Linked Data for the Life Sciences

Bio2RDF Release 2: Improved coverage, interoperability and provenance of Life Science Linked Data

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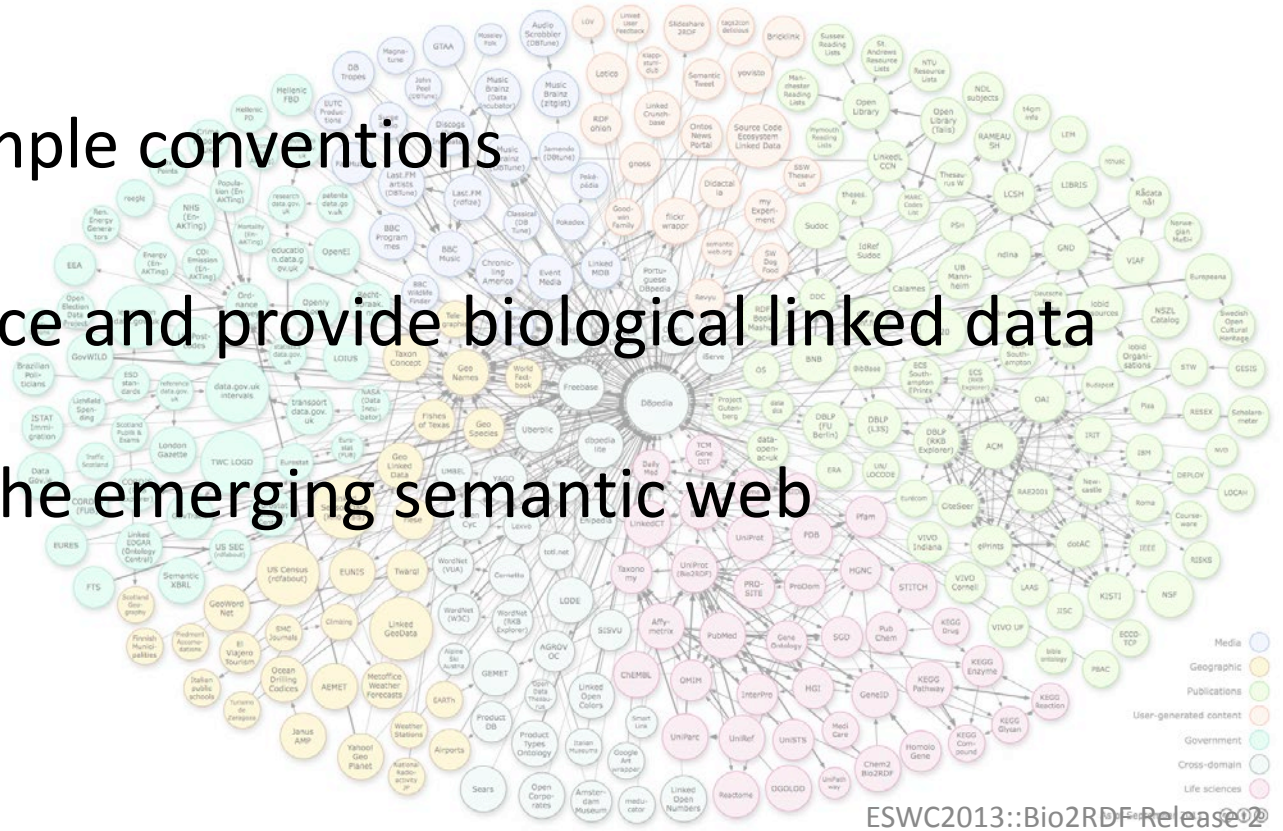
BIO2RDF

is an *open source* framework

that uses simple conventions

to produce and provide biological linked data

on the emerging semantic web



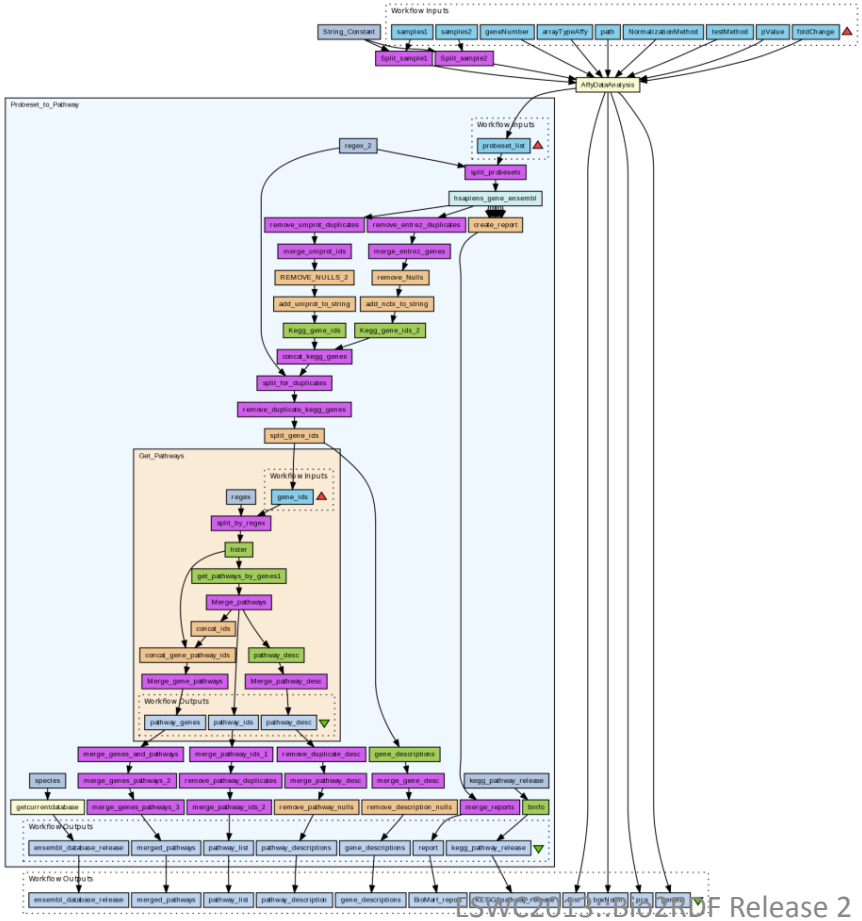
BIO2RDF

reduces the time and effort

involved in data integration

so that *you* can get to

doing **science**



Main features of Bio2RDF Release 2

- Bio2RDF conversion scripts, mapping files and web application are **open source** **and** **freely available** at http://github.com/bio2rdf

