chem-bla-ics

Taverna Workshop, Day 1 Update

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Abstract

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The second part of the morning session featured a presentation by Sirisha Gollapudi which spoke about mining biological graphs, such as protein-protein interaction networks and metabolic pathways. Patterns detection for nodes with only one edge, and cycles etc, using Taverna. An example data she worked on is the Palsson human metabolism (doi:10.1073/pnas.0610772104); she mentioned that this metabolite data set contains cocaine :) Neil Chue Hong finished with an introduction on the OMII-UK which is co-host of this meeting.

After lunch Mark Wilkinson introduced BioMoby, which we actually use in Wageningen already. I have tried to use jMoby to set up services based on the CDK, but failed sofar. Will talk with Mark on that. Next was my presentation, and I spoke about CDK-Taverna, Bioclipse and some peculiarities with chemoinformatics workflow, like the importance with intermediate interaction, the need to visualize the data and complex, information rich data. Bioclipse is seeing an integration of BioMoby and of Taverna.

After the coffee brake Marco Roos spoke about myExperiment and his work on text mining. I unfortunately missed this presentation, as I was meeting with people from the EBI who work on the MACiE database (see this blog item).

A discussion session afterwards introduced a few more Taverna uses, and encountered technical problems. Taverna2 is actually going to be quite interesting, with a data caching system between work processors, and a powerful scheme of annotation of processors, which will allow rating, finding local services, etc. More on that tomorrow. Dinner time now :)