

# ChEMBL 13 as RDF



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## Keywords

ChEMBL, Rdf, Semweb, Ontology, Cheminf

## Abstract

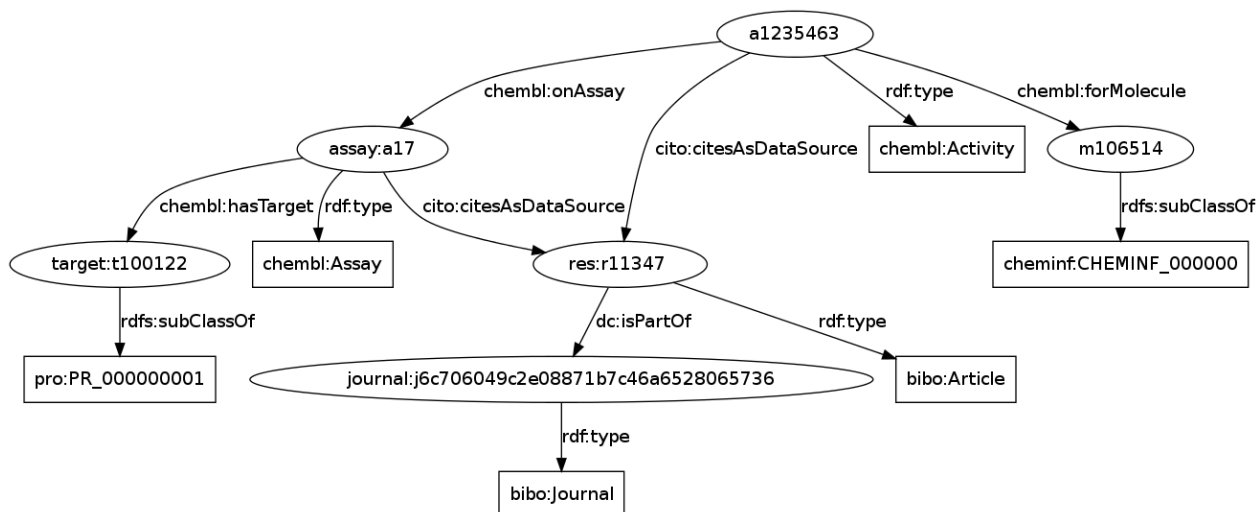
Update: this work is now described in this paper .

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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](#):

## List of all properties:

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

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](#).