BITS-PILANI, HYDERABAD CAMPUS
SUMMER TERM 2021-2022
Course Handout (Part II)

Date: 28/05/2022

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: DEBASHREE BANDYOPADHYAY

1. Course description:
Biomolecular Conformations, Structural genomics and proteomics, protein folding, Forcefield, Simulation, Conformational analysis, ab initio structure prediction, comparative modeling, 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 structure-function elucidation, and in cellular and structural biology. It describes the functionality, advantages, and limitations of standard computing strategies for the simulation of biomolecules.

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	Chapter in the Text Book
1-2	Introduction	What is modeling? Scope and application of modeling in modern biology	R-1 (1-2)
3-4	Protein structure and conformation	Protein structural hierarchy, Structural motifs, classification	R-1 (3-4)
5-7	Conformation and Variability in DNA structures	Conformational Flexibility, Canonical DNA Forms, DNA Sequence Effects, DNA local geometry, base pair parameters, base step parameters, DNA stiffness	R-1 (5-6)
8	Molecular graphics	Introduction to graphic representation, Representation of molecular structure: macromolecules Database of macromolecular structures	R-3 (4)
9-10	Visualization and modeling packages	Usages of freely available visualization packages like VMD, Rasmol, Pymol,	Class-notes/ websites

		SpdbViewer , Chimera, Cn3D	
11-12	Protein structure prediction and protein folding problem	First principle methods for predicting protein structure, comparative modeling, threading, CASP	T(10) R-4 (8-9)
13-14	Advanced homology modelling	Refined structure modeling by incorporation of experimentally derived spatial restraints	User guide to MODELLER
15-16	Forcefield	Forcefields in understanding protein structures (salt bridge, long range interactions etc.)	T (4)
17-21	Molecular mechanics	Theory and hands on sessions in Molecular Mechanics	T(5), class notes
22-27	Molecular dynamics	Basic and Advanced MD simulation techniques, simulated annealing, parallel tempering	T (6-7), class notes
28-29	Molecular Dynamics: Hands-on session	Exposure to NAMD software and usage	User guide of NAMD
30-36	Quantum chemical approaches	Basic quantum mechanics, H-F approximation, Basis set, application of quantum chemistry in Biological systems	T(2-3)
37-38	Quantum Chemistry: Hands-on session	GAMESS software and application of GAMESS to calculate optimized structure and energy of amino acids	User guide of GAMESS
39-42	Monte Carlo Simulation	Basics of Monte Carlo Sampling	T(8)

T=Text book, R=Reference book

6. Evaluation scheme:

Components	**Duration**	**Date &Time**	**Weightage (%)**	**Nature of Component**
Midsem	90 minutes	25/6 3:30-5:00PM	30%	Closed Book
Continuous evaluation (Assignments, projects, etc.)		To be announced	30%	Open book
Comprehensive Examination	3 Hours	22/7 AN	40%	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 departmental notice board and CMS

9. Make up Policy: Make up will only be given on genuine ground.

10. Academic Honesty and Integrity Policy: Academic honesty and integrity are to be maintained by all the students throughout the semester and no type of academic dishonesty is acceptable.

Instructor-in-charge
BIO F417