

MAD phasing on the SBC-CAT 19-ID undulator beamline at the APS

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With the availability of the third-generation synchrotrons, the multiple wavelength anomalous dispersion (MAD) technique is rapidly becoming a method of choice for initial phasing in macromolecular crystallography. Undulators (which produce high-flux, high-brilliance x-ray beams at these synchrotrons) have not been previously tested extensively for MAD phasing. Hence, the success of this method was a major criterion for the commissioning of the 19-ID undulator beamline of Structural Biology Center (SBC) at Advanced Photon Source (APS).

To date, wide variety of elements have been used as anomalous scatterers, with K and L₃ absorption edges in the energy range from 7.1 keV to 17.16 keV, utilizing undulator, first (fundamental), and third harmonic radiation. Typically, the fluorescence scans are taken from the macromolecular crystal, increasing the monochromator energy by small steps. The choice of wavelengths can be determined visually from the scans or from the plots of f' and f'' based on the Kromers-Libberman transformations. Then, 3–5 wavelength MAD data is usually collected from a fresh crystal. Thus far, eight successful MAD experiments have been carried out by the SBC staff; more than 20 experiments have been conducted by the user groups participating in the commissioning of the beamline. Various experimental configurations have been used, such as mirror plane and inverse beam geometry, data collection in the small rotational wedges or in one swipe for each wavelength, etc. Crystallographic statistics of these MAD experiments, along with the details of representative examples have been evaluated.