

Predicting Physicochemical Properties — Hands-on

Build reliable **physicochemical property predictors** for **pKa**, **logP/logD**, and **solubility**. This hands-on module spans data curation and standardization, **fragment-based/QM/COSMO-style** approaches, and **machine-learning regression** with microstate-aware calculations. You will generate **pH-dependent** property panels, calibrate against reference sets, quantify uncertainty, and craft design rules that translate to medicinal chemistry decisions.

Predicting Physicochemical Properties (pKa, logP/logD, Solubility)

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Session 1

Fee: Rs 19800 [Apply Now](#)

Endpoints, Data & Microstates

Definitions & measurement contexts

[pKa \(macro vs micro\)](#) [logP vs logD](#) [kinetic vs thermodynamic solubility](#)

Curation & standardization

[salts/tautomers/neutralization](#) [unit/condition harmonization](#) [scaffold/time-aware splits](#)

Tautomers & protonation states

microstate enumeration **population weighting** **pH-dependent properties**

Session 2

Fee: Rs 22800 Apply Now

Models: Fragment, QM & ML

Fragment/fragment-additivity baselines

H substituent constants **Hansch/Taft-style parameters** **descriptor engineering**

QM/COSMO-style methods (lite)

microspecies energies **implicit solvent ideas** **computational cost vs accuracy**

ML regressors for properties

RF/XGBoost/linear baselines **graph/transformer (optional)** **regularization & CV**

Session 3

Fee: Rs 25800 Apply Now

Calibration, pH-Dependence & Uncertainty

External calibration & transfer

holdout/external sets **domain shift checks** **bias/variance review**

pH profiles & logD curves

speciation vs pH **permeability & ionization** **biorelevant media notes**

Uncertainty & AD

ensembles/bootstrap **conformal intervals**

applicability domain flags

Session 4

Fee: Rs 29800 Apply Now

Mini Capstone: Property Panel & Design Rules

Build a property panel pipeline (pKa, logP/logD, Solubility)

Theory + Practical

pH-profiled outputs & flags

logD curves **ionization & permeability notes**

solubility risk bands

Deliverables

ranked compound sheet (CSV) **calibrated report**

(PDF/HTML) **configs/notebooks for reruns**