

Chemical Databases, Identifiers & Normalization — Hands-on

Build practical skills in working with chemical databases and identifiers. Starting from public sources such as PubChem and ChEMBL, you will learn how to retrieve, merge, de-duplicate and normalize compounds, assign stable identifiers and create registration-ready libraries for QSAR, ADMET and screening workflows.

Chemical Databases, Identifiers & Normalization

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Session 1

Fee: Rs 8800 [Apply Now](#)

Chemical Databases Landscape & Schemas

Major chemistry resources and use cases

[PubChem / ChEMBL / ChEBI](#) [vendor libraries](#) [in-house databases](#)

Data models, entities and relationships

[compound vs salt vs batch](#) [assay and activity tables](#) [metadata fields](#)

Toolchain and basic access

web UI and REST APIs **Python clients** **simple SQL views**

Session 2

Fee: Rs 11800 **Apply Now**

Querying & Integrating Public Repositories

Search strategies and filters

substructure / similarity **property filters** **activity based queries**

Bulk download and parsing workflows

SDF / CSV exports **compression and chunks** **incremental updates**

Merging multi-source compound sets

ID mappings **schema alignment** **basic FAIR checks**

Session 3

Fee: Rs 14800 **Apply Now**

Registration, IDs & Normalization Rules

Internal identifiers and primary keys

compound IDs **salt / batch IDs** **link to external IDs**

Normalization and de-duplication logic

parent / child relationships **salt stripping** **duplicate detection**

Audit trails and change tracking

versioned records **registration logs** **simple QC reports**

Session 4

Fee: Rs 18800 Apply Now

Mini Capstone: Clean, Linked Compound Set

Create a small registration-ready compound collection

Theory + Practical

Apply merge, normalization and ID assignment workflow

multi source merge **duplicate removal** **external cross references**

Deliverables: normalized table, mapping file and short QC summary

CSV tables **ID mapping file** **notebook or script**