chem-bla-ics

CDK Literature #3

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Keywords
Cdk

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

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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 webservices

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

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