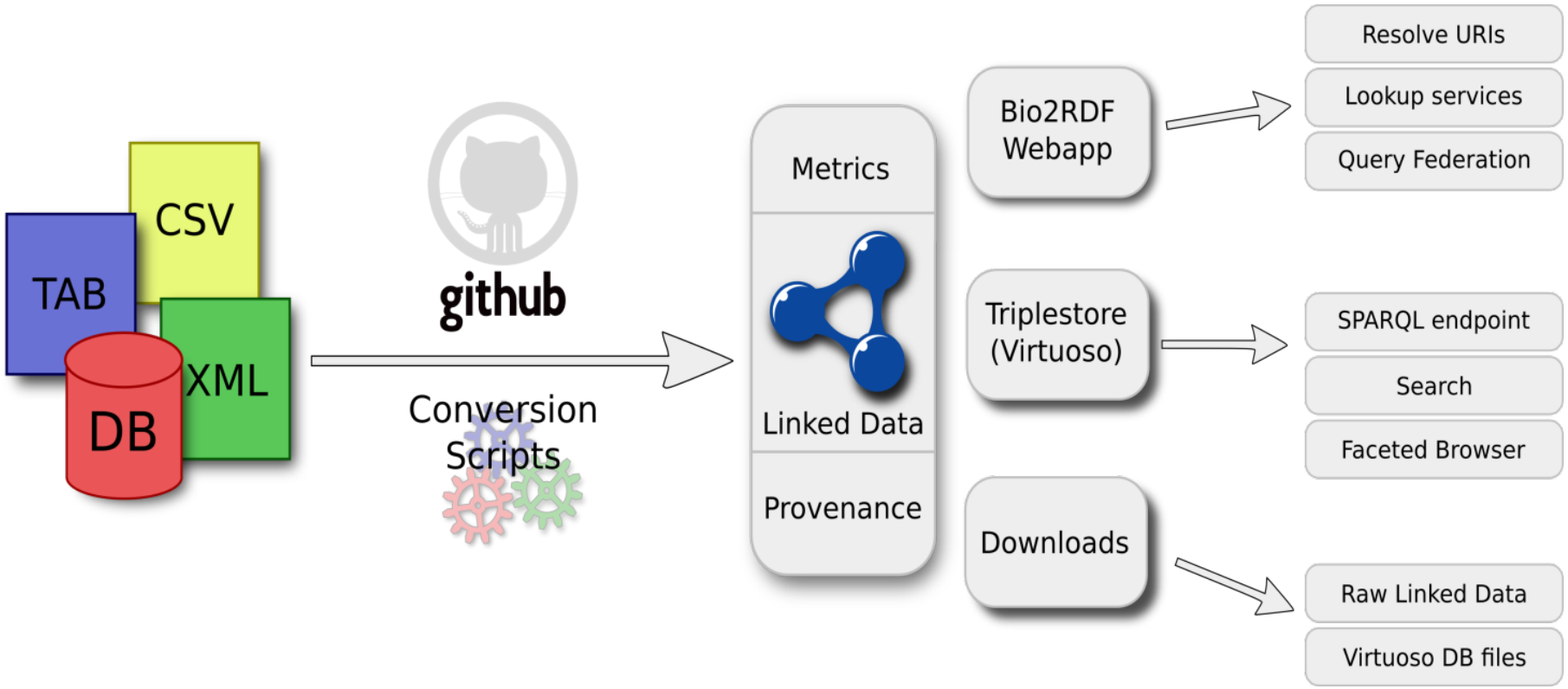
- Bio2RDF enables (syntactic) data integration within and across datasets by using one language (**RDF**), having a **common URI pattern** and a **common resource registry**

- 19 Release 2 datasets have **provenance** and endpoints feature pre-computed **graph summaries** for fast lookup

- Bio2RDF web application enables **entity resolution**, **query federation** across an **expandable distributed network of SPARQL endpoints**

BIO2RDF

At the heart of Linked Data for the Life Sciences



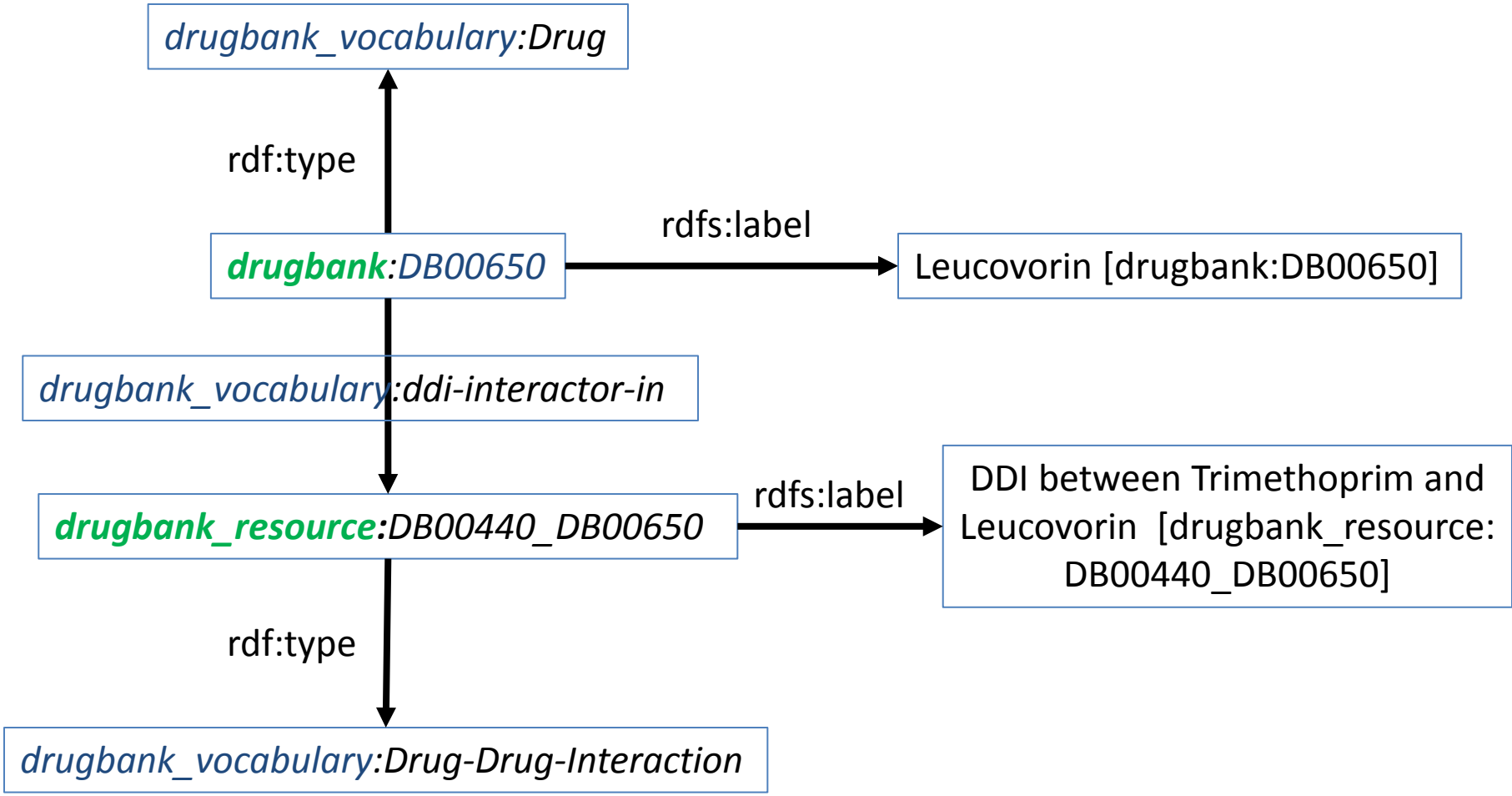
Bio2RDF data are identified using *simple* http URI patterns

