

chem-bla-ics

ACS Chicago - Day #3

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chem-bla-ics

Tuesday promised to be an interesting day: an interesting 'Scientific Communication' CINF session in the morning and early afternoon. And, rather important to me, the [Blue Obelisk](#) dinner that night, just after another CINF party, where I chatted with a few others about options of a chemistry equivalent of the [Google Summer of Code](#); who knows what happens this summer, but start thinking about ideas on how to increase the web experience of chemistry journal web pages.

The GSoC

Now that I am talking about the GSoC, you might have realized that the [CDK](#) and [Bioclipse](#) did not make it as mentoring organization. While I had not seriously expected it, all the enthusiasm from within both projects including several interested students, I was a bit hoping for getting accepted with at least one of them. Meanwhile, [KDE](#), as expected, is approved, and actually contains two interesting chemistry project ideas too. One is about a 3D viewer/editor for which 7 students send Google a proposal, and the other about text mining of chemical content on the desktop, using [Strigi](#) (two students). Both topics have one excellent proposal, who do good in the ranking process. So, we might have some chemistry in the GSoC after all.

CINF

OK, back to the ACS meeting. Fahrenbach had a presentation on blogging too, but don't remember anything special about it. The [CHED](#) session was more elaborate on the whole topic, and since you are a reader of chemical blogs, you all know about this anyway :) Loney introduced [biotechexchange.org](#) which is building a social network around biotechnology. There are other community sites like this, and my major *problem* with these community building efforts is that they are too well defined. I much prefer to work in a more open environment where I can get in contact just as easily with people outside some specific topic. For the rest, the set of technologies is rather comprehensive.

Frenkel spoke about the imminent success of [ThermoML](#), which is now being supported by vendors and publishers, smoothing the whole dissemination of data supported by this format. It is basically what [CML](#) is attempting to achieve in molecular structure data. Day is having a good go at this with crystal data, and [his CrystalEye project](#) is supposed to be launched next month.

Hey, at Microsoft.com, had a rather manager level presentation, with very little value for someone into the field of 'data lifecycle and curation'. Rather disappointing on a scientific conference, or am I judging the ACS conference here? If the Microsoft is getting interested in chemoinformatics that might be a good thing, as long as they are OK with open source, open data and open standards. Who knows...

Rzepa had his presentation on the semantic wiki, which he, in similar form, [held at the German Chemoinformatics Conference too](#). New, I think, were the sheets on reasoning based on the content of the wiki. That was rather interesting. If we all would make our chemical knowledge

chem-bla-ics

available as [RDF](#), then this can become a big thing very soon. I skipped the presentation of Renear on ontologies, though it was actually one that I had hand picked; but I was simply too tired. Will watch the podcast when available. (BTW, are they making podcasts for the CINF session only, or for the whole ACS meeting?)

In the afternoon, I also followed just a subset of the presentations. The last one was by Scott [who spoke earlier on Second Life](#). I'm really interested in seeing where this is going, though I have my reservations if this is the right medium for mining chemical knowledge. Today she spoke on the social bookmarking and podcasting initiatives at Nature and [Nature Network](#). The latter is a social site, like like BioTechExchange, but not limited to one specific topic, and more interdisciplinary (my account at [NN](#)). I blogged [about some early issues](#) some time ago.

Jmol

Jabri showed us how [Jmol](#) is adding value to the [ACS Chemical Biology](#) journal. Yes, that's what she said. An opensource tool, developed by people on their free time, is making an ACS journal more valuable. I am very happy to hear that, and it strongly supports our view that opensource chemoinformatics is very important. Some more support from established organizations might be in order indeed!

Blue Obelisk

It has become a habit to organize [Blue Obelisk](#) dinner to talk about opensource, opendata, openscience, and the future. Actually, we secretly talk about talking over the world, but I can't say that. (Neither can I tell anything about our secret rituals. The protocol for becoming member of our society is quite simple though: be clear about your opinion that ODOSOS is the future.) Dinner was great, and it was great talking to several older and newer members of the movement. Cheers all! Oh, there also was some awards involved, but I hope Peter and Christoph will blog about that and post the pictures.