Classical QSAR — Hansch, Free–Wilson & ML QSAR — Hands-on

Develop end to end QSAR skills starting from classical Hansch and Free–Wilson formulations through to modern ML based QSAR models. This module focuses on chemically sensible descriptor use, statistically sound model building, applicability domain, and transparent reporting that can survive peer review and regulatory scrutiny.

Classical QSAR — Hansch Free Wilson & ML QSAR

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Session Index

Session 1

Fee: Rs 8800 Apply Now

Classical QSAR Foundations (Hansch & Free–Wilson)

Historical perspective and QSAR problem framing

origin of QSAR | **structure activity relationships** | **when QSAR is appropriate**

Hansch analysis concepts

hydrophobic, electronic, steric terms | **linear and parabolic models** | **interpretation of coefficients**

Free–Wilson analysis and substituent constants

fragment contribution ideas **indicator variables** **link to modern fragment based design**

Session 2
Fee: Rs 11800 Apply Now

Linear Model Building, Validation & Domain

Regression setup and dataset partitioning

training vs test vs external set **response scaling / log transforms** **dealing with assay noise**

Internal validation and statistics

R^2, adjusted R^2, RMSE **Q^2, cross validation schemes** **Y randomization checks**

Applicability domain and outlier analysis

leverage plots (Williams) **influential points** **reporting prediction bounds**

Session 3
Fee: Rs 14800 Apply Now

ML QSAR: Nonlinear Models & Best Practices

From linear QSAR to ML QSAR

when linear models break down **nonlinearity and interactions** **choice of algorithms**

Common ML QSAR algorithms

Random Forest and gradient boosting **SVM and kNN QSAR** **simple neural networks**

Best practices and pitfalls in ML QSAR

data leakage and overfitting **hyperparameter search**

external test discipline

Session 4

Fee: Rs 18800 Apply Now

Mini Capstone: Build, Validate & Report a QSAR

Selecting a dataset and framing the QSAR objective

Theory + Practical

Implementing a complete QSAR workflow

descriptor subset and model choice validation stats and domain comparison of linear vs ML model

Deliverables: QSAR report and deployment ready model files

notebook or script with pipeline summary table of metrics model file and readme