Subject Code : P8BIE1

EC – I STRUCTURAL BIOINFORMATICS

UNIT – I

Overview of structural bioinformatics – understanding structural basis for biological phenomena – challenges in structural bioinformatics – integration of structural data with other data – Structure Databases – PDB, NDB, CCD - Structural Classification – SCOP, CATH, FSSP - Structural genomics

UNIT – II

Conformational Analysis of proteins– Forces that determine protein structure – polypeptide chain geometries – Ramachandran Map – potential energy calculations – observed values for rotation angles – structure comparison and alignment

UNIT – III

Conformational analysis of nucleic acids and carbohydrates – general characteristics of nucleic acid structure – geometries, glycosidic bond – rotational isomers and ribose puckering - forces stabilizing ordered forms – base pairing – base stacking.

UNIT – IV

Structure Prediction Methods – Homology Modeling – Fold Recognition Methods – a*b initio* methods –Rosetta – CASP – prediction of secondary structure – Chou-Fasman, Garnier-Osguthorpe-Robson (GOR) methods – transmembrane structure prediction – solvent accessibility calculations and prediction.

UNIT – V

Interactomes – macromolecular interactions - protein-protein interactions – protein-DNA interactions – protein-ligand interactions – interactions databases – BIND, ProNIT - Docking – principles and methods

Reference Books

1. C.R.Cantor & P.R.Schimmel, Biophysical Chemistry Part - I, W.H. Freeman & Co., in San Fransisco, 1980.
2. C. Branden and J. Tooze, Introduction to Protein Structure, Garland Publishing Inc., New York., 1999.
3. P.E. Bourne and H. Weissig (Eds.) Structural Bioinformatics, John-Wiley and Sons, 2003.