Molecular simulation study on the photochemical response and dynamics of photoactive yellow protein

Photoactive yellow protein (PYP) is thought to be a receptor responsible for negative phototaxis of *E. halophila*. The three-dimensional structure of PYP is recognized as the prototype for a large and diverse family of sensory and signaling proteins that generally contain the PAS domain. Upon absorption of a photon (446 nm), the chromophore (*trans*-*p*-coumaric acid) of PYP is isomerized to the cis form. This initial molecular event triggers the photocycle that contains several intermediates. In particular, a blue-shifted intermediate formed on submillisecond, called M intermediate, is physiologically important because it is a putative signaling state. In general, to understand the signal transduction mechanism of receptor proteins, it is necessary to know how external perturbations such as ligand binding, photon absorption induce the structural and dynamical changes of the whole proteins. In this study, molecular dynamics simulation is applied to investigate how the chromophore isomerization influences the dynamics of PYP. We revealed that the M intermediate has a characteristic hinge-bending motion, probably responsible for the interaction with an unknown transducer protein.