Journal of Cheminformatics

POSTER PRESENTATION Open Access

Revisiting the dataflow principle for chemical information processing

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From 7th German Conference on Chemoinformatics: 25 CIC-Workshop
Goslar, Germany. 6-8 November 2011

Dataflow systems, such as Pipeline Pilot or KNIME have become important mainstream tools for data processing in chemistry. These established systems are all implemented relying on a data model emphasizing a strict row/column-centric data table view which does not facilitate interaction with individual chemistry objects, or non-uniform data contents.

Resuming our pioneering work which resulted in the implementation of the first dataflow system for chemistry [1], we present in this contribution a different, object-centric approach for the design of re-usable chemical information processing sequences. Our system is based on the metaphor of a factory floor, instead of opaque pipelines. Individual machining stations perform configurable processing steps on objects such as structures, reactions, datasets or tables. Objects are transported between these - or temporarily set on the factory floor for storage or inspection. The combination of this general concept with the extensive scripting functionality of the Cactvs Chemoinformatics toolkit results in a system with capabilities notably different and more flexible than standard pipelining systems.

Published: 1 May 2012

Reference

1. Ihlenfeldt , Takahashi , Abe : . *Proc. 28th Annual Hawaii International Conference on System Sciences* 1995, 227-236.

doi:10.1186/1758-2946-4-S1-P15
Cite this article as: Ihlenfeldt: Revisiting the dataflow principle for chemical information processing. *Journal of Cheminformatics* 2012 **4** (Suppl 1):P15.

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