

# Migrating pKa data from DrugMet to Wikidata

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## Keywords

Wikidata, Chemistry

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## chem-bla-ics

In 2010 [Samuel Lampa](#) and I started a pet project: collecting pK<sub>a</sub> data: he was working on RDF extension of MediaWiki and I like consuming RDF data. We started [DrugMet](#). When you read this post, this MediaWiki installation may already be down, which is why I am migrating the data to [Wikidata](#). Why? Because data curation takes effort, I like to play with Wikidata (see [this H2020 proposal](#) by [Daniel Mietchen et al.](#)), I like Open Data, and it still [much needed](#).

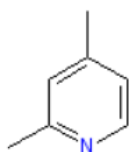
We opted for a page with the minimal amount of information. To maximize the speed at which we could add information. However, when it came to semantics, we tried to be as explicit as possible, and, e.g. use [the CHEMINF ontology](#). So, it collected:

1. InChIKey (used to show images)
2. the paper it was collected from (identified by a DOI)
3. the value, and where possible, the experimental error

A page typically looks something like this:

## 2,4-lutidine

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Facts about 2,4-lutidine ⓘ	
CHEMINF 000200	JYYNAJVZFGKDEQ-UHFFFAOYSA-N + 🔍
CHEMINF 000567	Q22266828 + 🔍
Equivalent URI	<a href="http://drugmet.rilspace.org/resource/2,4_lutidine">http://drugmet.rilspace.org/resource/2,4_lutidine</a> 🔗 + 🔍
HasPKaValue	An experimental pKa value from 10.1021/ed050p510 for 2,4-lutidine + 🔍
IsDiscussedBy	Paper with DOI 10.1021/ed050p510 + 🔍
Label	2,4-lutidine + 🔍
Original URI	<a href="http://drugmet.rilspace.org/resource/2,4_lutidine">http://drugmet.rilspace.org/resource/2,4_lutidine</a> 🔗 + 🔍
SubClassOf	CHEMINF 000000 + 🔍

While not used on all pages, at some point I even started using templates, and I used these two, for molecules and papers:

```
{{Molecule
|Name=
|InChIKey=
```

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```
|DOI=  
|Wikidata=  
}}
```

