Computational Drug Discovery: A One-Day Hands-On Online Workshop for Scholars and Researchers

9:30 AM to 4:00 PM, 11th March 2025 (Tuesday)

Registration Link: https://forms.gle/jS9gDyFpMzrd3cF16 (Last Date: 1st March 2025)

jointly organized by

Department of Chemistry
Manipur University
&
Schrödinger, Inc.

Registration Fee: Rs. 150/-
UPI No.: 84159 23983

Who Should Attend:

- **Research Scholars & Faculty** seeking to integrate computational techniques into their work.
- **Scientists & Professionals** looking to stay ahead in pharmaceutical research.

Requirement: Laptop/Desktop with internet connectivity

- **Molecular Modeling**
- **Structure-Based Drug Design**
- **Artificial intelligence driven drug design, and simulation techniques - essential skills for modern pharmaceutical and biomedical research**
- **Maestro GUI, a powerful interface for biologics visualization, molecular sketching, and protein selection**

Chairman:
Prof. N. Rajen Singh
Head, Department of Chemistry, MU

Convenor & Schrodinger Software In-charge (Dept.):
Dr. Francis A. S. Chipem
Department of Chemistry, MU

Speakers (Online):

Dr. Abhijit Kayal
Sr. Scientist, Schrodinger

Dr. Vinod Devaraji
Sr. Scientist, Schrodinger

Dr. Koushik Kasavajhala
Sr. Scientist, Schrodinger

Organizing Committee Members:

Prof. R. K. Hemakumar Singh
Prof. Naorem Homendra
Prof. R. K. Lonibala
Prof. Okram Mukherjee Singh
Prof. R. K. Bhubon Singh
Dr. K. Surjit Singh
Dr. W. Rameshwor Singh
Dr. Ningombam Yaiphaba
Dr. R. K. Sunil Singh
Dr. Th. Joymati Devi
Dr. Raju Laishram
Dr. N. Shantibala
Dr. Ng. Florence

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Venue: **Conference Hall (Second Floor), Department of Chemistry, Manipur University**

Program Details

Time	Workshop Topic/Item
9:30 AM	Technical set-up, Audio & Visual Check
9:40 AM	Introductory Note
10:00 AM	**Opening-Molecular Modelling Introductory Presentation**
10:30 AM	**Logging into Cloud instance**
10:45 AM	**Maestro GUI: Bio Macromolecules Visualisations, Building Molecules and Enumeration**
11:15 AM	**Ligand Preparation and ADME**
11:45 AM	**Protein Preparation of Protein Kinase A**
1:00 PM – 2:00 PM	Lunch Break Continue to use software during the break
2:00 PM	Welcome Back
2:10 PM	**Molecular Docking Analysis for hit identification**
2:40 PM	**Molecular Docking Analysis 1 – Pose visualization and evaluation**
3:00 PM	**Molecular Docking Analysis 2 – Protein-Ligand Interaction Diagram and Calculation of Interaction Fingerprints**
3.30 PM	**AI/ML Driven Toxicity Activity Predictions**
3:45 PM – 4:00 PM	Review of Day Activities