



GUJARAT TECHNOLOGICAL UNIVERSITY

Program Name: Bachelor of Engineering

Level: UG

Branch: Biotechnology

Subject Code: BE05004051

Subject Name: Structural Biology

w. e. f. Academic Year:	2024-2025
Semester:	5
Category of the Course:	Professional Elective Course - 1

Prerequisite:	None
Rationale:	Structural biology elucidates the 3D architecture of biological macromolecules, providing insight into function, dynamics, and molecular interactions—essential for rational drug design and protein engineering.

Course Outcomes:

Sr. No.	CO statement	Marks% weightage
CO-1	Explain structural organization of proteins and nucleic acids.	20
CO-2	Describe experimental methods like XRD, NMR, Cryo-EM.	15
CO-3	Model and visualize biomolecular structures.	15
CO-4	Analyze protein-ligand interactions.	15
CO-5	Correlate structure with function in biological systems.	15

Teaching and Examination Scheme:

Teaching / Learning Scheme (in Hours per semester)					Total Credits	Assessment Pattern and Marks					Total Marks
L	T	P	PBL	Total no of hours per semester		Theory		Tutorial / Practical			
						ESE (E)	PA / CA (M)	PA/ CA (I)	PBL (I)	ESE (V)	
45	0	30	15	90	3	70	30	20	30	50	200

Content:

Sr. No.	Content	Total Hrs
1	Basics of Macromolecular Structure Levels of protein structure, DNA/RNA conformations.	10
2	Structure Determination Methods X-ray crystallography, NMR spectroscopy, cryo-electron microscopy.	10
3	Structure Visualization and Modeling Molecular graphics, PyMOL, Chimera, energy minimization.	10
4	Molecular Dynamics and Docking Simulations using GROMACS, docking protocols, validation tools.	10



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5	Applications Structure-based drug design, enzyme engineering, mutational analysis.	05
TOTAL		45

Suggested Specification table with Marks (Theory): (For B.E. only)

Distribution of Theory Marks					
R Level	U Level	A Level	N Level	E Level	C Level
20	20	20	20	10	10

R: Remembrance; U: Understanding; A: Application, N: Analyze and E: Evaluate C: Create and above Levels (Revised Bloom's Taxonomy)

The syllabus of Advanced Power Electronics directly contributes to

SDG 3	The syllabus contributes to rational drug discovery, protein engineering, and understanding biomolecular interactions for improved disease diagnosis and therapeutic development.
SDG 4	Structural biology promotes interdisciplinary scientific learning by integrating molecular biology, computational biology, chemistry, and bioinformatics for advanced research skills.
SDG 9	The subject supports innovation in structure-based drug design, molecular modeling, protein engineering, and computational biotechnology applications.
SDG 3	Molecular docking and protein-ligand interaction studies contribute to personalized medicine and improved therapeutic targeting.
SDG 12	Computational modeling and molecular simulation reduce experimental resource usage by enabling predictive analysis before laboratory experimentation.

Reference Books:

1. Branden & Tooze, *Introduction to Protein Structure*.
2. Mount, *Bioinformatics: Sequence and Genome Analysis*.
3. Leach, *Molecular Modelling: Principles and Applications*.

List of Experiments / Practical Demonstrations

1. Visualization of protein structure in PyMOL.
2. Secondary structure prediction.
3. Molecular docking of enzyme-ligand complex.
4. MD simulation setup using GROMACS.

Major Equipment

1. High-performance computers



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2. Visualization workstation

Open-Source Software / Learning Websites

1. RCSB PDB, PyMOL, Chimera, GROMACS
2. NPTEL: Structural Bioinformatics

List of suggested activities for Project Based Learning (PBL):

Sr. No.	PBL Category	Name of the Activity	No. of Hours	Evaluation Criteria
1	Industry / Research Laboratory Visit	Visit to structural biology laboratory / bioinformatics center / molecular modeling or drug discovery research laboratory	Visit = 5 hrs, Report preparation = 5 hrs Total = 10 hrs	Based on report submitted. Report should contain observations on molecular visualization, structure determination methods, docking studies, and computational structural biology workflows.
2	Video Based Learning	Technical video-based learning related to protein structure, X-ray crystallography, NMR spectroscopy, Cryo-EM, molecular docking, and molecular dynamics (MOOC/NPTEL Video)	Duration of video = 5 hrs, Report preparation = 5 hrs Total = 10 hrs	Report/presentation based on video learning outcomes and understanding of structural biology concepts.
3	Assignment / Technical Writing / Research Writing	Numerical and theory-based assignments related to protein structure prediction, molecular visualization, docking analysis, and molecular dynamics	5 assignments of 2 hrs each Total = 10 hrs	Based on assignment submitted, technical understanding, structural interpretation, and scientific analysis.
4	Complex Problem-Solving targeting relevant SDGs / Mini Project	Comparative analysis of protein-ligand interaction using molecular docking and structural visualization tools (PyMOL/Chimera)	15 hrs	Based on problem-solving approach, docking interpretation, molecular interaction analysis, and scientific feasibility.
5	Research Paper Review / Analysis	Discussion on research paper related to protein structure, Cryo-EM, molecular docking, structure-based drug	5 research papers = 20 hrs	Summarize research paper and evaluate critical structural and computational parameters.



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		design, or molecular dynamics simulation (SCOPUS Indexed / reputed Journal)		
6	Poster / Chart / PowerPoint Presentation	Poster/chart/power point preparation on topics such as Protein Structure, X-ray Crystallography, Cryo-EM, Molecular Docking, Molecular Dynamics, Drug Design	Duration = 6 hrs	Based on poster/chart preparation, scientific understanding, technical depth, and presentation skills.
7	Mini Project	Working/non-working model or simulation of 3D protein structure visualization, molecular docking of enzyme–ligand complex, or secondary structure prediction	10 hrs	Based on internal/external evaluation, innovation, scientific understanding, and technical relevance.
8	Group Discussion / Quiz / Simulation	Group discussion on emerging topics such as AI in Drug Discovery, Protein Folding, Computational Structural Biology, and Rational Drug Design	Duration = 1 hr each	Based on participation, scientific understanding, technical knowledge, and communication skills.
9	Case Study Analysis / Seminar	Real-world case study on protein misfolding diseases, structure-based drug discovery, enzyme engineering, or biomolecular interactions	Data collection/study = 5 hrs, Report preparation = 5 hrs Total = 10 hrs	Based on in-depth scientific study, technical depth, fact-finding, and conclusions.
10	Other	Patent Search and Innovation Gap Identification in structural bioinformatics, protein engineering, molecular docking, or drug discovery	10 hrs (Search + Report)	Based on number of relevant patents analyzed and identification of innovation scope.

Note:

1. Mini Project – 10 Marks , Micro Project – 5 Marks
2. The hours allocated to specific activities should be proportionate to the total no. of PBL hours and marks.
