

**10th National Symposium cum Workshop on “Recent Trends in Structural Bioinformatics and Computer Aided Drug Design” [SBCADD’2018]
and**

1st Annual Meeting of Bioinformatics and Drug Discovery Society [BIDDS]

20th - 23rd February, 2018

PROGRAMME SCHEDULE

20 th February, 2018	
09:00-10:30 am	Registration
10:30-12:00 pm	Invocation and Vallal Vazhthu
	Lighting of Kuthuvilakku
	Welcome Address Prof. J. Jeyakanthan Organizing Secretary, SBCADD’2018
	Inaugural Address Prof. Arun K Pujari Vice-Chancellor Central University of Rajasthan, Rajasthan
	Presidential Address Prof. S. Subbiah Vice-Chancellor Alagappa University
	Thematic Address Prof. T. P. Singh Distinguished Biotechnology Research Professor Department of Biophysics All India Institute of Medical Sciences, New Delhi
	Keynote Address Prof. K. Suguna Molecular Biophysics Unit Indian Institute of Science, Bangalore
	Felicitation Address Prof. D. Velmurugan UGC - BSR Faculty CAS in Crystallography and Biophysics University of Madras, Chennai
	Vote of Thanks Prof. Sanjeev Kumar Singh Organizing Committee Member, SBCADD’2018
12:00-12:15 pm	HIGH TEA

Session I	
Chairperson: Prof. K. Suguna Co-Chairperson: Prof. Sanjeev Kumar Singh	
12:15-01:00 pm	Plenary Lecture – I: Dr. G. Narahari Sastry , Indian Institute of Chemical Technology, Hyderabad Title: Developing Disease Specific Web Portals: Molecular Property Diagnostic Suite
01:00-02:00 pm	LUNCH
Session II	
Chairperson: Prof. Michael Gromiha Co-Chairperson: Dr. M. Karthikeyan	
02:00-02:30 pm	Plenary Lecture – II: Dr. K. Suguna , Indian Institute of Science, Bangalore Title: Aspartic Proteinases as Drug Targets
02:30-03:00 pm	Plenary Lecture – III: Dr. H. A. Nagarajaram , Central University of Hyderabad, Hyderabad Title: Analysis of Human-viral protein-protein interaction networks
03:00-03:30 pm	Plenary Lecture –IV: Dr. D. Velmurugan , University of Madras, Chennai Title: Isolation, structural characterization, cell line studies and molecular modeling of four anti-cancer compounds from medicinally important herbs
03:30-03:45 pm	HIGH TEA
Session III	
Chairperson: Dr. Ritushree Kukreti Co-Chairperson: Prof. J. Jeyakanthan	
03:45-04:15 pm	Plenary Lecture – V: Dr. K. Sekar , Indian Institute of Science, Bangalore Title: Sequence motif and its three-dimensional structure: A data mining study
04:15-04:45 pm	Plenary Lecture – VI: Dr. T. P Singh , All India Institute of Medical Sciences, New Delhi Title: Search of Multiple Hot Spots on the Surface of Peptidyl-tRNA Hydrolase: Structural, Binding and Antibacterial Studies
04:45-05:15 pm	Plenary Lecture – VII: Dr. Michael Gromiha , Indian Institute of Technology - Madras, Chennai Title: Bioinformatics approaches for discriminating driver and passenger mutations in Cancer
05:30-06:30 pm	1st Annual Meeting of Bioinformatics and Drug Discovery Society [BIDDS]
07:00-08:00 pm	Cultural(s)
08:00-09:00 pm	Dinner

21st February, 2018

Session IV

Chairperson: **Prof. Shandar Ahmed**

Co-Chairperson: **Dr. RM. Vidhyavathi**

09:30-10:00 am	Plenary Lecture-VIII: Dr. Shailza Singh , National Centre for Cell Science, Pune Title: Signaling framework for Synthetic circuit immuno-modulation in <i>Leishmaniasis</i> : A Structural Perspective for Drug Delivery Systems
10:00-10:30 am	Plenary Lecture – IX: Dr. Suresh K. Rayala , Indian Institute of Technology - Madras, Chennai Title: Targeting DNA repair proteins in Cancer
10:30-11:00 am	Plenary Lecture – X: Dr. Ritushree Kukreti , CSIR-Institute of Genomics and Integrative Biology, New Delhi Title: Peripheral blood gene expression signatures determining valproate efficacy in patients with epilepsy
11:00-11:15 am	HIGH TEA
Session V	
Chairperson: Prof. Vikash Kumar Dubey Co-Chairperson: Dr. J. Joseph Sahayarayan	
11:15-11:45 am	Plenary Lecture – XI: Dr. Shandar Ahmed , Jawaharlal Nehru University, New Delhi Title: Big data analytics and deep learning applications for transcriptome based drug discovery.
11:45-12:15 pm	Plenary Lecture – XII: Dr. Ganesh Venkatraman , Sri Ramachandra University, Chennai Title: Pak1- a new molecular player in the arena of skin cancer
12:15-12:45 pm	Plenary Lecture – XIII: Dr. Poonam Singh , CSIR- Central Electrochemical Research Institute, Karaikudi Title: Repurposing of drugs for identifying new uses of existing drugs
01:00-02:00 pm	LUNCH & POSTER SESSION
Session VI	
Chairperson: Dr. Timir Tripathi Co-Chairperson: Dr. P. Boomi	
02:00-02:30 pm	Plenary Lecture – XIV: Dr. Vikash Kumar Dubey , Indian Institute of Technology, Guwahati Title: Exploiting mechanism of parasite manipulation of host immunity and key metabolic pathways for management of the disease
02:30-03:00 pm	Plenary Lecture – XV: Dr. A. Anand , Vellore Institute of Technology, Vellore Title: Gene and protein Network Analysis Tools for understanding the molecular basis of antibiotic resistance in pathogenic bacteria
03:00-03:15 pm	HIGH TEA

