chem-bla-ics

German Conference on Chemoinformatics 2006: Day 1 and 2

Published November 13, 2006

Citation
Willighagen, E. (2006, November 13). German Conference on Chemoinformatics 2006: Day 1 and 2. *Chem-bla-ics*. https://doi.org/10.59350/txr0z-6j242

Keywords
Cheminf, Conference, Openscience, Bioclipse, Cdk

Abstract
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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 form 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

Todays 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 understand 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 opensource chemoinformatics 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.