Poster Presentations

[MS5-P17] Low Multiplicity Sulfur SAD Phasing in the Home lab

<u>Séverine Freisz</u>¹, Juergen Graf², Matthew Benning and Vernon Smith

 ¹ Bruker AXS GmbH, Östliche Rheinbrückenstr.
49, 76187 Karlsruhe, Germany
² Incoatec GmbH Max-Planck-Straße 2 21502 Geesthach, Germany
³ Bruker AXS Inc., 5465 East Cheryl Parkway, Madison, WI 53711, USA Severine.freisz@bruker-axs.de

Advances in crystallographic hardware and software have enabled structural biologists to investigate more challenging projects. Recent developments have greatly increased the capabilities of in-house diffraction systems and made it easier to obtain de novo structural information in the home lab.

Single-wavelength anomalous diffraction (SAD) techniques with Cu radiation are now widely used for structure solution even in cases involving weak anomalous scatterers, like sulfur. 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 even far away from the absorption edge.

Higher multiplicity data sets are an established method for successful in-house SAD trials. This requires software which optimizes the collection strategy, for example with respect to overall datacollection time to minimize radiation damage.

We have now introduced the D8 VENTURE solution for structural biology with the PHOTON 100 detector featuring the first CMOS active pixel sensor in X-ray crystallography. The new very high brightness microfocus X-ray sources such as METALJET, Turbo Xray Srouce and IµS now deliver beam intensities comparable to those of typical bending-magnet beamlines. Here we present two low multiplicity sulfur-SAD phasing experiments on a small Thaumatin crystal collected on the D8 VENTURE with the Turbo Xray Source as well as with the new METALJET that allowed us to obtain nice high resolution structures.

Keywords: Phasing, biocrystallography, in House