

BridgeDb and Wikidata: a powerful combination generating interoperable open research

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Egon Willighagen (on behalf)
@egonwillighagen
0000-0001-7542-0286



Maastricht University

bridgedb.github.io



NWO Open Science grant

grant number: 203.001.121

BridgeDb and Wikidata: a powerful combination generating interoperable open research (BridgeDb)

▼ [Egon L. Willighagen](#), [Martina Kutmon](#), [Marvin Martens](#), [Denise Slenter](#)

Abstract ▲

Like humans have a unique social security number and different phone numbers from various providers, so do proteins and metabolites have a unique structure but different identifiers from various databases. BridgeDb is an interoperability platform that allows combining these databases, by matching database-specific identifiers. These matches are called identifier mappings, and they are indispensable when combining experimental (omics) data with knowledge in reference databases. BridgeDb takes care of this interoperability between gene, protein, metabolite, and other databases, thus enabling seamless integration of many knowledge bases and wet-lab results. Since databases get updated continuously, so should the Open Science BridgeDb project.

Keywords ▲

BridgeDb, Wikidata, open science, identifie

Dutch public summary ▲

Net zoals mensen een uniek Burgerservicenummer (BSN) hebben en verschillende telefoonnummers van diverse telecomaandbieders, zo hebben eiwitten en metabolieten een unieke structuur maar andere

[Article metadata](#)

[Dutch public summary](#)

[Project proposal](#)

— [The vision for your project](#)

— [Project plan](#)

— [Team members](#)

[Open Science track record of the main applicant](#)

[Data management](#)

— [Will this project involve re-using existing research data?](#)

— [Will data be collected or generated that are suitable for reuse?](#)

— [After the project has been completed, how will the data be stored for the long-term and made available for the use by third parties? Are there possible restrictions to data sharing or embargo reasons?](#)

— [Will any costs \(financial and time\) related to data management and sharing/preservation be incurred?](#)

[Software sustainability](#)

— [Will software be generated during the project?](#)

— [How will the software be licensed and be made available for re-use?](#)

— [What measures are needed to make the software appropriate for long-term \(re-\)use by third parties?](#)

Project Plan

The project plan is organized in three work packages (WP1, WP2, WP3), following the three output themes. Work package 1 (**WP1**) intends to upgrade the BridgeDb Java library. Currently, the main Java library is already built with Apache Maven, however, the build system should also be applied to related tools, and we will extensively use GitHub Actions for automation. Second, only a subset of library modules is currently available as OSGi bundles, which is essential for reuse in various third-party tools, like PathVisio ([Kutmon et al. 2015](#)) and Cytoscape ([Kutmon et al. 2013](#), [Shannon et al. 2003](#)). Therefore all modules will be extended to support OSGi bundles, something that is already done for five core BridgeDb modules. Furthermore, to improve maintainability, WP1 will continue extending the unit tests and integration tests. Particularly, the testing of the database backends that hold the ID mapping data (Apache Derby and MySQL) needs to become more comprehensive.

Work package 2 (**WP2**) focuses on the BridgeDb Webservice. This continuously running service is an ELIXIR *RIR* and daily supports projects like WikiPathways and Cytoscape to assist data analysis of omics datasets (transcriptomics, proteomics, metabolomics, etc.). The Webservice will be extended to support Compact Identifiers ([Wimalaratne et al. 2018](#)) as a new input and output format, in order to support persistent, machine-resolvable citation of research data in written material. Furthermore, we will introduce support for JavaScript Object Notation (JSON) as a serialization format for multiple application programming interface (API) calls. The OpenAPI (Swagger) interactive documentation will be updated accordingly. Furthermore, the Webservice itself will become even more FAIR, by adopting the DataCite standard, and providing provenance in the HCLS Community Profile for Dataset descriptions.

