

ChEMBL-RDF: Uploading data to Kasabi with pytassium



Published October 22, 2011

Citation

Willighagen, E. (2011, October 22). ChEMBL-RDF: Uploading data to Kasabi with pytassium. *Chem-bla-ics*. <https://doi.org/10.59350/k1860-kks41>

Keywords

Kasabi, ChEMBL, Semweb

Copyright

Copyright © None 2011. 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

I reported earlier how to I [uploaded the ChemPedia \(RIP\) data onto Kasabi](#). But for ChEMBL-RDF I have used the [pytassium](#) tool, not just because it has a cool name :) I discovered yesterday, however, that I did not write down in this lab notebook, what steps I needed to take to reproduce it. And I just wanted to uploaded new triples to the [ChEMBL-RDF data set on Kasabi](#).

The new triples I wanted to upload, link the [new public ChEMBL identifiers](#) (like [ChEMBL25 for aspirin](#)) to the internal ChEMBL database identifier I used for ChEMBL 09 for the URIs. So, I am adding a lot of triples like:

```
<http://data.kasabi.com/dataset/chembl-rdf/09/molecule/m517180> <http://  
www.w3.org/2002/07/owl#sameAs>  
<http://data.kasabi.com/dataset/chembl-rdf/09/chemblid/CHEMBL1>
```

And the pytassium code I use to upload this to Kasabi looks like:

```
import pytassium  
import time  
  
dataset = pytassium.Dataset('chembl-rdf','XXX')  
  
# Store the contents of a turtle file  
dataset.store_file('chemblids.nt', media_type='text/plain')
```

So, that omission in my log book has been corrected now.