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Cloud-based Hands-on Workshop:
Computational Structure-based Screening and Explicit Molecular Dynamics

Date: 05th & 06th Nov 2020 ~ Time: 10:00 - 16:00 IST

Outline: Two-day 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 - 05th Nov 2020

Time	Session
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 - 06th Nov 2020

Time	Session
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	**4. Desmond Trajectory Visualization**
11.50	**Breakout 4** - Participant analysis
12.15	Break - Continue to use software during the break
14.00	Welcome Back
14.05	**5. Desmond Molecular Simulation Analysis**
14.20	**Breakout 5** - Analyzing molecular dynamics 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

Workshop Speakers:

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

Registration:

Registration is open to 30 participants, please register here - **https://rb.gy/fy6s6x**

General Inquiries:

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