

## Peptide & Macrocycle Informatics — Hands-on

Master **peptide & macrocycle informatics** from sequence design to structure-aware screening. This hands-on module covers **cyclization strategies** (head-to-tail, side-chain, stapling), **conformation sampling** and property prediction (permeability, polarity, proteolysis), **macrocycle descriptors**, and **docking/MD-lite** evaluation. You will ship a **reproducible pipeline** to enumerate, filter, and prioritize peptide/macrocycle candidates with **synthesis-aware** constraints.

# Peptide & Macrocycle Informatics: Design & Screening

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### Session 1

**Fee: Rs 20800** [Apply Now](#)

## Building Blocks, Cyclization & Enumeration

AAs & non-canonical units

[L/D amino acids](#) [N-methyl,  \$\beta/\gamma\$ -AAs](#) [linkers & spacers](#)

Cyclization strategies

[head-to-tail / side-chain](#) [disulfide / lactam bridges](#)  
[hydrocarbon stapling](#)

Enumeration & constraints

**SMARTS rules** **position-specific libraries** **synthesis-aware filters**

### **Session 2**

**Fee: Rs 23800** Apply Now

## **Conformations, Descriptors & Permeability**

Conformational sampling

**distance geometry / ETKDG** **low-mode / torsion scans**  
**solvent-aware pruning**

Macrocycle descriptors

**PMI / 3D shape** **tPSA / HBD/HBA (exposed)** **intra-H bonds / chameleonicity**

Permeability & stability

**Caco-2 heuristics** **protease site flags** **serum stability hints**

### **Session 3**

**Fee: Rs 26800** Apply Now

## **Docking/Scoring & MD-lite Stability**

Pose generation for macrocycles

**conformer → docking** **induced-fit (lite)** **constraint docking (hotspots)**

Scoring & rescoring

**consensus scores** **interaction fingerprints**  
**strain/entropy notes**

MD-lite stability checks

**short relax simulations** **H-bond & RMSD traces**  
**binding mode persistence**

**Session 4**

**Fee: Rs 30800** Apply Now

## Mini Capstone: Library → Shortlist

Build an enumerate → sample → score → shortlist pipeline

**Theory + Practical**

Developability & synthesis awareness

**permeability & protease risk bands** **stapling/disulfide**  
**feasibility** **vendor BB coverage**

Deliverables

**ranked shortlist (CSV)** **poses & MD-lite plots**  
**configs/notebooks for reruns**