

# 9<sup>th</sup> Workshop on Bioinformatics and Molecular Modeling in Drug Design

March 25-27, 2019

Venue: Seminar Hall,  
Dr. B. R. Ambedkar Center for Biomedical Research (ACBR),  
University of Delhi, Delhi 110007

## Detailed Programme

### DAY 1

Monday, March 25, 2019

08:45 – 09:15 a.m. Registration

### Session I

09:15 – 09:25 a.m. *Welcome Address and Inauguration*  
*Prof. Daman Saluja, Director ACBR& Chairperson workshop*

09:25 – 09:30 a.m. *Introduction to speakers: Prof. K. Natarajan (Session Chair)*

09:30 – 10:30 a.m. **Dr. Dinesh Gupta**, Coordinator, Structural and Computational Biology Group, ICGEB, New Delhi;  
*Inaugural Address*  
*Expertise: Translational Bioinformatics*

10:30 – 11:30 a.m. **Dr. Gitanjali Yadav**, Coordinator, Sub DIC at NIPGR, New Delhi  
*Expertise: Computational ecology and system Biology*

11:30 – 11:45 a.m. HIGH TEA

### Session II

11:45 – 12:45 p.m. **Dr. Debasisa Mohanty**, Coordinator, DIC,NII, New Delhi  
*Expertise: Bioinformatics & Computational Biophysics; In silico analysis of genomes*

12:45 – 01:30 p.m. **Dr. Madhu Chopra**, ACBR, DU

- “Basics of Molecular Modeling, energy minimization and molecular dynamics”
- Introduction to molecular modeling software tools

01:30 – 2:30 p.m. LUNCH

<b>Session III</b>	
<b>02:30 – 03:15 p.m.</b>	<b><i>Hands on session. demonstration by Dr. Madhu Chopra</i></b> <ul style="list-style-type: none"> <li>• Building Molecules, Visualization and Analysis</li> <li>• Energy Minimization</li> <li>• Docking and scoring</li> </ul>
<b>03:15 – 03:30 p.m.</b>	<b>TEA</b>
<b>03:30 – 5:30 p.m.</b>	<b><i>Hands-on-training...</i></b> <ul style="list-style-type: none"> <li>• Building Molecules, Visualization and Analysis</li> <li>• Energy Minimization</li> <li>• Use of the Binding Site tool panel to define a binding site using receptor cavities or known ligands for use in the Receptor-Ligand Interactions protocols</li> <li>• Docking and scoring</li> </ul>
<b>DAY 2                      Tuesday, March 26, 2019</b>	
<b>Session I</b>	<i>Chairperson, Prof. Vani Brahmachari, ACBR</i>
<b>09:30 – 10:30 a.m.</b>	<b>Dr. Ankita Narang</b> , ACBR <i>Expertise: Computational Biology</i>
<b>10:30 – 11:00 a.m.</b>	<b>TEA</b>
<b>Session II</b>	<i>Chairperson, Prof. Vani Brahmachari, ACBR</i>
<b>11:00 – 12:00 noon</b>	<b>Dr. Lipi Thukral</b> , IGIB, Delhi <i>Title: How protein homologs have different functions but same binding sites?</i>
<b>12:00 – 1:00 p.m.</b>	<b>Dr. Arnab Bhattacharjee</b> , JNU, New Delhi <i>Expertise: Molecular simulations and biophysics</i>
<b>01:00 – 02:00 p.m.</b>	<b>LUNCH</b>
<b>02:00 – 03:00 p.m.</b>	<b>Dr. Madhu Chopra</b> <ul style="list-style-type: none"> <li>• Protein Homology Modeling and drug design strategies (Lecture &amp; Demonstration)</li> <li>• Introduction to Gromacs for setting up Molecular Dynamics</li> </ul>
<b>03:00 – 03:20 p.m.</b>	<b>TEA</b>

<b>Session III</b>	
03:20 – 04:20 p.m.	<b>Hands-on-Training session By Mr. Prakash Jha</b> <ul style="list-style-type: none"> <li>Molecular Dynamics using Gromacs</li> </ul>
<b>Session IV</b>	
04:20 – 5:30 p.m.	<b>Hands-on-Training session contd....</b> <ul style="list-style-type: none"> <li>Conformational Analysis</li> <li>Pharmacophore Modeling</li> </ul>
<b>DAY 3</b>	<b>Wednesday, March 27, 2018</b>
<b>Session I</b>	<i>Chairperson: Dr. P. M. Luthra, ACBR, DU</i>
09:30 – 11:00 a.m.	<b>Prof. B. Jayaram</b> , Supercomputing Facility for Bioinformatics and computational biology, IIT, New Delhi <i>Expertise: GENOME to DRUGS</i>
11:00 – 11:30 a.m.	TEA
<b>Session II</b>	
11:30 –12:30 p.m.	<b>Dr. P. M. Luthra</b> , ACBR, DU <i>Expertise: Medicinal Chemistry and Drug Discovery</i>
12:30 – 1:30 p.m.	<b>Dr. Anshu Bhardwaj</b> , IMTECH, Chandigarh <i>Expertise: Bioinformatics and Computational Biology, Genome annotation, Drug discovery, Crowd sourcing.</i>
01:30 – 02:30 p.m.	LUNCH
<b>Session III</b>	
02:30 – 3:30 p.m.	<i>Hands -on -training session continued...</i> Pharmacophore Modeling and virtual screening
<b>Session IV</b>	
03:30 – 04:00 p.m.	<b>Distribution of Certificates and Vote of Thanks</b>
04:00 – 04:30 p.m.	TEA