Cloud-based Hands-on Workshop on Molecular Docking, Pharmacophore Modeling and Machine Learning

15 – 16th March , 2022

Organized by

Bioinformatics Division
ICMR - National Institute of Cancer Prevention & Research, Noida
&
Schrodinger Inc.

Patron

Dr. Shalini Singh
MBBS, MS, FICOG
Director, ICMR-NICPR

INVITATION

Dear All,

We cordially invite you to the Cloud based Hands on Workshop organized by the Bioinformatics Division, ICMR – NICPR and Schrodinger Inc. from 15 – 16th March, 2022. This workshop includes lectures and hands on sessions by eminent Scientists from Schrodinger, Inc.

Convener:

Dr. Subhash Agarwal
Scientist E & Head, Bioinformatics Division
Ph.: 0120-2446925
E-mail: bioinformaticslabnoida@gmail.com

Speakers:

Dr. Pritesh Bhat, Senior Scientist
Dr. Prajwal Nandekar, Senior Scientist
Dr. Koushik Kasavajhala, Senior Scientist
Mr. Vinod D, Senior Scientist
Mr. Kishore and Ms Shelvia Malik
Schrodinger Inc.

OUTLINE: Two-days cloud-based hands-on workshop targeting ligand and structure-based drug designing. Participants will get practical experience and in-person guidance in using the Maestro GUI, covering the organic molecule sketching, protein preparation, and screening using Molecular Docking for hit identification of molecules against therapeutic targets. The lectures will also deal with a brief theory and practical experience on Pharmacophore Modelling, Shape based Screening & Core Hopping and Machine-Learning Model building using AutoQSAR

PROGRAM SCHEDULE

DAY 1
15th March 2022 (Tuesday)

Time	Session
9:30 – 9:40	Opening remarks by **Director, NICPR** **Dr. Shalini Singh, MBBS, MS, FICOG, MAMS.**
9:40 – 9:50	Overview of Research Activities at Bioinformatics Division **Dr Subhash Agarwal, Scientist-E, NICPR**
9:50 – 10.00	Welcome Note. **Mr. Raghu Rangaswamy, Vice President, Schrodinger**
10:00	**1. OPENING** – Agenda and split into breakout rooms
10:10	▪ **Breakout 1** – Introductions and open software.
10:30	**2. Maestro GUI: Building molecules and Enumeration**
11:00	▪ **Breakout 2** – Building Chalcones from SMILES
11:20	**3. Ligand preparation and ADME**
11:35	▪ **Breakout 3** – Launch LigPrep
11:45	**Introduction 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

DAY 1
15th March 2022 (Tuesday)

Time	Session
14:40	**6. Molecular Docking Analysis**
14:55	▪ **Breakout 6** – 2D molecular docking analysis
15:30	**7. Full Revision of Day1**
	▪ **Breakout 7** – Full session practice
15:55 – 16:15	Wrap-up and Q/A

DAY 2
16th March 2022 (Wednesday)

Time	Session
9:30	Technical set up and Audio & Visual Check
10:00	**1. OPENING** – Ligand-Based Drug Design
11:00	**2. Organic Molecules Enumeration**
11:15	▪ **Breakout 1** – Reaction-based enumeration, library enumeration, ADME
11:30	**3. Pharmacophore Modelling**
12:30	▪ Demo: Pharmacophore Modelling, Analysis & Validation
12:45	▪ **Breakout 2** – Pharmacophore Modelling
12:15	**Break** – Continue to use software during the break
14:00	Welcome Back
14:05	**4. Shape Screening & Core Hopping**
14:30	▪ **Breakout 3** – Hands-on Shape Screening & Core Hopping

DAY 2
16th March 2022 (Wednesday)

Time	Session
14:50	**5. Machine-Learning Model Building using AutoQSAR**
15:10	▪ **Breakout 5** – Participant hands-on AutoQSAR
15.30	**6. Full Revision of Day 2**
16.00	Wrap-up and Q/A

REGISTRATION DETAILS

Registration Fees: Rs 500/-
No. of seats: 100

Registration link:
https://forms.gle/RjoxpOqpYt8wrG5C6

Last date for registration: 11th March, 2022
Hardware Requirements: Computer/Laptop, Chrome browser, Internet Connection (~5Mbps)

General Inquiries:
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