

COURSE TITLE	BIOMOLECULAR MODELLING AND SIMULATION
COURSE CODE	01CB0707
COURSE CREDITS	3

Objective:

- 1 This course aims to equip students with interdisciplinary skills, bridging computational and biological sciences for advanced research and real-world applications.

Course Outcomes: After completion of this course, student will be able to:

- 1 Apply basic mathematical tools to model biological systems using computer software.
- 2 Analyze different bioinformatics models by comparing their use and accuracy.
- 3 Evaluate models by checking their limits, errors, and ethical concerns.
- 4 Design smart models for drug research using AI and cloud tools.

Pre-requisite of course: Basic understanding of Docking and Modelling

Teaching and Examination Scheme

Theory Hours	Tutorial Hours	Practical Hours	ESE	IA	CSE	Viva	Term Work
2	0	2	50	30	20	25	25

Contents : Unit	Topics	Contact Hours
1	Introduction to Biomolecular Modeling and Simulation Definitions, scope and application of modeling in modern biology, Energy landscape, Dimensionality reduction	6
2	Molecular graphics VMD, Rasmol, Pymol, SpdbViewer, Chime, Cn3D, Energetics and Forcefield: Different types of interactions and formulation of forcefield, Construction of molecular energy function	5
3	Molecular models Degrees of freedom, spatial boundary conditions, ingredients and parameterization of force fields, Water models	5
4	Molecular mechanics Basic algorithm of MM, Applicability and principles, Monte Carlo Simulation, Molecular dynamics: Basic MD algorithm, Applications of MD in Biomolecular system, Its limitation, Analysis of molecular dynamics trajectories	7
5	Emerging Trends AI/ML in modelling (QSAR), Cloud-based simulation, Validation and Ethical Considerations: Model validation techniques, and ethical issues in simulations	5
Total Hours		28

Suggested List of Experiments:

Contents : Unit	Topics	Contact Hours
1	Experiment 1 Interpret biomolecular structures using PyMOL, identifying and analyzing key structural motifs such as α -helices, β -sheets, and ligand-binding regions.	2
2	Experiment 2 Compare and evaluate protein structures using RasMol and SPDBViewer to assess conformational differences and structural quality from the PDB database.	2
3	Experiment 3 Analyze molecular structures in VMD by performing distance, angle, and dihedral measurements for structural validation.	2
4	Experiment 4 Validate and assess molecular models using Ramachandran plots, energy profiles, and stereochemical checks through PROCHECK or MolProbity to ensure structural integrity.	2
5	Experiment 5 Construct and optimize small molecules using Avogadro by applying classical force fields (e.g., MMFF94), followed by energy minimization and geometry optimization.	2
6	Experiment 6 Calculate the energy profile of a peptide using Chimera, applying internal force fields and assessing structural conformations.	2
7	Experiment 7 Interpret key molecular interactions (hydrogen bonds, ionic interactions, van der Waals forces) in protein-ligand complexes using visualization and analysis tools.	2
8	Experiment 8 Develop and simulate a molecular system using GROMACS: generate topologies, define periodic boundaries, and solvate the system with water and physiological ions.	2
9	Experiment 9 Analyze energy minimization of a biomolecular system in GROMACS, interpreting convergence data and potential energy landscapes.	2
10	Experiment 10 Equilibrate a solvated protein system using NVT and NPT ensembles, assessing temperature and pressure stability over time.	2
11	Experiment 11 Conduct and interpret short molecular dynamics (MD) production run in GROMACS and generate trajectory files for downstream analysis.	2
12	Experiment 12 Analyze MD trajectories using RMSD, RMSF, hydrogen bonding patterns, and radius of gyration to evaluate conformational dynamics and protein flexibility.	2

Suggested List of Experiments:

Contents : Unit	Topics	Contact Hours
13	Experiment 13 Simulate and assess the effect of point mutations on protein stability using computational mutagenesis tools and stability prediction algorithms.	2
14	Experiment 14 Develop, train, and validate a QSAR model using molecular descriptors and machine learning algorithms to predict biological activity or pharmacokinetic properties.	2
Total Hours		28

Textbook :

- 1 Simulation Algorithms for Computational Systems Biology, Luca Marchetti, Corrado Priami, and Vo Hong Thanh, Springer, 2017

References:

- 1 Modeling and Analysis of Bio-molecular Networks, Modeling and Analysis of Bio-molecular Networks, Jinhua Lü and Pei Wang, Springer, 2020
- 2 Mathematical Modeling in Systems Biology: An Introduction, Mathematical Modeling in Systems Biology: An Introduction, Brian P. Ingalls', MIT Press, 2013
- 3 Computational Biology: A Practical Introduction to BioData Processing and Analysis with Linux, MySQL, and R, Computational Biology: A Practical Introduction to BioData Processing and Analysis with Linux, MySQL, and R, Röbbe Wünschiers, Springer, 2013

Suggested Theory Distribution:

The suggested theory distribution as per Bloom's taxonomy is as follows. This distribution serves as guidelines for teachers and students to achieve effective teaching-learning process

Distribution of Theory for course delivery and evaluation					
Remember / Knowledge	Understand	Apply	Analyze	Evaluate	Higher order Thinking / Creative
0.00	0.00	35.00	35.00	30.00	0.00

Instructional Method:

- 1 The course delivery method will depend upon the requirement of content and need of students. The teacher in addition to conventional teaching method by black board, may also use any of tools such as demonstration, role play, Quiz, brainstorming, MOOCs etc.
- 2 The internal evaluation will be done on the basis of continuous evaluation of students in the laboratory and class-room.
- 3 A practical examination will be conducted at the end of the semester for the evaluation of the performance of students in the laboratory.

Supplementary Resources:

- 1 <https://nptel.ac.in/courses/103103036>
- 2 https://www.youtube.com/watch?v=vM58c_AKH8c