GI-MS46-P16 | Long-wavelength protein crystallography at Diamond Light Source

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The long wavelength I23 beamline at Diamond Light Source is a unique facility dedicated to streamline solving the crystallographic phase problem by conducting anomalous dispersion experiments close to the atomic absorption edges of light atoms naturally occurring in proteins. The beamline operates in a core wavelength range from 1.5 to 4 Å, offering an experimental setup complementing a suite of five MX beamlines at Diamond Light Source. To minimize absorption effects, the entire beamline including end station with goniometer and detector operate in vacuum environment ($<10^{-7}$ mbar). Cooling the samples during storage, transfer and data collection is realized through the manifold of conductive links connecting pulse tube cryocoolers with sample storage and kappa goniometer. A large cylindrical Pilatus 12M detector allows access to diffraction data up to 2theta = ±90◦ that in combination with the absence of X-ray scattering results in superior quality of diffraction data.

The unique wavelength range towards the sulfur and phosphorous K-absorption edges opens new opportunities for macromolecular crystallography. A multitude of native phasing experiments can be performed, including sulphur/phosphorus single wavelength anomalous dispersion (S/P-SAD). Additionally, access to the absorption edges of calcium, potassium and chlorine allows an unambiguous determination of ions from these biologically vital elements. Recent results from the beamline and the emerging novel applications from extending the wavelength range will be discussed. Examples will be shown on identification of using anomalous contrast as well as structures solved on the beamline based on the anomalous signal from S, Cl, I, K, Ca, V.