Bio2RDF data are identified by Internationalized Resource Identifiers (IRIs) of the form:

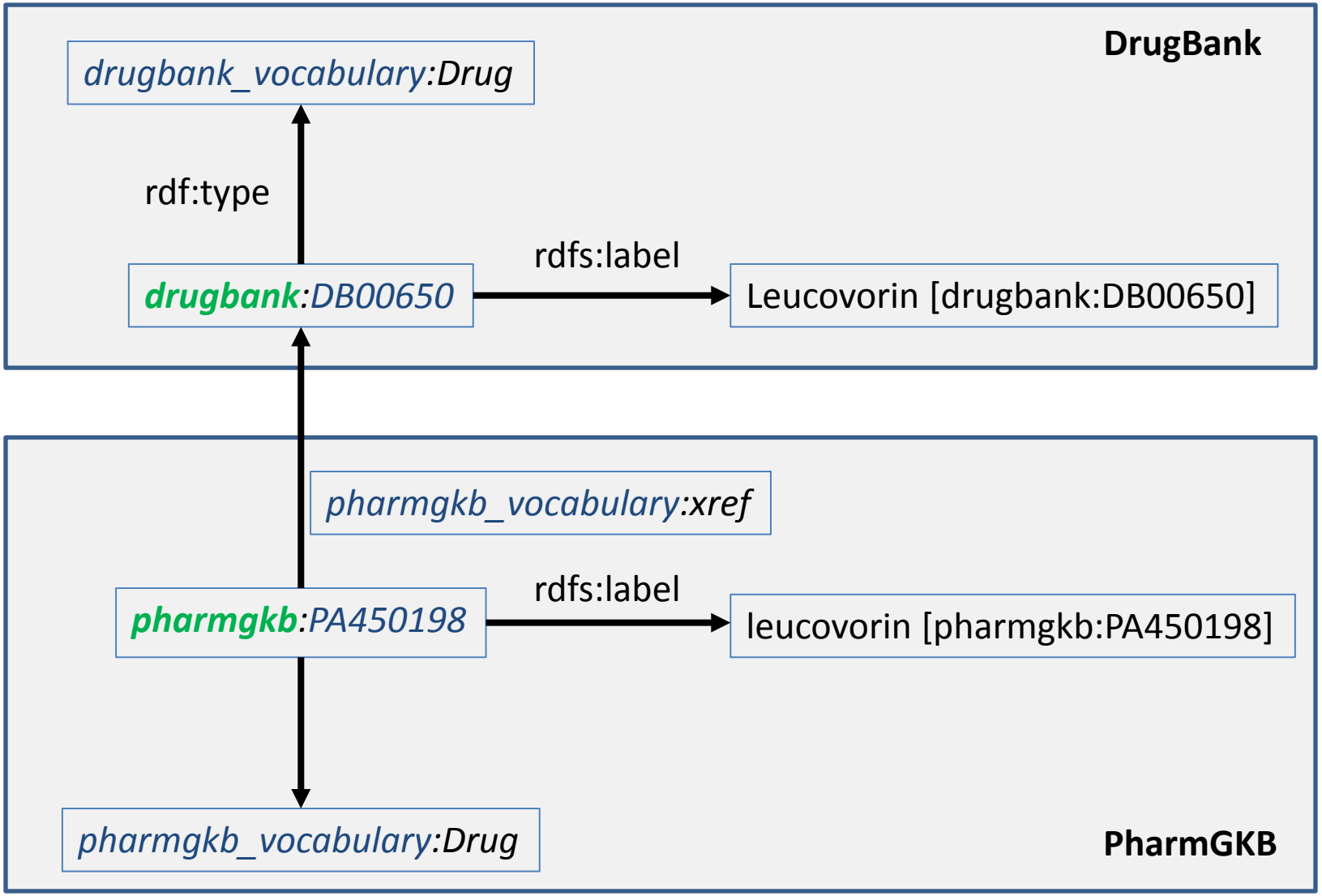
- *http://bio2rdf.org/namespace:identifier*
  for source data **with an assigned identifier**
- *http://bio2rdf.org/namespace_resource:identifier*
  for source data **without an assigned identifier**
- *http://bio2rdf.org/namespace_vocabulary:identifier*
  for dataset-specific **types and relations**

Where *namespace* comes from a curated registry of datasets, hence enabling simple syntactic-based integration in and across datasets.

Data are *described* through machine-understandable statements



The linked data network expands with inter-dataset statements



Linked Data: You can look it up

Leucovorin [drugbank:DB00650] at Bio2RDF

Search

Find intranamespace linksFind global linksLinks Namespace

Find links in namespace

http://bio2rdf.org/drugbank:DB00650

Leucovorin [drugbank:DB00650]

Subject	Predicate	Object
http://bio2rdf.org/drugbank:DB00650	http://bio2rdf.org/bio2rdf_resource:urlList	http://bio2rdf.org/html/drugbank:DB00650
	http://bio2rdf.org/drugbank_vocabulary:absorption	Following oral administration, leucovorin is rapidly absorbed. The apparent bioavailability of leucovorin was 97% for 25 mg, 75% for 50 mg, and 37% for 100 mg.
	http://bio2rdf.org/drugbank_vocabulary:affected-organism	Humans and other mammals
	http://bio2rdf.org/drugbank_vocabulary:biotransformation	Hepatic and intestinal mucosal, the main metabolite being the active 5-methyltetrahydrofolate. Leucovorin is readily converted to another reduced folate, 5,10-methylenetetrahydrofolate, which acts to stabilize the binding of fluorodeoxyridylic acid to thymidylate synthase and thereby enhances the inhibition of this enzyme.
	http://bio2rdf.org/drugbank_vocabulary:brand	Calcium citrovorum factor
	http://bio2rdf.org/drugbank_vocabulary:calculated-property	http://bio2rdf.org/drugbank_resource:calculated_property_DB00650_10
		http://bio2rdf.org/drugbank_resource:calculated_property_DB00650_11
		http://bio2rdf.org/drugbank_resource:calculated_property_DB00650_12
		http://bio2rdf.org/drugbank_resource:calculated_property_DB00650_13
		http://bio2rdf.org/drugbank_resource:calculated_property_DB00650_14

You can get what links to it

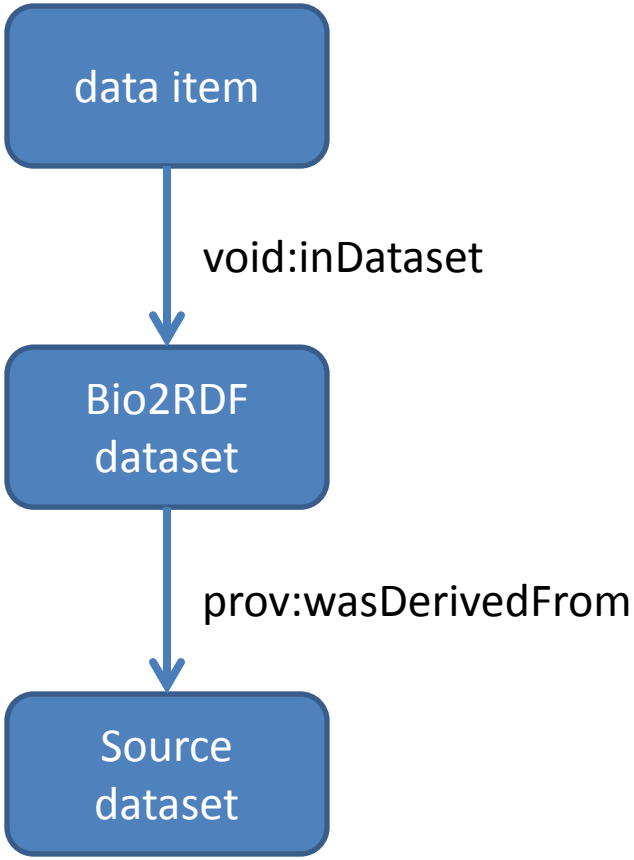
What links to DrugBank's Leucovorin?

