

ADMET & Toxicity Prediction — Hands-on

Build trustworthy **ADMET & toxicity prediction** models that accelerate medicinal chemistry while reducing late-stage attrition. This hands-on module covers endpoint design and data curation, classification/regression modeling, panel-based risk scoring, uncertainty estimation, and applicability domain — all delivered as **reproducible pipelines** suitable for audit and reuse.

ADMET & Toxicity Prediction (In Silico)

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Session 1

Fee: Rs 18800 [Apply Now](#)

Endpoints, Data & Curation

ADMET endpoints & study design

[absorption/permeability \(Caco-2/MDCK\)](#) [metabolism \(CYP inhibition/induction\)](#) [tox \(DILI/hERG/Ames\)](#)

Data sources & QC

[standardization \(tautomers/salts\)](#) [dedup & aggregations](#) [unit/threshold harmonization](#)

Feature spaces

[descriptors \(0D–3D\)](#) [fingerprints \(ECFP\)](#) [task-specific](#)

features

Session 2

Fee: Rs 21800 Apply Now

ADMET Modeling & Imbalance

Algorithms & calibration

logistic/RF/XGBoost regression for clearance/logS
probability calibration

Imbalanced learning & metrics

class weights/SMOTE PR-AUC/ROC-AUC/F1 threshold
tuning

Cross-validation & splits

scaffold/time-aware splits nested CV leakage
prevention

Session 3

Fee: Rs 24800 Apply Now

Toxicity Panels, Applicability Domain & Uncertainty

Toxicity endpoints & panels

hERG/Ames/SkinSens/DILI multi-task setups
consensus/rule filters

Applicability Domain (AD)

distance/leverage (Williams) density/nearest
neighbors confidence intervals

Uncertainty & interpretation

bootstrap/ensembles conformal prediction
permutation/SHAP

Session 4

Fee: Rs 28800 Apply Now

Mini Capstone: Risk Triage Pipeline

Build: ingest → model → AD/uncertainty → triage

Theory + Practical

Decisioning & reporting

traffic-light panel risk **model/AD cards** **config + seeds + env**

Deliverables

ranked compounds w/ risk bands **uncertainty & AD summary** **reproducible notebook/script**