Multi-component Analysis of Raw Diffraction Data

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Computational methods in macromolecular crystallography are pursued to enable structure solution of the most challenging molecular targets, where crystals inherently have low scattering power.

For such molecules, an optimal modeling of measured intensity is essential to extract and describe phasing signals. However, this analysis is not straightforward in the experiments pushing the limits, where phasing signal is correlated with non-isomorphism or radiation induced changes. Alternative solutions, like correcting for radiation damage with high-redundancy data that reduce the correlation, are not possible with heavy exposures limiting the crystal lifetime. Without the high-redundancy data, the current approaches to deal with radiation-induced changes are numerically unstable.

A statistical description was developed and implemented to solve this problem, making it possible to both correct for and/or recover the phasing signal from radiation damage changes, even from data of limited redundancy. This approach creates a new framework for an analysis of signal-to-noise ratio in many areas of macromolecular crystallography. The results and their potential consequences will be presented.

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