets. For particulate filtration and suspended matter separation a 3-unit prefilter assembly (consisting of spun, sediment, and activated carbon cartridges) has been incorporated.

Simulation Study for Carbon Dioxide Hydrogenation towards Methanol using Single and 2 Reactor Configurations

This work describes the detailed study of steady-state simulation by Aspen plus for methanol synthesis by CO_2 hydrogenation using an equilibrium reactor. In the first configuration, methanol synthesis is carried out in a single reactor which resulted in CO_2 conversion of 30.43%. Another configuration considered is a two-reactor system with separation of products (methanol and water) continuously from each reactor at the outlet of the reactors using separator to increase the conversion of CO_2 towards methanol. It is observed that 53.2% of CO_2 conversion took place in this reactor system. The study showed that the formation of methanol is also more with continuous removal of products compared to the single reactor system.

Ibuprofen Crystallization: Effect of Cooling Rate on Metastable Zone Width

The objective of this study is to carryout unseeded cooling crystallization of Ibuprofen in ethanol and study the effect of cooling regime on the metastable zone width (MSZW) through induction time experiments. It is observed that MSZW increases with sharper cooling rates, whereas controlled slow cooling results in considerably small MSZW. Such study can form a basis for crystallization modelling that can be ultimately used for optimization and control purposes.

Surfactant Degradation using Hydrodynamic Cavitation-based Hybrid Advanced Oxidation Technology: A Techno Economic Feasibility Study

The treatment of surfactant (sodium dodecyl sulphate, SDS) laden wastewater using hydrodynamic cavitation (HC) technology was investigated. 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). Further studies were conducted using HC coupled with other oxidizing agents. Around 56% degradation was achieved in 1 hour using HC alone, which was further accelerated to more than 80% degradation using the integration approach. (*Chem. Eng. J.*, **2020**, 125599).

Degradation of Organic Micropollutants in Wastewater by Hydrodynamic Cavitation

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***. Considering 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. Studies similar to cavitation were performed on the degradation MPs with standalone ozonation. 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. (*J. Environ. Chem. Eng.*, 9, **2021**, 105652.)

Zero Liquid Discharge Strategy for Dye-Contaminated Water Streams: A Green and Sustainable Approach Using Hydrodynamic Cavitation and Vacuum Membrane Distillation

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 were used as the cavitating device in the HC reactor. Improvement in the performance of HC was carried out using hybrid schemes and the maximum degradation of 91.45% was achieved. (*ACS Sustain. Chem. Eng*., 9, **2021**, 6707–6719).

Design, Development and Performance Evaluation of Skid-mounted Pilot Wastewater Treatment and Resource Recovery Unit for Mechanical Scavenging Vehicle

The process is working on the principle of hydrodynamic cavitation + ozonation based oxidation process that can be implemented in various active areas of research including recovery of the valuable resources from the waste streams, dye degradation in the textile industrial effluent. The intense physical and chemical changes associated with the cavitation process with an intensified effect by integrating ozonation would address many such challenging water related issues. The process is also feasible to be integrated with chemical precipitation process for degradation of organics, reduction in COD and recovery of nutrient rich water for irrigation.

Cavitation Technique for Extraction of Pectin from Fruit Industries Waste

For higher extraction of pectin from the ground peels, deep eutectic solvents (DES) was used which can be considered to be green solvents as they can be reused, recycled and in turn reduces the chemical demand. The slurry consisting of water, DES and ground biomass was subjected to cavitation. Further downstream processes give the purest form of pectin in good yields with a minimal amount of chemicals.

Non-Thermal Sterilization of Tender Coconut Water

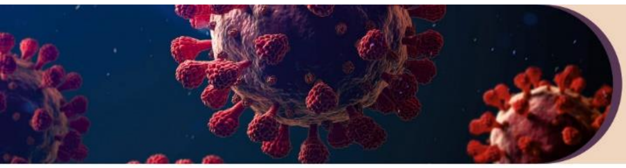
This work relates to the development of a technology based on hydrodynamic cavitation reactor alternative to conventional ultra-heat treatment for sterilization and preservation of liquid foods for conservation of the sensory characteristics, nutrition content and freshness of the food products at a reduced processing cost. The technology is applicable for processing a wide variety of fluid foods on a higher quality allowing for about 20% reduction in energy consumption.

Decolorization of Poly-tetrafluoroethene (PTFE)

PTFE being hydrophobic was dissolved in a solvent of choice and was cavitated for color reduction. Furthermore, several oxidation technologies were employed for the complete removal of color and improved aesthetic properties.

Adsorption: Packed Bed

Treatment of Real-life Washing Machine Streams: Cellulose Acetate based polymeric beads were prepared using phase inversion of polymeric drops in water bath. Extensive experiments to ascertain the practical applicability of the adsorbent using packed bed for COD and TOC reduction were carried out both as a batch process and as column studies as a function of contact time, solution pH (2-11), adsorbent dosage (0.5-5 g), bed height (6-10 cm), flow rate (10-50 ml/min) and temperature (293, 303 and 313 K). Results suggest that direct treatment with a



packed bed had a removal of 46.25 and 18.17% of COD and TOC, respectively.

Experimental Determination and Modelling of Co-Solvent and Anti-Solvent Behaviour of Binary Systems on Dissolution of Pharma Drug; L-Aspartic Acid and Thermodynamic Correlations

In this study, solubility of L-aspartic acid (L-ASP) in different binary mixtures (formic acid/ trimethylamine (TMA)/methanol/iso-propyl alcohol (IPA) + water) were carried out at temperatures from 283.15 to 328.15 K. Different thermodynamic models like Apelblat equation, Apelblat-Jouyban-Acree model, NRTL model, and general single model were applied to correlate the experimental data. It was found that Apelblat equation and general single model was the best-fit for correlating solubility of L-ASP in binary mixtures with average relative deviation (ARD) less than 2% and root mean square deviation (RMSD) are below 5.3E-04. It can also be concluded that formic acid and TMA act as co-solvent in dissolution of L-ASP in their respective binaries, whereas methanol and IPA exhibited anti-solvent effect in the aqueous solution. The generated SLE data would be helpful in technological research for production of drugs in purification and separation process (*J. Mol. Liq.*, **2020**, 314, 113657)

UNIFAC Predictions of Isobaric Vapor–Liquid Equilibrium Data for the Binary System of Dimethyl Carbonate+ Anisole at Different Pressures

In this work, isobaric vapor–liquid equilibrium (VLE) data for the binary system of dimethyl carbonate (DMC) (1) + anisole (2) at pressures of 33.33, 46.66, 59.99, 73.33, and 94.66 kPa were measured by using a Swietoslawski-type Ebulliometer. The binary VLE data are correlated by the NRTL and Wilson activity coefficient models, and binary interaction parameters are determined using Nelder–Mead simplex optimization method. The correlated results are in good agreement with the experimental data, liquid phase composition versus bubble temperature for both NRTL and Wilson models. A GC-based modified universal quasi-chemical functional-group activity coefficient (UNIFAC)–Lyngby (LBY) model is used to predict the binary VLE data of the present binary system. The predicted results are in reasonably good agreement with the experimental data, indicating that the selected patterns of group interaction parameters are valid for the present system. (*J. Chem. Eng. Data*, **2020**, 66, 3788-3801)

Salting-Out Assisted Liquid-Liquid Extraction (SALLE) for Separation of Morpholine from Aqueous Stream: Phase Equilibrium, Optimization and Modeling

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. 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. As the CO_3^{2-} anion shows more negative value of Gibb's free energy of hydration, ΔG_{hyd} than Cl^- revealed better salting-out ability of CO_3^{2-} ion. Further, the process parameters 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 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 (*J. Mol. Liq.*, 298, **2020**, 111884).

Development of Process for Production of Choline Hydroxide/ Choline Etchant

The overall objective of this project is to develop a suitable method for synthesis & purification of choline hydroxide and provide a basis for scale up to productionize the choline hydroxide. The method adopted for the synthesis of choline hydroxide, comprises of the direct reaction of TMA (trimethyl amine) and EO (ethylene oxide). The process is established at 1L & 2L scale reactor capacities with optimal process and operating conditions to achieve ultrapure grade choline hydroxide.

Experimental setup(a) 1L SS Reactor, and (b) 2L PTFE lined SS Reactor

Strategic Biorefinery Platform for Green Valorization of Agro-Industrial Residues: A Sustainable Approach Towards Biodegradable Plastics

The fractionation of tender coconut husks (TCH) to yield cellulose, hemicellulose and lignin fractions has been investigated by different pretreatment methodologies using conventional and novel reaction media. Excellent outcomes were obtained with the use of the deep eutectic solvent composed of choline chloride and oxalic acid dihydrate that led to the dissolution of 95.5% of the initial lignin in TCH to yield a cellulose fractional recovery of 87.5% at the optimal conditions attained by parametric variations. Interestingly, the same eutectic mixture also functionalized the obtained cellulose to cellulose nanocrystals (CNC) with 69% yield, crystallinity index of 88.6% and average particle size of 146 nm. Further, isolated starch from waste tamarind seeds was used as the polymer matrix wherein the CNC was added as a suitable bio-filler to cast bioplastic films using biodiesel by product glycerol as a plasticizer. The results elucidate that the huge dependence for petro-plastics could be reduced with the integrated valorization of solid wastes that can aid wide-ranging industries and align with the rising motto of a bioeconomy. (*J. Clean. Prod.*, **2021**, 290, 125184)

High proton conductivity dual modified ionic crosslink membrane for fuel cell application at low humidity condition with molecular dynamics simulations

Dual modified ionic cross-link polysulfone (PSF) polymer-based proton-conducting membrane is synthesized with an aim to provide low methanol permeability without sacrificing the proton conductivity for direct methanol fuel cell application. The modified membrane achieved a high proton conductivity of 0.072 Scm^{-1} (30 °C) and 0.178 Scm^{-1} (110 °C) in low humidity condition (40%). The membrane exhibits low methanol permeability (2.5×10^{-8} cm^2s^{-1}) with high selectivity (28.4×10^5 Scm^3s^{-1}). The higher diffusivity of hydronium ion (H_3O^+) with an increase in hydration level and temperature was studied by molecular dynamics simulation that agrees well with experimental results in terms of proton conductivity. The reduced electrostatic interactions between the sulfonic acid group and H_3O^+ ion were confirmed by the radial distribution function analysis. Moreover, the high interaction of amine group with H_3O^+ ion also contributes to the proton conductivity enhancement. The dual modified membrane achieved maximum power density of 0.19 Wcm^{-2} at 45 mA cm^{-2}, 42% higher compared to aniline treated polysulfone (APSF) membrane. (*Renewable Energy*, 2020, 160, 1036-1047)

Microporous Material Induced Composite Membrane with Reduced Oxygen Leakage for MFC Application

A novel composite membrane, with high proton conductivity and low oxygen diffusivity consisting 15 wt.% zeolite 4A incorporated in 2:1 blend ratio of sulfonated polyethersulfone (SPES) and polyvinylidene fluoride (PVDF) has been synthesized for energy generation. The membrane was found to have desired functional groups, with semi-crystalline nature, high thermal stability (490 °C), and uniform morphology. A maximum power density with high COD along with low oxygen diffusivity was obtained. The results showed that the K^+ cation has low oxygen diffusivity (4.50×10^{-8} m^2s^{-1}) with high H_3O^+ diffusivity (1.5×10^{-10} m^2s^{-1}). This result implies that potassium containing compound is more beneficial for the preparation of MFC solution, as K^+ cation shows the desired behavior required for MFC. (*J. Environ. Chem. Eng.*, **2020**, 8(5), 104117)

Design of a Mini Pilot Plant for Surface Water Purification based on Ultrafiltration Hollow Fibers (100 LPH)

Mini pilot plant of 100 LPH capacity with frontal, and lateral view

The consumption of surface water containing bacterial contamination and turbid substances ions causes various diseases such as gastrointestinal diseases. Ultrafiltration can be effectively used for clarification and disinfection of municipal water or surface water. The developed technology was deployed in rural areas in villages, schools, hostels, and small hamlets.

Design of Waste-Derived Affordable, Reusable, Washable, and Sustainable Multi-Layered Face Mask

A 3D design four-layered mask comprising a waste-derived PET was considered for the development low-cost, durable, high-quality multilayered face mask that can protect against virus and other pathogens. The waste-derived PET hydrophobic layer provides mechanical support to the mask and also barricades the particulate pollutants, bacteria and viruses from entering the respiratory tracts. The technology for production of protective multilayer facemask is commercialized and is now available in the market with the brand name "SaanS". The NGOs and Start-up have sold around 1 million masks to date across 20 States in India with employment generated for more than 500 senior citizens and self-help groups (SHGs)

Template of commercial SaanS mask

Ventilator

The designed emergency ventilator (EV) can control a patient's peak inspiratory pressure (PIP) and breathing rate while keeping a positive end-expiratory pressure (PEEP).

UV Disinfector

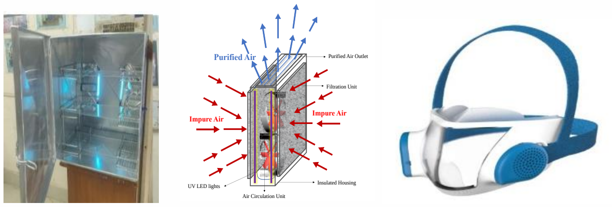
An UV disinfection cabinet prototype has been developed. Direct UV exposure is made possible through reflective surfaces and vertical light positions. The prototype is equipped with multistage transparent racks for uniform exposure and ease of use. An observation window is provided to avoid unwanted and direct exposure to the UV light.