http://bio2rdf.org/linksns/drugbank/drugbank:DB00650

Subject	Predicate	Object
http://bio2rdf.org/drugbank_resource:DB00650_359	http://bio2rdf.org/drugbank_vocabulary:drug	http://bio2rdf.org/drugbank:DB00650
	http://www.w3.org/1999/02/22-rdf-syntax-ns#type	http://bio2rdf.org/drugbank_vocabulary:Drug-Target-Interaction
	http://www.w3.org/2000/01/rdf-schema#label	drug-target interaction Leucovorin and Thymidylate synthase [drugbank_resource:DB00650_359]
http://bio2rdf.org/drugbank_resource:DB00650_drugbank_target:1709	http://bio2rdf.org/drugbank_vocabulary:drug	http://bio2rdf.org/drugbank:DB00650
	http://www.w3.org/1999/02/22-rdf-syntax-ns#type	http://bio2rdf.org/drugbank_vocabulary:Drug-Transporter-Interaction
	http://www.w3.org/2000/01/rdf-schema#label	drug-transporter interaction Leucovorin and Canalicular multispecific organic anion transporter 2 [drugbank_resource:DB00650_drugbank_target:1709]
http://bio2rdf.org/drugbank_resource:DB00650_drugbank_target:1735	http://bio2rdf.org/drugbank_vocabulary:drug	http://bio2rdf.org/drugbank:DB00650
	http://www.w3.org/1999/02/22-rdf-syntax-ns#type	http://bio2rdf.org/drugbank_vocabulary:Drug-Transporter-Interaction
	http://www.w3.org/2000/01/rdf-schema#label	drug-transporter interaction Leucovorin and Canalicular multispecific organic anion transporter 1 [drugbank_resource:DB00650_drugbank_target:1735]
http://bio2rdf.org/drugbank_resource:DB00650_drugbank_target:2164	http://bio2rdf.org/drugbank_vocabulary:drug	http://bio2rdf.org/drugbank:DB00650
	http://www.w3.org/1999/02/22-rdf-syntax-ns#type	http://bio2rdf.org/drugbank_vocabulary:Drug-Transporter-Interaction
	http://www.w3.org/2000/01/rdf-schema#label	drug-transporter interaction Leucovorin and Multidrug resistance-associated protein 4 [drugbank_resource:DB00650_drugbank_target:2164]
http://bio2rdf.org/pharmgkb:PA450198	http://bio2rdf.org/pharmgkb_vocabulary:xref	http://bio2rdf.org/drugbank:DB00650
	http://www.w3.org/1999/02/22-rdf-syntax-ns#type	http://bio2rdf.org/pharmgkb_vocabulary:Drug
	http://www.w3.org/2000/01/rdf-schema#label	leucovorin [pharmgkb:PA450198]

Powered by Bio2RDF/1.4-SNAPSHOT | View as RDF/XML | View as N3 | View as HTML | View as JSON

Every Bio2RDF dataset now contains provenance metadata



Features

- Entity-dataset link
- Creator
- Publisher
- Date created
- License & rights
- Source
- Availability
- SPARQL endpoint
- Data dump

