

Open Chemical Data #1: NMRShiftDB

Egon Willighagen 

Published September 10, 2009

Citation

Willighagen, E. (2009). Open Chemical Data #1: NMRShiftDB. In *chem-bla-ics*. chem-bla-ics. <https://doi.org/10.59350/g3jct-gta96>

Keywords

Opendata, Friendfeed, Chemistry

Abstract

As I reported earlier, progress is only possible if you can modify and redistribute. This is why Open Data, Open Source, and Open Standards are so important to us Blue Obelisk members. For data, proper licensing makes these two requirements possible, but more importantly, make those rights explicit. Rich is running the nice Zusammen blog, but most of his entries are not Open Data.

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.

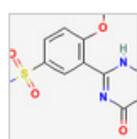
chem-bla-ics

As I reported earlier, progress is only possible if you can modify and redistribute. This is why Open Data, Open Source, and Open Standards are so important to us [Blue Obelisk](#) members. For data, [proper licensing](#) makes these two requirements possible, but more importantly, make those rights explicit. [Rich](#) is running the nice [Zusammen](#) blog, but most of his entries are **not** Open Data. Even larger chemistry data repositories can be vague and have seemingly contradicting statements.

One project which did it right, was the [NMRShiftDB](#). They were ahead of their time and did pick a proper Open license. By current standards not the best data license (the [GNU FDL](#)), but the best at the time. To push real Open Chemical Data a bit more, I will create a series much like Rich' series, but will make the restriction that the sources are clear about what rights they give users and that those include the rights to modify and redistribute the data without unreasonable restrictions.

I will not say much about the database itself, and even less now, as I think the *NMRShiftDB* is well-known amongst my readers.

Moreover, I have set up a [FriendFeed](#) room, [Open Chemical Data](#), where I will aggregate feeds of new molecules in these databases:



Open Chemical Data [edit settings](#)

1 subscriber

Feed of Open Chemical Data. Criterion: the data source must provide a (CML)RSS feed and the data must use an Open license (no public domain).

[add/edit](#)

Lists: [Home feed \(edit\)](#)

[✉ Invite](#) | [Email / IM ▾](#) | [Unsubscribe](#)

Add: [Photos](#) - [Files](#)

Post



InChI=1/H2O/h1H2 (INChI), XLYOFNOQVPJNP-UHFFFAOYSA-N (InChI Key), O (SMILES) - <http://www.ebi.ac.uk/nmrshif...>

Monday from NMRShiftDB - [Comment](#) - [Like](#) - [Share](#) - [Edit ▾](#)



1-[(2S,4R)-4-tert-butoxy-2-(methoxymethyl)pyrrolidin-1-yl]ethanone - <http://www.ebi.ac.uk/nmrshif...>

August 22 from NMRShiftDB - [Comment](#) - [Like](#) - [Share](#) - [Edit ▾](#)

1-[(2S,4R)-4-tert-butoxy-2-(methoxymethyl)pyrrolidin-1-yl]ethanone ([edit](#) | [delete](#))



(3-methyloxetan-3-yl)methyl (2Z)-3-iodoprop-2-enoate - <http://www.ebi.ac.uk/nmrshif...>

August 13 from NMRShiftDB - [Comment](#) - [Like](#) - [Share](#) - [Edit ▾](#)

Now, the only problem is, I need candidate for this series, and cannot actually think of a third entry (second being the [Open Notebook Science Solubility](#) data)... Want to help me out? Please let me know which chemical database is using a Open Data license.