Poster Presentation

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High-resolution and low-dose X-ray crystal structure of Photosytem II

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Photosystem II (PSII) is a large multi-subunit membrane protein embedded in thylakoid membranes as a dimeric form with molecular weight of 700 kDa. The oxygen-evolving complex (OEC) of PSII is the heart of photosynthesis to split water molecules and to produce electrons and protons. The X-ray crystal structure of PSII was reported recently at a resolution of 1.9 Å with an averaged coordinate error (DPI) of 0.11 Å [1]. The chemical composition of OEC was fixed to as Mn4CaO5(H2O)4, and the structure was unambiguously determined for the first time including all amino-acid residues and oxo-bridging oxygen atoms ligated to the metal atoms.After the structure determination, two problems are newly showed up. One is the resolution problem. The resolution of 1.9 Å is extremely high in comparison with that of crystal structure previously reported [2], however, it is not enough to obtain precise information for bond lengths between metals and oxo-bridging oxygen atoms in OEC. The other is the X-ray reduction problem on Mn atoms. The reflection intensities were measured by a slide-oscillation method at a low X-ray dose of 0.85 MGy. According to the EXAFS studies reported by Glöckner et al. [3], the dose value corresponded to that 25% of OEC in crystal was damaged into Mn(II) aqua complexes. In order to overcome these problems, we have succeeded to get high quality crystals of PSII, which show much higher resolution and isomorphism. The high isomorphism is very important to obtain low-dose data using multiple crystals. Sixteen partial datasets were reduced using XDS and merged to a resolution of 1.77 Å. The calculated X-ray dose was 0.11 MGy, only 13 % of that for the 1.9 Å resolution data. Based on the merged data, structure determination is underway.

[1] *Y. Umena, K. Kawakami, Shen J.-R, et al, Nature, 2011, 473, 55-60,* ***[2]*** *A. Guskov, et al. Nat. Struct. Mol. Biol., 2009, 16(3), 334-42,* ***[3]*** *C. Glöckner, et al. J. Biol. Chem., 2013, 288, 22607-22620*

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