Poster Presentation

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Big Methods for Small Molecules

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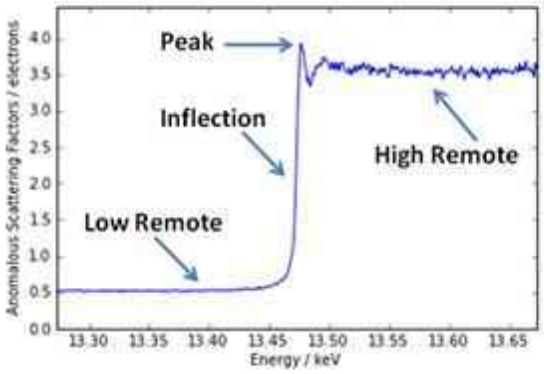
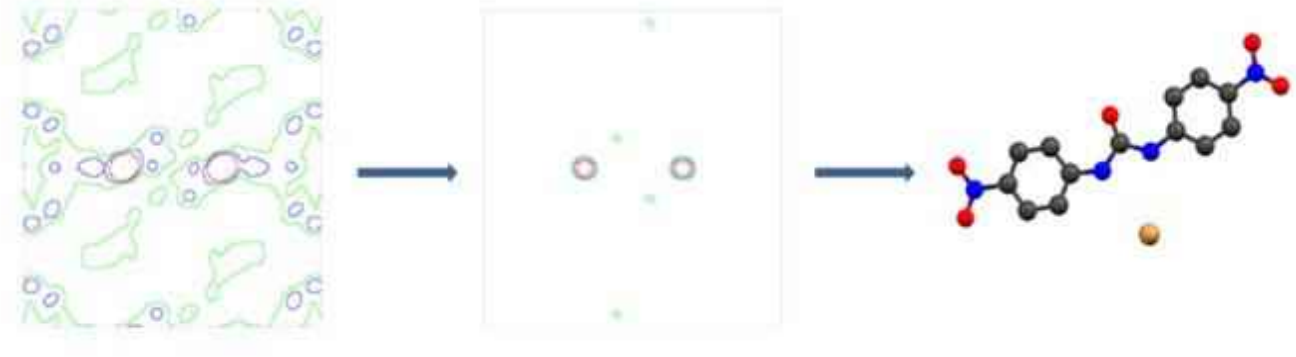
Since the early 70's, multiple wavelength experiments have been used to determine phases of proteins containing anomalous scatterers. The small molecule single crystal beamline, I19,[1] at Diamond Light Source, is designed to carry out single crystal anomalous dispersion studies using tunable wavelength. These experiments can differentiate between oxidation states; discriminate between atoms with near-identical X-ray scattering factors; and solve the phase problem for very low resolution X-ray data. We describe the application of MAD phasing (Karle and Hendrickson [2]) to determine the structure of large 'small molecules' where only low-resolution data is available. Initial studies were carried out on a known, (well diffracting) centrosymmetric bromide containing compound. The wavelength dependence of the anomalous signal from the bromide was calculated from fluorescence absorption data in DetOx.[3] Datasets were then collected at 4 wavelengths chosen to maximize differences in the anomalous signal. Using the MAD phasing equations we obtained estimates for the anomalous scattering contribution from all atoms in the structure and a phase difference between that and the normal scattering component. This allowed us to reduce noise in the Patterson map and locate only the heavy atom scatterers. We then use phase estimates from the heavy atom substructure to locate the rest of the atoms. Initial proof of concept experiments will now be extended to larger structures where data is not of sufficient resolution to be solved by direct methods alone.

[1] *H. Nowell et. al., J. Sync. Rad. 2012, 19, 435-441,* ***[2]*** *J. Karle, Int. J. Quant. Chem.: Quantum Biology Symposium 7, 1980, 357-367; W Hendrickson, Trans. ACA, 1985. 21: p. 11-21,* ***[3]*** *K. Sutton et. al., J. Sync. Rad. 2013, 20(1), 200-204*





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