

**W0356**

**A High Throughput Pipeline for Protein-ligand Complex Crystal Structure Determination.** Jian Xu, Zeljko Dzakula, Dan Berard, Accelrys Inc., 9685 Scranton Road, San Diego, CA 92121, USA.

Discovery Studio HT-XPIPE is a fully automated software pipeline that aims to accelerate and streamline the structure determination process for protein-ligand complex. The pipeline consists of all the individual stages that are normally required for determination of a protein-ligand structure, i.e., molecular replacement, initial refinement, identification of ligand density, ligand placement, complex refinement, water placement and refinement, and map generation. The user can customize the protocols in the pipeline including which stages are executed. DS HT-XPIPE incorporates the XLIGAND algorithm (Oldfield, 2001) and CNX with common protocols used by industrial crystallographers. Both intermediate and final results are stored in a project knowledge management system and experiments can be retrieved and re-run at any time. We have validated the pipeline using a wide set of data from PDB and our collaborators with a significant success rate.

Oldfield, T.J. *Acta Cryst.* 2001, D57, 696-705

Herb Klei, AccelrysWorld 2003