Wikidata and Scholia as hub linking metabolite knowledge

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BeNeLux Metabolomics Days
#NMCDays
Rotterdam, 2018-08-19

Maastricht University

Acknowledgements

- Finn Nielsen (Scholia inventor)
- Denise Slenter (BiGCaT PhD candidate)
- Others
  - Various Maastricht University research groups
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  - ChEBI team: Christoph Steinbeck (now Jena), Gareth Owen
  - PubChem, WikiGenomes teams: Evan Bolton, Gang Fu, Sebastian Burgstaller, Andra Waagmeester (Micelio)
  - SPLASH team: Gert Wolgemuth, Sajjan Singh Mehta
  - Wikidata & WikiCite teams: Daniel Mietchen, Dario Tataborelli
  - Wikidata:WikiProject Chemistry
  - Reactome: Robin Haw, Henning Hermjakob

WikiPathways: a multifaceted pathway database bridging metabolomics to other omics research

Denise N Slenter, Martina Kutmon, Kristina Hanspers, Anders Riutta, Jacob Windsor, Nuno Nunes, Jonathan Mélius, Elisa Cirillo, Susan L Coort, Daniela Digles ... Show more

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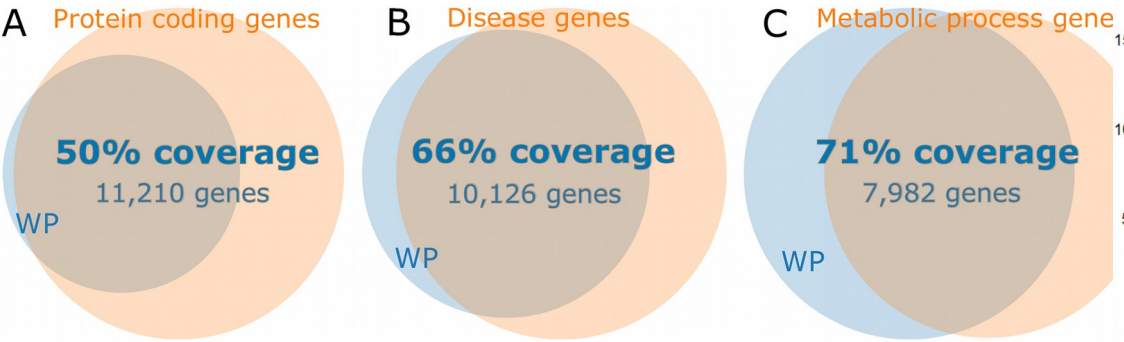
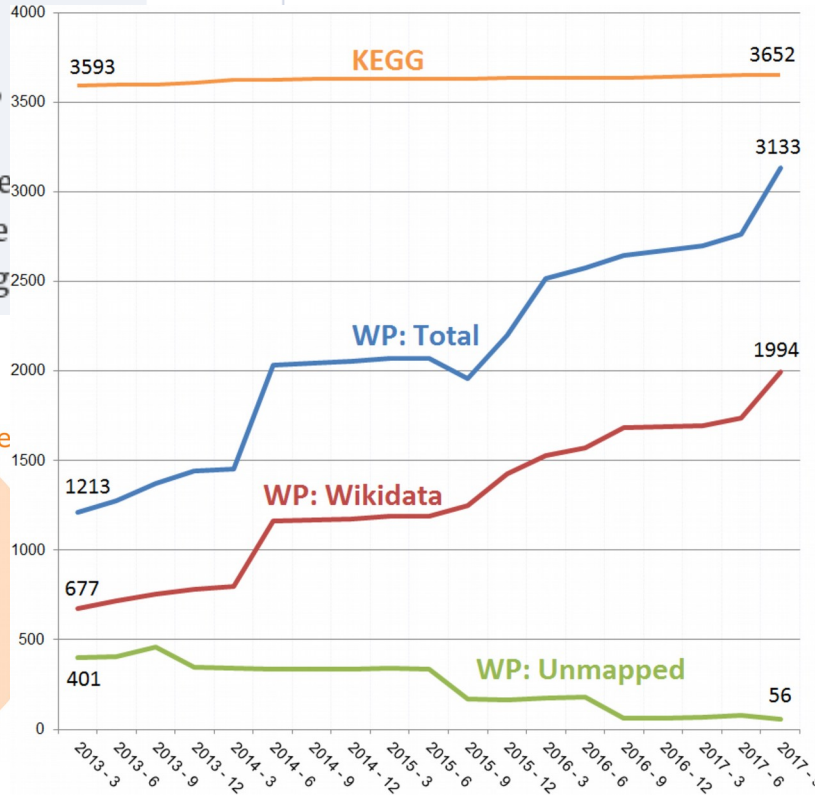
https://doi.org/10.1093/nar/gkx1064
Published: 10 November 2017 **Article history** ▾

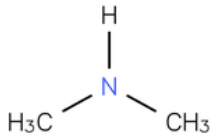
Abstract

WikiPathways (wikipathways.org) captures the collective knowledge represented in biological pathways. By providing a database in a curated, machine readable way, omics data analysis and visualization is enabled. WikiPathways and other pathway databases are used to analyze experime data by research groups in many fields. Due to the open and collaborative nature of the WikiPathways platform, our content keeps growing and is g





