【Grant-in-Aid for Specially Promoted Research】

Biological Sciences

Title of Project： Elucidation of the mechanisms of water-splitting in photosystem II

Jian-Ren Shen
(Okayama University, Graduate School of Natural Science and Technology, Professor)

Research Area：Biology, Biophysics
Keyword：Photosynthesis, Membrane proteins, Light-energy conversion, Water-splitting

【Purpose and Background of the Research】

The purpose of the present study is to elucidate the mechanism of light-induced water-splitting reaction catalyzed by photosystem II (PSII), the largest mystery remained unsolved in oxygenic photosynthesis, by means of a combination of structural biology, structural and functional characterization of various mutants, infra-red spectroscopy, electron spin resonance (EPR) measurement, and quantum mechanical (QM) and molecular mechanical (MM) calculations.

In oxygenic photosynthesis, PSII catalyzes light-induced water-splitting, leading to the evolution of dioxygen, protons and electrons. PSII is a multi-subunit membrane protein complex consisting of 20 subunits and a number of cofactors, with a total molecular mass of 350 kDa. We have succeeded in obtaining high quality crystals of PSII from a thermophilic cyanobacterium, and analyzed its structure at a 1.9 Å resolution. The structure we obtained, however, corresponds to the S_1-state in the S-state cycle (Fig. 1) of the water-splitting reaction. In order to fully unravel the mechanism of the water-splitting reaction, it is essential to solve the structures of the reaction intermediates, and to elucidate the structural and energetic changes accompanying each step of the reaction, along with the roles of individual subunits. We will accomplish these goals by using a combination of advanced technologies described above.

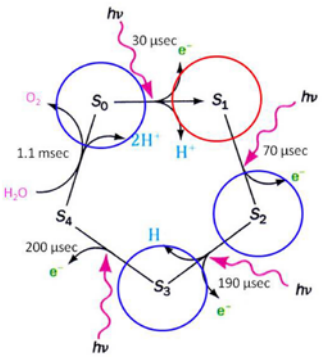

Fig. 1. S-state model of the water-splitting reaction taking place in PSII.

【Research Methods】

The research methods will be based mainly on crystal structural analysis of various reaction intermediates and mutants of PSII at atomic resolutions, but will also include visible, infra-red spectroscopy, EPR, QM/MM calculations, and various functional analysis of the mutants.

【Expected Research Achievements and Scientific Significance】

Water-splitting and oxygen evolution have been cited as the last and most important mystery in photosynthesis; the elucidation of this natural system will yield valuable information for not only natural but also artificial photosynthesis, since the natural system is highly efficient in utilizing visible light and uses only abundant, non-toxic metals for the catalytic reactions. PSII is the largest membrane protein complex whose structure has been solved beyond 2.0 Å resolution so far. Its refined structural and functional studies will inspire higher resolution structural studies of a vast number of other membrane proteins and their complexes, the structure of most of them, even if solved, have remained at a "medium" resolution.

【Publications Relevant to the Project】

Umena Y., Kawakami K., *Shen J.-R., *Kamiya N. Crystal structure of oxygen-evolving photosystem II at 1.9 Å resolution. *Nature* **473**, 55-60, 2011.

Kawakami K., Umena Y., Kamiya N., Shen J.-R. Location of chloride and its possible functions in oxygen-evolving photosystem II revealed by X-ray crystallography. *Proc. Natl. Acad. Sci. USA* **106**, 8567-8572, 2009.

【Term of Project】

FY2012-2016

【Budget Allocation】

399, 500 Thousand Yen

【Homepage Address and Other Contact Information】

http:// http://www.biol.okayama-u.ac.jp/shen2/ﾄｯﾌﾟ.htm
shen@cc.okayama-u.ac. jp