Protein–Ligand & Protein–Protein Docking Strategies — Hands-on

Learn how to plan and run docking studies that stand up to scrutiny. This module walks through receptor and ligand preparation, binding site identification, protein–ligand and protein–protein docking strategies, and rigorous scoring, rescoring and validation to deliver decision grade interaction models for discovery projects.

Protein–Ligand & Protein–Protein Docking Strategies

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Session Index

Session 1

Fee: Rs 17800 Apply Now

Docking Concepts, Search & Receptor Preparation

Docking problem and search space definition

- pose vs affinity prediction
- global vs local search
- rigid vs flexible components

Receptor preparation best practices

- protonation and tautomer states
- cofactors, metals and key waters
- cleaning alternate conformers

Binding site identification and grid setup

known ligand and pocket based sites cavity detection tools grid box design and resolution

Session 2

Fee: Rs 21800 Apply Now

Protein–Ligand Docking Workflows

Ligand preparation and conformer generation

ionization and tautomers stereochemistry and chiral centers conformer libraries for flexible ligands

Docking algorithms and sampling modes

genetic and stochastic search rigid receptor vs induced fit options ensemble docking concepts

Practical protein–ligand docking pipelines

set up, run and monitor jobs handling small libraries vs large campaigns basic post processing of poses

Session 3

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Protein–Protein Docking & Interface Modelling

Features of protein–protein interfaces

hotspots and contact patches shape and electrostatic complementarity transient vs obligate complexes

Global vs local protein–protein docking

blind docking vs guided docking symmetry and multimeric assemblies use of experimental restraints

PPI docking tools and refinement ideas

clustering of poses and ranking interface analysis and hotspot inspection preparing complexes for MD refinement

Session 4

Fee: Rs 28800 Apply Now

Scoring, Rescoring & Validation Strategy

Scoring functions and ranking poses

empirical vs knowledge based scores consensus scoring ideas interaction fingerprints and filters

Rescoring and physics based refinement options

MM GBSA and related approaches short MD relaxation of complexes stability and key contact checks

Validation, benchmarking and reporting of docking studies

enrichment, ROC curves and early recognition reproduction of known complexes protocol documentation and decision logs