WP 5.2: CCP4i Data Tracking in the PX Structure Determination Software Pipeline

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Introduction

A key part of the integrated technology platform being delivered by the BIOXHIT project is the development of automated structure determination software pipelines that cover the post-data collection stages of structure solution by protein X-ray crystallography (PX). These pipelines need to accurately record and track the data that they produce, both for their own operation and for final deposition of the determined structures.

BIOXHIT Workpackage 5.2 is principally concerned with developing a system for performing this data management in order to address the needs of ongoing to integrate the handler into CCP4i "def file" format. An SQLite backend is hidden within "client API" libraries. (So far Tcl implementation of the database from them.

The tracking database backend is based on the CCP4i "def file" format. An SQLite backend is also available which will be used for the proposed "knowledge database". Work is also ongoing to integrate the handler into CCP4i (the CCP4 graphical user interface).

Next steps

Over the next 12 months the aims are to:
• Make release 0.1 of dbCCP4i and the visualiser to users and developers
• Finish integrating dbCCP4i into CCP4i
• Work with users to identify improvements to the visualiser
• Work with developers to integrate dbCCP4i into their applications and pipelines
• Expand the tracking database, and develop and implement the "knowledge database"

Key considerations

• Implement a system for both manual and automated structure determination
• Allow multiple database back-ends
• Gather as much information from client programs as possible automatically
• Open architecture accommodating heterogenous software components

Availability

The initial version of the handler, database and visualiser will be available for release by the end of February 2007, and will be available at www.ccp4.ac.uk/projects/bioxhit_public/ along with other CCP4 BIOXHIT deliverables.

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See http://www.ccp4.ac.uk/projects/bioxhit.html for more information