chem-bla-ics

Chemo::Blogs #2



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Abstract

Because no one picked up my Chemo::Blogs suggestion, I will now officially claim the blog series title. However, unlike the original Bio::Blogs series, I will not summarize interesting blogs, but just spam you with websites I recently marked as toblog on del.icio.us.

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Semantics and Text Mining

Evan Prodromou wrote about RDFa vs microformats. The latter are commonly used in enhancing blog semantics, and for example used by PostGenomic.com. While RDFa is more explicit, e.g. by using namespaced markup, we have to wait until XHTML2 to see it working. I do not think chemists are using tags a log yet, but let me propose the following microformats: 1/CH4/h1H4 and methane. Standard JavaScripts and CSS scripts will then do the rest. (Think: addressing newlines, auto googling-for-inchi, etc).

The reason why using microformats is interesting, is text mining, of various kinds. Whether it is setting up a molecule-article link database, or find hot molecules in blogspace, adding semantics will help tools like OSCAR3 to mine chemistry. Some time ago OTMI was proposed by Nature, and they now set up a dedicated web site to explain there view on text mining. Zack Rosen has a good idea why RDF Semantic web research isn't working.

Blogspace

There are a few new chemistry blogs I want to mention (and already added to Chemical blogspace): ChemBark, lirico which has an interesting chemoinformatics section, and The Curious Wavefunction. Worth reading indeed.

Pierre's YOKOFAKUN deserves a paragraph of his own. He recently blogged about bio2rdf which provides an RDF interface to biochemical knowledge via Life Science Identifiers (LSID), OBOEdit which is a Java-based ontology editor, and Amadea which is a Taverna- and KNIME-like tool for setting up UNIX pipes.

Online EMBL Symposium

A few EMBL PhD students are having the First Online EMBL PhD Symposium (catchy name, or ...;) Anyway, discussions are held on IRC, and it has a rather interesting Web2.0 session. All media is available on the website but requires registration right now. After the conference it will become open access to all. Jean-Claude contributed *The UsefulChem Project: Open Source Chemistry Research using Blogs and Wikis* to the Participants' Contributions section, and I had a poster on *Distributing molecular information over the Internet*, discussing CMLRSS, blog aggregators, CML and other things. The IRC session was logged and is available here.

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Literature

Finally, I want to mention three recent articles. First one is a recent write up by Bourne and Friedberg about *Ten Simple Rules for Selecting a Postdoctoral Position* (DOI: 10.1371/journal.pcbi. 0020121). With the end of my current postdoc position nearing, rather useful reading. Some time ago I blogged about a New open access journal Source Code for Biology and Medicine, and the journal is now up and running. Details can be read in the first editorial (DOI: 10.1186/1751-0473-1-1). The third article I would like to mention is *Scientific Software Development Is Not an Oxymoron* by Baxter (DOI: 10.1371/journal.pcbi.0020087), though I do not think it has new insights.

OK, this was a rather lengthy write up, but really needed to clean up my toblog section :)