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Softer but stronger? Sulfur SAD with low energy X-rays of 2.7 Å

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Single wavelength anomalous diffraction (SAD) is a powerful experimental phasing technique used in macromolecular crystallography (MX). SAD is based on the absorption of X-rays by heavy atoms, which can be either incorporated into the protein (crystal) or naturally present in the structure, such as sulfur or metal ions. In particular, sulfur seems to be an attractive candidate for phasing, because most proteins contain a considerable number of S atoms. However, the K-absorption edge of sulfur is around 5.1 Å wavelength (2.4 keV), which is far from the optimal wavelength of most MX-beamlines at synchrotrons. Therefore, phasing experiments have to be performed further away from the absorption edge, which results in weaker anomalous signal. This explains why S-SAD was not commonly used for a long time, although its feasibility was illustrated by the ground-breaking study by Hendrickson and Teeter [1]. Recent developments in instrumentation, software and methodology made it possible to measure intensities more accurately, and, as a consequence, S-SAD has lately obtained more and more attention [2]. The beamline BL-1A at Photon factory (KEK, Japan) is designed to take full advantage of a long wavelength X-ray beam at around 3 Å to further enhance anomalous signals. We performed S-SAD experiments at BL-1A using two different wavelengths (1.9 Å and 2.7 Å) and compared their phasing capabilities. This methodological study was performed with ferredoxin reductase crystals of various sizes. In order to guarantee statistical validity and to exclude the influence of a particular sample, we repeated the comparison with several crystals. The novelty in the approach consists in using very long wavelengths (2.7 Å), not fully exploited in the literature so far. According to our study, the 2.7 Å wavelength shows - despite strong absorption effects of the diffracted X-rays - more successful phasing results than at 1.9 Å.

[1] *W. A. Hendrickson, M. M. Teeter, Nature, 1981, 290, 107-113,* ***[2]*** *Q. Liu, T. Dahmane, Z. Zhang, et al, Science, 2012, 336, 1033-1037*

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