

Molecular Descriptors & Fingerprints — Hands-on

Generate robust molecular features for cheminformatics and QSAR. This module covers descriptor theory and practice across 0D–3D properties and popular fingerprints, along with best practices for data hygiene, scaling, variance/collinearity diagnostics, and exportable, reproducible feature matrices.

Molecular Descriptors & Fingerprints (0D–3D, ECFP)

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Session 1

Fee: Rs 11800 [Apply Now](#)

Descriptor Landscape (0D–3D)

0D/1D/2D descriptors overview

[formulae, counts](#) [topological indices](#)
[physicochemical props \(logP, TPSA\)](#)

Tooling

[RDKit](#) [Mordred](#) [PaDEL-Descriptor](#)

Reproducibility & hygiene

standardization before calc missing/NaN handling
units & provenance

Session 2

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Fingerprints (ECFP/Morgan, MACCS, Paths)

Binary & count fingerprints

ECFP/Morgan radius & nBits MACCS keys
topological/Daylight-like

Similarity & diversity

Tanimoto/Jaccard Butina clustering scaffold splits

Sparse matrices & storage

CSR/COO formats feature hashing binary vs count
use-cases

Session 3

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Conformers, 3D Descriptors & QA

Conformer generation

ETKDG & MMFF/UFF energy minimization ensemble
selection

3D descriptors

WHIM & MoRSE autocorrelations pharmacophore
counts

Quality checks

variance/near-constant filters correlation heatmaps
missingness & imputation

Session 4

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Mini Capstone: Feature Matrix Build

Pipeline: standardize → compute → validate

Theory + Practical

Scaling & export

z-score/robust scaling **sparse FP matrices** **CSV/NPZ +
YAML config**

Deliverables

feature matrix & data dictionary **QA report**
(variance/corr) **reproducible notebook/script**