

Feature Selection & Model Reproducibility — Hands-on

Design robust QSAR/QSPR feature spaces and validation strategies that generalize. This module focuses on principled feature selection, collinearity control, leakage prevention, and reproducibility practices. You will implement end-to-end, audit-ready pipelines with nested cross-validation, proper reporting, and artifacts for reuse.

Feature Selection & Model Reproducibility for QSAR/QSPR

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Session Index

[Session 1 — Data Hygiene & Collinearity Control](#) [Session 2 — Filter/Wrappers/Embedded & Dimensionality Reduction](#) [Session 3 — Validation: Nested CV, Leakage & Stability](#) [Session 4 — Mini Capstone: Reproducible FS Pipeline](#)

Session 1

Fee: Rs 12800 [Apply Now](#)

Data Hygiene & Collinearity Control

Pre-FS checks & filters

[missingness & imputation](#) [variance/near-zero variance](#) [scaling/normalization](#)

Collinearity diagnostics

[correlation matrices](#) [VIF thresholds](#) [cluster-based pruning](#)

Train/test hygiene

scaffold/stratified splits no peeking policies
pipelines for transformations

Session 2

Fee: Rs 15800 Apply Now

Filter/Wrappers/Embedded & Dimensionality Reduction

Filter methods

univariate tests mutual information mRMR

Wrappers & embedded

RFE/RFE CV Boruta/SHAP Lasso/Elastic Net

Dimension reduction

PCA/PLS UMAP for EDA targets & scaling effects

Session 3

Fee: Rs 18800 Apply Now

Validation: Nested CV, Leakage & Stability

Leakage-safe pipelines

Pipeline/ColumnTransformer fit/transform
boundaries temporal/scaffold splits

Model selection the right way

nested cross-validation grouped CV bootstrap
stability

Sanity checks & AD

y-scrambling permutation tests applicability domain

Session 4

Fee: Rs 22800 Apply Now

Mini Capstone: Reproducible FS Pipeline

Build: filter → FS → model → validate

Theory + Practical

Report & artifacts

config YAML/JSON **random seeds & env lock**
model/FS cards

Deliverables

reproducible notebook/script **metrics + stability**
plots **pipeline diagram**