SMILES, CAS and InChI in blogs: Greasemonkey

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Abstract
As follow up on my Including SMILES, CML and InChI in blogs blog last week, I had a go at Greasemonkey. Some time ago already, Flags and Lollipops and Nodalpoint showed with two cool mashups (one Connotea/Postgenomic and one Pubmed/Postgenomic) that userscripts are rather useful in science too. I can very much recommend the PubMed/Postgenomic mashup, as PubMed has several organic chemistry journals indexed too!

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As follow up on my Including SMILES, CML and InChI in blogs blog last week, I had a go at Greasemonkey. Some time ago already, Flags and Lollipops and Nodalpoint showed with two cool mashups (one Connotea/Postgenomic and one Pubmed/Postgenomic) that userscripts are rather useful in science too. I can very much recommend the PubMed/Postgenomic mashup, as PubMed has several organic chemistry journals indexed too!

So, how does this relate to my blog of last week? Well, would it not be nice that if your blog uses the markup as suggested in that blog , that you automatically get links to PubChem and Google? That is now possible with a small GPL-ed Greasemonkey script called blogchemistry.user.js.

The Greasemonkey plugin requires Firefox to be installed. If ready, install the script by cli·cking this link earlier, and the Greasemonkey will ask you if you want to install the script. After, check the output for this RDFa markup content:

- a SMILES: [CCO]{.chem:smiles xmlns:chem="http://www.blueobelisk.org/chemistryblogs/"}
- a CAS registry number: [50-00-0]{.chem:casnumber xmlns:chem="http://www.blueobelisk.org/chemistryblogs/"}
- and an InChI: [InChI=1/CH4/h1H4]{.chem:inchi xmlns:chem="http://www.blueobelisk.org/chemistryblogs/"}

It should look like the output for this blog item:

Sunday, December 17, 2006

Counting stereoisomers from the molecular formula

We all know the combinatorial explosion when calculating the number of possible constitutional isomers (see wp:structural isomorphism) of a certain molecular formula. For example, C2H6 has only one constitutional isomer (ethane, InChI=1/C2H6/c1-2/h1-2H3 Google, PubChem), and C4H10 has only two. Especially, breaking symmetry by replacing one carbon by another element, or replacing a single by a double bond, increases the number sharply. For example, C7H16 has only nine constitutional isomers, while replacing two single bonds by two double bonds, creating C7H10, increases this number to 499! Then, replacing in the last formula, one carbon by an oxygen adds another few, totaling 747 isomers.

Now, C8H8NBr has at least **649 thousand** constitutional isomers, and I am quite interested in being able to know the number of isomers beforehand, without having to generate the structures itself (for example, using CDK's GENMDeterministicGenerator). InChI=1/C8H8BrN/c9-7-1-2-8-6(5-7)3-4-10-8/h1-2,5,10H,3-4H2 Google, PubChem is one of the isomers.

Note the superscript PubChem and Google links.