

Poster Presentations

[MS04-P14] CCP4 6.4, the Next Step in the MX Software Development and Distribution.

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The CCP4 [1] modernisation program has been launched two years ago and is currently in progress. Installer for Windows and Setup Manager for Linux systems have been developed and substantially simplified the installation procedure. The Update Manager was distributed separately just after 6.3.0 release and its improved version was integrated in the release 6.4.0. More than twenty updates were provided between the two releases to make updated versions of CCP4 components and bug fixes readily available for users. In 6.4.0, the update mechanism was extended to ARP/wARP model building suite [2], which is integrated in CCP4 user interface and distributed by CCP4. Starting from 6.4.0, the molecular graphics program Coot [3] was fully integrated in the CCP4 suite and versions for all platforms including various flavours of Linux were made available. JHbuild, a new building mechanism, allows easy maintenance of source CCP4 installations; nightly builds help external developers track compilation issues. Together with the update mechanism, these tools ensure efficient development and maintenance of the suite, and quick delivery of new or updated programs to users.

Here we also present key programs and new components included in the release 6.4. Mosflm and its user GUI iMosflm are tools for integration of diffraction images. The data reduction step is presented by programs Pointless, Aimless and CTruncate. The entire data processing is automated in Xia2 pipeline. The phasing step is presented in CCP4 by several programs and pipelines. New methods of scoring potential

molecular replacement solution was implemented in Phaser and made it faster in simple cases and improved success rate for difficult cases. Tools for molecular replacement now include Ample, a new pipeline using ab-initio search models. Improvement in phase estimates was achieved in Crank pipeline by means of covariant analysis of all available phase sets. Several new components for model building and refinement were added. The new program Nautilus and Coot 0.7 provide automatic and graphical facilities, respectively, for polynucleotides building. The Ligand Builder working in conjunction with ProDRG is another new feature in Coot. ProSMART is a new program for structure alignment and generation of external restraints for refinement. It was included in the suite along with the corresponding options in Refmac task interface. The program Zanuda for space group validation extended validation facilities of the Suite. The set of new components also include Dimple, a pipeline for structure solution and difference map analysis for nearly isomorphous structures containing ligands. Graphical functionality was extended to include QtRView, a new result viewer, ViewHKL for displaying general information on X-ray data sets, and graphical interface for structure analysis program PISA.

[1] M. D. Winn *et al.* (2011). *Acta Cryst.* D67, 235-248.

[2] G. Langer *et al.* (2008). *Nat. Protoc.* 3, 1171-1179.

[3] P. Emsley *et al.* (2010). *Acta Cryst.* D66, 486-501.

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