

Centre for Experimental Drug Design and Development

Our department has received a grant of Rs 11.33 Lakhs for the proposal entitled "Establishing Centre for Experimental Drug Design and Development" from All India Council for Technical Education (AICTE) under the Modernization and Removal of Obsolescence (MODROBS) scheme. The scheme aims to modernize and remove obsolescence in the Laboratories to enhance the functional efficiency of technical institutions for Teaching, Training, and Research purposes. The lab is fully equipped with an array of instrumentation necessary to support work in areas such as chemical synthesis, drug discovery, and medicinal chemistry. We are committed to giving our chemistry students hands-on experience using state-of-the-art equipment early their studies. Facilities available in the lab are

- *Monowave assisted reaction station*
- *Rotavapors*
- *Multiskan™ FC Microplate Photometer*
- *Wellwash™ Microplate Washer*
- *Fume Hood*
- *Vacuum pumps*
- *High Vacuum Pumps*
- *Magnetic stirrers*
- *Heat Gun*
- *Infrared thermometer*
- *FT-IR ATR Bruker*
- *Vacuum filtration assembly*



- *Analytical and other scales*
- *Dual wavelengths UV cabinets*
- *Rotamantles*

- *Centre for Molecular Simulations and Drug Design*

- *Centre for Molecular Simulations and Drug Design, under department of pharmaceutical chemistry was founded in November 2019. Over the last few years, computer aided drug design (CADD) has become a powerful technique because of its utility in various phases of drug discovery and development through various advanced features. This facility provides an ideal research environment for the complete spectrum of computer-assisted drug discovery for undergraduates, post graduates and research scholars. The students can understand how the drug discovery process works from the identification of molecular targets to the design of therapeutic candidates. The overall goal is to develop and apply innovative computational methodologies for drug design and discovery to address problems at the interface between chemistry, biology and medicine. Research activities of this laboratory focus on modelling protein-ligand interactions,*



structure-based drug design, molecular dynamics, Pharmacophore modelling, ADME prediction, homology modelling and QSAR. Among these, structure based drug design is our focus due to rapid growth in structural data (available in RCSB & Nucleic acid Data Bank). This structural data can be used in molecular modeling to design lead molecules based on the structural features of the active site to design several classes of bioactive compounds targeted to specific diseases. We are also interested to offer training programmes and research assistance to the students in areas like virtual screening based on the integration of docking, molecular dynamics, and free energy-based scoring functions.



Our team has strong experience in this field and we are also in tight cooperation with leading groups from academia around the globe and published several research articles in reputed international peer reviewed journals. The department has five computer with high end configuration and various commercial as well as open source softwares to train the process of drug design