

Remote Access Synchrotron: Small Molecule collection on Macro-instrument: **An Analysis of the software for integration.**

Dr. Richard J Staples

Michigan State University, Department of Chemistry, East Lansing MI 48824, USA,
staples@chemistry.msu.edu

We have been running small molecule crystal structures on the Life Science Collaborative Access beamline 21-ID-D at the Advanced Photon Source, Argonne National Laboratory for more than one year with limited success. The limit of the success appears to be with the integration and indexing of the data collected (HKL2000 and XDS). Indexing using the Macromolecular software is extremely challenging and often guess work. The use of standard small molecule packages (APEX3, HKL3000_SM, and CrysAlisPro) were used to determine which program might integrate the data to yield the best results. This poster will compare results of such analysis in hopes of creating discussion on potential changes or pitfalls that occur in collecting data in this manner.

This research used resources of the Advanced Photon Source, a U.S. Department of Energy (DOE) Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357. Use of the LS-CAT Sector 21 was supported by the Michigan Economic Development Corporation and the Michigan Technology Tri-Corridor (Grant 085P1000817). Use of Beam Line 21-ID-D.