chem-bla-ics

SWAT4LS: wrapping up #1

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Abstract
It's already been five days since the SWAT4LS meeting (matching blog), and finally got around to writing up my personal summary. I very much enjoyed the Blue Obelisk dinner on Thursday evening with Nico, Duncan, and Miguel (the CDK one).

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The SWAT4LS was fun, interesting, perhaps to short, but very much appreciated! Thanx to all organizers! During the day various people tweeted the meeting, using the #swat4ls2009 hashtag (forwarded to a FriendFeed room), while Nico covered things in various blog posts which I'll link to below where appropriate. Summaries I have seen so far are from Nico and Duncan (again :), and the organizers.

The day kicked off with a presentation by Alan Ruttenberg (Nico's coverage). It nicely demonstrated where the semantic web for life sciences is going too. Particularly interesting was the integration of SPARQL with Jmol in ImmPort/JmolViz: it uses Jmol to visualize a PDB entry, while using SPARQL to retrieve atomic and residue annotation, using Jmol script (we have to thank another Miguel (the Jmol one) for taking the scripting and visualization capabilities to the next level in 2002). It always makes me proud to see one of the projects I have worked on to hit a prominent place in keynote talks at conferences :)

Alan also clarified that CC0 is not a license, but a statement about the *public domain* nature of data; there is nothing to accept, nothing to live up to. The important is, and I am sure most of my readers are well aware of that, is that it formalized the public domain concept by wrapping it in a full CC0 statement. My recommendation to all who want to make (chemical data) available as *public domain*, use the CC0; just because the CC0 works in any country, and it will make a lot of your users very happy. **If you cannot claim CC0 because you are not really owner (as I have seen done), do not claim the data to be public domain either then (which was done)!**

There was also note of the Amino Acid Ontology, which comes closer to our groups proteochemometrics work, but I have yet to look if this can be used for or linked protein descriptors. Also interesting is the idea behind RDFHerd , a project aiming to distribute RDF data sets as installable packages. If I understood correctly, only Virtuoso is yet supported, but this thing can fly, particularly, if these packages are easily converted into Debian packages.

More wrapping up will follow, but got other business to do first now.