One ID in the pathway, many in the popup



MOL | SMILES | InChIKey

WikiPathways | KEGG Pathways | Reactome Pathways

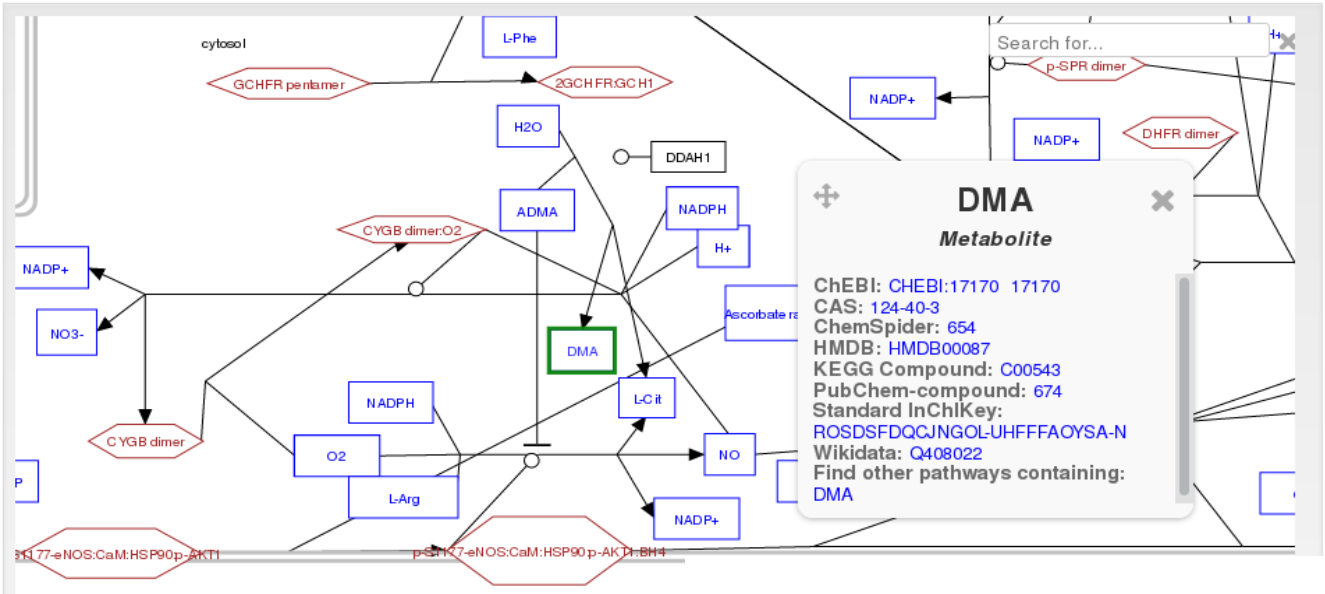
Select Species

Homo sapiens

Select Pathways

Metabolism of nitric oxide

This metabolite has been identified in the following MetaboLights studies. MTBLS100 MTBLS172



Maastricht University 1976 2016 reactome MetaboLights

Databases & identifiers

- HMDB: **H**uman **M**etabolome **D**ata**b**ase
- ChEBI: Database of **Ch**emicals **E**ntities of **B**iological **I**nterest
- ChemSpider, PubChem
- CAS: **C**hemical **A**bstracts **S**ervice
- InChI: **I**nternational **Ch**emical **I**dentifier
  - UniChem, …

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So, what IDs are used in WikiPathways?

2017

datasource	numberEntries
ChEBI	1923
HMDB	623
CAS	299
KEGG Compound	251
PubChem-compound	245
Chemspider	174
PubChem-substance	33
LIPID MAPS	10
Reactome	4
Wikidata	3
ChEMBL compound	2

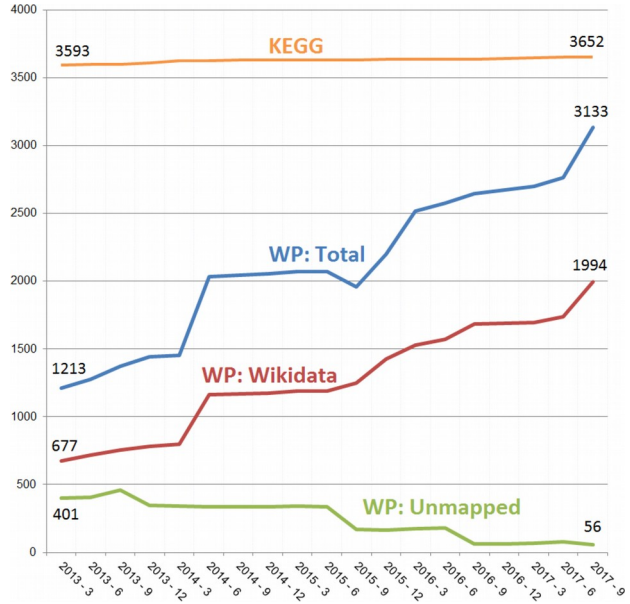
2015

source	count
HMDB	569
ChEBI	496
KEGG Compound	408
CAS	293
PubChem-compound	217
Chemspider	156
PubChem-substance	24
LIPID MAPS	11
Wikipedia	9
ChemIDplus	7
Reactome	4
ChEMBL compound	2
Other	1
CTD Chemical	1
ChemSpider	1

2012

source	count
HMDB	522
Kegg Compound	389
CAS	267
ChEBI	244
Entrez Gene	136
PubChem-compound	108
Chemspider	15
Wikipedia	11
PubChem-substance	8
ChemIDplus	7
ChEMBL compound	2
3DMET	1
LIPID MAPS	1

