a crystal of lower quality can be accepted if only a connectivity structure is needed but the requirements are more strict when a fully publishable result is required. The number of parameters considered in determining "rank" can be large. Algorithms may include the following parameters: resolution limits, $I/\sigma(I)$, spot sharpness, indexing quality, refinement quality, mosaicity, ice-ring detection, and others. The success of the experiment can be bolstered by the amount of information provided to the system, but a truly automatic system should be able to provide the necessary results with little or no human intervention. The ability to screen large numbers of crystals also allows tests for polymorphism, autoresolution of enantiomers, phase transformations, etc.

Keywords: robotics, automation algorithms, ranking

MS.10.3

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True walk-away automation in chemical crystallography

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The recent trend in the analytical instruments market towards compact benchtop systems spawned the development of fully automated low-cost X-ray diffractometers. This was made possible in part through advances in the analytical software, specifically new and improved algorithms and decision making expert systems. This paper presents an overview of the decision tree implemented in one such system and the individual steps involved in producing publication quality structures from single-crystals without user intervention. The design of the fully automated system is targeted primarily towards users who are not expert crystallographers. In addition to all decisions being made autonomously, this means keeping the user informed about the progression of the experiment in an easily comprehensible way. Equally important is to suggest remedies in case a problem is encountered that cannot be tackled in software, such as a poorly centered crystal, radiation induced crystal decay, or a temperature induced phase transition. The expert system proceeds through the following stages: quantify the crystal quality, determine the unit cell and the crystal symmetry, select a data collection strategy, acquire and reduce the diffraction data, scale the diffraction data, determine the space group, solve the phase problem, refine and validate the molecular structure, and finally generate a report. The results are provided as a Crystallographic Information File (CIF) and as a Hypertext Markup Language (HTML) report.

Keywords: automation, chemical crystallography, software

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Rapid synchrotron X-ray crystallography for drug discovery using the SGX-CAT beamline at the APS

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SGX Pharmaceuticals, Inc., a San Diego-based oncology drug discovery company, designed, built, and operates a protein crystallography beamline (SGX-CAT) at the Advanced Photon Source (APS). This insertion device beamline operates exclusively as a mail-in facility, providing high-throughput X-ray crystallographic data collection for SGX, its corporate partners, and APS General Users. Screening of crystal quality and diffraction data collection at SGX-CAT utilize a series of automated processes, including crystal screening and data collection, sample loop visualization/centering, removal of surface ice from the sample, crystal quality scoring, and diffraction data processing/reduction. For most samples, crystal quality is evaluated and diffraction data are recorded without human intervention. All operations are tracked using a custom database, which links beamline operations to those elsewhere in the company and provides real-time access to information from the beamline. Expert systems evaluate the contents of the database, determine the next experiments to be performed, and, via web-based displays, summarize results therefrom. With this high-throughput approach, SGX makes routine use of synchrotron-based crystallography for de novo structure determination and for its FAST fragment-based, structure-guided drug discovery platform. During 2005, 2006, and 2007, 9379, 9934, and 10895 crystals were automatically screened at SGX-CAT, respectively. The number of diffraction datasets recorded at SGX-CAT averaged in excess of 4000/annum during the same period. Rapid access to crystallographic data proved critical for discovery of SGX523, a potent, selective, and orally-bioavailable c-MET inhibitor now in Phase I clinical trials for treatment of cancer patients.

Keywords: drug discovery and design, data collection methods, protein kinases

MS.10.5

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The interdependence of wavelength, redundancy and dose on a sulfur sad experiment

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In the last decade popularity of sulfur SAD anomalous dispersion experiments spread rapidly among synchrotron users as a quick and streamlined way for solving phase problem in macromolecular crystallography. On beam line 10 at SRS (Daresbury, UK) data sets have been collected on HEWL at six wavelengths between 0.979 Å and 2.290 Å to evaluate the importance and the interdependence of experimental variables like Bijvoet ratio, wavelength, resolution limit, redundancy, and absorbed dose in the sample per image. All the crystals used for the experiments were of high quality, so that the results could be interpreted independently of that. A feature of these experiments was the use of the detector tilt capability of the beam line to preserve high diffraction resolution even at the long wavelengths we tested. Radiation damage was found to affect disulfide bridges after the crystals have been given a total dose 2.5 $\times$ 10^6 Gγ. However with such a total dose, for all the data sets, it was possible to find a strategy to collect data to determine the sulfurs sub-structure and produce good quality phases by choosing the optimum combination of wavelength, exposure time and redundancy. $<|\delta_{ano}|/\sigma_{ano}>$ bigger than 1.0 for all resolution shells was a necessary requirement for a successful sulfur SAD substructure location. This work expands the general vision of a single wavelength anomalous