

Molecular Docking Benchmarking & Validation Studies — Hands-on

Build trustworthy docking benchmarks and validation reports. Learn dataset curation, unbiased splits, proper metrics, statistical testing, and transparent reporting. Run multi-engine comparisons and summarize performance with reproducible evidence.

Molecular Docking Benchmarking & Validation Studies

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Session 1

Fee: Rs 6300 [Apply Now](#)

Benchmark Design & Datasets

Choosing targets and actives/decoys; leakage and analog bias control

[DUD-E](#) [DEKOIS](#) [PDBbind](#)

Chemistry hygiene: tautomers/protomers, duplicates & data standardization

[RDKit](#) [charge states](#) [salt stripping](#)

Protein prep, grids & binding site definition

cofactors/waters **box size/centers**

Session 2

Fee: Rs 8400 Apply Now

Metrics: Ranking & Poses

Virtual screening metrics & interpretation

ROC-AUC/PR-AUC **EF@1/5/10%** **BEDROC/RIE**

Pose prediction metrics & success criteria

RMSD $\leq$ 2.0 Å **top-n success** **interaction recovery**

Engines & consensus scoring (overview)

Vina/Smina **rDock** **GOLD*/Glide***

Session 3

Fee: Rs 11200 Apply Now

Bias, Stats & Reproducibility

Split strategies & bias checks

scaffold/time-split **property-matched decoys** **Y-randomization**

Statistical testing & uncertainty

bootstrap CI **DeLong for AUC** **paired tests**

Reproducible reports & provenance

configs/seeds/logs **Snakemake/Nextflow** **Quarto**

Session 4

Fee: Rs 14000 Apply Now

Mini Capstone: Build & Defend a Benchmark

Create a target-specific set, run multi-engine VS, and compute

ranking/pose metrics with CIs

Theory + Practical

Consensus/score fusion & sensitivity analyses

rank aggregation **threshold sweeps**

Deliverables: figures, tables, README & manifest

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