



NTHRYS WORKSHOPS

Molecular Modelling Of Enzymes

8:45 AM - 10:15 AM: Session 1: Enzyme Mechanism Modelling

Hands-on workshop on modelling enzyme mechanisms.
Protocols for simulating enzyme-catalyzed reactions and studying transition states and intermediates.

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

Networking and refreshments.

10:30 AM - 12:00 PM: Session 2: Modelling Enzyme-Substrate Complexes

Practical session on modelling enzyme-substrate interactions.
Protocols for building enzyme-substrate complexes and simulating their binding and reaction pathways.

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

Catered lunch and networking opportunity.

1:00 PM - 2:30 PM: Session 3: Computational Enzyme Design

Hands-on training on designing enzymes in silico.

Protocols for using computational tools to engineer enzymes with new or improved catalytic properties.

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

Time for a stretch and informal discussions.

2:45 PM - 4:15 PM: Session 4: Predicting Enzyme Kinetics Using Molecular Modelling

Practical session on predicting enzyme kinetics.

Protocols for using molecular modelling to calculate kinetic parameters like K_m , V_{max} , and catalytic efficiency.

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