chem-bla-ics

Adding chemical compounds to Wikidata

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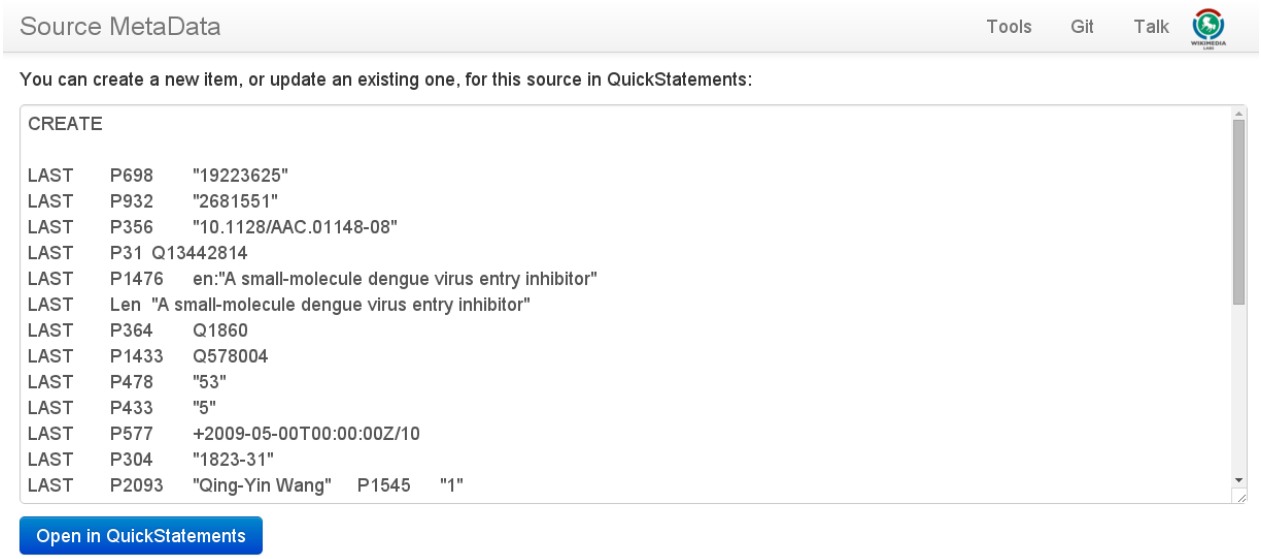
Abstract
Adding chemical compounds to Wikidata is not difficult. You can store the chemical formula (P274), (canonical) SMILES (P233), InChIKey (P235) (and InChI (P234), of course), as well various database identifiers (see what I wrote about that here]). It also allows storing of the provenance, and has predicates for that too.

Adding chemical compounds to Wikidata is not difficult. You can store the chemical formula (P274), (canonical) SMILES (P233), InChIKey (P235) (and InChI (P234), of course), as well various database identifiers (see what I wrote about that here]). It also allows storing of the provenance, and has predicates for that too.

So, to enter a new structure for a compound, you should enter the compound information to Wikidata. Of course, make sure to create the needed accounts, particularly one for Wikidata (create account) (not sure if the next steps needs a more general Wikimedia account too).

Entering the research paper:
Magnus Manske pointed me to this helper tool. If you have the DOI of the paper, it is easy to add a new paper. This is what the tool shows for doi:10.1128/AAC.01148-08 (but no longer when you try!):



You need permission to run this script and the tool will alert you about that, and give the instructions how to get permission. After I clicked the Open in QuickStatements I get this output, showing me an entry in Wikidata was created for this paper:

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1. Processing Q22309806 (Q22309806 P698 "19223625")
2. Processing Q22309806 (Q22309806 P932 "2681551")
3. Processing Q22309806 (Q22309806 P356 "10.1128/AAC.01148-08")
4. Processing Q22309806 (Q22309806 P31 Q13442814)
5. Processing Q22309806 (Q22309806 P1476 en:"A small-molecule dengue virus entry inhibitor")
6. Processing Q22309806 (Q22309806 Len "A small-molecule dengue virus entry inhibitor")
7. Processing Q22309806 (Q22309806 P364 Q1860)
8. Processing Q22309806 (Q22309806 P1433 Q578004)
9. Processing Q22309806 (Q22309806 P478 "53")
10. Processing Q22309806 (Q22309806 P433 "5")
11. Processing Q22309806 (Q22309806 P577 +2009-05-00T00:00:00Z/10)
12. Processing Q22309806 (Q22309806 P304 "1823-31")
13. Processing Q22309806 (Q22309806 P2093 "Qing-Yin Wang" P1545 "1")
14. Processing Q22309806 (Q22309806 P2093 "Sejal J Patel" P1545 "2")
15. Processing Q22309806 (Q22309806 P2093 "Eric Vangrevelinghe" P1545 "3")
16. Processing Q22309806 (Q22309806 P2093 "Hao Ying Xu" P1545 "4")
17. Processing Q22309806 (Q22309806 P2093 "Ranga Rao" P1545 "5")
18. Processing Q22309806 (Q22309806 P2093 "Deana Jaber" P1545 "6")
19. Processing Q22309806 (Q22309806 P2093 "Wouter Schul" P1545 "7")
20. Processing Q22309806 (Q22309806 P2093 "Feng Gu" P1545 "8")
21. Processing Q22309806 (Q22309806 P2093 "Olivier Heudi" P1545 "9")
22. Processing Q22309806 (Q22309806 P2093 "Ngai Ling Ma" P1545 "10")
23. Processing Q22309806 (Q22309806 P2093 "Mee Kian Poh" P1545 "11")
24. Processing Q22309806 (Q22309806 P2093 "Wai Yee Phong" P1545 "12")
25. Processing Q22309806 (Q22309806 P2093 "Thomas H Keller" P1545 "13")
26. Processing Q22309806 (Q22309806 P2093 "Edgar Jacoby" P1545 "14")
27. Processing Q22309806 (Q22309806 P2093 "Subhash G Vasudevan" P1545 "15")

