

Text mining for chemistry using OSCAR3

Egon Willighagen 

Published June 22, 2006

Citation

Willighagen, E. (2006). Text mining for chemistry using OSCAR3. In *chem-bla-ics*. chem-bla-ics. <https://doi.org/10.59350/wpk6m-d9y71>

Keywords

Oscar, Bioclipse, Textmining

Abstract

Peter Corbett from Peter Murray-Rust's group at the Unilever Cambridge Centre for Molecular Informatics visited Christoph Steinbeck's junior Research Group on Molecular Informatics at the CUBIC today, and spoke about the status of Oscar3, a chemistry text mining program with the Artistic License.

Copyright

Copyright © Egon Willighagen 2006. Distributed under the terms of the [Creative Commons Attribution 4.0 International License](#), which permits unrestricted use, distribution, and reproduction in any medium, provided the original author and source are credited.

chem-bla-ics

Peter Corbett from Peter Murray-Rust's group at the Unilever Cambridge Centre for Molecular Informatics visited Christoph Steinbeck's junior Research Group on Molecular Informatics at the CUBIC today, and spoke about the status of Oscar3, a chemistry text mining program with the Artistic License. Oscar3, the successor of version 1 and 2, can detect and extract molecular structures and experimental details from plain text articles, using a variety of text mining techniques.

The afternoon was spent on hacking Oscar3 into Bioclipse, with good success. It involved updating Oscar3 for the latest CDK and setting up a plugin infrastructure for Bioclipse. This plugin will allow mining (scientific) articles for chemical compounds and their properties from within Bioclipse. The outcome of today's hacking session was somewhat less ambitious and focused on the general infrastructure, and getting the OPSIN functionality in Oscar3 available as a wizard. OPSIN is a IUPAC name to structure tool and, amongst many other names, is able to recognize caffeine (InChI=1/C8H10N4O2/c1-10-4-9-6-5(10)7(13)12(3)8(14)11(6)2/h4H,1-3H3):

The screenshot displays the Bioclipse software interface. The main window shows a chemical structure of caffeine (1,3,7-trimethylpurine-2,6-dione) in the center. On the left, a BioResource Navigator pane lists various files, with '1,3,7-trimethylpurine-2,6-dione.cml' selected. Below the structure, a Properties pane shows details for the selected molecule:

Property	Value
CDK	
Atom count	14
Bond count	15
File format	Chemical Markup Language
Formula	C8H10N4O2
Mass	194.08035
Natural m.	194.19353
SMILES	O=C2c1c(ncn1C)N(C(=O)N2C)C
Strand count	
General	
Format	Chemical Markup Language
Name	1,3,7-trimethylpurine-2,6-dione.cml

A 'New Molecule from name' dialog box is open in the foreground, prompting the user to enter a molecule name. The name '1,3,7-trimethylpurine-2,6-dione' is entered in the text field, and the file type is set to 'cml'. The dialog box includes 'Back', 'Next', 'Finish', and 'Cancel' buttons.