The last work package (**WP3**) translates the new functionalities to practical use cases. In this WP, existing ID mapping databases will be updated, using the new releases of BridgeDb Java library and tested in applications using the new BridgeDb version. We intend to widen the scope of ELIXIR resources supported in the ID mapping databases, to make more resources interoperable (and therefore more FAIR). Here, we will increasingly use Wikidata and its international scientific collaborations ([Waagmeester et al. 2021](#), [Waagmeester et al. 2020](#)). These mapping databases will continue to be released via public archives (e.g. Figshare, Zenodo) under open licenses, and indexed on the BridgeDb website annotation at bridgedb.github.io/data/gene_database/. To do so, WP3 will develop a tool that takes DOIs of the mapping databases as input to extract metadata from the respective repositories and generate this indexing website. WP3 will test the resulting mapping databases with downstream tools (PathVisio, WikiPathways, Cytoscape, etc.). Docker Images of the various tools will be developed to simplify dissemination and reuse. Practically, this work will involve two hackathons involving the senior scientific employees (Slenter, Kutmon, Martens) and the full-time non-scientific personnel (see the Section *Team members* and Table [1](#)).



BridgeDb

SOFTWARE

Open Access

The BridgeDb framework: standardized access to gene, protein and metabolite identifier mapping services

Martijn P van Iersel^{1*}, Alexander R Pico², Thomas Kelder¹, Jianjiong Gao³, Isaac Ho², Kristina Hanspers², Bruce R Conklin^{2,4}, Chris T Evelo³

Abstract

Background: Many complementary solutions are available for the identifier mapping problem. This creates an opportunity for bioinformatics tool developers. Tools can be made to flexibly support multiple mapping services or mapping services could be combined to get broader coverage. This approach requires an interface layer between tools and mapping services.

Results: Here we present BridgeDb, a software framework for gene, protein and metabolite identifier mapping. This framework provides a standardized interface layer through which bioinformatics tools can be connected to different identifier mapping services. This approach makes it easier for tool developers to support identifier mapping. Mapping services can be combined or merged to support multi-omics experiments or to integrate custom microarray annotations. BridgeDb provides its own ready-to-go mapping services, both in webservice and local database forms. However, the framework is intended for customization and adaptation to any identifier mapping service. BridgeDb has already been integrated into several bioinformatics applications.

Conclusion: By uncoupling bioinformatics tools from mapping services, BridgeDb improves capability and flexibility of those tools. All described software is open source and available at <http://www.bridgedb.org>.

Background

Many interesting problems in bioinformatics require the integration of experimental data from different sources. Examples include merging two independently created protein-protein interaction networks in Cytoscape[1] and visualizing microarray data on a collection of biological pathways in GenMAPP[2] or PathVisio[3]. More often than not, data of different types and from different sources are annotated with different identifiers. Thus, an important step in the analysis workflow is deducing which identifiers from one set correspond to which identifiers in the other set.

This problem of identifier mapping has been recognized, and a number of resources have been developed to solve it, including DICT[4], CRONOS[5], MatchMiner[6], AliasServer[7], PICR[8], Synergizer[9] and

Ensembl BioMart[10]. For the most part, these resources accurately map identifiers and provide an interface, usually a web site, to the mappings. However, each resource necessarily has a focused domain of application based on limitations in resources and in the interest of its developers. Mapping services differ in aspects, such as coverage of species, coverage of identifier types, access speed and frequency of database updates. This has created two challenges for developers of bioinformatics applications. The first challenge is to develop software that is not tied to a single identifier mapping service. Tools that are built around a single service would have to be adapted with considerable effort if a more suitable service comes along. Optimally, switching should be a simple matter of configuration. The second challenge is to combine mapping services to get the benefits of each. For example, one could combine a small mapping table of probe identifiers of a custom microarray with a large mapping resource, such as Ensembl BioMart, or one could combine metabolite

* Correspondence: martijn.vaniersel@bigcut.unima.nl

¹Department of Bioinformatics - BiGCaT, Maastricht University, Maastricht, the Netherlands



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* Correspondence: martijn.vaniersel@biocat.unima.nl

¹Department of Bioinformatics - BiGaT, Maastricht University, Maastricht, the Netherlands



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Maastricht University

BridgeDb

F1000Research

F1000Research 2016, 7(ELIXIR):1960 Last updated: 10 OCT 2019



SOFTWARE TOOL ARTICLE

Providing gene-to-variant and variant-to-gene database identifier mappings to use with BridgeDb mapping services.

