4th IIT Madras – Tokyo Tech Joint Symposium on "Frontiers in Bioinformatics: Large scale data analysis, Resources and Drug Design"

10th-11th November, 2017

IC&SR Auditorium, IIT Madras

SCHEDULE

November 10, 2017, Friday

08:00 -09.00 ***Registration***

09:00-09:30 ***Inauguration***

09:30- 10:00 ***Coffee break***

SESSION 1 (10:00 – 12:00): Protein sequence/Structure/Function Analysis

Chairpersons: Dr. Masakazu Sekijima / Prof. D. Velmurugan

10:00 - 10:30 ***Sequence motif and its three-dimensional structure: A data mining study***
Prof. K. Sekar, Indian Institute of Science, Bangalore

10:30 - 11:00 ***Implications of glycosylation in proteins through genetic and proteomic sequence analysis***
Prof. K. Veluraja, Vellore Institute of Technology, Vellore

11:00 - 11:30 ***Evolution of structure-function relationships in the carbohydrate esterase family 7***
Dr. N. Manoj, IIT Madras

11:30 - 12:00 **Oral presentations**

12:00 - 13:00 ***Lunch and Discussions***

SESSION 2 (13:00 – 15:00): Computer Aided Drug Design - I

Chairpersons: Prof. K. Sekar / Dr. Takashi Ishida

13:00 - 13:30 ***Compound screening contest method for identifying target protein inhibitors using the tyrosine-protein kinase Yes***
Dr. Masakazu Sekijima, Tokyo Institute of Technology, Tokyo

13:30 - 14:00 ***Computational studies on Hexokinase II: Targeting the old foeas a potential candidate for cancer***
Dr. M. Elizabeth Sobhia, NIPER, Chandigarh

14:00 - 14:30 ***In silico, in vitro, X-ray crystallography, and integrated strategies for discovering spermidine synthase inhibitors for Chagas disease***
Dr. Ryunosuke Yoshino, Tokyo Institute of Technology, Tokyo

14:30 - 15:00 **Oral presentations**

15:00 - 15:30 ***Tea break***

SESSION 3 (15:30 - 16:30): Bioinformatics databases/algorithms
Chairpersons: Dr. Athi Narayanan / Dr.Kazuki Izawa

15:30 - 16:00 ***Prediction of Protein-Protein Interactions with MEGADOCK: Parallelization, Application, and Open Database***
Dr. Masahito Ohue, Tokyo Institute of Technology, Tokyo

16:00 - 16:30 **Oral presentations**

SESSION 4 (16:30 - 18:30) Poster presentations I

Evaluators: Prof. D. Velmurugan, Dr. Takashi Ishida, Dr. Masakazu Sekijima and Prof. K. Sekar

16:30-17:30 ***Odd numbered posters***

17:30-18:30 ***Even numbered posters***

November11, 2017, Saturday

SESSION 5 (09:00 - 11:00) Computer Aided Drug Design - II

Chairpersons: Dr. Karthik Raman / Dr. Nobuyuki Uchikoga

09:00 -09:30 ***Isolation, structural characterisation and molecular modelling studies of four anticancer compounds from medicinally important herbs***
Professor D. Velmurugan, University of Madras

09:30 - 10:00 ***Ensembling multiple molecular finger print based predictions for improvement of ligand base drug discovery***
Dr. Takashi Ishida, Tokyo Institute of Technology, Tokyo

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

10:30 - 11:00 **Oral presentations**

SESSION 6 (11:00 - 12:00) Poster presentations II/Coffee break

SESSION 7 (12:00 - 13:00) Bigdata/ NGS analysis/ Networks - I

Chairpersons: Prof. K. Veluraja / Dr. Ryunosuke Yoshino

12:00 - 12:30 ***Analysis for protein-protein interaction surfaces: exploring docking space and biological protein networks***
Dr. Nobuyuki Uchikoga, Tokyo Institute of Technology

12:30 - 12:50 ***Large scale data analysis and discrimination of driver and passenger mutations in cancer***
Dr. M. Michael Gromiha, IIT Madras

12.50 - 13.00 **Oral Presentation**

13:00 - 14:00 ***Lunch and Discussions***

SESSION 8(14:00 - 15:20) Bigdata/ NGS analysis/ Networks - II

Chairpersons: Prof. Mukesh Doble / Dr. Masahito Ohue

14:00 - 14:30 ***Learning and Predicting Novel Metabolic Pathways through Subgraph Mining***
Dr. Karthik Raman, IIT Madras

14.30 - 14.50 ***Computationally Driven Drug Discovery In Structure-Enabled Programs: Free Energy Calculations***
Mr. R Raghu, Schrodinger, Bangalore

14:50 - 15:20 **Oral presentations**

15:30 - 16:30 ***Valedictory and Presentation of poster awards***

16:30 - 17:30 ***High Tea and Discussions***