

chem-bla-ics

German Conference on Chemoinformatics 2006: Day 1 and 2

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The [2nd German Conference on Chemoinformatics](#) started yesterday, with two chemoinformatics tutorials: one on industrial chemoinformatics (I saw this presentation before... not sure when), with a good overview on integrating different information sources; the second one was about opensource chemoinformatics by [Christoph Steinbeck](#) (being involved in opensource chemoinformatics for almost 10 years now!), which included a [Bioclipse](#) demo (by me) and a demo by Thomas Kuhn on the [CDK](#) based chemoinformatics plugin to [Taverna](#). Other opensource projects of the [Blue Obelisk](#) movement were mentioned and a few outside it too.

The conference is in honor of the life work by [Prof. Gasteiger](#), who gave an overview of chemoinformatics in his group, Germany and Europe. He stressed the need of education in chemoinformatics, like in [Obernai](#). He also highlighted that we, today, are still solving the same problem as 30 years ago. Which is true, which is why this channel is called [Chem-bla-ics](#), trying to solve that problem. When asked if opensource chemoinformatics from the start would have addressed this, he replied that he requires people to cooperatively do research with his group; opensource clearly cannot enforce that.

Day 2

Today's program had a number of interesting presentations (I, unfortunately, missed the first presentation, so have to visit that group soon now, to make up for that.) [Prof. Aires-de-Sousa](#) showed his work on MOLMAP for mapping metabolic networks ([KEGG](#) really, see my [earlier blog](#)), and showed, just as proof of principle, classification of organisms based on this.

J. Weisser talked about docking, still an obligatory topic. This work really showed two new approaches: the use of QM partial charges (the example showed an improvement in RMSD of a factor 10, not very statistical, but promising indeed); the second was the fact that water does not like to be in tight spots, because of reduced possibilities for hydrogen bonding. A concept common in understanding supramolecular phenomenon, but I have not seen this applied to docking before. But I am no expert in that field. M. Wagner showed work on using KEGG data to estimate likely metabolites, and the use in reducing effects of metabolic degradation. T. Schroeter introduced me to [gaussian processes](#), a new data modeling method. Quite embarrassing to get introduced to such, as being specialized in modeling methods for chemical problems.

The poster session was, as normally, really exhausting, talking to a lot of people. Having a booth at the exhibition on open-source cheminformatics added a nice twist to this. I therefore skipped the FIZ-award winner lectures, so I hope someone else will blog about those.

One last note: [Sun started releasing their Java platform under the GPL license](#). [Jim](#), seems that they [proved me wrong](#). The class library is still not GPL, but is expected to become licensed such somewhere in the first half of next year.