



NTHRYS WORKSHOPS

Molecular Modelling In Drug Design

8:45 AM - 10:15 AM: Session 1: Structure-Based Drug Design

Hands-on workshop on structure-based drug design techniques.
Protocols for designing small molecule inhibitors by leveraging the 3D structures of target proteins.

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

Networking and refreshments.

10:30 AM - 12:00 PM: Session 2: Ligand-Based Drug Design Approaches

Practical session on ligand-based drug design.
Protocols for developing pharmacophores and QSAR models to guide the design of new compounds.

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

Catered lunch and networking opportunity.

1:00 PM - 2:30 PM: Session 3: Fragment-Based Drug Discovery

Hands-on training on fragment-based drug discovery techniques.

Protocols for screening and growing small molecular fragments to optimize drug binding.

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

Time for a stretch and informal discussions.

2:45 PM - 4:15 PM: Session 4: ADMET Modelling in Drug Development

Practical session on ADMET (Absorption, Distribution, Metabolism, Excretion, and Toxicity) modelling.

Protocols for predicting drug pharmacokinetics and toxicity using computational methods.

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