Poster Presentation

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Facilities for macromolecular crystallography at the HZB

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The Helmholtz-Zentrum Berlin operates three beamlines for macromolecular crystallography at the electron storage ring BESSY II [1,2]. BL14.1 and BL14.2 are tunable in the photon energy range from 5 keV to 15.5 keV, while BL14.3 is a fixed-energy side station (13.8 keV). They feature state-of-the-art experimental stations and ancillary facilities, serving more than 100 research groups across Europe. More than 2000 protein structures measured at BESSY II have resulted in PDB depositions so far, and with more than 450 PDB depositions in 2016, they are currently among the most productive MX-stations in Europe.

The experimental endstation of BL14.1 provides high degree of automation and is equipped with a very large Pilatus 6M pixel detector, a CATS sample changer robot and an MD2 microdiffractometer with mini-kappa-capabilities. In 2016 also BL14.2 underwent a comprehensive endstation upgrade to increase the performance in terms of sample throughput, allowing for large automated fragment-screening campaigns in the near future. BL14.2 now features a Pilatus3S 2M detector, a G-Rob sample changer robot and an in-house built piezo-controlled nanodiffractometer. Its large sample dewar can accommodate up to 294 samples, supporting both, SPINE- and UNIPUCKS. In addition to the standard MX-setup a high-resolution UV/Vis microspectrophotometer can be attached to the goniometer in order to perform spectro-photometric measurements of crystals during diffraction data collection, e.g. to account for radiation damage (Figure).

Both beamlines are operated using MXCuBE V2 and various data processing software including the data processing expert system XDSAPP [3] are available. All standard data collection procedures, such as SAD and MAD, are possible, as well as long-wavelength measurements and element identification using an X-ray fluorescence detector. Further experimental possibilities are radiation induced phasing experiments using a pulsed UV-laser, in situ crystal screening, crystal annealing and controlled crystal dehydration using an HC1 dehydration device on BL14.3. Furthermore, the HZB-MX group operates an S1 BioLab which supports the complete workflow from protein purification to crystallization.

Figure: Absorbance spectra of the redox indicator Resazurin in the oxidized state (blue) and the reduced state (red) measured with the microspectrophotometer. The absorbance maxima are 25 nm apart and can clearly be distinguished.

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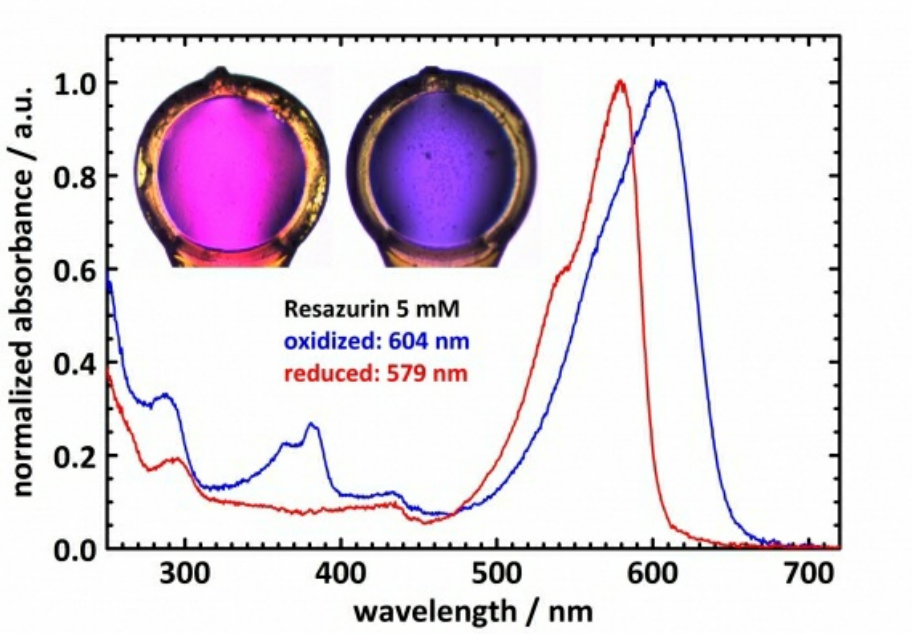
[2] Mueller, U. et al. (2015). Eur. Phys. J. Plus 130, 141.
[3] Sparta, K. et al. (2016). J. Appl. Cryst. 49, 1085-1092.



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