IV Year B.Tech. Bioinformatics I - Semester	L	T	P	To	C
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BI 415 STRUCTURAL BIOINFORMATICS

Course Description and Objectives :

This course aims to study the strategy and tactics of biophysical concepts of macromolecules and the conformational analysis and forces that determine the protein and nucleic acid structure and ligand interaction with macromolecules. Study of the size and shape of the macro molecule using different techniques using various tools like X-ray Crystallography and NMR is explained in the course.

Course Outcomes :

1. Student will learn the different structural levels of biological macromolecules, its size, shape, their conformations and the forces that are involved in stabilizing these molecules.
2. They will be able to utilize the tools by which this analysis is done will be learned.
3. The student would also learn about the ligand interaction with macromolecules.
4. They will understand the basic principles of various methods of spectroscopy and its applications
5. They will understand the concepts behind X-ray diffraction and X-ray crystallography.

Unit I : Introduction: Levels of structures in Biological macromolecules :

Basic strategies in biophysics- Principles and concepts used in biophysical analysis of life processes - Biomolecules and their interactions, size and shape of macromolecules.

Unit II: Conformational Analysis :

Forces that determine protein and nucleic acid structure, basic problems, polypeptide chains geometries, potential energy calculations, observed values for rotation angles, hydrogen bonding, hydrophobic interactions and ionic interactions, disulphide bonds.

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Unit III : Structural Analysis of Macromolecules :

Prediction of proteins structure, nucleic acids, general characteristics of nucleic acid structure, geometries, glycosidic bond rotational isomers and those puckering backbone rotational isomers and ribose puckering forces stabilising ordered forms, base pairing, base stacking tertiary structure of nucleic acids.

Unit IV : Spectroscopy and methods of visualization :

Absorption spectroscopy, Linear and Circular Dichroism, Emission spectroscopy, Nuclear Magnetic Resonance spectroscopy. Methods of direct visualisation, macromolecules as hydrodynamic particles, macromolecular diffusion, ultracentrifugation, viscometry.

Unit V : X-ray diffraction :

X-ray crystallography - X-ray diffraction, determination of molecular structures, electron microscopy, neutron scattering, light scattering.

Text Book :

1. Cantor R., Schimmel P.R., Biophysical Chemistry, Vol. I, II, W.H. Freeman & Co., 1985.

Reference Books :

1. Daniel. M, Basic Biophysics for Biologists, 1998.
2. Kensal E. van Holde, W. Curtis Johnson and P. Shing Ho, Principle of Physical Biochemistry, Prentice Hall, New York, 1998.

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