significantly slow. There is also a critical hydration level below which proteins do not function. Those facts indicate that the dynamics of water play an important role for proteins to function. However, its underlying molecular mechanism has not been clarified yet. To understand it, it is vital to understand the role of water molecule for proteins to change their conformations, since the function of the proteins can be understood as the consecutive conformation changes of the proteins triggered by the external stimuli.

In order to understand the mechanism, we do molecular dynamics simulation of a peptide, Met-Enkephalin, which consists of 5 amino acids, in explicit water solvent. The conformational changes of the peptide can be classified into the following two cases. One is water assisting, that is, the surrounding water performs major mechanical work for the peptide to change its conformation. The other is water hindering, that is, the water prevents peptide from changing its conformation. The difference between the two can be understood in terms of the cooperative behavior of the water. We extract the cooperative behavior from density, momentum and energy density of the water by using our coarse-grained method, GAIO extended to non-stationary dynamical system due to Froiland.

14:00-17:00 C 会場 / Room C

蛋白質:機能 1

2C1412

Photo-induced structural change of the blue-light sensor phototropin “LOV1-LOV2 Domain”

Kengo Nishiumi, Tilo Mathes, Masahide Terazima (Grad. Sch. Sci., Kyoto Univ., Fac. Sci., FU)

Phototropin is a blue-light sensor protein which exists in plants and regulates phototropism or stomal opening and so on. The N-terminal photosensory domain of the phototropins contains two very similar domains of 110 amino acids designated LOV1 and LOV2. These domains bind the cofactor flavin mononucleotide (FMN) and act as blue-light sensors. For understanding the functional mechanism of the full-length phototropin, the photochemistry of the LOV2 domain has been extensively studied, because this LOV2 domain is thought to play an important role in regulating phototropin activity. A next logical step could be revealing the photochemistry of the extended domain “LOV1-LOV2 tandem”. In this study, we used the LOV1-LOV2 tandem from Chlamydomonas reinhardtii, ~34kDa and the transient grating (TG) method for this purpose. The LOV1 domain of the tandem was inactivated by mutation of the reactive cysteine 57 to serine to prevent overcrowding of the spectra. The TG signal after the photoexcitation showed a typical “LOV2 signal”; the formation of cysteine adduct (~2 μs) and the thermal grating signal. However, after the thermal grating, the behavior was different from that of the LOV2 domain reaction. The signal consists of several phases of protein diffusion. One of significant differences is the diffusion rate of this protein. The rate is much slower than that of LOV2. This is thought to be caused by the formation of higher aggregates (larger than decamer). Details will be presented in the conference.

2C1424

光化学反応の観察からみたYIVな光流動体の系内反応

Seokwoo Cho1, Yusuke Nakasone1, Helfenberg Klaas J2, Masahide Terazima1 (Department of Chemistry, Graduate school of Science Kyoto University, Univ Amsterdam, Swammerdam Inst Life Sci, Mol Microbial Physiol Grp, Amsterdam, Netherlands)

YIVa is a blue light sensor protein composed of the N-terminal LOV (Light-Oxygen-Voltage) domain, linker domain, and the C-terminal STAS (Sulphate Transporter and Anti Sigma factor antagonists) domain. By physiological experiments, YIVa is believed to act as a positive regulator for stress response regulated by the sigma-B factor. However, the signal transduction process is not yet revealed. For understanding the signal transduction mechanism, the photochemical reaction dynamics has to be elucidated. In this report, we study the photochemistry of the LOV domain of YIVa by the time-resolved transient grating (TG) method. The TG signal after the photoexcitation of the LOV domain showed a typical phototropin-LOV domain signal; an adduct formation, volume change, and diffusion change. However, the analysis is very complicated, because the signal was dependent on the observation time range, concentration, excitation light intensity, and temperature in a complex manner. Preliminary, we found that the ground state of the LOV domain is in equilibrium between the dimer and the tetramer. When the LOV domain absorbs blue light, the tetramer dissociates into the dimer. However, when the dimer absorbs the light, it associates into the tetramer. This dissociation/association processes are dependent on the temperature and laser power. We will discuss the reaction in more detail in the conference.

2C1436

Photo-reaction of the LOV domain of phototropin under high pressure

Kunisato Kuro1, Francielle Sato2, Yusuke Nakasone1, Kazunori Zikihara2, Satoru Tokunom2, Masahide Terazima1 (Grad. Sch. Sci., Univ. Kyoto, 2UEM (Universidade Estadual de Maringa), 3Otsuka. Pref. Univ)

For biological function of proteins, their structural fluctuations could play an important role. However, the importance has not been well recognized, because it is difficult to detect such fluctuations during reactions. In particular, there has been no useful technique to measure the fluctuation of transient intermediates. On this point, our group has been showing that the transient grating (TG) technique is a powerful time-resolved method to determine the various thermodynamical parameters, including the volume change of intermediates. If the TG signal can be measured under high-pressures, it will provide the isothermal compressibility of intermediates, which is directly related to the volume fluctuation. Recently we succeeded in detecting such transient volume fluctuations by constructing a high-pressure optical cell. In this study, we applied this TG technique to blue light sensor, phototropin LOV2-linker protein reaction under various pressures from 0.1 MPa to 400 MPa. This reaction has been studied extensively so far at the ambient pressure, and we extended this approach to high pressures. We found that the molecular diffusion signal of LOV2-linker showed very interesting pressure dependence; its intensity increased up to 100 MPa and considerably decreased in the range from 100 MPa to 400 MPa. This pressure dependence may be related to the pressure dependent reaction mechanism and intermediate fluctuations. Details will be presented at the conference.

2C1448

Statistical Mechanical Model of Signaling Pathways in Phototactic Yellow Protein

Taishi Suhata, Kazunito Ishii, Masaki Sasa1 (Department of Applied Physics, Nagoya University, 2Department of Computational Science and Engineering, Nagoya University)

Phototactic yellow protein (PYP) is a water-soluble photo-sensor protein found in purple photosynthetic bacteria. When a p-coumaric acid (pCA) bound to Cys69 absorbs a photon, the subsequent isomerization of pCA results in the partial unfolding of the N-terminal domain, which should be recognized by the partner protein to transmit the photo-signal. Since there is no direct interaction between pCA and the N-terminal domain, it is important to resolve the pathway within PYP to convey the signal between them. We examine this problem by using a statistical mechanical model of PYP and comparing the results with the experiments and simulations. The model shows that the structural loosening around pCA, which is induced by the isomerization, changes the vibration modes of PYP, so that the coupled process of change in the vibration modes and perturbation of the structural stability determines the main features of the pathway.

2C1512

NIRS in 1D size scale: the application to Group II Chaperonin using Diffraction X-ray Tracking


Group II chaperonin, found in archaea and in the eukaryotic cytosol, is an indispensable protein that captures an unfolded protein and refolds it to the correct conformation in an ATP dependent manner. Chaperonin-mediated protein folding is critically dependent on the closure and opening of a built-in lid, which is triggered by ATP. Recent study with cryo-EM study and computer modeling suggest that the ring structure of chaperonin twist to seal off the central cavity under ATP cycle. However such dynamic could not be traced