

# Jamia Millia Islamia

## One Week Workshop on Advanced Drug Designing and Computational Biology

September 16<sup>th</sup>-22<sup>nd</sup>, 2024



### Day 1 – 16/09/2024 Monday (Venue: - FTK-CIT Conference Hall, JMI)

9:00 - 10:00	<ul style="list-style-type: none"> <li>Registration</li> </ul>	
10:00 - 10:10	<ul style="list-style-type: none"> <li>Recitation of the Holy Quran and Tarana-e-Jamia</li> </ul>	
10:10 - 10:20	<ul style="list-style-type: none"> <li>Welcome Address, Introduction to the Workshop and the Dept. of Chemistry</li> </ul>	<b>Prof. Saeed Uddin</b> , Chairperson Dean (Faculty of Sciences)
10:20 - 10:30	<ul style="list-style-type: none"> <li>Address by SPARC Co-Ordinator</li> </ul>	<b>Prof. Zahid Ashraf</b> Institute SPARC Co-Ordinator, JMI
10:30 - 10:35	<ul style="list-style-type: none"> <li>Address by Guest of Honor</li> </ul>	<b>Prof. G.P.S. Raghava</b> Director, IIIT, Delhi
10:35 - 10:40	<ul style="list-style-type: none"> <li>Address by Guest of Honor</li> </ul>	<b>Dr. Saman Habib</b> , Chief Scientist CSIR-CDRI, Lucknow
10:40 - 10:45	<ul style="list-style-type: none"> <li>Address by Guest of Honor</li> </ul>	<b>Prof. Ramesh Chandra Deka</b> Vice-Chancellor, Cotton University
10:45 - 10:50	<ul style="list-style-type: none"> <li>Message from Prof. Jonathan L. Vennerstrom, UNMC, USA</li> </ul>	
10:50 - 11:00	<ul style="list-style-type: none"> <li>Presidential Address</li> </ul>	<b>Prof. Mohammad Shakeel</b> Chief-Patron, Vice-Chancellor
11:00 – 11:10	<ul style="list-style-type: none"> <li>Vote of thanks</li> </ul>	
11:10 – 11:15	<ul style="list-style-type: none"> <li>National Anthem</li> </ul>	
11:15 - 11:40	<b>High Tea</b>	
11:40 - 12:20	<ul style="list-style-type: none"> <li>Keynote Lecture: <b>Advances in Computer-Aided Protein Therapeutics</b></li> </ul>	<b>Prof. G.P.S. Raghava</b> Guest of Honor, IIIT, Delhi
12:20 - 13:00	<ul style="list-style-type: none"> <li>Plenary Lecture: <b>Organelle Biology and Targets for Intervention Against Malaria</b></li> </ul>	<b>Dr. Saman Habib</b> , Guest of Honor CSIR-CDRI, Lucknow
13:00 - 14:00	<b>Lunch</b>	
14:00 - 14:40	<ul style="list-style-type: none"> <li>IL-1</li> </ul>	<b>Prof. Suvendra K. Ray</b> Tezpur University, Assam
14:40 - 18:00	<ul style="list-style-type: none"> <li>Software Installation and Introduction to Linux Command</li> </ul>	

### Day 2 – 17/09/2024 Tuesday (Venue: Auditorium, University Polytechnic, Gate No.7, JMI)

10:00 - 10:50	<ul style="list-style-type: none"> <li>IL-2: <b>Structure-Based Drug Discovery: Principles and Protocol</b></li> </ul>	<b>Prof. Imtaiyaz Hassan</b> JMI, New Delhi
10:50 - 11:00	<b>Tea Break</b>	

11:00 -11:50	<ul style="list-style-type: none"> <li>IL-3</li> </ul>	Dr. Mohammad Sufian Badar Jamia Hamdard, New Delhi
11:50 -12:40	<ul style="list-style-type: none"> <li>IL-4: Probing Multivalent Centers in Cholera Prophylaxis: Catalytic Applications and Mechanistic Insights</li> </ul>	Dr. Imran A. Khan Jamia Hamdard, New Delhi
12:40 -13:40	Lunch	
<b>(Venue: - FTK-CIT Conference Hall, JMI)</b>		
13:40 -14:30	<ul style="list-style-type: none"> <li>Introduction to Molecular File Formats</li> </ul>	
14:30 -15:00	<ul style="list-style-type: none"> <li>Introduction to Modern Drug Discovery Pipeline</li> </ul>	
15:00 -16:00	<ul style="list-style-type: none"> <li>Structure Prediction; Active Site Prediction and Virtual Screening</li> </ul>	
16:00 -16:15	Tea Break	
16:15 -17:00	<ul style="list-style-type: none"> <li>Molecular Docking</li> </ul>	
<b>Day 3 – 18/09/2024 Wednesday (Venue: - FTK-CIT Conference Hall, JMI)</b>		
9:30 -10:30	<ul style="list-style-type: none"> <li>IL-5</li> </ul>	Prof. B. Jayaram, IIT Delhi
10:30 -11:00	<ul style="list-style-type: none"> <li>IL-6: Structural and Functional Studies, Inhibitor Development Against Cysteine Biosynthetic Pathway Enzymes of <i>E. histolytica</i></li> </ul>	Prof. Samudrala Gourinath JNU, New Delhi
11:00 -11:10	Tea Break	
11:10 -12:40	<ul style="list-style-type: none"> <li>IL-7: Structure-Based Drug Designing of Antimalarial and Antituberculosis Agents</li> </ul>	Prof. Naidu Subbarao JNU, New Delhi
12:40 -13:10	<ul style="list-style-type: none"> <li>IL-8: AI and Machine Learning in Drug Design: From Data to Therapeutics</li> </ul>	Dr. Khalid Raza JMI, New Delhi
13:10 -14:00	Lunch	
13:40-14:30	<ul style="list-style-type: none"> <li>Recap of Previous Hands-on Session</li> </ul>	
14:30 -16:00	<ul style="list-style-type: none"> <li>Introduction to MD Simulation</li> </ul>	
16:00 -16:15	Tea Break	
16:15 -17:30	<ul style="list-style-type: none"> <li>Minimization, Heating, Equilibration</li> </ul>	
<b>Day 4 – 19/07/2024 Thursday (Venue: - FTK-CIT Conference Hall, JMI)</b>		
10:00 -10:50	<ul style="list-style-type: none"> <li>IL-9: New Anti-Malarial Development: Basic Research to Drug Development</li> </ul>	Dr. Pawan Malhotra ICGEB, New Delhi
10:50 -11:00	Tea Break	
11:00 -11:50	<ul style="list-style-type: none"> <li>IL-10</li> </ul>	Dr. Dhiraj Kumar ICGEB, New Delhi
11:50 -12:40	<ul style="list-style-type: none"> <li>IL-11: Organelle Dynamics and Lipid Biogenesis in Human Malaria Parasite: Discovering Novel Drug Targets and New Antimalarial Candidates</li> </ul>	Dr. Asif Mohmmmed ICGEB, New Delhi
12:40 -13:40	Lunch	
13:40 -16:00	<ul style="list-style-type: none"> <li>Production-MD Simulation</li> </ul>	

