

## Integration optimization, triage and analysis tools for serial crystallography

Artem Y. Lyubimov, Monarin Uervirojnangkoorn, Aina E. Cohen and Axel T. Brunger

Serial crystallography (SX), whereby still (zero-rotation) diffraction images are collected from multiple crystals at randomized orientations, is rapidly emerging as a useful tool for structural analysis of radiation-sensitive samples at microsecond (synchrotron) or femtosecond (XFELs) scale. As SX is rapidly becoming accessible to the broader crystallographic community, a need has developed for versatile, powerful, and user-friendly data processing software. The **i**ntegration **o**ptimization, **t**riage and **a**nalysis (*IOTA*) toolkit serves as a front-end for both *cctbx.xfel* or *DIALS*, with integration optimization tools available for the former and in development for the latter. Pairing the optimization tools in *IOTA* with the **p**ost-**r**efinement and **m**erging program *PRIME*, researchers can obtain interpretable merged datasets from very limited (< 1000) amounts of diffraction images, making this technique most suitable for projects where crystalline material is in limited supply. The rapid, easy-to-read graphical feedback allows users to make on-the-spot adjustments to experimental parameters, thus increasing the success of high-rate SX experiments.