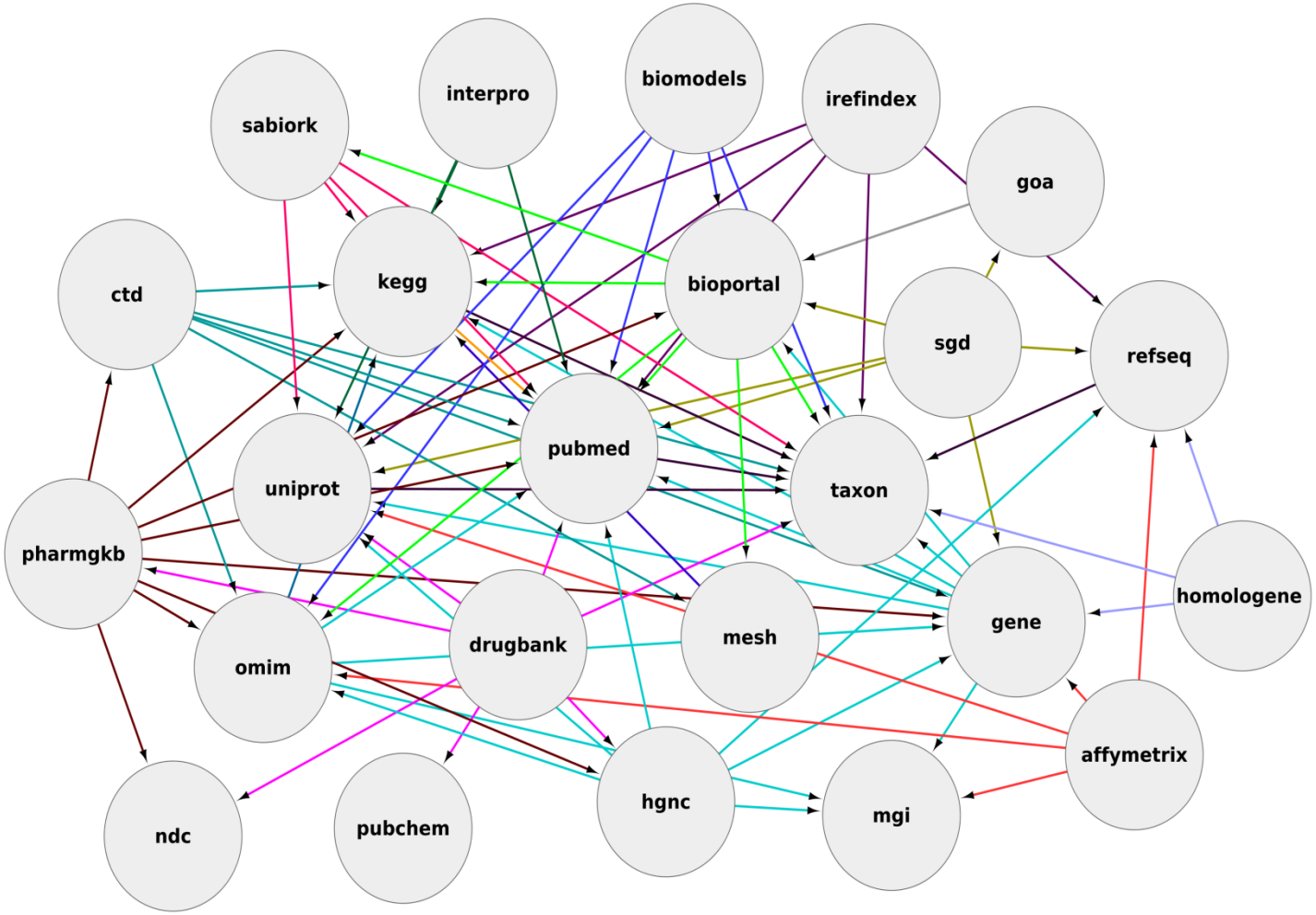
Vocabularies

VoID
Dublin Core
W3C Provenance
Bio2RDF vocabulary

Bio2RDF Release 2 – New and Updated Datasets

Dataset	Namespace	# of triples
Affymetrix	affymetrix	44469611
Biomodels*	biomodels	589753
Comparative Toxicogenomics Database	ctd	141845167
DrugBank	drugbank	1121468
NCBI Gene	ncbigene	394026267
Gene Ontology Annotations	goa	80028873
HUGO Gene Nomenclature Committee	hgnc	836060
Homologene	homologene	1281881
InterPro*	interpro	999031
iProClass	iproclass	211365460
iRefIndex	irefindex	31042135
Medical Subject Headings	mesh	4172230
NCBO BioPortal*	bioportal	15384622
National Drug Code Directory*	ndc	17814216
Online Mendelian Inheritance in Man	omim	1848729
Pharmacogenomics Knowledge Base	pharmgkb	37949275
SABIO-RK*	sabiork	2618288
Saccharomyces Genome Database	sgd	5551009
NCBI Taxonomy	taxon	17814216
Total	**19**	**1,010,758,291**

Inter-dataset connectivity

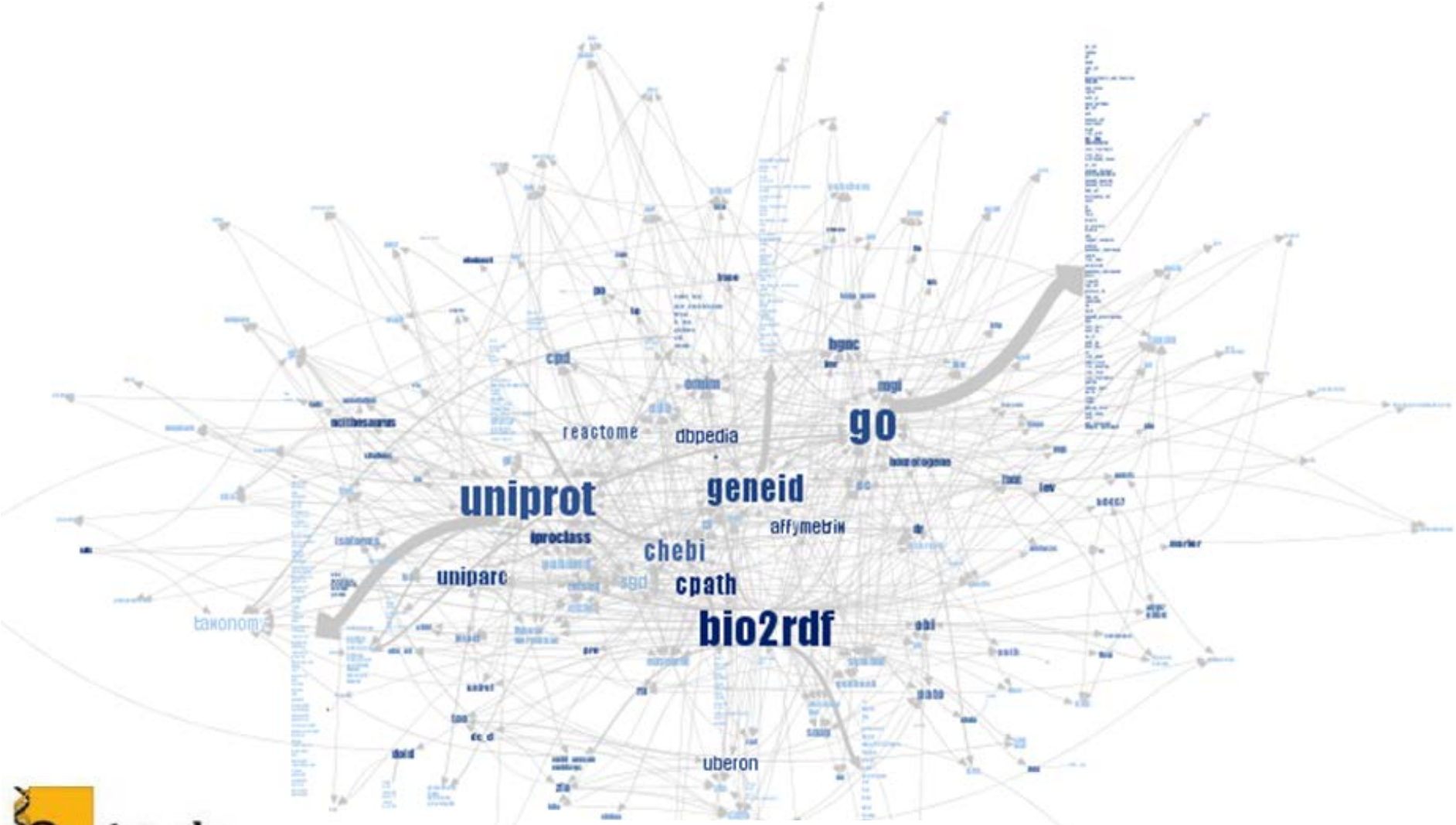


Inter and Intra dataset namespace links

Search:

Namespace	Namespace	Counts
http://bio2rdf.org/gi	http://bio2rdf.org/geneid	66560550
http://bio2rdf.org/geneid	http://bio2rdf.org/refseq	64873849
http://bio2rdf.org/taxon	http://bio2rdf.org/geneid	61059037
http://bio2rdf.org/genbank	http://bio2rdf.org/geneid	31429478
http://bio2rdf.org/geneid	http://bio2rdf.org/bio2rdf_dataset	10363740
http://bio2rdf.org/geneid	http://bio2rdf.org/pubmed	9886627
http://bio2rdf.org/go	http://bio2rdf.org/geneid	1377620
http://bio2rdf.org/eco	http://bio2rdf.org/geneid_resource	1359362
http://bio2rdf.org/geneid	http://bio2rdf.org/geneid_resource	1359362
http://bio2rdf.org/geneid	http://bio2rdf.org/geneid_resource	1359362
http://bio2rdf.org/geneid_resource	http://bio2rdf.org/bio2rdf_dataset	1359362
http://bio2rdf.org/geneid_vocabulary	http://bio2rdf.org/geneid_resource	1359362
http://bio2rdf.org/go	http://bio2rdf.org/geneid_resource	1359362
http://bio2rdf.org/unists	http://bio2rdf.org/geneid	1109358
http://bio2rdf.org/geneid	http://bio2rdf.org/ensembl	844168
http://bio2rdf.org/geneid	http://bio2rdf.org/unigene	561022
http://bio2rdf.org/pubmed	http://bio2rdf.org/geneid_resource	446186
http://bio2rdf.org/vega	http://bio2rdf.org/geneid	156033
http://bio2rdf.org/geneid_vocabulary	http://bio2rdf.org/dataset_resource	97
http://bio2rdf.org/geneid	http://bio2rdf.org/dataset_resource	12
http://bio2rdf.org/dataset_vocabulary	http://bio2rdf.org/dataset_resource	1

The Wider Network of Bio2RDF Linked Data



Centre de Recherche du CHUL (CHUQ)
Université Laval
CHUQ
QUT Queensland University of Technology
Microsoft QUT eResearch Centre
Carleton University
Powered by Virtuoso
LinkingOpenData

BIO2RDF

Linked Data for the Life Sciences

–Release 2–

[website][datasets][documentation]

NCBI Gene

NCBI Gene provides information for genes from a wide range of species. A record may include nomenclature, Reference Sequences (RefSeqs), maps, pathways, variations, phenotypes, and links to genome-, phenotype-, and locus-specific resources worldwide.

