ESRF	**Experiment title: FRANKFURT BAG**	**Experiment number**: MX135
Beamline: ID14-4	**Date of experiment**: from: 8.12.2003 to: 9.12.2003	**Date of report**: 21.1.2004
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Report:

1. Cyclohexandiol dehydratase (CDH)

CDH from was crystallized in the space group $P4_{1/3}2_12$ with cell axis of 122.9 Å and 143.5 Å. Most likely, a dimer is present in the asymmetric unit.

a) Native data were collected to 1.2 Å. Due to limited area of the detector and the large size of the crystals the data indicated a high degree of overlap and data processing is not completed. But it appears that data evaluation is feasable.

b) A second native data set was collected at 1.7 Å resolution with a smaller crystals. The overall R_{sym} of 5.4% and the completeness is 94.7 %. This data appears to be well suitable as reference data set for the MIR phasing procedure.

c) A MAD data set of CDH soaked with 0.5 mM $HgAc_2$ was measured at 2.5 Å resolution.
The peak data set provided an R_{sym} of 4.5% and a completeness of 99.6%. Two mercury binding site could be clearly detected. Phase determination is in progress.
The inflection data set had an R_{sym} and completeness of 3.9% and 99.6%, respectively and remote data set of 3.7% and 99.6%, respectively.

d) An SAD data set was meassured with crystals soaked with 0.5 mM thimerosal were also measured to 2.5 Å (R_{sym} =4.6%; completeness= 99.6%) but no mercury binding site could be found.

e) Crystals were very sensitive to K_2PtCl_4 but a soak with 0.2 M after a soaking time of 2h could be measured to 2.8 Å (R_{sym}=5.4%; completeness=100%). Three platinium binding sites could be detected. A further evaluation is in progess.

2. Formaldehyde-activating enzyme (FAE)

FAE was cocrystallized with its substrate H_4MPT (2.5 mM) in a new crystal form. The space group was $P2_1$ and the cell parameters 48.9 Å, 112.6 Å, 72.0 Å and 91.6°. The crystals diffracted to around 2.5 Å. A complete data set could be collected that resulted in an R_{sym} was 7 % and the completeness 87%. The structure could be solved by molecular replacement procedures and H_4MPT could be clearly localized between the 5 subunits.
FAE crystals (space group $P4_12_12$, cell axis 119.5 Å and 205.8 Å) were soaked with the second substrate formalaldehyde. A complete data set was measured at 2.6 Å resolution. The R_{sym} was 7.4% and the completeness 100%. The data were not further evaluated so far.

3. Formyl-methanofuran: H_4MPT-Formyltransferase (Ftr)

Ftr was cocrstallized with formyl-methanofuran and H_4MPT using PEG 8000 as precipitant. The crystals were with around 40 μm very thin such a highly intense and focussed synchrotron radiation was essential for data collection. Data were collected to a resolution of 2.5 Å. The R_{sym} was 6.6 % and the completeness 95%. So far molecular replacement calculations failed and it was not possible to find out, whether the substrates had bound.

4. ATP binding domain of a phosphate ABC transporter (CysA)

CysA crystals were soaked with ATP prior to data collection. The obtained data set to 2.8 Å was of high quality (Rsym = 5.7%; completeness = 98.9%) but a subsequent structure determination indicated that ATP has not bound.

5. Heme domain of cytochrome oxidase (Cyt)

Crystals of Cyt were soaked with 5 mM DTT for about 30 min and flash-frozen. A data set was collected up to 1.5 Å resolution. The resulting R_{sym} was 6.7% and the completeness 98.3%. Data were not further evaluated so far.

6. Methanol-H_4MPT methyltransferase (Mta)

Mta was crystallized in space group $P2_1$ with cell parameters of 101.7 Å, 172.9 Å, 190.5 Å and 98.9°. However the cell parameters can vary considerably between crystals. Native data were collected at 2.5 Å resolution. The R_{sym} and the completeness was 8.0% and 97.5%. This structure could not be solved so far.