chem-bla-ics

CDK Literature #2

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Cdk

Abstract
Second in a series of articles summarizing articles that cite one of the main CDK articles for CDK News. The first CDK Literature was already half a year ago, so it was about time.

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Bioclipse

Nothing much I have to say about that. Just browse my blog and you'll see that it heavily uses CDK, JChemPaint and Jmol. See also the Bioclipse blog.
Ola Spjuth, Tobias Helmus, Egon Willighagen, Stefan Kuhn, Martin Eklund, Johannes Wagener, Peter Murray-Rust, Christoph Steinbeck, Jarl Wikberg, Bioclipse: an open source workbench for chemo- and bioinformatics, BMC Bioinformatics, 2007, 8(59), doi:10.1186/1471-2105-8-59

Proteomics in 2005/2006

Review article on proteomics which mentions the CDK and JChemPaint in the data analysis section, but it does not cite them. It does cite the Bioclipse article though.
Jeffrey Smith, Jean-Philippe Lambert, Fred Elisma, Daniel Figeys, Proteomics in 2005/2006: Developments, applications and challenges, Analytical Chemistry, 2007, 79(12):4325-4343, doi: 10.1021/ac070741j

Combinatorial Enumeration

Article by Andreas on SmiLib (BSD-like license) which is library for combinatorial enumeration using building blocks. The CDK is used for the addition of explicit hydrogens and the creation of MDL SD files. Andreas mentions in the article that the CDK's SMILES parser ignores stereo chemistry.
Andreas Schüller, Volker Hänke, Gisbert Schneider, SmiLib v2.0: A Java-Based Tool for Rapid Combinatorial Library Enumeration, QSAR & Combinatorial Science, 2007, 26(3):407-410, doi: 10.1002/qsar.200630101

Molecular Query Language

This article is also from the group of Gisbert. Ewgenij introduces an open standard SMARTS replacement, covered in CDK News in 2005 . There is an interface to the CDK, but the license of the reference implementation makes it impossible to distribute it with the CDK itself. This is rather unfortunate, because if it would have been possible, a number of implementations in the CDK, such as atom type perception, could be based on MQL. See also Jörgs blog on MQL.
Ewgenij Proschak, Jörg Wegner, Andreas Schüller, Gisbert Schneider, Uli Fechner, J. Chem. Inf. Model., 2007, 47(2):295-301, doi:10.1021/ci600305h

Golden Rules in Mass Spectroscopy

Tobias Kind wrote about structure elucidation using mass spectra, and discusses MolGen and CDK's `DeterministicStructureGenerator`, and mentions problems with both generators. He

has been in contact with the CDK and recently did extensive tests.
Tobias Kind and Oliver Fiehn, Seven Golden Rules for heuristic filtering of molecular formulas obtained by accurate mass spectrometry, BMC Bioinformatics, 2007, 8:105, doi: 10.1186/1471-2105-8-105