Fumio Hirata, J Proteomics Bioinform 2016, 9:10(Suppl)
http://dx.doi.org/10.4172/0974-276X.C1.088

Structure, fluctuation and function of biomolecules in solution explored by the 3D-RISM/RISM theory

Fumio Hirata
Toyota Physical & Chemical Research Institute, Japan

There are two physicochemical processes which are essential for living bodies to maintain their life: "self-organization" and "molecular recognition." Protein folding and formation of cell-membrane are typical examples of the former process, in which biomolecules have to overcome the entropy barrier to organize them into some characteristic structure. On the other hand, a molecular recognition process concerns whenever a biomolecule performs its function as a "molecular-machine." For examples, in order for the enzymatic reaction to occur, substrate molecules should be accommodated first by the protein in its reaction pockets to form so-called an enzyme-substrate (ES) complex. The two processes may not proceed spontaneously if biomolecules and ligand molecules existing by themselves in "vacuum," because those are not in favor with respect to entropy. For instance, the protein folding is a process in which a protein folds into a native conformation, the state of least entropy, from the random coil, the state of largest entropy. Then, why do those processes occur spontaneously in our body? It is because there is always "aqueous solution" in the real environment of a living body. We have been developing a statistical mechanics theory called "3D-RISM/RISM" for past few decades, which has proven it to be capable of handling such processes stated above in biosystems. The latest development of the theory has brought the structural fluctuation of biomolecules within scope of the science, which plays a crucial role in any biological activities. The talk includes the following two topics; both are related to protein functions and drug discovery. (i) A 3D-RISM/RISM study of the oseltamivir binding efficiency with the wild-type and resistance-associated mutant forms of the viral influenza-B neraminidase. (ii) Theoretical and biochemical determination of ammonia pathway in the purine biosynthetic enzyme: formylglycinamide ribonucleotide amidotransferase.

Biography

Fumio Hirata has completed his PhD from Hokkaido University and Post-doctoral studies from State University of New York, University of Texas and Rutgers University. He was an Associate Professor in Kyoto University and a Professor in Institute for Molecular Science. Later he became a Professor Emeritus of the institute. Currently he is working at Toyota Physical & Chemical Research Institute. He has published more than 200 papers in reputed journals and has served as an Editorial Board Member of repute.

fumiothinksnowhirata@gmail.com

Notes: