

chem-bla-ics

ChEMBL RDF #1:SPARQL end point

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Keywords

Rdf, ChEMBL, Sparql

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In a [series of SPARQL end points](#), I am happy to present a new [Virtuoso 6.1](#)-hosted SPARQL end point for the [ChEMBL database \(CC-BY-SA\)](#), at our groups new [rdf.farmbio.uu.se](#) server. The server is hosting [23.8M triples](#), with the data based on [ChEMBL 02](#). There is a [SPARQL end point](#), as well as a [SNORQL interface](#):

Snorql: Exploring <http://rdf.farmbio.uu.se/chembl/sparql>

SPARQL:

```
PREFIX rdf: <http://www.w3.org/1999/02/22-rdf-syntax-ns#>
PREFIX rdfs: <http://www.w3.org/2000/01/rdf-schema#>
PREFIX owl: <http://www.w3.org/2002/07/owl#>
PREFIX dc: <http://purl.org/dc/elements/1.1/>
PREFIX foaf: <http://xmlns.com/foaf/0.1/>
```

```
SELECT DISTINCT ?class
WHERE { [] a ?class }
ORDER BY ?class
```

Results:

Browse:

- [Classes](#)
- [Properties](#)

List of all classes:

class
http://rdf.farmbio.uu.se/chembl/onto/#RelationType
http://rdf.farmbio.uu.se/chembl/onto/#Compound
http://rdf.farmbio.uu.se/chembl/onto/#Target
http://purl.org/ontology/bibo/Article
http://purl.org/ontology/bibo/Journal
http://rdf.farmbio.uu.se/chembl/onto/#Assay
http://rdf.farmbio.uu.se/chembl/onto/#Activity
http://www.openlinksw.com/schemas/virtrdf#array-of-QuadMap

There are 2.4M [activities](#), 34k [papers](#), 517k [compounds](#), 416k [assays](#), associated with 7k [targets](#) (proteins etc):

class	count
"http://purl.org/ontology/bibo/Article"	33956
"http://purl.org/ontology/bibo/Journal"	13
"http://rdf.farmbio.uu.se/chembl/onto/#Activity"	2404622
"http://rdf.farmbio.uu.se/chembl/onto/#Assay"	416284
"http://rdf.farmbio.uu.se/chembl/onto/#Compound"	517261
"http://rdf.farmbio.uu.se/chembl/onto/#RelationType"	4
"http://rdf.farmbio.uu.se/chembl/onto/#Target"	7192

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I will not discuss any cool mashups with the rich data set and [Bioclipse](#), as that is the main topic my student [Annzi's Masters project](#).