RGCB
DISCOVERIES FOR A BETTER TOMORROW

BASICS OF MOLECULAR DYNAMIC SIMULATIONS

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WHO IS THIS COURSE FOR?

This course is for those interested in learning the basics of molecular dynamics simulations and a hands-on approach to the capabilities of GROMACS and free energy calculations. No previous experience in the field of structural bioinformatics is required, but a basic knowledge of protein structure is an advantage. Experience with a UNIX-like command-line environment is not required, but it helps to type the commands into the modeling concepts and biology.

1. **Basics of MD simulations**
2. **Key concepts of molecular interactions**
3. **Binding free energy calculations**
4. **Hands-on training**

09:30 AM
Basics of MD simulations

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

11:30 AM - 12.30 PM
Binding free energy calculations

12:30 PM - 1.30 PM
Hands-on training

FEES

500 INR *for Students and Academicians*
2500 INR *for Non-Academics*
100 $ *for Foreign Participants*

More Info
Register

rgcb.res.in

Bioinformatics Facility
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