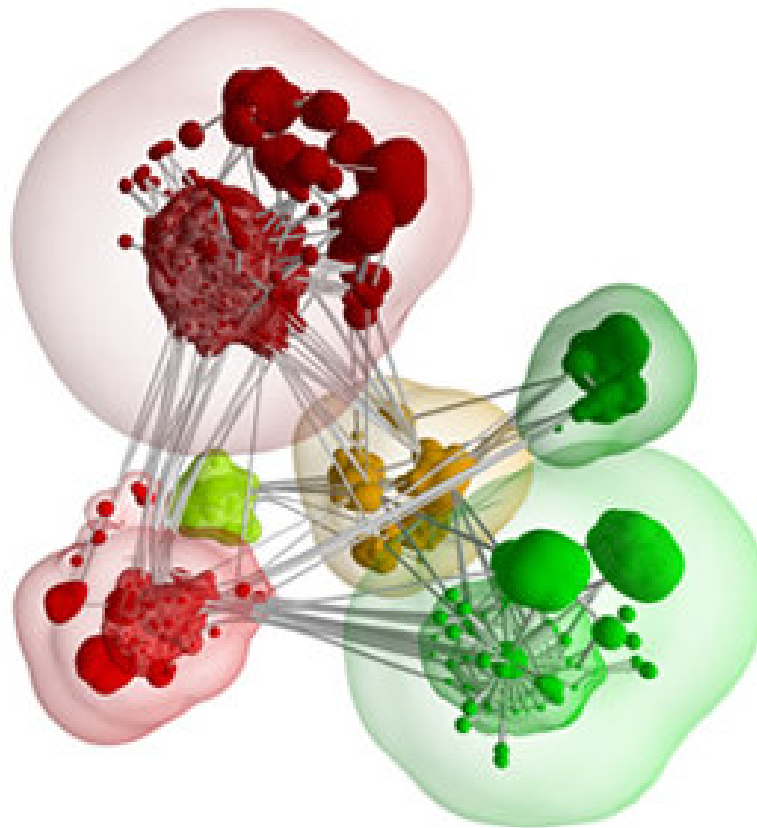# A Visual Query Editor
for Sparql and Prolog

Jans Aasman, Ph.D.
CEO Franz Inc
Ja@Franz.com

Content

- Why writing SPARQL queries is challenging

- The datasets that we will use

- A demo of our Visual Query Editor

- Installing Gruff

- A little bit of federation

- Latest news about 4.1 and TBC

So you want to do a query

Select two clinical trials that discuss Morphine or Morphine Sulfate and discuss at least the target Cytochrome c3 but also other targets and discusses the same side effects.

