De Novo Design & Generative Chemistry — Hands-on

Build a practical understanding of de novo molecular design and generative chemistry for discovery projects. You will work with SMILES and graph based representations, explore generative model concepts, use simple scoring and property filters to steer design, and assemble a transparent, reproducible generative loop that hands over realistic ideas to medicinal chemistry teams.

De Novo Design & Generative Chemistry

Help Desk · WhatsApp

Session Index

Session 1 — De Novo Design Concepts & Representations | Session 2 — Generative Models for Molecules | Session 3 — Scoring, Property Biasing & Filters | Session 4 — Mini Capstone: Generative Design Loop

Session 1

Fee: Rs 8800 Apply Now

De Novo Design Concepts & Representations

Roles of de novo design in discovery

idea generation **scaffold exploration** **design make test cycles**

Molecular representations for generation

SMILES and canonical SMILES **molecular graphs fragments and scaffolds**

Toolchain and quality checks for generated molecules

RDKit sanitization | basic property panels | invalid and duplicate handling

Session 2

Fee: Rs 11800 Apply Now

Generative Models for Molecules

Families of generative models (high level)

RNN and sequence based | autoencoder style models | graph oriented ideas

Sampling strategies and diversity handling

temperature and top k sampling | random seeds | duplicate and analogue control

Simple workflows for model usage

scripted generation runs | saving and reusing samples | logging parameters and outputs

Session 3

Fee: Rs 14800 Apply Now

Scoring, Property Biasing & Filters

Scoring functions for generated molecules

simple property scores | QSAR model scores | basic docking score usage

Multi objective and constrained design ideas

potency and ADMET trade offs | score aggregation | simple desirability functions

Filtering and triage of generated sets

PAINS and reactive groups | property and rule filters | diversity aware down selection

Session 4

Fee: Rs 18800 Apply Now

Mini Capstone: Generative Design Loop

Set up a small generative design cycle

Theory + Practical

Generate, score and filter candidate molecules

generation runs | property and ADMET scoring | hit list triage

Deliverables: scored idea set and documented workflow

SMILES list with scores | short ranking report | notebook or script for reruns