# Theoretical studies on the structures and functions of metalloproteins

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Proteins themselves are polymers of amino acids, which are purely organic molecules. However, they are not always functionally adequate on their own, and it is essential to enhance their functions by cofactors, especially metal ions and complexes. This is the reason why proteins have acquired more diverse functions and regulation mechanisms. Metalloenzymes catalyze various chemical reactions such as synthesis, degradation, and redox reactions under mild conditions, and the elaborate combinations of these reactions maintain the activities of life. In other words, the essence of life phenomena is a series of chemical reactions driven by them. To elucidate their reaction mechanisms at the atomic level, it is necessary to theoretically clarify the three-dimensional structure of proteins, especially the roles of amino acid residues, water molecules, and cofactors that constitute the active center. Then, the unique functions of proteins can be elucidated by comparing them with the findings by conventional biochemical and molecular biological methods. Our research group has been analyzing the functions of various metalloproteins with mutual collaborations with experimental groups. In this presentation, I will focus on the following three themes:

**(1) Structural Diversity Analysis of Metallothionein by Molecular Dynamics Simulations**
**(2) Mutational effects on the stability of Mb 3D domain swapping dimers**
**(3) Theoretical Elucidation of the Mechanism of Semiquinone Radical Formation in CAO**

**References**

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