Curated subset



+ Reactome

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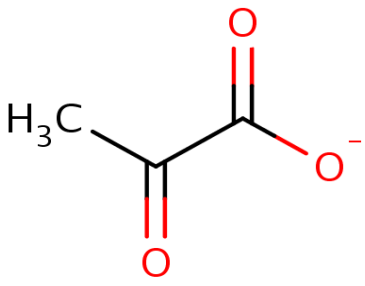
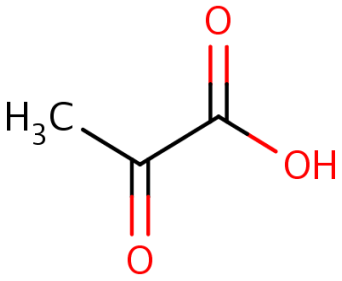
Expression chemistry in metabolic pathways

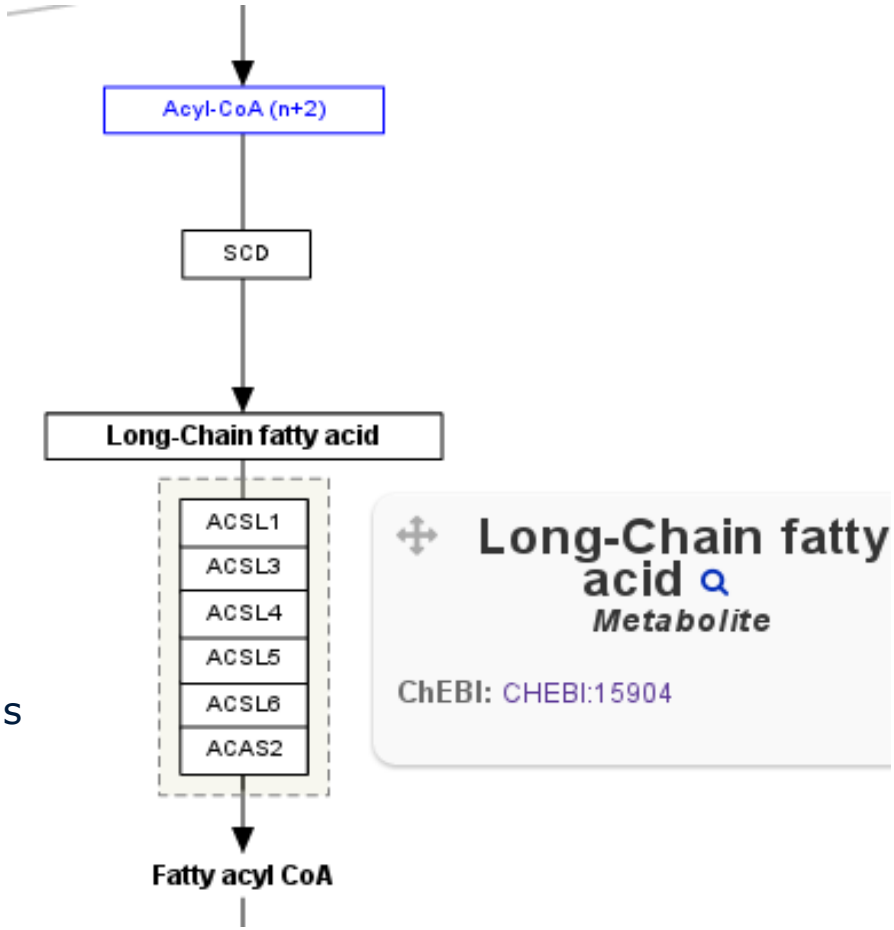
CHEBI:15361 (Pyruvate) -> Ce:CHEBI:32816 (conjugate) -> Ck:C00022 -> [WP2456 HIF1A and PPARG regulation of glycolysis, WP2453 TCA Cycle and PDHc]



