Poster Presentation

Low Multiplicity Sulfur SAD Phasing in the Home lab

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Advances in crystallographic hardware and software are enabling structural biologists to investigate more challenging projects. Recent developments in hardware and software are greatly increasing the capabilities of in-house diffraction systems making it more routine to obtain de novo structural information in the home lab. Single-wavelength anomalous diffraction (SAD) techniques with Cu Ka or Ga Ka radiation are now widely used for structure solution even in cases involving weak anomalous scatterers, like sulfur. We have now introduced the D8 Venture solution for structural biology with the PHOTON 100 detector featuring the first CMOS active pixel sensor for X-ray crystallography. Our new microfocus source, the METALJET delivers beam intensity exceeding those of typical bending-magnet beamlines. The very high intensity, the small beam focus and the lower air scatter produced by Gallium K help to greatly reduce the background scatter. This provides greater signal to noise essential to identify weak anomalous signal. Due to the very weak anomalous scattering of S, data multiplicities in the order of 40 are typically necessary to obtain phases by S-SAD. Collecting high-multiplicity data minimizes systematic experimental errors to measure with very high accuracy the minute intensity difference between Friedel Pairs (1.0 - 1.5 %) [1]. This requires software which optimizes the collection strategy, for example with respect to overall data collection time to minimize radiation damage. The combination of a brighter, more stable X-ray source with a high sensitivity low noise detector have greatly improved the quality of data collected in-house. The high quality allows successful SAD measurements far away from the absorption edge. Here we present a low multiplicity sulfur-SAD phasing experiment on a small Thaumatin crystal showing the high quality of the data collected on the D8 VENTURE with the METALJET.

[1] Doutch, J. synchrotron Rad. 2012

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