| SNBL | **Experiment title**: Studies of the haem containing proteins: myoglobin, haemoglobin, nitrogen oxide synthase and cytochrome c with main interest on different reactive intermediates. | **Experiment number**: 01-02-360 |
|---|---|---|
| **Beamline**: BM01 | **Date of experiment**: from: 04-SEP-02 07:00 to: 06-SEP-02 07:00 | **Date of report**: 30-Sep-02 |
| **Shifts:** 6 | **Local contact(s)**: Silvia CAPELLI | *Received at UNIL:* |

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## Investigation of myoglobin:

The myoglobin project was this time further developed:

We have previous let myoglobin react with hydrogen peroxide or other organic peroxides at different pH-values. We have in these studies trapped the intermediate called compound II, and looked on the pH dependence.

This time two data sets were collected of the compound II at different pH's by using a short wavelength of 0.72 Å. The short wavelength was used to try to avoid for possible reduction of the oxidized reaction centre. Also a data set of myoglobin reaction with peracetic acid was collected.

Data sets were:

Rection with $H_2O_2$ – pH 6.8 – 0.72 Å wavelength

Resolution: 25-1.45 Å $R_{merge}$: 4.5% Completeness: 86% (scalepack) not fully scaled

Rection with $H_2O_2$ – pH 8.7 – 0.72 Å wavelength

Resolution: 25-1.50 Å not processed

Rection with peracetic acid – 0.90 Å wavelength

Resolution: 25-1.35 Å $R_{merge}$: 4.1% Completeness: 99.5%

## Other proteins :

Crystals of a few other proteins were also tested. These include small crystals of ribonucleotide reductase p53R2 that did not diffract beyond 10Å, the amyloid fibrous Bence Jones protein, of which only very thin needles are available. No useful diffraction was obtained for BJ protein. Finally, the double mutant e165q/d166n of Malate Dehydrogenases from the thermophilic bacteria *Chloroflexus aurantiacus* were mounted. The crystals diffracts beyond 2.25Å but have a large mosaicity, making the diffraction data more or less useless.

**Related Publications in this periode:**


- Strand, K. R., Karlsen, S. and Andersson, K. K. (2002). Cobalt substitution of mouse R2 ribonucleotide reductase as a model for the reactive diferrous state. Spectroscopic and structural evidence for a ferromagnetically coupled dinuclear cobalt cluster. *J. Biol. Chem*. **277**, 34229-34238
- Strand K.R., Karlsen, S., Gørbitz, C. H. and Andersson, K. K. (2002). Spectroscopical and crystallographic studies of the dinuclear metal cluster of ribonucleotide reductase r2 from mouse. *Proceedings of the 6th European Biological Inorganic Chemistry Conference, July 29- August 3, Lund, Sweden/ Copenhagen, Denmark*, p. 224
- Hersleth, H.-P., Dalhus, B., Görbitz, C. H. and Andersson, K. K. (2002). pH Dependence of Peroxide Derived High Valent Haem in Myoglobin Studied by X-Ray Crystallography. *XIX Congress and General Assembly of the International Union of Crystallography*, 6th–15th August 2002, Geneva, Switzerland. *Acta Cryst*. A**58** (Suppl.), C117
- Hersleth, H.-P., Uchida, T., Teschner, T., Shünemann, V., Görbitz, C. H., Kitagawa, T., Trautwein, A. X. and Andersson K. K. (2002). Crystallographic and Spectroscopical Studies of Peroxide-Derived Myoglobin Compound II. *Proceedings of the 6th European Biological Inorganic Chemistry Conference, July 29- August 3, Lund, Sweden/ Copenhagen, Denmark*, p. 256
- Dalhus, B., Bjørk, A., Mantzillas, D., Eijsink, V. and Sirevåg, R. (2002). Analysis of an Ionic Network Within a Protein Oligomer and Engeneering Towards Higher Thermostability. *XIX Congress and General Assembly of the International Union of Crystallography*, 6th–15th August 2002, Geneva, Switzerland. *Acta Cryst*. A**58** (Suppl.), C371