Protein Ligand & Protein Protein Docking Principles — Hands-on

Learn end to end principles of protein–ligand and protein–protein docking for real projects. From receptor and ligand preparation, search space definition and docking runs to pose inspection, scoring, rescoring and validation against experimental data, you will create docking workflows that are transparent, reproducible and suitable for hypothesis generation and follow up simulations.

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Session Index

Session 1

Fee: Rs 12320 Apply Now

Docking Concepts & Receptor Preparation

Docking theory and use cases

search vs scoring separation **rigid vs flexible docking ideas** **protein–ligand vs protein–protein focus**

Choosing and cleaning receptor structures

selecting experimental or modeled structures | removing clashes and artifacts | handling alternate conformations

Receptor preparation for docking engines

adding hydrogens and assigning protonation | assigning charges and atom types | keeping or removing waters, cofactors and ions

Session 2

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Ligand / Partner Preparation & Search Space

Small molecule ligand preparation

2D to 3D conversion and tautomers | protonation and charge states | conformer generation concepts

Protein–protein docking partners

interface knowledge and restraints | global vs local docking setups | coarse grained vs atomistic approaches

Binding site and search space definition

using known ligands and pockets | grid boxes and search radii | blind docking caveats

Session 3

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Docking Runs, Scoring & Pose Inspection

Docking engines and search algorithms

grid based and shape based ideas | stochastic search concepts | exhaustiveness vs speed tradeoffs

Scoring functions and rescoring

empirical and knowledge based scores | rank vs absolute energy interpretation | rescoring and consensus scoring ideas

Visual inspection and interaction analysis

H bonds, salt bridges and hydrophobic contacts | clashes and unrealistic geometries | pose clustering and representative selection

Session 4

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Validation, Best Practices & Reporting

Redocking, cross docking and controls

redocking known complexes | RMSD based pose assessment | negative controls and decoy ligands

From docking scores to hypotheses

prioritizing poses and compounds | linking to SAR and mutagenesis data | deciding when MD or free energy is needed

Documentation, figures and reproducibility

recording parameters and software versions | interaction diagrams and 3D views | tables and checklists for reviewers