

Introduction to Molecular Dynamics Simulations

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Who is this course for?

This course is designed for students interested in learning the fundamentals of molecular dynamics simulations and gaining practical experience with GROMACS software package. No prior expertise in structural bioinformatics is necessary, however a fundamental understanding of protein structure is advantageous. Experience with a command-line environment like UNIX is not essential, although it is helpful for inputting the MD simulations instructions.

- 1 Basics of MD simulations
- 2 Key concepts of molecular interactions
- 3 Hands-on training
- 4 MD Analysis

09:30 AM
Basics of MD simulations

10:00 AM - 11.00 AM
Key concepts of molecular interactions

11:30 AM - 12.30 PM
Hands on Training

12:30 PM - 1.30 PM
MD analysis

FEES

750 INR for Students and Academicians
2500 INR for Non-Academics
100 \$ for Foreign Participants



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Bioinformatics Facility

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