

chem-bla-ics

Text mining for chemistry using OSCAR3

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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 application window. The main workspace shows the chemical structure of caffeine (1,3,7-trimethylpurine-2,6-dione). A 'New Molecule from name' dialog box is open, prompting the user to enter a name. The name '1,3,7-trimethylpurine-2,6-dione' is entered in the 'Enter name' field, and the file type is set to 'cml'. The background interface includes a BioResource Navigator on the left, a JChemPaint toolbar at the top, and a Properties panel at the bottom right showing various chemical and general properties 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)N2)C
Strand count	
General	
Format	Chemical Markup Language
Name	1,3,7-trimethylpurine-2,6-dione.cml