Schrodinger workshop Schedule

Agenda

Participants will receive practical online training sessions with guidance, covering various topics over the course of three days. On day 1, we will focus on organic molecule sketching, protein selection, and data management functions of the Maestro GUI. The goal will be to identify hit molecules against therapeutic targets through preparation and screening. Day 2 will concentrate on the application of Ligand-based drug discovery for molecular dynamics drug discovery. We shall also showcase case study on using machine learning based hit/lead optimization protocols. A brief review of the background theory will be provided during the workshop, and industrial case studies will be used to incorporate the theory into the sessions.

Day 1: Structure based molecular docking (molecular modelling)

Time	Topics to be covered
10:00 AM	Introduction to Molecular Modelling & Logging into Cloud instance
10:45 AM	Maestro GUI: Exploring enumeration of Mycobacterium tuberculosis lead molecules – Hands on
11:45 AM	Protein Preparation of inhibitors Protein Kinases A in Mycobacterium tuberculosis. - Hands on
12:15 PM	Binding Pocket Identification of Protein Kinases B.
1.00-2.00 PM	Lunch Break
2:00 PM	One step Molecular Docking
2:40 PM	Molecular Docking Analysis 1 – Pose visualization and evaluation
3:15 PM	Molecular Docking Analysis 2 – Ligand Interaction Diagram and Calculation of Interaction Fingerprints
3.30	Ligand Designer for Protein Kinase A for antimycobacterial design.
3:45 – 4:00 PM	Review of Day 1 activities

Day 2: Application of molecular dynamics in drug discovery and AutoQSAR

Time	Topics to be covered
10:00 AM	Role of Molecular dynamics in drug discovery
10:30 AM	Protein preparation of Aurora kinase- Molecular Dynamics
10:45 AM	System building on Aurora Kinase- Hands on
11:45 AM	Thermodynamics molecular dynamics setup on Aurora kinase.
1.00-2.00	Lunch Break
2:00 PM	Qualitative Molecular dynamics trajectory analysis
2:10 PM	Quantitative Molecular dynamics trajectory analysis
3.30	Machine learning using AutoQSAR- Activity based hit/lead optimization
3:45 – 4:00 PM	Review of Day 3 activities