Structure Based Virtual Screening & Docking Workflows — Hands-on

Gain practical skills in structure based virtual screening and molecular docking workflows. This module covers receptor and binding site preparation, ligand library preparation, docking setup, scoring and enrichment analysis so that you can design, execute and interpret in silico screens that feed into hit finding and lead discovery programs.

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Session Index

Session 1

Fee: Rs 8800 Apply Now

Docking Foundations & Receptor Concepts

Principles of molecular docking and virtual screening

search in pose and conformation space **scoring functions overview** **screen vs refine mindsets**

Receptor structures and sources

PDB and predicted models **holo vs apo structures** **selecting a docking template**

Binding site identification and representation

co crystallized ligand based sites | pocket detection tools | grid boxes and constraints

Session 2

Fee: Rs 11800 Apply Now

Receptor & Binding Site Preparation

Protein preparation workflows

adding hydrogens and assigning bonds | protonation and tautomer states | resolving missing side chains

Handling water molecules, cofactors and metals

retained vs removed waters | essential cofactors and ions | binding site specific decisions

Defining docking grids and constraints

grid size and resolution choices | centering on ligand or residues | pharmacophore and hydrogen bond constraints

Session 3

Fee: Rs 14800 Apply Now

Ligand Preparation & Docking Protocols

Ligand library preparation

enumerating tautomers and protonation states | 3D conformer generation | filtering by simple rules

Docking search algorithms and settings

exhaustiveness and number of poses | flexible ligand and side chain options | reproducibility and random seeds

Running a small scale docking job

setting up input files and folders **basic parallelization options** **log files and error checks**

Session 4

Fee: Rs 18800 Apply Now

Mini Capstone: Screening Run & Enrichment

Designing a focused virtual screen and success criteria

Theory + Practical

Post processing docking results and enrichment analysis

ranking by score and filters **visual inspection of top poses** **enrichment curves and hit rates**

Deliverables: documented workflow and ranked hit list

notebook or script for docking run **CSV with top ranked compounds** **summary slides for project teams**