Centre of Excellence in Pharmaceutical Sciences

Workshop on

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

In collaboration with Schrödinger

Date: 01- 02December 2022

Venue: CEPS, GGSIPU, Dwarka Campus, New Delhi

Post-event Report

CEPS organized a Workshop on "Cloud-based Hands-on: Computer Aided Drug Design Workflow" on 1st – 2nd December 2022, to have practical experience on Molecular Modeling programs implemented in Maestro. The need of *in-silico* based drug discovery makes the whole process fast paced by utilizing sophisticated computational tools/algorithms to study the molecular mechanism(s) of various diseases which could be dealt in detail at atomic level. This workshop helped the students to understand and discover various approaches that could be used for drug discovery process.

The Event started with a warm welcome to our guest speakers Dr. Prajwal Nandekar, Scientist II and Dr. Koushik Kasavajhala, Scientist I from Schrödinger, Bangaluru. Bouquets were presented to our eminent speakers and lamp was lighted by the speakers and Director of CEPS, Prof. A.K. Narula to take blessings of Almighty.



Objective of Event:

This Event was organized for post graduate and PhD students to bring awareness and some hands on practical applications used in Computational Biology and Bioinformatics, specifically on Maestro by Schrödinger. Science has become interdisciplinary in nature and computational Biology/Bioinformatics is playing greater roles in studying various diseases. Scientists from diverse background expertise, work on a common problem and in the current scenario, with the advent of newer technologies and techniques, interdisciplinary and integrative scientific research skills are in high demand. The Workshop was open to students from all disciplines of Sciences, on first come first serve basis.



Program:

It was a two-day cloud-based hands-on workshop targeting structure-based drug designing. Participants had 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 also included a brief recap of background theory for Molecular mechanics, Molecular Docking, and Molecular Dynamics, etc. via case studies on the real-time industrial projects.

Important Key Points:

- They were given tasks related to Molecular modeling Applications and those who obtained good results were motivated by giving them a token of appreciation by Schrödinger Scientists.
- Students finished the tasks with great zeal and enthusiasm and the results were analyzed and discussed.
- Looking at their keen interest to learn more, the students were provided Cloud space for four days on which all the modules of Maestro, Schrödinger were made available from 1st – 4th Dec 2022. The students were keen on using the cloud based services on weekend to explore more in the field of Bioinformatics/Computational Biology.

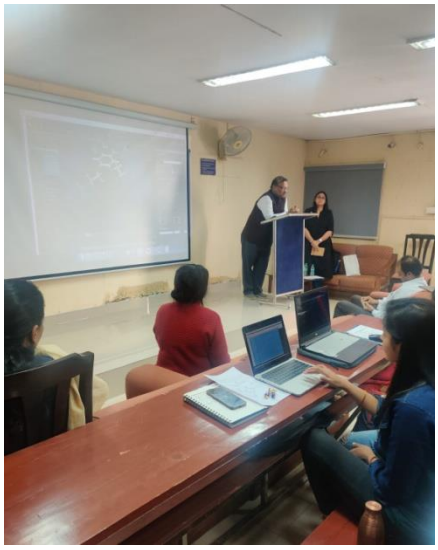
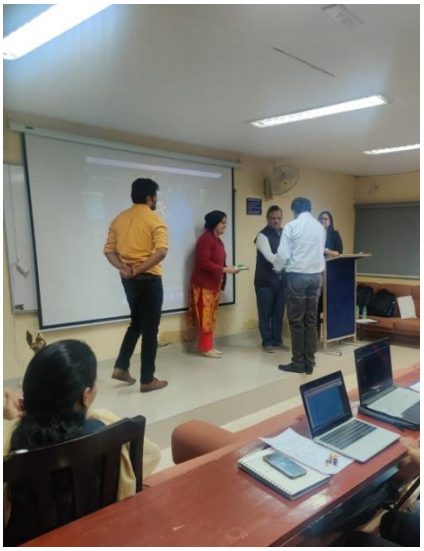
Feedback:

All the students attended the two-day workshop with sincerity and dedication. It was a great learning experience for the participants and they showed tremendous enthusiasm for more future workshops to learn advance techniques and applications.

CEPS Mood: Happy and excited students can't stop discussions regarding various modeling applications with the speakers to learn and understand more during tea break.

On behalf of CEPS faculty, we would like to extend Thanks to our Hon VC Prof. (Dr.) Mahesh Verma.

Vote of Thanks: Vote of thanks was delivered by Our Director Sir, Prof A.K. Narula and the speakers were presented with a small token of thanks for taking their time out from their busy schedules to come and train our students on *in-silico* Molecular modeling drug discovery aspects.


With this, CEPS successfully Organized a two-day Cloud based Hands-on workshop and look forward to do more Workshops in near future.