Workshop on

"Cloud-based Hands-on Workshop:

Computationally Driven Drug Design Workflows"

Date: Jan 19-20, 2023

Venue: Online, Cloud Based Workshop

Deadline for Registration: Jan 10, 2023

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: To register, kindly send an e-mail to Ms **Lara Alzyoud**: **lara.alzyoud@aau.ac.ae**

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, etc. via case studies on the real-time industrial projects.

Coordinators:

Dr. Mohammad Ghattas, Professor, College of Pharmacy, Al Ain University

Ms Lara Alzyoud, Master student, College of Pharmacy, Al Ain University

Workshop Speakers from Schrödinger:

Dr. Pritesh Bhat, Dr. Koushik Kasavajhala

Program Details

Day 1	
Time	**Workshop Topics**
1:45 PM	**Technical set-up, Audio & Visual Check**
2:00 PM	**1. Opening-Molecular Modelling Introductory Presentation**
2:30 PM	**2. Logging into Cloud instance**
2:40 PM	**3. Maestro GUI: Building Molecules 2D and 3D**
3:00 PM	**4. Maestro GUI: SMILES**
3:15 PM	**5. Maestro GUI: Protein Visualization**
3:45 PM	**Break - Continue to use software during the break**
4:00 PM	**6. Protein Preparation**
4:20 PM	**7. Grid Generation**
4:30 PM	**8. Ligand Preparation**
4:45 PM	**9. Molecular Docking**
5:00 PM	**Review Day 1 activities and Finish**

Day 2	
Time	**Workshop Topics**
8:00 AM	**1. Docking Analysis**
9:00 AM	**2. Opening - Molecular dynamics theory presentation**
9:30 AM	**3. Logging into cloud instance**
9:35 AM	**4. Protein Preparation**
10:00 AM	**5. Desmond Introduction and building your MD simulation system**
10:30 AM	**6. Desmond Molecular Dynamics Submission**
10:50 AM	**Break - Continue to use software during the break**
11:10 AM	**Welcome Back**
11:10 AM	**7. Desmond Molecular Simulation Analysis 1 – Visual Analysis**
11:40 AM	**8. Desmond Molecular Simulation Analysis 2 – Quantitative Analysis using Simulation Interaction Diagram**
12:20 PM	**9. Organic Molecules Enumeration and ADME – Ligand Designer**
12:50 – 1:00 PM	**Review Day 2 Activities and Finish with Concluding Remarks**