Protein Dynamics and Structure Studied by Neutron Scattering

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Protein is a functional biological macromolecule and plays an essential role in almost all vital phenomena. Protonation/deprotonation is one of the most essential chemical processes in biological reactions. Proteins work in an aqueous milieu at room temperature, indicating that proteins cannot escape from thermal fluctuation. Therefore, the understanding of the position and the dynamics of hydrogen atom is the most essential and significant subject in molecular biophysics. Neutron is one of the most effective probes for the purpose.

We have been studying protein dynamics using Staphylococcal nuclease as a sample with neutron scattering [1-5]. Our study covers wide range of protein dynamics from protein dynamical transition to dynamical heterogeneity and the effect of hydration water to protein dynamics.

We also carried out neutron crystallography on photoactive yellow protein which contains two abnormal short hydrogen bonds. We identified ~87% (819/942) of the hydrogen positions in PYP, and revealed the existence of a low barrier hydrogen bond [6].

Based on these results, the expectation for J-PARC from the view point of biophysics will be discussed.

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