[version 1; peer review: 1 approved, 1 not approved]

Friederike Ehrhart^{1,2}, Jonathan Melius¹, Elisa Cirillo¹, Martina Kulmon^{1,3}, Egon L. Willighagen¹, Susan L. Coort¹, Leopold M.G. Curfs², Chris T. Evelo^{1,3}

¹Department of Bioinformatics - BiGaT, NUTRIM, Maastricht University, Maastricht, 6200 MD, The Netherlands

²R&C-Part Expertise Centre, Maastricht University Medical Center, Maastricht, 6200 MD, The Netherlands

³Maastricht Centre for Systems Biology (MacSBo), Maastricht University, Maastricht, 6200 MD, The Netherlands

V1 First published: 03 Sep 2016, 7(ELIXIR):1960 (<https://doi.org/10.12688/f1000research.15706.1>)
Latest published: 03 Sep 2016, 7(ELIXIR):1960 (<https://doi.org/10.12688/f1000research.15706.1>)

Abstract

Database identifier mapping services are important to make database information interoperable. BridgeDb offers such a service. Available mapping for BridgeDb link 1. genes and gene products identifiers, 2. metabolite identifiers and InChI structure description, and 3. identifiers for biochemical reactions and interactions between multiple resources that use such IDs while the mappings are obtained from multiple sources. In this study we created BridgeDb mapping databases for selections of genes-to-variants (and variants-to-genes) based on the variants described in Ensembl. Moreover, we demonstrated the use of these mappings in different software tools like R, PathVisio, Cytoscape and a local installation using Docker. The variant mapping databases are now described on the BridgeDb website and are available from the BridgeDb mapping database repository and updated according to the regular BridgeDb mapping update

Open Peer Review

Reviewer Status

Invited Reviewers	
1	2
version 1 published 03 Sep 2016	report report

1 **Patrice Godard** , UCB (Union Chimique Belge), Brussels, Belgium

2 **Osman Ugur Sezerman**, Acibadem University, Istanbul, Turkey

Any reports and responses or comments on the

Increasing the nanopublication recall with a BridgeDb Identifier Mapping Service

Egon Willighagen¹ [0000-0001-7542-0286]

Dept. Bioinformatics - BiGaT, NUTRIM, Maastricht University, NL
egon.willighagen@maastrichtuniversity.nl

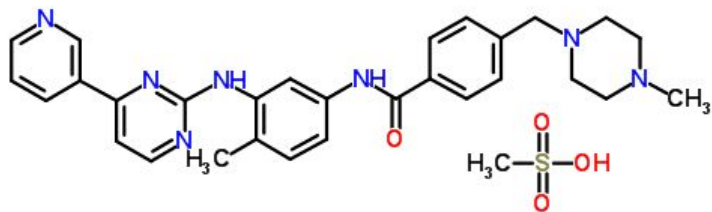
Abstract. The volume of literature in the life sciences is continuously growing and keeping up with it is a problem. While review articles and databases help us by summarizing vast amounts of research, dissemination of core research outcomes is still mostly restricted to scholarly journal. Nanopublications have been proposed as a solution to capture scientific statements. This led to a 2010 proposal to serialize nanopubs in the Resource Description Framework (RDF) and in 2016 to an international network of nanopublication servers. However, RDF has a limitation that the Internationalized Resource Identifier (IRI) for resources does not have to be normalized and unique. To overcome this issue, the Open PHACTS project developed an Identifier Mapping Service and an approach called *scientific lenses* for mapping of equivalent IRIs. We here demonstrate the application of this approach to improve the recall of

What is BridgeDb exactly?

