Centre of Excellence in Pharmaceutical Sciences (CEPS)

Guru Gobind Singh Indraprastha University (GGSIPU)
Sector 16-C, Dwarka, New Delhi.

F.15/GGSIPU/CEPS/2022/ 485 Dated: 24/11/2022

NOTICE

Subject: Invitation for Two day workshop on "Cloud-based Hands-on Workshop: Computational Aided Drug Design Workflow"

Centre of Excellence in Pharmaceutical Sciences (CEPS), Guru Gobind Singh Indraprastha University, Dwarka, Delhi, in collaboration with Schrödinger is going to organize two-day workshop **"Cloud-based Hands-on Workshop: Computational Aided Drug Design Workflow"** for masters and PhD students.

Requirements: Own laptops are required for the workshop and with appropriate internet speed will be provided by CEPS, GGSIPU. Users can get connected to their laptops by their mobile hotspots as well as Cloud space will be provided and your login credentials will be used for hands-on experiments.

Interested participants would have to fill the registration form for the workshop latest by 28th November, 2022. Participants will be selected on **first come first serve** basis.

https://forms.gle/nyLAKG7uWy9aSd2UA

Note: Event Brochure (Copy Attached)
Date and Day: 1st (Thursday) and 2nd (Friday) December 2022
Time: 9:30 onwards
Venue: CEPS, GGSIP University

Prof. A.K. Narula
(Director, CEPS)

Centre of Excellence in Pharmaceutical Sciences (CEPS), GGSIPU, New Delhi
in
Collaboration with
Schrödinger

Organising

Two days Workshop on "Computer Aided Drug Design Workflow"

For Masters / Ph.d Students

on

01st & 02nd December 2022

Time: 09.30 a.m. to 04.30 p.m

Venue: CEPS, GGSIPU Campus.

Patron:
Prof. (Dr.) Mahesh Verma
Vice Chancellor
Padma Shri Awardee
National Science and
Technology Awardee
DR. B. C. Roy Awardee

Speakers:
Dr. Prajwal Nandekar
Senior Scientist –II
Schrödinger, Banglaore
Dr. Koushik Kasavajhala
Senior Scientist –I
Schrödinger, bangalore

Coordinators
Prof. A.K Narula, Director, CEPS,
Dr. Parul Sharma,
Dr Deepa Deswal,
Dr Shruti Peshoria,
Dr Preeti Sehgal,
Dr Ruchi Sharma

Workshop on

"Cloud-based Hands-on Workshop:
Computational Aided Drug Design Workflow"

Date: 01- 02December 2022

Venue: Centre of Excellence in Pharmaceutical Sciences (CEPS), Guru Gobind Singh Indraprastha University (GGSIPU)

Deadline for Registration: **28th November 2022**

Research Scholars and postgraduate students are eligible to register for the workshop.

Registration Fee: N/A

Requirements: Laptop/Desktop with at least 10 Mbps Internet connection (mobile hotspots can also be used), and Google Chrome browser

Workshop Highlights: 2-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 A.K. Narula, Director CEPS, GGSIPU, Dr. Parul Sharma, Dr. Deepa Deswal, Dr. Shruti Peshoria, Dr. Preeti Sehgal and Dr. Ruchi Sharma, CEPS GGSIPU

Workshop Speakers from Schrödinger: Dr. Prajwal Nandekar, Scientist II, Dr. Koushik Kasavajhala, Scientist I

Program Details

Day 1	
Time	**Workshop Topics**
9:30-10:00 AM	**Technical set-up, Audio & Visual Check and**
9:40 AM	**Introduction of Speakers Inauguration**
10:00 AM	**1. Opening-Molecular Modelling Introductory Presentation**
10:30 AM	**2. Logging into Cloud instance**
10:45 AM	**3. Maestro GUI 1: 2D Sketcher and 3D Builder**
11:15 AM	**4. Maestro GUI 2: Building DNA and Importing SMILES**
11:45 AM	**5. Maestro GUI 3: Protein Visualization 6B2Q**
12:15 PM	**6. Protein Preparation and Grid Generation 6B2Q**
1:00 PM	**Lunch Break**
2:00 PM	**7. Ligand Preparation for 6B2Q**
2:10 PM	**8. Molecular Docking 6B2Q**
2:40 PM	**9. Molecular Docking Analysis 1 – Pose visualization and evaluation**
3:15 PM	**10. Molecular Docking Analysis 2 – Ligand Interaction Diagram and Calculation of Interaction Fingerprints**
3:45 – 4:00 PM	**Review Day activities and Finish**

Day 2	
Time	**Workshop Topics**
10:00AM	**1.Opening-Molecular dynamics theory presentation**
10:30AM	**2.Logging into cloud instance**
10:45AM	**3.Protein Preparation**
11:15AM	**4. Desmond Introduction and building your MD simulation system**
11:45AM	**5.Desmond Molecular Dynamics Submission**
12:15PM	**Break-Continue to uses of software during the break**
2:00PM	**Welcome Back**
2:10PM	**6.Desmond Molecular Simulation Analysis1– Visual Analysis**
2:40PM	**7. Desmond Molecular Simulation Analysis 2 – Quantitative Analysis using Simulation Interaction Diagram**
3:30PM	**8.Ligand Designer**
3:50 – 4:00 PM	**Review Day 2 Activities and Finish with Concluding Remarks**