

Pharmacophore Modeling — Hypothesis Generation & Validation — Hands-on

Build practical skills in pharmacophore modeling for ligand and structure based design. This module covers pharmacophore concepts, feature definition, hypothesis generation and alignment, validation with actives/decoys and pharmacophore based virtual screening so that you can design and defend campaigns for hit discovery, expansion and scaffold hopping.

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Session 1

Fee: Rs 8800 [Apply Now](#)

Pharmacophore Concepts & Feature Types

Role of pharmacophores in discovery workflows

[link between ligands and targets](#) [orthogonal to QSAR and docking](#) [hit finding and scaffold hopping](#)

Pharmacophore feature definitions and chemistry

[H bond donors and acceptors](#) [aromatics, hydrophobes, charges](#) [exclusion volumes and](#)

vectors

Ligand based vs structure based pharmacophores

from aligned active ligands **from protein ligand complexes** **hybrid approaches and use cases**

Session 2

Fee: Rs 11800 Apply Now

Hypothesis Generation & Alignment

Selecting actives and preparing input for models

choosing representative actives **activity thresholds and labels** **tautomers, protonation and 3D conformers**

Ligand alignment and common pharmacophore hypotheses

alignment strategies and reference choice **automatic vs manual hypothesis building** **mandatory vs optional features**

Structure based pharmacophore derivation

extracting features from complexes **interaction pattern guided feature choice** **mapping to known SAR trends**

Session 3

Fee: Rs 14800 Apply Now

Pharmacophore Screening & Enrichment

Preparing libraries and search settings

3D conformer ensembles **feature tolerances and distances** **exclusion volume options**

Running pharmacophore based virtual screening

search modes and hit thresholds **score interpretation** **visual inspection of mapped hits**

Enrichment analysis and hypothesis refinement

actives/decoys based enrichment metrics **feature pruning or tightening** **multiple hypothesis strategy**

Session 4

Fee: Rs 18800 Apply Now

Mini Capstone: End-to-End Pharmacophore Campaign

Designing a pharmacophore campaign for a target

Theory + Practical

Building, validating and deploying a hypothesis

active set and decoy design **screening and enrichment evaluation** **linking results to chemistry ideas**

Deliverables: hypothesis file, screening hits and summary

pharmacophore model export **prioritized hit list (CSV)** **one page report for project teams**