Classical QSAR/QSPR Modeling — Hands-on

Develop trustworthy QSAR/QSPR models using well-established linear and nonlinear algorithms. This hands-on module emphasizes sound validation (CV, external test), applicability domain (AD), and transparent reporting aligned with OECD principles. You will implement leak-free pipelines that can be audited, reused, and transferred across projects.

Classical QSAR/QSPR Modeling (Linear & Nonlinear)

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Session Index

Session 1

Fee: Rs 13800 Apply Now

Linear Models (MLR/PLS) & Metrics

Modeling with descriptors & fingerprints

MLR (OLS) basics | **PLS/PLS-DA** | **regularization overview**

Error functions & fit quality

RMSE/MAE/R^2 | **Q^2 (CV)** | **residual analysis**

Pipelines & preprocessing

scaling/centering train/validation/test stratified/scaffold splits

Session 2

Fee: Rs 16800 Apply Now

Nonlinear Models (kNN/SVM/Tree Ensembles)

Algorithms & hyperparameters

kNN (distance/ks) SVM (C, gamma, kernels) RF/GBM (trees, depth)

Tuning & calibration

grid/random/Bayesian search probability calibration class imbalance strategies

Interpretation & fairness

permutation/SHAP feature effects bias checks

Session 3

Fee: Rs 19800 Apply Now

Validation, OECD Principles & Applicability Domain

Validation toolkit

k-fold/nested CV external test set Y-randomization

OECD & transparent reporting

defined endpoint unambiguous algorithm measures of goodness

Applicability Domain (AD)

leverage/Williams plot distance-based AD confidence intervals

Session 4

Fee: Rs 23800 Apply Now

Mini Capstone: End-to-End QSAR

Build & compare linear vs nonlinear models

Theory + Practical

Document & deliver

model cards + AD plots **config + seeds + env** **reproducible notebook/script**

Deliverables

trained models & metrics **external-test report** **Williams plot & AD summary**