Compound Library Design, Diversity & Enrichment — Hands-on

Learn how to organise and review compound libraries from a cheminformatics perspective. You will explore diversity and chemical space concepts at a high level, use simple selection and enrichment ideas, and prepare concise views that support screening ready and focused library decisions without giving any synthesis or procurement guidance.

Compound Library Design, Diversity & Enrichment

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Session 1
Fee: Rs 8800 Apply Now
Library Concepts & Strategy Overview

Types of libraries and high level strategy

screening, focused and follow up sets broad vs targeted coverage ideas series and scaffold based views

Basic inputs for library design discussions

structures and key properties simple annotation

fields assay and project context snapshots

High level objectives for library design work

coverage of ideas and chemotypes reasonable property profiles clear and concise summaries

Session 2
Fee: Rs 11800 Apply Now

Chemical Space & Diversity Views

Simple representations of library chemical space

property distributions conceptually scatterplots and map style views regions of interest and gaps

Diversity and similarity thinking at series level

fingerprint based similarity ideas clusters and neighbourhoods overview simple measures of spread and overlap

Scaffolds, subseries and coverage views (conceptual)

core and decoration based grouping representation of subseries coverage of chemotype families

Session 3
Fee: Rs 14800 Apply Now

Selection, Enrichment & Prioritisation

Concepts for selecting subsets from a library

balanced subsets vs minimal sets property and scaffold filters (idea) subsets for pilots and screens

Enrichment views for targets or themes (high level)

annotated subsets and tags simple hit rate style summaries heatmap and table style reports

Library triage and prioritisation narratives (non prescriptive)

ranking subsets with clear caveats highlighting strengths and gaps suggesting follow up review points

Session 4
Fee: Rs 18800 Apply Now
Mini Capstone: Library Design & Enrichment Brief

Prepare a small virtual compound library overview

Theory + Practical

Create diversity and chemical space views for the set

property and similarity plots simple scaffold and subset maps coverage and gap highlights

Deliverables: library design and enrichment summary pack

overview table of compounds 2–3 key plots or grids PDF/HTML narrative brief