All done!.

Later, I can use the new Q-code (Q22309806) to use as source for statements about the compound (formula, etc).

Draw your compound and get an InChIKey:
The next step is to draw a compound and get an InChIKey. This can be done with many tools, including Bioclipse. Rajarshi opted for alternatives:

> • @collabchem @egonwillighagen OSRA or https://t.co/ZIQdgrYsmr?
> — Rajarshi Guha (@rguha) January 27, 2016

Then check if the compound is not already in Wikidata. You can use this SPARQL query for that using the InChIKey of the compound (it's for acetic acid, so it will be found):

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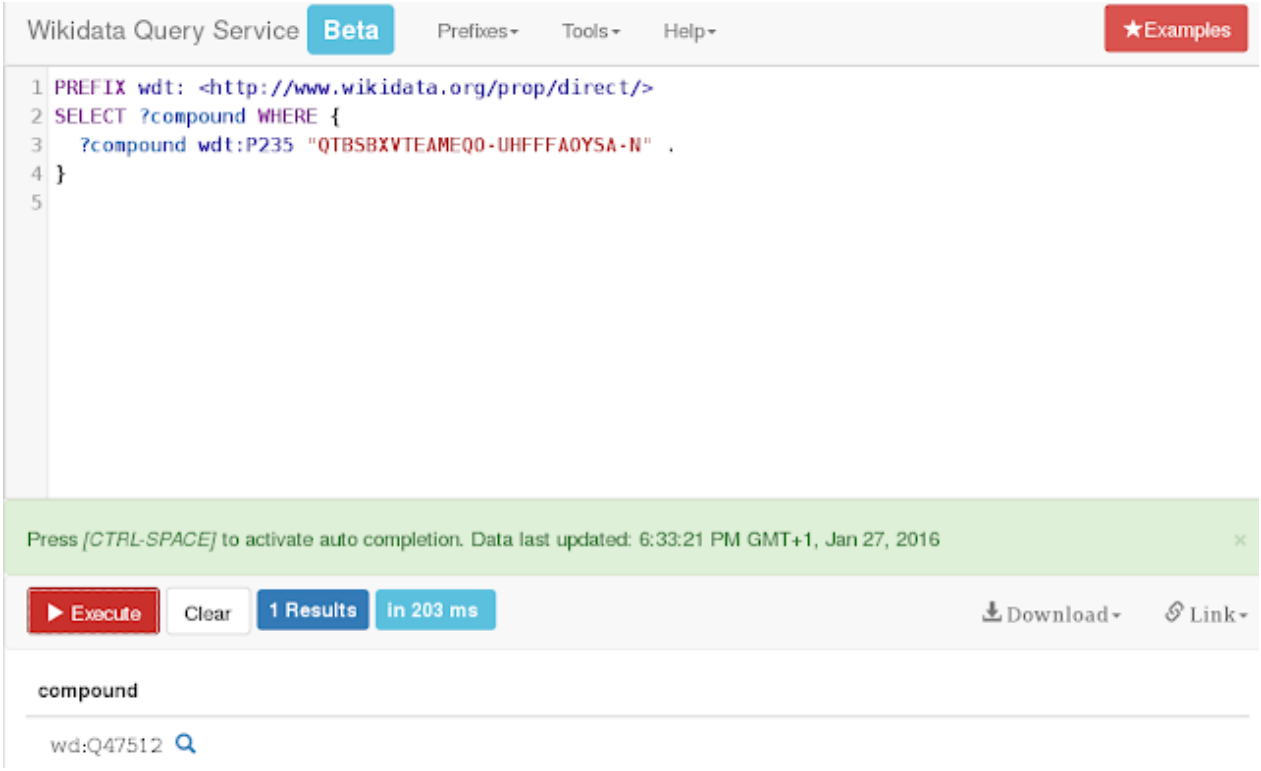


