Course Title: Computational Drug Design

Course Code CSE- 873

Course Objectives:

This course is designed to introduce the students with the different challenges in drug discovery and to use the advanced computational tools in drug design.

Course Outcomes

After completing this course student will be able to understand the application and algorithms of different computational tools in drug discovery. Additionally, students will get awareness regarding current challenges in global pharmaceutical industry.

Course Contents:

Introduction: Pharmacoinformatics and Drug Discovery, Molecular Representation, File formats, Quantitative Structure Activity Relationship (QSAR), Molecular Descriptors, (1D, 2D, 3D), Fragment-based Drug Design, Target-based drug design, Pharmacophore Modeling, Data Base Search, High throughput screening

Recommended / Reference Books:

- QSAR: Hansch Analysis and Related Approaches in Methods and Principles in Medicinal Chemistry by Hugo Kubinyi, Volume 1, 1993, VCH Publishers, New York, NY (USA).
- 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 Design in 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.
- Pharmacophore and Pharmacophore Search in Methods and Principles in Medicinal Chemistry, Edited by Thierry Langer and Rémy D. Hoffmann, Volume 32, 2006.