Overview

Bio-organic Chemistry is one of the most productive research groups of the institute making significant contributions in the area of drug development, natural products, biocatalysis, organocatalysis, glyco-chemistry, organic synthesis etc. Prospecting the plant as well as microbial biodiversity of the region as well as other parts of the country is one of the broad objectives of the group. The natural plant biodiversity specifically related to medicinal plants used in the traditional medicine is one of the major activities comprising detailed chemistry, identifying bioactive components/fractions/marker molecules, standardization etc. besides, generation of focused libraries based on natural product scaffolds, which has resulted in identifying several bioactive lead molecules.

Mission and Goals

In concordance with the missions and goals of the institute, the bio-organic group strives to contribute towards its development and recognition as one of the premier national institutes in the area of drug development, natural products and bio-catalysis. Some important goals set by the group include:

- Development of unique centre of repository of natural products (2500 or more molecules) and chemical libraries based upon them. The chemical library thus created can cater to the needs of the scientists across the country involved in drug development besides being a recurring source of income to the institute.
- Identification of new lead molecules in anti-cancer, anti-inflammatory, anti-arthritic, anti-bacterial, anti-fungal, anti-diabetic, anti-oxidant, immunomodulation, efflux pump inhibition, bio-enhancers etc.
- Generation of IPR as well as patenting of the bioactive molecules as NDEs or INDs is envisaged.
- New developments in synthetic chemistry, organocatalysis and glycochemistry.
- Development of novel industrial biocatalysts and processes based on them.
- Development of green methodologies.

Competencies

- Natural product Chemistry (medicinal and aromatic plants)
  (Extraction using conventional and non-conventional approaches, isolation, characterization, standardization, quality evaluation of plant based formulations, extracts, fractions and pure isolates)
- Compound library generation (chemical modifications) based on natural products and establishment of structure activity relationships
- Molecular structure elucidation.
- Development of new and novel methodologies for the preparation of chemicals of importance using Organic synthesis, Glycochemistry, Organocatalysis etc.
- Biotransformations aided through lipases, esterases, dehydrogenases, nitrilases, peroxidases and glycosidases

People

Name	Expertise	E-mail
S.C. Taneja	Drug Development, Natural Product Chemistry, Synthetic Chemistry, Enzyme Chemistry, Perfumery Chemistry, Molecular Modeling, Glycochemistry and Organocatalysis.	sctaneja@iiim.res.in
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D. Mukherjee	Medicinal Chemistry, Glyco-Chemistry, Development of novel synthetic methodologies, Biotransformations and Catalysis	dmukherjee@iiim.res.in
P.L. Sangwan	Natural Product Chemistry, Drug Development and Synthetic Chemistry	plsangwan@iiim.res.in
Bhahwal A. Shah	Drug Development, Natural Product Chemistry, New synthetic methodologies, Biocatalysis and Organocatalysis.	bashah@iiim.res.in
B. Singh	Chemo-enzymatic Studies of biologically active intermediates, Natural Product Chemistry and Synthetic Chemistry	bsingh@iiim.res.in
S. Singh	Technical Assistance	

Area of Research

- Drug Development
- Rational drug design using Molecular Modeling
- Development of focused semi-synthetic libraries based upon natural product scaffolds and establishment of possible SARs, molecular modes of action etc
- Synthesis of bio-molecules
- New developments and methodologies in carbohydrate chemistry
- Organo- and Heterogenous catalysis for diversity oriented synthesis (DOS).
- Identification of novel biocatalysts
- Development of biocatalytic process for molecules of industrial importance

Facilities

- HPLC units with normal, reverse phase and chiral columns.
- Centrifuge.
- Freeze drier.
- Hydrogenation apparatus.
- Flash chromatographs bench as well as fully automatic with loading capacity up to 100 g batch.
- Low temperature deep freezers (up to multiliter capacity).
- Sonicators.
- High and low temperature probes for carrying out reaction at desired temperature.
- Ice-Maker
- TLC Spraying cabinets with plate heating facility.

Current Research

- Generation of focused libraries based upon following natural product scaffolds such as terpenoids (mono-, di- and triterpenoids), alkaloids, withanolide, steroids, amides, coumarins, flavonoids, lignans, phenolics etc. for identifying lead molecules, optimization, identification of their molecular targets, mode of action in the area of cancer, inflammation, anti-bacterial, anti-fungal, immunomodulation, CNS/CVS, , efflux pump inhibition, bio-enhancers etc.
- Isolation and characterization of novel natural products of plant origin
- Development of novel protection methodologies, glycosylation, chemical transformation for the preparation of bioactive molecules
- Application of organocatalysis in useful chemical transformations
- Generation of a biocatalytic toolbox comprising lipases, esterases, dehydrogenases, nitrilases, peroxidases and glycosidases for the biotransformation of industrially important drugs, their precursors, auxiliaries, perfumery chemicals etc.
- Development of chemo-enzymatic methods for the preparation of chiral biomolecules
- Identification and development of endophytic sources for industrially important molecules
- 3D-structure prediction cum determination of proteins/w enzymes using *in silico* lab facility, QSAR studies of bioactives

Current Projects

- Development of novel target based anticancer therapeutics (SIP-0027)
- Exploitation of India's rich microbial diversity (NWP-006)
- Screening of microorganisms for the development of a biocatalyst tool box with emphasis on novel bacterial cellulase, cold active protease and lipase enzymes for important bio-transformations (MLP-007).
- Golden Triangle Project (CSIR, AYUSH and ICMR)
- Development of anti-bacterial agent for oral health care (SSP-0415)
- Discovery and pre-clinical studies of new bioactive molecules (natural and semi-synthetic) and traditional preparations (NWP-0037)
- Isolation and identification of bioactive principle/s from plant source for rheumatoid arthritis (CLP-0304)
- Drug target development using *in silico* biology (CMM-0017)
- Exploring botanicals for Malaysia-Tonkat Ali (SSP-0414)
- Enzymatic Screening of molecules (CNP-1300)