DEPARTMENT OF BIOINFORMATICS
ALAGAPPA UNIVERSITY
*(A **State University Reaccredited with 'A' Grade by NAAC**)*
KARAIKUDI-630 004, TAMIL NADU

6th National Symposium cum Workshop on "Recent Trends in Structural Bioinformatics and Computer Aided Drug Design"

SBCADD-2014

18th -21st February, 2014

PROGRAMME SCHEDULE

DAY I

18th February, 2014

Venue: Department of Bioinformatics, Science Block

Workshop on "Computational Methods in Drug Discovery"

09:00 – 10:00 am	**REGISTRATION**
10:00-11:30 am	Methods and Advances in Structure and Ligand Based Drug Design ***Presentation***
11:30 - 11:45 am	**TEA**
11:45 -12:30 pm	Selection and refinement of crystal structure of target for SBDD; Preparation of ligands for SBDD ***Presentation and Hands-on***
12:30 - 1:15 pm	Importance of Binding site for Structure based lead identification and optimization ***Presentation and Hands-on***
01:15 - 02:00 pm	**LUNCH**
02:30 - 3:15 pm	Recent Developments in Docking Scoring Functions; Structure Based Virtual screening of IRAK4 (Oncology target) Inhibitors using ***Presentation and Hands-on***
03:15- 4:00 pm	Protein-Protein docking methods and applications in BiologicsDocking of FAB13B5 antibody to HIV-1 Capsid Protein ***Presentation and Hands-on***
04:00 - 04:15 pm	**TEA**
04:15 - 5:00 pm	Exercise on modeling the compounds using Sitemap and Docking ***Exercise***

DAY II

19th February,2014

INAUGURAL FUNCTION

Venue: L.C.T.L. Palaniappa Chettiar Memorial Auditorium, Alagappa University

09:30-10:30 pm	Invocation and VallalVazhthu
	Lighting of Lamp
	Welcome Address **Dr. J. JEYAKANTHAN** Convener Professor and Head, Department of Bioinformatics
	Presidential address **Dr. S. KALIYAMOORTHY** Convener Vice Chancellor Officiating Committee
	Inaugural Address **Dr. T.P. SINGH** Distinguished Biotechnology Research Professor Department of Biophysics All India Institute of Medical Sciences New Delhi
	Keynote Address **Dr. B. JAYARAM** Coordinator School of Biological Sciences IIT Delhi, New Delhi
	Special Address **Dr. MANJU BANSAL** Molecular Biophysics Unit Indian Institute of Science Bangalore

	Thematic Address **Dr. D. VELMURUGAN** Professor & Head CAS in Crystallography and Biophysics University of Madras Chennai
	Vote of Thanks **Dr. SANJEEV KUMAR SINGH** Organizing Secretary Associate Professor Department of Bioinformatics
10:30-10:45 am	**HIGH TEA**

Plenary Lecture-Session I

10:45-11:25 am	Innate Immune Proteins as Protein-Antibiotics - A Structural basis **Prof. T.P. Singh** All India Institute of Medical Sciences, New Delhi
11:25 – 12:05 pm	DNA structural features and gene expression **Prof. Manju Bansal** Indian Institute of Science, Bangalore
12:05 – 12:45 pm	Genomes to Hit Molecules *In Silico*: A country path today, a highway tomorrow **Prof. B. Jayaram** Indian Institute of Technology, Delhi

12:45 – 01:45 pm	**LUNCH**

Plenary Lecture-Session II

01:45-02:25pm	Inhibitors for cell division protein – A theoretical and experimental approach **Prof. MukeshDoble** Indian Institute of Technology Madras, Chennai
02:25 -03:05 pm	Divalent N(I) compounds in anti-malarial drug design **Prof. P.V. Bharatam** National Institute of Pharmaceutical Education and Research (NIPER)
03:05-03:45pm	Molecular informatics and its impact on Drug Discovery **Dr. V. N.Balaji** Consultant&Ex-CEO, Jubilant Biosys Limited

03:45 –04:00 pm	**HIGH TEA**

04:00-04:40 pm	Protein engineering and structural analysis of *Staphylococcus typhi*OmpFporin **Prof. S. Krishnaswamy** Madurai Kamaraj University, Madurai
04:40–05:20 pm	Design of peptide inhibitors as potential anti-viral drugs for Dengue virus **Prof. D. Velmurugan** University of Madras, Chennai
05:20-06:00 pm	Redefining Psychiatric Diseases: A Systems Biology Approach **Dr. Basant K. Tiwary** Pondicherry University, Pondicherry

06:00-06:45pm	**CULTURALS**

DAY III

20th February, 2014

Venue: Department of Bioinformatics, Science Block

Plenary Lecture-Session III

10:00-10:40 am	Data mining in Protein Structures **Prof. K. Sekar** Indian Institute of Science, Bangalore
10:40-11:20 am	Non-canonical H-bonds in β- lactamases **Prof. AnandAnbarasu** Vellore Institute of Technology, Vellore
11:20 – 11:35 am	**TEA**
11:35 – 12:15 pm	Drug Repositioning - Challenges and Opportunities **Dr. G. Ramesh Kumar** AU KBC Research Centre, MIT Campus of Anna University
12:15 -12:55 pm	Thermodynamic analysis of water and its applications in Drug discovery **Mr. R. Raghu** Schrodinger (USA), Bangalore
12:55 – 02:05 pm	**LUNCH& POSTER SESSION**

Workshop

02:05 – 03:30 pm	Advances in Homology Modeling Homology modeling of MK5 (mitogen-activated protein kinase [MAPK]-activated protein kinase 5) ***Presentation and Hands-on***
03:30- 03:45 pm	**TEA**
03:45 – 05:30 pm	Structure and Ligand Pharmacophore modeling and virtual screening of Anti-cancer compounds ***Presentation and Hands-on***

SCHRÖDINGER.

DAY IV

21st February, 2014

Venue: Department of Bioinformatics, Science Block

Workshop

10:00 -11:30 am	Methods in QSAR modeling; 3D-QSAR modeling of anti-cancer compounds ***Presentation and Hands-on***
11:30 -11:45 am	**HIGH TEA**
11:45 - 1:15 pm	Optimizing the virtual screening hits obtained from docking and pharmacophore models using: MMGBSA, constraint-filters, clustering methods, structural interaction fingerprints (SIFt) and Chemoinformatics ***Presentation and Hands-on***

01:15- 2:30 pm	**LUNCH & POSTER SESSION**
02:30- 3:15 pm	**VALEDICTORY FUNCTION & PRIZE DISTRIBUTION**