

powerful combined approach to model rebuilding. It is available in the Crystallography and NMR System (CNS) v1.3, and will also be available in phenix.refine in the near future.

The Phenix software (including phenix.mr_rosetta and phenix.morph_model) is available at <http://www.phenix-online.org> and Rosetta is available at <http://depts.washington.edu/uwc4c/express-licenses/assets/rosetta>.

- [1] DiMaio, et al., Nature 473, 540-543 (2011).
 [2] Brunger, et al., Acta Cryst D68, 391-403 (2012).

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MS4-02 Classical-style MAD phasing with wavelength interleaving and kappa goniometry on PROXIMA-1.

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In the early days of the MAD method, Hendrickson et al. (see e.g. [1]) used carefully designed protocols to maximise the signal-to-noise (S/N) ratio of anomalous and dispersive signals. Optimal anomalous S/N was achieved by re-orienting crystals on a multi-axis goniometer to record Bijvoet pairs on the same image, or by the interleaving of thin wedges (typically, 5 to 10 degrees) of data collected 180 degrees apart in rotation angle (“inverse-beam” method). High-S/N dispersive differences were obtained by similarly interleaving thin wedges of data at inflection-point and remote wavelengths. The special accuracy of these phasing differences was then exploited via the MADSYS software suite [2]. The advent of third-generation synchrotron sources and of CCD detectors created strong pressure towards data collection strategies that would be devoid of the complications of inverse-beam and wavelength-interleaving protocols, after it was shown that simpler strategies involving the collection of full datasets, for one wavelength at a time, around a single axis, were capable of yielding MAD-phased structures in remarkably short times [3]. From that point on, although many beamline GUIs still offered their users options to program inverse-beam and/or wavelength-interleaved experiments, these protocols rapidly fell into disuse except in the hands of a few devotees. We have revisited the original complex protocols with modern approaches to data processing, substructure solution and phasing (in particular the Bayesian approach to phasing implemented in SHARP [4]) and assessed the gains in phasing power provided by these protocols over the conventional ones. Our studies have been performed mostly on structures phased experimentally by anomalous scattering effects at the Tantalum L-III edge. Besides presenting our specific results, we will discuss prospects for implementing these protocols and the associated processing and phasing procedures in the form of integrated workflows suitable for the modern context of high-speed beamline operation and requiring little or no expertise from the users.

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