Air Purifier

The compact domestic air purification unit enables low-cost purification of airborne pollutants, virus, bacteria, and particulate matter. Acoustic panels for noiseless operation and multi-layer filtration system with inline UV sterilization are incorporated in the compact unit.

Respiratory Device

A Portable Personal Air Purifying Respiratory Device with a centrifugal dual fan technology, equipped with 5-layered unit was developed. The device intakes ambient air through a frontal layer with 100% BFE. The heart of the Melt Blown PP layer filtration is 99.35% BFE and 99.5% PFE sandwiched between two nonwoven PP layers. The life of the battery withstands for 8-10 hours with an external power bank.



UV Cabinet, air purification unit, and respiratory device

Central Workshop Support to Grass Root Innovations across Telangana & Andhra Pradesh

5- Speed Power Tiller

An innovator from Khammam, Telangana came up with an innovation of 8 speed power tiller, and the institute provided support in the form of design of gear box for a 5-speed tiller. After due authentication of the design, the tiller was fabricated at the institute, and tested in the field, demonstrated to the innovator and the engineering drawings of the new designs were handed over to the innovator along with the costing of the product.

5-Speed Power Tiller Prototype

Hand Operated Multiple Brick Maker

An innovator from Guntur district, Andhra Pradesh (AP) developed a hand operated multiple brick maker. However, the innovation was not commercially viable. The institute worked on the operational issues that included re-designing the entire brick making unit considering cost of the unit while retaining the other features such as rate of production. A prototype was fabricated and was demonstrated to Palle Srujana team.

Low-Cost Hand Operated Multiple Brick Maker

Mastless Wind Mill

The coast line of Andhra Pradesh is full of salt fields and prawn farms which require lot of water pumping as part of its operation and maintenance. To mitigate the demand for power during water pumping, an innovator from Guntur District, AP, came up with an innovation of Mastless Wind Mill for harnessing wind power from sea breeze throughout the day. The institute designed a plunger pump that was fabricated and integrated into the newly designed prototype mastless windmill. It was installed at West Gogulapalli, Nellore District, AP.

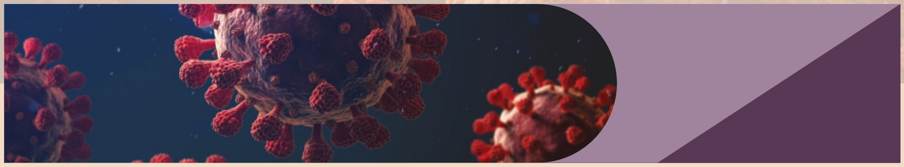
Mastless windmill designed, fabricated at CSIR-IICT and installed at West Gogulapalli

Facility Creation and Modernization of Pilot Plant

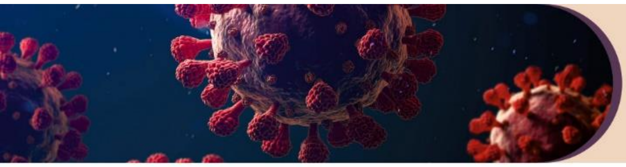
Up-gradation and modernization to facilitate safe and speed up technology transfer of pilot plant processes was initiated. Replacement of existing equipment has been completed. The state-of-the-art facility will help in scale up studies of the lab to commercial scale. Pilot plant is fully operational during COVID pandemic, and the works related to preparation of APIs such as dry potassium fluoride, an intermediate for preparation of covid drugs, demonstration of cinnamic acid of 1 kg batch and separation of solid and liquid were carried out.

Activities of Instrumentation Group

The instrumentation group is involved in Process control & automation (lab scale, pilot scale, interventions during technology transfer), Repair & maintenance of measuring & control equipment, instruments & utilities, Component of building renovation works, Comprehensive management of audio, visual & telephones systems. Major tasks include, hydrazine hydrate commercial plant at client site, agro mission kilo lab at PPC Moula Ali, upgradation of PP-II and 2G bio ethanol.



BUSINESS DEVELOPMENT & RESEARCH MANAGEMENT



BUSINESS DEVELOPMENT & RESEARCH MANAGEMENT

BASIC RESEARCH

The Business Development and Research Management Division is the Institute-Industry-Societal Interaction Facilitation wing. The division aims to promote expertise and capabilities of the institute, enable technology/ know-how/licensing to industry and cater to societal needs. The department also coordinates and manages activities related to IPR, ISTAD, CSIR funded projects, CSR activities and skill development and capacity building programs.

The following encompass the major activities of the Division:

- Business Development and Management
- Project Coordination of CSIR funded projects
- Research Planning Activities
- Skill Development and Capacity Building Activities
- Intellectual Property Rights (IPR) Management and Awareness Activities
- Corporate Social Responsibility (CSR) initiatives
- International S & T Affairs - clearances for projects & foreign deputations of staff

Activities

Business Development

The department facilitates seamless interaction with industry and identifies R&D areas of collaboration that match the business interests of the clients, while addressing issues that appeal the society. To this end, BDRM works closely with the research groups and organizes Industry Interactive Meets. This industry outreach program, aims to facilitate one-to-one interaction between industry personnel and scientists of the Institute.

The core strengths of the institute classified under three major sectors - Pharma and agro chemicals; Catalysis and fine chemicals; and Energy & environmental - are mapped against prospective industries for building business. Connects with major associations such as 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.

Strategy for business development and marketing

Adopted a comprehensive and coherent strategy of business development for translating and valorising IP and non-IP protected knowledge and cater to the market's demand leading to financial self-sufficiency. Some of the initiatives in this direction are:

- **Co-opting BD Champions from Departments -** The BD champions would target clients in their specific sector and pitch in for knowledge transfer in their domain of expertise.
- **Engaging consultants for aggressive marketing** Identifying promising business and technological white spaces without prejudice needs professional help from outside organizations.
- **Campaigning Organisation's Strengths & Capabilities** – Promoted technologies (FTT's/MMP's – Low Hanging Fruits (LHF's)) and patent strengths at industry meetings to bring commitments from stakeholders both technical and financial.
- **Networking & Nurturing Start Up's -** Networking and nurturing the start-ups created by CSIR-IICT alumni and offering incubation to more applicants has increased the revenues through collaboration for analytical services in particular.
- **Customer-Friendly Business Models –** The contract options offered were simple, swift, flexible, transparent, and participative
- **Tapping Corporate Social Responsibility Funds -** Liaison with corporate houses to tap the CSR funds for deployment of socially relevant technologies and collaborate on R & D projects of mutual interest under CSR.

Business Management

The division provides an interface between management, R&D departments and user agencies such as industries (National and Overseas), government departments, public sector organizations to offer R&D services and contemporary technological solutions.

The division is also actively involved in marketing CSIR-IICT knowledge base and R&D capabilities to user agencies and prospective clients and plays a key role in catalyzing External Cash Flow (ECF) (Non-Grant-in-Aid projects) earnings of the institute, facilitating IP & technology transfer, tapping CSR funds and conducting skill development programs. The activity in turn enhances the image of the institute and catalyses its performance.

- Scientific framework of collaboration
- Conducting negotiations with industries for identifying and finalizing new research collaborations.
- Arranging Non-Disclosure Agreements for exchange of information.
- Preparation of financial estimates and present the financial aspects of collaboration to management and clients.

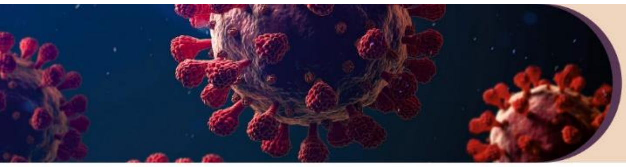
Drafting, negotiating and finalizing agreements for sponsored, consultancy, and collaborative projects with scientific, technical, Intellectual Property Rights, financial, administrative aspects of collaboration by coordination with clients and scientists.

- Obtaining necessary approvals from management, Management Council and CSIR Hq, wherever necessary.
- Facilitating 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.

Major activities 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.
- Facilitating prospective clients' visits and exploring new research collaborations by projecting R&D capabilities and expertise.
- Negotiating with Industrial Clients to Explore New Research Collaborations
- Facilitating interactions between management, scientists and industrial clients to finalise the
- Raising of tax invoices against the testing services offered to clients.
- Preparation of tax e-invoices against the samples received for sampling and analysis of Coal and forwarding to clients.
- Follow up with clients for release of due payments
- Preparation of receipts with calculation of GST, TDS, GST-TDS etc., and forwarding to the Department of Accounts for lodgement in respective projects
- Reconciliation on daily basis – Invoice(s) raised *vis-à-vis* payment released
- Accounting of ECF of all receipts from industry
- Coordinating GST payments with the accounts department
- Attending audit queries related to industry projects whenever necessary.
- Facilitating vendor registration forms, receipts and TDS forms with clients

Information support to C-DIS (CSIR-Data Infographics System) portal of CSIR Hq



Business Development and Management Efforts at a Glance:

Sl.No	BD Efforts	2020	2021
1	Technologies		
	- Developed	16	19
	- Transferred	16	19
2	New projects undertaken	49	74
3	MoU's signed	6	5
4	Industry Interaction Meetings held	29	56
5	Queries received	118	151
6	NDA's signed	36	34
7	Patents Out licensed	01	01
8	Non GAP ECF (Rs. Lakhs)	2167.7	4847.88

Best practices followed for Research planning

The institute has a tradition of viewing the challenges related to globalization, industrialization and competitiveness as opportunities to innovate and contribute to the vision of the Nation. Accordingly, the Institute revisits its focus-areas from time-to-time and constantly aligns them to meet the global demands with the aid of effective management strategies.

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) COVID 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

Commitment with individual targets: Specific goals and financial targets are assigned to scientists and technical staff for equitable distribution of responsibility to achieve the set targets.

Three tier project management with three teams a) Business team b) Technical team & c) Support team, for swift response, technical discussions and timely delivery so as to address the requirements of the clients on fast track mode.

Research Advisory & Project Implementation Department (RAPID) was constituted with a team of scientists covering all the research areas of the institute, who will provide advice and encourage scientists for submission of project proposals to CSIR and other funding agencies. RAPID also pools up the expert teams with requisite skill sets to meet the needs of the industrial projects and facilitates BDRM in addressing such project enquiries, and also helps in making collaborations with Academic institutions.

Mapping of Human Resources – Identified a pool of technical support staff for ready deployment of the HR based on the skill set required for the project that saves time on the process of recruitment or induction of HR.

Project Management of CSIR funded projects

with the committee of experts constituted 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 new R & D proposals as per the protocols of scrutiny by three-member committee and obtaining necessary approvals and liaison with Headquarters. 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 2020-21 & 2021-22

Project Type	Total No. of projects Handled in 2020-21	Total No. of projects Handled in 2021-22
Mission Mode	5	8
FTT	5	5
FBR	10	12
Covid	3	1
NMITLI	1	-
TKDL		2
Total budget released	24	28

Training Programmes under CSIR Integrated Skill Initiative:

The skill development programmes aim to create opportunities in areas of Chemistry, Chemical engineering and allied sciences for upskilling the talented youth so as to achieve better employment and entrepreneurial goals. The idea is to mainly improve the participants' confidence through skills and provide platforms for growth in all the related sectors.

As part of CSIR-Integrated Skill initiative, current programmes are focussed in providing Skill Development Training on Analytical Skill Development, Advanced Synthetic Organic Chemistry, Quality Control Chemist, Lab Technician – R & D, Basic Cheminformatics and Bioinformatics, Water Purification Systems and Analysis, Process Plant Drafting using Autocad, Basic Cell and Molecular Biology, Data Analysis etc. The department is identifying new areas of skill development as required by the industry so that placement for students can be guaranteed.

A total of 10 skill development trainings / programmes were conducted during 2021-2022 and around 413 participants benefitted. Out of these, majority of them have pursued higher studies (191), while some were benefitted in their career progress (208) and few of them (09) got employment opportunities.

Table – 2: SDP Details During 2020-21

Sl. /No	Sponsoring industry/ Govt agency name	Name of the course	From date	End date	No. of candidates trained
01	Advertisement, CSIR-IICT	International Virtual Training Program on "Generic Drugs"	19-11-2020	19-11-2020	84
02	Dissertation or Internship	Dissertation or Internship	01-04-2020	31-03-2021	65
			Total		**149**

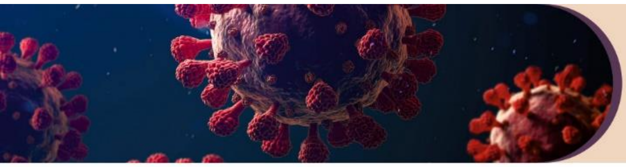


Table – 3: SDP Details During 2021-2022

Sl. No	Sponsoring industry/ Govt agency name	Name of the course	From Date	End Date	No. of candidates trained
01	Bhavan's College, Secunderabad	Certificate Course in Basic Bioinformatics and Cheminformatics (Online)	13-09-2021	24-09-2021	33
02	CRCL, New Delhi	Modern Methods of Chemical Analysis Including Spectroscopic & Chromotographic Methods of Analysis	27-09-2021 04-10-2021 22-11-2021 13-12-2021 07-02-2022 28-02-2022	01-10-2021 08-10-201 10-12-2021 24-12-2021 25-02-2022 11-03-2022	60
04	CSIR-Integrated Skill Initiative	National Level FDP on IPR for Academia (in association with CKBC College, Jorhat)	20-09-2021	25-09-2021	148
05	CSIR-Integrated Skill Initiative	Process Plant Drafting using Autocad	08-11-2021	03-12-2021	8
06	CSIR-Integrated Skill Initiative	Water Purification & Water Analysis	24-09-2021 22-10-2021 06-03-2022	24-10-2021 22-11-2021 05-04-2022	8
07	CSIR-Integrated Skill Initiative	Advanced Analytical Chemistry Training	04-10-2021	29-10-2021	12
08	CSIR-Integrated Skill Initiative	Advanced Synthetic Organic Chemistry Training	06-12-2021	21-01-2022	2
09	CSIR-Integrated Skill Initiative	Upskilling to Post Graduate students in Chemistry	01-01-2022	31-03-2022	21
10	Cipla Foundation	Orientation cum Skill Training programme to Post Graduate Students in Chemistry from North Eastern states of India	02-01-2022	31-03-2022	26
11	CSIR-Integrated Skill Initiative	Analytical Food Chemistry	21-03-2022 28-03-2022	23-03-2022 01-04-2022	21
12	Dissertation or Internship	Dissertation or Internship	01-04-2021	31-03-2022	74
Total					413

The R&D achievements 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.

