s1.m2.o5 **A Fully Automated Diffraction System for the Small Molecule Laboratory.** Mark Light, Michael Hursthouse and Yang Li, *School of Chemistry, University of Southampton, Southampton, Hampshire, SO17 1BJ, UK. E-mail: light@soton.ac.uk*

Keywords: Automation; Robotics; Software

The advent of CCD detectors and bright lab X-ray sources has accelerated the diffraction experiment to a point where a small molecule data set can be collected in as little as a few minutes, or more routinely in a few hours. Thus, to fully utilise the instruments capability some level of automation is essential. In our lab in Southampton we have taken the approach of automating the entire process, from mounted crystal to refined structure. A pre-mounted sample from a rack of 24 is loaded onto a Kappa CCD diffractometer by a BruNo sample changing robot. Prescans are performed to asses the crystal diffraction quality and, if favourable, a unit cell is determined. Data collection is carried out using a calculated strategy based on the diffracting power of the crystal and the unit cell dimensions. Data reduction takes place as a parallel process and finally the structure is solved and refined. Key points in the development of the system included the automation of the diffraction experiment, intelligent decision making, integration of the diffractometer and sample changing robot, automation of structure solution and refinement, and development of a controlling GUI. The automation software is written in PYTHON and utilises the documented diffractometer control and data collection software modules of COLLECT [1]. This made possible the full integration of the system flow between the robot and diffractometer and substitution of all required user inputs. A user interface, X-Tray, has been written to initialise the experiment and set various global parameters. The structure solution and refinement program, SYSTEM-Y, is written in FORTRAN and is based on the SHELX [2] suite of programs.

[1] "Collect" data collection software, Nonius B.V., 1999.
[2] SHELX97, *Programs for Crystal Structure Analysis* (Release 97-2). G. M. Sheldrick, Institüt für Anorganische Chemie der Universität, Tammanstrasse 4, D-3400 Göttingen, Germany, 1998.

s1.m3.o1 **Statistical Phase Improvement Without a Solvent Boundary.** Kevin D Cowtan, *University of York, UK. E-mail: cowtan@ysbl.york.ac.uk*

Keywords: Density Modification; Likelihood; Protein

A new technique has been developed for phase improvement using prior knowledge concerning the electron density to construct updated posterior phase probability distributions[1]. This approach has been implemented in the 'pirate' phase improvement software, available in beta release from CCP4.

The new approach involves description each point in the current electron density map in terms of a position in a two-dimensional continuum which differentiates between electron sparse and dense regions and between ordered and disordered regions. A similar classification is performed for a simulated map for a known reference structure, which has been constructed to have similar scaling, resolution and noise levels as the unknown map. The features of the simulated map and the true map for the known structure and used to construct density probability distributions for features in that region of the classification continuum. These distributions are then applied to the unknown structure, and used to provide additional phase information, which may be combined with the existing phase probability distributions.

This approach avoids the problems inherent in existing methods when dealing with ordered solvent and disordered protein. It may also be applied to awkward problems, such as metalloproteins, by the appropriate choice of reference structures. Initial results suggest that the method is highly competitive with other work in the field.

[1] Cowtan K. (2000). *Acta Cryst.* **D56**, 1612-1621.