Why writing SPARQL queries can be challenging

- Remembering (and reconstructing) namespaces
- Finding the constants in expressions
- Remembering the filter syntax
- Seeing the structure of you query

```
PREFIX drugbanktarget:  <http://www4.wiwiss.fu-berlin.de/drugbank/resource/targets/>
PREFIX drugbankdrug:  <http://www4.wiwiss.fu-berlin.de/drugbank/resource/drugs/>
PREFIX franz: <http://www.franz.com/>
SELECT ?ct2 ?ct ?target ?sideeffect WHERE
{ ?ct franz:discusses-target ?target ,
                             drugbanktarget:4968 ;
      franz:discusses-drug drugbankdrugs:DB00295 ;
      franz:discusses-side-effect ?sideeffect .
  ?ct2 franz:discusses-drug drugbankdrugs:DB00295> ;
       franz:discusses-side-effect ?sideeffect .
  FILTER ( ?ct2 != ?ct )
  FILTER ( drugbanktargets:4968 != ?target ) }
LIMIT 32
```
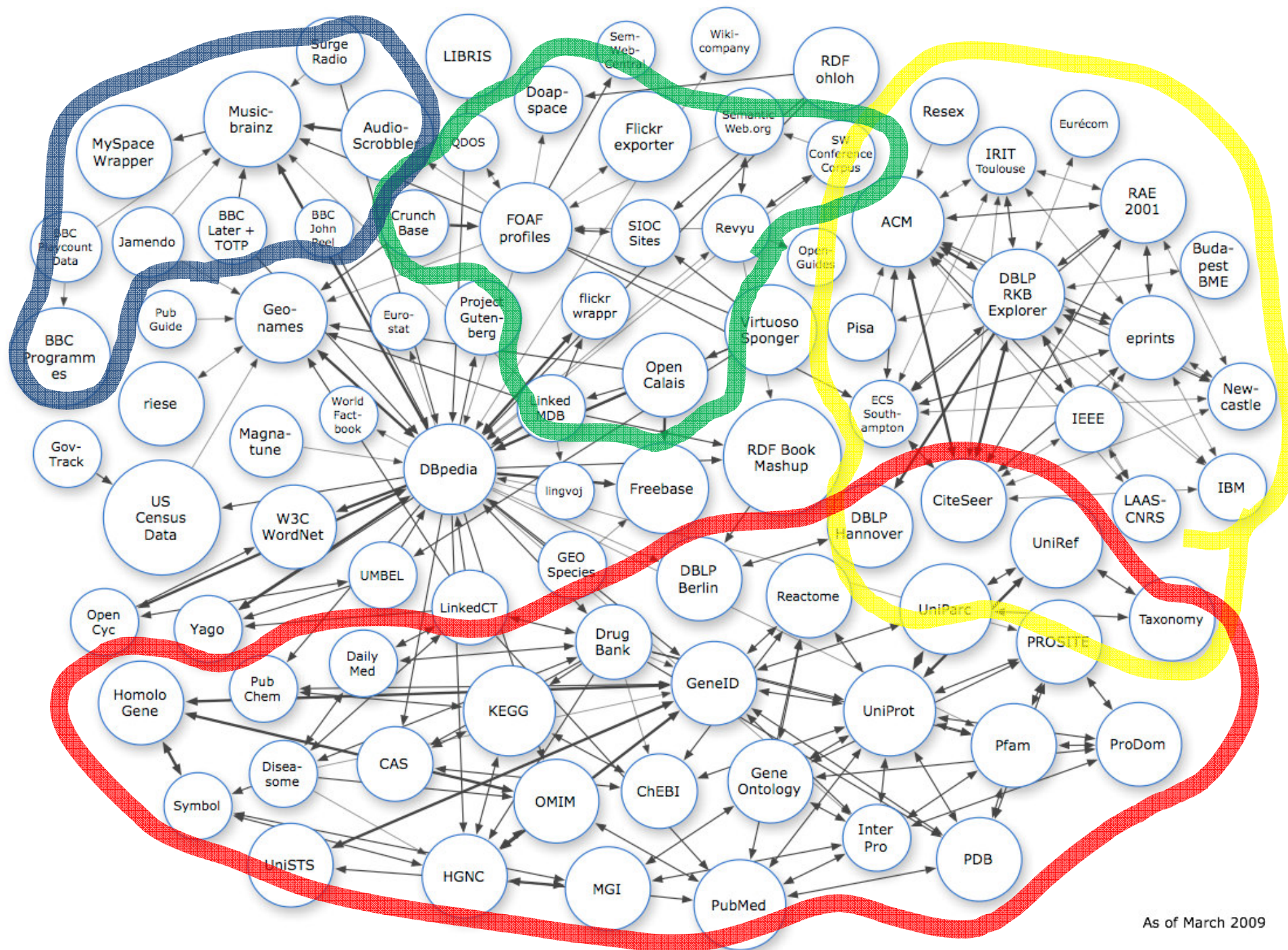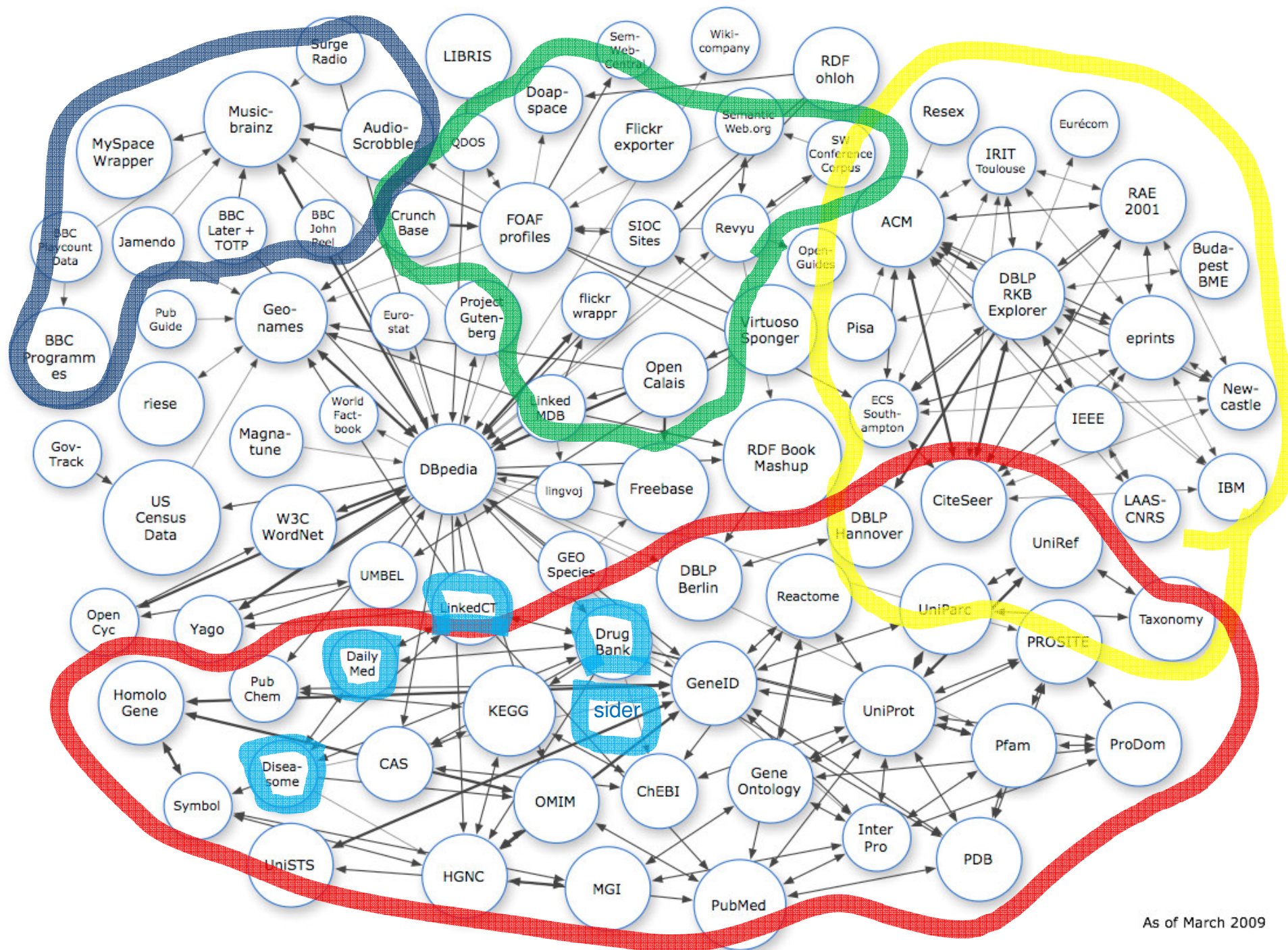
Wouldn't this be easier...

