

Drug Discovery Fundamentals & Cheminformatics Basics — Hands-on

Build a strong foundation in modern small-molecule drug discovery and cheminformatics. From the R&D pipeline and target selection to chemical space, molecular properties and in-silico thinking, this module prepares you for downstream QSAR, virtual screening, docking and ADMET workflows in later tracks.

Drug Discovery Fundamentals & Cheminformatics Basics

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Session 1

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Drug Discovery Landscape & R&D Pipeline

Pharma R&D lifecycle and discovery pipeline

[discovery](#) → [preclinical](#) → [clinical](#) [attrition & decision gates](#) [small vs large molecules](#)

Target product profiles and modality choices

[TPP & unmet need](#) [small molecules / biologics / peptides](#) [risk/benefit framing](#)

Role of in-silico methods in discovery

virtual screening **QSAR & property prediction** **ADMET & risk triage**

Session 2

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Targets, Ligands & Chemical Space

Target selection and validation concepts

genetic & pathway evidence **phenotypic vs target-based** **druggability**

Ligand types and binding basics

agonist / antagonist / inhibitor **affinity & potency** **selectivity & off-targets**

Chemical space and libraries

fragments & scaffolds **HTS vs focused sets** **diversity vs depth**

Session 3

Fee: Rs 14800 Apply Now

Cheminformatics Foundations & Toolchain

Molecular file formats and identifiers

SMILES / canonical SMILES **InChI / InChIKey** **SDF / MOL2**

Basic molecular properties and rules

MW, logP, HBD/HBA **Lipinski & Veber rules** **alerts & red flags**

Open-source toolchain overview

RDKit (Python) **KNIME workflows** **Open Babel & CDK**

basics

Session 4

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Mini Capstone: From Brief to Design Sketch

Framing a simple discovery problem and constraints

Theory + Practical

Searching and curating a small virtual library

PubChem / ChEMBL concepts **basic filters & rules**
simple prioritization grid

Deliverables: rationale, library sheet and next-step plan

spreadsheet with key properties **one-page design**
note **link to future QSAR/VS modules**