

Pharmacophore Modeling — Hands-on

Create actionable pharmacophore models that capture the essential interaction patterns driving activity. In this hands-on module you will derive hypotheses from aligned actives and protein–ligand contacts, validate with decoys, and execute ligand-based virtual screening workflows with robust enrichment and triage practices.

Pharmacophore Modeling: Hypothesis Generation & Screening

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Session 1

Fee: Rs 15800 [Apply Now](#)

Concepts, Features & Hypothesis Building

Pharmacophore basics & SAR inputs

[essential vs optional features](#) [exclusion volumes](#)
[feature tolerance/radii](#)

Feature perception & types

[HBD/HBA](#) [aromatic/hydrophobe](#) [pos/neg ionizable](#)

Tooling & workflow setup

RDKit/Pharmit **Open3DAlign/Align-it** **PLIP for contacts**

Session 2

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Alignment, Constraints & Validation

Active set alignment & hypothesis generation

shape/pharmacophore/MCS **multi-conformer handling**
constraints & optionality

Hypothesis scoring & pruning

coverage & selectivity **RMSD/tolerances** **pose sanity checks**

Validation with decoys

DUD-E style decoys **ROC-AUC/EF_{1%}** **early enrichment metrics**

Session 3

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Virtual Screening & Hit Triage

Database prep & multi-conformer libraries

enumeration & protonation **ETKDG conformers**
diversity curation

Search & ranking

pharmacophore fit score **shape/3D similarity**
rescoring & filters (PAINS/Lipinski)

Triage & follow-up

clustering & representative picks **basic docking**
cross-check **synthetic feasibility notes**

Session 4

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Mini Capstone: Enrichment Workflow

Build & validate a hypothesis, then screen

Theory + Practical

Measure enrichment & report

ROC/PR & EF curves **top-N precision** **reproducible
configs**

Deliverables

pharmacophore model file **ranked hit list + clusters**
enrichment report & notebook/script