CENTRE OF BIOINFORMATICS RESEARCH & TECHNOLOGY

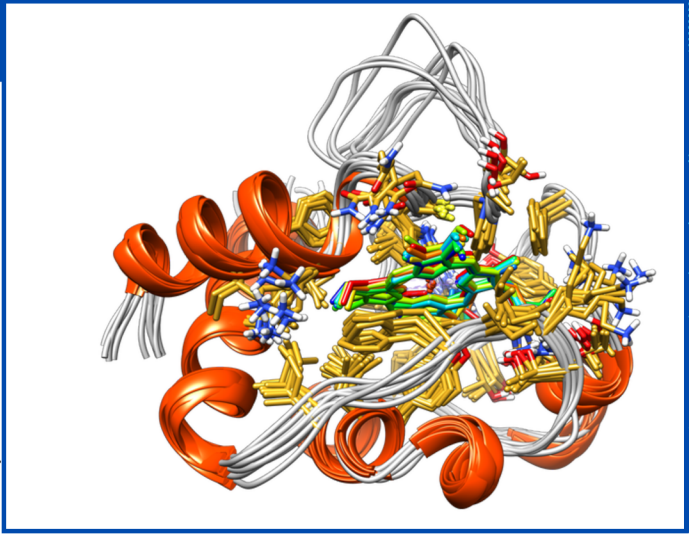
Hands-on Training

Molecular Dynamics (MD) Simulations

OF PROTEIN-LIGAND COMPLEX

ONLINE

From Setup to Insight: Master MD Simulations for Drug Discovery



About the Training

This comprehensive program covers Molecular Dynamics simulations of protein-ligand complexes, from system preparation and force field parameterization to running production simulations. Participants will master trajectory analysis, protein-ligand interaction studies, and visualization techniques, gaining practical skills to independently conduct MD simulations and generate publication-quality results for drug discovery applications.

Topics

- Introduction to Molecular Dynamics Simulations
- Force Fields & Parameterization
- System Preparation & Setup
- Ligand Parameterization & Topology Generation
- Solvation & Ion Placement
- Energy Minimization & System Equilibration
- Production MD Simulations
- Trajectory Analysis - Basic Properties
- Protein-Ligand Interaction Analysis
- Advanced Trajectory Analysis
- Visualization & Reporting
- Troubleshooting & Best Practices

Program Benefits

- Certificates
- Access to Live Sessions
- Recordings
- Workshop Materials
- Online Technical Support Post Training

Tools/Software

AMBER, VMD, CHARMM-GUI, Molstar, Python-Jupyter, NGLView/MolStar, ProLIF, Bio3D, R/Python scripts, PyMOL, ChimeraX, matplotlib,

Registration Process

To get the application form and fee details, and for any other queries, write to us at info@cbirt.net or call us at +91 6398142849.

SCAN HERE

Course Instructors

- Dr. Pawan Kumar, Bioinformatics Trainer, CBIRT
- Dr. Tamanna Anwar, Training Organizer & CoFounder, CBIRT

Duration, Date & Time	2 Weeks 15 Dec.-26 Dec. 2025	Monday – Saturday 6:00 PM – 7:00 PM	Registration Closes 14 Dec. 2025

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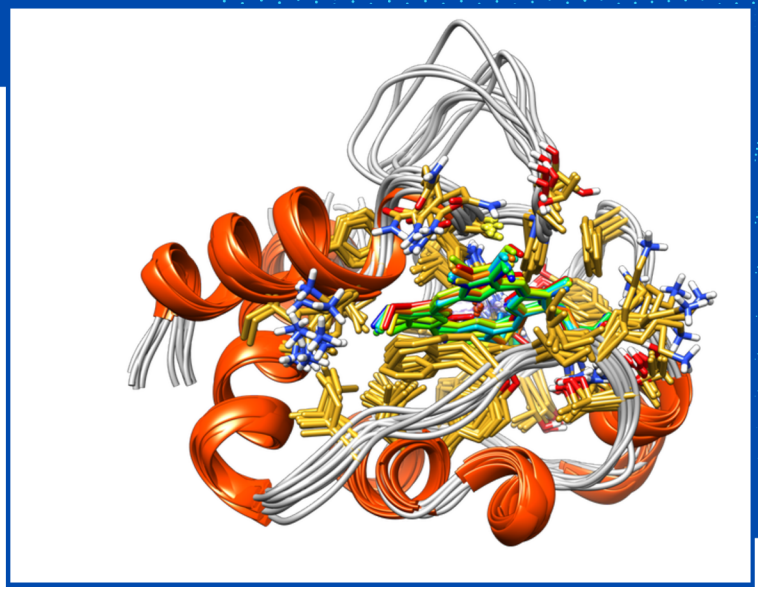

To register for the workshop, please submit the registration form along with your payment details. We accept multiple payment methods to ensure a convenient and secure registration process.

SCAN THE QR CODE FOR THE REGISTRATION FORM

Registration Process

STUDENTS

Upto Masters	PH.D
INR-2249	INR-2499

POSTDOC/RESEARCH SCHOLARS

INR-2749

STAFF/FACULTY

INR-2999

INDUSTRY PROFESSIONALS

INR-3499

INTERNATIONAL PARTICIPANTS

(Including all Living, Working, or Studying Abroad at the time of the Workshop).

STUDENTS		POSTDOC/ RESEARCH SCHOLARS	STAFF/FACULTY	INDUSTRY PROFESSIONALS
Upto Masters	PH.D			
USD 40	USD 45	USD 50	USD 60	USD 70

Payment Methods

SCAN QR CODE

UPI ID

BHIM UPI

centreofbioinformaticsresearch@cnrb

PAYPAL ID

PayPal

PayPal.Me/cbirt1

ONLINE TRANSFER

Account No. - 120023770387
Bank Name - CANARA BANK
IFSC Code - CNRB0002336
Branch Code - 002336
Branch - Kelangar, Aligarh

Payable to: Centre of Bioinformatics Research and Technology

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