CHEBI:15361



CHEBI:32816

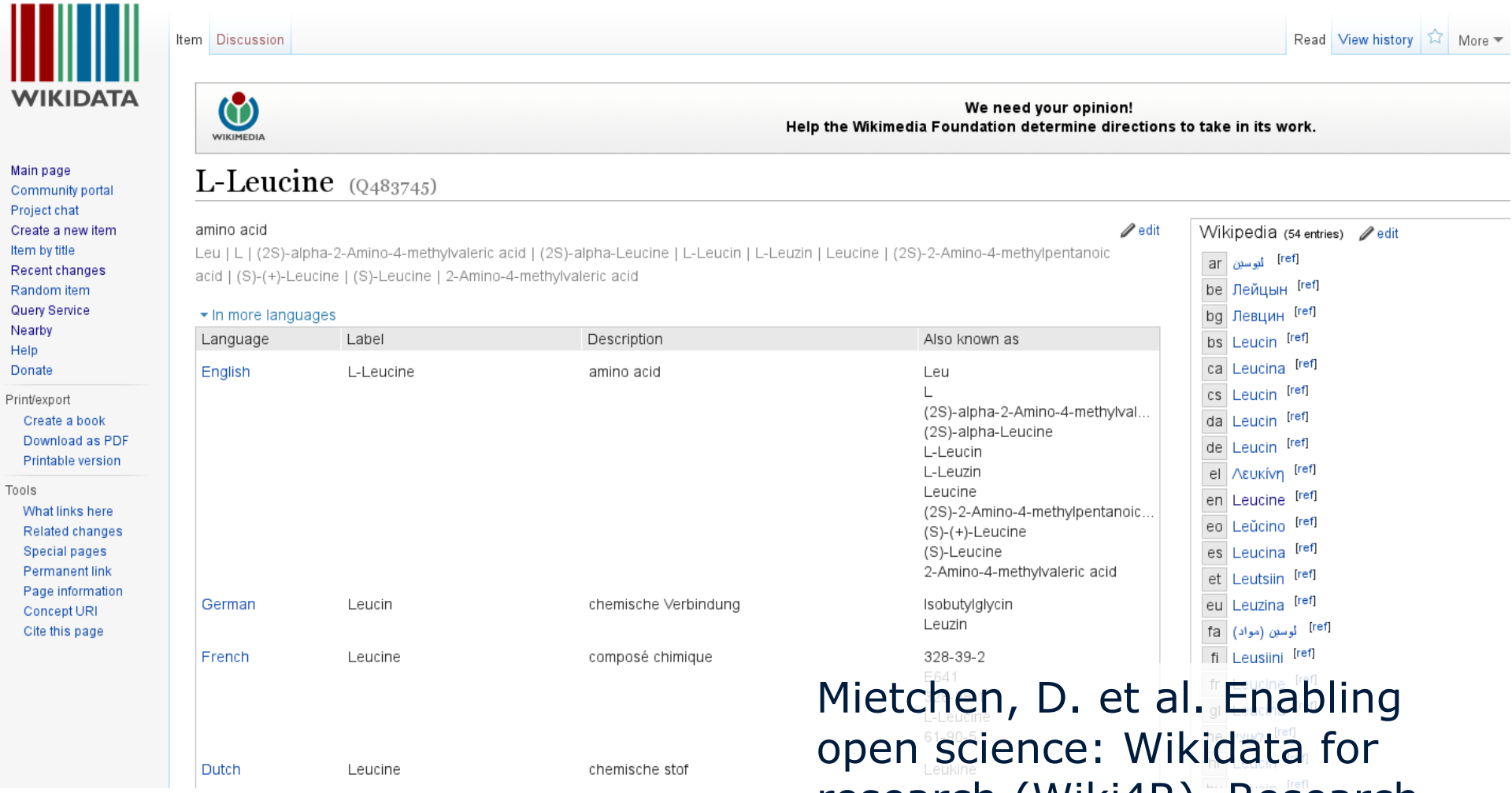


Brenninkmeijer, CYA, et al. "Scientific Lenses over Linked Data: An approach to support task specific views of the data. A vision." Proceedings of 2nd International Workshop on Linked Science. 2012.

What if we had more metabolite info?

- more CAS registry numbers?
- more physchem properties?
- more literature references?

Wikidata



Mietchen, D. et al. Enabling open science: Wikidata for research (Wiki4R). Research Ideas and Outcomes 1, e7573+ (2015)

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Wikidata: external (database) identifiers

Identifiers

Freebase ID	/m/0h1wg ▸ 1 reference
ChEBI ID	57427 ▾ 1 reference stated in: ChEMBL ChEMBL ID: CHEMBL291962 language of work or name: English title: L-Leucine (English) retrieved: 19 January 2016
ChEMBL ID	CHEMBL291962 ▸ 1 reference

WIKIDATA

Main page
Community portal
Project chat
Create a new item
Item by title
Recent changes
Random item
Query Service
Nearby
Help
Donate

Tools
What links here
Related changes

Property | Discussion

DSSTOX substance identifier (P3117)

DSSTox substance identifier used in the Environmental Protection Agency (
DTXSID

▾ In more languages

Language	Label	Description
English	DSSTOX substance identifier	DSSTox substar Environmental F Dashboard
German	DSSTOX-Identifikator	No description d
French	No label defined	No description d
Dutch	No label defined	No description d
Swedish	No label defined	No description d

