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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 5.2.18 Implementation of a “smart logfile browser”

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Organisation name of lead contractor for this deliverable: CCP4/STFC
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De 5.2.18 Implementation of “smart logfile browser”

The “baubles” program has been developed by extending the “smartie” library previously developed for the starKey program (deliverable 5.1.4), to provide “smart logfile browser” functionality.

Baubles is a Python program which takes a logfile from a CCP4 program, SHELX run or CCP4i task, analyses it using the functions in the smartie module, and generates an “annotated” version of the information in the file which can be viewed in a HTML web browser.

The annotated logfile provides an interactive view of the file contents, with significant data from each step in the log promoted to prominent positions. Tables found in the file are displayed inline using CCP4’s “Jloggraph” Java applet, and different views of the output of individual programs is available (for example the “summary” view shows a limited amount of output based on tags in the logs, while a “full” view allows the entire content to be viewed).

An initial version of baubles was released to the community via the CCP4bb mailing list in late 2007 and has subsequently been incorporated into the CCP4 graphical user interface CCP4i for the CCP4 6.1 release.

A CCP4 newsletter article outlines the principle features of baubles:

- “Baubles: Making the World a Better Place for Logfile Viewing”, Peter Briggs and Kevin Cowtan, *CCP4 Newsletter on Protein Crystallography* **47** (Summer 2007)
<http://www.ccp4.ac.uk/newsletters/newsletter47/articles/baubles.html>

Baubles annotated logfiles are now automatically generated at the end of a CCP4i run, and can be accessed from both CCP4i and from the dbviewer visualisation tool (developed for deliverable 5.2.7). Both programs also give the option of generating an annotated logfile if one doesn’t already exist, or regenerating an existing file e.g. when it was produced by an earlier version of the Baubles software.

A version of the visualiser application with the extension to incorporate baubles can be found in the dbccp4i-0.4.6 files at http://www.ccp4.ac.uk/projects/bioxhit_public:

- de5.2.18_dbccp4i-0.4.6.tar.gz
- de5.2.18_dbccp4i-0.4.6.zip

A version of the baubles software can be found in the following supplementary file from the same location:

- de5.2.18_baubles-0.0.7.zip
- de5.2.18_baubles-0.0.7.tar.gz

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