chem-bla-ics

Christmas presents...

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Bioclipse, Userscript

Abstract

Our Christmas tree has not been decorated yet, but the presents are there: the BMC Bioinformatics paper on userscripts in life sciences, Bioclipse 1.2.0, a long list of blogs to rate, and a very nice overview from Wendy Warr on workflow environments, discussing and comparing different offerings like Pipeline Pilot, Taverna, and KNIME.

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Userscripts

The paper on userscripts describes how Greasemonkey scripts can be used to combine different information sources (DOI:10.1186/1471-2105-8-487). A trailer:

> ***Background***
> *The web has seen an explosion of chemistry and biology related resources in the last 15 years: thousands of scientific journals, databases, wikis, blogs and resources are available with a wide variety of types of information. There is a huge need to aggregate and organise this information. However, the sheer number of resources makes it unrealistic to link them all in a centralised manner. Instead, search engines to find information in those resources flourish, and formal languages like Resource Description Framework and Web Ontology Language are increasingly used to allow linking of resources. A recent development is the use of userscripts to change the appearance of web pages, by on-the-fly modification of the web content. This pens possibilities to aggregate information and computational results from different web resources into the web page of one of those resources.*

Peter et al. have been using this technology for CrystalEye too, but the paper was in a finalizing state when the userscript was announced , unfortunately.

Bioclipse 1.2.0

The other present is the Bioclipse 1.2.0 release, for which the QSAR feature is a great new feature addition (see my blog the other day with an overview of blog items detailing my participation in that feature). Ola et al. have done a great job with the plot functionality, which is very nice to scatter plot calculated descriptors. This release is likely going to be the last one in the Bioclipse 1 series, except for bug fix releases, so, this release also means I can start contributing to the Bioclipse 2 series. Recent items in the Bioclipse blog show a bright future, with project based resource handling, better scripting (R, ruby, JavaScript, BeanShell?).

BTW, we never have presents under the tree; we have Sinterklaas.