3rd IIT Madras – Tokyo Tech Joint Symposium on
"Algorithms and Applications of Bioinformatics"
5th–6th November, 2015
IC&SR Auditorium, IIT Madras

Tentative schedule

November 5, 2015, Thursday

8.30 – 9.00	Registration
9.00 – 9:30	Inauguration
9:30 – 10:00	Coffee break

Session 1: 10:00 – 12:00 **Protein sequence/structure/function analysis**

Chairpersons: Professor Yutaka Akiyama/ Prof. D. Velmurugan

10:00 – 10:30   Dr. N. Srinivasan, Indian Institute of Science, Bangalore
Bridging the islands of protein families in sequence space using artificial sequences

10:30 – 11:00   Dr. Takashi Ishida, Tokyo Institute of Technology, Tokyo
Protein structure prediction based on machine learning

11:00 – 11:30   Dr. N. Manoj, IIT Madras
Evolutionary history of the Neuropeptide S Receptor/Neuropeptide S system

11:30 – 12:00   Dr. Nobuyuki Uchikoga, Chuo University, Tokyo
Analysis of protein docking decoys in terms of physicochemical properties of protein interaction surfaces using rigid-body docking process

12:00 – 13:00   Lunch and Discussions

Session 2: 13:00 – 15:00 **Bioinformatics databases/algorithms**
Chairpersons: Prof. N. Srinivasan/ Dr. Sekijima

13:00 – 13:30   Prof. Yoshihiro Taguchi, Chuo University, Tokyo
Principal component analysis based unsupervised feature extraction applied to various bioinformatic analyses

13:30 – 14:00   Dr. M. Michael Gromiha, Department of Biotechnology, IIT Madras
Development of databases and algorithms for identifying aggregating peptides: applications to neurodegenerative diseases

14:00 – 14:30	Dr. Shuntaro Chiba, Tokyo Institute of Technology, Tokyo
	Systematic Approach to Force Field Determination for Solution Based on Kirkwood-Buff Theory

14:30 – 15:00	Dr. Yuri Matsuzaki, Tokyo Institute of Technology, Tokyo
	MEGADOCK: A high-performance protein-protein interaction prediction software for petascale supercomputing environments

15:00 – 15:30	Tea break

Session 3: 15:30 – 16:30 High performance computing/genome sequencing
Chairpersons: Prof. Y-h. Taguchi/ Prof. Srinivasa Chakravarthy

15:30 – 16:00	Prof. Yutaka Akiyama, Tokyo Institute of Technology, Tokyo
	GHOST-MP: an ultra-fast and high-sensitive homology search software for metagenome analysis

16:00 – 16:30	Dr. R. Sowdhamini, NCBS Bangalore
	Genome sequencing of Tulsi – a medicinally important herb

Session 4: 16:30 – 18:30　　　Poster presentations I
Evaluators: Prof. D. Velmurugan, Prof. Y-h. Taguchi, Dr. Sekijima and Dr. Sowdhamini

16:30-17:30:	Odd numbered posters
17:30-18:30:	Even numbered posters

November 6, 2015, Friday

Session 5: 9:00 – 10:30 Drug design
Chairpersons: Dr. Athi Narayanan/ Dr. Nobuyuki Uchikoga

9:00 – 09:30	Professor D. Velmurugan, University of Madras
	Inhibition of drug efflux mechanism of NorM-A Multidrug and Toxic compound extrusion Transporter- An insilico molecular modeling and simulation studies

09:30 – 10:00	Dr. Masakazu Sekijima, Tokyo Institute of Technology, Tokyo
	Molecular Dynamics Simulation and Docking Simulation for Drug Discovery

10:00 – 10:30   Professor Mukesh Doble, IIT Madras
Design of Anti inflammatory drugs targeting the arachidonic acid pathway

10:30 – 11:30   **Session 6: Poster presentations II/** Coffee break

Session 7: 11:30 - 13:00 **Molecular dynamics simulations**
Chairpersons: Dr. Karthik Raman/ Dr. Shuntaro Chiba

11:30 – 12:00   Dr. V. Subramanian, Central Leather Research Institute
Studies on the structure and dynamics of collagen like peptides with interruption and their interaction with matrix metalloproteinase using molecular modeling techniques

12:00 – 12:30   Prof. K. Veluraja, Vellore Institute of Technology
Structural insights of Hemagglutinin complexed with derivatives of sialyldisaccharides –MD simulation Approach

12:30 – 13:00   Dr. S. Senapati, Department of Biotechnology, IIT Madras
Mechanism of Activation and Inhibition of Cyclin Dependent Kinase 2

13:00 – 14:00   Lunch and Discussions

Session 8: 14:00 – 15:00 **Oral presentations**
Chairpersons: Prof. Veluraja/ Dr. Ishida

15:00 – 16:00   Valedictory and Presentation of poster awards
Valedictory address: Prof. K.K. Balasubramanian, INSA Senior Scientist, IIT Madras

16:00 – 17:00   High Tea and Discussions