Intellectual Property Rights (IPR) Management and Awareness Activities

CSIR-IICT is one of the leading IP portfolio holders in CSIR. During the last five years, it has demonstrated a significant increase in patent out-licensing thereby transforming it into an IP driven R&D institute. The department looks after IPR management, awareness and other matters relating to IPR including patents. CSIR-IICT also facilitates in commercialisation of patents and technology know-how. The major activities contributed by this wing are as follows:

i. IPR coordination & management (coordination between IICT, CSIR-IPU and attorneys/patent agents-both India & abroad)

ii. Coordination with CSIR-URDIP to obtain various IP services or to execute tasks related to Patinformatics (e.g. patentability assessment, patent landscaping, FTO/clearance search)

iii. Examination and applying for the approval of National Biodiversity Authority (NBA) for obtaining IPR using biological materials as per Biological Diversity Act-2002

iv. Execution of Access and Benefit Sharing (ABS) agreement with National Biodiversity Authority (NBA) for obtaining IPR using biological materials as per Biological Diversity Act-2002

v. Patentability assessment and preparation of search report of new patent proposals to place before IPR Management Committee before taking a call on filing by the Committee

vi. Assistance in drafting of patent specification and revising the Claims with techno-legal inputs as per prescribed rules

vii. This wing acts as IP MIS support for the institute to provide replies to the queries of various agencies and bodies seeking inputs through RTI, audits, parliament, PMO etc

viii. Providing additional IP support to the institute like portfolio assessment, rating/ranking, patent valuation etc

ix. Promotion of IPR/Patents & IP Commercialisation activities:

- Patent valorisation & negotiation and out-licensing
- Assisting/reviewing in preparation of various licensing agreements, MoUs, project proposals etc.
- Drafting of IP agreements for national and international collaboration/sponsorship

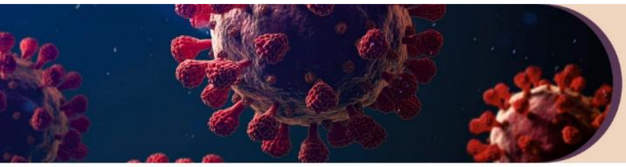
x. IPR awareness activities:

This department is also involved in various IPR awareness programs for the scholars and researchers in line with the coherent objectives of the institute and Govt of India. Having expertise in managing one of the highest IP portfolios among CSIR labs, various institutes approach the department for training and awareness on IPR, patent processing and management. In addition to other awareness initiatives, this department conducted a one week Faculty Development Program (FDP) in September 2021.

Corporate Social Responsibility (CSR) Initiatives and Management:

The Government of India through Gazette notification has allowed 2% of the net profit as Corporate Social Responsibility (CSR) funds to be contributed towards the incubators or the Public Sector undertakings of Central or State Government to conduct research in science, technology, engineering and medicine for promoting the Sustainable Development Goals. Additional resources for funding R&D projects at national institutions of eminence and excellence are now available collaboratively to boost the R&D investments in the country. CSIR-IICT welcomes corporates to invest their CSR funds in various R&D and related activities in the institute.

CSIR is registered under Societies Registration Act, 1860 with the Prime Minister of India as President and Minister of Science and Technology as Vice



President is the having u/s 12A certification of the Income Tax Act, 1961. CSIR has been approved under Section 10(23C) (IV) of Income Tax Act 1961 for assessment year 2010-11 onwards as implementing/Executing body. CSIR is eligible for CSR funding support from corporates under Section 13, Schedule VII of Companies Act, 2013 after the amendment dated 11th October 2019 vide gazette notification number G.S.R 776(E). Therefore, CSIR-IICT being a constituent laboratory of CSIR is eligible for CSR funding support from corporates.

Our focus area to collaborate with the industries primarily but not exclusively adhered with healthcare, eenergy environmental sustainability, food & nutrition, materials, specialty chemicals, fluoro & agro chemicals, capacity building aiming at promoting various Sustainable Development Goals (SDGs).

The department takes a lead role in tapping CSR funds, which mainly started at CSIR-IICT since 2020. The department conceptualises and prepares proposals in a synergistic manner in association with PI as per the prescribed provisions of CSR. This division executes the management, follow-up, drafting & negotiation of agreement, fund request, fund processing and monitoring of utilisation of the fund.

The following projects are executed under CSR funding during 2020-22.

S.No	Title of the Project	Sponsor/ Collaborator	Status
1	Develop the Multi-layered face mask model technology and to manufacture an inexpensive, washable facemasks with antimicrobial properties for the common man in villages under CSR Funds (Project SAANS)	Cipla Foundation (CF) C/o Cipla Limited, Mumbai. Ambuja Cement Foundation (ACF) Mann Deshi Foundation Help Age India Halo Medical Foundation	COMPLETED
2	Transfer of Mercaptan free Profenofos synthesis technology	Pesticides Manufacturers & Formulations Associations of India (PMFAI), Mumbai -400053	COMPLETED
3	Orientation cum training programme for MSc (Chemistry) Students from North Eastern States of India	Cipla Foundation (CF) C/o Cipla Limited, Mumbai.	COMPLETED
4	Development of video learning materials on (a) Bio-fuel cells and (b) Sustainable Energy For students of Class VI to XII	Kewaunee Labway India PVT Limited, Bengaluru.	ONGOING
5	Providing Sustainable access to High Quality Portable Water to communities using water from air kiosks through Atmospheric Water Generator (AWG) Technology	SEWA-THDC, Rishikesh	ONGOING

CSR initiatives of this division had shown its flying colour as an implementation agency by securing **CSR India Award 2021** from **Green Tech Foundation, India under the health care theme** for the Four-ply Face Mask Project with several innovative features useful in prevention of COVID-19. This award was received by Chair, BDRM along with other team members at Mahabalipuram, Chennai in December 2021.

Efforts made in other activities at a Glance:

Sl.No	BD Efforts	2020	2021
1	CSIR funded Projects undertaken	24	28
2	Digitization through CDIS Portal	133	165
3	Patents Filed & Granted	Filed India : 20 Granted in India :26 Total : 49	Filed Abroad : 29 Granted Abroad :24 Total : 50
4	Skill Development Programmes	2 Programmes 149 Trained	10 Programmes 413 Trained
5	No.of National MoUs signed	6	5
6	No.of International MoUs signed	3	1
7	No.of Sensitivity and Security Clearance for International Projects	3	3
8	No. of Monthly reports submitted to CSIR Hqtrs	12	12
9	No. Quarterly reports submitted to CSIR Hqtrs	4	4
10	No. of CSR projects undertaken	2	3

Snapshot

Favipiravir as Ciplenza developed by Cipla & CSIR-IICT

Adjuvant for Covaxin developed by BBIL with CSIR-IICT

CSIR-IICT has licensed an Indian patent on immune adjuvant to industry partner (M/s BBIL, Hyderabad)

Participants of Skill Development Training on "Analytical Techniques in Food and Nutritional Chemistry"

MoU with Yonsei University, South Korea

Come, join us to celebrate

FIRST YEAR ANNIVERSARY OF SAANS FACE MASK PROJECT

A unique collaborative initiative that is saving lives & livelihoods in Covid

WEDNESDAY, 11TH AUGUST 2021 | 3.00PM – 4.00 PM

ZOOM MEETING ID - 838 9619 2051 | PASSCODE - 654321

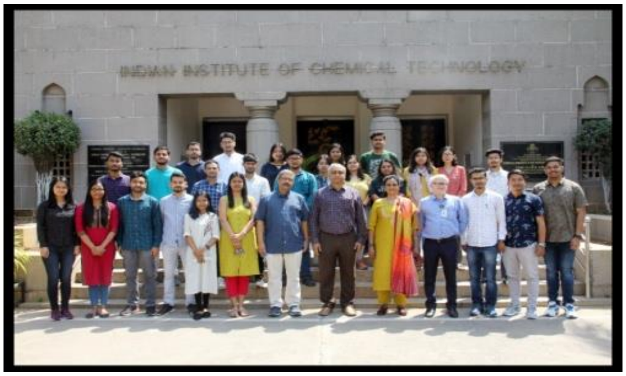
Click here to join

GUESTS OF HONOUR

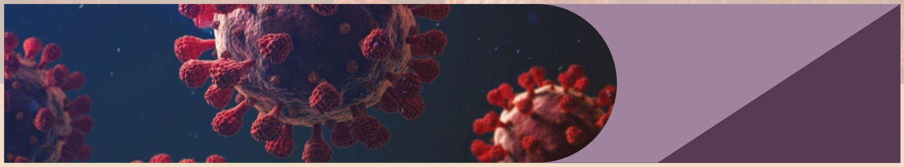
Dr Shekhar C Mande Secretary, DSIR & Director General, Council of Scientific & Industrial Research, New Delhi	Dr S Chandrasekhar Director, CSIR-Indian Institute of Chemical Technology, Hyderabad	Mr M K Hamied Trustee (Chairman) Cipla Foundation	Ms Rumana Hamied Managing Trustee Cipla Foundation

SAANS Mask project under CSR with CIPLA Foundation

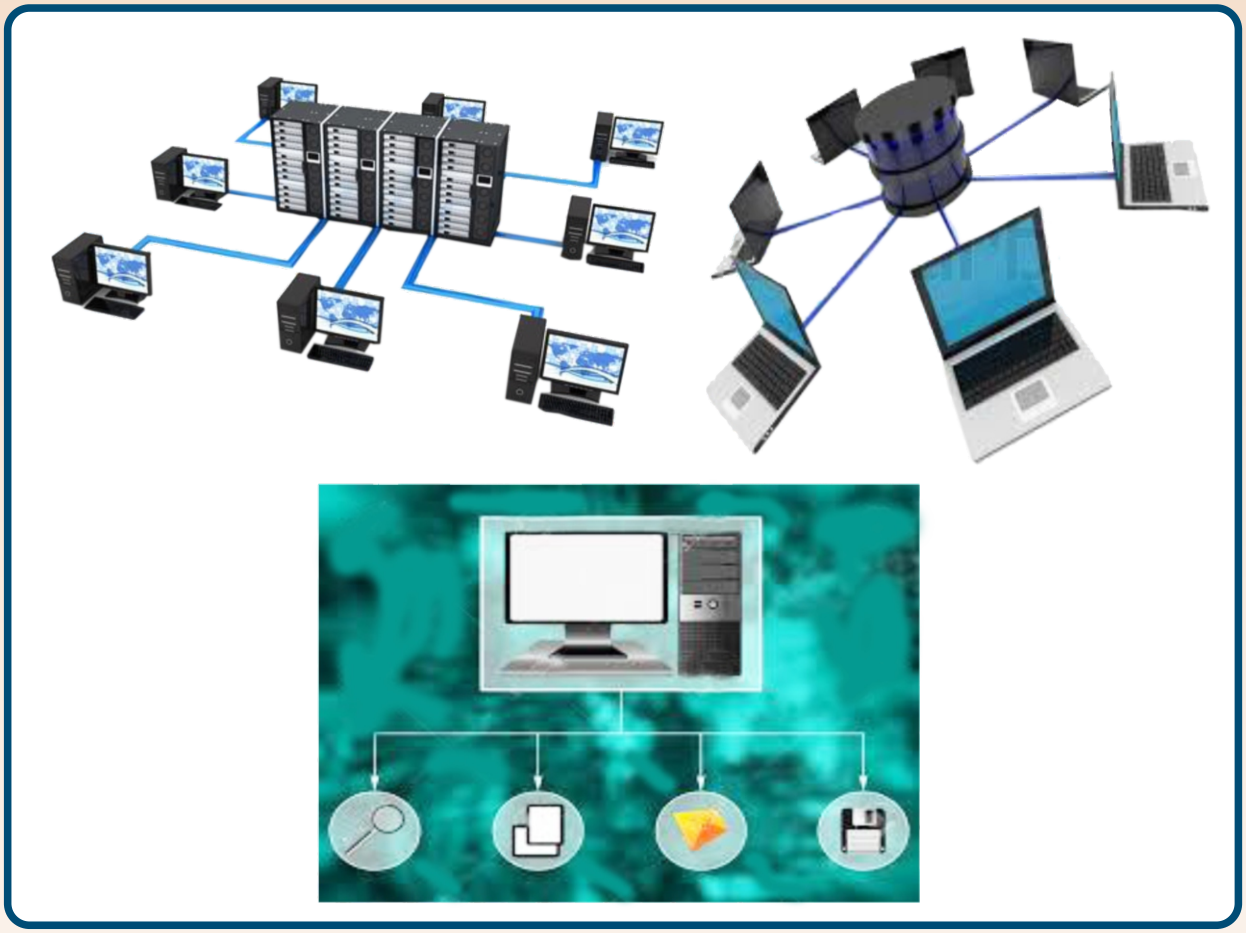
Participants of Skill Development Training to "CRCL Officers"



Participants of Orientation Skill Development Training for students of North Eastern states under CSR by CIPLA Foundation



CENTRE FOR IT SERVICES



CENTRE FOR IT SERVICES

The Computer Centre of IICT started in the year 1966 and is one of the earliest in CSIR Labs. It is the centralized resource facilitator for entire Campus. The main aim of computer centre is to provide IT enabled facilities for the ongoing R & D projects.

