

ChEMBL 13 as RDF

Egon Willighagen 

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Keywords

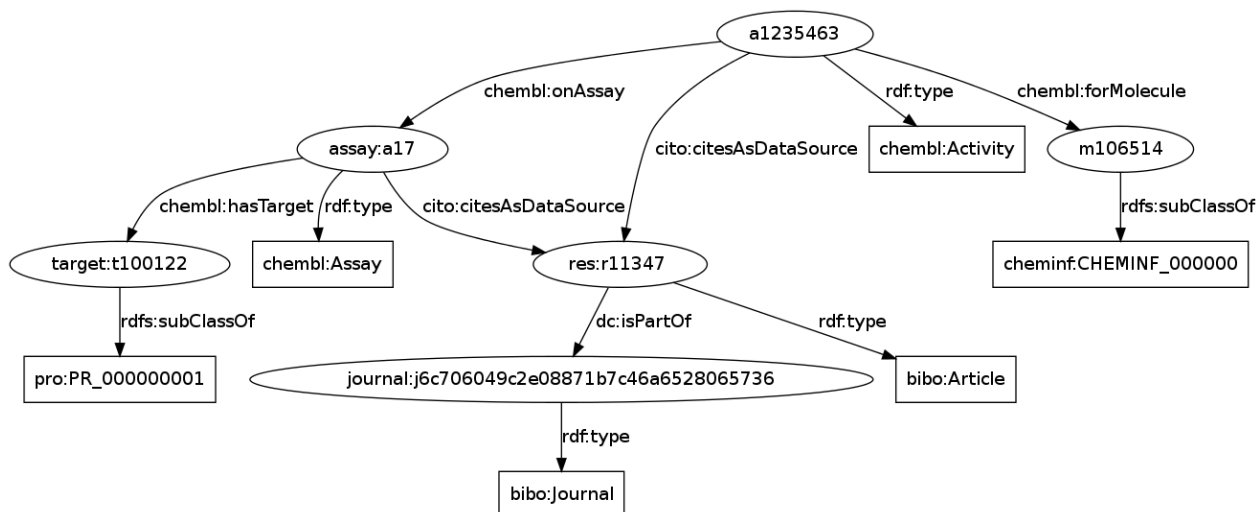
Chembl, Rdf, Semweb, Ontology, Cheminf

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Update: this work is now described in [this paper](#).

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](#):

List of all properties:

property
dc:date
dc:identifier
dc:isPartOf
dc:title
<http://purl.org/dc/terms/created>
<http://purl.org/dc/terms/modified>
<http://purl.org/ontology/bibo/doi>
<http://purl.org/ontology/bibo/issue>
<http://purl.org/ontology/bibo/pageEnd>
<http://purl.org/ontology/bibo/pageStart>
<http://purl.org/ontology/bibo/pmid>
<http://purl.org/ontology/bibo/volume>
<http://purl.org/spar/cito/citesAsDataSource>
chembl:activeCompound
chembl:classL1
chembl:classL2
chembl:classL3
chembl:classL4
chembl:classL5
chembl:classL6
chembl:classL7
chembl:classL8
chembl:forMolecule
chembl:hasAssayType
chembl:hasConfScore
chembl:hasDescription
chembl:hasKeyword
chembl:hasTarget
chembl:hasTaxonomy

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_0000000001` from the [PRotein Ontology](#).

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