

10th Workshop on Bioinformatics and Drug Design: Artificial Intelligence (AI) and Machine Learning (ML) Based Methods

March 12-14, 2020, Venue: Seminar Hall, Dr. B. R. Ambedkar Center for Biomedical Research (ACBR), University of Delhi, Delhi 110007

Time	DAY 1 (12-03-2020)	DAY 2 (13-03-2020)	DAY 3 (14-03-2020)
08:45 – 09:15 a.m.	Registration		
09:15 – 09:30 a.m.	<i>Welcome Address and Inauguration</i> Prof. Daman Saluja , Director ACBR & Chairperson workshop		
09:30 – 10:30 a.m.	Dr. Debasisa Mohanty , Coordinator, DIC, NII, New Delhi <i>Expertise:</i> Bioinformatics & Computational Biophysics; <i>In silico</i> analysis of genomes	Dr. Dinesh Gupta , Coordinator, Structural and Computational Biology Group, ICGEB, N. Delhi; <i>Expertise:</i> <i>Translational Bioinformatics</i>	Dr. Salma Jamal , Jamia Hamdard, N. Delhi <i>Expertise:</i> Cheminformatics and bioinformatics <ul style="list-style-type: none"> • Introduction to machine learning based drug design methods • Data retrieval and pre-processing, descriptor generation
10:30 – 11:30 a.m.	Dr. Gitanjali Yadav , Coordinator, Sub DIC at NIPGR, New Delhi <i>Expertise:</i> Computational ecology and system Biology	Dr. Arun Sharma , DBT Apex Centre, ICGEB, New Delhi	Dr. Salma Jamal <ul style="list-style-type: none"> • Training and test set, predictive classification model generation • Model Evaluation: Cross validation & statistical evaluation
11:30 – 11:45	Tea	Tea	Tea
11:45 – 12:45 p.m.	Prof. Shandar Ahmad , JNU, New Delhi <i>Expertise:</i> Machine Learning, big data analysis, Deep learning through NN	Dr. G. Pillai , Scientist, Nyro Research India, Kochi <ul style="list-style-type: none"> • Role of Machine Learning in Drug Design 	Dr. Tavpritesh Sethi , IIIT Delhi <i>Expertise:</i> Computational Biology-AI, ML & DL
12.45 – 1.30 p.m.	Dr. Anshu Bhardwaj , IMTECH, Chandigarh <i>Expertise:</i> Bioinformatics and Computational Biology, Genome annotation, Drug discovery, Crowdsourcing.	Dr. G. Pillai , Hands on Demonstration: <ul style="list-style-type: none"> • RDkit libraries and Machine Learning in CADD. 	Dr. Tavpritesh Sethi , IIIT Delhi Hands-on-training session
01.30 – 2.30 p.m.	LUNCH	LUNCH	LUNCH
02:30 – 03:15 p.m.	Dr. Madhu Chopra , ACBR, DU <i>Expertise:</i> Computer aided drug design and development <ul style="list-style-type: none"> • Introduction to molecular modeling, QSAR and virtual screening software tools 	<i>Hands-on-Training session By</i> Mr. Prakash Jha <ul style="list-style-type: none"> • Molecular Dynamics using Gromacs 	Dr. Tavpritesh Sethi , IIIT Delhi Hands-on-training session continued
03:15 – 03.30 p.m.	Tea	Tea	Tea
03.30 – 5.30 p.m.	Hands-on-training... <ul style="list-style-type: none"> • Energy Minimization • Define a binding site using receptor cavities or known ligands • Docking and scoring 	<i>Hands-on-Training session contd....</i> <ul style="list-style-type: none"> • Conformational Analysis • QSAR and Classification Methods • Pharmacophore Modeling • Virtual screening methods 	Distribution of Certificates and Vote of Thanks