chem-bla-ics

German Conference on Chemoinformatics 2006: Day 3

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Abstract
Just some short quites note about the third day (see day 1 and 2). Today's program of the German Conference on Chemoinformatics started with a presentation by Rzepa about his work on a semantic wiki (DOI:10.1021/ci060139e), which might be online here. (He recorded a podcast, but I have not seen it online yet.) I wish I could see the sources of those wiki pages, to see how that system integrates RDF, but at least Jmol is running fine.

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After the coffee break, Kuhn showed a coarse grained force field, approximating molecules by hacking them up in fragment of 3-10 heavy atoms. I guess, a bit like some small molecules force fields do for methyls. Fragments within a molecule are tied together by springs, and intra- and intermolecular force field parameters by running MD runs on fragment pairs. Varnek argued that QSPR for melting point prediction has reached a fundamental limited, with an RMSE of around 30 to 40 degrees Celsius, which makes it quite unreasonable to decide whether a compound with a predicted melting point of 40 degrees is solid or fluid at room temperature.

You have to forgive me for not reporting on the afternoon session; I was tied up talking with people at our booth, talking about the CDK, Taverna, Bioclipse, Jmol, other opensource chemoinformatics tools, and chemoinformatics in general. Very nice, but exhausting. I might advise the organization to set up a blog aggregator next year, though I am not sure whether there are others blogging about this conference.