Session VII	
Chairperson: Dr. Shailza Singh Co-Chairperson: Dr. V.K. Langeswaran	
03:15-03:45 pm	Plenary Lecture – XVI: Dr. Basant Kumar Tiwary , Pondicherry University, Puducherry Title: A search for Network Biomarker among Heterogeneity of Cancer
03:45-04:15 pm	Plenary Lecture – XVII: Dr. Timir Tripathi , North-Eastern Hill University, Shillong Title: Understanding the role of structurally distant amino acids in modulating the structure and activity of <i>Mycobacterium tuberculosis</i> isocitrate lyase.
04:15-04:45 pm	Plenary Lecture – XVIII: Dr. Md. Imtiyaz Hassan , Jamia Millia Islamia University, New Delhi Title: A Newer Therapeutic Approach to Target Cancer Cell Progression by Inhibiting Human Protein Kinases using Natural Products
04:45-05:15 pm	Plenary Lecture – XIX: Dr. Asimul Islam , Jamia Millia Islamia University, New Delhi Title: Macromolecular crowding induces stabilization of proteins: A study to understand the significance of the size of crowder
05:15-05:45 pm	Talk from Mr. Ranganathan Raghavan , GE Healthcare Life Sciences Title: The Highway: From University to a Lab to a Business

Workshop on <i>In Silico</i> Structure and Ligand Based methods in Drug Discovery		
22nd February, 2018		
Day 1: Structure & Ligand Based Drug Discovery		
09:30-10:30 am	Session I	Computational methods and advances in the discovery of small drug designing: <i>Advanced In silico methods in Lead identification and Optimization</i> <i>Examples of success stories: Clinical candidates designed using modeling methods</i> Presentation
10:35-01:00 pm	Session II	Selection and refinement of crystal structure of target for SBDD; Preparation of ligands for SBDD: Includes selection of PDB structures (target structures) and explanations about the pitfalls in structures and how to refine the structures for SBDD Presentation and Hands on
11:15-11:30 am	HIGH TEA	
11:30-12:15 pm	Session III	Binding site analysis and its importance in Structure based lead identification and optimization: Presentation and Hands on
12:15-02:00 pm	LUNCH & POSTER SESSION	
02:00-04:00 pm	Session IV	Recent Developments in Docking Scoring Functions: Docking studies of FXa inhibitors

		Structure Based Virtual Screening of novel FXa <i>Presentation and Hands on</i>
04:00-04:15 pm	HIGH TEA	
04:15-05:00 pm	Session V	Method in achieving the Protein flexibility upon ligand binding (INDUCED FIT): Case study with MK5 receptor <i>Presentation and Hands on</i>
05:00-05:30 pm	Chairperson: Dr. Ravikumar Muttineni	Co-Chairperson: Prof. J. Jeyakanthan Beckman Coulter Centrifugation Solution for Biomolecules <i>Presentation</i>
05:00-08:00 pm	Schrodinger Practice session	
23rd February, 2018		
09:30-11:30 am	Session VI	Homology modeling of unknown targets: case study with kinase receptor: Homology modeling of MK5 (Mitogen-Activated protein kinase [MAPK]-activated protein kinase 5): Starting with the selection of sequence, searching the proper homologous template, model building and refinement. Further validation of final model. Advances in Homology Modeling of GPCRs. <i>Presentation and Hands on</i>
11:30-11:45 am	HIGH TEA	
11:45-12:30 pm	Session VII	Pharmacophore modeling and virtual screening of Anti-cancer compounds: Case study with AT1 receptor inhibitors: Identification of common pharmacophore, scoring and validation of pharmacophore, virtual screening of database with diverse compounds. <i>Presentation and Hands on</i>
12:30-01:15 pm	Session VIII	Methods in QSAR modeling 3D-QSAR modeling of anti-cancer compounds <i>Presentation and Hands on</i>
01:15-02:00 pm	LUNCH	
02:00-03:30 pm	Session IX	Calculation of physiochemical properties and ADME modeling: <i>Presentation and Hands on</i>
	Session X	Protein-Protein Docking Protein-protein docking and building complex of Trypsin-trypsin inhibitors Understanding protein-protein interface using Schrödinger PPI tool <i>Presentation and Hands on</i>
	Session XI	Residue scanning and associated property predictions Protein aggregation predictions and analysis of results <i>Hands on</i> Protein Aggregation Analysis Residue-scanning and associated property predictions, Cysteine scanning, Reactive hot spots prediction and Affinity Maturation in peptide designing and vaccine modeling <i>Hands on</i>

03:30-03:45 pm	HIGH TEA
03:45-04:45 pm	Crystallization Techniques <i>Hands on</i>
05:00- 05:30 pm	VALEDICTORY FUNCTION
05:30-09:00 pm	Schrodinger Practice session