MS2-O4 Macromolecular Crystallography at SwissFEL

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X-ray free electron lasers (XFELs) bear the promise of providing damage-free protein structures in a "diffract-before-destroy" approach. The Swiss free electron laser (SwissFEL) is currently under construction at the Paul Scherrer Institute, Switzerland. In the standard operation mode, the hard X-ray beamline will deliver 2-20 fs (rms) pulses at 100 Hz repetition rate, with photon energies in the range 2-12.4 keV and up to about 1 mJ/pulse. The start of operation is foreseen at the end of 2017. The hard X-ray experimental stations are conceived to offer state-of-the-art possibilities for femtosecond protein crystallography, with a variety of sample delivery methods and experimental conditions. At each station, femtosecond pump lasers will be available for time resolved studies.

The SwissFEL hard X-ray experimental station A (ESA) is designed for time resolved X-ray spectroscopy and serial femtosecond crystallography (SFX). It will cover the full photon energy range 2-12.4 keV, and the beam can be focused down to a size of 1 μm. The experiments are done within a chamber at pressures ranging from vacuum to ambient. The chamber can host injectors to perform SFX measurements while delivering the sample with a liquid or viscous jet [1]. Simultaneous acquisition of diffraction images and single-shot X-ray emission spectra will be possible.

The SwissFEL hard X-ray experimental station B (ESB) is designed for time-resolved X-ray diffraction studies in the field of condensed matter physics. The beam can be focused down to a size of 2 μm. The station also includes a general purpose table for alternative setups, one of which will be an in-house developed instrument for fixed-target protein crystallography, an important recently developed alternative to sample injection. The possible data acquisition schemes include synchrotron-like rotation measurements on a relatively small set of large crystals [2], as well as SFX on microcrystals deposited on a solid support [3] with fast scanning data acquisition, in the photon energy range 5-12.4 keV. An automatic sample changer will ensure high-throughput use of the XFEL beam. In-air and in-helium sample environments, as well as cryogenic and room-temperature conditions will be available.

[1] Kang, Y., et al. (2015). *Nature*, *523*(7562), 561–567

[2] Cohen, A. E., et al. (2014), Proc. Natl. Acad. Sci. U. S. A., 111(48), 17122–17127.

[3] Hunter, M. S., et al, (2014). Sci. Rep., 4, 6026.

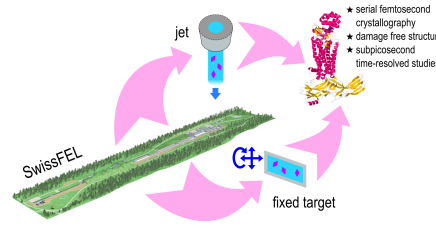

Figure 1. Sample delivery possibilities at SwissFEL. Structure of the rhodopsin-arrestin complex by femtosecond X-ray laser (PDB 4ZWJ, ref [1]).

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