SNBL	**Experiment title**: BAG proposal in Macromolecular Crystallography for the University of Oslo	**Experiment number**: 01-02-928
Beamline: BM01A	**Dates of experiments**: From: 02-JUN-11 08:00 to: 06-JUN-11 08:00	**Date of report**: 30-FEB-12
Shifts: 12	**Local contact(s)**: Volodymyr SVITLYK	*Received at UNIL:*

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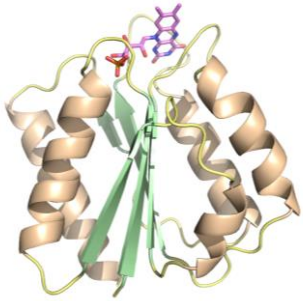
1. MYOGLOBIN

The main goal of this project has been to investigate the peroxidase reaction cycle in myoglobin (Mb) by trapping intermediates in the cycle. Two of the intermediates have been determined, the so-called compound II equivalent and the compound 0 equivalent as well as the resting state. Several of these states experience some radiation damage of the metal site as investigated by light absorption microspectrophotometry and online Raman spectroscopy at SNBL previously. This time we continued to study radiation damage effect with both UV-vis and Raman spectroscopy in combination with crystallography.

2.RIBONUCLEOTIDE REDUCTASE

The enzyme Ribonucleotide Reductase (RNR) converts the four ribonucleotides to their corresponding deoxyribonucleotides that are necessary for DNA synthesis. The Class Ib Ribonucleotide Reductase system in *Bacillus cereus* consists of at least 4 proteins; NrdE, NrdF, NrdH, and NrdI. We have performed studies of the flavine co-factor in NrdI at SNBL. This time we collected an initial data set of a complex between NrdI and NrdF.

2. FLAVODOXIN



There are three flavodoxins in *B. Cereus* that, and they represent the electron delivering system for both ribonucleotide reductase and nitric oxide synthase. The flavodoxin named BC1376 diffracted to 0.97 Å at SNBL, but collecting data to 0.97 Å would according to strategy programs have required an oscillation of 0.1°. This would have been very time consuming due to the image plate detector, so initial data was collected to only 1.2 Å. The structure was solved, and later higher resolution data was collected on other beamlines. The data collection was accompanied by Raman spectra of the crystals.

3. CYTOCHROME C

Nitrosomonas europea Cytochrome c is an electron transfer protein with some special electronic properties. We have obtained initial structures of the native and delN64 mutant of the protein. This time new data sets was accompanied by single crystal UV-vis and Raman spectroscopy.

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4. CATALASE-PEROXIDASE

Mycobacterium tuberculosis KatG is the enzyme responsible for activation of the anti-TB drug isoniazid in use for over fifty years, and mutations in this enzyme are the primary source of drug resistance in clinical strains of the TB pathogen throughout the world. The protein has both peroxidase and catalase activity, and an important question is to understand the correspondence between specific structural features and catalytic function in KatG. This time new data sets was accompanied by single crystal UV-vis and Raman spectroscopy.