

Open Notebook Science Solubility: the SPARQL end point

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Keywords

Chemistry, Rdf, Sparql

Abstract

The Open Notebook Science Solubility challenge is an project crowd sourcing solubility of organic compounds in non-aqueous solvents.

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chem-bla-ics

The [Open Notebook Science Solubility](#) challenge is an project crowd sourcing solubility of organic compounds in non-aqueous solvents. I have been working on RDF-ing this data:

- [Solubility Data in Bioclipse #1](#)
- [Solubility Data in Bioclipse #2: handling RDF](#)
- [Solubility Data in Bioclipse #3: Finding ChEBI IDs](#)
- [Solubility Data in Bioclipse #4: Finding ChEBI IDs \(Again, but better\)](#)

And this resulted in a joint chapter in the nice [Beautiful Data](#) book.

What I had not done so far, is set up a SPARQL end point for this data, like I did for the [NMRShiftDB data](#) .

Now, however, a Virtuoso-powered [SPARQL end point](#) is available, and I hope this will seen get picked up by the other nodes on the ONS Solubility project. It is not a auto-synchronized link, though.

Possible advantages include that the client can perform any query and get these results in various formats, including JSON. For example, follow this link to get all [solutes in JSON format](#).

The matching SPARQL looks like:

```
prefix dc: <http://purl.org/dc/elements/1.1/>
prefix ons: <http://spreadsheet.google.com/plwwufp30hfhq0udnEmRD1aQ/onto#>

select distinct ?s ?title where {
  ?s a ons:Solute ;
    dc:title ?title .
}
```