Keywords: genome, gene, DNA

Namespace: gene

Homepage: http://www.ncbi.nlm.nih.gov/gene

Organization: NCBI

License: Public domain information on the National Library of Medicine (NLM) Web pages may be freely distributed and copied. However, it is requested that in any subsequent use of this work, NLM be given appropriate acknowledgment.

Identifier Regex Pattern: ^\d+$

SPARQL Endpoint URL: http://cu.gene.bio2rdf.org/sparql

Faceted Browser URL: http://cu.gene.bio2rdf.org/fct

Conversion Script URL: http://github.com/bio2rdf/bio2rdf-scripts/tree/master/gene

Download URL: http://download.bio2rdf.org/release/2/gene

Contents

Basic data metrics

Search:

Endpoint URL	http://cu.gene.bio2rdf.org/sparql
Unique Predicate count	60
Number of Triples	394026267
Unique Subject count	12543449
Unique Object count	121538103

List of unique types and their frequencies

Search:

Type URI	Count
http://bio2rdf.org/geneid:vocabulary:Gene	10363740
http://bio2rdf.org/geneid:vocabulary:protein-coding-gene	9696194
http://bio2rdf.org/geneid_vocabulary:Gene-process-Association	555519
http://bio2rdf.org/geneid_vocabulary:Gene-function-Association	361870
http://bio2rdf.org/geneid:vocabulary:pseudo-gene	322624
http://bio2rdf.org/geneid_vocabulary:Gene-component-Association	322122
http://bio2rdf.org/geneid:vocabulary:tRNA-gene	181973
http://bio2rdf.org/geneid:vocabulary:unknown-gene	41476

List of the unique predicate-object links and their counts

Search:

Predicate URI	Object Count
http://bio2rdf.org/geneid_vocabulary:has_protein_accession	45183309
http://bio2rdf.org/geneid_vocabulary:has_taxid	36614440
http://bio2rdf.org/geneid_vocabulary:has_genomic_nucleotide_accession	34159091
http://bio2rdf.org/geneid_vocabulary:has_genomic_nucleotide_gi	34080237
http://bio2rdf.org/geneid_vocabulary:has_protein_gi	25129500
http://www.w3.org/1999/02/22-rdf-syntax-ns#type	21966993
http://rdfs.org/ns/void#inDataset	11603251
http://bio2rdf.org/geneid_vocabulary:has_pubmed_id	9886627
http://bio2rdf.org/geneid_vocabulary:has_rna_nucleotide_genbank_accession	3983786
http://bio2rdf.org/geneid_vocabulary:has_rna_gi	3983785
http://bio2rdf.org/geneid_vocabulary:has_rna_nucleotide_accession	3215317
http://bio2rdf.org/geneid_vocabulary:has_rna_nucleotide_gi	3163309
http://bio2rdf.org/geneid_vocabulary:evidence	1358492
http://bio2rdf.org/geneid_vocabulary:go_term	1239511
http://bio2rdf.org/geneid_vocabulary:gene	1239511

List of the unique predicate-literal links and their counts

Search:

Predicate URI	Literal Count
http://bio2rdf.org/geneid_vocabulary:has_start_position	23237101
http://bio2rdf.org/geneid_vocabulary:has_end_position	23235859
http://bio2rdf.org/geneid_vocabulary:has_orientation	20727859
http://bio2rdf.org/geneid_vocabulary:has_status	20616926
http://www.w3.org/2000/01/rdf-schema#label	11603253
http://bio2rdf.org/geneid_vocabulary:has_locus_tag	10363740
http://bio2rdf.org/geneid_vocabulary:has_symbol	10363740
http://bio2rdf.org/geneid_vocabulary:modification_date	10363740
http://bio2rdf.org/geneid_vocabulary:has_description	10355316
http://bio2rdf.org/geneid_vocabulary:has_chromosome	2664327

Graph summaries in query formulation

List of the total number of subject type-predicate-object type links

Search:

Subject Type	Subject Count	Predicate	Object Type	Object Count
http://bio2rdf.org/drugbank_vocabulary:Dosage	230	http://bio2rdf.org/drugbank_vocabulary:route	http://bio2rdf.org/drugbank_vocabulary:Route	42
http://bio2rdf.org/drugbank_vocabulary:Drug	6511	http://bio2rdf.org/drugbank_vocabulary:calculated-property	http://bio2rdf.org/drugbank_vocabulary:f8167ecb8671078eb5d5a76d3a977e76	6511
http://bio2rdf.org/drugbank_vocabulary:Drug	6094	http://bio2rdf.org/drugbank_vocabulary:target	http://bio2rdf.org/drugbank_vocabulary:Target	4081
http://bio2rdf.org/drugbank_vocabulary:Drug	1266	http://bio2rdf.org/drugbank_vocabulary:dosage	http://bio2rdf.org/drugbank_vocabulary:Dosage	230
http://bio2rdf.org/drugbank_vocabulary:Drug	1127	http://bio2rdf.org/drugbank_vocabulary:product	http://bio2rdf.org/drugbank_vocabulary:Pharmaceutical	11512
http://bio2rdf.org/drugbank_vocabulary:Drug	1074	http://bio2rdf.org/drugbank_vocabulary:ddi-interactor-in	http://bio2rdf.org/drugbank_vocabulary:Drug-Drug-Interaction	10891

```
PREFIX drugbank_vocabulary: <http://bio2rdf.org/drugbank_vocabulary:>
PREFIX rdfs: <http://www.w3.org/2000/01/rdf-schema#>
SELECT ?ddi ?d1name ?d2name
WHERE {
        ?ddi a drugbank_vocabulary:Drug-Drug-Interaction .
        ?d1 drugbank_vocabulary:ddi-interactor-in ?ddi .
        ?d1 rdfs:label ?d1name .
        ?d2 drugbank_vocabulary:ddi-interactor-in ?ddi .
        ?d2 rdfs:label ?d2name.
    FILTER (?d1 != ?d2)
}
```

