

## Experimental report, MX-304

### 30.11- 1.12 2004

#### 1. Enterocin A immunity protein

We tried to collect data for a large number of crystals, however no sample gave diffraction to a resolution useful for structural elucidation. Since we have no in-house diffractometer, assesment of crystal quality prior to visits to ESRF is currently not possible. The EntAim crystals are thin, needleshaped crystals with low diffracting volume. The station was further running in 16-bunch mode with low intensity.

#### 2. MAD iron-edge data collection of a cytochrome from *Methylococcus capsulatus*

The methanotropic organism *Methylococcus capsulatus* is can be utilized to produce biomass from natural gas resources. A large portion of its soluble protein consists of a c-type cytochrome which we have isolated and purified. This cytochrome is believed to be involved in the methane metabolism of the cell, but its interaction partners are so far unknown.

We collected two full datasets (peak and inflection wavelength) for each of 2 crystals of this haem-containing protein, trying to utilize the iron edge for SAD-phasing. Analysis of the integrated frames shows, however, that the anomalous signal is too weak for SAD-phasing. XPREP statistics shows that the anomalous difference at the iron edge is insignificant.

	Peak(1)	Inflection(1)	Peak(2)	Inflection(2)
Resolution	2.75	2.75	2.75	2.75
I/sI	18.3	12.1	17.5	13
R(sym)	0.173	0.169	0.071	0.072
R(anomal)	0.191	0.183	0.080	0.079
Completeness	95.7	93.7	92.9	86

#### 3. Peroxidase reaction cycle intermediate in the haem protein myoglobin

The main goal of this project has been to investigate the peroxidase reaction cycle in myoglobin by trapping intermediates in the cycle. Some of the states are subjected to reduction of the haem-iron due to radiaton damage. The highly oxidized intermediate compound II (stable at a wavelength of 0.9 Å) was now subjected to a longer wavelength of 1.7 Å to see if this could induce reduction. The state was checked by microspectrophotometry (available at SNBL) before and after data collection, which showed no reduction of the reaction center. A full set of the oxidized intermediate compound II was collected.

Dataset	Completeness	R(sym)	Resolution	I/sI
mb7	85.9% (71.1%)	0.041 (0.131)	2.8 Å	15.4 (5.6)