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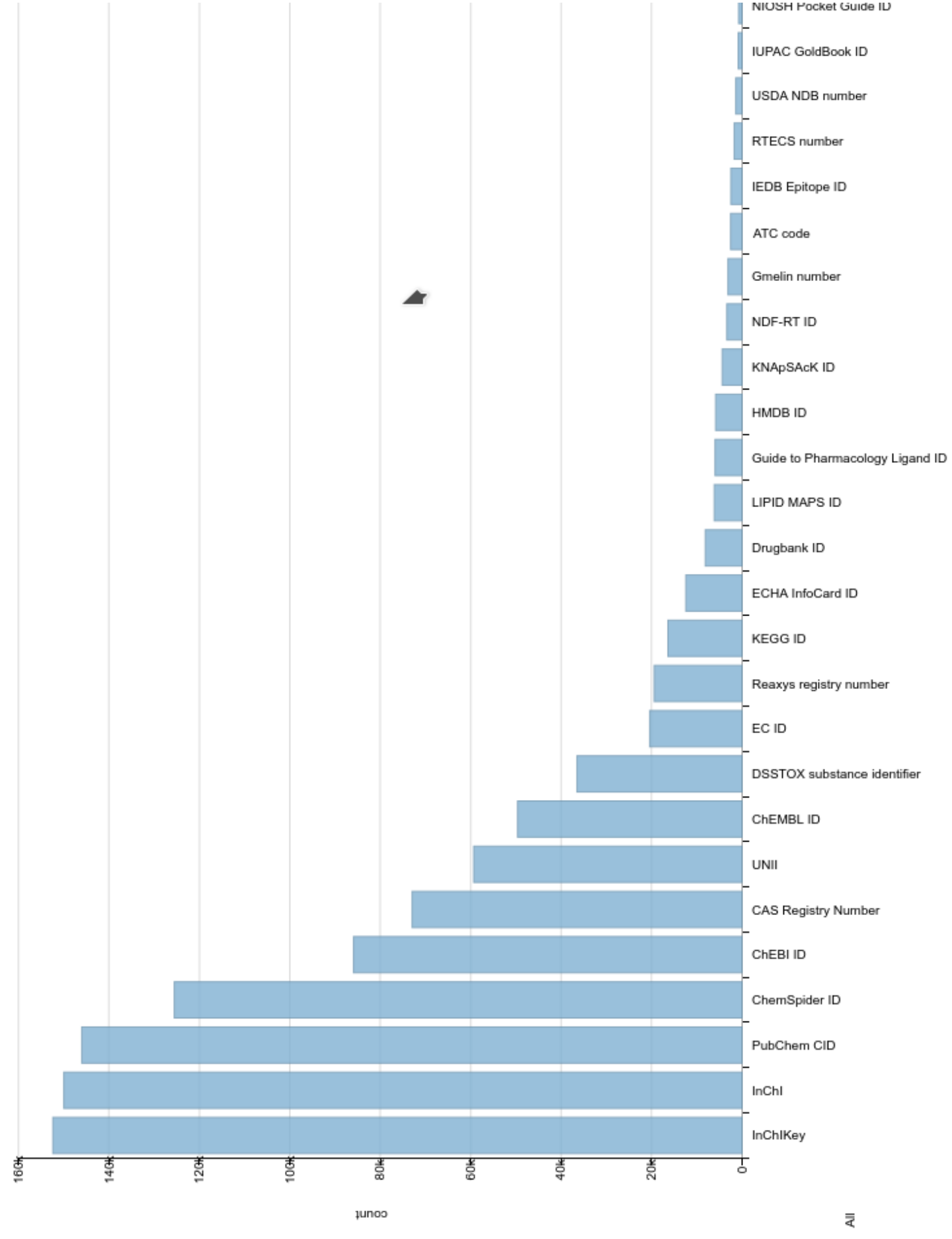
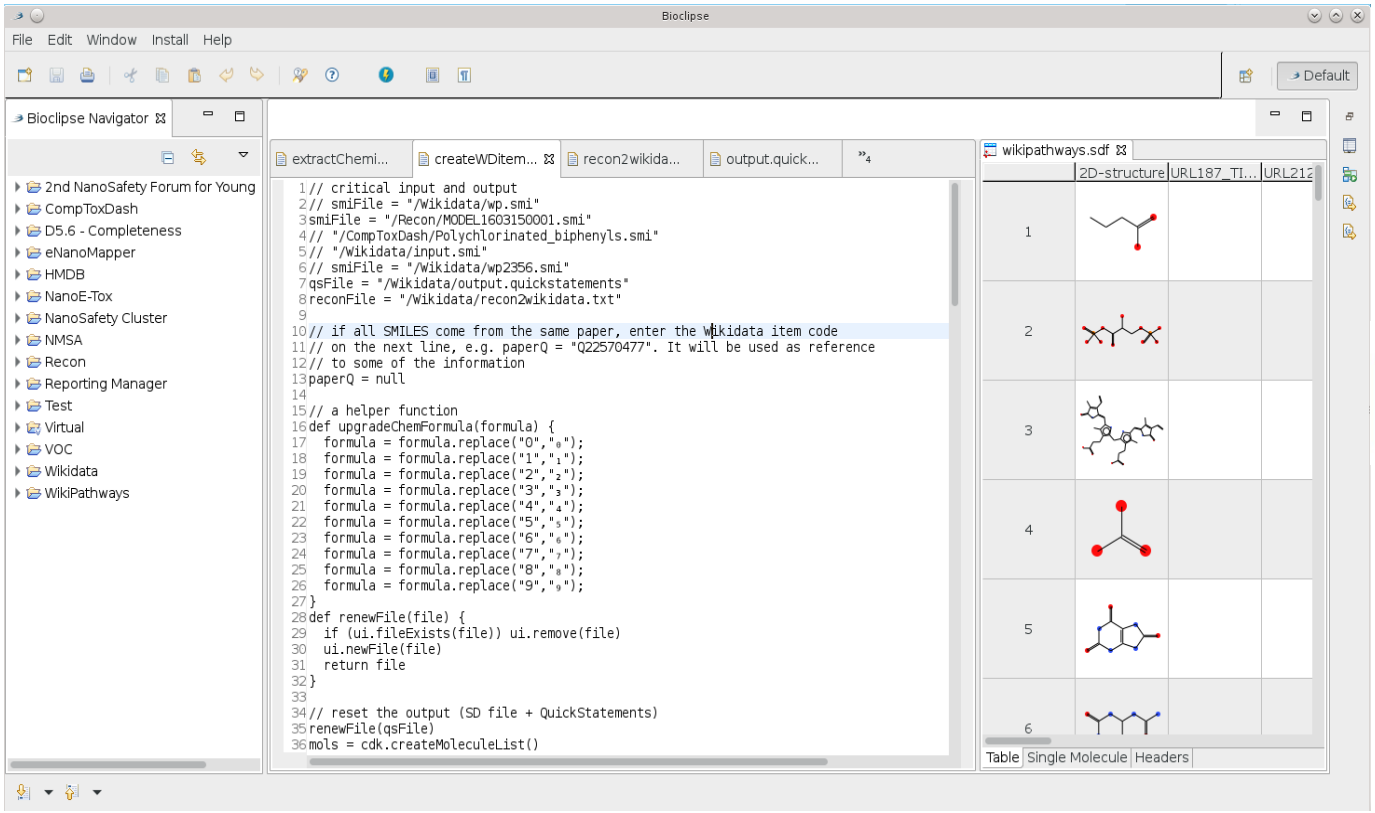
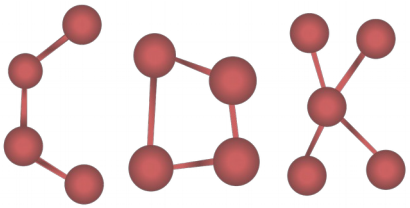

