

## E0009

**Automation for Solving Protein Structures.** G. Winter, C.C. Ballard, P.J. Briggs, CCLRC Daresbury Lab., Warrington, UK.

This poster describes an initiative for the automation of part of the software pipeline for macromolecular structure determination via X-ray crystallography. This is a collaboration between e-HTPX<sup>[1]</sup> and CCP4<sup>[2]</sup> and builds on work done as part of the DNA project<sup>[3]</sup>.

Automation in this context means following the same procedures and making the same decisions as a “normal” user would, and covers the structure determination process from data collection to model building.

The effort aims to build on the existing computational units (programs, scripts & libraries) within the CCP4 suite to provide an environment for the development of automated procedures.

This includes wrapping existing programs to provide generic programming interfaces which can be accessed from scripting languages and a toolbox of utility functions for manipulating and analysing data. This toolbox will incorporate functionality already found in the suite and new functions where gaps have been identified.

As the analysis of program output (for example assessing data quality from statistics) is of critical importance in decision making, part of the project will focus on marking up program output in a machine readable form.

Expansion of the existing CCP4i database, which is being done as part of the BioXHit project (4), will be used to store and retrieve project and data history.

Ultimately the project will provide a programming framework which is modular and will enable rapid prototyping of automated procedures. Separate layers of knowledge will be provided, so that sophisticated expertise can be called upon when needed by sequential knowledge encoded for example in scripts.

The initiative will make use of open standards, and the resulting components will be made available to users and developers via CCP4.

[1] <http://www.e-htpx.ac.uk>

[2] <http://www.ccp4.ac.uk>

[3] <http://www.dna.ac.uk>

[4] <http://www.bioxhit.org>