Course Title: Molecular Modeling and Drug Design

Course Code CSE-874

Course Objectives:

- To understand the critical relationship among biomolecular structure, function and force field models.
- To be able to utilize basic modeling techniques to explore biological phenomena at the molecular level.
- To emphasize drug/receptor interactions in detail by molecular dynamics simulations and homology modeling.

Course Outcomes:

- Students are introduced to the principles and practice of Molecular modeling and modern drug discovery.
- An awareness of rational drug design, based on understanding of three-dimensional (3D) structures and physicochemical properties of drugs and receptors will be created.

Course Contents:

- Introduction to Molecular Modeling
- Ligand Representation
- Conformational Analysis
- Force Fields
- Types of Drug/Receptor Interaction
- Homology Modeling
- Docking
- Classical MD Simulation
- Classification (Machine Learning) Methods.

Recommended / Reference Books:

- Advanced Computer- Assisted Techniques in Drug Discovery in Methods and Principles in Medicinal Chemistry by Han van de Waterbeemd (ed.) Volume 3, 1994, VCH Publishers, New York, NY (USA).
- Molecular Modeling in Methods and Principles in Medicinal Chemistry by Hans-Dieter Holtje and Gerd Folkers, Third edition, Volume 5, 1996, VCH Publishers, New York, NY (USA).
- Structure-Based Ligand Designing Methods and Principles in Medicinal Chemistry by Klaus Gubernator, Hans-Joachim Bohm, Volume 6, 1997, VCH Publishers, New York, NY (USA).
- Virtual Screening for Bioactive Molecules by in Methods and Principles in Medicinal Chemistry, Edited by Hans-Joachim Bohm and Gisbert Schneider, Volume 10, 2000.