```
{{Paper  
|DOI=  
|Year=  
|Wikidata=  
}}
```

These templates, as well as the above screenshot, already contain a spoiler, but more about that later. Using MediaWiki functionality it was now easy to make lists, e.g. for all pK<sub>a</sub> data (more spoilers):

## All pKa values

Below is a list of all pKa values extracted from [All papers](#).

Page	Wikidata	Molecule	pKa	Error	InChIKey
<a href="#">2,4-lutidine</a>	<a href="#">Q22266828</a>	2,4-lutidine	6.46	0.20	JYYNAJVZFGKDEQ-UHFFFAOYSA-N
<a href="#">2,5-lutidine</a>	<a href="#">Q23636061</a>	2,5-lutidine	6.18	0.07	XWKFPIODWVPLX-UHFFFAOYSA-N
<a href="#">2,6-lutidine</a>	<a href="#">Q209284</a>	2,6-lutidine	6.67	0.04	OISVCGZHLKNMSJ-UHFFFAOYSA-N
<a href="#">3,4-lutidine</a>	<a href="#">Q23636064</a>	3,4-lutidine	6.28	0.21	NURQLCJSMXZBPC-UHFFFAOYSA-N
<a href="#">3,5-lutidine</a>	<a href="#">Q23636070</a>	3,5-lutidine	5.85	0.35	HWWYDZCSSYKIAD-UHFFFAOYSA-N
<a href="#">3-chloropyridine</a>	<a href="#">Q223069</a>	3-chloropyridine	4.09	0.11	PWRBCZZQRRPXAB-UHFFFAOYSA-N
<a href="#">4-bromopyridine</a>	<a href="#">Q229935</a>	4-bromopyridine	3.96	0.09	BSDGZUDFPKIYQG-UHFFFAOYSA-N
<a href="#">4-pyridinecarboxaldehyde</a>	<a href="#">Q23636732</a>	4-pyridinecarboxaldehyde	4.72	0.37	BGUWFUJQJCDRPTL-UHFFFAOYSA-N
<a href="#">Acetic acid</a>	<a href="#">Q47512</a>	acetic acid, Acetic acid			QTBSBXVTEAMEQO-UHFFFAOYSA-N
<a href="#">Acetoacetic acid</a>	<a href="#">Q409692</a>	Acetoacetic acid	3.58		WDJHALXBUFZDSR-UHFFFAOYSA-N
<a href="#">Acetylthiazolidine-4-carboxylic acid</a>	<a href="#">Q23636743</a>	acetylthiazolidine-4-carboxylic acid	2.96		JJEJMHHLICERIA-UHFFFAOYSA-N
<a href="#">Acrylic acid</a>	<a href="#">Q324628</a>	Acrylic acid	4.25		NIXOWILDQLNWCW-UHFFFAOYSA-N
<a href="#">Adipamic acid</a>	<a href="#">Q23637022</a>	Adipamic acid	4.63		NOIZJQMZRULFFO-UHFFFAOYSA-N
<a href="#">Alanine</a>	<a href="#">Q218642</a>	alanine	2.61		QNAYBMKLOCPYGG-UHFFFAOYSA-N

I find a database like this very important. It does not capture all the information it should be capturing, though, as is clear from [the proposal](#) some of use worked on a while back. However, this project got on hold; I don't have time for it anymore, and it is not core to our department enough to spend time on write grant proposals for it.

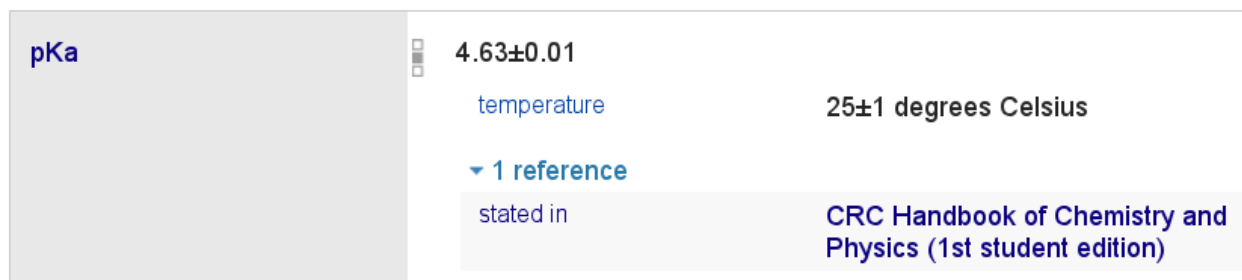
But I still do not want to get this data get lost. Wikidata is something I have started using, as it is a machine readable CCZero database with an increasing amount of scientific knowledge. More and more people are working on it, and you must absolutely [read this paper](#) about this very topic (by [a great team](#) you should track, anyway). I am using it myself as source of identifier mappings and more. So, migrating the previously collected data to Wikidata makes perfect sense to me:

1. if a compound is missing, I can easily [create a new one using Bioclipse](#)

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2. if a paper is missing, I can easily [create a new one using Magnus Manske's QuickStatements](#)
3. Wikidata has a pretty decent provenance model

I can annotate data with the data source (paper) it came from and also experimental conditions:



The screenshot shows the Wikidata property page for pKa. The value is 4.63±0.01, with a temperature of 25±1 degrees Celsius. There is one reference listed: CRC Handbook of Chemistry and Physics (1st student edition).

