Protein Protein and Protein Nucleic Acid Docking — Hands-on

Learn how to design and run docking workflows for protein–protein and protein–nucleic acid complexes. This module covers interface biology, complex preparation, docking search strategies, scoring and pose inspection so that your PPI and protein–DNA/RNA models are suitable for interpretation, MD and design.

Protein Protein and Protein Nucleic Acid Docking

Help Desk · WhatsApp

Session Index

Session 1

Fee: Rs 8800 Apply Now

Interface Biology and Complex Preparation

Interfaces in protein protein and protein nucleic acid complexes

hotspots and contact residues | **electrostatics and shape complementarity** | **transient vs obligate interactions**

Preparing individual partners for docking

removing clashes and poor geometry | **protonation and**

charge states | choosing constructs and truncations

Defining binding regions and restraints from data

mutagenesis and crosslink hints | co evolution and conservation patches | experimental and literature derived restraints

Session 2

Fee: Rs 11800 Apply Now

Protein Protein Docking Strategies and Scoring

Global and local PPI docking approaches

global search on whole surface | local docking near known patches | rigid body vs flexible side chains

PPI specific scoring concepts

shape complementarity and desolvation | electrostatic and hydrophobic balance | interface area and packing

Pose clustering and near native selection

clustering by RMSD or interface similarity | filtering steric clashes and artifacts | shortlisting poses for refinement

Session 3

Fee: Rs 14800 Apply Now

Protein DNA or RNA Docking and Specificity

Nucleic acid structure basics for docking

DNA and RNA geometry | backbone flexibility and grooves | sequence dependent shape features

Protein nucleic acid docking considerations

electrostatics and phosphate groups | base readout

and indirect readout handling backbone flexibility in docking

Scoring, footprint and contact pattern analysis

hydrogen bond and salt bridge networks base specific contacts and motifs sequence and structure based specificity checks

Session 4

Fee: Rs 18800 Apply Now

Mini Capstone: Complex Docking and Analysis

Select a PPI or protein nucleic acid system and define the problem

Theory plus Practical

Perform docking, refine and interpret candidate complexes

pose clustering and ranking interface contact and footprint analysis selection for MD or further design

Deliverables: docked complex set and analysis report

complex PDB files interface maps and plots written interpretation and caveats