SCHRÖDINGER

RCMS A NUST Research Centre

Workshop on

"Cloud-based Hands-on Workshop:

Rational Computational Drug Design Approaches"

15-16 June 2021

Venue: Online, Cloud Based Workshop

Deadline for Registration: 10 June 2021

Note: The registration is first come first basis and the seats are limited
Faculty members, research scholars and postgraduate students are eligible to register for the workshop.

Registration Fee: ….

Requirements: Laptop/Desktop with at least 5 Mbps Internet connection, and Google Chrome browser

Workshop Highlights: 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 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.

Coordinator:

Dr. Ishrat Jabeen, National University of Science & Technology (NUST), Pakistan

Workshop Speakers from Schrödinger:

Dr. Pritesh Bhat, Dr. Prajwal Nandekar

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Program Details

Day 1	
Time	**Workshop Topics**
9:30 AM	**Technical set-up, Audio & Visual Check**
9:40 AM	**Inauguration**
10:00 AM	**1. Opening-Molecular Modelling Introductory Presentation**
10:30 AM	**2. Logging into Cloud instance**
10:45 AM	**3. Maestro GUI: Building Molecules and Enumeration**
11:15 AM	**4. Ligand Preparation and ADME**
11:45 AM	**5. Protein Preparation**
12:15 PM	**6. Binding Pocket Identification**
12:30 PM	**Break - Continue to use software during the break**
2:00 PM	**Welcome Back**
2:10 PM	**7. Molecular Docking**
2:40 PM	**8. Molecular Docking Analysis 1 – Pose visualization and evaluation**
3:15 PM	**9. Molecular Docking Analysis 2 – Ligand Interaction Diagram and Calculation of Interaction Fingerprints**
3:45 – 4:00 PM	**Review Day 1 activities and Finish**

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Day 2

Time	Workshop Topics
10:00 AM	**1. Opening - Molecular dynamics theory presentation**
10:30 AM	**2. Logging into cloud instance**
10:45 AM	**3. Protein Preparation**
11:15 AM	**4. Desmond Introduction and building your MD simulation system**
11:45 AM	**5. Desmond Molecular Dynamics Submission**
12:15 PM	**Break - Continue to use software during the break**
2:00 PM	**Welcome Back**
2:10 PM	**6. Desmond Molecular Simulation Analysis 1 – Visual Analysis**
2:40 PM	**7. Desmond Molecular Simulation Analysis 2 – Quantitative Analysis using Simulation Interaction Diagram**
3:20 PM	**8. Organic Molecules Enumeration and ADME**
3:50 – 4:00 PM	**Review Day 2 Activities and Finish with Concluding Remarks**

Registration: Registration is open to 100 participants, please register here – https://forms.gle/Lg4xytEbB88cbhjN8