

AI-Driven Biomolecular Modeling — Hands-on

Use state-of-the-art AI to predict, assess, and apply protein structures. Learn how to craft MSAs, select templates, interpret confidence metrics, run monomer/multimer jobs, and prepare AI models for downstream tasks like docking, design, and variant analysis—with reproducible, automated pipelines.

AI-Driven Biomolecular Modeling (AlphaFold, RoseTTAFold, ESMfold)

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Session Index

[Session 1 — Foundations: MSAs, Templates & Metrics](#)

[Session 2 — Running](#)

[AlphaFold/RoseTTAFold](#)

[Session 3 — ESMFold, Multimers & Refinement](#)

[Session 4 — Mini](#)

[Capstone: AI Model → Application](#)

Session 1

Fee: Rs 6300 [Apply Now](#)

Foundations: MSAs, Templates & Metrics

MSA and template strategy for robust predictions

[HHblits/JackHMMER](#) [MMseqs2](#) [PDB templates](#)

Confidence metrics and model selection

[pLDDT](#) [PAE](#) [iptm/ptm \(multimer\)](#)

Pitfalls: disorder, repeats, low-depth MSAs, domain splits

[domain segmentation](#) [linkers](#)

Session 2

Fee: Rs 8400 Apply Now

Running AlphaFold/RoseTTAFold

Local, server and cloud options; hardware & caching tips

GPU/CPU choices **databases mgmt** **batch runs**

Tuning inputs: MSAs, templates, recycles, ensembles

num_recycles **num_ensembles** **template filters**

Interpreting outputs, ranking, and preparing models for use

relaxation **B-factor/pLDDT mapping**

Session 3

Fee: Rs 11200 Apply Now

ESMFold, Multimers & Refinement

ESMFold for fast predictions; when MSA-free helps

LM-only inference **throughput vs accuracy**

Complexes & interfaces: AlphaFold-Multimer/RoseTTAFold2

chain pairing **iptm scoring** **interface QC**

Relaxation, cleanup & docking-readiness

amber_relax **clash/geometry checks** **missing loops**

Session 4

Fee: Rs 14000 Apply Now

Mini Capstone: AI Model → Application

Predict, assess and use a model for a downstream task
(docking/design/variants)

Theory + Practical

Pipeline automation & provenance (batch runs, configs, logs)

Snakemake/Nextflow **Conda/Mamba** **Quarto summary**

Deliverables: figures, tables, README & manifest

PDF **CSV/TSV** **checksums**