ESRF	**Experiment title: Studies of the structure-function relationship of proteins investigated at the MPI Dortmund**	**Experiment number**: LS-1677
Beamline: ID14-2	**Date of experiment**: from: 24-Feb-00 to: 26-Feb-00	**Date of report**: 15.8.2000
Shifts: 6	**Local contact(s)**: Rasmussen Bjarne	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Alexandru-Tudor Constantinescu*, Karsten Goedecke*, Dr. Oleksii Rak*, Dr. Axel J. Scheidig*, Dr. Nicolas Thomä*

Report:
The following projects were investigated:

1. Crystal structure determination of photosystem II

We have crystallized the active, dimeric form of PS II. Using beamline ID14-2 (and test beam time on ID13) we were able to collect a first native data set up to 4.3 Å resolution (overall 85 % completeness). This data set allowed us an evaluation of the space group and the suggestion of a hypothetical crystal packing model. Different potential heavy atom derivatives were collected with different resolutions. The evaluation of these data sets is in progress.

Kuhl, H., Kruip, J., Seidler, A., Krieger-Liszkay, A., Bünker, M., Bald, D., Scheidig, A.J. & Rögner, M. (2000). Towards structural determination of the water-splitting enzyme:Purification, crystallization and preliminary crystallographic studies of photosystem II from a thermophilic cyanobacterium. J. Biol. Chem. 275, 20652-20659.

2. Proteins involved in vesicular transport

Rab GGTase II. **The protein crystallizes in very thin plates which diffract in house up to 8 Å resolution. At ID14-2 we could collect data sets up to 2.5 Å resolution. However, due to multiple overlapping reciprocal lattices it was not possible to process the data. In the meantime the structure of Rab GGTase II was solved by the group of Deisenhofer and we stopped the project.**

Rab GGTase II in complex with Rab7 and REP-1. **This 200 kDa ternary complex is the functional unit of Rab GGTase II which prenylates Rab7 if complexed with REP-1. The crystals diffract in house up to 10 Å resolution. After optimization of the freezing conditions at ID14-2 the maximum diffraction was around 5 Å. Improvement of the crystal quality is in progress.**

Ypt7p**. This small GTP-binding protein forms very thin hexagonal needles. We were able to collect a complete data set up to 2.3 Å resolution (space group P61). Structure refinement is in progress.**

Gyp7:Ypt7p**. Gyp7p is the GTPase activating protein of Ypt7p. The binary complex with the transitions state analogue GDP-AlF_3 diffracted up to 4.5 Å resolution. We were not able to solve the structure using molecular replacement with Gyp1-46p and Ypt7p as a search model. Optimization of the crystals and expression as Se-Met substituted protein is in progress.**

3. Proteins involved in DNA methylation

DAM**. We have crystallized the DNA-methyltransferase DAM from *E. coli* in complex with a specific double stranded DNA and a modified cofactor. The crystals belong to space group P212121. A complete data set (95 %) with a maximum resolution of 2.5 Å could be collected. Since molecular replacement with other known DNA-methyl-transferases as models did not work we have to search for heavy atom derivatives. This 35 kDa protein contains two methionines and we plan the modification of the DNA with iodine and bromine in order to derive MIR and MAD phasing possibilities.**