

**LHSG-CT-2003-503420**

**BioXHIT**

**A European integrated project to provide a highly effective  
technology platform for Structural Genomics.**

**Life Sciences, Genomics and Biotechnology for Health**

**WP5.2: De 5.2.16** Extended visualiser capabilities to show data stored in the  
knowledge base schema

**Due date of deliverable: 31.12.2007**  
**Actual submission date: 30.06.2008**

**Start date of project: 1.1.2004**                      **Duration: 60 months**

**Organisation name of lead contractor for this deliverable: CCP4/STFC**  
Daresbury **Author: Peter Briggs**

## De 5.2.16 Extended visualiser capabilities to show data stored in the knowledge base schema

The demonstration knowledge base schema and implementation was delivered as part of D 5.2.8. Deliverable 5.2.16 provides a CCP4i task interface which can be accessed from the visualiser application “dbviewer” (D 5.2.7) in order to provide a way for the user to interact easily with the demonstration knowledge base.

### Description

Figure 1 shows an example of the task interface window when no SQLite crystallographic database is available.

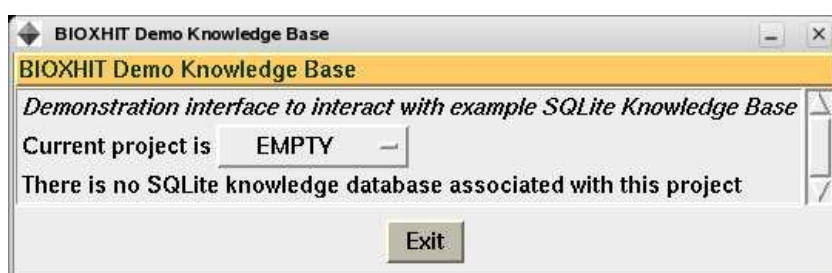


Figure 1: "bioxhit\_db" CCP4i task interface to the crystallographic database when no SQLite database is associated with the current project.

Figure 2 shows an example of the task interface window when an SQLite crystallographic database is available for the project.

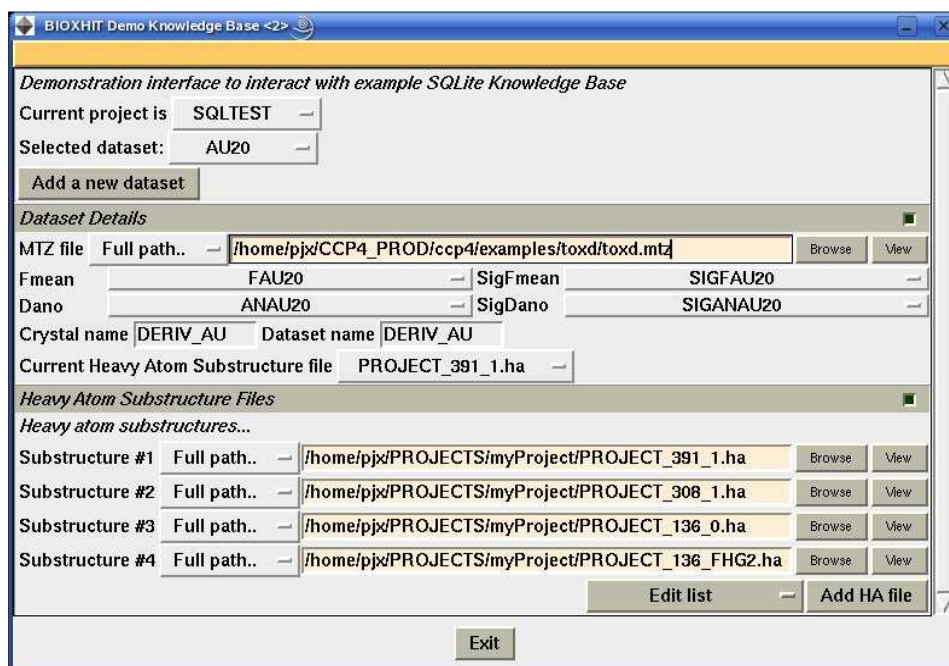


Figure 2: the "bioxhit\_db" task interface showing the content of an SQLite database attached to a CCP4i project.

The interface allows the user to browse the list of available datasets for the current project, and to define new datasets using the “Add a new dataset” button.

The data associated with the selected dataset (including associated MTZ file and data columns and none or more possible heavy atom substructures) are shown. New heavy atom substructure files can be associated with each dataset using the “Add HA file” button. Each dataset can also have a “current” heavy atom substructure file, which can be updated using a menu which lists all available files attached to that dataset.

(For more detail on the data and their relationships, see the documentation for deliverable D 5.2.8).

The interface can be accessed via the dbviewer (version 0.4.6 or later) from the option “Access demo SQLite db” under the “File” menu. Alternatively on UNIX platforms it is possible to launch the task interface using

```
> ccp4i -t bioxhit_db
```

at the command line prompt.

### **Availability**

The task interface files are included in dbccp4i 0.4.6, which is available from [http://www.ccp4.ac.uk/projects/bioxhit\\_public](http://www.ccp4.ac.uk/projects/bioxhit_public):

- de5.2.16\_dbccp4i-0.4.6.tar.gz
- de5.2.16\_dbccp4i-0.4.6.zip

Alternatively they can be obtained alone from the same location in the following files:

- de5.2.16\_bioxhit\_db\_interface.zip
- de5.2.16\_bioxhit\_db\_interface.tar.gz

in which case they must be manually installed by copying the files to the `.../ccp4i/tasks` subdirectory or folder of the current CCP4 installation on the system being used.

---

Peter Briggs, CCP4