SAD Phasing at Bijvoet Ratio below 0.6%

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SAD method is getting more and more important in high-throughput determination of protein structures. An important factor affecting SAD phasing is the Bijvoet ratio $\langle|\Delta F|\rangle/\langle F\rangle$. This makes sulfur-SAD data a challenge in diffraction phasing. B.C. Wang [1] has demonstrated that the error-free sulfur-SAD data of Rhe with Bijvoet ratio at 0.6% can be successfully phased by the ISAS procedure. Ramagopal *et al.* [2] reported the test on phasing three sets of experimental sulfur-SAD data, glucose isomerase at λ=1.54Å, xylanase at λ=1.74Å and xylanase at λ=1.49Å. Bijvoet ratios are respectively 0.68%, 0.69% and 0.55%. In their test, SAD phasing was successful for the first two data sets but failed with the third one. Here we report the successful phasing of the xylanase SAD data at λ=1.49Å kindly supplied by Dr. Z. Dauter, Brookhaven National Laboratory, USA. *SHELXD* and *SOLVE* were used to locate and refine the sulfur atoms. *OASIS-2004* was used for the iterative SAD phasing, which incorporates dynamically known structure fragment(s). *DM* was used for density modification. *RESOLVE-BUILD* and *ARP/wARP* were used for automatic model building. The result is a structure model from *ARP/wARP* containing 300 of the total 303 residues.

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[1] Wang B.-C. *Methods Enzymol.* **,** 1985, **115**, 90-112. [2] Ramagopal U. A., Dauter M., Dauter Z., *Acta Cryst.*, 2003, D**59**, 1020-1027.

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