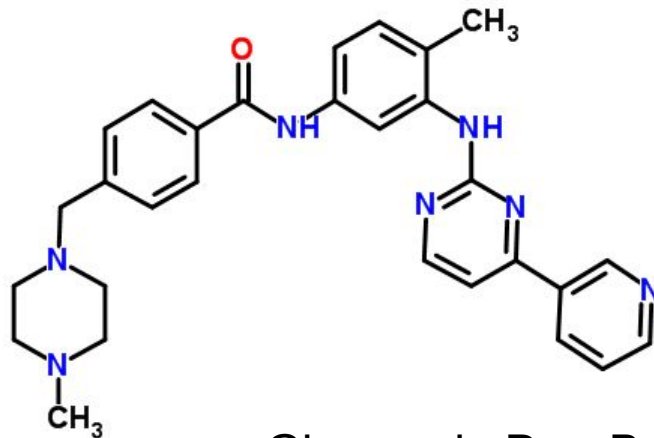
- A real-world need
- Java library
- A webservice
- identifier mappings
- integrations into other platforms



Motivation

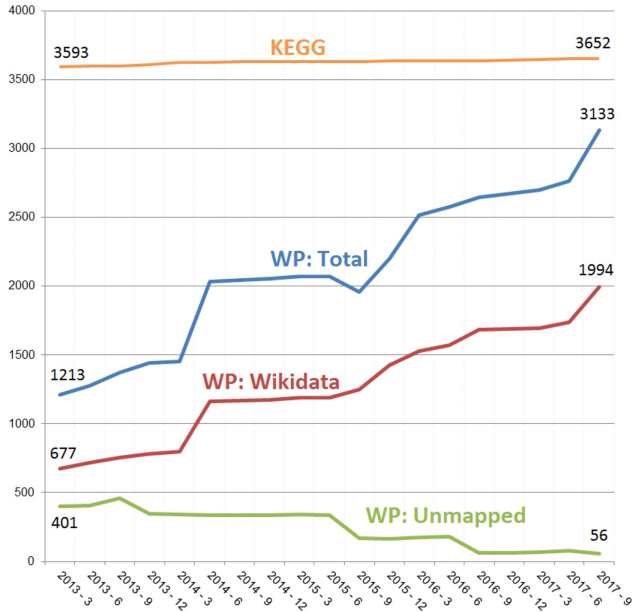
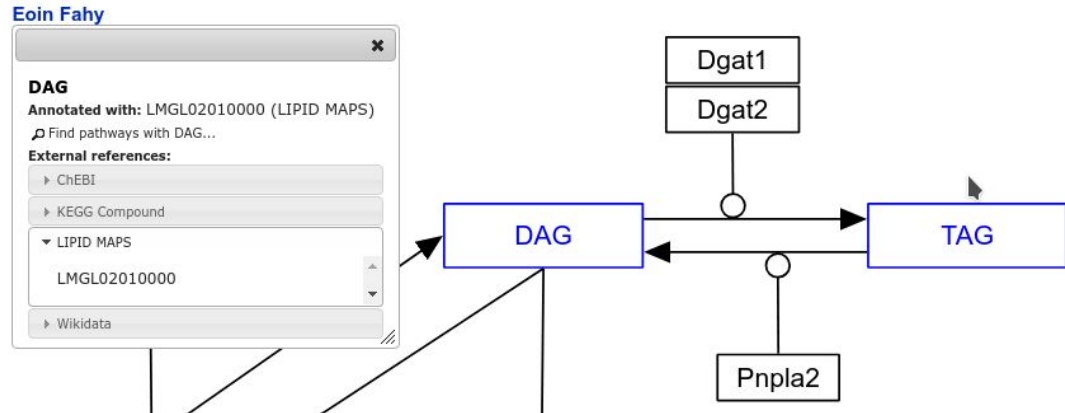
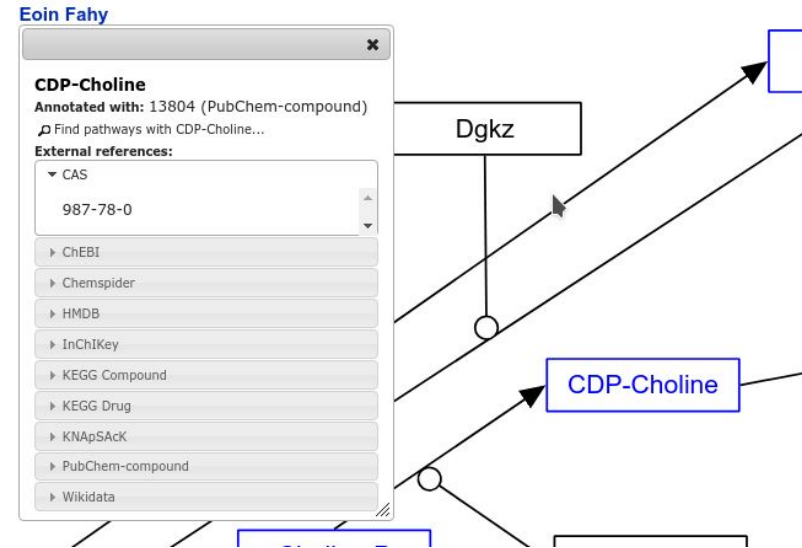


