Protein Ligand Docking Scoring and Consensus — Hands-on

Design and execute robust protein–ligand docking workflows for hit finding, pose prediction and prioritization. This module covers receptor and ligand preparation, docking search strategies, scoring functions, pose inspection, enrichment metrics and consensus docking strategies that improve decision confidence.

Protein Ligand Docking Scoring and Consensus

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Session Index

Session 1

Fee: Rs 8800 Apply Now

Docking Concepts, Receptors & Ligands

Docking goals and use cases in discovery projects

virtual screening cascades | **pose prediction and SAR support** | **triaging HTS and fragment hits**

Receptor preparation principles

protonation states and tautomers | **missing side chains and loops** | **waters, cofactors and metal ions**

Ligand preparation and chemical sanity checks

valence, chirality and formal charges | ionization and tautomers windows | 3D conformer generation overview

Session 2

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Search Algorithms, Scoring & Poses

Binding site definition and grids

known pockets and co crystal based boxes | cavity detection concepts | grid generation parameters overview

Docking search strategies and flexibility models

rigid receptor, flexible ligand | side chain flexibility concepts | stochastic and systematic searches

Scoring functions, rescoring and pose inspection

empirical, knowledge based and force field scores | interaction fingerprints and contacts | visual checks and red flag poses

Session 3

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Consensus Docking, Enrichment & QA

Pose and score based consensus strategies

multi program docking ideas | rescoring and rank aggregation | interaction pattern consensus

Using actives and decoys to measure performance

ROC and enrichment curves | early enrichment metrics | retrospective validation concepts

Quality assurance and reproducibility in docking runs

seed and determinism considerations **logging parameters and versions** **storing poses and scores with metadata**

Session 4

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Mini Capstone: Docking & Ranking Campaign

Define a docking problem and prepare receptor and library

Theory + Practical

Run docking, analyze poses and apply consensus strategy

primary docking and rescoring **interaction fingerprint review** **shortlist generation and sanity checks**

Deliverables: ranked hit list and docking report

pose files and score tables **enrichment and performance plots** **methodology and parameter appendix**