13:15-, 26-OCT-2018
G201, KPSI, Kyoto, JAPAN
The 43rd KPSI Seminar, KPSI-QST

フラグメント分子軌道法に基づく計算生命科学

福澤薫(星薬科大学 薬学部)

In Silico Life Science Based on the Fragment Molecular Orbital method

Dr. Kaori Fukuzawa
School of Pharmacy and Pharmaceutical Sciences, Hoshi University

The Fragment molecular orbital (FMO) method is one of the high-potential approach to analyze molecular interaction in atomic level. It is suitable for analysis of intermolecular interactions of combinations of bio-macromolecules such as protein-ligand, protein-protein, and nucleic acids containing systems. As a methodology for drug discovery, detailed information on the interaction between the ligand and the target protein can be obtained based on a quantum mechanical calculation. Interaction between a ligand and each amino acid residue can also be quantitatively evaluated using the inter fragment interaction energies (IFIEs) and their energy components. The FMO method has been applied to many protein-ligand systems, and recent activities that have evolved these researches have been rapidly progressing. Here we will introduce the recent research on the development mainly in ″FMO Drug Design Consortium (FMODD)″ through industry-academia-government collaboration.

Through the use of K-supercomputer, FMO calculation of more than 2,000 protein-ligand complex structures have been done over the past three years, using X-ray crystal structures. The results have been used to understand protein-ligand interactions, predict their binding affinities, and compare the calculated binding energies to experimental activity values. We are constructing the “FMO database” to store these calculation results and plan to release it widely as a basic data of FMO based drug design. In the future, we are aiming for rational drug design with high reliability in cases where electronic effects are important, which cannot be solved by conventional classical approaches.