You can use the SPARQLed query assistant with updated endpoints

http://sindicetech.com/sindice-suite/sparqled/

```
1  PREFIX rdf: <http://www.w3.org/1999/02/22-rdf-syntax-ns#>
2
3  SELECT ?drugname ?genename WHERE {
4     ?s a <http://bio2rdf.org/pharmgkb_vocabulary:Drug-Gene-Association> .
5     ?s <
6  }
7  LIMIT 1
8
```

```
<http://bio2rdf.org/pharmgkb_vocabulary:association_type>
<http://www.w3.org/2000/01/rdf-schema#label>
<http://bio2rdf.org/pharmgkb_vocabulary:drug>
<http://bio2rdf.org/pharmgkb_vocabulary:gene>
<http://rdfs.org/ns/void#inDataset>
<http://bio2rdf.org/pharmgkb_vocabulary:article>
<http://bio2rdf.org/pharmgkb_vocabulary:pd_relationship>
<http://bio2rdf.org/pharmgkb_vocabulary:pk_relationship>
```

```
1  PREFIX rdf: <http://www.w3.org/1999/02/22-rdf-syntax-ns#>
2
3  SELECT ?drugname ?genename WHERE {
4     ?s a <http://bio2rdf.org/pharmgkb_vocabulary:Drug-Gene-Association> .
5     ?s <http://bio2rdf.org/pharmgkb_vocabulary:drug> ?drug .
6     ?s <http://bio2rdf.org/pharmgkb_vocabulary:gene> ?gene .
7     ?drug <http://www.w3.org/2000/01/rdf-schema#label> ?drugname .
8     ?gene <http://www.w3.org/2000/01/rdf-schema#label> ?genename .
9  }
10 LIMIT 10
```

graph: http://sindicetech.com/analytics

Use virtuoso's built in faceted browser to construct increasingly complex queries with little effort

OPENLINK SOFTWARE

Displaying List of Distinct Entity Names ordered by Count where:

Entity1 is a **http://bio2rdf.org/d...ug-Drug-Interaction** . Drop
Entity2 **<http://bio2rdf.org/d...y:ddi-interactor-in>** Entity1 . Drop Entity2

View query as SPARQL Facet permalink

Go to: Show 20 1 - 20 of 1109 total

Entity		Count
Voriconazole [drugbank:DB00582]	Describe	246
Triprolidine [drugbank:DB00427]	Describe	200
Telithromycin [drugbank:DB00976]	Describe	195
Trimipramine [drugbank:DB00726]	Describe	174
Warfarin [drugbank:DB00682]	Describe	174

Federated Queries over independent SPARQL endpoints

get all biochemical reactions in biomodels that are kinds of "protein catabolic process“, as defined by the gene ontology (in bioportal endpoint)

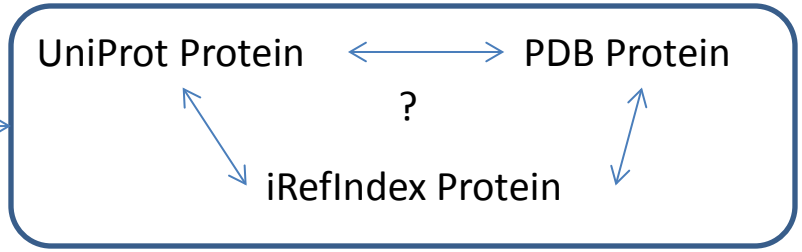
SPARQL Endpoint: http://bioportal.bio2rdf.org/sparql

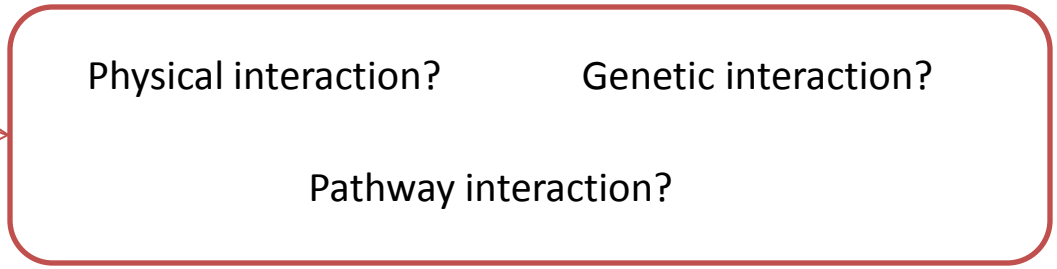
```
SELECT ?go ?label count(distinct ?x)
WHERE {
   ?go rdfs:label ?label .
   ?go rdfs:subClassOf ?tgo OPTION (TRANSITIVE) .
   ?tgo rdfs:label ?tlabel .
   FILTER regex(?tlabel, "^protein catabolic process")
   service <http://biomodels.bio2rdf.org/sparql> {
    ?x <http://bio2rdf.org/biopax_vocabulary:identical-to> ?go .
    ?x a <http://www.biopax.org/release/biopax-level3.owl#BiochemicalReaction> .
   } # end service
}
```

Heterogeneous biological data on the semantic web is difficult to query

Question: Find all proteins that interact with beta amyloid

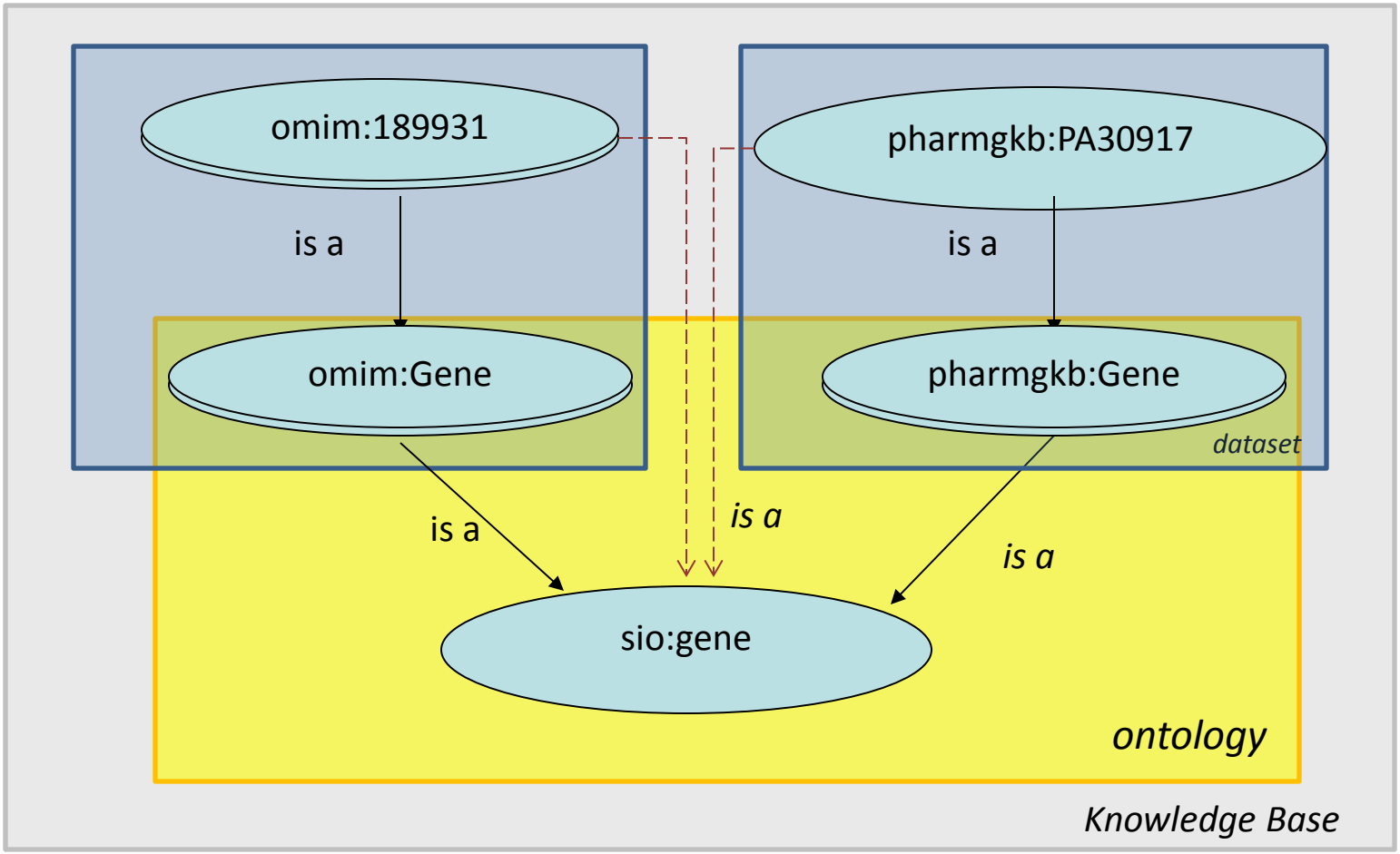
```
SELECT * WHERE {
    ?protein a bio2rdf:Protein .
    ?protein bio2rdf:interacts_with bio2rdf:beta-amyloid
    .
}
```





