

Molecular Docking & Energy Minimization Techniques — Hands-on

Practical docking from target prep to minimized poses. Learn clean receptor/ligand preparation, grid/box design, rigid vs flexible docking, constraints, consensus rescoring, and fast energy minimization for better pose quality and figures.

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Session 1

Fee: Rs 6300 [Apply Now](#)

Preparation: Receptor & Ligands

Receptor clean-up, protonation and pocket definition

[pdbfixer](#) [PDB2PQR/propka](#) [fpocket](#) [grid/box setup](#)

Ligand standardization: stereochemistry, tautomers, charges

[RDKit](#) [Open Babel](#) [Gasteiger/AM1-BCC](#)

Cofactors, waters and metal handling; restraints & exclusions

[keep/remove rules](#) [pharmacophore hints](#)

Session 2

Fee: Rs 8400 Apply Now

Docking: Rigid/Flexible & Constraints

Search algorithms, parameters and reproducibility settings

AutoDock Vina/Smina **rDock** **GOLD***
exhaustiveness/seeds

Flexible side chains & induced fit strategies (overview)

rotamer sampling **soft potentials** **constraints**
(HB/metal)

Pose clustering and diversity control for top-N selection

RMSD-based clusters **centroid representatives**

Session 3

Fee: Rs 11200 Apply Now

Rescoring & Energy Minimization

Consensus scoring and contact-based sanity checks

Vina/GOLD/rDock scores **PLIP fingerprints** **strain**
flags

Pose relaxation and quick minimization pipelines

MMFF94/UFF/GAFF **OpenMM** **GROMACS (steepest/CG)**

Exporting scenes, tables and 2D diagrams

PyMOL/ChimeraX **LigPlot+** **CSV/TSV bundles**

Session 4

Fee: Rs 14000 Apply Now

Mini Capstone: Dock → Minimize → Report

Dock a small set, relax top poses, and assemble a report bundle

Theory + Practical

Provenance, parameter files and reproducibility checklist

YAML/JSON configs **Conda/Mamba** **Quarto**

Deliverables: figures, tables, README & manifest

PDF **CSV/TSV** **checksums**