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Using in situ single-crystal UV-vis and Raman spectroscopy to study the effect of X-ray radiation damage on the crystal structures of haem proteins

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To be able to correctly interpret the crystal structure of redox- and metalloproteins caution must be employed. The influence of X-ray radiation damage to protein crystals is well known to occur even at cryogenic temperatures, and redox active sites like metal sites seem especially vulnerable for radiation-induced reduction [1,2,3]. We have used in situ (online) UV-vis and Raman spectroscopy to study how different haem and flavoproteins are influenced by X-rays during crystallographic data collection [1,2]. The spectroscopic changes have been monitored as a function of X-ray exposure (dose absorbed), Our studies show that these redox states are very fast reduced by X-rays resulting in very short lifedoses. Structurally we have observed for haem proteins a lengthening of the Fe-O bond, and for flavoproteins a bending of the flavin ring during X-ray induced radiation damage, in agreement with DFT [1,2,3]. We have recently started to investigate if varying the doserates and wavelengths can increase the lifedoses. In general our studies show the need of combining protein crystallography with in situ single-crystal spectroscopy when redox and metalloproteins are studied.

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Primary author: Dr HERSLETH, Hans-Petter (Department of Molecular Biosciences, University of Oslo, P.O.Box 1041 Blindern, 0316 Oslo, Norway)

Co-authors: Dr POMPIDOR, Guillaume (Swiss Light Source, Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland); Prof. ANDERSSON, K. Kristoffer (Department of Molecular Biosciences, University of Oslo, P.O.Box 1041 Blindern, 0316 Oslo, Norway); Ms LOFSTAD, Marie (Department of Molecular Biosciences, University of Oslo, P.O.Box 1041 Blindern, 0316 Oslo, Norway); Dr VAN BEEK, Wouter (Swiss–Norwegian Beamlines at ESRF, BP 220, 38043 Grenoble Cedex, France); Dr RØHR, Åsmund K. (Department of Molecular Biosciences, University of Oslo, P.O.Box 1041 Blindern, 0316 Oslo, Norway)

Presenter: Dr HERSLETH, Hans-Petter (Department of Molecular Biosciences, University of Oslo, P.O.Box 1041 Blindern, 0316 Oslo, Norway)

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