ESRF	**Experiment title:** Structural studies of chloroplast F_1-ATPase	**Experiment number**: LS-1755
Beamline: ID14-2	**Date of experiment**: from: 03-11-00 to: 04.11.00	**Date of report**: 1.2.01
Shifts: 3	**Local contact(s)**: Stéphanie Monaco	*Received at ESRF:*

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Report:

The chloroplast ATP synthase, a complex multi-subunit enzyme of the thylakoid membrane, catalyses ATP synthesis and ATP hydrolysis coupled with a transmembrane proton transport. The enzyme consists of 2 distinct structural domains. The membrane integrated CF_o-complex mediates proton transport across the thylakoid membrane and provides specific sites for the attachment of the membrane extrinsic, catalytic CF_1-complex which contains five different polypeptides in a stoichiometry of $\alpha_3\beta_3\gamma\delta\varepsilon$. The chloroplast ATP synthase shares many structural and functional characteristics with the homologous bacterial and mitochondrial ATPases, but is unique is several aspects of enzyme activation and sensitivity towards specific energy transfer inhibitors [1].
In order to understand these structural and functional differences we study the chloroplast ATPase from spinach and various inhibitor complexes of the membrane extrinsic CF_1-domain.

We have recently solved the structure of a $\alpha_3\beta_3$-core complex from spinach chloroplast ATPase [2] by molecular replacement using atomic coordinates derived from the homologous bovine mitochondrial F_1 [3]. The structure probably reflects a unique latent state of the chloroplast enzyme which is not found in bacterial and mitochondrial ATPases. The chloroplast γ and ε subunits which control the activation of the CF_1-complex were not resolved in this native structure.

In order to obtain additional structural information on these subunits and to analyse the mechanism and the binding sites of certain energy transfer inhibitors we have started to study various CF_1-inhibitor complexes.

Data sets of CF_1-LuciferYellow, CF_1-OPDM and CF_1-Quinacrine were collected during 3 shifts on ID14-2. Data were processed by DENZO/SCALEPACK on site. All crystals showed high mosaicity, belong to the space group *R32* and have unit cell parameter similar to the native CF_1-complex.

CF_1-LuciferYellow	3.5 Å, 12.1 % R-merge, 93.3 % completeness, 2.7 I/σI (outer shell)
CF_1-OPDM	3.5 Å, 13.3 % R-merge, 96.2 % completeness, 2.0 I/σI (outer shell)
CF_1-Quinacrine	3.6 Å, 11.0 % R-merge, 98.5 % completeness, 3.0 I/σI (outer shell)

Refinement of the CF_1-inhibitor complexes is in progress. In addition to the data sets collected on the various inhibitor-complexes diffraction of several CF_1-tentoxin crystals was tested in order to optimise cryo-conditions.

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] Abrahams, J.P.,Leslie, A.G.W., Lutter, R. and Walker, J.E. (1994) *Nature* 370, 621-628