Gleevec in ChemSpider and ChEMBL
(imatinib mesylate)



Gleevec in DrugBank
(actually imatinib)

Use Case: WikiPathways

Denise Slenter *et al*, 10.1093/nar/gkx1064

*WP4351.r98614.gpml - PathVisio 3.4.0

File Edit Data View Plugins Help

Zoom: 127,6%

Title: Omega-9 FA synthesis
Organism: Mus musculus

metaboliite annotation

Identifier:	LMFA01010012
Database:	LIPID MAPS

Cross references

CAS
143-07-7

ChEBI
30805
41882
CHEBI:30805
CHEBI:41882

Gene database: ...Derby_Ensembl_91.bridge | Metabolite database: ...data_metabolites.bridge | Interaction database: null

one entity, one
identifier

entities and
interactions can
cite literature

BridgeDb ID mapping files:

1. genes/proteins
2. metabolites
3. interactions

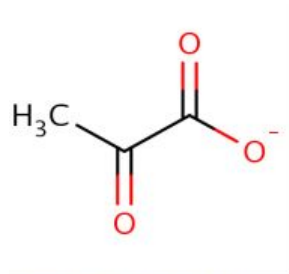
links to other
databases

Identifier mapping complexity

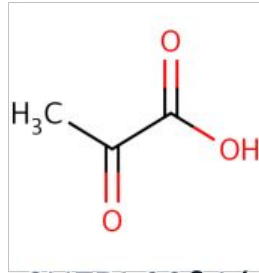


Chemistry in metabolic pathways

CHEBI:15361 (Pyruvate) -> Ce:CHEBI:32816 (conjugate) -> Ck:C00022 -> [WP2456 HIF1A and PPARG regulation of glycolysis, WP2453 TCA Cycle and PDHc]

