# 理工学研究所
# 国際交流・公開研究セミナー

Prof. M. Michael Gromiha（インド, インド工科大学マドラス校）が来日される機会に, 最近その応用が注目されているタンパク質相互作用の機械学習を用いた予測について, 基礎となるタンパク質相互作用の性質と機械学習手法に関してご講演をお願いしました. 是非ご参集ください.

題　目：　Integrating computational methods and experimental data for understanding the binding affinity of protein-protein complexes
講演者：　Prof. M. Michael Gromiha
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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 (1,2). 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–□, electrostatic and aromatic interactions. Our observations have been verified with the experimental binding specificity of protein-protein complexes and found good agreement with experiments (3). Further, we have developed algorithms for discriminating protein-protein complexes based on their binding affinities, (4) predicting the binding affinity (5) and constructing protein-protein interaction networks (6). We have also analyzed the integrative role of amino acid residues involved in both stability and binding (7). Recently, we developed a database for binding affinity of protein-protein complexes and their mutants (8). Utilizing the database, we analyzed the factors influencing the affinity of single mutants and the additivity effects of double mutants (9). The salient features of the results will be discussed
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