

Drug Discovery Informatics & Virtual Screening Workflows — Hands-on

Build a rigorous virtual screening pipeline from raw compound libraries to prioritized hits. Learn curation, filtering, cheminformatics, docking-based HTVS, ML re-ranking, and objective enrichment evaluation with clean, reproducible outputs.

Drug Discovery Informatics & Virtual Screening Workflows

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Session 1

Fee: Rs 6300 [Apply Now](#)

Library Curation & Rule-based Filters

Source libraries and normalization (vendors & public sets)

[ZINC](#) [ChEMBL](#) [Enamine*](#) [PubChem](#)

Standardization, dedupe & salt/tautomer handling

[RDKit](#) [Open Babel](#) [InChI/SMILES](#)

Medicinal chemistry rules & alert filters

[Lipinski/Veber](#) [PAINS/BRENK](#) [REOS/lead-likeness](#)

Session 2

Fee: Rs 8400 Apply Now

Cheminformatics & ML (QSAR/Re-rank)

Descriptors & fingerprints for similarity and QSAR

ECFP4/FCFP MACCS Physchem panel

Modeling & re-ranking strategies (overview)

RF/XGBoost logistic/PLS cross-validation

Data hygiene: balancing, decoys and leakage checks

DUD-E style decoys scaffold split Y-randomization

Session 3

Fee: Rs 11200 Apply Now

Docking HTVS & Enrichment Analytics

High-throughput docking pipelines & batching

AutoDock Vina/Smina rDock GOLD* array jobs

Hit selection & re-scoring with contacts/fingerprints

PLIP/LigPlot+ consensus ranks

Objective evaluation & early recognition metrics

ROC-AUC/PR-AUC EF1%/EF5% BEDROC

Session 4

Fee: Rs 14000 Apply Now

Mini Capstone: VS → Hits → Report

Run a focused VS, re-rank with ML/contacts, and pick top hits

Theory + Practical

Workflow automation & provenance

Snakemake/Nextflow **Conda/Mamba** **Quarto report**

Deliverables: figures, tables, README & manifest

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