

## Library Design, Synthesis Prioritization & DQA — Hands-on

Learn how to design, score and prioritize small molecule libraries that are both chemistry realistic and project relevant. This module focuses on focused and diverse library strategies, multiparameter profiles, synthesis feasibility signals and practical design quality assessment (DQA) so that project teams receive libraries they can actually progress.

# Library Design Synthesis Prioritization & DQA

[Help Desk · WhatsApp](#)

### Session Index

[Session 1 — Library Design Strategies & Chemotypes](#) [Session 2 — Scoring, Ranking & Multiparameter Profiles](#) [Session 3 — Synthesis Feasibility, Retrosynthesis & DQA](#) [Session 4 — Mini Capstone: Library Design & Prioritization](#)

### Session 1

**Fee: Rs 8800** [Apply Now](#)

## Library Design Strategies & Chemotypes

Roles of libraries across discovery stages

[HTS, fragment, focused and follow up sets](#) [hit expansion vs exploratory libraries](#) [library objectives and constraints](#)

Chemotypes, scaffolds and enumeration basics

[core scaffolds and R group positions](#) [enumeration rules and patterns](#) [chemical space coverage vs focus](#)

Diversity, similarity and property space views

**similarity metrics and clustering** **physchem filters**  
**and sweet spots** **balancing novelty with known space**

## **Session 2**

**Fee: Rs 11800** Apply Now

### **Scoring, Ranking & Multiparameter Profiles**

Scoring functions for library members

**simple potency or activity proxies** **physchem and**  
**ADMET score components** **synthetic accessibility**  
**signals at high level**

Multiparameter optimization and MPO style scores

**combining properties into MPO functions** **visualizing**  
**trade offs and Pareto ideas** **rule based cutoffs vs soft**  
**scores**

Ranking, clustering and representative selection

**rank lists with diversity constraints** **picking cluster**  
**representatives** **shortlists for screening and**  
**synthesis**

## **Session 3**

**Fee: Rs 14800** Apply Now

### **Synthesis Feasibility, Retrosynthesis & DQA**

Synthesis feasibility concepts for library design

**building block availability thinking** **simple route**  
**complexity signals** **what synthetic teams typically**  
**flag**

Retrosynthesis hints and simple feasibility scores

**rule based and ML style feasibility scores** **using**

**vendor and building block catalogs** **flags for difficult functional groups**

Design Quality Assessment (DQA) for libraries

**checklists for design quality** **traffic light views for risk dimensions** **summary metrics for project review**

#### **Session 4**

**Fee: Rs 18800** Apply Now

### Mini Capstone: Library Design & Prioritization

Framing a small library brief for a target or series

**Theory + Practical**

Designing, scoring and filtering a candidate library

**enumeration of a focused set** **MPO scoring and diversity checks** **feasibility and DQA traffic lights**

Deliverables: library proposal and DQA summary

**spreadsheet or table of candidates** **plots for property and diversity views** **two to three slide library summary deck**