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: 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. Provide a working knowledge of freely available software to carry out independent research projects in biomolecular modeling. Explore the possibilities of modeling to complement 3D structure determination, analysis, evaluation and data retrieval in a research or industry based laboratory.

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	Book (Sec/Chap)
1-2	Introduction	What is modeling? Scope and application of modeling in modern biology	R-1 (1-2)
3-7	Protein structure and conformation	Amino Acid Building Blocks, Rotameric Structures Protein Conformation Framework, Ramachandran Plots, Conformational Hierarchy, Structural motifs	R-1 (3-4)
8-10	Conformation and Variability in DNA structures	Basic Building Blocks, Conformational Flexibility, Canonical DNA Forms, DNA Sequence Effects,	R-1 (5-6)
11	Molecular graphics	Introduction to graphic representation,	R-3 (4)

		Representation of molecular structure: macromolecules Database of macromolecular structures	
12	Visualization and modeling packages	Usages of freely available visualization packages like VMD, Rasmol, Pymol, SpdbViewer , Chimera, Cn3D	Class-notes/websites
13-15	Protein structure prediction and protein folding problem	First principle methods for predicting protein structure, comparative modeling, threading , CASP	T(10) R-4 (8-9)
16	Comparative Modeling: Hands-on session	Exposure to MODELLER software and its usage	User guide to MODELLER
17-23	Quantum chemical approaches	Basic quantum mechanics, H-F approximation, Basis set, application of quantum chemistry in Biological systems	T(2-3)
24-25	Quantum Chemistry: Hands-on session	Exposure to GAMESS software and its usage	User guide of GAMESS
26-27	Energetics and Forcefield	Different types of interactions and formulation of forcefield	T (4)
28-32	Molecular mechanics	Basic algorithm of MM and their utilities , Hand on sessions	T(5)
33-38	Molecular dynamics	Basic MD algorithm, Its limitation, treatment of long range forces, conformational analysis from MD simulation, advanced techniques in MD simulations	T (6-7)
39-40	Molecular Dynamics: Hands-on session	Exposure to NAMD software and usage	User guide of NAMD
41-42	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
Test 1	1 hr	8/9 2:30PM-3:30PM	20%	Closed Book
Test 2	1 hr	25/10 2:30PM-3:30PM	20%	Closed Book
Assignment/Seminar/ Project		To be announced in the class	25%	Open book
Comprehensive examination	3 Hours	6/12 AN	20% 15%	Closed book Open 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.

Instructor-in-charge
BIO F417