The datasets

As of March 2009

As of March 2009

As of March 2009
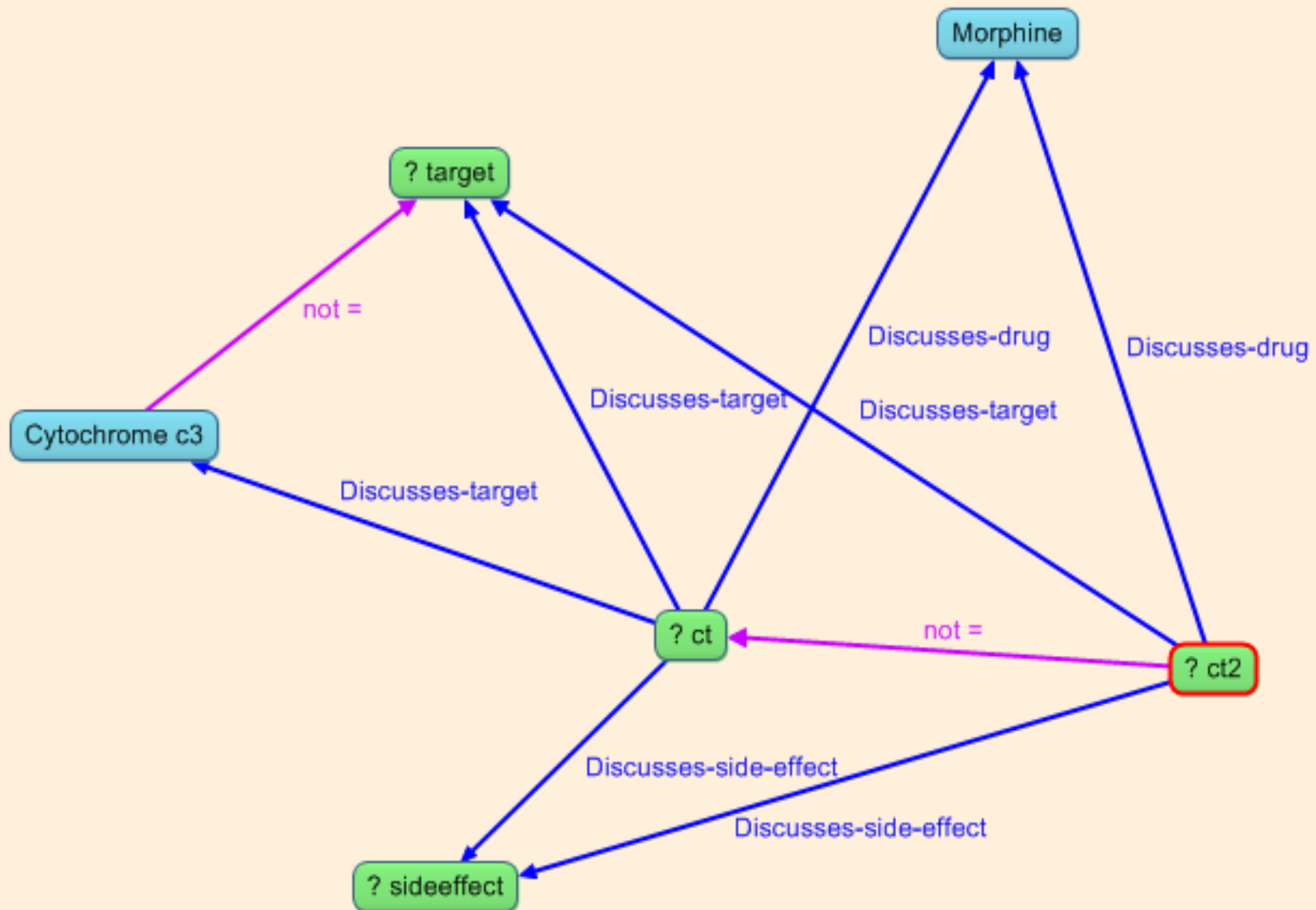
DrugBank

Search: [_____] [Search] [Advanced]

The DrugBank database is a unique bioinformatics and cheminformatics resource that combines detailed drug (i.e. chemical, pharmacological and pharmaceutical) data with comprehensive drug target (i.e. sequence, structure, and pathway) information. The database contains nearly 4800 drug entries including >1,350 FDA-approved small molecule drugs, 123 FDA-approved biotech (protein/peptide) drugs, 71 nutraceuticals and >3,243 experimental drugs. Additionally, more than 2,500 non-redundant protein (i.e. drug target) sequences are linked to these FDA approved drug entries. Each DrugCard entry contains more than 100 data fields with half of the information being devoted to drug/chemical data and the other half devoted to drug target or protein data.

DrugBank is supported by David Wishart, Departments of Computing Science & Biological Sciences, University of Alberta.

More about DrugBank

What's New?

- You can now set the maximum number of results returned from a structure search on the ChemQuery page. The limit used to be 100, which missed some important drugs in the search results.
- We have implemented the ChemAxon solution for structure searches. You can now perform similarity (tanimoto), substructure, and exact searches via the ChemQuery function. This system replaces an outdated structure search and should be faster and more accurate. We have only added the most basic features for this release, so if you would like to see more/different features added, please let us know.

D2R Server publishing the DrugBank Database
Running at http://www4.wiwiss.fu-berlin.de/drugbank/

Home | drug_interactions drugs enzymes references targets

DrugBank is a repository of almost 5000 FDA-approved small molecule and biotech drugs. It contains detailed information about drugs including chemical, pharmacological and pharmaceutical data; along with comprehensive drug target data such as sequence, structure, and pathway information.
This is a D2R Server publishing the DrugBank data as linked data on the Semantic Web. The database can be accessed using

1. your plain old web browser
2. Semantic Web browsers
3. SPARQL clients.

1. HTML View

You can use the navigation links at the top of this page to explore the database.

2. RDF View

You can also explore this database with **Semantic Web browsers** like Tabulator or Disco. To start browsing, open this entry point URL in your Semantic Web browser:

http://www4.wiwiss.fu-berlin.de/drugbank/all

3. SPARQL Endpoint

SPARQL clients can query the database at this SPARQL endpoint:

http://www4.wiwiss.fu-berlin.de/drugbank/sparql

The database can also be explored using this AJAX-based SPARQL Explorer.

LinkedCT: Clinical Trials

Up-to-date information for locating federally and privately supported clinical trials for a wide range of diseases and conditions.

It contains 81,571 trials sponsored by the National Institutes of Health, other federal agencies, and private industry

ClinicalTrials.gov receives over 40 million page views per month 50,000 visitors daily.

Finding entities in Clinical Trials

- Clinical trials has too much text

- We searched for drugs, diseases, targets and side effects in Clinical trials and created new triples

    - CT100385   discusses-side-effect   headache
    - CT100385   discusses-drug   aspirin
    - CT100385   discusses-disease   alcohol-addiction
    - CT100385   discusses-target   some-protein

Installing Gruff

- And how to do federation

Latest news

- AllegroGraph 4.1 now available
  - Warm standby
  - Replication
  - Point in time recovery
  - User controlled indices

- Integration with TopBraidComposer now working for 4.1
  - Create triple stores with TBC
  - Use Gruff to write sparql queries (that can be used in TBC)