NIOSH Pocket Guide ID
IUPAC GoldBook ID
USDA NDB number
RTECS number
IEDB Epitope ID
ATC code
Gmelin number
NDF-RT ID
KNApSAcK ID
HMDB ID
Guide to Pharmacology Ligand ID
LIPID MAPS ID
Drugbank ID
ECHA InfoCard ID
KEGG ID
Reaxys registry number
EC ID
DSSTOX substance identifier
ChEMBL ID
UNII
CAS Registry Number
ChEBI ID
ChemSpider ID
PubChem CID
InChI
InChIKey
160k
140k
120k
100k
80k
60k
40k
20k
0
count
All

QuickStatements: scriptable adding of content



Spjuth, O. et al., 2007, BMC Bioinformatics

Bioclipse



Willighagen, E. et al., 2017, J. Cheminformatics

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QuickStatements: scriptable adding of content, here, the SPLASH

convert2rdf.groovy | wikidataMashup.groovy | mona-identifier-table.csv

```
ID,SPLASH,InChIKey,SMILES
AU100601,splash10-0a4i-1900000000-d2bc1c887f6f99ed0f74,QKLPUVXBJHRFQZ-UHFFFAOYSA-N,C=1C=C(C=CC1N)S(N=C2C=NC=C(Cl)N2)(=O)=O
AU100701,splash10-0a4i-1900000000-d2bc1c887f6f99ed0f74,XOXHILFPRYWFOD-UHFFFAOYSA-N,C=1C=C(C=CC1N)S(NC=2C=CC(Cl)=NN2)(=O)=O
AU100801,splash10-0pk9-2970000000-abb9e31dc053c1d21884,ASWVTGNCAZCNNR-UHFFFAOYSA-N,CC1=CC(C)=NC(=N1)NS(C2=CC=C(C=C2)N)(=O)=O
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AU100903,splash10-0a4i-0910000000-7b5873eb9276bcb413be,ZZORFUFYDOWNEF-UHFFFAOYSA-N,COC=1C=C(N=C(N1)OC)NS(C2=CC=C(C=C2)N)(=O)=O
AU100904,splash10-0k96-0910000000-24de656de5a8714caacb,ZZORFUFYDOWNEF-UHFFFAOYSA-N,COC=1C=C(N=C(N1)OC)NS(C2=CC=C(C=C2)N)(=O)=O
AU100905,splash10-0udl-0900000000-cf83e971f45b0faf66d2,ZZORFUFYDOWNEF-UHFFFAOYSA-N,COC=1C=C(N=C(N1)OC)NS(C2=CC=C(C=C2)N)(=O)=O
AU101001,splash10-0a4i-2901000000-8862dd6e93b57f07349b,PJSFRIWCGOHTNF-UHFFFAOYSA-N,COC1=C(N=CN=C1OC)NS(C2=CC=C(C=C2)N)(=O)=O
AU101101,splash10-0udi-0090000000-1bc83eabade65dc8953a,SEEPANYCNGTZFQ-UHFFFAOYSA-N,C1=CN=C(N=C1)NS(C2=CC=C(C=C2)N)(=O)=O
AU101102,splash10-0a4i-0910000000-bd163c77861c5a8afa49,SEEPANYCNGTZFQ-UHFFFAOYSA-N,C1=CN=C(N=C1)NS(C2=CC=C(C=C2)N)(=O)=O
AU101103,splash10-0a4i-0900000000-260a572b5c7f3c070c26,SEEPANYCNGTZFQ-UHFFFAOYSA-N,C1=CN=C(N=C1)NS(C2=CC=C(C=C2)N)(=O)=O
AU101104,splash10-052r-0900000000-580f983ba2
AU101201,splash10-0a4i-1900000000-95dc6d24a8
AU101302,splash10-0a4i-3900000000-23eed4bc89
AU101501,splash10-001i-0090000000-eef21c4c7e
```

mona-identifier-table.csv | convert.groovy | mappings.txt

```
Q55167836   P4964   "splash10-0f89-0950000000-117ad116d5ac14a5be9c"
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Q55167836   P4964   "splash10-001i-0900000000-daa82fab29c3bc26425a"
Q55167836   P4964   "splash10-0g5i-0900000000-56c0d97c8ede7a0f5121"
Q4596780    P4964   "splash10-00di-4900000000-73bfbb6a2b2ba59e4f4f"
Q4596780    P4964   "splash10-00di-0900000000-2370c00b72994e6aa54f"
Q11751639   P4964   "splash10-00di-0910000000-74bd5c8746b39b3c0420"
Q11751639   P4964   "splash10-014i-0900000000-7ac1f98cc9b9752a76d6"
Q11751639   P4964   "splash10-014i-0900000000-f5c899766b4d912df5ce"
Q11751639   P4964   "splash10-014i-0900000000-5e5ee374be357b4e26a4"
Q55177068   P4964   "splash10-0059-0900000000-d1e136c596eda61fdad6"
Q55177068   P4964   "splash10-001i-1900000000-d9c4b6edb79ec7db500c"
Q55177068   P4964   "splash10-000i-9500000000-ec02387ba0107a9f05cb"
Q55177068   P4964   "splash10-000i-9100000000-c1e7be64cc9ef25c1291"
Q55177068   P4964   "splash10-0006-9000000000-d90115a5ff29ff776135"
```

