BIRLA INSTITUTE OF TECHNOLOGY AND SCIENCE, PILANI
INSTRUCTION DIVISION
FIRST SEMESTER 2016-2017
Course Handout (Part II)

Date: 02/08/16

In addition to part -I (General Handout for all courses appended to the time table) this portion gives further specific details regarding the course.

Course No. BIO F417
Course Title: Biomolecular Modeling
Instructor in Charge: SHIBASISH CHOWDHURY

1. Course description:
Biomolecular Conformations, Structural genomics and proteomics, protein folding, Forcefield, Simulation, Conformational analysis, ab initio structure prediction, comparative modeling, lattice models, usage of modeling packages.

2. Scope and objective of the course:
The course is designed to provide students the first hand experience of potential utility of biomolecular modeling especially in concurrent pharmaceutical research, and in cell and structural biology. It describes the functionality, advantages, and limitations of standard computing strategies for the simulation of biomolecules. Provide a working knowledge of freely available software to carry out independent research projects in biomolecular modeling and explore the possibilities for modeling to assist in the process of determination, analyzing, evaluating, displaying, and retrieving of 3D structure data in a research or industry laboratory environment.

3. Text Book: "Molecular modeling: Principles and Applications" By Andrew R Leach, 2nd Edition, 2001, Pearson Education Lim.

4. Reference Book: (1) "Molecular Modeling and Simulation - An Interdisciplinary Guide" By Tamar Schlick, Springer, New York, 2002
(2) "Principles of protein structure" By Schulz, G.E. and Schirmer, R.H., New York, Springer-Verlag, 1979
(3) "An Introduction to Computational Biochemistry" – By C. Stan Tsai, Wiley-Liss, Inc, 2002.
(4) " Bioinformatics: genes, proteins and computers" – Edited by C. Orengo, D. Jones, J. Thronton, BIOS Scientific Publishers Ltd., UK, 2003.

5. Course Plan:

Lecture No.	Learning Objectives	Topics to be covered	Reference Chap/Sec. (Book)
1-2	Introduction	What is modeling? Scope and application of modeling in modern biology	R-1 (1-2)
3-8	Protein structure and conformation	Amino Acid Building Blocks, Rotameric Structures Protein Conformation Framework, Ramachandran Plots, Conformational Hierarchy, Structural motifs	R-1 (3-4)

9-12	Conformation and Variability in DNA structures	Basic Building Blocks, Conformational Flexibility, Canonical DNA Forms, DNA Sequence Effects,	R-1 (5-6)
13-14	Molecular graphics	Introduction to graphic representation, Representation of molecular structure: both small molecules and macromolecules Database of macromolecular structures	R-3 (4)
15-17	Visualization and modeling packages	Usages of freely available visualization packages like VMD, Rasmol, Pymol, SpdbViewer , Chime, Cn3D	Class-notes/websites
18-22	Protein structure prediction and protein folding problem	First principle methods for predicting protein structure, comparative modeling, threading , CASP, Protein folding theories	R-4(8-9)
23-25	Energetics and Forcefield	Different types of interactions and formulation of forcefield	T (4)
26-30	Molecular mechanics	Basic algorithm of MM and their utilities , Hand on sessions	T(5)
31-32	Monte Carlo Simulation	Basics of Monte Carlo Sampling	T(8)
33-35	Molecular dynamics	Basic MD algorithm, Its limitation, treatment of long range forces	T (6-7)
36-38	Conformational analysis	Analysis of molecular dynamics trajectories	T (9)
39-40	Lab on MD	Hand on session on molecular Dynamics	Amber package

6. Evaluation scheme:

Components	Duration	Date &Time	Weightage (%)	Nature of Component
Mid-semester test	90 min	<TEST_1>	25%	Closed Book
Assignment/seminar (several)			15%	
Surprise Quiz (several)	15 min		10%	Closed/open Book
Project			15%	Open Book
Comprehensive examination	3 Hours	<TEST_C>	35%	Partially closed Book

7. Chamber Consultation Hour: To be announced in the class.

8. Notices: Notices, if any concerning the course will be displayed on the notice Board of Biology Group.

9. Make up Policy: Make up will be given on genuine grounds as determined by the Instructor-in-charge

Instructor-in-charge
BIO F417