Journal of Cheminformatics

POSTER PRESENTATION Open Access

CDK-Taverna 2.0: migration and enhancements of an open-source pipelining solution

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From 6th German Conference on Chemoinformatics, GCC 2010
Goslar, Germany. 7-9 November 2010

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.

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) [2,3] or Bioclipse [4]. A first integrated version of CDK-Taverna was recently released to the public [5].

Current developments in CDK-Taverna refactor all workers as well as the complete setup on the basis of Taverna 2.2 and CDK 1.3.5 which themselves introduce major improvements to the whole platform. In addition the CDK is enhanced with specific functions and options for reaction enumeration based on a reaction template and corresponding reactant libraries. Reaction enumeration supports combinatorial chemistry approaches in the drug discovery process of the pharmaceutical industry. The CDK enhancements are applied and illustrated by corresponding CDK-Taverna-workflows.

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doi:10.1186/1758-2946-3-S1-P5
Cite this article as: Truszkowski *et al.*: CDK-Taverna 2.0: migration and enhancements of an open-source pipelining solution. *Journal of Cheminformatics* 2011 **3**(Suppl 1):P5.

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Published: 19 April 2011

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