

NMRShiftDB enters rdf.openmolecules.net

Egon Willighagen 

Published March 18, 2009

Citation

Willighagen, E. (n.d.). In *chem-bla-ics*. chem-bla-ics. <https://doi.org/10.59350/yk97t-8s820>

Keywords

Nmrshiftdb, Rdf, Opendata, Nmrshiftdb

Copyright

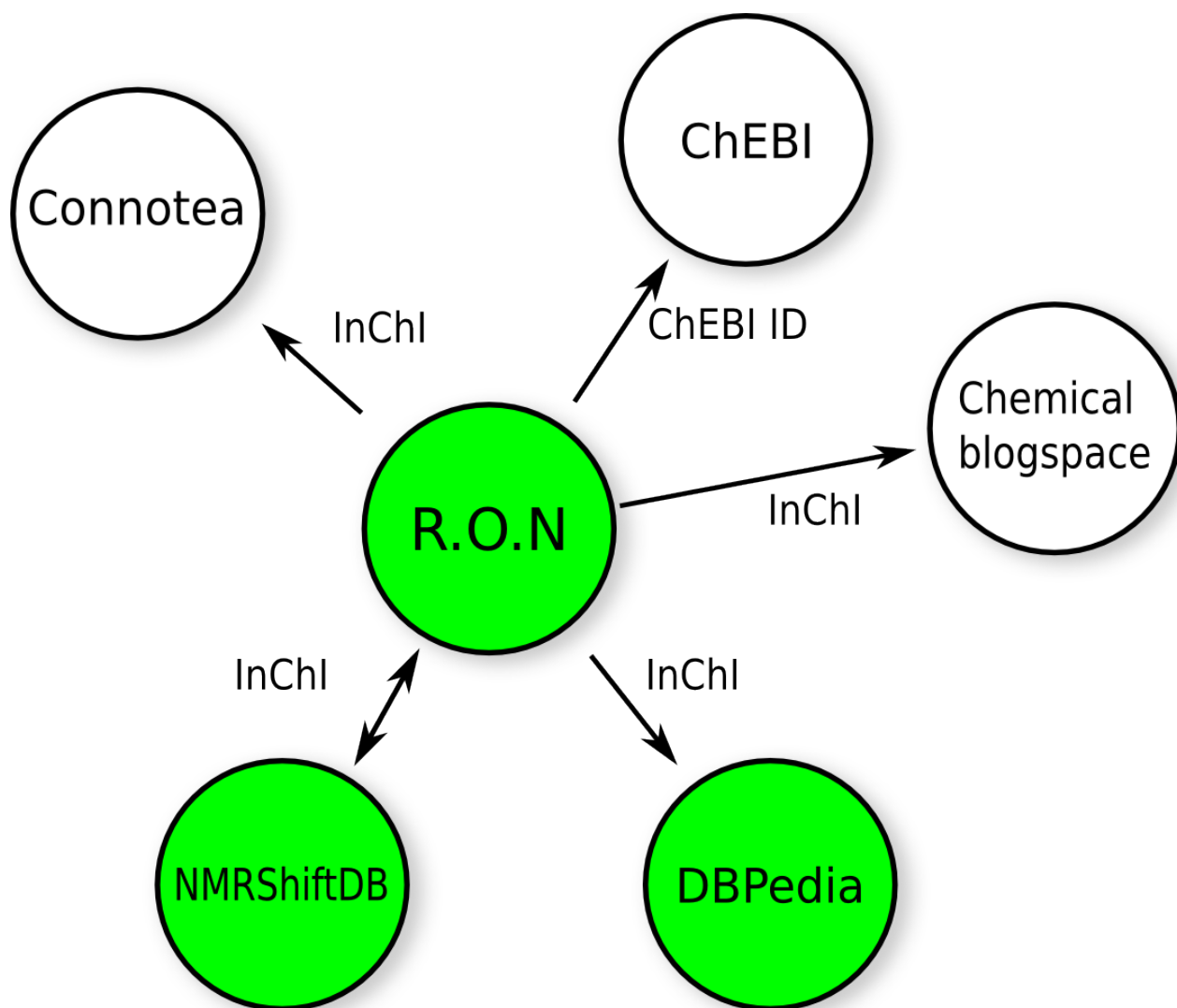
Copyright © Egon Willighagen 2009. Distributed under the terms of the [Creative Commons Attribution 4.0 International License](#), which permits unrestricted use, distribution, and reproduction in any medium, provided the original author and source are credited.

chem-bla-ics

This morning I finished setting up a [RDF](#) interface to the [NMRShiftDB](#) data (see [nmr:234](#)):

```
-<rdf:RDF>
  -<rdf:Description rdf:about=".">
    <nmr:moleculeId>234</nmr:moleculeId>
    <foaf:homepage rdf:resource="http://nm:
      /234"/>
    <chem:casnumber>62994-47-2</chem:cas
  -<chem:inchi>
    InChI=1/C15H22O3/c1-13(2)7-4-8-14(3)12(1
    </chem:inchi>
    <owl:sameAs rdf:resource="http://rdf.ope
      /h5,9-10,12,18H,4,6-8H2,1-3H3/t12-,14-,15+/r
    <chem:inchikey> QGMWDUUHVVLHNP-AE
    <nmr:hasSpectrum rdf:resource="#spec
    <dc:title>warburganal</dc:title>
  </rdf:Description>
  -<rdf:Description rdf:about="#spectrum4735">
    <nmr:spectrumId>4735</nmr:spectrumI
    <nmr:spectrumType>13C</nmr:spectru
  </rdf:Description>
</rdf:RDF>
```

And made links between the new frontend and rdf.openmolecules.net, make the *Linked Open Chemistry Data* (LOCD) network grow (naming following [Linked Open Drug Data](#)). In comparison with the previous depiction, I added arrows to indicate the direction of the linking. Green nodes still indicate sources with an RDF interface; therefore, the LOCD network consists really only of those green nodes:



The link with DBPedia is discussed in [DBPedia enters rdf.openmolecules.net](#). The [source code for the NMRShiftDB-RDF frontend](#) can be found at [GitHub](#).