QuickStatements: Magnus Manske, WT Sanger Institute in Cambridge

SPLASH: G. Wolhgemuth, 10.1038/nbt.3689

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More identifiers: EPA CompTox Dashboard, LIPID MAPS, PDB ligand identifiers

DSSTOX substance identifier DTXSID30678817

1 reference

stated in Mapping file of InChIStrings, InChIKeys and DTXSIDs for the EPA CompTox Dashboard

PDB ligand ID ACY

Egon Willigh@gen
@egonwillighagen

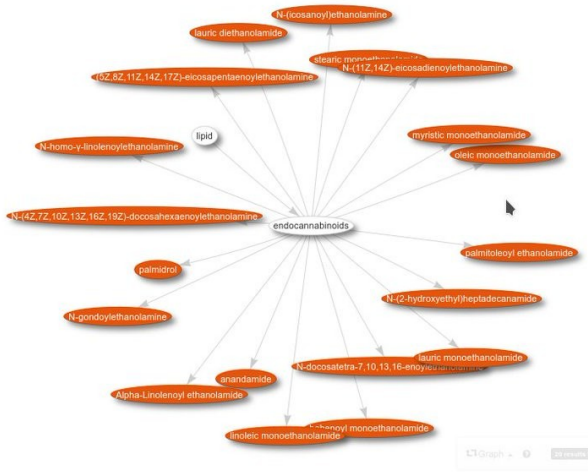
ok, we had 2333 @lipidmaps identifiers in @wikidata this morning... the current count is 6099 :) tinyurl.com/y8g3zwas #endocannabinoidSaturday

11:05 PM - Jun 30, 2018

See Egon Willigh@gen's other Tweets

endocannabinoids (Q55282178)

Class Hierarchy



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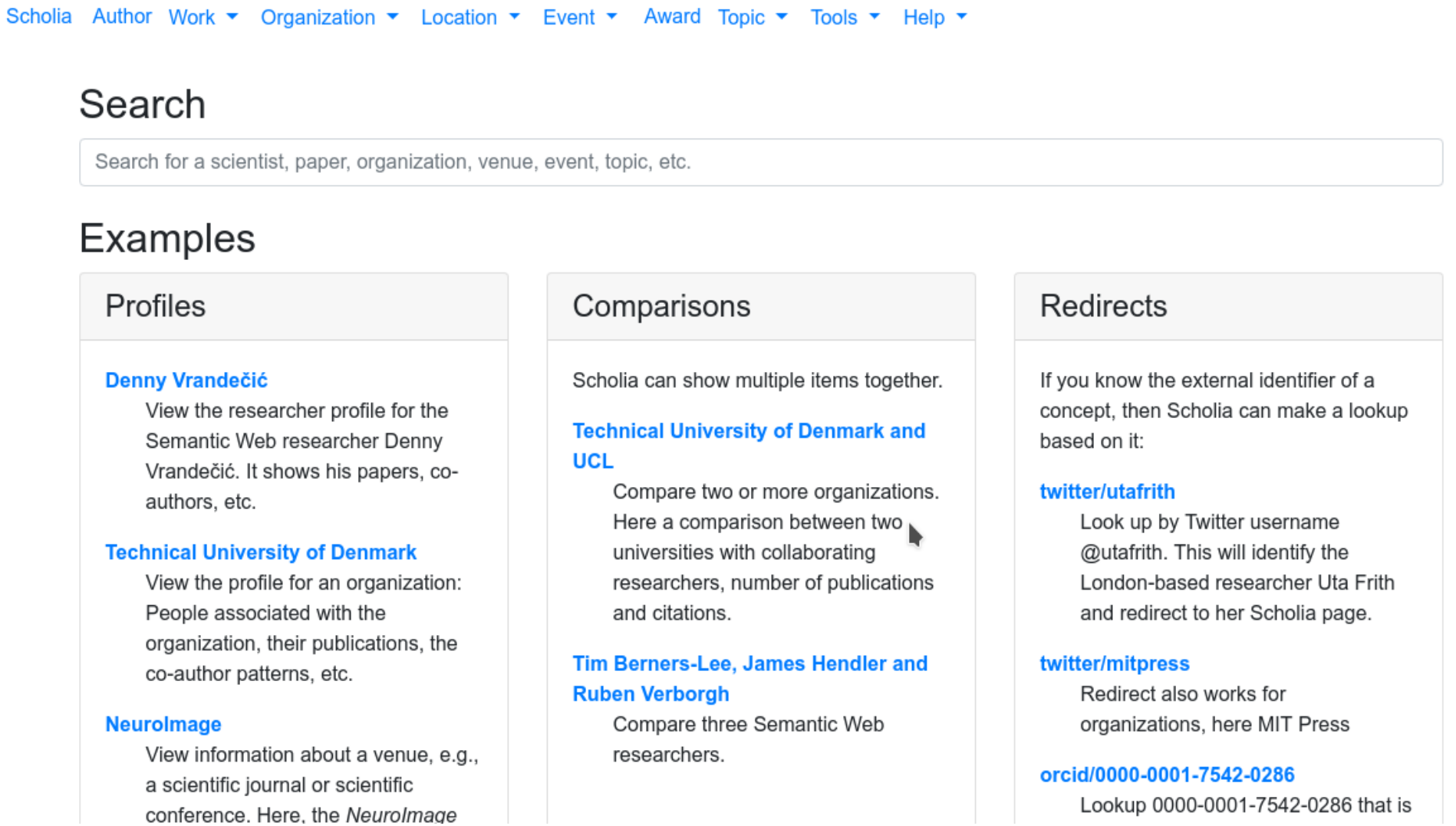
Scholia: visualizing data