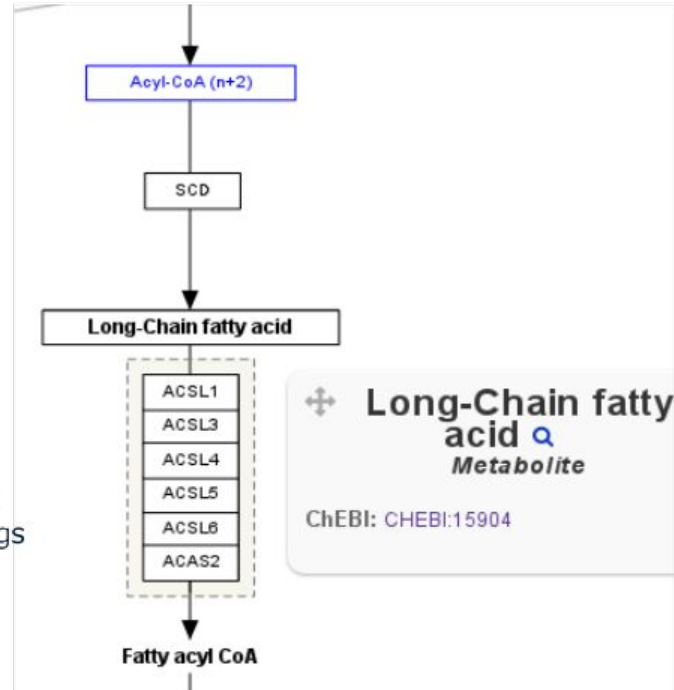


CHEBI:15361



CHEBI:32816

Brenninkmeijer, CYA, et al. "Scientific Lenses over Linked Data: An approach to support task specific views of the data. A vision." Proceedings of 2nd International Workshop on Linked Science. 2012.



Metabolite Identifier Mapping

Related Compounds

Show entries

Search:

Mol	InChIKey	CAS	ChemSpider	PubChem CID
acetate ion	QTBSBXVTEAMEQO-UHFFFAOYSA-M	71-50-1	170	175
acetic acid c-14	QTBSBXVTEAMEQO-HQMMCQRPSA-N	2845-03-6	144444	164769
deuterated acetic acid	QTBSBXVTEAMEQO-GUEYOVJQSA-N	1186-52-3	2006083	2723903
acetic acid	QTBSBXVTEAMEQO-UHFFFAOYSA-N	64-19-7	171	176
acetic acid c-13	QTBSBXVTEAMEQO-VQEHIDDOSA-N	1563-79-7	8329490	10153982
acetic acid c-11	QTBSBXVTEAMEQO-JVVVGQRLSA-N	78887-71-5	396653	450349

[Edit on query.Wikidata.org](#)

Showing 1 to 6 of 6 entries

Previous

1

Next



What about genes/proteins?

- UniProt/Ensembl
 - focuses on the concept gene/protein
 - no DNA variations (single nucleotide polymorphism)
- Protein Data Bank
 - proteins with specific SNPs
- Post-translational modifications
 - phosphorylation, etc
- Book equivalent:
 - book with ISBN, and the physical book in the library

Where do the mappings come from?

Sources of identifier mappings

- genes and proteins
 - **Ensembl**, NCBI, HGNC, UniProt, ...
- metabolites
 - **HMDB**, **ChEBI**, PubChem, **Wikidata**, ...
- publications
 - DOI, PubMed (from **Wikidata**)
- interactions
- SARS-CoV-2 proteins
 - before UniProt; from **Wikidata**



When using these files in studies, please cite the data following the [DataCite](#) standard. And thanks to [Zenodo](#) and [Figshare](#) for hosting the data.

Requests for additional identifier mapping files can be posted [here](#).

Gene / Protein ID mapping databases

JSON source

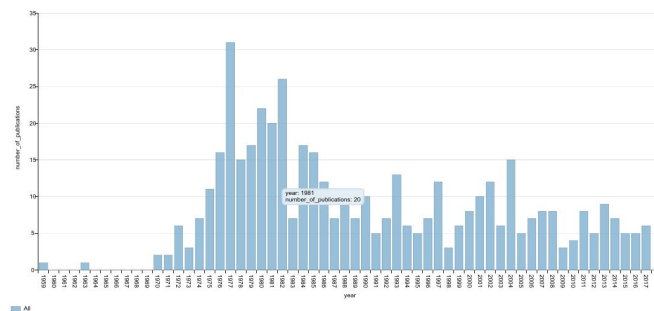
Species	BridgeDb Download	QC report	Size	DOI	License	Date	Tested with
Anopheles gambiae	Ag_Derby_Ensembl_Metazoa_49.bridge	QC	45.0 MB	(doi:10.5281/zenodo.6500401)	license	2022-04-28	PathVisio 3.3
Aspergillus niger	An_Derby_Ensembl_Fungi_49.bridge	QC	32.2 MB	(doi:10.5281/zenodo.6502081)	license	2022-04-28	PathVisio 3.3
Arabidopsis thaliana	At_Derby_Ensembl_Plant_49.bridge	QC	199.7 MB	(doi:10.5281/zenodo.6502052)	license	2022-04-28	PathVisio 3.3
Bacillus subtilis	Bs_Derby_Ensembl_91.bridge			(doi:10.5281/zenodo.3667670)	license		
Bos taurus	Bt_Derby_Ensembl_105.bridge	QC	160.8 MB	(doi:10.5281/zenodo.6502115)	license	2022-04-28	PathVisio 3.3
Caenorhabditis elegans	Ce_Derby_Ensembl_105.bridge	QC	177.0 MB	(doi:10.5281/zenodo.6502115)	license	2022-04-28	PathVisio 3.3
Canis familiaris	Cf_Derby_Ensembl_105.bridge	QC	146.1 MB	(doi:10.5281/zenodo.6502115)	license	2022-04-28	PathVisio 3.3



