# Cloud-based Hands-on Workshop on Computational Structure based Screening and Explicit Molecular Dynamics

## 23 – 24th March , 2021

***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 on Computational Structure based Screening and Explicit Molecular Dynamics organized by the Bioinformatics Division, ICMR – NICPR and Schrodinger Inc. from 23 – 24th March, 2021. This workshop includes lectures and hands on sessions by eminent Scientists from Schrodinger, Inc.


**Convener:**

**Dr. Subhash Agarwal**
Scientist E, 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**
**Schrodinger Inc.**

ICMR INDIAN COUNCIL OF MEDICAL RESEARCH | NICPR NATIONAL INSTITUTE OF CANCER PREVENTION AND RESEARCH

SCHRÖDINGER®

**OUTLINE: Two-days 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 the 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 via case studies on the real - time industrial projects.**

# PROGRAM SCHEDULE

| DAY 1<br>23rd March 2021 (Tuesday) | |
|---|---|
| **Time** | **Session** |
| 9.30 – 9.45 | Opening remarks by **Director, NICPR**<br>**Dr. Shalini Singh, MBBS, MS, FICOG, MAMS.** |
| 9.45 – 9.55 | Overview of Research Activities at Bioinformatics Division<br>**Dr Subhash Agarwal, Scientist-E, NICPR** |
| 9.55 – 10.00 | Welcome Note.<br>**Mr. Raghu Rangaswamy, Vice President, Schrodinger** |
| 10.00<br>10.10 | **1. OPENING** – Agenda and split into breakout rooms<br>▪ **Breakout 1** – Introductions and open software. |
| 10.30<br>11.00 | **2. Maestro GUI: Building molecules and Enumeration**<br>▪ **Breakout 2** – Building Chalcones from SMILES |
| 11.20<br>11.35<br>11.45 | **3. Ligand preparation and ADME**<br>▪ **Breakout 3** – Launch LigPrep<br>Intro to Molecular Docking, protein and Ligand Preparations |
| 12.10<br>12.30 | **4. Protein Preparation and Grid Generations**<br>▪ **Breakout 4** – Prepare protein and Grid generations and molecular docking |
| 13.00<br>14.00 | **Break** – Continue to use software during the break<br>Welcome Back |
| 14.10<br>14.25 | **5. Molecular Docking**<br>▪ **Breakout 5** – Analyzing 3D molecular docking analysis |

| DAY 1<br>23rd March 2021 (Tuesday) | |
|---|---|
| **Time** | **Session** |
| 14.40<br>14.55 | **6. Molecular Docking Analysis**<br>▪ Breakout 6 – 2D molecular docking analysis |
| 15.30 | **7. Full Revision of Day1**<br>▪ **Breakout 7** – Full session practice |
| 15.55 – 16.00 | Wrap-up and Finish |

| DAY 2<br>24th March 2021 (Wednesday) | |
|---|---|
| **Time** | **Session** |
| 9.30 | Technical set up |
| 9.50 | Audio & Visual Check |
| 10.00<br>10.30 | **1. OPENING** – Agenda and molecular dynamics theory<br>▪ **Breakout 1** – Docking results and ligand sketching |
| 10.45<br>11.00 | **2. Desmond Introduction**<br>▪ **Breakout 2** – Protein ligand complex formation, system building |
| 11.15<br>11.25 | **3. Molecular Dynamics Demo**<br>▪ **Breakout 3** – MD submission |
| 11.35<br>11.50 | **4. Desmond Trajectory Visualization**<br>▪ **Breakout 4** – Participant analysis |

| DAY 2<br>24th March 2021 (Wednesday) | |
|---|---|
| **Time** | **Session** |
| 12.15<br>14.00 | **Break** – Continue to use software during the break<br>Welcome Back |
| 14.05<br>14.20 | **5. Desmond Molecular Simulation Analysis**<br>▪ **Breakout 5** – Analyzing 3D molecular docking analysis |
| 14.45<br>15.00 | **6. Organic Molecules Enumeration**<br>▪ **Breakout 6** – Reaction-Based enumeration, library enumeration, ADME |
| 15.30 | **7. Full Revision of Day 2** |
| 15.55 – 16.00 | Wrap-up and Finish |

## REGISTRATION DETAILS

**Registration Fees: Rs 500/-**
**No. of seats:** 70
**Registration link:**
https://forms.gle/RjoxpQqpYt8wrG5C6
**Last date for registration: 18th March, 2021**
**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
***bioinformaticslabnoida@gmail.com***