



	Experiment title: Crystallographic Investigations on Structure and Function of Photoactive Proteins	Experiment number: MX-134
Beamline: ID14 2	Date of experiment: 18 July 2003 to: 21 July 2003	Date of report: 28.02.2005
Shifts: 9	Local contact(s): Dr. Ingar LEIROS	<i>Received at ESRF:</i>
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Report:

Photosystem II (PSII) is located in the thylakoid membrane of higher plants, algae and cyanobacteria that catalyzes the oxidation of water to atmospheric oxygen.

We are elucidating the three-dimensional structure of the PSII purified from the thermophilic cyanobacterium *Thermosynechococcus elongatus*. Up to now we obtained electron density maps at relatively low resolutions (Zouni *et al.* 2001), the most recent model determined at 3.2 Å (Biesiadka *et al.*, 2004), collected during the same proposal (MX 134) period.

This higher resolution data of native PSII inspired us to study herbicide binding to PSII. A huge variety of herbicides were reported to bind to PSII, i.e. Phenol-type and atrazin derivatives. We applied different approaches to incorporate herbicide into PSII. We either co-crystallized PSII in the presence of PSII or we soaked PSII crystals over night in a solution with herbicides. We collected several datasets of PSII in complex with different kind of herbicides. For many collected datasets a lower diffraction power (< 5.0 Å resolution) and an increased mosaicity was observed. These latter difficulties were reflected in rather bad data statistics and the low resolution of the data did not permit us to locate the herbicides.

Nevertheless were able to collect one dataset to 4.0 Å resolution in complex with a bound herbicide and we could locate the bound ligand. Attempts to optimize the herbicide soaking are initiated.

During the same experiment we were able to collect further partial datasets of PSII which will be used to fill the segments of data which are missing in the native 3.2 Å dataset.

Additional native datasets were collected on major histocompatibility complexes, which are related to Ankylosing Spondylitis (AS) an autoimmune disease genetically linked to HLA-B*27. The subtype HLA-B*2705 of this MHC class I molecule is strongly associated with AS while HLA-B*2709 is not. The only difference between the two alleles is the HLA heavy chain (HC) at position 116. During the MX134 proposal we already collect datasets of both subtypes with a nonapeptide (pGR) to atomic resolution. We addressed the question whether a change in the pH might have an influence on the conformation of the bound peptide, as a lowered pH was reported for inflamed tissues. Therefore we collected for each subtype high resolution dataset of HLA-B*2705:pGR at HLA-B*2709:pGR at 1.7 Å resolution, respectively.

Reference

Zouni, A., Witt, H.-T., Kern, J., Fromme, P., Krauß, N., Saenger, W., Orth, P. (2001) Crystal structure of photosystem II from *Synechococcus elongatus* at 3.8 Å resolution. *Nature* **409**, 739-743.

Biesiadka, J., Loll, B., Kern, J., Irrgang, K.-D. and Zouni, A. (2004) Crystal structure of cyanobacterial photosystem II at 3.2 Å resolution: a closer look at the Mn-cluster. *Phys Chem Chem Phys*, **6**, 4733-4736.