Explore how cheminformatics can be applied to natural products and their semi-synthetic analogs. You will work with natural product style datasets, annotate structures and scaffolds, and examine simple derivatization and analog design concepts in silico to support discovery and property optimization, without performing laboratory synthesis guidance.

Cheminformatics for Natural Products & Derivatization

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Session 1
Fee: Rs 8800   Apply Now

Natural Products Space & Data Foundations

Natural products in discovery (conceptual overview)

structural diversity and complexity   privileged motifs and scaffolds   semi synthetic analogs idea

Data sources and formats for natural products (high level)

library and database style collections   structure plus basic metadata   curation and consolidation ideas

Simple views of natural products chemical space

property distributions (conceptual) NP like vs synthetic like regions series and families of interest

Session 2
Fee: Rs 11800 Apply Now

Structures, Scaffolds & Annotation for Naturals

Handling complex natural product structures (idea level)

rings, stereocenters and macrocycles basic representation concerns consistency checks conceptually

Scaffold and fragment views for natural products

core vs decoration thinking motif annotation (informal) families and clusters

Simple annotation of origin and context (non lab)

source type fields (conceptual) target or pathway tags (overview) linking to reference metadata

Session 3
Fee: Rs 14800 Apply Now

Analog Design, Derivatization & Profiling

Analog and derivatization thinking (non procedural)

site of modification ideas decoration vs core changes simple chemotype exploration

In silico property and similarity profiling of NP analogs

basic descriptors and property grids similarity to parent and series distribution views (conceptual)

Communicating NP analog and derivatization options (high level)

maps of analog sets simple prioritization tables non prescriptive suggestion notes

Session 4
Fee: Rs 18800 Apply Now

Mini Capstone: Natural Product Series Pack

Assemble and annotate a small natural product style series

Theory + Practical

Create scaffold, analog and property overview views (in silico only)

scaffold and decoration map property distribution plots simple similarity panels

Deliverables: natural product series informatics summary pack

curated dataset snapshot plots and scaffold diagrams PDF/HTML narrative overview