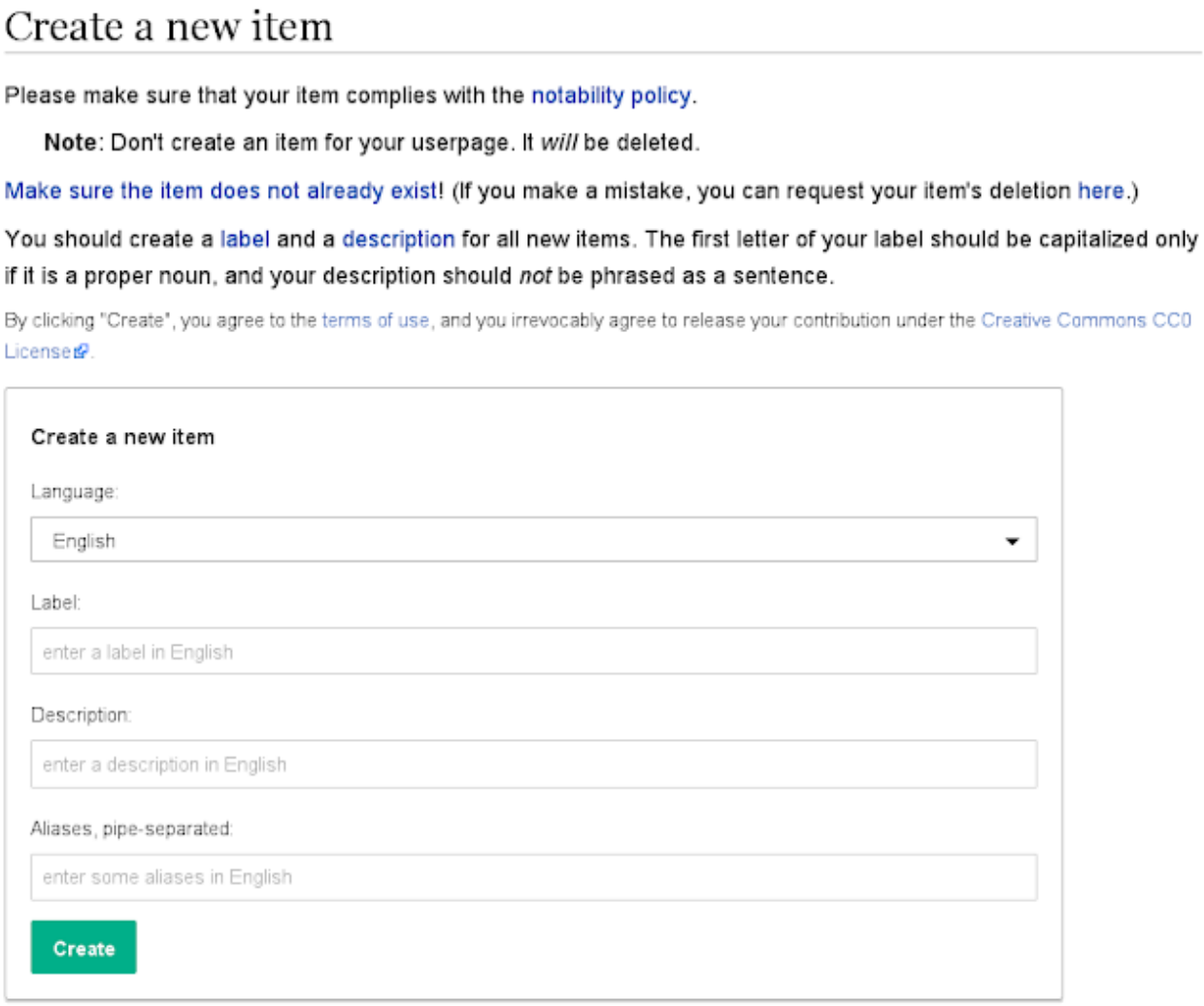
For convenience, here the copy/pastable SPARQL:

```
PREFIX wdt:
SELECT ?compound WHERE {
  ?compound wdt:P235 "QTBSBXVTEAMEQO-UHFFFAOYSA-N" .
}
```

Entering the compound:
So, the compound is not already in Wikidata, so time to add it. The minimal information you should provide is the following:

- mark the new entry as 'instance of' (P) 'chemical compound (Q)
- the chemical formula and SMILES (use as reference the paper)
    - add the reference to the paper you entered above
- add the InChIKey and/or InChI

The first step is to create a new Wikidata entry. The Create new item menu in the left side panel can be used, showing a page like this:



As a label you can use the name used in the paper for the compound, even if a code, and as description ‘chemical compound’ will do for now; it can be changed later.

Feel free to add as much information about the compound as you can find. There are some chemically rich entries in Wikidata, such as that for acetic acid (Q47512).