

Overview

The recently established in-silico facility encompasses activities like Molecular Docking, QSAR studies and 3-D structure prediction using Homology Modeling and Threading techniques. The software used to carry out the sophisticated experiments include Cerius2 and Insight-II from Accelrys, Schrodinger suite, Hyperchem and several other public domain software. Molecular modeling approach is being utilized to minimize the animal sacrifice to develop more potent, less toxic drug like molecules. Various targets such as TNF- α , NF- κ B, Histone deacetylase, Topoisomerase I & II and bacterial efflux pumps like NorA, TetK, MSRA, Bmr etc. are being used for drug development by studying the ligand-receptor interaction mechanisms. The group has an active interaction with the wet lab researchers in the institute, which thereby, further strengthens the *in silico* activities and should help in contributing to the Open Source Drug Discovery (OSDD) project. The group also interacts with all other major research groups of the institute in order to provide the mechanistic and informatics inputs to their respective research problems.

Mission and goals

Applications in Drug Designing Process using *in silico* approach and be a participant in the OSDD consortium.

- Identification of potent molecules from natural products/ semi-synthetic repository of IIIM, Jammu using *in silico* biological approaches for various activities against various molecular targets.
- Development of therapeutics from discovery leads.
- Generate qualified and trained IT professionals for pursuing research in the area of bioinformatics.
- Location-specific development of databases based on Microbial Biodiversity of North Western Himalayas.
- Web-site development and maintenance of the Institute & Bioinformatics centre.
- To evolve and implement programmes on education of users, training of information scientists in the area of Bioinformatics thereby, contributing towards the Human Resource Development.
- To build up information resources, prepare databases and develop relevant information handling tools and techniques.

Competencies

- State-of-the-art in silico facility with Silicon Graphics and HP Intel Xeon based workstations equipped with software like Cerius-2, Insight-II, Schrodinger suite and Hyperchem to carry out molecular modeling activities.
- Development of QSAR models with the objective of developing potent bioactive molecules.
- 3D structure prediction, using homology modeling and Threading techniques, of important therapeutic targets whose crystal structure is not known.
- Molecular docking experiments and result analysis with sophisticated software tools.

People (list of people)

S.No	Name	Expertise	Email ID
1.	S.Koul	Drug development, natural product chemistry, synthetic chemistry, enzymatic chemistry and molecular modeling	skoul@iiim.res.in
2.	Amit Nargotra	Molecular modeling and drug designing, QSAR studies, in silico 3D structure prediction, fragment based drug discovery, software programming and database development	anargotra@iiim.res.in

Area of Research

- In silico 3D structure prediction of various therapeutic targets and its functional effect analysis with in silico site directed mutagenesis
- Identification and development of potent bioactive molecules through QSAR studies.
- Studies related to ligand-receptor interaction mechanisms for several important targets like anti-cancer, anti-inflammatory, anti-bacterial and other areas of the interest of the Institute.
- Understanding the complexity of proteins viz-a-viz with the biological activity eg. Role of Protein knots and their effect on biological activity.

Facilities

- Silicon Graphics Fuel with Accelrys package (Cerius-2 and Insight-II) installed. The same software would also be installed on the Windows HP (Dual AMD Opteron Processor) Workstation.
- Linux HP workstations (Intel Xeon Dual Core Processor) with the software suite Schrodinger installed.

Current Research

- Screening of compounds from IIIM repository against several identified cancer targets viz., Topoisomerase I & II, Histone deacetylase, Inose, Tubulin etc.
- In silico structure prediction of bacterial efflux pump NorA, Bmr, Tetk and MSRA.
- QSAR model development of identified efflux pump inhibitors and design of new more potent inhibitors based on the predictive model.
- Understand the mechanism of action of TB drugs onto specific targets and identification of new potent molecules from IIIM that may be effective against these targets.
- Elaborate upon the complex structure of proteins e.g, knots with respect to its functionality/activity.

Projects

- Establishment of Sub-DIC under BTIS Net programme – GAP 0141
- Drug Target Development using *in silico* biology – CMM 0017