

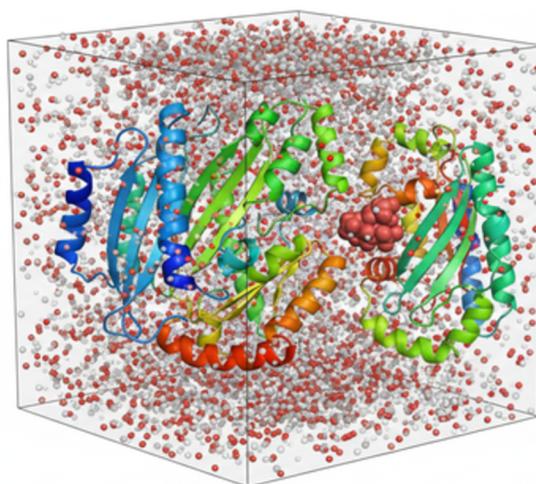
Hands-on Training

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
- ✓ Results and Interpretation



Program Benefits

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



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



Tools/Software

GROMACS, PyMOL/Chimera, VMD, Avogadro, CGenFF server, MDAnalysis, ProLIF, Bio3D, R/Python scripts, ChimeraX, matplotlib, Command-line tools.



Course Instructors

- Dr. Petrina Jebamani, Bioinformatics Trainer, CBIRT
- Dr. Tamanna Anwar, Organizer & Founder, CBIRT

Duration, Date & Time

2 Weeks
06-17 Apr. 2026

Monday – Saturday
7:15 PM – 8:15 PM

Registration Closes
05 Apr. 2026

Call us for registration & queries



+91 6398142849



info@cbirt.net



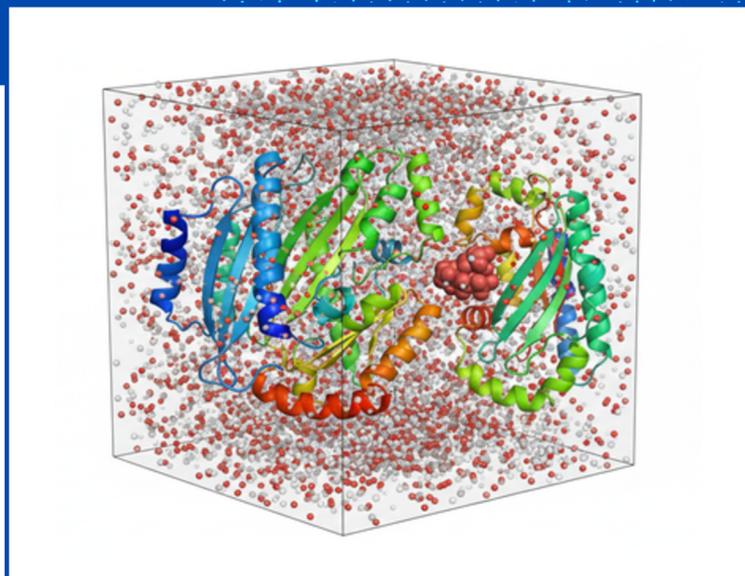
www.cbirt.net

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

Payment Methods

SCAN QR CODE



centreofbioinformaticsresearch@cnrb

UPI ID



PAYPAL ID



[PayPal.Me/cbirt1](https://www.paypal.com/Me/cbirt1)

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Payable to: Centre of Bioinformatics
Research and Technology

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