ESRF	**Experiment title:** Structural studies of chloroplast F_1F_o-ATPase	**Experiment number**: LS-2010
Beamline: ID14-2	**Date of experiment**: from: 01-10-01 to: 02-10-01 from: 21-11-01 to: 22-11-01	**Date of report**: 1.2.02
Shifts: 5	**Local contact(s)**: Edward Mitchell and Dominique Bourgeois	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

G. Groth*, C. Schnick*, **J. Voet van Vormizeele***, **C. Zobel***

Heinrich-Heine-Universität, Biochemie der Pflanzen, D-40225 Düsseldorf, GERMANY

Report:

The chloroplast ATP synthase, a multi-subunit enzyme of the thylakoid membrane, shares many structural and functional characteristics with the homologous bacterial and mitochondrial enzymes, but is unique is several aspects of enzyme activation and sensitivity towards specific energy transfer inhibitors [1]. In order to understand these differences we are trying to solve the structures of the chloroplast ATPase and of the membrane extrinsic CF_1-domain of the spinach enzyme complexed with inhibitors or with transition state intermediates.

We have recently solved the structure of the $\alpha_3\beta_3$-core complex of the chloroplast ATPase [2] and of the spinach chloroplast F_1-ATPase complexed with the phytopathogenic inhibitor tentoxin [3] which does not affect bacterial or mitochondrial F_1-ATPases. However, F_1-subunits γ and ε which are supposed to control the activation of the chloroplast ATPase were not resolved in these structures. In order to obtain further structural information on these subunits and to resolve binding sites and mechanism of additional CF_1-inhibitors we have crystallized the soluble chloroplast F_1-domain in the presence of the transition state intermediate fluoroscandium (ScFx) or in the presence of the inhibitors N,N'-dicyclohexylcarbodiimide (DCCD) or dequalinium chloride (DQ), respectively.

Data sets of CF_1-ScFx, CF_1-DCCD and CF_1-DQ were collected during 5 shifts on ID14-2. Data were processed by DENZO/SCALEPACK on site. All crystals showed mosaicity of 0.7-0.8, belong to space group *R32* and have unit cell parameter similar to the native CF_1-complex (a = 147 Å, b = 147 Å, c = 385 Å).

Data set	Resolution [Å]	R-merge [%]	Completeness [%]	I/σI (outer shell)
CF_1-ScFx	3.5	13.5	99.8	4.6
CF_1-DCCD	3.6	8.9	93.6	3.2
CF_1-DQ	3.6	10.9	98.5	3.6

Refinement of the CF_1-inhibitor complexes is still in progress. In addition to the data sets collected on the various inhibitor-complexes we have also collected diffraction data on crystals of the CF_1CF_o-complex which contains the membranous subunits of the chloroplast ATPase in addition to the soluble membrane extrinisic CF_1-complex.

References:

[1] Groth, G. und Strotmann, H. (1999) *Physiologia Plantarum* 106: 142-148.

[2] Groth, G. and Pohl, E. (2001) *J. Biol. Chem.* 276, 1345-1352

[3] Groth, G. (2002) *Proc. Natl. Acad. Sci. USA*, (- in press -)