

Efficiency of Light Atoms on the Low Energy SAD Phasing

Yusuke Yamada^a, Tadashi Satoh^a, Kentaro Ihara^a, Noriyuki Igarashi^a, Naohiro Matsugaki^a, Nobuhisa Watanabe^b, Mamoru Suzuki^c, Soichi Wakatsuki^a, ^a*Struct. Biol. Res. Cent., Photon Factory, KEK, Japan.* ^b*Grad. Sch. Sci., Hokkaido Univ., Japan.* ^c*Inst. Prot. Res., Osaka Univ., Japan.* E-mail: yusuke.yamada@kek.jp

Recent advancements in the X-ray data-acquisition techniques and phasing algorithms have enabled structure determination using weak anomalous signals from light elements such as sulfur that are naturally present in most proteins. This is rapidly becoming a useful technique for high-throughput protein crystallography because it does not require preparation of heavy atom derivatives. Photon Factory is building a new insertion device beamline BL-17 with emphasis on diffraction experiments with microcrystals and low X-ray energy phasing (around 6 keV) [1]. To establish a standard experimental protocol of the low energy SAD, we carried out diffraction experiments on two lectins [2] and a small GTPase with low energy X-ray beams. In the case of the lectins, it was found that the number of potassium ions in the crystal is critical for the phasing. The crystal structure containing two potassium ions were solved successfully, but crystals with only one potassium ion were not. In the case of the small GTPase, phasing was successful despite the fact that it contains fewer sulfur atoms than the proteins whose structures have been solved by the low energy SAD so far. This is because the phosphates of GDP and the calcium ion bound to the GDP contributed significantly to the anomalous signal. This suggests that the low energy SAD is a successful method especially for nucleotide binding proteins.

[1] Igarashi N., et al., *IUCr2005*, Florence. [2] Satoh T., et al., *IUCr2005*, Florence.

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