Three-day workshop on Advanced Drug Design and Medicinal Chemistry (ADDMC 2nd to 4th February 2022)

About the NIPER Guwahati

National Institute of Pharmaceutical Education and Research (NIPER) is the first national level institute in pharmaceutical sciences with an objective of becoming a center 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, training and perform research with a focus on the applications 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 centers at NIPER-G are continuously fulfilling the need and requirements.

Workshop theme and objective

Discovery of effective treatment options for many diseases (e.g., diabetes, malaria, NAFLD, and cancer) remains a challenging problem even in the 21st century. Computational drug design concepts and technologies have already delivered drugs (e.g., Oseltamivir and Zanamivir) and continue to give vital insights into many more. Nonetheless, the ever-evolving nature of the human genetics, pathophysiology and emergence of resistance requires continuous progress in our scientific and technologies capabilities. This has driven the latest revolution in modern data science and drug discovery methods. Artificial Intelligence (AI) coupled with an exponential increase in the GPU cloud infrastructure, software, have made exascale computations possible. Thus, a reinvention and revolution in the drug discovery timelines is once again on the horizon. The job market for AI supported drug design and discovery is already expanding rapidly.

Thus, it is essential that the young generation actively learns and participates in these activities to ensure the bright future for the nation and meet the make-in-India objectives in the drug discovery sector. The know-how and expertise in modern computational and AI based drug discovery methods is indispensable for medicinal chemistry students and discovery scientists in general.

This workshop aims to introduce young medicinal chemists to modern AI based drug discovery process, get hands-on experience in the tools used for drug design and provide a platform to interact with leading experts across the globe. The sessions are planned such that experts will 1) Introduce the fundamental concepts in AI, computational chemistry, and drug design, 2) Give real-life examples of how these concepts are applied in modern drug discovery settings and last but not the least, 3) Participants will get hands-on training using modern drug design tools. Our focus will be on teach basics of molecular modelling techniques including applications of Quantum Chemical methods, drug design concepts: virtual screening, pharmacophore mapping, molecular docking, QSAR, and dynamics. Eminent speakers will also discuss the role of AI in drug discovery and recent developments in the field.

Dates:

3-5 February 2022. (Thur, Fri, Sat)

Last date for registration:

15th January 2022.

Registration fees:

No fees

Workshop Mode:

Mixed: online-offline mode. Due to COVID-19 related restrictions we have limited capacity to accommodate participants thus a hybrid

mode has been chosen. Those unable to travel can join online for lectures and hands-on sessions. Details will be shared near the time of the workshop.

Patron

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

Chief-Guest

Prof. E. D. Jemmis, IISc

Proposed list of invited speakers.

Names of confirmed speakers

Prof. P. V. Bharatam, NIPER Mohali
Prof. G Narahari Sastry, NESIT Jorhat
Prof. Sam de Visser, University of Manchester, UK
Prof. Evan Coutinho, BCP, Mumbai
Prof. G. P. S. Raghava, IIIT Delhi
Prof. Kunal Roy, JadavpurUniversity, Kolkata
Prof. Prashant Kharkar, ICT Mumbai
Dr. Prakash Rathi, AstraZeneca, UK
Dr. Jaimeen Majamudar, Pfizer, US
Dr. Pankaj Soni, Pfizer, US
Prof. Lalitha Guru Prasad, University of Hyderabad
Prof. Sandip Paul, IIT Guwahati
Dr. Madhavi Sastry, Schrodinger
Dr Suman Sirimulla, UTEP, US
Dr. Jagannath Mondal, TIFR Hyderabad
Prof. A. K. Chakraborti, IACS, Kolkata,
Dr. Devendra Dhakad, NIPER Kolkata

Institutional Advisory Board

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Ms. Sanjana Roychowdhury,
Ms. Monika Verma,

Convener

Dr. Vaibhav A. Dixit,

Assistant Professor, Department of Medicinal Chemistry, NIPER-G.

Contact

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Schedule

Theme: Basics of methods/tools used in Molecular modelling, Drug Design and Medicinal Chemistry

Day/date	Theme	Time	Speaker	Title/Agenda
Day 1 **2nd Feb 2022**	Inaugural session	10.00 to 10.15 am	Prof. USN Murty, Director NIPER-G	Welcome Address and introduction to the Chief Guest
		10.15 to 10.25 am	The Chief Guest	Opening address by the Chief Guest
	Basics of methods/tools used in Molecular modelling	10.30 to 11.10 am	Prof. G Narahari Sastry, NESIT Jorhat	To be announced
		11.15 to 11.55 am	Prof. Evan Coutinho, BCP, Mumbai	The Art and Science of QSAR
		12.00 to 12.55 pm	Prof. P. V. Bharatam, NIPER SAS Nagar	3D thinking in anti-cancer drug design
		13.00 to 14:00 pm	---	Lunch Break
		2:30 to 3:10 pm	Prof. Lalitha Guru Prasad	Sequence and structure analysis of SARS CoV-2 spike protein.
		3:30 to 5:30 pm	Hands-On session	Prof. Prashant Kharkar. OpenEye software for Drug Discovery
Day 2 **3rd Feb 2022**	Applications of AI and QSAR in Drug Design and more…	10.00 to 10.40 am	Prof. G. P. S. Raghava	Advances in computer-aided protein therapeutics
		10:50 to 11:30 am	Prof. Sandip Paul	To be announced
		11:40 to 12:10 pm	Prof. Kunal Roy	
		12:15 to 12:55 pm	Dr. Madhavi Sastry	To be announced
		13.00 to 14:00 pm	---	Lunch Break
		2:30 to 3:10 pm	Dr. Sam de Visser	To be announced
		3:30 to 5:30 pm	Hands-On session	Dr Suman Sirimulla
Day 3 **4th Feb 2022**	Case studies and selected real-world applications	10.00 to 10.40 am	Dr. Jagannath Mondal	Computer simulation of protein/small-molecule binding kinetics in real time
		10:50 to 11:30 am	Dr. Devendra Dhakad	To be announced
		11:40 to 12:10 pm	Prof. A. K. Chakraborti	New Anti-inflammatory Scaffolds: Sustainable Medicinal Chemistry

				Approaches
		12:15 to 12:55 pm	Dr. Pankaj Soni	To be announced
		13.00 to 14:00 pm	---	Lunch Break
		2:30 to 3:10 pm	Dr. Prakash Rathi	To be annouched
		3:20 to 4:00 pm	Dr. Jaimeen Majmudar	Role of Chemical Biology in Drug Discovery
		4:00 to 5:30 pm	Hands-On session	Discovery studio