

W0061

Software for Efficient Co-crystal Structure Determination. J. Badger, P. Collins, R. Rosenfeld, B. Smith, R. Atha, D.E. McRee, Molecular Images and ActiveSight, 4045 Sorrento Valley Blvd., San Diego CA 92121 USA.

Iterative drug design projects that include protein crystallographic data typically require that structure results are returned to synthetic chemists within weekly cycles. Similarly, the viability of crystallographic fragment-based lead discovery projects depends on being able to analyze 100's of data sets within a few weeks. ACTOR/FR-E systems provide the hardware for unattended repetitive data collection but automated software is required for structure determination.

To manage the raw data processing needs of high volume co-crystallography projects, we have developed *PyDInt* (Python Distributed Integration system). This client-server software system uses D*TREK as its processing engine and only requires a target list of image directories to automatically process multiple data sets in the expected space group. We have also developed a Python application (*BNG*) for automating structure solution from multiple data sets. *BNG* takes the integrated data and runs molecular replacement and refinement programs (CCP4) to solve each structure. *BNG* outputs include logs of the structure solution history and session files for the MIFit model-building program. These session files enable immediate viewing of each structure in the context of its electron density map.