Division of Life Science: Biological Function and Information Group

Chief: SHIGETA Yasuteru, Professor, Ph.D.

Biological phenomena are governed by a series of chemical reactions driven by biological molecules such as proteins, nucleic acids, lipids, and sugars. As such, the fundamental molecular mechanisms of biological phenomena can be understood by examining the changes in electronic states and the spatial arrangement of atoms during chemical reactions. In the Biological Function and Information Group, we use computational methods such as first-principles calculations based on quantum theory and molecular dynamics (MD) calculations based on classical (statistical) mechanics to understand the inherent dynamic structure–function relationships in biological molecules and to understand the essence of biological phenomena.

Check it now!
Our Research Movie

"Comprehensive in silicon drug repositioning for COVID-19 related proteins"

Development of an efficient structure sampling method using MD and machine learning

Protein conformational change is a phenomenon that operates over extremely long timescales, making it difficult to track using conventional MD simulations. We have developed Parallel Cascade Selection MD (PaCS-MD) to efficiently explore protein folding pathways (Fig. 1). Furthermore, we have found that the sampling efficiency can be significantly increased by using machine learning—a method rooted in information science. This method has proven to be suitable for massively parallel environments. We are using the supercomputer at the Research Center for Computational Science to perform such calculations.

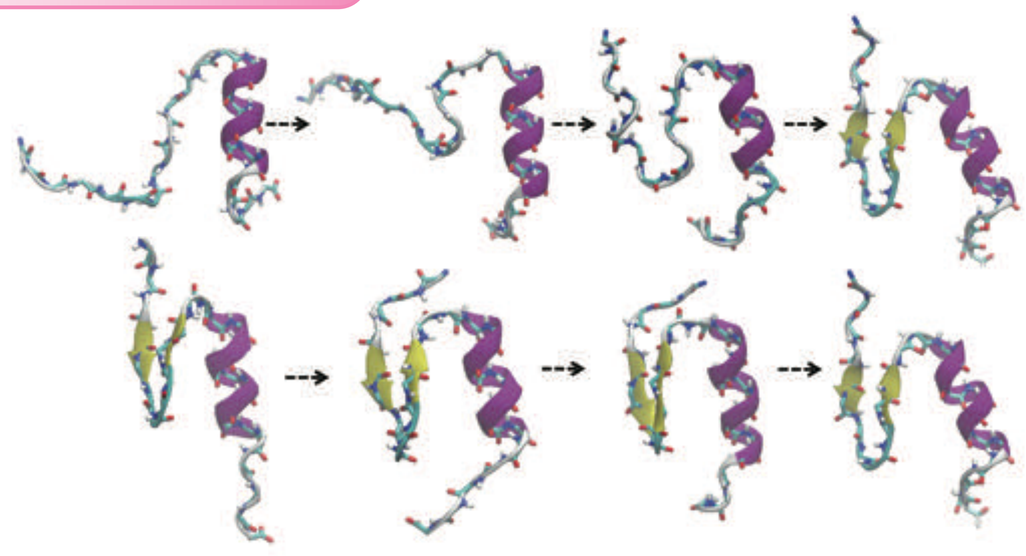
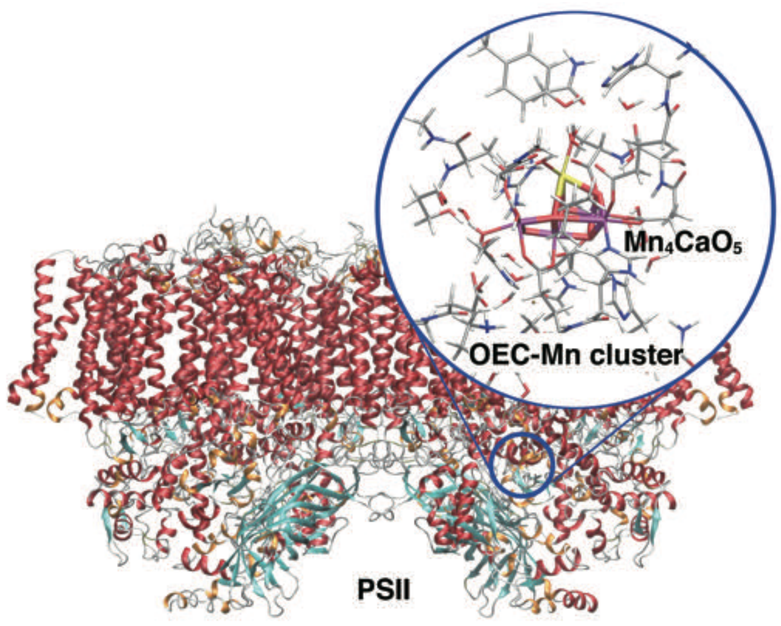


Fig.1 Tryptophan cage folding simulation

Reaction analysis of proteins using hybrid QM/MM methods



Photosystem II has a highly characteristic reaction active center composed of manganese, calcium, and oxygen atoms (Fig. 2) and produces oxygen molecules from water molecules in a multi-step chemical reaction using light energy. We identified the structure–electron–proton transfer changes in this reaction (water-splitting reaction) using a hybrid QM/MM method.

Fig.2 Overall structure and active center structure of photosystem II

Clarifying the mechanism of amino-acid formation in interstellar space and the origin of L-body excess formation

Because some of the biomolecules that constitute life have been found in meteorites, there is a possibility that life originated in interstellar space. We are using high-precision ab initio methods to comprehensively analyze various reaction pathways for prebiotic amino-acid synthesis and degradation. In collaboration with the Division of Astrophysics, we are studying the molecular evolutionary processes related to the origins of life.

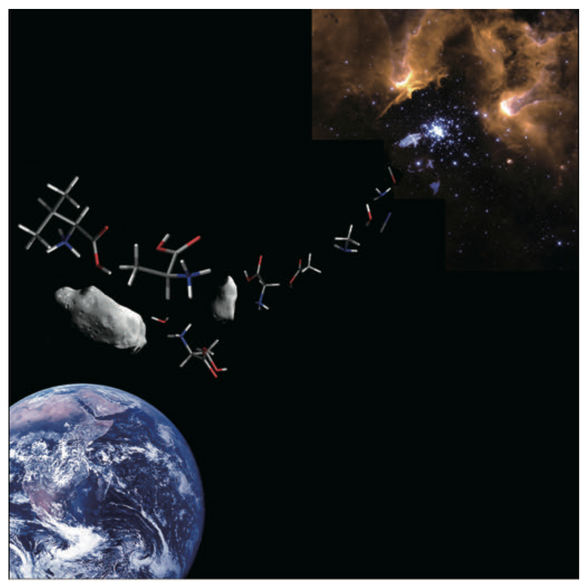


Fig.3 Image of molecular evolution and amino-acid synthesis in interstellar space