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Energy Flow Analysis of Photoactive Yellow Protein TAKAKAZU ISHIKURA, KAZUTOMO KAWAGUCHI, HIROSHI WATANABE, Nagoya Univ, TAKAHISA YAMATO, Nagoya Univ / CREST, JST — The signal transduction of photosensory receptors is intimately related to the energy relaxation associated with the relevant functional motion. To understand this energy conversion process, it is useful to analyse the energy flux vector field in a polypeptide chain matrix. Recently, we developed a new formalism for energy flux, J_{AB} , between two different sites A and B in a protein. Flexibility is one of the attractive points of this method, namely, sites A/B can be consisted of an atom or any groups of atoms. In addition, huge computation resource is not required for this method. Since this method is based on the linear response theory, the energy flux, J_{AB} , can be obtained from a classical molecular dynamics simulation trajectory. We can define energy conductivity between the sites A and B in terms of the time-correlation function of J_{AB} . This quantity corresponds to the transport coefficient of heat and potential energy, representing the strength of the direct energetic coupling between the two sites. We applied this method to a photosensory receptor, photoactive yellow protein (PYP). We calculated the energy conductivity between the chromophore and the surrounding amino acid residues, Tyr42, Glu46, Thr50, Arg52, and Tyr98. As a result, we observed the values of energy conductivity decreased in this order. We will discuss the possibility of finding energy transfer pathway in PYP with this method.

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