SCHRÖDINGER

RGCB
DISCOVERIES FOR A BETTER TOMORROW

COMPUTATIONAL STRUCTURE-BASED SCREENING AND EXPLICIT MOLECULAR DYNAMICS

3 & 4 AUG 2021

Two-days cloud-based hands-on workshop targeting structure-based drug designing. Participants will get practical experience and in-person guidance in using the Maestro GUI, covering the organic molecule sketching, protein selection, preparation, and screening for hit identification of molecules against therapeutic targets. The workshop will also include a brief recap of background theory for Molecular mechanics, Molecular Docking, and Molecular Dynamics via case studies on the real-time industrial projects.

DAY 1

9.30
Technical set-up

9.50
Audio & Visual check

10.00
1. Opening -
Agenda and split into breakout rooms

10.10
Breakout 1 -
Intoductions and open software

10.30
2. Maestro GUI:
Building Molecules and Enumeration

11.00
Breakout 2 -
Build Chalcones from SMILES

11.20
3. Ligand Prepartion and ADME

11.35
Breakout 3 -
Launch LigPrep

11.45
Intro to Molecular Docking, Protein and Ligand Preparations

12.10
4. Protein Preparation and Grid Generations

12.30
Breakout 4 -
Prepare protein and grid generations and molecular docking

13.00
Break -
Continue to use software during the break

14.00
Welcome Back

14.10
5. Molecular Docking

14.25
Breakout 5 -
Analyzing 3D molecular docking analysis

14.40
6. Molecular Docking Analysis

14.55
Breakout 6 -
2D molecular docking analysis

15.30
7. Full Revision of Day 1

Breakout 7 -
Full session practice

15.55
Wrap-up

16.00
Finish

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DAY 2

9.30
Technical set-up

9.50
Audio & Visual check

10.00
1. Opening -
Agenda and molecular dynamics theory

10.30
Breakout 1 -
Docking results and ligand sketching

10.45
2. Desmond Introduction

11.00
Breakout 2 -
Protein ligand complex formation, system building

11.15
3. Molecular Dynamics Demo

11.25
Breakout 3 -
MD submission

11.35
Desmond Trajectory Visualization

11.50
Breakout 4 -
Participant analysis and molecular docking

13.00
Break -
Continue to use software during the break

14.00
Welcome Back

14.05
5. Desmond Molecular Simulation Analysis

14.20
Breakout 5 -
Analyzing 3D molecular docking analysis

14.45
6. Organic Molecules Enumeration

15.00
Breakout 6 -
Reaction-based enumeration, library enumeration, ADME

15.30
7. Full Revision of Day 2

15.55
Wrap-up

16.00
Finish

Speakers:

Dr. Pritesh Bhat
Dr. Prajwal Nandekar
Dr. Koushik Kasavajhala
Ms. Shelvia Malik
Mr. Kishore V
Mr. Vinod D
Mr. Sivakumar K C

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More Info

Register

FEES
500 INR *for Students and Academicians*
2500 INR *for Non-Academics*
100 $ *for Foreign Participants*