

Direct Use of SAD Phase Information in Automated Model Building and Refinement

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The incorporation of prior phase information in a maximum likelihood formalism has been shown to strengthen model refinement. However, the currently available likelihood refinement target using prior phase information has shortcomings: the refinement target considers experimental phase information indirectly and statically in the form of Hendrickson-Lattman coefficients. Furthermore, the current refinement target implicitly assumes that the prior phase information is independent from the calculated model structure factor.

We have derived a multivariate likelihood function that overcomes these shortcomings and directly incorporates experimental phase information from a single-wavelength anomalous diffraction (SAD) experiment allowing for the simultaneous refinement of heavy atom and model parameters [1]. We have implemented this SAD function in the refinement program REFMAC5 [2]. The SAD function has been tested on many different real test cases yielding consistently better results than currently available functions. In some cases, the automated model building program ARP/wARP [3] can only successfully build a model when using the SAD function.

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