NMRShiftDB RDF #3: Bio2RDF

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Published October 9, 2009

Citation

Willighagen, E. (2009). NMRShiftDB RDF #3: Bio2RDF. In *chem-bla-ics*. chem-bla-ics. https://doi.org/10.59350/rnjv0-tj350

Keywords

Nmrshiftdb, Rdf, Bio2rdf

Copyright

chem-bla-ics

My might have seen my efforts to convert the NMRShiftDB data into RDF:

- NMRShiftDB RDF #2: Some statistics
- NMRShiftDB RDF #1: Spectra by InChI
- NMRShiftDB enters rdf.openmolecules.net #2: SPARQL end point with Virtuoso

Peter Ansell has shortly after that copied the data into Bio2RDF, but I had not blogged about that yet. So, here goes. If you have not looked at Bio2RDF yet, this is a good time to do that. The structure of the exposed triples is not perfect, and I just realized I made a beginners mistake, to use a domain name in a namespace I have not control over (bad me). The Virtuoso6 faceted browser allows you to navigate the data in Bio2RDF by molecule (e.g. molecule 234):

warburganal at **Bio2RDF**

Search

Find intranamespace linksFind global links Links Namespace   Find links in namespace

http://bio2rdf.org/nmrshiftdb_molecule:234

Subject	Predicate	Object
http://bio2rdf.org/nmrshiftdb_molecule:234	http://purl.org/dc/elements/1.1/title	warburganal
	http://www.blueobelisk.org/chemistryblogs/casnumber	62994-47-2
	http://www.blueobelisk.org/chemistryblogs/inchi	InChI=1/C15H22O3/c1-13(2)7-4-8-14(3)12(13)6-5-11(9-16)15(14,18)10-17/h5,9-10,12,18H,4,6-8H2,1-3H3/t12-,14-,15+/m0/s1
	http://www.blueobelisk.org/chemistryblogs/inchikey	QGMWDUUHVVLHNP-AEGPPILIBL
	http://www.nmrshiftdb.org/onto#hasSpectrum	http://bio2rdf.org/nmrshiftdb_spectrum:4735
	http://www.nmrshiftdb.org/onto#moleculeId	234
	http://www.w3.org/2002/07/owl#sameAs	http://bio2rdf.org/cas:62994-47-2
		http://bio2rdf.org/inchi:1/C15H22O3/c1-13(2)7-4-8-14(3)12(13)6-5-11(9-16)15(14,18)10-17/h5,9-10,12,18H,4,6-8H2,1-3H3/t12-,14-,15+/m0/s1
		http://pele.farmbio.uu.se/nmrshiftdb/?moleculeId=234 (External link)
	http://xmlns.com/foaf/0.1/homepage	http://nmrshiftdb.ice.mpg.de/portal/js_pane/P-Results/nmrshiftdbaction/showDetailsFromHome/molNumber/234 (External link)

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And by spectrum too (e.g. spectrum 4735):

(No title found) at **Bio2RDF**

Search

Find intranamespace linksFind global links Links Namespace   Find links in namespace

http://bio2rdf.org/nmrshiftdb_spectrum:4735

Subject	Predicate	Object
http://bio2rdf.org/nmrshiftdb_spectrum:4735	http://bio2rdf.org/ns/bio2rdf:linkedToFrom	http://bio2rdf.org/nmrshiftdb_molecule:234
	http://www.nmrshiftdb.org/onto#field	50
	http://www.nmrshiftdb.org/onto#solvent	Chloroform-D1 (CDCl3)
	http://www.nmrshiftdb.org/onto#spectrumId	4735
	http://www.nmrshiftdb.org/onto#spectrumType	13C
	http://www.nmrshiftdb.org/onto#temperature	298
	http://www.w3.org/2002/07/owl#sameAs	http://pele.farmbio.uu.se/nmrshiftdb/?spectrumId=4735 (External link)

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