Keeping in view the major activities of the department in providing Internet enabled technical support services, the Computer Centre was renamed as **Centre of IT Services (CITS)** in 2020.

Vision & Mission:

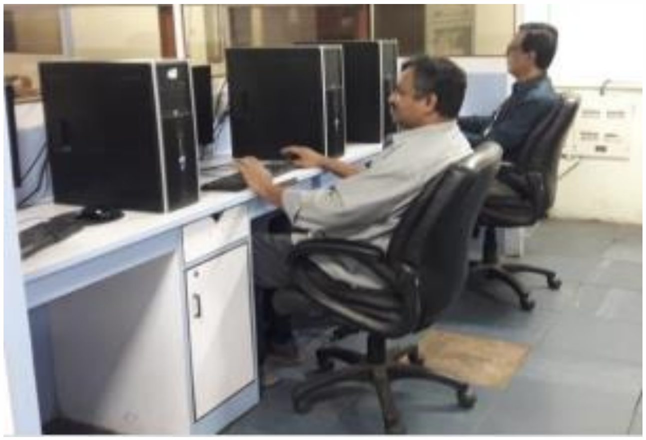
Vision:

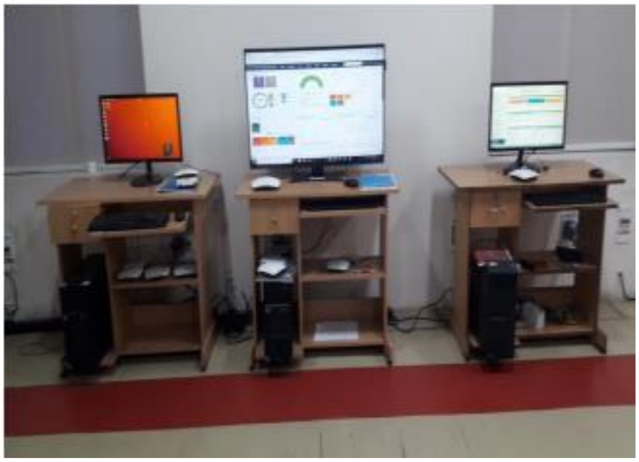
To establish a secure, reliable and high-quality Information Technology infrastructure to facilitate the scientists and research students in carrying out their Research & Development activities,

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. The NKN is designed and implemented by the National Informatics Centre (NIC), Department of Information Technology, Govt. of India, with 1 GB Network Bandwidth that interconnects leading Scientific and Technical Institutions across India was commissioned at IICT.

INFRASTRUCTURE FACILITIES: IICT has the following infrastructure to cater to novel research facilities in a 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 X65670 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

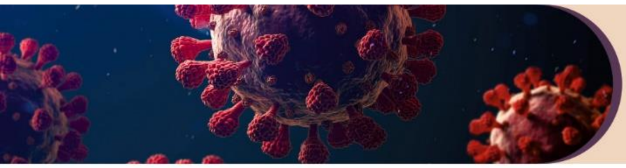
CORE COMPETENCIES:

- Security Management (UTM in High Availability, Servers, Clients)
- High Performance Computing
- Windows/Linux Server Administration
- Virtualization
- Database management: RDBMS: Oracle/MSSQL/ MY-SQL
- Syslog management for network devices
- ISPs: NIC/TATA Now this year IICT is planning for BSNL ISP also
- 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



- CCNET: an Intranet web portal for various maintenance modules/software installations/software patches/ general instructions etc.
- Adminsalchemy for internal circulars and OMs etc.

Support	Ongoing software projects
• Research Instruments IT support • NEERI Zonal lab IT support • MPDS: Molecular Modelling • Bio-Envis • Computational Chemistry • Software support for Admin Groups	• Implementation of e-Notebook, Chem-Draw Professional software • Online Recruitment Portal • Continuous Network vulnerability assessment

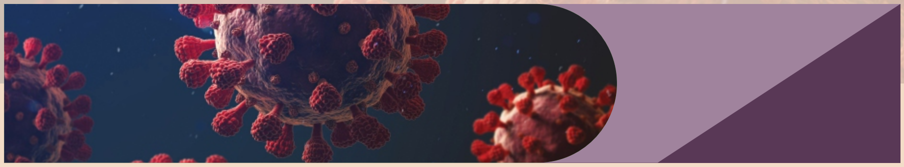
IT Services:

The Centre for IT Services is providing following services to the staff of the institute

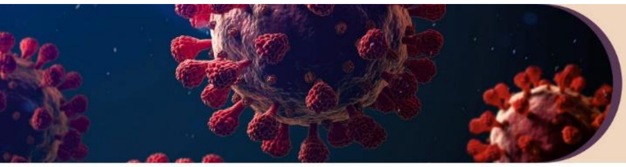
1. Information Technology support services like
    - VPN services
    - Virtual conferencing and meetings using MS-TEAMS, Zoom meeting services etc.
    - LIVE streaming of important events in social media applications like YouTube and Face book.
    - Campus wide CCTV network
    - Face-reading attendance system
2. Multimedia support services
    - Online/ Offline/ hybrid events
    - Video Conference/ virtual conference
    - Public Address System for meetings, seminars, workshops, conferences, etc.
    - Multimedia presentations
3. 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/ up gradation/ Hard Disk Error fixing
- Managing user e-mail accounts
- Personal folder management for user email accounts
- Providing service like HTTP, FTP, TELNET, VPN etc to Power Users
- All the client modules of Scientific Software implementation

Application Software Installation and User training



DEPARTMENT OF KNOWLEDGE & INFORMATION MANAGEMENT



KNOWLEDGE & INFORMATION MANAGEMENT

In the interest of the Institute's growth and to ensure better recognition and visibility, the Department of Knowledge & Information Management (DKIM) was created on February 1, 2018. The primary responsibility of the Department of Knowledge & Information Management (DKIM) is to ensure smooth functioning of research activities of the institute by providing reliable and secure information. The effective and transparent information assist in promotion, dissemination and exchange of knowledge.

DKIM is also associated with Human Resource Development and management which include facilitating temporary and permanent staff in the projects and other research work. New Project Proposals are forwarded to various agencies under the Grant-in-Aid (GAP) schemes for funding. Processing and monitoring of temporary manpower requisitions and their induction are checked and facilitated as per the requests of the respective principal investigators (PIs). 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 with internationally acclaimed reference collections in frontier areas of chemical, engineering and life sciences and plays a vital role in acquisition, organization, and dissemination of knowledge. The library is equipped with an impressive collection in both print and electronic resources, including books, journals, technical reports, standards, patents, theses and other materials supported by an adequate infrastructure. The main thrust of the library is continuous improvement of quality services and facilities to achieve higher degree of user satisfaction. Print holdings include books, dictionaries, handbooks, encyclopaedias, 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 inception i.e. 1907 and the same is now available online from January 2012 onwards. The Library's computer infrastructure is upgraded and user rooms are created to facilitate the usage of CD-Rom databases and browsing of E-Resources. Online databases and E-Journals are made available at the desktops of users. 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: SciFinder is a paid online database from American Chemical Society. It is a research discovery to explore CAS databases that contain literature from many scientific disciplines including biomedical sciences, chemistry, engineering, materials science, agricultural science etc. Thus, 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.

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, this information is available on CDs and from January 2012 onwards available online.

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: The patent database is available to the researchers namely Derwent World Patents Index through NKRC. It is searchable to give patent titles and abstracts using clear, descriptive, industry-specific terms and is made available at the desktops of users.

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 also get 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, users have access to multiple journals at their desktops.

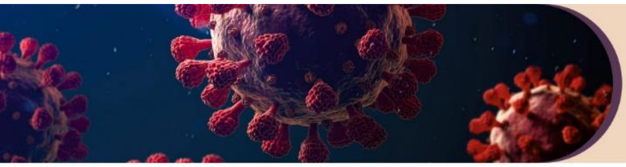
Library Home Page: Library Home page http://libdoc has also been designed and maintained, serving as one-point access to all the above mentioned E-Resources. The features of the page are enhanced by updating utilities from time to time.

Digital Repository (DRI): DRI is a digital archive of research output of the scientists at the institute. 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 are provided here. Publications from the year 1947 and bibliographic details of Ph.D thesis from the year 1945 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, PostgreSQL and Apache Tomcat on Linux OS. This Software has the facility to upload preprints by users themselves into the DRI.

Activities:

Scientometric analysis of research publications: Information on the bibliographical details along with the Impact factors of the research papers are regularly communicated to the management and CSIR-NIScPR for assessing the research output of the Institute there by assisting the top management in evaluating quality and quantity of research.

Archiving of Publications: It is essential to preserve the research outputs, and make it readily available for reference. Reprints of research papers are collected/ downloaded from source publications, indexed and bound into volumes and displayed in the library.



Services: The department 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 subscribers through the paid membership of the library.

Project Management & HR Management:

Scientists are informed about the announcement of calls for new proposals from various National and International funding agencies and timely submission of the proposals are facilitated. GAP proposals are processed following guidelines of the Institute and approval from 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 information related to the proposals is updated on "RMANET", an internal database. DKIM also maintains all the related documents of sanctioned, ongoing and completed GAP projects. Allotment of numbers to the sanctioned GAP projects and informed to the PI, Finance and Purchase departments for smooth management of the project. Preparation of utilization certificates/statement of expenditure, replying to audit queries on GAP projects, forwarding UCs and SEs to funding agencies is being done in coordination with Finance and Accounts apart from uploading scanned copies of UCs and SEs in PFMS and updating information in One CSIR.

Manpower requirements of GAP Projects are processed and coordinated with administration / PI. Deputation of Ph.D Students/Project assistants to attend Conference / Workshop under GAP Projects are processed in coordination with the PI. SRF applications are processed for Ph.D and Research Associate programs. Temporary manpower is requisitioned and their induction is facilitated 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.

Certificates are designed and issued to the students who complete their Ph.Ds and Projects (JRF, SRF, RA, NPDF, TWAS, Ramanujan, Ramalingaswamy and Inspire, etc).

GAP ECF for April 2020 – March 2022

	April 2020 – March 2021	April 2021 - March 2022
Projects	85	82
Fellowships	119	86
Amount (Rs. in lakhs)	2795.89	1732.52

Drafting of Agreements/ MOU's/MOAs for Academic and Joint Collaborations

The visibility of an institute is immensely enhanced by collaborations with other academic, research institutes and national and international universities of repute. The PIs are assisted in drafting and executing Inter-institutional and inter-disciplinary joint collaboration agreements between CSIR-IICT and other national universities and research institutions.

Event Management:

Weekly Lab Strategic Group (LSG) Meetings: On every Wednesday, LSG meetings are scheduled to review ongoing research projects. A calendar for two months is shared with PIs and a detailed confirmation is shared to the concerned PIs through mail. The meetings are conducted regularly on a fixed time and day. The project technical progress, project management, purchase, admin and finance issues are discussed and resolved. Course corrections if any are advised to the PI by Chairman and members.

Organizing Institutional Science Events: The department organizes Seminars, Conferences, Symposia's (National and International), Guest Lectures and Retirement events and also provides assistance to events that are organized by other departments. Correspondence with regard to Chief Guest lecture invitation, raising sanction order, approvals from competent authority, printing of invitation cards & posting them to retirees, universities, CSIR Headquarters, Directors of other CSIR institutes and also other eminent personalities are facilitated by DKIM. The department also makes arrangement of logistics. Arrangements are made for guided tours in the campus for 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 organized on the designated dates.

1. February 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

Awards Information:

The scientists of CSIR-IICT receive many Awards, Honors and Accolades throughout the year. Congratulatory notes are prepared to acknowledge the staff and students' recognitions and honors. In case of prestigious awards, press notes are issued for publicizing the achievement to the common people.

The department plays a key role in selection and announcement of the IICT annual appreciation awards and rewards for staff members and selection of the annual CSIR awards to meritorious wards of the staff members.

Documentations:

CSIR-IICT Brochure: A colorful, glossy brochure was prepared with pictures of the Institute and various instruments housed with persuasive notes attracting the attention of the potential clients with a view to boost the transfer of technology and knowhow.

Branding & Promotional Activities: DKIM takes active interest in preparing posters, brochures, handouts, periodicals, biennial reports, and social media posts including facebook and Twitter.

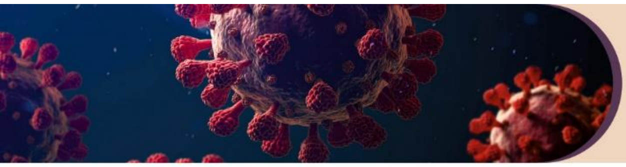
Press related Activities:

Branding and publicity of CSIR-IICT is a major function. The responsibility of projecting correct image of the institute and staff is of paramount importance. Besides, the public are informed about the R&D activities/achievements of our institute through various media platforms.

