

## W0149

**Automated Data Processing at SGX-CAT.** John Badger<sup>1</sup>, Jon Christopher<sup>2</sup>, Thomas S. Peat<sup>2</sup>, Stephen Wasserman<sup>1</sup>, <sup>1</sup>SGX Inc., 10505 Roselle St., San Diego, CA92121, USA, <sup>2</sup>OpenEye Scientific Software Inc., 101 N Acacia Ave., Solana Beach, CA 92075.

SGX runs a dedicated beam-line (SGX-CAT) at the APS, Chicago to provide x-ray data collection capabilities for internal drug discovery activities and partnered structure determination projects. SGX-CAT receives daily shipments of crystals from the laboratories at SGX in San Diego. To efficiently process the large numbers of data sets taken at the beam line and rapidly return the reduced data to the home laboratory requires the use of almost completely automated procedures.

A fully automated data processing system (AMAP) was developed at SGX to meet this need. This system incorporates MOSFLM for data indexing and integration and CCP4/SCALA and CCP4/TRUNCATE for merging and reduction to structure factor amplitudes. Experience with AMAP is that almost all data sets capable of yielding structural models can be reduced from frames to structure factor amplitudes with minimal human interaction. The main factors that have led to this level of success are the incorporation of robust multi-trial auto-indexing procedures capable of detecting and recovering from poor initial peak selections and, more generally, ongoing evaluation against a wide variety of new crystal data sets.