SNBL	**Experiment title**: BAG proposal in Macromolecular Crystallography for the University of Oslo - Studies of proteins in the Oslo region.	**Experiment number**: 01-02-633
Beamline: BM01	**Date of experiment**: from: 18-JUN-03 07:00 to: 21-JUN-03 07:00	**Date of report**: 30-OCT-03
Shifts: 12	**Local contact(s)**: Jon Are BEUKES	*Received at UNIL:*

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Three dimensional structure determination of enterocin A immunity protein (EntA-im).

Dalhus, B., Johnsen, L. & Nissen-Meyer, J.

We have previously obtained native diffraction data for two crystals of enterocin A immunity protein (see previous report). The enterocin A immunity protein crystals belong to the monoclinic crystal system with unit cell dimensions a = 116.59, b = 42.37 and c = 66.19 Å and with β = 111.27°. The symmetry and systematic absences in the diffraction pattern is consistent with space group C2. The presence of two molecules in the asymmetric unit with a molecular weight around 12.2 kDa gives a crystal volume per protein mass (V_m) of about 3.1 $Å^3$ Da^{-1} and a solvent content around 60 % by volume (1).

We collected three datasets of heavy-atom derivatives of EntA-im in order to solve the phase problem by MIR. Each set where of resonable quality:

Derivative	Resolution	R-merge	Completeness (Scalepack statistics)
#1	2.1Å	0.06(0.29)	97(90)%
#2	2.5Å	0.08(0.22)	98(92)%
#3	2.6Å	0.07(0.21)	92(72)%

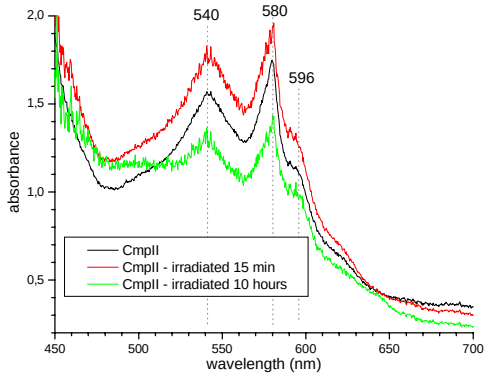
Scaling against the native data shows strong and probably unspecific binding of the heavy atom ions. Patterson difference maps where uninterpretable. Producation of Se-Met mutant is in progress.

Investigation of myoglobin:

Hersleth, H.-P., Görbitz, C. H. & Andersson, K. K.

The myoglobin project was further developed. We have previously let myoglobin react with hydrogen peroxide and other organic peroxides at different pH-values. We have in these studies trapped the intermediates called compound II and compound 0, and looked on the pH dependence.

This time the prime focus was on radiation damage of the reaction site in the protein. We measured light absorption on crystals before and after irradiation to check for changes. (We used the microphotospectrometer in connection with ID9.) As shown in the figure we could not observe any reduction of compound II after irradiation.



	Resolution	R-merge	Completeness
#1	1.3Å	0.05(0.31)	98(98)%
#2	1.4Å	0.06(0.28)	96(94)%

Related Publications in this periode:

- Dalhus, Johnsen & Nissen-Meyer (2003), Acta Crystallographica, Biological Crystallography, **D59,** 1291-1293**.**
- Lectures – *2nd Swiss-Norwegian Beam Lines Highlights Meeting, Tromsø, 23rd-25th June 2003.*
  - Hersleth, H.-P. – Trapping reaction intermediates in the myoglobin-peroxide reaction. A crystallographic study supported by single crystal light absorption spectroscopy.
  - Andersson, K. K. – Crystallographic and spectroscopical (EPR, MCD, Raman) studies of Ribonucleotide reductase from mouse show new carboxylate/tyrosyl radical shifts of the Di iron-oxygen cluster