

Cheminformatics for Natural Products & Phytochemicals — Hands-on

Work end-to-end on **natural products (NP)** and **phytochemicals** with the right informatics. This hands-on module covers **dereplication** (formula/adduct logic, MS/MS library search), **molecular networking**, **NP-likeness/scaffold analysis**, stereochemistry & conjugates (glycosides/terpenoids), **bioactivity annotation**, and **reproducible curation** workflows for discovery and nutraceutical R&D.

Cheminformatics for Natural Products & Phytochemicals

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Session 1

Fee: Rs 18800 [Apply Now](#)

NP Data, Curation & Stereochemistry

Sources & ontologies

[COCONUT](#), [NP Atlas](#), [ChEBI](#) [taxonomic & botanical metadata](#) [bioactivity & assay tags](#)

Curation specifics for NPs

[mixtures/extracts handling](#) [glycosides/conjugates](#)

stereocenters & macro stereochemistry

ID & normalization

SMILES/InChI for NPs **tautomers/adduct notes**

vendor/collection mapping

Session 2

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Dereplication & Molecular Networking

Formula/adduct-aware dereplication

exact mass & isotopes **[M+H]⁺ / [M-H]⁻ heuristics**
library/MS/MS search

Molecular networking (GNPS-style)

spectral similarity graphs **annotation levels &**
propagation **cluster to scaffold hints**

Feature → structure triage

in-silico fragments **derep hit ranking** **reporting**
templates

Session 3

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NP-Likeness, Scaffolds & Bioactivity Maps

NP-like space & scaffolds

scaffold trees/rings **NP-likeness score** **chemotype**
tagging

Bioactivity & pathway context

target/mechanism links **assay harmonization**
polypharmacology hints

Synthesis/derivatization ideas

semi-synthetic derivatives **de-glycosylation**
strategies **IP/novelty flags (lite)**

Session 4

Fee: Rs 28800 Apply Now

Mini Capstone: From Extract to Candidates

Build an extract → derep → network → shortlist pipeline

Theory + Practical

Reporting & deliverables

candidate list + NP-likeness **network & derep report**
metadata pack (taxonomy/assays)

Optional next steps

semi-synthesis proposals **in silico ADMET screen** **IP**
scan pointers