



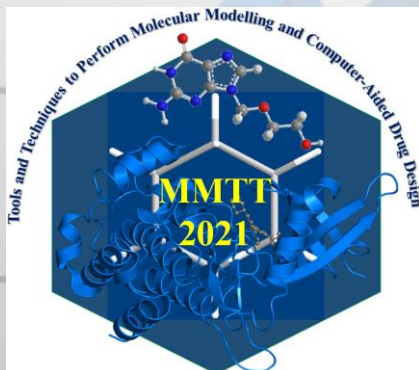
INTERNATIONAL WORKSHOP

on

Tools and Techniques to Perform Molecular Modelling and Computer-Aided Drug Design

(MMTT-2021)

11th - 17th January 2021 (Virtual Mode)



Organized by:

Department of Medicinal Chemistry

National Institute of Pharmaceutical Education and Research (NIPER) Guwahati
(Dept. of Pharmaceuticals, Ministry of Chemicals and Fertilizers, Govt. of India)
Sila Katamur (Halugurisuk), Changsari, Kamrup, Guwahati 781101, Assam (India)

About the NIPER Guwahati

National Institute of Pharmaceutical Education and Research (NIPER) is the first national level institute in pharmaceutical sciences with a proclaimed objective of becoming a centre of excellence for advanced studies and research in pharmaceutical sciences. NIPER is given the Institute of National Importance (INI) status by an act of Parliament of India. NIPER-Guwahati is the only National Institute in Pharmaceutical Sciences in the entire North Eastern Region of India. It was established in the year 2008 to provide high quality education and research with a focus on the exploitation of natural and synthetic products of this region for drug discovery and development. Currently, NIPER-G offers postgraduate as well as doctoral studies in various discipline of Pharmaceutical science. To meet the scientific as well as social responsibilities, six national level centres are continuously fulfilling the need and requirements under the flagship of NIPER-G.

About the Workshop

The workshop on “Tools and techniques to perform molecular modelling and computer-aided drug design” (MMTT-2021), aims to provide a platform for medicinal/computational researchers to utilize the knowledge for computer-aided drug design, discovery, and development. The basic idea is to teach how we perform modern molecular modelling, why we should do it, and most importantly, explain the basics behind the mouse clicks to the beginners.

Salient features of the workshop are as follows:

- Basic introduction to drug design
- Molecular docking using different tools such as Autodock, Glide, etc.
- Introduction to PYMOL, VMD, Openbabel, and Maestro interfaces
- Theoretical methods and algorithms to determine protein structure. Major pitfalls or challenges in determining protein structure. Open-source tools for homology modelling (MODELLER)
- Introduction and applications of force field
- Deciding reaction centre in covalent docking, ligand-based approaches like QSAR, pharmacophore modelling and machine learning, etc.
- Introduction to freely available molecular dynamic engines like NAMD, GROMACS, and DESMOND
- Reaction modelling, QM/MM studies. Introduction to Gaussian and Jaguar
- Case studies on Drug discovery

Who should attend?

The participants of the workshop may be students, research scholars, post doctoral fellows, and young faculties with a background in medicinal/computational chemistry and biology.

How to Apply

Please visit <https://niperguwahati.ac.in/mmtt-2021/>
(no registration fee)

Participants

Lectures are open to all attendees and hands-on training will be provided to 20 invited participants.

Important Dates

Last Date of Registration: 08th January 2021
Workshop Dates: 11th-17th January 2021

Awards

The group with the best hands-on project will be honoured with a prize.

Invited Speakers

Prof. G Narahari Sastry, NESIT Jorhat
Prof. G P S Raghava, IIIT Delhi
Prof. P V Bharatam, NIPER Mohali
Prof. A Shurki, The Hebrew University of Jerusalem, Israel
Prof. Sam de-Visser, University of Manchester, UK
Prof. Etienne Derat, Sorbonne Université Paris, France
Prof. Devesh Kumar, BBAU Lucknow
Prof. Hajime Hirao, City University, Hong Kong
Prof. Sandip Paul, IIT Guwahati
Prof. Aditya Narayan Panda, IIT Guwahati
Prof. Kunal Roy, Jadavpur University, Kolkata
Dr. Madhavi Sastry, Schrodinger
Dr. Deva Priyakumar, IIIT Hyderabad
Dr. F A Pasha, CRD, SABIC, Saudi Arabia
Dr. Jagannath Mondal, TIFR Hyderabad
Dr. Rajat Desikan, Invictus Oncology, Delhi
Dr. Avital Sharir-Ivry, McGill University, Canada
Dr. Priyadarshi Satpati, IIT Guwahati
Dr. Nihar Ranjan Jena, IIIT-DM Jabalpur
Dr. Manavalan Balachandran, Ajou University Medical Center, South Korea
Dr. Harinder Singh, JCVI, USA
Dr. Sandeep Kumar Dhanda, St. Jude Children's Research Hospital, USA
Dr. Chinmayee Choudhury, PGIMER Chandigarh
Dr. Priyanka Banerjee, Charite and Freie University, Berlin
Dr. Hemant Kumar Srivastava, NIPER Guwahati

Patron

Dr. USN Murty, Director
National Institute of Pharmaceutical Education and Research (NIPER)
Guwahati. Sila Katamur (Halugurisuk), Changsari, Kamrup, Guwahati 781101,
Assam (India)

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