ontology as a strategy to formally represent and integrate knowledge

Semantic data integration, consistency checking and query answering over Bio2RDF with the Semanticscience Integrated Ontology (SIO)



Querying Bio2RDF Linked Open Data with a Global Schema. Alison Callahan, José Cruz-Toledo and Michel Dumontier. Bio-ontologies 2012.

- entity
  - attribute
  - object
    - 'information content entity'
    - 'material entity'
      - 'chemical entity'
        - atom
        - 'chemical substance'
        - 'covalently connected entity'
          - molecule
            - antigen
            - catalyst
            - drug
            - isomer
            - ligand
            - 'molecular regulator'
            - 'organic molecule'
            - 'pharmaceutical component'
            - polymer
            - primer
            - product
            - 'signal transducer'
            - substrate
            - target
        - 'specialized chemical entity'
        - 'submolecular entity'
      - 'heterogeneous substance'
      - wave
    - 'spatial region'
  - process

- topObjectProperty
  - 'is related to'
    - 'has attribute'
    - 'is attribute of'
    - 'is comparable to'
      - 'is numerically comparable to'
      - 'is variant of'
        - 'is dissimilar to'
        - 'is homologous to'
        - 'is similar to'
          - 'is broader than (t)'
            - 'is broader than'
          - 'is match to'
          - 'is narrower than (t)'
        - 'is version of'
    - 'is generically related with'
    - 'is mutually related to'
    - 'is referred to by'
    - 'is spatiotemporally related to'
    - 'refers to'

SRIQ(D)
10700+ axioms
1300+ classes
201 object properties (inc. inverses)
1 datatype property

Annotations

description
"An isomer is a molecule that is compositionally identical to another molecule as a result of a different atomic connectivity."@en

label
"isomer"@en

Description: isomer

Equivalent classes

molecule
and ('is variant of' some molecule)

Superclasses

Inherited anonymous classes

'has part' some
(atom
and ('is covalently connected to' some atom))

'has component part' some 'covalent chemical bond'

'physical entity'
or 'abstract entity'

'has proper part' only 'material entity'

'has quality' some mass

'has quality' only 'physical quality'

'spatiotemporal region'
or ('is located in' some 'spatiotemporal region')

'has proper part' only 'physical entity'

'processual entity'
or 'material entity'
or region

'has part' some atom

Bio2RDF and SIO powered SPARQL 1.1 federated query: Find chemicals in CTD and proteins in SGD that participate in the same GO process

```
SELECT ?chem, ?prot, ?proc
FROM <http://bio2rdf.org/ctd>
WHERE {
    ?chemical a sio:chemical-entity.
    ?chemical rdfs:label ?chem.
    ?chemical sio:is-participant-in ?process.
    ?process rdfs:label ?proc.
   FILTER regex (?process, "http://bio2rdf.org/go:")
    SERVICE <http://sgd.bio2rdf.org/sparql> {
        ?protein a sio:protein .
        ?protein sio:is-participant-in ?process.
        ?protein rdfs:label ?prot .
    }
}
```

Bio2RDF RDFization guidelines are available at our wiki

PUBLIC bio2rdf / bio2rdf-scripts

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RDFization Guide v1.1

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The linked data that forms part of **Bio2RDF** ascribes a to simple set of modeling patterns that permit our different datasets to syntactically interoperate. The *best practices* here presented have been inspired by the Banff Manifesto, Tim Berner-Lee's design principles and the collective experience of our community. This document provides a simple set of guidelines to guide *Bio2RDF* users and contributors in the creation and querying of our data.

This guide will assume that you have working experience in creating RDF documents programatically. If this describes you, then read on!

Table of Contents

Reusing known identifiers

The over 1800 biological databases that are currently available usually provide unique identifiers for every record that they contain. For example, the Protein Databank uses a four character string to represent their unique entries (e.g. 1Y26), similarly PubMed uses an integer to identify publication records (e.g. 22359647).

https://github.com/bio2rdf/bio2rdf-scripts/wiki/RDFization-Guide-v1.1

What the future holds

- Aiming for twice yearly release schedule. Next release will include large datasets (>15B RefSeq, Genbank, PubMed, PDB)
- Working with **identifiers.org** to create a common registry with 2200 entries
  - Spiking in identifiers.org and original data uris, where available
- Consolidating provenance/metrics with **OpenPHACTS**
- Incorporate W3C Linking Open Drug Data (LODD) effort
  - **OMIM** (released), **SIDER** (beta), CHEMBL (beta), **LinkedCT** (beta), DailyMed (RDF available), TCM (RDF available),
- Extended dataset coverage by tapping into existing endpoints (uniprot, bioportal, ebi-rdf?)
- Showcase with other third party tools

Bio2RDF Release 2 – A summary

- Updated data conversion source code to use PHP API (all available through GitHub)
  - http://github.com/bio2rdf/bio2rdf-scripts
  - https://github.com/bio2rdf/bio2rdf-scripts/wiki/RDFization-Guide-v1.1
- Simple Bio2RDF IRI design patterns that facilitate syntactic consistency and interoperability backed by simple registry
- Dataset provenance and metrics
- We welcome comments, suggestions and contributions
  - **Join our mailing list at bio2rdf@googlegroups.com**

Acknowledgements

Bio2RDF Release 2

Allison Callahan, Jose Cruz-Toledo, Peter Ansell

Bio2RDF

Francois Belleau, Marc-Alexandre Nolin

Alex De Leon, Steve Etlinger, Nichealla Keath

Jacques Corbeil, James Hogan Jean Morissette, Nicole Tourigny, Philippe Rigault and Paul Roe

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