CorA families [2], which show functional [3] and apparently structural differences.

Both full-length protein and its truncated version, comprising the soluble domain, were successfully overexpressed in *E.coli* and purified using Immobilized Metal Ion Affinity (IMAC) chromatography. Crystallization trials with several commercially available screens (JSCG+, Morpheus, PGA) gave a number of hits, optimization of which, yielded crystals suitable for data collection at synchrotron.

Several datasets with varying resolution from 3.5Å to 5 Å were collected at National Synchrotron Radiation Research Center (Taiwan), Diamond Synchrotron (UK) and Australian Synchrotron (Australia).

Initial analysis of collected data as well as future steps of structure determination will be presented.

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The catalytic architecture of leukotriene C_4 synthase with two arginine residues

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Leukotriene (LT) C_4 and its metabolites, LTD_4 and LTE_4, are the lipid mediators involving in inflammatory and immunoresponses. These lipid mediators are collectively called cysteinyl leukotrienes (Cys-LTs). The therapeutic effects of the intervention with the Cys-LT biosynthesis or the antagonist of the specific receptor of Cys-LT suggests that Cys-LT plays an important role as a pathogenic factor of bronchial asthma.

LTC_4 synthase (LTC_4S) is the nuclear membrane-embedded enzyme responsible for LTC_4 biosynthesis, catalyzing the key reaction to conjugate glutathione (GSH) and LTA_4 at the first step of Cys-LTs metabolism as a branch in the arachidonic acid cascade. A previous crystal structure revealed important details of GSH binding, and implied a GSH activating function for Arg104. In addition, Arg31 was also proposed to participate in the catalysis based on the putative LTA_4 binding model [1].

To elucidate structural and functional relationship of LTC4S, we constructed mutants at several arginine residues including Arg104 and Arg31, and the catalytic architecture of LTC4S was thoroughly analyzed by enzyme kinetics and X-ray crystallography of these mutants [2]. Both the arginine mutants showed decreased catalytic activities, indicating concerted catalysis with Arg104 and Arg31 described as follows. Arg104 as the base catalyst binds to thiol group of GSH, and generates thiolate anion. The activated thiolate attacks the carbon atom of the epoxide group of LTA4 to form the covalent bond between GSH and LTA4. Synchronously, guanidino group of Arg31 as the acid catalyst donates a proton to the oxygen of the epoxide group, and its positive charge accelerates the propagating reaction by the neutralization of the emerging negative charge of oxyanion generated from epoxide ring-opening.

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Crystal structures of photosystem II complexed with electron-transfer inhibitors

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Oxygen-evolving Photosystem II (PSII) is a multi-subunit membrane protein complex performing light-induced electron transfer and water-splitting reactions, leading to the formation of molecular oxygen. After initial light excitation and charge separation in PSII, an electron is transferred to a bound plastoquinone molecule Q_A, and subsequently to an exchangeable plastoquinone Q_B. Q_B is the final electron acceptor of PSII, and leaves PSII at the stromal side to cytochrome b_6f as plastoquinol (PQH_2) after uptake of two protons and two electrons. A non-heme iron is located between Q_A and Q_B, and is coordinated by four histidine residues and one bicarbonate ion. Based on XAS experiment and DFT calculation, it was suggested recently that the coordination number of the non-heme iron changes from six to five in the electron transfer from Q_A to Q_B [1]. A class of herbicides is well-known to inhibit the electron transfer beyond Q_A by binding to the Q_B site of PSII . These herbicides have been classified into several types, namely, phenolic, triazine, uracil, and urea types. The corresponding representatives of the four types of herbicides are bromoxynil, terbutryn, bromacil, and DCMU, respectively. PSII crystals were soaked into each of 1 mM solutions of the four herbicides to prepare the electron transfer inhibitor complexes, and X-ray diffraction data were collected at BL44XU, SPring-8, Japan. The four crystal structures were solved independently with the molecular replacement technique, using the 1.9 Å resolution structure (PDB code: 3ARC) determined recently by our group [2] as a search model, and refined at resolutions of 2.3 Å-1.9 Å. All of the four herbicides were modeled into the Q_B site. The crystal structure of PSII-terbutryn complex has been reported at a resolution of 3.2Å with PDB codes 3PRQ and 3PRR [3], in which no water molecules were assigned. In contrast, our structure of PSII-terbutryn complex, determined at a resolution of 2.0 Å, consisted of many water molecules, and some of them were hydrogen-bonded to terbutryn. Furthermore, we found that the bicarbonate ion was coordinated to the non-heme iron as a monodentate ligand, resulting in a coordination number of five for the non-heme iron. This is apparently different from the coordination number of six in native PSII. Thus, the coordination number of the iron may be different in different herbicide complex of PSII. This is the first crystallographic result showing that the bicarbonate ion is able to change its coordination pattern for the non-heme iron.

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