chem-bla-ics

ChEMBL 13 as RDF

Egon Willighagen

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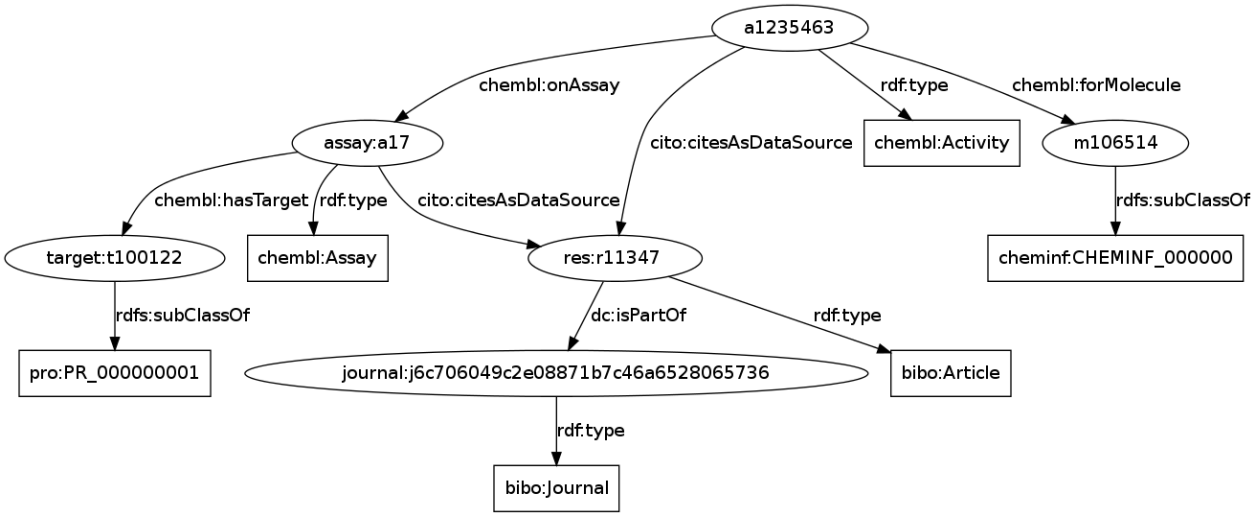
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Keywords
Chembl, Rdf, Semweb, Ontology, Cheminf

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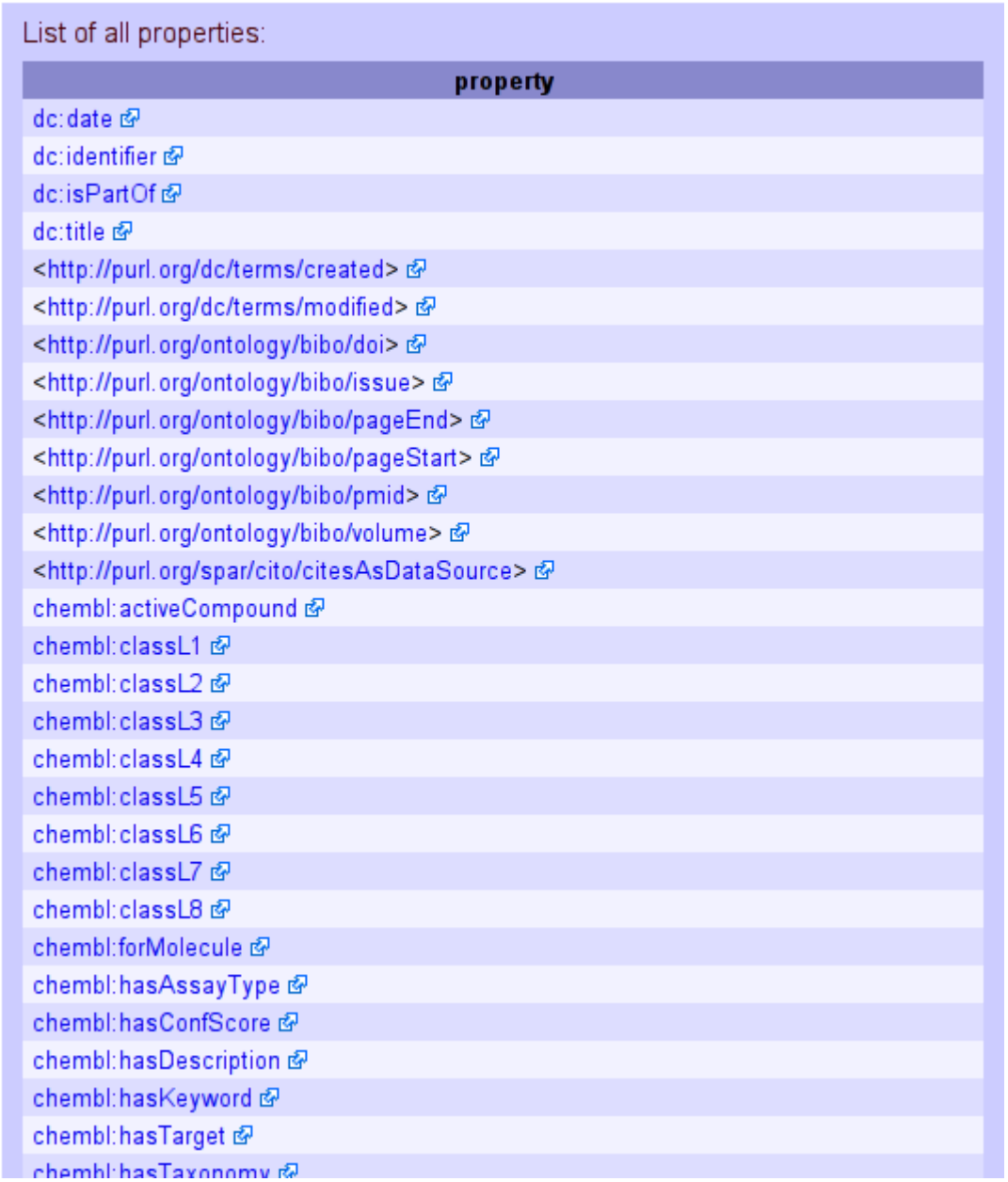
Update: this work is now described in this paper .

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:

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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_000000001` from the PRotein Ontology.

A paper dedicated to the ChEMBL-RDF is in preparation. Existing use cases can be found here.