ESRF	**Experiment title: Studies of the structure-function relationship of proteins investigated at the MPI Dortmund**	**Experiment number**: LS-1677
Beamline: ID14-1	**Date of experiment**: from: 27-Apr-00 to: 29-Apr-00	**Date of report**: 15.8.2000
Shifts: 6	**Local contact(s)**: Burmeister, Wilhelm	*Received at ESRF:*

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Report:
The following projects were investigated:

1. Crystal structure determination of photosystem II

Different potential heavy atom derivatives were collected with different resolutions (4.2 – 5.5 Å). The evaluation of these data sets is in progress.

2. Proteins involved in vesicular transport

Rab GGTase II in complex with Ypt7p and REP-1. **The crystals could not be evaluated in house due to size limitations. After optimization of the freezing conditions at ID14-1 the maximum diffraction was around 6 Å. Improvement of the crystal quality 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 modified at two, three and five positions, respectively with iodine. From the five-times iodinated complex we could collect a complete data set (93 %) with a maximum resolution of 3.2 Å and of the three-times iodinated complex up to 3.5 Å resolution (98 % complete). The Patterson maps indicate the incooporation of heavy atoms (iodine), however, the evaluation is still in progress.**

4. Photoreceptor pSR II

pSR II is a photoreceptor in the plasma membrane of archaeon Natronobacterium pharaonis and functions as a sensor for phototactic avoidance. This 7-helix transmembrane protein crystallizes in very small cubic prisms of around 0.03 x 0.03 x 0.02 mm^3. The diffraction limit of these crystals is at ID14-1 at around 8 Å. In the meantime we could collect a complete data set with maximum resolution of 3.5 Å at the micro focus beamline ID13.

5. Rap guanine-nucleotide exchange factor directly activated by cAMP (Epac II)

We have crystallized the 45kda regulatory domain of Epac II, which contains two cAMP-binding domains and a DEP domain for membrane targeting. The crystals belong to space group P212121 and diffract to 3.6Å at the home source. At ID14-1 we collected a complete (93%) dataset at 2.6Å resolution. Molecular replacement using the cAMP binding domains of PKA as search models failed. The crystallized domain contains 10 Methionines and we are therefore currently persuing the structure determination by SeMet – MAD phasing.

6. Inducibly expressed GTPase (IGTP)

IGTP is a representative of the 47kda–family of interferon-γ-inducable GTPases. We have crystallized full length IGTP. The crystals belong to space group P212121 and diffract to 3.2Å at the home source. At ID14-1 we were able to collect a complete (99%) dataset at 2.3Å resolution. Since no homologous structures to IGTP are known and the IGTP-molecule contains 11 Methionines, we are now persuing the de novo structure determination by SeMet–MAD phasing.

7. Human Thymidylate Kinase (TmpK)

Human TmpK is the rate limiting enzyme in the activation pathway of the AIDS prodrug AZT. The slow phosphorylation rate of AZT-monophosphate (AZTMP) to its diphosphate results in the accumulation of the toxic monophosphate metabolite and in a very low concentration of the antiviral triphosphate metabolite. We generated a mutant ("small lid") that has greatly improved activity towards AZTMP phosphorylation. To understand the structural reasons we collected data to 1.8Å resolution of the AZTMP ADP complex of the mutant (completeness 99.7% (99.9%) , Rsym 6.4% (35.8 %), I/sigma(I) 12.6 (3.2)). Structure refinement is under way.