



NTHRYS WORKSHOPS

Introduction To Molecular Modelling

8:45 AM - 10:15 AM: Session 1: Fundamentals of Molecular Modelling

Hands-on workshop covering the basic concepts of molecular modelling.
Protocols for building molecular structures, understanding force fields, and setting up simulations.

10:15 AM - 10:30 AM: Coffee / Tea / Snacks Break

Networking and refreshments.

10:30 AM - 12:00 PM: Session 2: Molecular Dynamics Simulations

Practical session on setting up and running molecular dynamics simulations.
Protocols for simulating molecular behavior over time and analyzing trajectory data.

12:00 PM - 1:00 PM: Lunch Break

Catered lunch and networking opportunity.

1:00 PM - 2:30 PM: Session 3: Energy Minimization and Optimization

Hands-on training on energy minimization techniques.
Protocols for optimizing molecular structures to find the lowest energy conformations using various algorithms.

2:30 PM - 2:45 PM: Short Break

Time for a stretch and informal discussions.

2:45 PM - 4:15 PM: Session 4: Visualization of Molecular Models

Practical session on visualizing molecular structures.

Protocols for using molecular graphics software to render 3D models and analyze molecular interactions.

4:15 PM - 4:30 PM: Coffee / Tea / Snacks Break

Last networking opportunity with snacks.

4:30 PM - 5:30 PM: Closing Session: Implementing Changes and Technology Adoption

Group discussions on implementing new techniques learned today.

Dialogue on overcoming challenges in adopting new technologies in similar sectors.

Feedback session and closing remarks.

Certificate Issue

5:30 PM: Workshop Concludes