Build practical skills in ligand based pharmacophore modeling and 3D alignment, from identifying key interaction features to building, validating and applying pharmacophore hypotheses. You will work through conformer generation, alignment strategies and screening workflows to design focused libraries and support hit expansion and early lead optimization.

Pharmacophore Modeling & 3D Alignment

Help Desk · WhatsApp

Session Index

Session 1 — Pharmacophore Concepts & Feature Types Session 2 — Conformers, Alignments & Hypothesis Building Session 3 — Pharmacophore Screening & Scoring Session 4 — Mini Capstone: From Actives to Pharmacophore Screen

Session 1
Fee: Rs 8800 Apply Now

Pharmacophore Concepts & Feature Types

Pharmacophore theory and applications

ligand based design   hit expansion   scaffold hopping

Pharmacophore feature definitions

H bond donors and acceptors   aromatic rings and hydrophobes   positive and negative centres

Toolchain overview for pharmacophores

RDKit pharmacophore features   open source viewers

basic project setup

Session 2
Fee: Rs 11800 Apply Now

Conformers, Alignments & Hypothesis Building

Conformer generation for ligand sets

force field based methods | number and pruning of conformers | energy windows

3D alignment strategies

pairwise and multi ligand alignment | shape and feature alignment | reference driven workflows

Building initial pharmacophore hypotheses

common feature extraction | edit and refine hypotheses | constraints and tolerances

Session 3
Fee: Rs 14800 Apply Now

Pharmacophore Screening & Scoring

Setting up pharmacophore based screens

query building | database preparation | conformer ensembles

Scoring, ranking and enrichment checks

fit scores and thresholds | enrichment and hit rates | early recognition thinking

Visual inspection and hypothesis refinement

aligned poses review | add or relax features | iteration with chemists

Session 4
Fee: Rs 18800 Apply Now

Mini Capstone: From Actives to Pharmacophore Screen

Build a pharmacophore from a small active set

Theory + Practical

Run a screening workflow on a compound collection

conformer and alignment setup **hit list generation**
basic enrichment evaluation

Deliverables: pharmacophore model, aligned hits and workflow notebook

pharmacophore file **hit list with poses** **reproducible script or workflow**