

chem-bla-ics

# CiTO / CiteULike: publishing innovation

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## Keywords

Citeulike, Cito, Rdf

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**Citations (CiTO) [edit] [Show as list]**

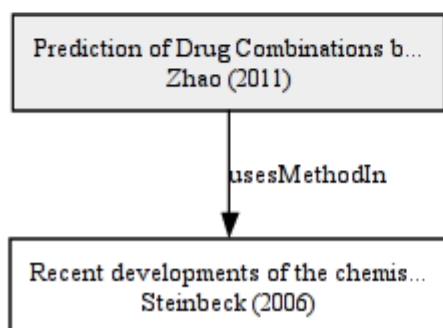
usesMethodIn

### Recent developments of the chemistry development kit (CDK) - an open-source java chemo- and bioinformatics.

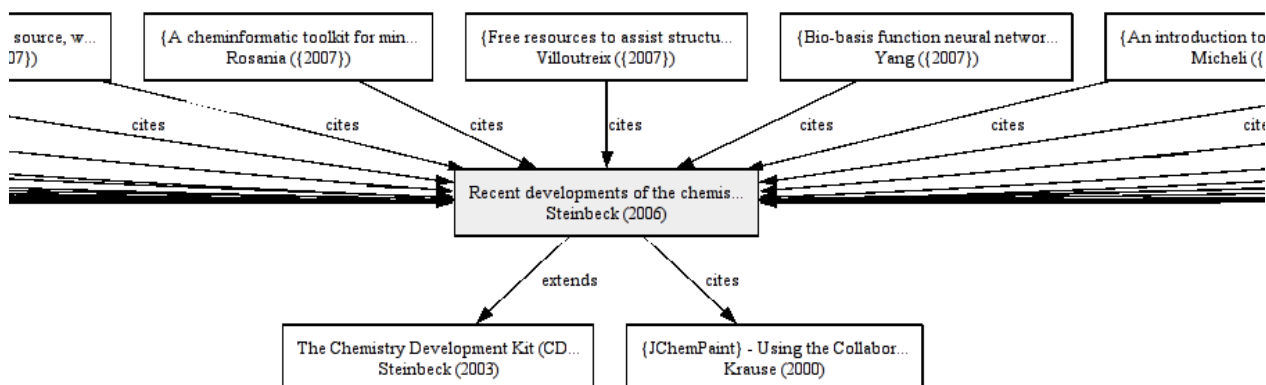
*Current pharmaceutical design*, Vol. 12, No. 17. (2006), pp. 2111-2120, [doi:10.2174/1381612067775852](https://doi.org/10.2174/1381612067775852) by [C. Steinbeck](#), [C. Hoppe](#), [S. Kuhn](#), [M. Floris](#), [R. Guha](#), [E. L. Willighagen](#) posted to [papers](#) [opensource](#) [java](#) [cheminformatics](#) by [egonw](#) keyed Steinbeck2006 on 2007-06-09 09: with 5 people and 1 group

#### Abstract

The Chemistry Development Kit (CDK) provides methods for common tasks in molecular informatics and 3D rendering of chemical structures, I/O routines, SMILES parsing and generation, ring searches checking, structure diagram generation, etc. Implemented in Java, it is used both for server-side core services, possibly equipped with a web interface, as well as for applications and client-side applets. This introduces the CDK's new QSAR capabilities and the recently introduced interface to statistical software.



Because CiteULike takes advantage of the [inverse function](#) of the CiTO predicates, they show up with the cited paper too, which is less suitable for the top-down flow graphics:



To make this advertorial a bit balanced, not all [my wishes](#) have been implemented yet, and the next up from my perspective should be Linked Data. There is some Linked Data embedded as RDFa, but the latter is not turning out to be the killer I had hoped, and regular RDF entry points should be used.

Each CiteULike entry (post) should get a unique [IRI](#) (or [URI](#)) and opening that link should give RDF about that post ([wish #10](#)). That's is [dereferencibility](#). The RDF can be, for example, in [BIBO](#)

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but there are many alternatives, and I have not been keeping up with which is the best (please leave a comment, if you have an opinion on that).

But I like where this is going! Thanx, CiteReallyLikeThis!