The efforts 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 the 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 R&D activities initiated in the institute and thus 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. The Director and concerned scientists interact with the media and disseminate information about their work.

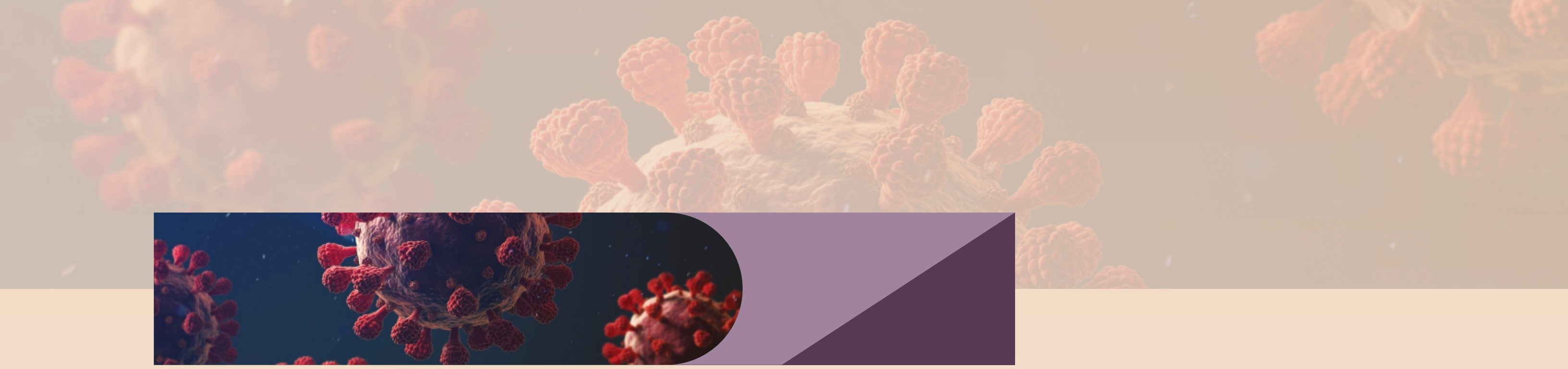
Press Releases, Content Generation: A press release details important points of the events held in the institute and it is shared to media houses for publication. There are two kinds of press releases – one is an after-event release, and the other is an announcement of awards, achievements of individual scientists and signing of MoUs and other related significant events of the institute. The after-event press release ensures that the information about the programme reaches various media houses. 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 the institute is projected correctly in the public platforms, and also gains visibility through special write-ups. In many instances, special articles are prepared on achievements of scientists and this is shared with the media for publication. Increased coordination with media personnel ensures that the articles are published promptly.

Coordination with Vigyan Prasar (DST): Another important step towards communication by the Institute is coordinating with Vigyan Prasar to disseminate activities of the institute reach to a wider audience. Work with Vigyan Prasar involves forwarding 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

HUMAN RESOURCE DEVELOPMENT



ACADEMY OF SCIENTIFIC AND INNOVATIVE RESEARCH

AcSIR | Academy of Scientific & Innovative Research

ACADEMY OF SCIENTIFIC AND INNOVATIVE RESEARCH

The AcSIR was established in 2010 (by a resolution of GOI on July 17, 2010) and formalized by an Act of Parliament *vide* The Gazette of India (dated February 7, 2012) which was notified on April 3, 2012 as an *Institution of National Importance*.

AcSIR has been set up based on a 'Hub and Spoke' model where hub (AcSIR-HQ at Ghaziabad) is responsible for centralized administrative functions. The spokes are located in the 45 CSIR Laboratories (AcSIR Academic Centres) and 12 non-CSIR Institutes (AcSIR Associate Academic Centres) spread along the length and breadth of India, which act as the academic campuses of AcSIR. In addition, AcSIR has collaborative academic programs with other national and international educational institutions. The AcSIR has been mandated to undertake high quality teaching and research in frontier areas of Science and Technology. This mission is to be achieved through AcSIR students, who are engaged in research in the broad areas of Biological Science, Chemical Science, Engineering Science, Mathematical & Information Science, Physical Science, and other Inter- & trans-disciplinary areas of study.

Currently, AcSIR has about 6000 Students enrolled in Ph.D, Integrated Dual Degree Program (M.Tech+Ph.D), Integrated M.Sc-Ph.D, M.Tech, M.Sc. and PG Diploma courses and about 3769 students have already graduated from AcSIR. Presently, AcSIR is ranked 2nd by "Scimago Institutions Ranking" (2021), 13th by "Nature index" (2020-21) and 22nd "NIRF (2021) in the Research Category, among the academic institutions in India.

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 2022, for Ph.D programme 914 students enrolled. About 157 scientists of CSIR-IICT, Hyderabad, are associated as faculty members in the disciplines of Chemical, Biological and Engineering Sciences.

AcSIR Functionaries:

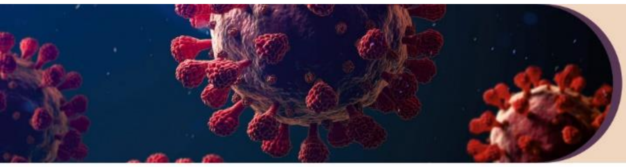
Dr. Ramanuj Narayan	Dean, Chemical Sciences (From January 2021)
Dr. Ch. Raji Reddy	AcSIR Coordinator, CSIR-IICT (from February 2016)
Dr. Pradosh P. Chakrabarti	AcSIR Coordinator, Designate (from February 2022)

- **STUDENTS ENROLLED FOR AcSIR Ph.D PROGRAM_SESSION WISE**

Discipline	August 2020	January 2021	August 2021	January 2022	Total
Chemical Sciences	30	15	20	25	**90**
Biological Sciences	04	08	17	10	**39**
Engineering Sciences	04	03	04	NIL	**11**
Total	**38**	**26**	**41**	**35**	**140**

- **NUMBER OF STUDENTS SUBMITTED Ph.D THESIS**

Discipline	Thesis Submitted April 2020-March 2021	Thesis Submitted April 2021-March 2022	Total
Chemical Sciences	59	36	95
Biological Sciences	17	20	37
Engineering Sciences	03	04	07
Total	**79**	**60**	**139**



- **NUMBER OF Ph.D STUDENTS AWARDED**

Discipline	PhD AWARDED April 2020-March 2021	Thesis Submitted April 2021-March 2022	Total
Chemical Sciences	43	34	77
Biological Sciences	19	11	30
Engineering Sciences	02	02	04
Total	**64**	**47**	**111**

- **COURSES OFFERED IN ALL DISCIPLINES**

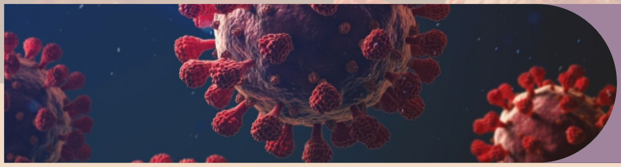
S. N	Course Code	Course Name
1.	BIO-IICT-1-0004	Research Methodology
2.	BIO-IICT-1-0001	Biostatistics
3.	BIO-IICT-1-0002	Computation/bioinformatics
4.	BIO-IICT-1-0003	Basic Chemistry
5.	BIO-IICT-2-2901	Biotechniques & Instrumentation
6.	BIO-IICT-2-2902	Chemical Biology
7.	BIO-IICT-3-2901	Seminar course
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

- **NUMBER OF PROJECT ASSOCIATE/SPA/NPDF ETC**

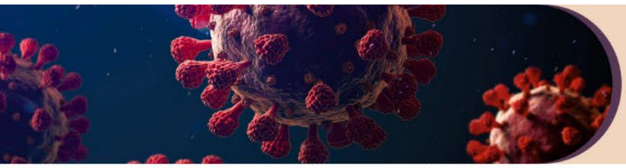
Category	2020-2021	2021-2022	Total
SPA/NPDF etc.	16	34	50
Project Associate	39	138	177
Total	**55**	**172**	**227**

- **NUMBER OF DISSERTATION/INTERNSHIP**

Qualification	2020-2021	2021-2022	Total
B. Tech	7	18	25
B. Sc	01	NIL	01
M. Pharm	28	07	35
M. Tech	05	14	19
M. Sc	24	47	71
Others (p)	NIL	09	09
Total	**65**	**95**	**160**



DISTINGUISHED LECTURES



DISTINGUISHED LECTURES

2020-22

- Webinar on "Mitigation of COVID-19: Testing, Drugs, Vaccines, PPEs & Self Hygiene". **June 12, 2020**

- Webinar on "Drug Discovery, Safety Gear for COVID-19". **June 15, 2020**

- Webinar on "Catalysis interventions for Green chemistry & sustainable development" by Dr. Darbha Srinivas, CSIR-Bhatnagar Fellow, CSIR-NCL. **July 24, 2020**

- Webinar on "Role of Biology and Chemistry in mitigating COVID-19". **August 27, 2020**

- CSIR Foundation Day Lecture by Dr. A. V. Rama Rao FNA, Former Director, CSIR-IICT, Founder Avra Labs. **September 26, 2020**

- International women's day Webinar on "Choose to challenge". **March 08, 2021**

- Panel discussion on "Campaign for COVID-19 Appropriate Behaviour and Vaccination" in Telugu. **April 28, 2021**

- "A.V. Rama Rao Technology Award Lecture" on "Peptide-based Palette in Chemical Biology and Structured Materials: Approaches for Chemical Neuroscience, Stem Cell Engineering, and Applied Coloration" (virtual mode) by Dr. Sandeep Verma Secretary SERB, New Delhi. **May 11, 2021**

- "A. V. Rama Rao Young Scientist Award Lectures" by Dr. Chandra Mouleeswara Rao Volla, Associate Professor, Department of Chemistry, IIT-Mumbai & Dr. Pazhamalai Anbarsan, Associate Professor, IIT-Madras". **May 11, 2021**

- 79th CSIR Foundation Day Lecture-2021 by Prof. B. J. Rao, Vice-Chancellor, University of Hyderabad. **September 26, 2021**

As part of **AZADI KA AMRIT MAHOTSAV** celebrations, following online lectures were organized by virtual mode:

- Online Lecture of LS-SERIES on "Radiative impacts of black carbon aerosols on climate" by Dr. S Suresh Babu, Head & Scientist SG, Vikram Sarabhai Space Centre, ISRO. **October 05, 2021**

- Lecture on "Wi-Fi Security: Threats & Solutions" by Prof. Bheemarjuna Reddy Tamma, Dept. Computer Science Engg, IIT Hyderabad. **October 06, 2021**

- Lecture on "Sustainable Plastic Waste Valorisation" was delivered by (Padma Shri) Prof. R Vasudevan, Coordinator TCE ENVIS RP, Dean ECA and Professor, Thiagarajar College of Engineering. **October 08, 2021**

- Lecture on "National Strategy on Unified Blockchain Framework- Providing Trust and Transparency in Citizen Services" by Dr. BK Murthy, Senior Director & Group Head R & D IT, MeitY GOI. **October 11, 2021**

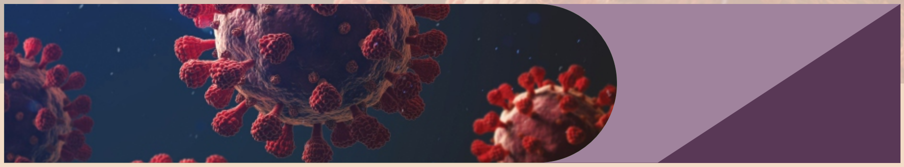
- Lecture on "Development of Nanocrystalline Materials with Exciting properties through Particulate Technologies" by Prof. BS Murty, Director, IIT Hyderabad. **October 11, 2021**

- Lecture on "Drone Technologies For Human Welfare" by Prof. Abhishek, Associate Professor, Dept. of Aerospace Engineering, IIT Kanpur. **October 18, 2021**

- Lecture on "BLOCKCHAIN: A Disruptive Technology for security beyond Cryptocurrency" by Prof. Naveen Chilamkurti, Head of Cyber security Discipline, Director, La Trobe University, Melbourne, Australia. **October 20, 2021**
- Lecture on "A Future Hydrogen Economy – Reality or a Pipe Dream?" by Dr. S. Srikanth, Formerly Outstanding Scientist CSIR and Director CSIR-NML Jamshedpur. **October 22, 2021**
- Lecture on "Process Modelling and Simulation" by Prof. Viswanathan Nurni Neelakantan, Professor & In-Charge, Centre of Excellence in Steel Technology, Dept IIT Mumbai. **October 26, 2021**
- Lecture on "AI/ML and Data Science - A Unified Theory "by Prof. Vadlamani Ravi, IDRBT, Hyderabad. **October 27, 2021**
- National Science Day lecture on "Excellence Towards S&T" by Prof. Vinod K Singh, Chair Professor, Department of Chemistry, IIT Kanpur, and former Director of IISER Bhopal. **February 28, 2022**
- International women's day Lecture on "Big potential in tiny bugs: From ailment to health & from waste to wealth" by Dr. (Mrs.) Sharmila Mande, Chief Scientist, TCS Research. **March 08, 2022**
- Delivered a lecture in Hindi on " महामारी से सीख और आगे की राह " (Lessons learnt from the pandemic and the way forward) by Dr Rakesh K Mishra, Director, Tata Institute of Genetics & Society (TIGS), Benguluru and formerly Director, CSIR-CCMB. **March 11 2022**

