

SRM UNIVERSITY
FACULTY OF ENGINEERING & TECHNOLOGY
DEPARTMENT OF BIOINFORMATICS
BI0403- SYSTEMS APPROACH TO BIOLOGY
LESSON PLAN

SEMESTER: VII

Course: Systems Approach to Biology

CODE: BI0403

Staff Handling: Arnab Sarkar

Total Hours: 45

Unit No.	Contents / Topics	Hours Required	Learning Outcome
I	MOLECULAR DYNAMICS AND SIMULATION METHODS		Various dynamics aspect of protein Models. This unit deals with various statistical Methods applicable for bioinformatics Various conformational analysis techniques For studying protein structures Various sequence alignment methods are Discussed in this unit Various kind of free energy techniques and Other thermodynamics aspects are Discussed in the various topics
	Simple models and continuous potentials	1	
	Running Molecular Dynamics simulation	1	
	Constraint Dynamics	2	
	Time dependent properties	2	
	Conformational changes	2	
Chain Amphiphiles	1		
II	MONTE CARLO SIMULATION METHODS		
	Calculating properties by integration	1	
	Metropolis methods	1	
	Metropolis Monte Carlo methods	1	
	Simulation of molecules	1	
	Biased methods	1	
	Different Ensembles	2	
Calculating Chemical potentials	1		
III	CONFORMATIONAL ANALYSIS		
	Gibbs Ensemble methods	1	
	Systematic methods	1	
	Model building approaches	1	
	Random search methods	1	
	Distance geometry	1	
	Conformational space variations	1	
	Global energy minimization	1	
	Molecular fitting	1	
	Clustering algorithm	1	
Dimension reduction	1		
IV	IN PROTEOMICS		
	First principle methods	1	
	Comparative modeling	1	
	Sequence alignment	2	
	Threading CASP	1	
V	CHALLENGES IN MOLECULAR MODELING		
	Protein folding and unfolding	2	
	Free energy calculations	1	
	Free energy differences and applications	1	
	Enthalpy and Entropy differences	1	
	Partitioning free energies	1	
	Free energy methods	2	
	Continuum representation of solvents	1	
	Born and Onsager models	2	
Solvation models	1		
Chemical reactions and solid state defects	1		