NATIONAL UNIVERSITY OF SINGAPORE

School of Computing

C S S E M I N A R

Title: **Protein interactions-integrating computational methods and experimental data for understanding the binding specificity**

Speaker: Professor M. Michael Gromiha
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Date/Time: 19 June 2017, Monday, 11:00 AM to 12:30 PM

Venue: SR7, COM1-02-07

Chaired by: Dr Wong Lim Soon, KITHCT Chair Professor, School of Computing
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Abstract:

Protein-protein interactions play crucial roles in many biological processes and responsible for smooth functioning of the machinery in living organisms. Predicting the binding affinity of protein-protein complexes and understanding the recognition mechanism are challenging problems in computational and molecular biology. We have developed a generalized energy-based approach for identifying the binding site residues and interacting pairs in all types of protein complexes. We observed that the residues with charged and aromatic side chains are important for binding in protein-protein complexes. These residues influence to form cation-p, electrostatic and aromatic interactions. Our observations have been verified with the experimental binding specificity of protein-protein complexes and found good agreement with experiments. Further, we have developed algorithms for discriminating protein-protein complexes based on their binding affinities and predicting the binding affinity. These methods have been used for analyzing protein-protein interaction networks in different organisms. Recently, we developed a database for the binding affinity of protein-protein complexes and their mutants and utilizing the data for understanding the factors influencing the specificity of mutants. The salient features of the results will be discussed.

Biodata:

M. Michael Gromiha received the PhD degree in physics from Bharathidasan University, India, and served as a STA fellow, RIKEN researcher, research scientist, and senior scientist at Computational Biology Research Center, AIST, Japan, till 2010. He is currently an associate professor at the Indian Institute of Technology (IIT) Madras, India. His main research interests are structural analysis, prediction, folding and stability of globular and

membrane proteins, protein interactions and development of bioinformatics databases and tools. He has published over 180 research articles, 40 reviews, five editorials, and a book entitled Protein Bioinformatics: From Sequence to Function by Elsevier/Academic Press. His papers received more than 8,000 citations and h-index is 50. He is an associate editor of BMC Bioinformatics as well as editorial board member of Scientific Reports, Biology Direct, the Journal of Bioinformatics and Computational Biology, and Current Computer Aided Drug design. He has received several awards including the Oxford University Press Bioinformatics prize, Okawa Science Foundation Research Grant, Young Scientist Travel awards from ISMB, JSPS, AMBO, ICTP, etc., Best Paper Award at ICIC2011, ICTP Associateship award, ICMR International fellowship for Senior Biomedical Scientists, INSA Senior Scientist Award, Best Paper Award in Bioinformatics by Department of Biotechnology, India, Outstanding Performance award from Initiative for Parallel Bioinformatics (IPAB), Tokyo Institute of Technology, Japan and Institute Research and Development Award, IIT Madras. He is a member of the National Academy of Sciences, India.