

UNIT-I

PROTEIN-PROTEIN INTERACTIONS: Database for Protein-Protein interactions (DIP), Structural analysis, Solvent accessibility interactions of protein-protein interactions, Hydrogen bonds and salt bridges across PPI, Prediction of binding sites in protein-protein complexes, Energy-based approach for understanding the recognition mechanism of protein-protein complexes, Prediction of PPI pairs.

UNIT-II

PROTEIN-DNA INTERACTIONS: Structural analysis of interactions, DNA stiffness and protein-DNA binding specificity, Inter-and Intramolecular interactions, Discrimination of DNA-binding domains/ proteins, Prediction of DNA-binding sites, Databases for protein-DNA interactions.

UNIT - III

PROTEIN-RNA INTERACTIONS: Prediction of RNA-binding sites, Structural analysis, Methods for detecting Protein-RNA interactions, Databases for predicting protein-DNA interactions.

UNIT-IV

PROTEIN-LIGAND INTERACTIONS: Prediction of ligand-binding sites, Protein-ligand docking, Estimation of protein-ligand binding free energy, Scoring functions, Validation ligand and active site residues in protein structures, Protein-ligand databases.

UNIT-V

TOOLS AND SOFTWARES: Cytoscape for visualizing molecular interaction networks and biological pathways, SAPIN / Structural Analysis of Protein Interaction Networks, BindML, AutoDOCK, PatchDOCK, RPISeq, NUCPLOT, CAD-score, LigPlot.