Course number: **BSE6XX**

Course name: **Molecular Biophysics**

Prerequisite: **None**

Credits: **[3-0-0-9]**

Duration of Course: **Full Semester**

Proposing Department/IDP: **Biological Sciences and Bioengineering**

Proposing Instructor(s): **Sai Chaitanya Chiliveri**

Objectives:

The primary objective of this course is to provide postgraduate students with a strong and coherent foundation in molecular biophysics, emphasizing how physical principles govern the structure, stability, interactions, and functional dynamics of biological macromolecules. The course aims to help students view biomolecules such as proteins and nucleic acids not only as chemical entities, but also as dynamic physical systems shaped by thermal fluctuations and noncovalent forces. Through biologically relevant examples, students will gain an understanding of key processes, including protein folding and misfolding, molecular recognition, binding equilibria, cooperativity, and allosteric regulation. The course also aims to train students to interpret and critically evaluate experimental data obtained from widely used biophysical techniques. In addition, students will be introduced to modern computational tools, including molecular docking, molecular dynamics simulations, and AI-based structure-prediction methods, enabling them to appreciate how computational and experimental approaches complement each other in contemporary biomolecular research. Overall, the course is designed to strengthen conceptual understanding, develop quantitative intuition, and prepare students to apply molecular biophysics approaches in interdisciplinary research areas, including biology, biotechnology, medicine, and drug discovery.

Contents:

S.No	**Broad topic**	**Specific topics**	**Lecture (in hr)**
1	Introduction to Molecular Biophysics	Scope of molecular biophysics; biological length/time/energy scales; thermal motion and fluctuations; noncovalent forces (electrostatics, hydrogen bonding, van der Waals, hydrophobic effect); concept of free energy and stability; effects of salt, pH and temperature; forces shaping protein and nucleic acids structure; protein folding, misfolding and aggregation.	8
2	Molecular Recognition and Binding	Protein–ligand binding; protein–protein interactions; DNA/RNA binding proteins; binding affinity (K_d), binding curves and saturation; cooperativity and Hill model; allostery and	6

		molecular switching; multimerization and formation of macromolecular complexes.	
3	Biomolecular Dynamics and Functional Motions	Protein flexibility and motion across time scales; conformational exchange; induced fit vs conformational selection; coupling of structure, motion and function; experimental signatures of dynamics; introduction to NMR spectroscopy for studying biomolecular motions.	10
4	Experimental Tools in Molecular Biophysics	Circular dichroism and thermal melting; dynamic light scattering for size and aggregation; SEC-MALS for molecular weight and oligomeric state; SAXS basics for shape and flexibility; Isothermal titration calorimetry; Surface plasmon resonance; Biolayer interferometry.	9
5	Computational and AI tools in Molecular Biophysics	Molecular docking; molecular dynamics simulations and trajectory analysis; AI-based structure prediction (AlphaFold & Rosetta); integration of computational predictions with experimental observations.	6

References:

1. Physical Biology of the Cell by Rob Phillips, Garland Science, 2nd Edition.
2. Methods in Molecular Biophysics by Nathan Zeccai, Cambridge University Press, 2nd Edition.
3. Introduction to Protein Structure by Carl Branden & John Tooze, Garland Publishing, 2nd Edition.
4. Research Papers & Review Articles.

Dated: _______________ Proposer: ___________________________

Dated:_______________ DPGC Convener: ___________________

This course is approved /not approved

Chairman, SPGC

Dated:______________________