ID mapping sources: HMDB, ChEBI, and Wikidata



Publications per year



Show **10** entries

Search:

Mol	InChIKey	CAS	ChemSpider	PubChem CID
acetic acid	QTBSBXVTEAMEQO-UHFFFAOYSA-N	64-19-7	171	176
deuterated acetic acid	QTBSBXVTEAMEQO-GUEYOVJQSA-N	1186-52-3	2006083	2723903
acetic acid c-14	QTBSBXVTEAMEQO-HQMMCQRPSA-N	2845-03-6	144444	164769
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acetate ion	QTBSBXVTEAMEQO-UHFFFAOYSA-M	71-50-1	170	175

[Edit on query.Wikidata.org](#)

Showing 1 to 6 of 6 entries

Previous

1

Next

IDpred	IDpredLabel	count
Q wd:P235	InChIKey	152393
Q wd:P233	canonical SMILES	152233
Q wd:P234	InChI	149944
Q wd:P662	PubChem CID	145798
Q wd:P661	ChemSpider ID	125510
Q wd:P2017	isomeric SMILES	84844
Q wd:P683	ChEBI ID	84011
Q wd:P231	CAS Registry Number	72475
Q wd:P652	UNII	59293
Q wd:P592	ChEMBL ID	49622
Q wd:P3117	DSSTOX substance identifier	36373
Q wd:P232	EC ID	20335
Q wd:P1579	Beilstein Registry Number	19083
Q wd:P665	KEGG ID	15065
Q wd:P2566	ECHA InfoCard ID	12362
Q wd:P715	Drugbank ID	7786
Q wd:P595	Guide to Pharmacology Ligand ID	5950
Q wd:P2057	HMDB ID	5705
Q wd:P2064	KNapSAck ID	4272

Willighagen, Egon; Slenter, Denise; Mietchen, Daniel; Evelo, Chris; Nielsen, Finn (2018) figshare.
<https://doi.org/10.6084/m9.figshare.6356027.v1>

Integrations

BridgeDb can be used in multiple platforms

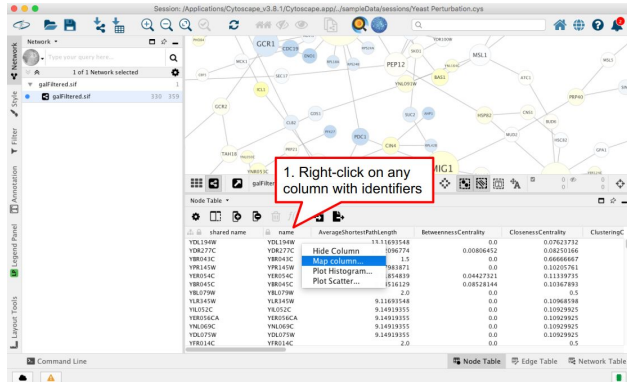
WikiPathways

Python

BridgeDb Webservice
(REST, JavaScript, ...)

