

Tagging Molecules: a mashup of Connotea and RDF



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Using the InChI and the new rdf.openmolecules.net website, it is now possible to tag molecules. And if you use [Connotea](#) for that, your tags will even show up on the rdf.openmolecules.net website. For example, at the time of writing, [methane](#) was tagged with *alkanes* and *gas*.

The trick I use, is that the rdf.openmolecules.net gives every molecule a unique HTTP [URL](#). This simply web2.0 approach offers an enormous amount of possibilities. The simplest application is that you can tag your molecules with a set label, such as *my-tomato-set*; after all, Connotea is account based. In this way, you can do open notebook QSAR studies (though the activities would still be missing).

The aforementioned example, however, give two classifications. *Methane is an alkane* and *Methane is a gas* (at room temperature). Not very well determined semantics, but it is web2.0, not the semantic web.

Interestingly, given some loosely defined semantics, use Connotea to link a molecule to a certain publication. For example, I can define *Estrone is cited in the article with PubMed ID 15659855* using the tag *pmid:15659855*. I'm sure using the DOI would work too, using the tag [doi:10.1107/S0108768104028344](#). I have not used these informal semantics in the rdf.openmolecules.net website yet, but if there is such interest, I can have such functionality hacked in minutes.

BTW, did anyone see [Gene Ontology](#) terms being used in social bookmarking services? For example, seeing a link to the PDB database with a tag *go:0008152*? Would be a bit cryptic, and, really, in this case rather minimalistic on information.

What's next?

Now comes the tedious task of converting the QSAR data sets I used in my PhD research with these tags. It's really something I wanted to do for a while now. Next on my [TODO](#) list is the Greasemonkey script that adds the tags from Connotea to PubChem.