National Science Day Lecture by Prof. Vinod K Singh

International Women's Day Lecture by Dr. Sharmila Mande



CONFERENCES / SEMINARS / TRAINING PROGRAMMES/ WORKSHOPS

Conferences/Seminars/Training Programmes/Workshops Organized by CSIR-IICT

2020-22

- Virtual Training Program to NAM Countries 12 -countries participants on "Development and use of genericdrugs & Popularize the Use of Generic drugs in the developing countries". **November 19, 2020**

- SCO-Young Scientist Forum organized in a virtual mode on "Developing a Roadmap for cooperation between the research institutions of the SCO member States in order to intensify the scientific and technical partnership for joint research of solutions to common challenges". **November 24-28, 2020**

- Ten days Skill Development Course on "Basic certificate course in Bioinformatics and Cheminformatics" under CSIR Integrated Skill Initiative (online) for the Students of Bhavans Vivekananda College, Secunderabad. **September 13-24, 2021**

- The five week Training Program to the fifth batch of CRCL officers on "Chromatographic, Spectroscopic & Spectrometric methods of analysis". **October 01, 2021**

- Seminar on "Sustainable Technological Innovations in Engineering, Science and Management". **October 25, 2021**

- Importance of "Science Popularization" among school children and general public. (An outreach program at IICT ZM School as a IISF pre event) **November 27, 2021**

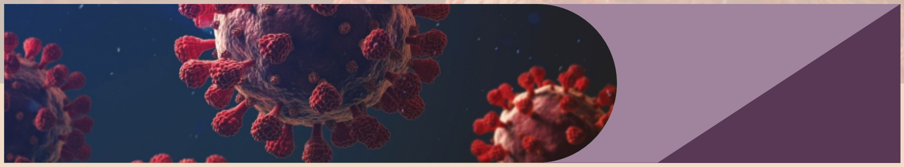
- A five week hybrid Training Course to the sixth batch of CRCL officers from ten CRCL laboratories across India on "Modern methods of Chemical Analysis including Spectroscopic & Chromatographic Methods of Analysis". **November 22 -December 24 2021**

- A five week hybrid Training Course to the seventh batch of CRCL officers on "Modern methods of Chemical Analysis including Spectroscopic & Chromatographic Methods of Analysis" **February 07 -11 March 11, 2022**

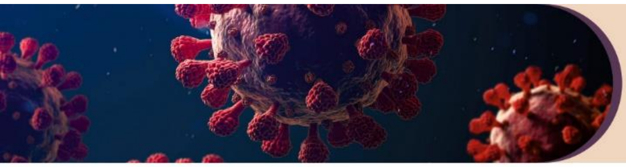
- The On-Campus "Orientation cum Skill Enhancement Program" for the M. Sc. (Chemistry) students from the North Eastern States sponsored by Cipla Foundation**. March 16-31, 2022**

Seminar Lecture by Dr. Nirmalya Bagchi

Training Course for CRCL officers



Awards & Honors



AWARDS & HONORS

2020-2021

Name of the Awardee (s)	Prize/Award/Honor
CSIR-IICT	Best Institute Award in New Generation Ideation Contest-2020
OSPC Division	Golden Peacock Innovative Product/Service Award (Team award)-2020, for the contribution of technology for Hydrazine Hydrate (HH), by IOD Global
Dr.S.Chandrasekhar; Dr.Prathama S. Mainkar; Dr. Ch. Raji Reddy; Dr. P. Nagender	CSIR Technology Award for Life Sciences-2020
Dr. Alka Kumari	IEI Young Engineer Award-2020 by Institute of Engineers India, Telangana Centre
Dr. Chittraranjan Patra	Editorial Board Member of Biomedical Materials & MedComm
Dr. L. Giribabu	Fellow of Royal Society of Chemistry (FRSC)-2020
Dr. Mohana Krishna Mudiam	Fellow of A.P. Academy of Sciences - 2020
Dr. Pradosh P. Chakrabarti	Prof. J. G. Kane Memorial Award-2020
Dr. S. Prasanth Kumar	Associate Fellow of A.P. Academy of Sciences (APAS) - 2020
Dr. Prathama S. Mainkar	Best Woman Senior Scientist Award by Genesin of Educational Impressions-2021
Dr. Sistla Ramakrishna	Fellow of Telangana Academy of Sciences-2020; Editorial Board Member of Cardiovascular Toxicology
Dr. Rambabu Chegondi	AVRA Young Scientist award -2020
Dr. Ram Chandra Reddy Jala	S. D. Tirumala Rao Memorial Award by OTAI-2020
Dr. Ch. Raji Reddy	NASI- Reliance Industries Platinum Jubilee Award -2020; SynOpen Associate Editor -2020
Dr. Sumana Chakravarty	SERB- POWER (Promoting Opportunities for Women in Exploratory Research) Fellowship-2021
Dr. S. Sridhar	The ICI India Ltd. Award Excellence in Process or Product Development - 2020 by IIChE; SRISTI-GYTI Appreciation 2020; 10th CIPET National Award-2021; HPCL New Generation Ideation Award 2021 by HPCL Green R&D Center, Bangalore; ONGC Award 2021 from IIChE, Kolkata ; Eminent Scientist of the Year Award- 2021 from the National Environmental Science Academy (NESA)
Dr. Vineet Aniya	Amar Dye-Chem Award-2020 by IIChE

2020-2021

Name of the Awardee (s)	Prize/Award/Honor
CSIR-IICT	8th CSR India Winner Award for IICT's first CSR project on Face Masks Saans by Greentech foundation
Dr.S.Chandrasekhar; Dr.Prathama S. Mainkar; Dr. Ch. Raji Reddy; Dr.M.Mohana Krishna Reddy; Dr.N.Jagadeesh Babu; Dr. P. Nagender	CSIR Technology Award for Innovation-2021
Dr. Alka Kumari	Executive Committee (EC) member of the IIChE-Hyderabad Regional Centre 2021-2023
Dr. Nivedita Sahu	Dr. B. P. Pal Memorial Award 2021
Dr. Ramanuj Narayan	First Place in TECHBHARAT Hackathon 2021
Dr. S. Sridhar	Life Fellow, Indian Desalination Association-2021; Distinguished Alumnus by OUCT Alumni Association – 2021; 8th CSR India Award-2021 by Greentech Foundation; Fellow, RJS International Multidisciplinary Research Foundation- 2021; Lifetime Achievement Award in the field of Chemical Engineering Indian Glory Award 2022
Dr. P. Srihari	CRSI Bronze Medal-2021
Dr. V. M. Tiwari Director CSIR-NGRI and Director (Additional Charge) CSIR-IICT	Sir JC Bose fellowship by SERB (DST)-2022
Dr. S. Venkata Mohan	Dr.C.V.Raman Memorial Award-2020

80th CSIR Foundation Day

CSIR Technology Awards 2021

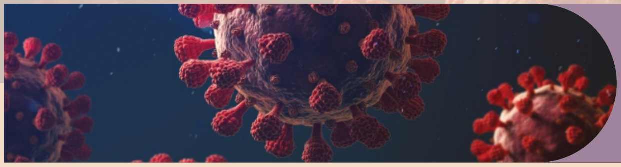
S Chandrasekhar, Ch. Raji Reddy, Prathama S. Mainkar, M. Mohana Krishna Reddy, N. Jagadeesh Babu, Punna Nagender

CSIR-Indian Institute of Chemical Technology , Hyderabad

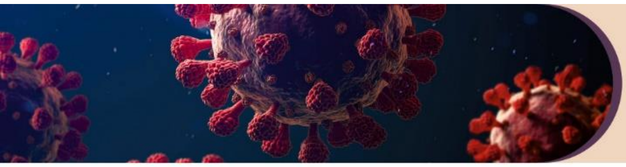
For developing a cost-effective and scalable process for the synthesis of TLR 7/8 agonist molecule (IMDG), used as an adjuvant in COVAXIN® (COVID-19 vaccine).

CSIR- IICT Team receiving CSIR Technology Award-2021

Dr. P. Srihari receiving CRSI-Bronze Medal



Other Events



OTHER EVENTS

2022

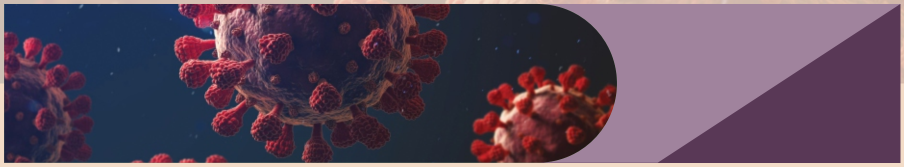
- Celebrated 74th Independence Day. **August 15, 2020**
- Conducted serological testing of antibodies against SARS-COV 2 in a first phase as part of CSIR cohort study initiated by IGIB, New Delhi. **September 4, 2020**
- Hindi Day Celebrations organised through MS teams with the chief guest Prof. Arun Kumar Tiwari, Scientist, Writer and Speaker. **September 16, 2020**
- Dr. Tamilisai Soundararajan, Governor of Telangana, visited the biogas plant set up at the Dr. B. R Ambedkar Vegetable Market Yard, Bowenpally. Technology provider, CSIR-Indian Institute of Chemical Technology (CSIR-IICT). **February 2, 2021**
- CSIR-IICT Post Card released at GPO, Hyderabad. **March 10, 2021**
- Organized World Tuberculosis (TB) Day. SaanS masks were distributed at the Gandhi Medical College and Hospital. **March 24, 2021**
- CSIR-IICT and Cipla Foundation distributed 1 Lakh Free Face Masks in Rural Telangana under Project 'SaanS'. **April 1, 2021**
- 7th International Yoga Day 2021 was celebrated at IICT. **June 21, 2021**
- CSIR IICT pavilion at Handlooms expo on the eve of National Handlooms day at People's Plaza, Necklace Road, Hyderabad. **August 7, 2021**
- Celebrated First Anniversary of the unique SAANS face mask project which was launched in partnership with Cipla Foundation and CSIR-IICT Hyderabad. **August 11, 2021**
- Fit India Freedom Run 2.0 to commemorate Azadi Ka Amrit Mahotsav was held at CSIR-IICT. **August 13-October 02, 2021**
- Celebrated 75th Independence Day. **August 15, 2021**
- A high level delegation from the Republic of Colombia visited to discuss technologies that may help in developing health programme in Columbia. **Sept 29, 2021**
- CSIR Jigyasa Virtual Lab inaugurated at Zilla Parishad High School, Chatakonda & Nava Bharat High School, Paloncha in Kothagudem, Telangana. **December 18, 2021**
- Dr V.M. Tiwari, Director, and staff felicitated Dr. Srivari Chandrasekhar on assuming charge as the Secretary, Department of Science & Technology, Government of India. **December 20, 2021**
- Acharya P.C.Ray Kilo Lab Facility at CSIR-IICT Moulali Complex, Hyderabad was dedicated to the Nation. Shri Jayant Sahasrabudhe, National Organising Secretary at Vijnana Bharati, unveiled the bust of Acharya Prafulla Chandra Ray at the facility. **December 25, 2021**
- Taiwanese delegation representing S&T Division of Taipei Cultural and Economic Centre (TECC), New Delhi, set up by the Ministry of Science & Technology visited. **February 17, 2022**
- The first Vision India@2047 Science Leaders Conclave at CSIR-IICT organized by Ministry of Science and Technology and Vijnana Bharati as a part of 75 years of India's independence celebrations – Azadi ka Amrut Mahotsav. Shri G. Kishan Reddy, Hon'ble Union Minister for

Culture and Tourism addressed on the concluding day. **March 26 & 27, 2022**

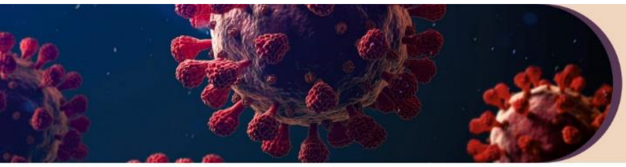
Dr.Tamilisai Soundararajan, Governor of Telangana, visited the biogas plant set up at the Dr. B. R. Ambedkar Vegetable Market Yard, Bowenpally

Inauguration of Acharya P.C.Ray Kilo Lab Facility at CSIR-IICT Moulali Complex, Hyderabad

Inaugural and Concluding Ceremony of Science Leaders Conclave at CSIR-IICT, Hyderabad



Staff List



STAFF LIST (AS ON 31/03/2022)

Chief Scientist
Dr. S. Chandra Sekhar
Dr. D. Shailaja
Dr. K. Yamuna Rani
Dr. K. Nagaiah
Sri. G.A. Raju
Dr. T. Shekharam
Dr. Sunkara V. Manorama
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Dr. A. Seshu Kumar
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Dr. B.L.A. Prabhavathi Devi
Dr. Pravin R. Likhar
Dr. Ashok Kumar Tiwari
Sri. Hari Shyamsunder Simha

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Dr. Shasi Vardhan Kalivendi
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Dr. Pavuluri Srinivasu
Dr. Sreepriya Vedantam
Sri. P. Anil Kumar

Senior Scientist
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Sri. S. Chandra Sekhar
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Dr. Ramesh Ummanni
Dr. Ram Chandra Reddy Jala
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Sri. Samuel L. Ralte
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Dr.Debabrata Maity

Scientist
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Dr. Arindam Chakrabarty
Dr. G.H. Gunasekar

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. K. Bhuvaneswari
Sri. Damodar Joshi
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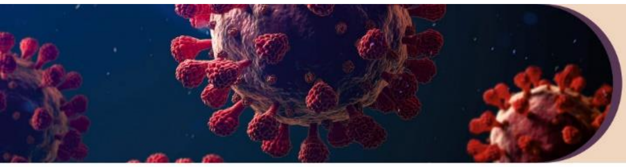
Sri. S. Srikamal
Sri. A. Radhakrishna



