



NTHRYS WORKSHOPS

Advanced Molecular Modelling Techniques

8:45 AM - 10:15 AM: Session 1: Quantum Mechanics in Molecular Modelling

Hands-on workshop on quantum mechanical calculations in molecular modelling. Protocols for applying quantum chemistry techniques to small molecules and reaction mechanisms.

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

Networking and refreshments.

10:30 AM - 12:00 PM: Session 2: Hybrid QM/MM Simulations

Practical session on hybrid quantum mechanics/molecular mechanics (QM/MM) approaches. Protocols for simulating complex systems that combine quantum and classical mechanics.

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

Catered lunch and networking opportunity.

1:00 PM - 2:30 PM: Session 3: Free Energy Calculations in Molecular Modelling

Hands-on training on free energy calculations.

Protocols for estimating binding free energies and analyzing molecular interactions using advanced simulation techniques.

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

Time for a stretch and informal discussions.

2:45 PM - 4:15 PM: Session 4: Coarse-Grained Modelling

Practical session on coarse-grained modelling techniques.
Protocols for simplifying large molecular systems to study their behavior over longer timescales.

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