

Molecular Descriptors 0D–3D & Feature Engineering — Hands-on

Develop a strong working knowledge of molecular descriptors from 0D counts to 3D shape indices, and how they feed into QSAR, ADMET and virtual screening workflows. You will generate, inspect and engineer descriptors and fingerprints using RDKit and KNIME, and learn how to prepare a high quality feature matrix that is ready for cheminformatics modeling and analytics.

Molecular Descriptors 0D–3D & Feature Engineering

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Session Index

[Session 1 — Descriptor Landscape & Physicochemical Properties](#) [Session 2 — Structural, Topological & 3D Descriptors](#) [Session 3 — Fingerprints & Feature Engineering](#) [Session 4 — Mini Capstone: Descriptor Matrix for Modeling](#)

Session 1

Fee: Rs 8800 [Apply Now](#)

Descriptor Landscape & Physicochemical Properties

Types of molecular descriptors and use cases

[0D / 1D / 2D / 3D](#) [global vs local](#) [QSAR / ADMET / VS](#)

Basic physicochemical descriptors

[molecular weight](#) [logP / logS](#) [HBA / HBD / TPSA](#)

Toolchain and calculation basics

RDKit descriptor modules **KNIME nodes** **simple descriptor sanity checks**

Session 2

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Structural, Topological & 3D Descriptors

2D structural and fragment descriptors

atom and bond counts **ring systems** **substructure flags**

Topological and connectivity indices

Wiener index **Balaban index** **kappa / chi indices**

3D and conformation based descriptors

shape descriptors **3D polar surface** **conformer generation basics**

Session 3

Fee: Rs 14800 Apply Now

Fingerprints & Feature Engineering

Circular and path based fingerprints

ECFP / FCFP **Morgan fingerprints** **MACCS keys**

Scaling, transforms and encoding strategies

standardization / normalization **log transforms** **one hot and binning**

Feature quality and reduction

variance and correlation filters **PCA overview** **basic feature selection ideas**

Session 4

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Mini Capstone: Descriptor Matrix for Modeling

From curated structures to descriptor table

Theory + Practical

Apply descriptor calculation and feature processing

physicochemical panel **fingerprint generation** **scaling**
and basic filtering

Deliverables: descriptor matrix and reproducible workflow

feature matrix CSV **RDKit or KNIME workflow**
environment or node list