

7th International Conference on

Proteomics & Bioinformatics

October 24-26, 2016 Rome, Italy

GNM 2.0 - A database housing protein dynamics data of >11,000 PDB structures revealing dynamics prerequisites for protein functions and interactions

Lee Wei Yang

National Tsing Hua University, Taiwan

Proteins function through advantageously utilizing a repertoire of possible modes of intrinsic motions. Understanding such motions, of which the importance has been acknowledged in year 2013's Nobel Prize in Chemistry, is essential to accurately predict two body interactions, channel gating mechanisms and enzyme catalysis. Here, we present the only dynamics database that houses dynamics data (vibrational normal modes) of protein structures in a size commensurate with Protein Data Bank (PDB). The interface that presents such data is state of the art of its kind. Given the wealth of the data, we are able to find dynamics traits for enzyme active sites. Such traits are later used to predict the locations of enzyme active sites for protein structures of a resolution as low as 20Å. We further data-mined the database and develop the concept of intrinsic dynamics domains (IDDs), including a domain plane (D-plane) and a domain axis (D-axis). It is found that a protein interacts with another at the interface where D-plane cuts through and forming a near-vertical angle between two intersecting D-axes from the two proteins over a set of 68 protein-protein complexes. The findings are then used to define quantitative criteria to filter out docking decoys unlikely to be native whereby the chance to find near-native hits is doubled. Our results also show that in 95% of the DNA-protein complexes, the DNA is cut through by protein's D-plane. The dynamics database, GNM 2.0, is made available at <http://dyn.life.nthu.edu.tw/gnmdb> and IDD website is provided at <http://dyn.life.nthu.edu.tw/IDD/IDD.php>.

Biography

Lee Wei Yang is currently an Associate Professor at Institute of Bioinformatics and Structural Biology, National Tsing Hua University, received his PhD degree in Molecular Genetics and Biochemistry from School of Medicine, University of Pittsburgh (2005) and his Post-doctoral training in University of Tokyo (2006-2009), La Jolla Bioengineering Institute and Department of Chemistry, Harvard University (2010-2011) before joining NTHU in 2011. He has published more than 30 papers in reputed journals and has an H-index of 16.

lwyang@life.nthu.edu.tw

Notes: