7th Workshop on Bioinformatics and Molecular Modeling in Drug Design

March 23-25, 2017

Venue: Seminar Hall, ACBR, University of Delhi

Detailed Programme	
DAY 1	Thursday, March 23, 2017
08:45 – 09:15 a.m.	Registration
09:15 – 09:30 a.m.	*Welcome and Administrative Announcements*
09:30 –11:00 a.m.	**Dr. Madhu Chopra**, ACBR *Basics of Bioinformatics, Molecular Modeling and its applications*
11:00 – 11:30 a.m.	**Tea**
11:30 – 12:30 p.m.	**Prof. K. Natarajan, Welcome Address & Introduction to speakers** **Dr. Dinesh Gupta**, ICGEB, New Delhi *Inaugural Address,* *Computational tools for exploration of interacting proteins as drug targets*
12:30 – 01:30 p.m.	**Dr. Debasisa Mohanty,** NII, New Delhi *Keynote Address,* *In silico analysis of protein interaction networks using multi-scale modelling approach*
01:30 – 02 :30 p.m.	**Lunch**
02:30 – 03:30 p.m.	*Hands on training session by Dr. Madhu Chopra (Demonstration)*
	• Building Molecules, Visualization and Analysis • Energy Minimization and Dynamics • 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
03:30 – 03:45 p.m.	Tea
03:45 – 05:00 p.m.	Hands –on –Training session on above tools
DAY 2	Friday, March 24, 2017
09:30 – 11:00 a.m.	***Webinar by Dr. Rae Lawrence,*** *Technical Expert from M/s Cresset, Cambridgeshire, UK* 1) *Introduction to Cresset's science and overview of applications* 2) *Introduction to scaffold-hopping and lead optimization by bioisosteric substitutions (Spark)* 3) *Introduction to ligand-based drug design and SAR analysis (Forge)* 4) *Overview of field based virtual screening (Blaze Demo Server)*

11:00 – 11:30 a.m.	**TEA**
11.30 – 12.30 p.m.	**Webinar by Dr. Rae Lawrence Continued……**
12.30 – 1.30 p.m.	**Dr. Anshu Bharadwaj, IGIB** *Understanding Natural Product Chemical Space for New Drug Discovery: Tuberculosis as a case study*
01:30 – 02.30 p.m.	**LUNCH**
02:30 – 03:30 p.m.	**Dr. Madhu Chopra** *Process of Drug Discovery and Development: Inventing drugs through use of Computational methods*
03.30 – 03.45 p.m.	**Tea**
03.45 – 05.00 p.m.	Hands – on – training session *Protein Structure Modeling and Protein –Protein Interaction Network Analysis*
DAY 3	**Saturday, March 25, 2017**
09:30 – 10:30 a.m.	**Prof. P. V. Bharatam,** NIPER, Mohali, Punjab **Keynote Speaker** *Design, Synthesis and Biological Evaluation of GSK-3β Inhibitors as Anti-Alzheimer's Agent*
10:30 – 11:00 a.m.	**TEA**
11:00 – 11:45 a.m.	**Dr. Shubhra Chaturvedi, INMAS,** *INMAS perspective on the application of molecular modeling in the development of neurological radiopharmaceuticals*
11:45 – 12:30 p.m.	**Prof. Vani Brahamachari, ACBR,** *Distinguishing between biochemical and cellular function: Are there peptide signatures for cellular function of proteins?*
12:30 – 1.30 p.m.	***Hands-on-Training session By Dr. Madhu Chopra*** • Docking and scoring • Pharmacophore Modeling
01:30 – 02:30 p.m.	**LUNCH**
03:00 – 4:00 p.m.	**Prof. Punit Kaur , AIIMS New Delhi,** *Valedictory Address* *The role of Structural Bioinformatics in BioMedical Sciences*
04.00 – 04.15 p.m.	***Distribution of Certificates and Vote of Thanks***
04:15 – 04:30 p.m.	***TEA***