

Computational Structural Biology Workflows & Automation

— Hands-on

Productionize your structural bioinformatics work. Design robust, auditable pipelines that run on laptops, HPC, or cloud with consistent results. Orchestrate multi-tool workflows (MD, docking, modeling, analysis), track provenance and data versions, and publish report bundles automatically.

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Session 1

Fee: Rs 6300 [Apply Now](#)

Workflow Design & Environments

Pipelines for modeling, docking, MD & analysis: DAGs, tasks, artifacts

Theory

Environment management & portability

[conda/mamba](#) [Docker](#) [Singularity/Apptainer](#)

Parameterization & configuration patterns

YAML/JSON **secrets & profiles**

Session 2

Fee: Rs 8400 Apply Now

Orchestration: Snakemake/Nextflow/CWL

Choose a workflow engine; rules/processes, resources & checkpoints

Snakemake **Nextflow** **CWL/WDL (overview)**

Scaling: local → HPC/cloud; schedulers & executors

Slurm/SGE/PBS **AWS/GCP/Azure** **profiles & queues**

Retry, caching & checkpointing; long MD/docking tasks

job arrays **resume & re-entrancy**

Session 3

Fee: Rs 11200 Apply Now

Reproducibility, Data & Deployment

Version control & data lineage

Git/GitHub/GitLab **DVC/artifact stores** **metadata manifests**

Testing, CI/CD & packaging for pipelines

pytest/unit checks **GitHub Actions/GitLab CI** **container registries**

FAIR outputs & automated reports

Quarto/Markdown **checksums/provenance** **release tagging**

Session 4

Fee: Rs 14000 [Apply Now](#)

Mini Capstone: Template → Automated Pipeline

Automate a mini workflow (prep → docking/MD → analysis) with
configs, containers & scheduler profile

Theory + Practical

Push-button run: CI trigger, artifact upload & Quarto report
bundle

release assets **manifest/checksums**

Deliverables: figures, tables, README & manifest

PDF **CSV/TSV** **HTML**