

Foundations of Cheminformatics & Molecular Representations — Hands-on

Build a rock-solid foundation in cheminformatics by learning how molecules are represented, validated, standardized, and exchanged across tools and pipelines. You will work hands-on with RDKit and Open Babel to parse, sanitize, canonicalize, and export structures in industry-standard formats with best practices for reproducibility.

Foundations of Cheminformatics & Molecular Representations (SMILES/InChI)

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Session Index

Session 1 — SMILES, InChI & Stereochemistry Session 2 — File Formats, Parsing & Sanitization
Session 3 — Canonicalization & Standardization Session 4 — Mini Capstone: Library Curation

Session 1

Fee: Rs 9800 [Apply Now](#)

SMILES, InChI & Stereochemistry

SMILES fundamentals & tokens

rings & branches **aromaticity models** **charges & isotopes**

InChI & InChIKey

layers & normalization **use in de-duplication**
identifier hygiene

Stereochemistry

R/S, E/Z **@ / @@ in SMILES** **double bond stereo**

Session 2

Fee: Rs 12800 Apply Now

File Formats, Parsing & Sanitization

Exchange formats & interop

SDF / MOL / MOL2 **SMI / CSV** **PDBQT basics**

RDKit & Open Babel toolchain

parsing & sanitization **valence/kekulization** **error handling**

Metadata & properties

SDF data fields **round-tripping** **SMILES canonical vs. input**

Session 3

Fee: Rs 15800 Apply Now

Canonicalization & Standardization

Canonical SMILES & uniqueness

hashing & IDs **tautomers & protonation** **salt/solvent stripping**

Normalization workflows

neutralization **aromaticity model choice** **standard tautomers**

InChI/InChIKey in pipelines

de-dup & merge **cross-database linking** **identifier QA/QC**

Session 4

Fee: Rs 19800 Apply Now

Mini Capstone: Library Curation

Curate a vendor/HTS library

Theory + Practical

Deduplicate, standardize & export

InChIKey de-dup **descriptor precompute** **SDF/SMI/CSV**
deliverables

Deliverables: standardized set & report

QA/QC checklist **pipeline script/notebook** **method**
notes