De Novo Design — Generative Models & Constraint Learning — Hands-on

Learn how to use modern generative models to propose molecules from scratch under realistic discovery constraints. This module covers de novo design concepts, sequence and graph based architectures, conditioning and constraint learning, multi objective scoring and human in the loop triage so that you can prototype small generative campaigns that plug into your docking, QSAR and ADMET workflows.

De Novo Design — Generative Models & Constraint Learning

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Session Index

Session 1

Fee: Rs 8800 Apply Now

Foundations of De Novo Design & Generative Chemistry

From library screening to de novo proposals

design space and chemical space ideas **when generative design adds value** **fit with docking QSAR and ADMET tools**

Molecular representations for generative models

SMILES and SELFIES strings | graph based representations | 3D aware ideas at a high level

Data sets and curation for generative chemistry

public chemistry collections | basic filtering and sanitization rules | splits, leakage and realistic benchmarking

Session 2

Fee: Rs 11800 Apply Now

Generative Architectures, Objectives & Constraints

Model families used in de novo design

RNN and auto regressive models | VAEs, GANs and reinforcement loops | transformer and diffusion style approaches

Conditioning and goal directed generation concepts

conditioning on targets, scaffolds or properties | reward functions and policy style updates | controlling exploration vs exploitation

Constraint learning and chemistry aware rules

physchem and structural alerts as constraints | SMARTS based forbidden patterns | simple synthesis and liability aware rules

Session 3

Fee: Rs 14800 Apply Now

Scoring, Filtering & Human in the Loop Design

Scoring functions for de novo molecules

QSAR and property predictors | docking and pharmacophore scores | simple ADMET and MPO style scores

Filtering, diversity and novelty checks

rule based and property filters | similarity, diversity and clustering views | novelty vs known chemistry balance

Human in the loop design and shortlists

interactive review and chemist input | shortlists for synthesis discussion | logging rationale and constraints used

Session 4

Fee: Rs 18800 Apply Now

Mini Capstone: De Novo Campaign Prototype

Framing a realistic de novo design brief

Theory + Practical

Running a small generative loop with constraints and scoring

generate and filter a focused set | apply multi objective scores | select shortlists for discussion

Deliverables: de novo design notebook and idea shortlist

workflow notebook or script | ranked molecule table with scores | one to two slide summary for project teams