

Cloud-based Hands-on Workshop

on

Molecular Docking, Pharmacophore Modeling and Machine Learning

15 – 16th March , 2023

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 from 15 – 16th March, 2023. 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

Schrodinger Inc.



SCHRÖDINGER®

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 15 th March 2023 (Wednesday)	
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 15 th March 2023 (Wednesday)	
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 16 th March 2023 (Thursday)	
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 16 th March 2023(Thursday)	
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/hYhTB1dszxxaVLxv8>

Last date for registration: 10th March, 2023

Hardware Requirements: Computer/Laptop, Chrome browser, Internet Connection (~5Mbps)

General Inquiries:

Dr. Subhash Agarwal, Scientist E and Head,
Mr Agneesh Pratim Das (+917321060674),
Bioinformatics Division

Phone: 0120-2446925

bioinformatics@labnoida@gmail.com