One Week Workshop on Advanced Drug Designing and Computational Biology

(Under the Aegis of SPARC Scheme)

16th-22nd September 2024

SPARC
Scheme for Promotion of Academic and Research Collaboration

सत्यमेव जयते
Ministry of Education
Government of India

Organized By

Department of Chemistry

Faculty of Sciences

Jamia Millia Islamia (A Central University)

New Delhi-110025, India

www.nasimulhodajmi.com

About the SPARC

Scheme for Promotion of Academic and Research Collaboration (SPARC) is designed by the Ministry of Education, Government of India, to elevate India's research landscape. By fostering collaborations with top international institutions from 28 selected countries, SPARC facilitates joint research and student and faculty exchange and attracts international talent to Indian institutions. Its goal is to address national and international challenges, enhance India's global research standing, and create a robust research ecosystem through developing high-quality academic resources and promoting international academic partnerships.

Overview of Programme

This workshop is designed to equip participants with in-depth knowledge and practical experience in the most advanced techniques and tools in drug design. Participants will gain insights into the integration of computational methods with experimental data, enhancing the efficiency of drug discovery and development.

Key components of the workshop include:

An introduction to molecular docking tools such as **AutoDock**, **AMDOCK**, and **CBDOCK**. Practical exercises in docking small molecules into protein targets. Protein-protein docking using **ClusPro** and **Rosetta** Server. Fundamentals of molecular dynamics (MD) simulations with **NAMD** and **GROMACS**, including the analysis of MD simulation results. The role of bioinformatics in deciphering disease mechanisms. Systems biology approaches to drug discovery.

About the Department of Chemistry

The Department of Chemistry at Jamia Millia Islamia is a prominent part of the Faculty of Sciences. It offers undergraduate (B.Sc. Hons.), postgraduate (M.Sc.), and doctoral (Ph.D.) programs with specializations in Inorganic, Organic, Physical, and Materials Chemistry. The Department comprises highly competent faculty members, including seven Professors, five Associate Professors, and eight Assistant Professors. Each faculty member is actively engaged in research and has published more than 400 research papers in reputed peer-reviewed journals over the last five years. The department has received research funding of 2.4 crore during the last three years from National and International funding agencies like ICMR, DBT, DST, SERB, etc. The department provides excellent research facilities and encourages collaboration with other research institutions.

Workshop Objectives

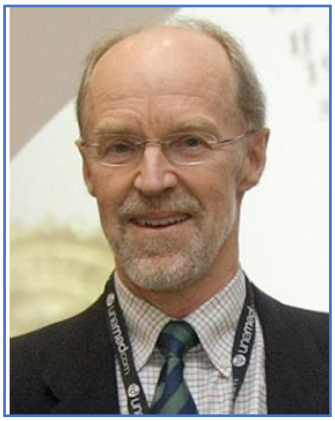
- **Structure-Based Drug Design (SBDD):** Learn to design drug candidates using 3D structures of biological targets through molecular docking, molecular dynamics (MD) simulations, and fragment-based drug design (FBDD).
- **Ligand-Based Drug Design (LBDD):** Explore techniques like Quantitative Structure-Activity Relationship (QSAR), Pharmacophore Modelling, and Virtual Screening to design new drugs based on known active molecules.
- **Molecular Modeling and Simulation:** Gain hands-on experience in building, refining, and simulating molecular structures using tools such as Gabedit, ORCA and GAMESS.
- **Predicting Drug Properties:** Use computational approaches to predict pharmacokinetics (ADME), pharmacodynamics, and toxicological effects with software like **ProTox** and **QSAR ToolBox**.
- **Generative AI/ Machine Learning Based Drug Design**

Learning Outcomes

Upon completing this workshop, participants will be able to:

1. Attain a comprehensive understanding of the fundamentals of drug design using computational approaches.
2. Achieve proficiency in structure- and ligand-based drug design techniques to develop potent drug candidates.
3. Develop expertise in refinement of molecular models, performing simulations, and interpreting results to assess the behavior and properties of drug candidates.
4. Critically evaluate the results of molecular docking and simulations, thereby optimizing the design and development of therapeutic agents and enhancing the probability of successful drug development.

International Experts



Prof. Jonathan L. Vennerstrom
(University of Nebraska Medical Center, USA)

Prof. Jonathan L. Vennerstrom, a medicinal chemist in UNMC's College of Pharmacy, has significantly contributed to the global fight against malaria. Through his work with Medicines for Malaria Venture, he and his team created a new malaria drug approved for use in India in 2012 and another drug candidate which has shown potential as a one-dose cure for malaria. This work was recognized with the prestigious 2019 American Chemical Society Award for Creative Invention. In addition, a panel of world health experts selected it in 2015 as one of 30 high-impact innovations that can save lives and transform global health within 15 years. Current projects include drug discovery for schistosomiasis, tuberculosis and other neglected disease. He has more than 200 publications and several patents to his credit.

