

ChEMBL 13 as RDF

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Citation

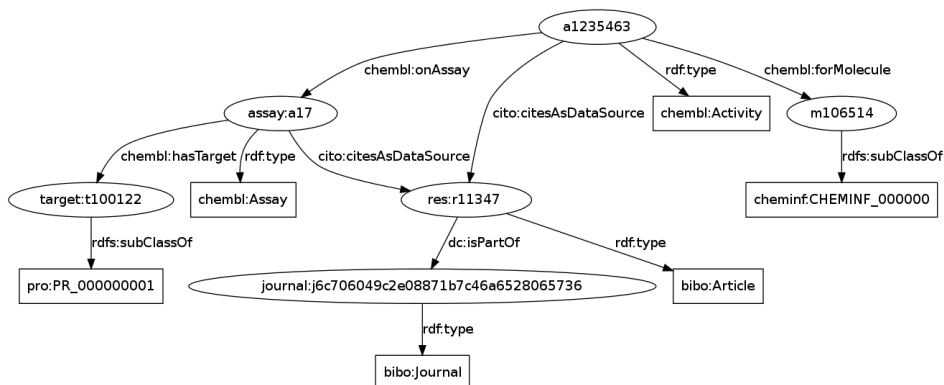
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Keywords

Chembl, Rdf, Semweb, Ontology, Cheminf

Abstract

Update: this work is now described in this paper.



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chem-bla-ics

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Last week, ChEMBL 13 was [released](#), with even more data, data fixes, [etc](#). Since my RDF for [ChEMBL 09](#) my workflow has become [more solid](#) and uses more common ontologies, started using more common ontologies and ontologies I just like, such as [CHEMINF](#) and [CiTO](#). Below is an overview of the resource types present in the RDF: activities (almost 7M now), chemical entities, assays, targets, and documents.

The [data on Kasabi](#) will be updated soon, and the [SPARQL end point](#) hosted by Uppsala University was updated yesterday, including the [SNORQL frontend](#):

The new data is not fully backwards compatible. The changes to the RDF include the use of `cito:citesAsDataSource`, more typing using existing ontologies, e.g. with `cheminf:CHEMINF_000000` and `pro:PR_000000001` from the [PRotein Ontology](#).

A paper dedicated to the ChEMBL-RDF is in preparation. Existing use cases can be found [here](#).

References

- [10.1371/JOURNAL.PONE.0025513](#)
- [10.1186/2041-1480-1-S1-S6](#)
- [10.1186/2041-1480-2-S1-S6](#)