AI-Assisted Medicinal Chemistry & Active Learning — Hands-on

Build **AI-assisted medicinal chemistry** workflows that prioritize the right compounds faster. This hands-on module teaches **active learning** for design–make–test–analyze (DMTA), **uncertainty quantification**, **acquisition strategies** for single/multi-objective optimization, and **human-in-the-loop** review. You will ship a **closed-loop pipeline** that proposes compounds under **synthesis-aware constraints** and learns from each experimental round.

AI-Assisted Medicinal Chemistry & Active Learning

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Session Index

Session 1

Fee: Rs 19800 Apply Now

DMTA, Data & Baselines

Design–Make–Test–Analyze (DMTA) loop

campaign framing **labels & assay QC** **bias & leakage checks**

QSAR baselines & featurization

ECFP/physchem/3D (lite) **linear/RF/XGB** **scaffold/time-aware CV**

Toolchain & orchestration

RDKit, scikit-learn, PyTorch | modAL/ALiPy (AL) | notebooks + configs

Session 2

Fee: Rs 22800 Apply Now

Uncertainty, Applicability Domain & Model Lifecycle

Uncertainty quantification (UQ)

ensembles/MC-dropout | conformal prediction | prediction intervals

Applicability domain (AD) & drift

distance/knn density | feature & label drift | retrain triggers

Labeling strategies & HIL review

expert loop & overrides | ELN/LIMS hooks (lite) | audit & provenance

Session 3

Fee: Rs 25800 Apply Now

Acquisition Functions & Multi-Objective (MPO)

Exploration vs exploitation policies

EI/UCB/Thompson | ε-greedy/uncertainty pick | batch/balanced AL

MPO & constraints

Pareto/weighted sums | ADMET & selectivity | synthesis & BB coverage

Campaign patterns

HTS triage & follow-ups | HTE plate designs | diversity quotas

Session 4

Fee: Rs 29800 Apply Now

Mini Capstone: Closed-Loop AL Campaign

Simulate budgeted AL rounds with an oracle

Theory + Practical

Evaluation & reporting

enrichment @k & hit rate | Pareto front & MPO score | chemist-readable rationale

Deliverables

round-wise picks (CSV) | plots & decision cards | configs/notebooks for reruns