B.S. Abdur Rahman Crescent Institute of Science and Technology

School of Life Sciences

Introduction to Molecular Modeling and Graphics

Course Description

This course is targeted at undergraduate level but is also suitable for graduate students wanting a background in modern computational and modeling approaches to solve biophysical/ biochemical problems in modeling.

Objectives

The course is designed to introduce future Biochemists, Biophysicists and Bioinformaticians to a wide range of techniques and applications in molecular modeling and computational drug design. Upon successful completion of the course, students will be able to:

1. **Recognize the basics of Molecular Modeling**
2. **Create Molecular visualization images of publication quality**
3. **List the modeling tools available to study Protein – ligand interactions**
4. **Explain various steps involved in Molecular Docking and Dynamics**
5. **Design a mini project to combine the proper application of modeling tools.**

Books and References

1.Molecular Modeling – Principles and Applications, 2nd Ed., Andrew Leach, 2001.

2.C.Mura, C.M. McCrimmon, J.Vertrees, M.R. Sawaya; "An Introduc.on to Biomolecular Graphics"; PLoS Computa<onal Biology 8 (2010) Vol. 6, pp 1-11

Prerequisites:

3.We will assume some background in Chemistry, Biochemistry and Physics. There are no computer science prerequisites for this course.

Lecture (Topics covered):

Introduction to Molecular Modeling; Potential Energy Surfaces and Optimization Methods; Molecular mechanics; Force fields, Types of force fields; Finding equilibrium structures: Geometry optimization; Conformational search; Solvation; Visualization and molecular properties; Molecular Docking and Molecular Dynamics

Hands-on Session:

1. Introduction to PDB and small molecule databases.
2. Introduction to computational visualization with PyMol and Generating publication images
3. Working with Chimera for performing analysis and modeling experiments
4. Molecular Docking using AudoDock VINA
5. Macromolecular structure preparation: Modeling missing loops, Homology Modeling
6. Molecular dynamics using NAMD and analysis

Course Instructors

Dr. Nehru Viji Sankaranarayanan
Dr. Umesh R. Desai Lab
Computational Research Scientist
Institute for Structural Biology, Drug Discovery and Development,
Department of Medicinal Chemistry
Virginia Commonwealth University
Richmond, VA 23219, USA
Email: (nvsankaranar@vcu.edu)

Dr. Balaji Nagarajan
Dr. Umesh R. Desai Lab
Institute for Structural Biology, Drug Discovery and Development,
Department of Medicinal Chemistry
Virginia Commonwealth University
Richmond, VA 23219, USA
Email: (bnagarajan@vcu.edu)

Coordinator
Dr. Ashok Kumar Pandurangan
Associate Professor
School of LifeSciences

Convener
Dr. S. Hemalatha
Professor & Dean
School of LifeSciences