SAD Phasing using a Home Source, What is the Limit?

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With a diffraction system combining a high-brilliance rotating anode source, graded multilayer optics, a 3- or 4-circle goniostat and a sensitive CCD detector it is possible to solve protein structures from Cu-Kα native data only using SAD (single-wavelength anomalous diffraction) [1].

With highly redundant data this can be done with proteins that only contain Sulfur as the anomalous scatterer, despite the relatively low anomalous scattering contribution (f″) at Cu-Kα of only 0.56 electrons.

The possibility to solve a structure using SAD phasing depends on the number of anomalous scatterers and the strength of the anomalous signal. These are expressed in the Bijvoet factor $\langle \Delta F\pm \rangle / \langle F \rangle$.

In this study we will show a number of cases of structure determination using SAD phasing on native data collected on a home source and how the Bijvoet factor can be used to predict the success of SAD phasing.

[1] Debreczeni J.E., et al*., Acta Cryst.,* 2003, D**59**, 686-696

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