Tentative schedule of 3-days On-site Hands-on Workshop: Computational Structure-based Drug Design and Molecular Dynamics

Date: 10th - 12th Aug 2022; Time: 9:30 am - 4:30 pm IST

Outline: 3-day cloud-based hands-on workshop targeting structure-based drug designing and molecular dynamics simulations. 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, CADD, Structure-based design approaches, and molecular dynamics simulations *via* case studies on the real-time industrial projects.

Registration:

Registration is open to 50 participants. **Please register here:** ***t.ly/C2Ve***

Last date of registration: 5th Aug 2022.

Hardware Requirement for Participant:

Computer/Laptop, Chrome browser, Internet connection (~5Mbps)

Day 1

Time	Session
14.00	Technical set-up
14.15	Opening - Agenda and Introduction to CADD
14.45	Open software Maestro GUI: Building Molecules
15.15	Ligand Preparation
16.00	Protein Preparation
16.30	Grid Generations
17.00	Molecular docking job submission
17.30	Wrap-up and Q/A

Day 2

Time	Session
9.30	Technical set-up
10.00	2D molecular docking analysis
10.30	3D molecular docking analysis
11:00	HITS identification
11.30	Lead optimization with Ligand designer
12:30	Practice and Q/A
13.00	Lunch Break - Continue to use software during the break
14.00	Molecular dynamics simulations - Introduction
14.30	Protein ligand complex formation
14.45	Complex preparation
15.15	System building
15.45	MD job submission
16:30	Practice session and Q/A

Day 3

Time	Session
9.30	Technical set-up
10.00	Desmond Trajectory Visualization
10.30	Simulation Interaction Diagram Analysis
11.30	Organic Molecules Enumeration and Ligands library generation
12.00	ADME predictions
12.30	Practice session
13.00	Wrap-up and Q/A

Workshop Speakers:

Dr. Prajwal Nandekar
Dr. Koushik Kasavajhala

Coordinators and General inquiries:

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