

Where can I host my experimental data? Open Submission Chemistry Databases #1

Egon Willighagen 

Published February 5, 2009

Citation

Willighagen, E. (2009). Where can I host my experimental data? Open Submission Chemistry Databases #1. In *chem-bla-ics*. *chem-bla-ics*. <https://doi.org/10.59350/24q7a-eg105>

Keywords

Chemistry, Opendata

Abstract

Rich just posted an interesting read on Web-Centric Science, after a gauntlet thrown down by The Realm of Organic Synthesis (TROS).

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

Rich just posted an interesting read on [Web-Centric Science](#), after a [gauntlet thrown down by The Realm of Organic Synthesis](#) (TROS).

I agree that this still is a problem: where can (organic) chemists host their data? TROS hints at [Wikipedia](#), but an encyclopedia is not always the most suited place for cutting edge chemistry (article can easily be biased, contain (science) political views, etc...). I would suggest a blog would be a good start, and if proper markup would be used services like [Chemical blogspace](#) would automatically aggregate it.

However, something less volatile might be interesting. So, what we need is an overview of web databases where experimental chemistry data can be hosted. I'll start one, and annotate resources with license, on [delicious.com](#), using the tags [chemistry](#) [+web](#) [+database](#) [+open](#) [+submission](#), and regularly summarize things here.

In the below table, the last column indicated the most liberal license you can use to host your data:

database	data type	license
NMRShiftDB	NMR spectra	GNU FDL
ChemSpider	Structures, links to papers, spectra	open data
SORD	Organic Reactions	?

There are some obvious gaps here, if you consider a typical experimental section. What to do with an measure melting point, IR spectra, mass spectral information, and measured elemental composition.