ESRF	**Experiment title:** X-Ray Crystallographic Investigations on the Structures and Functions of the Photosystem I and II	**Experiment number**: LS-1802
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Shifts: 6	**Local contact(s)**: Dr. Bill Shepard	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Peter Orth*, Norbert Krauß and Wolfram Saenger

Institut für Chemie/Kristallographie, Freie Universität Berlin, Takustr. 6, D - 14195 Berlin

Athina Zouni*, Jan Kern*, Petra Fromme* and Horst Tobias Witt

Max-Volmer-Institut für Biophsykalische Chemie und Biochemie, Technische Universität Berlin, Strasse des 17. Juni 135, D - 10623 Berlin

Report:

The reduction of the secondary bound quinone (Q_B) is an important step in the energetics of photosynthetic cyanobacteria. The Q_B site is also a well-established site of herbicide binding. A lot of commercially available herbicides function by inhibition of higher plants at the Q_B site of the D1 polypeptide. The crystal structure of reaction centre from purple bacteria in complex with the herbicide Atrazin was already solved.

Crystallographic studies have shown that co-crystallisation of proteins with inhibitors could lead to a more compact and stable state, because the conformational degree of freedom is decreasing.

PSII from the thermophilic cyanobacteria *Synechococcus elongatus* was co crystallised with different herbicides. The herbicide Ioxynil (4-hydroxy-3,5-diiodobenzonitrile) belonging to the family of halo-benzonitriles was used for the first trials. Crystals (0.4 x 0.4 x 0.8 mm) were grown under the same crystallisation conditions (Zouni, et al., 2000) like the native ones. The crystals belong to had the same space group and almost the same cell dimensions ($P2_12_12_1$, a=130 Å, b=228 Å, c=308 Å).

At the beamline ID 14 3 several partial data sets of crystals soaked in different herbicides were collected to determine the diffraction quality and the unit cell dimension of the crystals. On the best of the herbicide-PSII-co-crystals we collected a complete data set (99.4 %) at the beamline ID 14 3 at a wavelength of λ=0.933 under cryogenic conditions.. The crystals

diffract to ~ 4.2 Å resolution. The resulting data set after processing with DENZO and SCALEPACK had a maximum resolution of 4.2 Å with R_{sym}=0.08 and <I/σ(I)>=12.4 (R_{sym}=0.64 <I/σ(I)>=1.8)
In the difference electron density map, we identified additional density. We saw two peaks in the density belonging to the two iodine-atoms of Ioxynil. Also a deformation in the protein backbone around the Q_B binding pocket could be observed. But the resolution is still not sufficient to reveal the interaction between herbicide and the surrounding protein.

This result gave first indication, that the established crystallisation condition could be optimised by adding herbicides. This opens a new route towards to higher resolution.

References:

Zouni, A., Jordan, R., Schlodder, E., Fromme, P.,Witt, H.-T. (2000) First photosystem II crystals capable of water oxidation. *Biochim. Biophys. Acta* **1457**, 103-105.