

QSAR / QSPR Modeling & Validation — Hands-on

Acquire practical skills in designing, building and validating QSAR/QSPR models for potency, ADMET and physicochemical properties. Starting from curated datasets and descriptor matrices, you will explore linear and nonlinear algorithms, internal and external validation strategies, applicability domain assessment and best practices for transparent, reproducible and regulatory-aware QSAR workflows.

QSAR / QSPR Modeling & Validation

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Session 1

Fee: Rs 8800 [Apply Now](#)

QSAR/QSPR Concepts & Data Preparation

Foundations of QSAR/QSPR modeling

[endpoint definitions](#) [QSAR vs QSPR](#) [applicability & limits](#)

Dataset assembly and curation

[activity units & scaling](#) [structure concordance](#)
[outliers and noise](#)

Train/validation/test strategy

random vs rational splits | time and series aware splits | class balance checks

Session 2

Fee: Rs 11800 | Apply Now

Model Building: Linear & Nonlinear Methods

Classical QSAR and regression models

MLR / PLS | logistic models | regularized linear models

Machine learning QSAR/QSPR

Random Forest | Gradient Boosting | SVM and k-NN

Hyperparameters and feature handling

cross validation grids | descriptor selection basics | overfitting warning signs

Session 3

Fee: Rs 14800 | Apply Now

Validation & Applicability Domain

Internal and external validation metrics

R^2 / Q^2 / RMSE | ROC-AUC / accuracy | Y randomization checks

Applicability domain concepts and methods

leverage and distance plots | k-NN based domain descriptor space coverage

Guidelines and reporting expectations

OECD QSAR principles (high level) | transparency of models | basic uncertainty discussion

Session 4

Fee: Rs 18800 Apply Now

Mini Capstone: End-to-End QSAR/QSPR Model

From curated descriptors to validated model

Theory + Practical

Build, tune and test a QSAR/QSPR model

train/validation/test workflow **AD and Y-scrambling**
checks **prediction for new compounds**

Deliverables: model file, metrics sheet and short QSAR summary

notebook or script **CSV with predictions** **PDF/HTML**
model report