Design, execute, and document **virtual screening (VS)** campaigns that translate into actionable hit lists. You will implement **ligand-based** (similarity, shape, pharmacophore) and **structure-based** (docking, consensus rescoring) workflows with rigorous enrichment analytics, filtering, and triage — all packaged as reproducible, audit-ready pipelines.

Virtual Screening Workflows (Ligand-Based & Structure-Based)

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Session 1 — Ligand-Based VS (Similarity/Shape/Pharmacophore) Session 2 — Structure-Based VS (Protein Prep & Docking) Session 3 — Scoring, Re-Scoring & Enrichment Analytics Session 4 — Mini Capstone: VS Campaign & Hitlist

Session 1
Fee: Rs 16800 Apply Now
Ligand-Based VS (Similarity/Shape/Pharmacophore)

Libraries & preparation

enumeration & protonation conformers (ETKDG) diversity/cluster sets

Similarity & shape screening

ECFP/Tanimoto 3D shape overlays pharmacophore fit

Filtering & triage basics

PAINS/Lipinski/Veber dup removal scaffold splits

Session 2
Fee: Rs 19800 Apply Now
Structure-Based VS (Protein Prep & Docking)

Targets & preparation

structure selection & cleanup protonation/tautomer state binding site detection

Docking workflow

search params & exhaustiveness pose clustering constraints & waters

QC & sanity checks

redocking/ROC-Screen decoys & benchmarks pose inspection

Session 3
Fee: Rs 22800 Apply Now
Scoring, Re-Scoring & Enrichment Analytics

Scoring & consensus

empirical vs knowledge-based rescoring & MM/GBSA-lite rank aggregation

Enrichment & metrics

ROC/PR curves EF@1%, BEDROC AUC CI & statistics

Triage & medicinal rules

ADMET & tox filters alerts & liability notes cluster reps & novelty

Session 4

Fee: Rs 26800 Apply Now

Mini Capstone: VS Campaign & Hitlist

Design & execute a hybrid VS campaign

Theory + Practical

Rank, filter & cluster

consensus scoring **PAINS/Lipinski/ADMET**
representative selection

Deliverables

ranked hit list + clusters **enrichment report (ROC/EF)**
reproducible configs/notebook