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Third Generation of On-axis in situ Optical Spectroscopy – Extending the Scope of Macromolecular Crystallography

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Macromolecular Crystallography of proteins is one of the fundamental tools of a structural biologist. However, this method does not yield information on, for example, the chemical state of co-factors, the redox state of metal centers or disulphides, or the identity of bound ligands. Many of these observations can be directly or indirectly linked to radiation damage, one of the central limitations of synchrotron X-ray diffraction data collection [1]. To be able to better quantify the extend of this effect and obtain additional complementary data on the sample, the on-axis geometry for in-situ combination of optical spectroscopic methods with the diffraction experiment has proven highly effective [2].
At beamline X10SA at the Swiss Light Source we now are commissioning the third generation of an on-axis multi-mode micro-spectrophotometer (SLS-MS3). It is fully integrated into the completely rebuild beamline endstation and designed to remain always online, thereby dramatically reducing setup times for the support UV/Vis, Fluorescence,Raman and Resonance Raman spectroscopic modes.
We also present quantitative mappings of the on-axis sampling geometry to demonstrate its advantages for aligning the sampling volumes. We show applications of UV/Vis spectroscopy and resonant and non-resonant Raman spectroscopy toward monitoring the photo reduction of metal centers, ligand abstraction and bond breakage.

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