chem-bla-ics

Back from the 1st GCC



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Abstract

OK, just back from the first German Chemoinformatics Conference, which I enjoyed very much. A rather interesting program, and lots of interesting posters too. You can read the programme online, and will not spend too many words on that (at least not now). But what I will do is point out some interesting posters here.

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One poster was on the Molecular Query Language (MQL) by Ewgenij Proschak from Frankfurt. You can read more on this in the latest CDK News as it is implemented for the CDK too. The opensource implementation is expected next year.

Another interesting poster was on the use of ontologies to connect chemistry and biology. This poster was by Juergen Harter from BioWisdom, a Cambridge, UK based company.

Marc Zimmermann had a poster on the chemical OCR variant, called chemical structure recognition (CSR). This process converts images, for example scanned from literature, into a connectivity table. Difficult task, indeed. This page contains some information about this project.

There were other interesting posters too, so will probably report on those later too. But do feel free to leave comments to this blog post, discussing other interesting posters.