Sr. Superintending Engineer
Sri. P. Narayana Rao
Sri. Ch. Srinivas

Sr. Technical Officer (3)
Sri. S. Hemantha Kumar
Sri. A. Vishnu Vardhan
Dr. M. Syamala
Dr. Ch. Ramesh
Sri. K. Shiva Kumar
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Dr. B. Renuka
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Sri. Sunil Kumar
Sri. Arsid Niranjan
Sri. B.V. Devendra Rao
Ms. M. Preethi

Sr. Technical Officer (2)
Dr. Kuncha Madhusudana
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Ms. L. Kiranmayi
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Sri. P. Sivanarayanan
Sri. R. Boopathy
Dr. Rathod Aravind Kumar
Dr. Punna Rajendra Prasad

Executive Engineer
Sri. Mirza Mohd. Habeeb

Assistant Executive Engineer
Sri. D. Satish Kumar

Sr. Technical Officer (1)
Sri. K. Narsingh
Sri. P.V.S.S. Srinivas
Dr. M.G. Bhagya Lakshmi
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Sri. Chandrashekar Pendem

Technical Assistant
Sri. Amit Kumar Rajak

Sr. Technician (3)
Sri. J.V.S.N. Murthy
Dr. M. Shyam Sunder
Sri. P.V. Ravi
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Sri. B. Satyanarayana
Sri. Aziz Pasha
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Technician (1)
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Sri. Ganji Ashok
Sri. Jarupula Shankar
Dhanavath Venu
Abhilash G.R.
Prasanta Swain
Varun Pandit
Rajesh Jammana
Bobbili Hari Babu
Gulshan Kumar Gupta
Daripalli Srinivasa Rao
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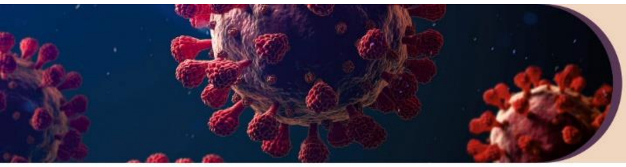
Ritanshi Kumar
V.K. Jaya Kumar
Amit Bhalkar Gurudeo
Ramteke Sujit Jaypal
Shamnad S.
Aditi Chaturvedi
Alok Kumar Yadav
Rohit Bamaniya
Samir Kumar Meher
Sangam Hari Krishna Sai
Merigi Somunaidu
Aqueeb Javed
Susanta Patra
Umesh R. Dasar
Ampolu Simhachalam
Bimagani Naresh Goud
Patlolla Mallareddy
Bandi Chaitanya
Ashirbad Mishra
Pyda Chandraseker
Nikesh Manjhi

Lab. Assistant
Sri. D. Narsing Rao
Sri. K. Sathyanarayana
Sri. J.Mallesh / Ramaiah
Sri. D.Gopalakrishna
Sri. Mohd. Odud / Md.Younus
Sri.Alimullah Khan
Sri. Md. Yousuf / Ismail Khan
Sri. K.Ramesh
Sri.Razak Ali / Sadiq Ali
Sri.Mir Mumtaz Ali



Sri. Gajula Sai Ganesh
Sri. Mohd. Ahemed/Akbar
Sri. C.Ganeshwar
Ms.Asghari Banu
Sri. G.Damodar
Sri.Mohd. Khaja Moinuddin
Sri. P.Ramulu
Sri. Mushtaq Ahmed
Sri. J.Venkatesh
Sri.Ghulam Taher
Sri. K.M. Eashwar Rao

Lab. Attendant (2)
Ms. B. Durga Bai
Ms. T. Padma

Controller of Administration
Smt. Sailaja Maddaly
Pradip Kumar

Controller of Finance & Accounts
Sanjeev Shekhar

Controller of Stores & Purchase
Sri. Uma Sankar Das
Sudhanshu Shekhar Choudhary
Shri. Dharmendra Kumar

Finance & Accounts Officer
A. Deenadayalan

Administrative Officer
Satish Kumar
Chandra Mohan Tudu

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Sri. Balaram Musunuri
Sri. G. Srikanth
Sri. S. Praveen Raju
Chandan Kumar
K.K. Saxena

Section Officer (F&A)
Dr. D.S. Sujatha
Shri. R.P.B.N. Kishore

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Ms. V. Jaishi Rani
Sri. R.R. Yadu Krishna
Ms. M. Saritha Kumari
Ms. D. Shamantha
Sri. P. Sailendra Rao

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Sri. Gattem Sainadh

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Sri. P. Shankar
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Sri. Praful Paswan

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Sri. Syed Shujat 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

Sr. Sec. Assistant (Gen)
Sri. Vellala Srinivas Karthik
Sri. Kalagatha Panidhar
Sri. Ulasala Jaya Prakash

Sr. Sec. Assistant (F&A)
Sri. T. Madhava Subrahmanya Kumar
Sri. Rakesh Doure
Sri. Thommandrula Suneel Kumar

Sr. Sec. Assistant (S&P)
Sri. Duduku Madhusudhan
Sri. G.L.S. Prasad

Jr. Hindi Translator
Shri. Aadrash Kumar

Security Officer
Sri. Dharmarao Kaspa

Staff Car Driver
Sri. B. Muralikrishna
Sri. B. Siddaramulu
Sri. P. Venkatesham

Assistant Halwai
Sri. E. Krishna

Coupon Clerk
Sri. M. Parushaiah
Ms. M. Swarna Latha

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Sri. M. Mohan Rao

Bearer (Canteen) (ACP)
Sri. K. Satyanarayana
Sri. M. Dasrath

Bearer (GH) (ACP)
Sri. Shaik Jahangir

Washboy/ Dish Cleaner (ACP)
Sri. M. Balaiah

Sweeper (Canteen)
Ms. C. Nagamani

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Ms. V. Sumathi
Sri. D. Rajesh
Sri. E. Arun Kumar
Sri. B. Mahender Kumar
Ms. D. Anuradha

Trainee
Sri. K. Rajasekhar

Farrash Gr. B (ACP)
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Farrash Gr. B
Sri. Shaik Ismail/Afzal

Safaiwala (ACP)
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Sri.Masood Ali
Mrs. K.C.Yesupadamma
Mrs. J.Laxmi
Mrs. A. Shashikala
Sri. D. Meghanath
Smt. M. Padma

ANNEXURES

PATENTS FILED IN INDIA & OVERSEAS

2020-2022

A Chemo-Enzymatic Process for the Preparation of (R)-2-Hydroxy-4-Phenylbutyric Acid Esters; **Application No.** 202111025039; 04-06-2021(IN)

A Chemo-Enzymatic Process for the Preparation of Eribulin Intermediates Thereof; **Application No.** PCT/IN2020/050533; 17-06-2020(WO)

A Chemo-Enzymatic Process for the Preparation of Eribulin Intermediates Thereof; **Application No.** 17/621052; 20-12-2021(US)

A Chemo-Enzymatic Process for the Preparation of Eribulin Intermediates Thereof; **Application No.** 2021-576357; 21-12-2021(JP)

A Continuous Flow Micro-Total Process System for Preparation of Celecoxib and Analogs Thereof; **Application No.** 20747897.5; 14-07-2021(EP)

A Continuous Flow Micro-Total Process System for Preparation of Celecoxib and Analogs Thereof; **Application No.**17/426906; 29-07-2021(US)

A Hydrodynamic Cavitation Reactor for Non-Thermal Sterilization of Liquid Food Products; **Application No.** 202011051434; 10-11-2021(IN)

A Nanoformulation for Glioma Treatment and Process for Its Preparation Thereof; **Application No.** 202111015505; 31-03-2021(IN)

A Nanoformulation for Glioma Treatment and Process for Its Preparation Thereof; **Application No.** PCT/IN2022/050317; 29-03-2022(WO)

A Process for Isolation of Saponinsuttroside B and Uttroside A from Solanumnigrum Linn; **Application No.** 202211028459; 17-05-2022(IN)

A Process for Mechano-Chemical Extraction of Vegetable Oil; **Application No**. 202010697429.6; 20-07-2020(CN)

A Process for Preparation Of 3 N-(3-((4-Amino-2-Butyl-1h-Imidazo [4,5-C]Quinolin-1-Yl) Methyl) Benzyl) -3,4,5-Trihydroxybenzamide, Intermediates and Derivatives Thereof; **Application No.** 202111052655; 16-11-2021(IN)

A Process for Preparation of 3,6-Dichlorocyano Pyrazine, 3,6-Dioxopiperazine Derivatives and Production of Favipiravir Thereof; **Application No.** 202011024682; 11-06-2021(IN)

A Process For Preparation Of 3,6-Dichlorocyano Pyrazine, 3,6-Dioxopiperazine Derivatives And Production Of Favipiravir Thereof; **Application No**. PCT/ IN2021/ 050571; 11-06-2021(WO)

A Process for the Preparation of Diamino Intermediates for the Production of Chloroquine, Hydroxychloroquine and Mepacrine Thereof; **Application No.** 202111047807; 20-10-2021(IN)

A Process for the Production of Dienes by Candida Sp; **Application No.** 202211022882 (IN)

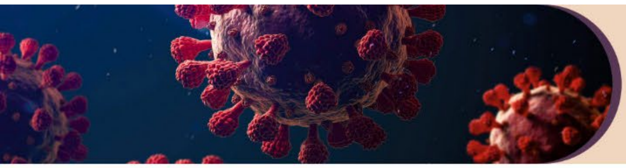
A Synergistic Formulation against Acne and a Process for the Preparation Thereof; **Application No.** 17/598105; 24-09-2021(US)

A Synergistic Formulation against Acne and a Process for the Preparation Thereof; **Application No.** 2020245333; 27-09-2021(AU)

A Synergistic Formulation against Acne and a Process for the Preparation Thereof; **Application No.** 20777202.1; 28-09-2021(EP)

A System and a Process for Simultaneous Removal of Ammoniacal Nitrogen and Oxidizable Carbon (Bio-Sac) From Wastewaters; **Application No.** 202111027593 (IN)

An Instantaneous Water Electrolyser and a Method for Ionizing Water; **Application No.** 202011028347; 03-07-2020(IN)



An Instantaneous Water Electrolyser and a Method for Ionizing Water; **Application No.** PCT/IN2021/050512; 26-05-2021(WO)

An Integrated Continuous Flow Machine Process System for the Synthesis of Daclatasvir Free Base and Analog Thereof; **Application No.** 202011024499; 14-08-2020(IN)

An Integrated Continuous Flow Process for the Preparation of Potent Inhibitors of Phosphodiesterase Type-5 [Pde-5] and Analogs Thereof; **Application No.** 202011029345; 08-07-2021(IN)

Anti-Inflammatory Compounds for the Treatment of Dermal Disorders; **Application No.**1189018; 20-11-2020(AR)

Anti-Inflammatory Compounds for the Treatment of Dermal Disorders; **Application No.** PCT/IB2020/061043; 23-11-2020(WO)

Anti-Inflammatory Compounds for the Treatment of Dermal Disorders; **Application No.** 109141014; 23-11-2020(TW)

Automated Diazomethane Generator, Reactor and Solid Phase Quencher; **Application No.** 202011036463; 24-08-2021(IN)

Automated Diazomethane Generator, Reactor and Solid Phase Quencher; **Application No.** PCT/IN2021/050811; 24-08-2021(WO)

Azirine Containing Compounds as Anti-Angiogenesis Agents and Preparation Thereof; **Application No.** 202011023422; 04-06-2021(IN)

Azirine Containing Compounds as Anti-Angiogenesis Agents and Preparation Thereof; **Application No.** PCT/IN2021/050544; 04-06-2021(WO)

Bimetallic Fluorescent Nanocomposites for Cancer Theranostics; **Application No.** PCT/IN2021/050215; 05-03-2021(WO)

Blue Emissive Nitrogen Doped Carbon Dots from Thevetiaperuviana; **Application No.** 202111044178; 29-09-2021(IN)

Catalytic Solvent and Stripping Media for Production and Purification of Furfural; **Application No.** 202111024754; 03-06-2021(IN)

Catalytic Vapor Phase Ammoxidation Process for the Preparation of O-Chloro Benzonitrile; **Application No.** 202111047811; 20-10-2021(IN)

Gem-Dimethyl Bicyclic [3.10] Proline Intermediate Compound and Production of Small-Molecule Inhibitor of the Sars-Cov-2 Main Protease Thereof; **Application No.** 202211019417; 31-03-2022(IN)

Hdac Inhibitors for Idiopathic Pulmonary Fibrosis; **ApplicationNo.**202011038497; 03-09-2021(IN)

Hdac Inhibitors for Idiopathic Pulmonary Fibrosis; **Application No.**PCT/IN2021/050851; 03-09-2021(WO)

Indole (Sulfomyl) N-Hydroxy Benzamide Derivatives as Selective Hdac Inhibitors; **Application No.** 18880632.7; 14-05-2020(EP)

Indole (Sulfomyl) N-Hydroxy Benzamide Derivatives as Selective Hdac Inhibitors; **Application No.** 2020/02786; 14-05-2020(ZA)

Indole (Sulfomyl) N-Hydroxy Benzamide Derivatives as Selective Hdac Inhibitors; **Application No.** 3082972; 19-05-2020(CA)

Indole (Sulfomyl) N-Hydroxy Benzamide Derivatives as Selective Hdac Inhibitors; **Application No.** 201880075426.X; 21-05-2020(CN)

