

Chemical RDFa with Operator in the Firefox toolbar

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Abstract

December last year I proposed the use of microformats and RDFa for simple semantic markup of molecular information.

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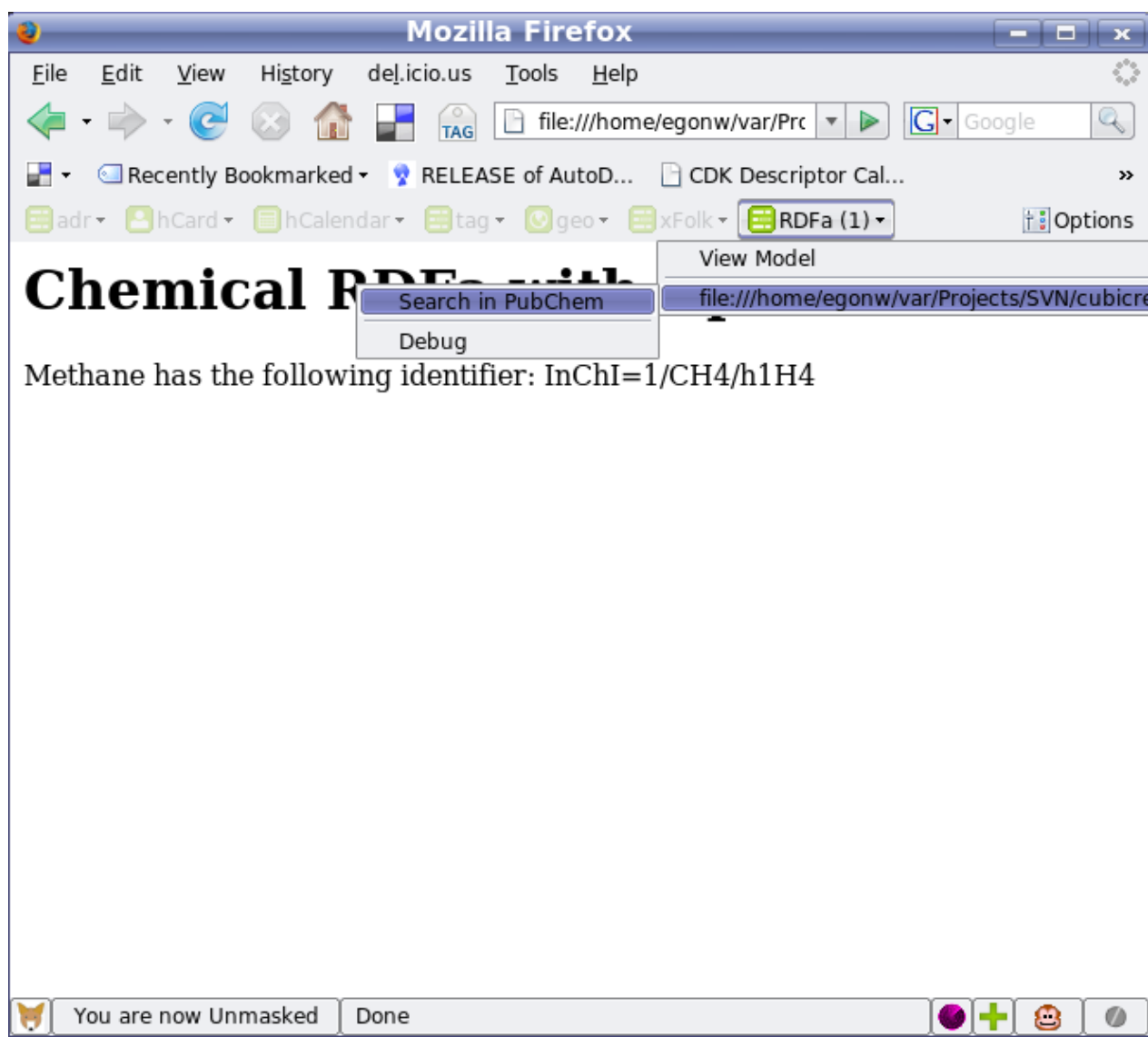
December last year I [proposed the use of microformats and RDFa](#) for simple semantic markup of molecular information. I linked that with the [InChI extension for the Postgenomic.com software](#) for [Chemical blogspace](#) and wrote these tools to work with the markup:

- [wrote a Greasemonkey script to automatically link to webservice](#) ,
- [explained how that script can be used on the server](#) , and
- [adapted a Greasemonkey script to show blog items related to molecules](#) .

All using the new semantic markup.

Of the two, I think RDFa has the best future. Then I [discovered Operator](#) , written by [Mike](#). While the Greasemonkey scripts already allow me to link to, for example, PubChem and eMolecules, the [Operator Firefox Addon](#) allowed me to open vCards incorporated in HTML pages directly to my address book client. Thus, I could open chemistry directly in [Bioclipse](#) too!

That was the idea, at least. I contacted Mike, and he asked me to wait until the first 0.8 releases, which he [announced earlier this month](#). This version allows user scripts to be written, which define how RDFa should be handled. And with his patience and help, this was the result:



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The HTML is almost [as explained before](#) , and looks like:

```
<html xmlns="http://www.w3.org/2002/06/xhtml12/">

<h1>Chemical RDFa with Operator</h1>

<div about="#chem_123" xmlns:chem="http://www.blueobelisk.org/chemistryblogs/">
  Methane has the following identifier: <span property="chem:inchi">InChI=1/CH4/h1H4</span>
</div>

</html>
```

It is important here to wrap the statement in a `<div>` element and to add the `@about` attribute to it, defining the Subject. Moreover, you need to use the `@property` attributes instead of `@class`. The content of this attribute defined the Predicate, and the content of the `` element is the Object, completing the RDF triple.

Operator detects these RDFa statements from the HTML, and creates a new menu item *Search in Pubchem* using this piece of code:

```
var pubchem_inchi = {
  description: "Search in PubChem",
  short: "PubChem",
  scope: {
    semantic: {
      "RDFa" : {
        property : "http://www.blueobelisk.org/chemistryblogs/inchi",
        defaultNS : "http://www.blueobelisk.org/chemistryblogs/"
      }
    }
  },
  doAction: function(semanticObject, semanticObjectType) {
    if (semanticObjectType == "RDFa") {
      return "http://www.ncbi.nlm.nih.gov/entrez/query.fcgi?CMD=search&DB=pccompound&term="
    }
  }
};
```

```
SemanticActions.add("pubchem_inchi", pubchem_inchi);
```

You can reproduce this by installing Operator 0.8a in Firefox, saving the script to a file in your home directory, and reading it via the Operator "Options" dialog. Make sure to also set the *Display Style* in the *General* tab of the dialog to *Data formats*. Only then will the RDFa magic kick in.

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Adding support for eMolecules, ChemSpider and whatever else we like is easy now. What I still need to explore (or ask Mike), is how I can trigger the *Open With/Save As* dialog of Firefox.