Prof. Apurba Dutta
(The University of Kansas, USA)

Prof. Apurba Dutta is a seasoned medicinal chemist at the University of Kansas. Prof. Dutta's academic journey includes extensive experience in India and Germany, enriching his global perspective on drug discovery. Dutta received a doctoral degree from North-Eastern Hill University in India. He was an Alexander von Humboldt Postdoctoral Fellow at the University of Konstanz, Germany, before serving as a scientist for several years at the Indian Institute of Chemical Technology in Hyderabad, India. At Kansas, he has received the Teaching Excellence Award from the Center for Teaching Excellence and served as a Senior Administrative Fellow.

His primary research expertise lies in medicinal and organic chemistry, which is used to develop anti-cancer and anti-infective agents. An important tool in his synthetic endeavors has been the utilization of readily available enantiopure amino acids as chiral building blocks towards stereoselective synthesis of desired target compounds. Prof. Dutta has been the principal investigator or co-investigator on 10 National Institutes of Health research grants and has over 80 peer-reviewed research publications, reviews, book chapters, and patents. Currently serving as the Interim Chair of the Department of Medicinal Chemistry, School of Pharmacy at KU.

Speakers

Prof. J. L. Vennerstrom
UNMC, USA

Prof. Apurba Dutta
KU, USA

Prof. B. Jayaram
IIT, Delhi

Prof. Punit Kaur
AIIMS, New Delhi

Prof. G.P.S. Raghava
IIIT, Delhi

Dr. Pawan Malhotra
ICGEB, New Delhi

Dr. Dhiraj Kumar
ICGEB, New Delhi

Prof. Zahid Ashraf
JMI, New Delhi

Dr. Ashok K Varma
ACTREC, Mumbai

Dr. Saman Habib
CSIR-CDRI, Lucknow

Prof. Imtiyaz Hassan
JMI, New Delhi

Prof. Suhel Parvez
Jamia Hamdard,
New Delhi

Prof. Suvendra K. Ray
Tezpur University,
Assam

Dr. Asif Mohmmed
ICGEB, New Delhi

Prof. Samudrala Gourinath
JNU, New Delhi

Prof. N. Senthil Kumar
Mizoram Central
University, Mizoram

Prof. Subbarao Naidu
JNU, New Delhi

Dr. Shane K. Naqvi
JMI, New Delhi

Prof. Shashank Deep
IIT, Delhi

Prof. M. Mumtaz Alam
Jamia Hamdard,
New Delhi

Dr. Rajan Patel
JMI, New Delhi

Dr. Pradeep Pant
Bennett University
Greater Noida

Dr. Imran A. Khan
Jamia Hamdard
New Delhi

Dr. Khalid Raza
JMI, New Delhi

ORGANIZING COMMITTEE

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Offg. Vice-Chancellor
Jamia Millia Islamia, New Delhi

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Dean (Faculty of Science)
Jamia Millia Islamia, New Delhi

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Supercomputing Facility for Bioinformatics Computational Biology, IIT Delhi

Prof. Jonathan L. Vennerstrom
Department of Pharmaceutical Sciences
University of Nebraska Medical Center, USA

Prof. Apurba Dutta
Department of Medicinal Chemistry, School of Pharmacy
The University of Kansas, USA

Registration Form

The participants are required to complete **online registration *via* google form** and pay the registration fee via the given account transfer. The registration fee is non-refundable, and it includes full participation, workshop kit, and lunch/refreshments.

Important Date

Deadline of Registration and Fee Payment: **10th September, 2024**

Eligibility to Participate

Students of Postgraduate Onwards, Researchers, Working Professionals in Drug Design and Medicinal Chemistry or Allied Areas, and Young Faculty Members.

Registration Fees Rs. 1500/-

*Student Accommodation Charges are applicable separately

***Note:** **Limited Seats Available (40)**
First Come First Served!
Please bring your laptop. No TA/DA will be provided
Shortlisted candidate will be informed.

**Register here by clicking the link or scanning the QR

https://bit.ly/4dzGmUD

Bank Account Details

Beneficiary Name (A/c Name)	JMI-Seminar and Symposium
Name of bank	Indian Bank
Branch	Jamia Millia Islamia
Saving Bank A/c No.	**6767690486**
IFSC Code	**IDIB000J029**
Branch Code	01622
MICR-Code	110019041
SWIFT CODE	IDIBINBBTSY
ZONE	Delhi
Branch Address	Moulana Mohd. Ali Jauhar Marg, Sports Complex, (Bhopal Ground), Jamia Nagar, New Delhi-110025

Venue

FTK-CIT Conference Hall,
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Contact

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