Learn to build and deploy **generative models for molecular design** using **RNNs, VAEs, and Diffusion**. This hands-on module covers dataset curation/tokenization, model training and sampling, **goal-directed optimization** with property predictors, and **synthesis-aware triage** (rules, SA/SCScore, basic retrosynthesis stubs). Deliverables include a reproducible pipeline that generates, filters, and prioritizes novel compounds.

# Generative Models for Molecule Design (RNN/VAE/Diffusion)

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## Session 1
**Fee: Rs 20800**   Apply Now

## Data, Tokens & Foundations

### Design datasets & curation

standardization (salts/tautomers)  dedup/scaffold splits  train/val/test hygiene

### Representations & tokens

SMILES/SELFIES  graphs (optional)  validity/uniqueness/novelty

Pipelines & infra

`config/seed mgmt` `checkpointing` `reproducible runs`

**Session 2**
**Fee: Rs 23800** Apply Now

## RNN/VAE/Diffusion: Training & Sampling

Model architectures & losses

`RNN (LSTM/GRU) LM` `VAE (KL, β-VAE)` `Diffusion (noise sched.)`

Training & sampling controls

`teacher forcing/temp/top-k` `validity/uniqueness checks` `diversity/novelty metrics`

Conditioning hooks (optional)

`property-conditional inputs` `scaffold/fragment control` `prompted generation`

**Session 3**
**Fee: Rs 26800** Apply Now

## Goal-Directed & Multi-Objective Design

Property prediction in the loop

`QSAR surrogates` `ADMET panels` `docking-in-the-loop (lite)`

Optimization strategies

`reinforcement learning (policy)` `Bayesian/iterative selection` `Pareto & weighted sums`

Constraints & controls

`PAINS/Lipinski/Veber` `scaffold retention/avoid` `novelty vs similarity`

**Session 4**
**Fee: Rs 30800** Apply Now

## Mini Capstone: Design → Filter → Prioritize

Generate a targeted library & screen

**Theory + Practical**

Synthesis-aware triage

**SA/SCScore** **fragment/BB coverage** **basic retrosynthesis stubs**

Deliverables

**generated set + validity/novelty** **ranked list (multi-objective)** **report + configs/notebooks**