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Migrating pKa data from DrugMet to Wikidata

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Abstract

In 2010 Samuel Lampa and I started a pet project: collecting pKa 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?

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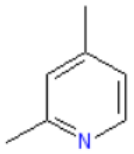
In 2010 Samuel Lampa and I started a pet project: collecting pK_a data: he was working on RDF extension of MediaWiki and I like consuming RDF data. We started DrugMet. When you read this post, this MediaWiki installation may already be down, which is why I am migrating the data to Wikidata. Why? Because 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



Facts about 2,4-lutidine

CHEMINF 000200	JYYNAJVZFGKDEQ-UHFFFAOYSA-N
CHEMINF 000567	Q22266828
Equivalent URI	http://drugmet.rilspace.org/resource/2,4_lutidine
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	http://drugmet.rilspace.org/resource/2,4_lutidine
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_a data (more spoilers):

All pKa values

Below is a list of all pKa values extracted from All papers.

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

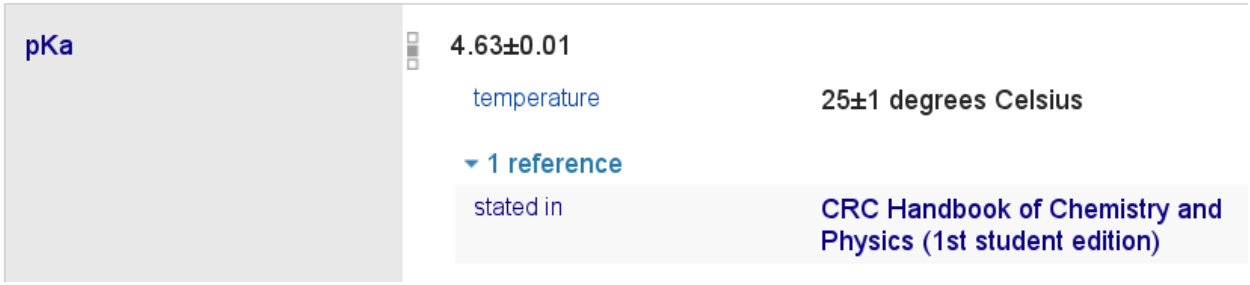
I find a database like this very important. It does not capture all the information it should be capturing, though, as is clear from the proposal some of use worked on a while back. However, this project got on hold; I don't have time for it anymore, and it is not core to our department enough to spend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

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:



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_a 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
Paper 10.1021 ja01252a028	10.1021/ja01252a028	Q23571227	1943
Paper with DOI 1.1000/1	1.1000/1	Q23572123	1937
Paper with DOI 1.1000/2	1.1000/2	Q23576506	1988
Paper with DOI 1.1000/3	1.1000/3	Q23577944	1986
Paper with DOI 10.1007/BF00652082	10.1007/BF00652082	Q23571358	1981
Paper with DOI 10.1021/ed050p510	10.1021/ed050p510	Q22262588	1973
Paper with DOI 10.1021/ed071pA6	10.1021/ed071pA6	Q23571464	1994
Paper with DOI 10.1021/ja01280a050	10.1021/ja01280a050	Q23571594	1937
Paper with DOI 10.1021/ja01489a008	10.1021/ja01489a008	Q22251355	1960
Paper with DOI 10.1021/ja01577a030	10.1021/ja01577a030	Q23571040	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_a statements, including literature source if available:

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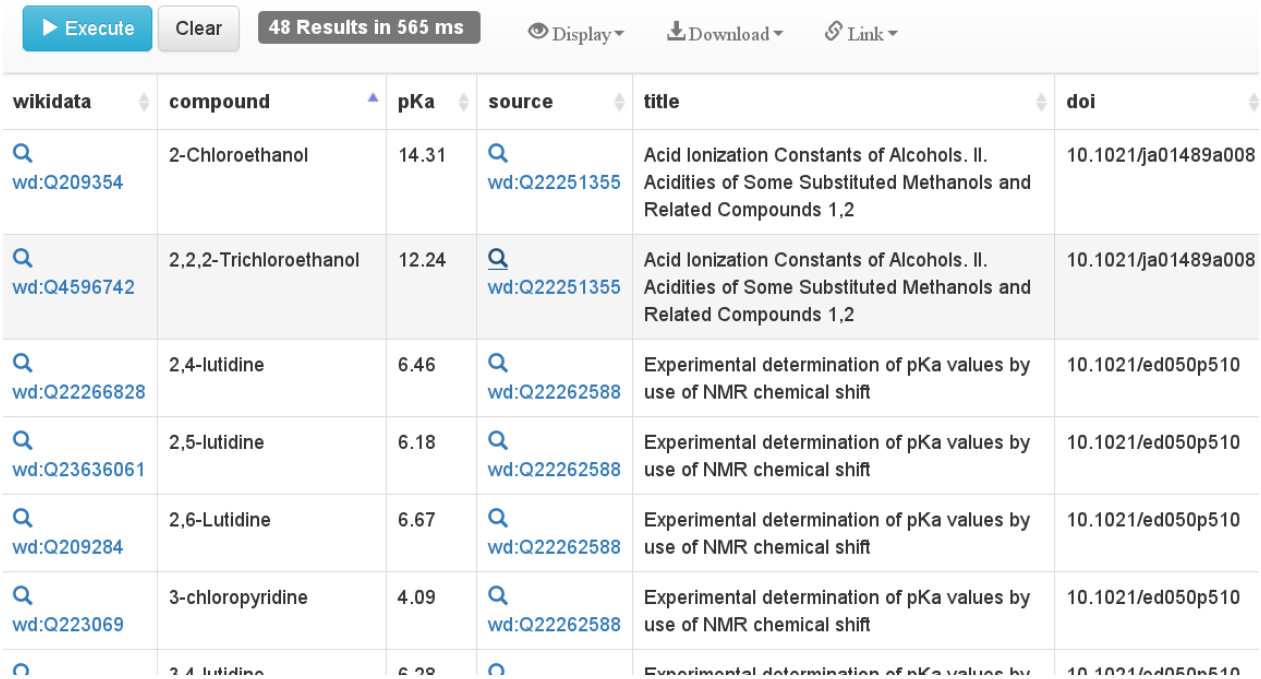
If you run that query on the Wikidata endpoint, you get a table like this:



▶ Execute | Clear | 48 Results in 565 ms | Display | Download | Link

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