In fact, you'll note that the the book is a separate Wikidata entry in itself. Better even, it's an 'edition' of the book. This is the whole point we make in the above linked H2020 proposal: Wikidata is not a database specific for one domain, it works for any (scholarly) domain, and seamlessly links all those domains.

Now, to keep track of what data I have migrated, I am annotating DrugMet entries with links to Wikidata: everything with a Wikidata Q-code is already migrated. The above pK<sub>a</sub> table already shows Q-identifiers, but I also created them for all data sources I have used (three of them are two books and [one old paper without a DOI](#)):

Paper	DOI	Wikidata	Publication Date
<a href="#">Paper 10.1021/ja01252a028</a>	10.1021/ja01252a028	<a href="#">Q23571227</a>	1943
<a href="#">Paper with DOI 1.1000/1</a>	1.1000/1	<a href="#">Q23572123</a>	1937
<a href="#">Paper with DOI 1.1000/2</a>	1.1000/2	<a href="#">Q23576506</a>	1988
<a href="#">Paper with DOI 1.1000/3</a>	1.1000/3	<a href="#">Q23577944</a>	1986
<a href="#">Paper with DOI 10.1007/BF00652082</a>	10.1007/BF00652082	<a href="#">Q23571358</a>	1981
<a href="#">Paper with DOI 10.1021/ed050p510</a>	10.1021/ed050p510	<a href="#">Q22262588</a>	1973
<a href="#">Paper with DOI 10.1021/ed071pA6</a>	10.1021/ed071pA6	<a href="#">Q23571464</a>	1994
<a href="#">Paper with DOI 10.1021/ja01280a050</a>	10.1021/ja01280a050	<a href="#">Q23571594</a>	1937
<a href="#">Paper with DOI 10.1021/ja01489a008</a>	10.1021/ja01489a008	<a href="#">Q22251355</a>	1960
<a href="#">Paper with DOI 10.1021/ja01577a030</a>	10.1021/ja01577a030	<a href="#">Q23571040</a>	1957

I have still quite a number of entries to do, but all the protocols are set up now.

On the downstream side, Wikidata is also great because of [their SPARQL end point](#). Something that I did not get worked out some weeks ago, I did manage yesterday (after [some encouragement from @arthursmith](#)): list all pK<sub>a</sub> statements, including literature source if available:

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If you [run that query on the Wikidata endpoint](#), you get a table like this:

wikidata	compound	pKa	source	title	doi
<a href="#">Q209354</a>	2-Chloroethanol	14.31	<a href="#">Q22251355</a>	Acid Ionization Constants of Alcohols. II. Acidities of Some Substituted Methanols and Related Compounds 1,2	10.1021/ja01489a008
<a href="#">Q4596742</a>	2,2,2-Trichloroethanol	12.24	<a href="#">Q22251355</a>	Acid Ionization Constants of Alcohols. II. Acidities of Some Substituted Methanols and Related Compounds 1,2	10.1021/ja01489a008
<a href="#">Q22266828</a>	2,4-lutidine	6.46	<a href="#">Q22262588</a>	Experimental determination of pKa values by use of NMR chemical shift	10.1021/ed050p510
<a href="#">Q23636061</a>	2,5-lutidine	6.18	<a href="#">Q22262588</a>	Experimental determination of pKa values by use of NMR chemical shift	10.1021/ed050p510
<a href="#">Q209284</a>	2,6-Lutidine	6.67	<a href="#">Q22262588</a>	Experimental determination of pKa values by use of NMR chemical shift	10.1021/ed050p510
<a href="#">Q223069</a>	3-chloropyridine	4.09	<a href="#">Q22262588</a>	Experimental determination of pKa values by use of NMR chemical shift	10.1021/ed050p510
<a href="#">Q22266828</a>	2,4-lutidine	6.46	<a href="#">Q22262588</a>	Experimental determination of pKa values by use of NMR chemical shift	10.1021/ed050p510

We here see experimental data from two papers: [10.1021/ja01489a008](#) and [10.1021/ed050p510](#). This can all be displayed a lot fancier, like make histograms, tables with 2D drawings of the chemical structures, etc, but I leave that to the reader.