16:00 -16:15	<b>Tea Break</b>	
16:15-17:30	<ul style="list-style-type: none"> <li>• Q &amp; A Session and Quiz</li> </ul>	
<b>Day 5 – 20/09/2024 Friday (Venue: - FTK-CIT Conference Hall, JMI)</b>		
10:00 -10:40	<ul style="list-style-type: none"> <li>• IL-12</li> </ul>	<b>Prof. Suhel Parvez</b> Jamia Hamdard, New Delhi
10:40 -10:50	<b>Tea Break</b>	
10:50-11:30	<ul style="list-style-type: none"> <li>• <b>IL-13: Disarming Pathogens: The Role of RNA Aptamers in Targeting Bacterial Ribosomes and Viral Counter-Defense Protein</b></li> </ul>	<b>Dr. Pradeep Pant</b> Bennett University, Greater Noida
11:30-12:10	<ul style="list-style-type: none"> <li>• <b>IL-14: Augmented Antibacterial Performance of Pyrrolidinium-Based Ionic Liquids with Melittin</b></li> </ul>	<b>Dr. Rajan Patel, JMI, New Delhi</b>
12:10-14:00	<b>Lunch Break</b>	
14:00-17:30	<ul style="list-style-type: none"> <li>• MD Simulation Results Analysis</li> </ul>	
<b>Day 6 – 21/09/2024 Saturday (Venue: - FTK-CIT Conference Hall, JMI)</b>		
09:00-11:00	<ul style="list-style-type: none"> <li>• <b>BIOVIA Discovery Studio overview, Discovery Studio Visualizer-Introduction &amp; hands-on practice</b></li> </ul>	BIOVIA Discovery Studio Team
11:00-11:15	<b>Tea Break</b>	
11:15-12:00	<ul style="list-style-type: none"> <li>• <b>Sequence and Structure Alignment Study (Theory and Demo)</b></li> </ul>	BIOVIA Discovery Studio Team
12:00-13:00	<ul style="list-style-type: none"> <li>• <b>Structure Drawing and Protein Preparation (Theory and Demo)</b></li> </ul>	BIOVIA Discovery Studio Team
13:00-14:00	<b>Lunch</b>	
14:00-14:30	<ul style="list-style-type: none"> <li>• <b>Data Exchange and Changing File Formats</b></li> </ul>	BIOVIA Discovery Studio Team
14:30-15:15	<ul style="list-style-type: none"> <li>• <b>Molecular Docking, Validation, and Interaction Analysis (Theory and Demo)</b></li> </ul>	BIOVIA Discovery Studio Team
15:15-16:00	<ul style="list-style-type: none"> <li>• <b>Molecular dynamics and trajectory analysis (Theory and demo)</b></li> </ul>	BIOVIA Discovery Studio Team
16:00-16:15	<b>Tea Break</b>	
16:15-17:00	<ul style="list-style-type: none"> <li>• <b>Running Protocol, Editing Protocols, Writing Script (Perl Script) (Theory and Demo)</b></li> </ul>	BIOVIA Discovery Studio Team
17:00-17:30	<b>Q&amp;A Session</b>	
<b>Day 7 – 22/09/2024 Sunday (Venue: - FTK-CIT Conference Hall, JMI)</b>		
10:00-10:30	<ul style="list-style-type: none"> <li>• IL-15</li> </ul>	<b>Dr. Shashank Shekhar, IIT Delhi</b>
10:30-10:45	<b>Tea Break</b>	
10:45-11:15	<ul style="list-style-type: none"> <li>• <b>Valedictory Function</b></li> </ul>	<b>Mr. M. Nasim Haider, Chief Guest</b>
11:15-11:30	<ul style="list-style-type: none"> <li>• <b>Vote of Thanks</b></li> </ul>	<b>Prof. Nasimul Hoda, Convenor</b>
12:30-13:30	<b>Lunch</b>	
<b>End of Workshop</b>		