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CDK Literature #3

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Keywords

Cdk

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Third in a series summarizing literature citing one of the two CDK articles. See also [#1](#) and [#2](#) .

Reviews

Two reviews have recently appeared which cite the CDK. Ricard Stefani has written a review in Portuguese of the many NMR-based elucidation tools on computer-aided structure elucidation. The CDK is cited as a general chemoinformatics tool. It also cites [SENECA](#) which uses CDK's [structure generators](#).

Ricardo Stefani, Paulo Nascimento, Fernando Da Costa, Computer-aided structure elucidation of organic compounds: Recent advances, Quimica Nova, 2007, 30(5):1347-1356, 2007, doi:10.1590/S0100-40422007000500048

Dimitris Agrafiotis has written a overview of the current state of chemoinformatics, and the CDK is cited as tool to calculate molecular descriptors. ([Jörg](#) is co-author, and [he blogged about this article](#) too).

Dimitris Agrafiotis, Deepak Bandyopadhyay, Jörg Wegner, Herman van Vlijmen, Recent advances in chemoinformatics, J. Chem. Inf. Model., 2007, 47(4):1279-1293, doi:10.1021/ci700059g

1H proton coupling prediction

I wrote up a separate blog item on this the article [Janocchio: Jmol and CDK based 1H coupling constant prediction](#) written by David Evans at Eli Lilly.

David Evans, Michael Bodkin, Richard Baker, Gary Sharman, Janocchio - a Java applet for viewing 3D structures and calculating NMR couplings and NOEs, Magnetic Resonance in Chemistry, 2007, 45(7):595-600, doi:10.1002/mrc.2016

QSAR

Quantitative-structure-activity-relationship (QSAR) modeling projects are finding their way to the CDK too. Dmitry Konovalov cites the CDK as a free source (as in gratis) for descriptor calculation and touches the problem of reproducibility of descriptor calculations. Unfortunately, it does not discuss initiatives like the descriptor ontology as is [discussed in the second CDK article](#) , or the efforts discussed in the [Blue Obelisk](#) paper (doi:10.1021/ci050400b), such as the Blue Obelisk Data Repository which aim to improve this reproducibility.

Dmitry Konovalov, Danny Coomans, Eric Deconinck, Yvan Vander Heyden, Benchmarking of QSAR models for blood-brain barrier permeation, J. Chem. Inf. Model., 2007, 47(4):1648-1656, doi:10.1021/ci700100f

SOAP webservice

Xiao Dong and the rest of the [Indiana team](#) have set up SOAP webservices, among many wrapping CDK functionality, such as descriptor alculatoin, 2D similarity and fingerprint calculations, and 2D structure depiction. They also set up a service for [toxTree](#), which itself uses

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the CDK too.

Xiao Dong, Kevin Gilbert, Rajarshi Guha, Randy Heiland, Jungkee Kim, Marlon Pierce, Geoffrey Fox, David Wild, *Web service infrastructure for chemoinformatics*, *J. Chem. Inf. Model.*, 2007, 47(4):1303-1307, doi:[10.1021/ci6004349](https://doi.org/10.1021/ci6004349)