Molecular Docking: Protein–Ligand & Protein–Protein — Hands-on

Gain hands-on experience in molecular docking workflows for both small-molecule ligands and protein–protein complexes. This module walks through structure preparation, binding site definition, docking protocols, scoring and rescoring, pose inspection and validation, so that you can design docking studies that are reproducible, interpretable and suitable for medicinal chemistry or mechanistic follow-up.

Molecular Docking: Protein–Ligand & Protein–Protein

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Session Index

Session 1

Fee: Rs 8800 Apply Now

Docking Concepts & Structure Preparation

Fundamentals of molecular recognition and docking

- search space vs scoring function
- rigid vs flexible docking
- use cases: screening vs pose prediction

Protein structure curation for docking

- selecting PDB entries and chains
- adding hydrogens

and protonation states handling missing loops, waters and cofactors

Ligand and partner preparation

2D to 3D conversion tautomer / stereochemistry issues charge and conformation generation

Session 2

Fee: Rs 11800 Apply Now

Protein–Ligand Docking Protocols & Scoring

Binding site identification and grid definition

using co-crystal ligands and pockets grid box placement and size orthosteric vs allosteric sites

Docking workflows and search algorithms

stochastic / genetic search ideas rigid receptor vs induced-fit flavors ensemble docking concepts

Scoring, rescoring and pose ranking

empirical vs knowledge-based scores visual inspection of poses rescoring and consensus strategies

Session 3

Fee: Rs 14800 Apply Now

Protein–Protein Docking & Interface Analysis

Principles of protein–protein recognition

shape and electrostatic complementarity hot spots and interface residues rigid body vs flexible interfaces

Protein–protein docking workflows

global vs local docking modes FFT/grid based search concepts use of restraints and bioinformatics clues

Analysing and refining docked complexes

interface contacts and buried surface area energy minimization and clashes choosing representative solutions

Session 4

Fee: Rs 18800 Apply Now

Validation, Benchmarking & Best Practices

Validating docking protocols on known complexes

Theory + Practical

Metrics, enrichment and pose reproducibility

RMSD to crystal poses enrichment curves and ROC-like plots retrospective vs prospective docking

Reporting, limitations and integration with MD / FEP

figure panels for docking studies common pitfalls and red flags when to follow up with MD or free energy