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Automated Determination of Protein: Ligand Structures From Image Data. J. Badger, C. Hansen, J. Hendle, C. Kissinger, M. Parlee, S. Wasserman, SGX, 10505 Roselle St., San Diego, CA 92121.

SGX operates a data collection facility at the APS (SGX-CAT) that communicates directly with both an Oracle-based information management system and the crystallographic computing capabilities at SGX/San Diego. This infrastructure has provided a unique opportunity to develop a high throughput system that integrates our automated data collection/reduction processes with automated co-crystal structure determination software into a single operation.

The rapid solution of large numbers of co-crystals is required for *(i)* lead discovery via crystallographic fragment screening (FASTTM), and *(ii)* lead optimization in aid of ongoing drug development projects. Since a single drug development project might easily generate 10-20 usable data sets/day, automated procedures extending well beyond raw data processing are needed to avoid creating an overwhelming load of structure determination work. With our system, automated data processing and structure determination procedures are automatically triggered at the conclusion of data collection. The endpoint of these procedures, prior to any human intervention, is a refined model, including the optimal conformer of a density-fitted ligand, together with a set of electron density maps, density images of the active site and structure validation diagnostics.