Indole (Sulfomyl) N-Hydroxy Benzamide Derivatives as Selective Hdac Inhibitors; **Application No.** 2020117075; 25-05-2020(RU)

Indole (Sulfomyl) N-Hydroxy Benzamide Derivatives as Selective Hdac Inhibitors; **Application No.** BR 11 2020 010564-3; 26-05-2020(BR)

Indole (Sulfomyl) N-Hydroxy Benzamide Derivatives as Selective Hdac Inhibitors; **Application No.**16/767389; 27-05-2020(US)

Indole-Ynone Mediated Benzoannulation Process for the Preparation of Carbazoles- Carbazomycin A, Calothrixin B and Staurosporinone; **Application No.** 20783102.5; 22-09-2021(EP)

Indole-Ynone Mediated Benzoannulation Process for the Preparation of Carbazoles- Carbazomycin A, Calothrixin B and Staurosporinone; **Application No.** 17/442828; 24-09-2021(US)

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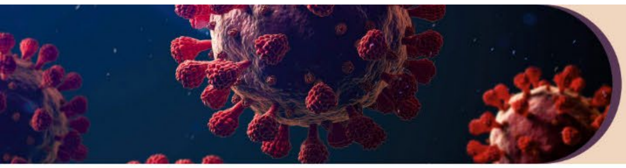

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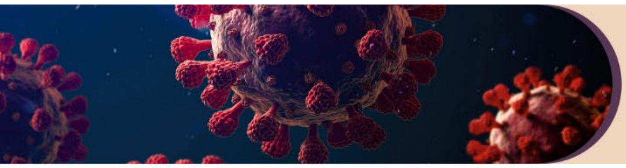

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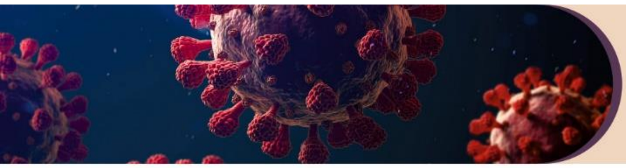

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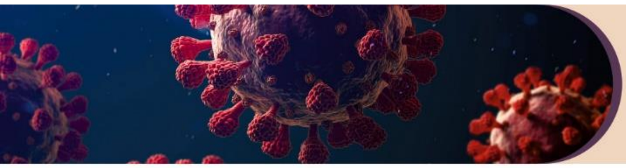

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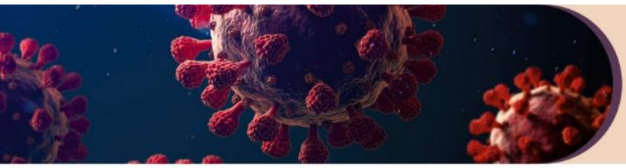

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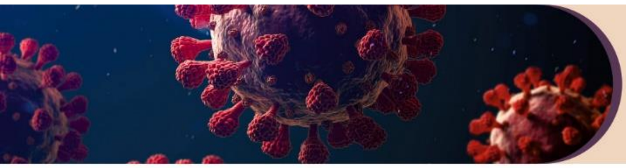

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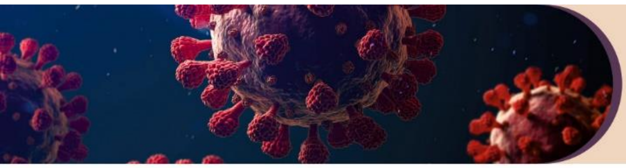

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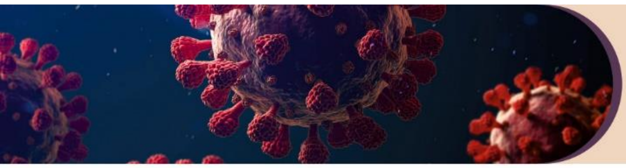

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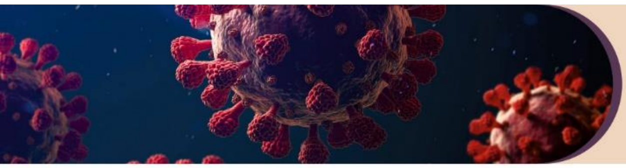

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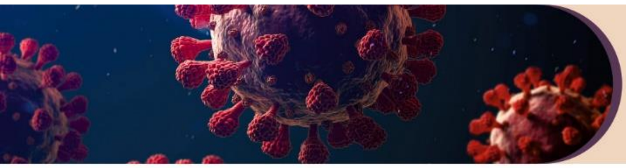

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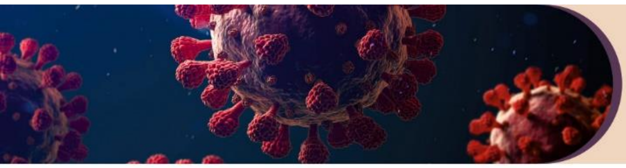

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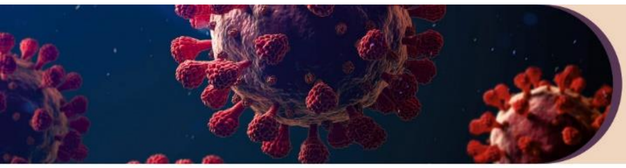

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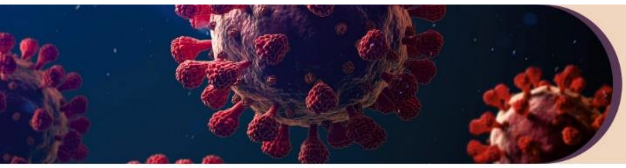

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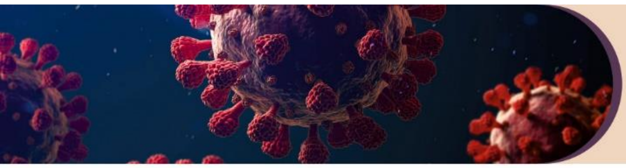

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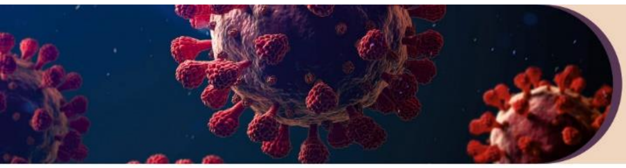

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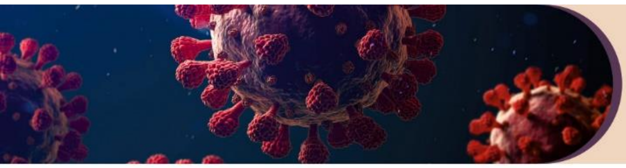

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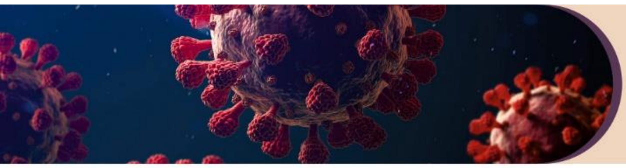

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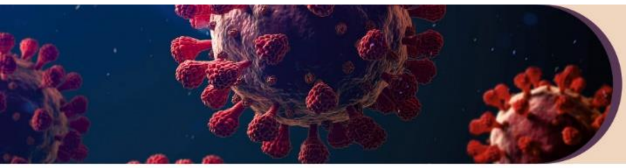

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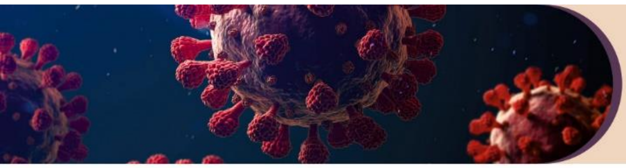

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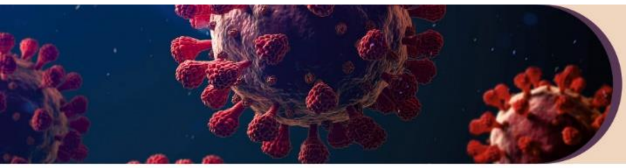

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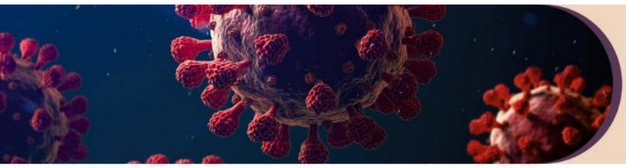

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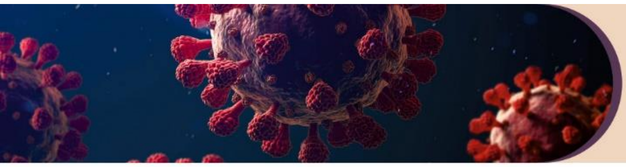

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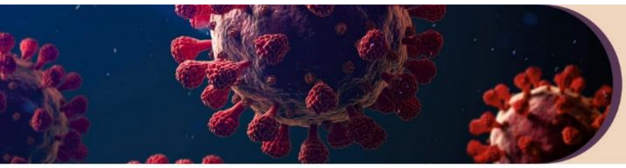

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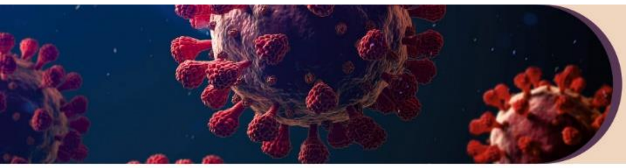

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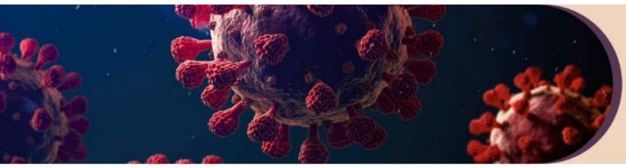

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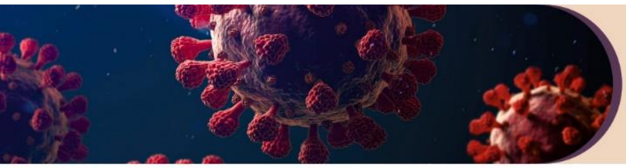

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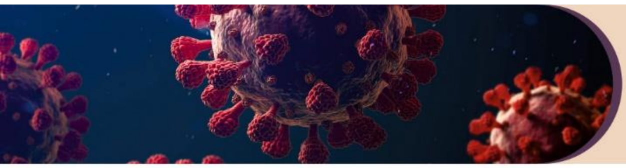

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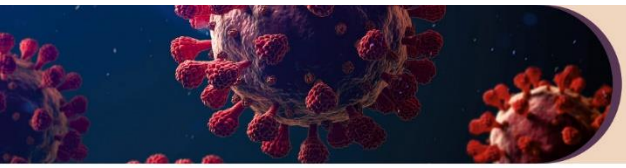

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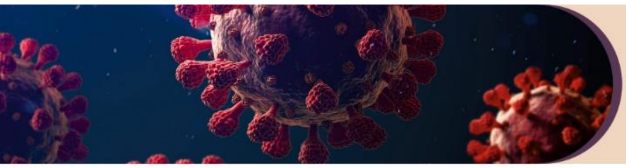

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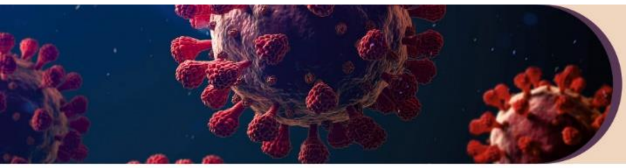

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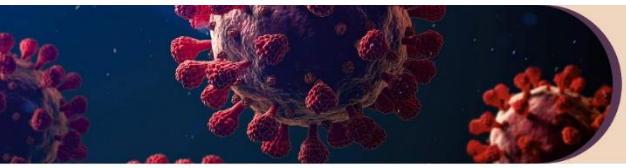

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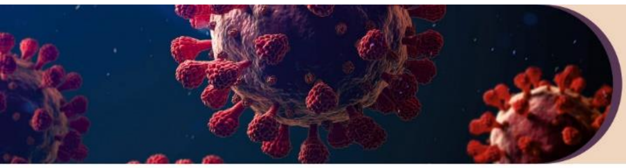

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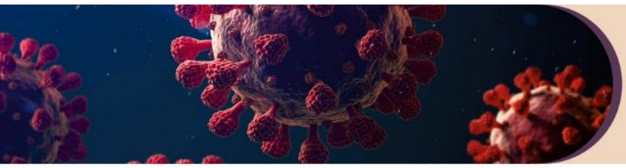

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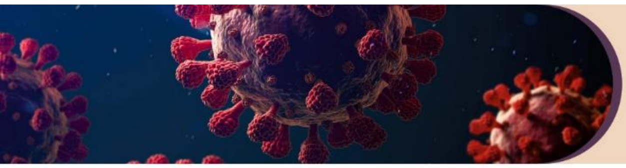

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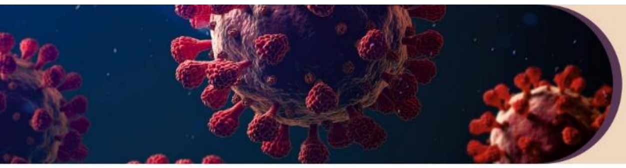

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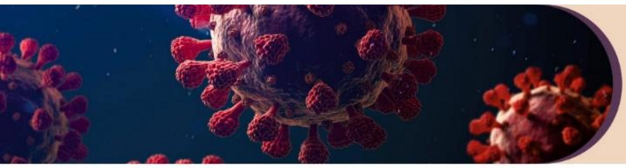

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