

Advance Molecular Dynamics Simulation Trajectory Analysis

From raw simulations to mechanistic insight — Visualization, Kinetics, Allostery,
Enhanced Sampling, and Reproducible Research Workflows.

STRUCTURE → DYNAMICS → ENERGETICS → KINETICS → INSIGHT

BITS BioCyTiH Foundation
W-207, BITS Pilani Hyderabad Campus, Jawahar Nagar, Kapra Mandal, Medchal District, Telangana, 500078,
Email: training@biocytihi.co.in Ph: 040-68012033, 9779441636
www.training.biocytihi.co.in

PROGRAM CURRICULUM

Five Days · Five Dimensions of MD Analysis

DAY

1

**Visualization &
Trajectory Fundamentals**

TOPICS

VMD · ChimeraX · Frame
navigation · Alignment ·
Movie-making

LAB

Load a protein trajectory;
clean movie; figure panel

Inspect trajectories
confidently; export
publication-quality visuals

DAY

2

**Stability, Flexibility &
Local Interactions**

TOPICS

RMSD · RMSF · Rg · SASA ·
H-bonds · Contact maps ·
MDAnalysis

LAB

Analyze protein–ligand
trajectory; plot time series;
compare replicas

Full stability report with
plots and interpretation

DAY

3

**Global Motion &
Conformational Landscapes**

TOPICS

DCCM · PCA · dPCA · TICA ·
Clustering · Free-energy
surfaces

LAB

Build feature sets; perform
PCA/TICA; cluster frames;
project to FES

Identify major
conformational states and
dominant motions

DAY

4

**Function, Allostery &
Binding Mechanisms**

TOPICS

Dynamic networks · Cryptic
pockets · Water networks ·
MM/PBSA · GBSA

LAB

Network analysis; compute
residue hotspots; inspect
water-mediated bridges

Connect structure to
mechanism, druggability,
and hotspots

DAY

5

**Kinetics, Enhanced
Sampling & Research
Workflows**

TOPICS

MSMs · HMMs ·
Metadynamics · PyEMMA ·
ML features · TDA · GNN

LAB

Mini kinetic model; bias
reweighting; capstone
analysis notebook

Complete research-grade
pipeline and final
presentation

YOUR INSTRUCTORS

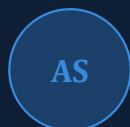
20 Years at the Frontier of Molecular Simulation



Dr. Sajeesh Chacko

Lead developer of advanced MD analysis techniques

25+ years in computational biophysics. Quantum Physics, Developed allosteric analysis methods



Dr. Ashutosh Shandilya

Expert in Enhanced sampling & ML-driven MD workflow

Lead developer of pocket detection and bias-reweighting techniques.
Expert in kinetics, MSMs, and reproducible pipelines.

SOFTWARE ECOSYSTEM

Tools You'll Master

VISUALIZATION

VMD · ChimeraX

MD ANALYSIS

GROMACS · CPPTRAJ ·
MDAnalysis

PYTHON & ML

PyEMMA · MDTraj ·
Scikit-learn

NETWORKS & POCKETS

AADS · fpocket · VolSurf

ENHANCED SAMPLING

aMD · ABPS · GNN
reweighting

KINETICS

PyEMMA MSMs · HMMs
· TICA

WHAT YOU'LL TAKE HOME

Concrete Deliverables, Every Single Day

Day 1



Clean trajectory movies and publication-ready figure panels

Day 2



Full protein stability report with annotated time-series plots

Day 3



PCA / TICA conformational landscape with clustered states

Day 4



Allosteric network map and druggability assessment

Day 5

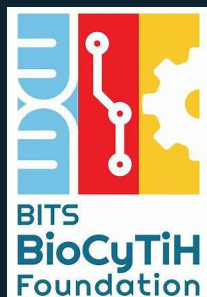


Mini kinetic model and bias-reweighted free-energy surface

Repo



Reproducible capstone notebook ready from our GitHub repository



REGISTRATION & RESOURCES

Join the Workshop



All input and output datasets available via our website and GitHub.

Start your analysis on day one — zero setup friction.

[Register Now →](#)

DURATION

5 days · Full day each

FORMAT

Hands-on labs + lectures

DATA REPO

GitHub + workshop website

CERTIFICATE

Issued on completion

[github.com /BBF-MD-Workshop](https://github.com/BBF-MD-Workshop)