Cytoscape (ht Alex Pico)

R (stats)



2. Identifier mapping with BridgeDb

Recipe Overview

Reading Time: 30 minutes | Executable Code: Yes

Difficulty: 3/5

Identifier mapping with BridgeDb

Recipe Type: Hands-on

Audience: Principal Investigator, Data Manager, Data Scientist

Maturity Level & Indicator: DOM-4-C4

Bioconductor

OPEN SOURCE SOFTWARE FOR BIOINFORMATICS

BridgeDbR

platforms: R6 rank: 638 / 2140 | support: D / 0 | in BioC: 8 years

build: OK | updated: before release | dependencies: 3

DOI: 10.18129/B3.bio.BridgeDbR

Code for using BridgeDb identifier mapping framework from within R

Bioconductor version: Release (3.15)

Use BridgeDb functions and load identifier mapping databases in R. It uses GitHub, Zenodo, and Figshare if you use this package to download identifier mappings files.

Author: Christ Leemans <christleemans@gmail.com>, Egon Willighagen <egon.willighagen@gmail.com>, Anwesha Bohler <anweshaohler@gmail.com>, Lars Eijssen <leijssen@maastrichtuniversity.nl>

Maintainer: Egon Willighagen <egon.willighagen@gmail.com>

Citation: (from within R, enter `<stat>lon("BridgeDbR")`):

Leemans C, Willighagen E, Slijter D, Bohler A, Eijssen L (2022). BridgeDbR: Code for using BridgeDb identifier mapping framework from within R. R package version 2.6.6, <https://github.com/bioconductor/BridgeDbR>.

Installation

To install this package, start R (version "4.2") and enter:

```
if (!require("BiocManager", quietly = TRUE))
  install.packages("BiocManager")
```

BridgeDb Docker Container and EOSC



BridgeDb **Explore**

bridgedb webservices 0.9.0
[Base URL: webservice.bridgedb.org]
</swagger/swagger.json>

Schemes
HTTPS ▾

Identifiers (Genes, proteins, metabolites, interactions) ▾

- GET** `/ {organism} /xrefs / {systemCode} / {identifier}`
- POST** `/ {organism} /xrefsBatch / {systemCode}`
- POST** `/ {organism} /xrefsBatch`
- GET** `/ {organism} /xrefExists / {systemCode} / {identifier}`
- GET** `/ {organism} /search / {query}`

OpenRiskNet

RISK ASSESSMENT E-INFRASTRUCTURE



<https://hub.docker.com/r/bigcatum/bridgedb/#!>

BridgeDb for NWO Open Science

wishlist: we love to hear identifier mapping needs from the other NWO Open Science grants



Maastricht University

A screenshot of the RIO (Research Ideas and Outcomes) grant proposal page. The page is titled "BridgeDb and Wikidata: a powerful combination generating interoperable open research (BridgeDb)". The author is listed as "Egon L. Willighagen, Martina Kutmon, Marvin Martens, Denise Slenter". The page includes an abstract, keywords, and a Dutch public summary. The abstract discusses the unique structure of proteins and metabolites and how BridgeDb is an interoperability platform that allows combining these databases. The keywords are "BridgeDb, Wikidata, open science, identifier". The Dutch public summary mentions the unique Burgerservicenummer (BSN) and the unique structure of proteins and metabolites. The page also features a sidebar with navigation links and a table of contents.

Acknowledgments

BridgeDb Community / mapping sources (Ensembl)

Manchester University: Carole Goble, Alasdair Gray,
Christian Brenninkmeijer

Maastricht University: Freddie Ehrhart, Jonathan Mélius,
Andra Waagmeester, *Marvin Martens*, Nuno Nunes, Chris
Evelo, *Denise Slenter*, Manas Awashti, Lucas Uberti-Bona,
Martina Kutmon, Finterly Hu

New UM: *Tooba Abbassi Dalooi*, ***Helena Basaric***



OpenRiskNet

RISK ASSESSMENT E-INFRASTRUCTURE



GLADSTONE
INSTITUTES

DATA2DISCOVERY^{INC.}



BridgeDb and Wikidata: a powerful combination generating interoperable open research

Open Science in Practice Webinar Series
2022-09-15

Egon Willighagen (on behalf)
@egonwillighagen
0000-0001-7542-0286



Maastricht University

bridgedb.github.io

