Structural change of ß core domain at the M intermediate of photoactive yellow protein.

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Photoactive yellow protein (PYP) is a putative water-soluble photoreceptor protein for negative phototaxis of *Ectothiorhodospira halophila*. PYP undergoes a cyclic photoreaction including several intermediates. Among the intermediates, PYP_M with blue-shifted spectrum is considered to be a physiological active state. A structural model of PYP_M had been proposed by x-ray crystallographic study. However, the discrepancies between the crystal structure and the solution structure have been pointed out by many spectroscopic studies performed under physiological solution conditions. In order to elucidate the structural properties of the active state in solution, we are trying to clarify the solution structure of PYP_M using solution x-ray scattering method.

In the previous experiments at BL40B2, we found the characteristic x-ray scattering profile with bimodal shape in higher angle region ($0.25<Q<1$ A^{-1}) in the dark state (b) and the change of the profile during PYP_M formation. To clarify the origin of the bimodal shape, the scattering profiles were calculated based on the crystal structure of the dark state PYP, suggesting that the bimodal shape is due to the correlation between the N-terminal domain and the ß core domain (a). In the present experiments, in order to confirm the origin of bimodal shape and to elucidate the structural changes at PYP_M, we carried out the solution x-ray scattering experiments on the truncated PYP (T23) which is digested the N-terminal 23 amino acid residues by trypsin. The obtained profile with a single peak (b) is quite similar to the calculated profile (a), indicating that the bimodal shape of dark state comes from the N-terminal domain. The profile of PYP_M of T23 is shown in (c). T23 loses the entire N-terminal domain. Therefore, the profile change observed here corresponds to the structural change in the rest domain (ß core domain). The profile with a single peak in the dark state split into the bimodal shape during PYP_M formation, suggesting that the ß core domain undergoes characteristic structural change (e.g. being two domains spatially separated). This observation is the first precise description about the structural change in the ß core domain.

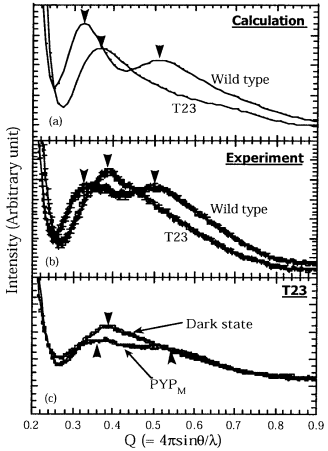

Fig. X-ray scattering profiles in higher angle region.

X-ray crystallography of peptide deformylase from *Thermus thermophilus* HB8

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Peptide deformylase is an essential metalloenzyme required for the removal of formyl group at the N terminus of nascent polypeptide chains in eubacteria as well as in mitochondoria and chloroplasts. For *Escherichia coli*, deletion of peptide deformylase gene proves to lethal. This formylation and deformylation cycle, which appears to be characteristic feature of eubacteria, does not occur in the cytoplasm of eukaryotic cells. Therfore, peptide deformylase is an attractive target for the design of new antibiotics.

The primary structure, tertiary structure and the coordination of a cystein suggest that *E. coli* peptide deformylase belongs to a new subfamily of metalloproteases..

T. thermophilus peptide deformylase has 36 % sequence homology to *E. coli* deformylase. Proteins from *T. thermophilus* have highly thermostable structures.

To elucidate structural features of thermostable proteins and the reaction mechanism, we have crystallized *T. thermophilus* deformylase. The crystal belongs to a hexagonal space group $P3_12_1$ with unit cell parameters a=b=103.0 Å and c=70.0 Å . However, the reproduction of high-resolution diffractions are quite difficult. During this beamtime, we collected 3.0 Å resolution native data