

Poster presentation

Open Access

## Creating chemo- & bioinformatics workflows, further developments within the CDK-Taverna Project

Thomas Kuhn\*<sup>1,2</sup>, Achim Zielesny<sup>1</sup> and Christoph Steinbeck<sup>1</sup>

Address: <sup>1</sup>Cologne University Bioinformatics Center (CUBIC), Cologne, Germany and <sup>2</sup>University of Applied Sciences of Gelsenkirchen, Institute for Bioinformatics and Chemoinformatics, Recklinghausen, Germany

\* Corresponding author

from 3rd German Conference on Chemoinformatics  
Goslar, Germany. 11-13 November 2007

Published: 26 March 2008

Chemistry Central Journal 2008, 2(Suppl 1):P27 doi:10.1186/1752-153X-2-S1-P27

This abstract is available from: <http://www.journal.chemistrycentral.com/content/2/S1/P27>

© 2008 Kuhn et al.

The CDK-Taverna project aims at building an open-source pipelining solution through combination of different open-source projects such as Taverna [1], the Chemistry Development Kit (CDK) [2] and Bioclipse [3].

Pipelining or workflow tools allow for the Lego™-like, graphical assembly of I/O modules and algorithms into a complex workflow which can be easily deployed, modified and tested without the hassle of implementing it into a monolithic application.

Current developments in CDK-Taverna focus on a soft computing framework which allows a flexible use of different methods from, for example, the WEKA [4] library. Here, properties of chemical substances may be calculated using descriptors from the QSAR / QSPR package of the Chemistry Development Kit (CDK).

Further, a reaction enumeration algorithm for combinatorial chemistry based on existing methods of the Chemistry Development Kit is being developed. This algorithm allows for the enumeration of a reaction given that reactants and products are provided as "Markush" structures.

### References

1. Oinn T, Addis M, Ferris M, Marvin D, Senger M, Greenwood M, Carver T, Glover K, Pocock M, Wipat A, Li P: **Taverna: A tool for the composition and enactment of bioinformatics workflows.** *Bioinformatics* 2004, **20(17)**:3045-3054.
2. Steinbeck C, Han YQ, Kuhn S, Horlacher O, Luttmann E, Willighagen E: **The Chemistry Development Kit (CDK): An open-source Java library for chemo- and bioinformatics.** *J Chem Inf Comput Sci* 2003, **43**:493-500.

3. Spjuth O, Helmus T, Willighagen EL, Kuhn S, Eklund V, et al.: **An open rich client workbench for chemo- and bioinformatics.** . submitted.
4. Witten IH, Frank E: **Data-Mining Practical machine learning tools and techniques.** 2nd Edition edition. *Morgan Kaufmann, San Francisco*; 2005.
5. Hassan M, Brown RB, Varma-O'Brien , Rogers D: **Cheminformatics analysis and learning in a data pipelining environment.** *Molecular Diversity* 2006, **10**:283-299.