## chem-bla-ics

# **ACS Chicago - Day #1**



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I was happy to notice just a minute ago that the first blog items covering the ACS meeting are popping up: C&EN has set up a dedicated blog about the meeting, Nature's Sceptical Caterine wrote she has reached the meeting too, Richard wrote about the scent of bugs in wine (or so), and Kyle won't make it other than tomorrow. Additionally, Nature is running a coverage of the ACS meeting. On the reader side, Paul is hoping that Whitesides will be blogged about.

My first day at the conference was interesting. The huge facility makes navigation a bit problematic, and we seemed to make it a habit to explore the wrong end of the building before heading in the right direction. There are a lot of maps in the ACS On-Site Meeting Program, but a nice overview map is lacking. Anyway, I spent the morning session in the 'blog, wiki, and podcast session', and the afternoon in CINF session honoring Prof. Wiggins.

# **CHED**

Vogel was the first speaker in the CHED C Section morning session, and spoke about blogs and RSS feeds in general. Mitch' Yahoo Pipes hackup was mentioned in one of the talks in this morning session. Currano followed with a discussion on social bookmarking, and so did Pence who focussed on the function in education. Francl put chemical blogging in some perspective which led to a short discussion on the difference in idea between blogs and wiki's. Gelder and Picione spoke about podcasting as multimedia blogs. Scott represented recent work by Nature in exploring Second Life technologies, and mentioned the chemistry on their island, which happened to host a session of the First Online EMBL PhD Symposium last year. Bradley spoke about how he integrated blogs and wiki's into there practicals. The atmosphere of the session was relaxed and the discussion lively.

# **CINF**

The downside of all these parallel sessions is that it is bound to give clashes. It's apparently even supposed to, because the ACS website private schedule assistant is made to make you aware and resolve such clashes. So, while I had to skip the CINF morning session honoring Wiggens, I had to skip the CHED session on social networking continuing on the CHED morning session. For example, I has to miss the presentation by Rzepa on the semantic wiki (Henry, I hope to have made up for it, by plugging your work here:)

Murray-Rust was the first speaker of the CINF Section A afternoon session, and talked about mashups, text mining and other things done in Cambridge. He also mentioned recent Greasemonkey scripts using comments from and enhancing our chemical blogs, now described at the Blue Obelisk website. (Especially the Chemical blogspace enhanced TOC of chemistry journals is nice.) Wild spoke about integrating text mining and chemoinformatics tools, and showed a mockup of a 'by the way' system for PubChem, where a PubChem entry would be enhanced with 'BTW, did you know that these 7 articles mention this molecules, and that ... etc'. These things are going to happen this year. Heller held his usual talk on InChI and PubChem, though the content has slightly changed since the last two versions I've seen (not the message, though). Doman gave a practical example showing backing up earlier statements that too much

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information is lost in the publication process. Heritage showed Elsevier/MDL's view on the future of chemoinformatics, and accurately touched where it is currently failing. Amusingly, he pointed out that Elsevier, the publisher, would love to see more accurate QSAR/QSPAR/VS/etc models; ironically, it is, actually, for a large part caused by data not ending up in publications that predictive models are not as accurate as they could be. So, while looking at the chemoinformaticians/metricians, they should really be looking at themselves.

Some of these presentations mentioned directly or indirectly things I worked on. Thanx for doing that! Because I knew that there was funding for going to this meeting, only after the poster submission deadline was closed, I am not in the opportunity to present my work myself.

The evening is for the traditionally parties, time to eat, drink, network, make deals and try to convince others about the virtues of ODOSOS.

A last reminder: tomorrow afternoon at 13:00 at Laptop Lane in the exposition area is a meeting of chemical bloggers. Please join and chat IRL for once! :)