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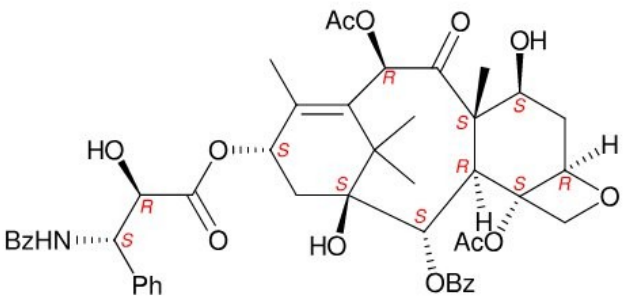
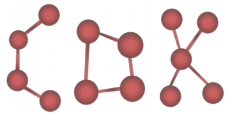
doi:10.1007/978-3-319-70407-4_36

Scholia: compounds

paclitaxel (Q423762)

Paclitaxel (PTX), sold under the brand name Taxol among others, is a chemotherapy medication used to treat a number of types of cancer. This includes ovarian cancer, breast cancer, lung cancer, Kaposi sarcoma, cervical cancer, and pancreatic cancer. It is given by injection into a vein. ... (from the English Wikipedia)





Identifiers

Show 10 entries Search:

IDpred	Id
ATC code	L01CD01
CAS Registry Number	33069-62-4

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
acetic acid c-13	QTBSBXVTEAMEQO-VQEHIDDOSA-N	1563-79-7	8329490	10153982
acetic acid c-11	QTBSBXVTEAMEQO-JVVVGQRLSA-N	78887-71-5	396653	450349
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

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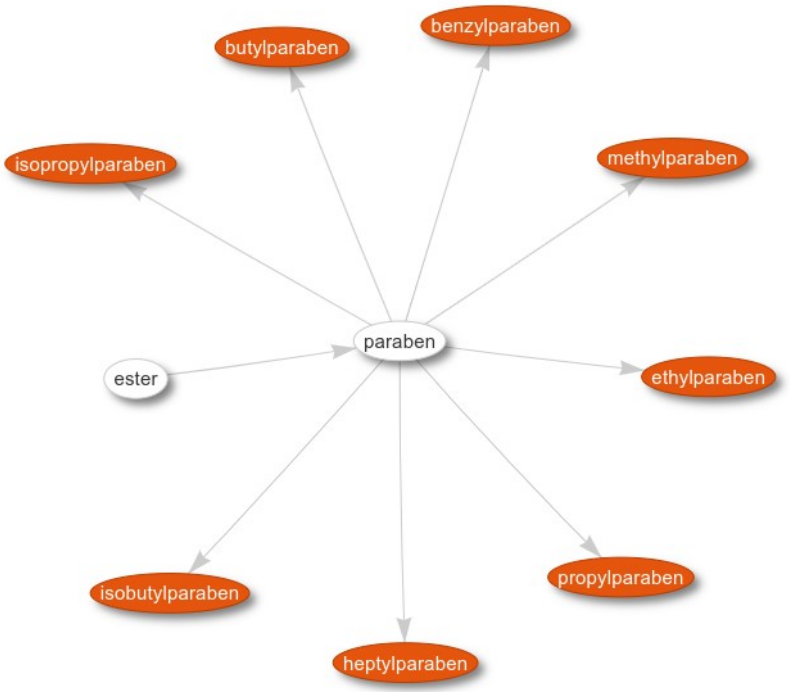
Scholia: visualizing data (compound classes)

Scholia | Author | Work | Organization | Venue | Series | Publisher | Sponsor | Award | Topic | Tools | About

paraben (Q410780)

Parabens are a class of widely used preservatives in cosmetic and pharmaceutical products. Chemically, they are a series of parahydroxybenzoates or esters of parahydroxybenzoic acid (also known as 4-hydroxybenzoic acid). Parabens are effective preservatives in many types of formulas. ... (from the English Wikipedia)

Class Hierarchy



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doi:10.1007/978-3-319-70407-4_36

Scholia: physical-chemical properties

Physchem Properties

Show 10 entries Search:

PropEntity	Value	Units	Qualifiers	Source	Doi
acid dissociation constant	4.74	1		Small Scale Determination of the pKa Values for Organic Acids	10.1021/ED071PA6
mass	60.021129	atomic mass unit		PubChem	
acid dissociation constant	4.756	1	temperature: 25	CRC Handbook of Chemistry and Physics (95th edition)	
boiling point	117.9	degrees Celsius	pressure: 101325	CRC Handbook of Chemistry and Physics (95th edition)	
density	1.0446	gram per cubic centimetre	temperature: 25	CRC Handbook of Chemistry and Physics (95th edition)	

Scholia: keeping up with literature

Recently published works on the chemical

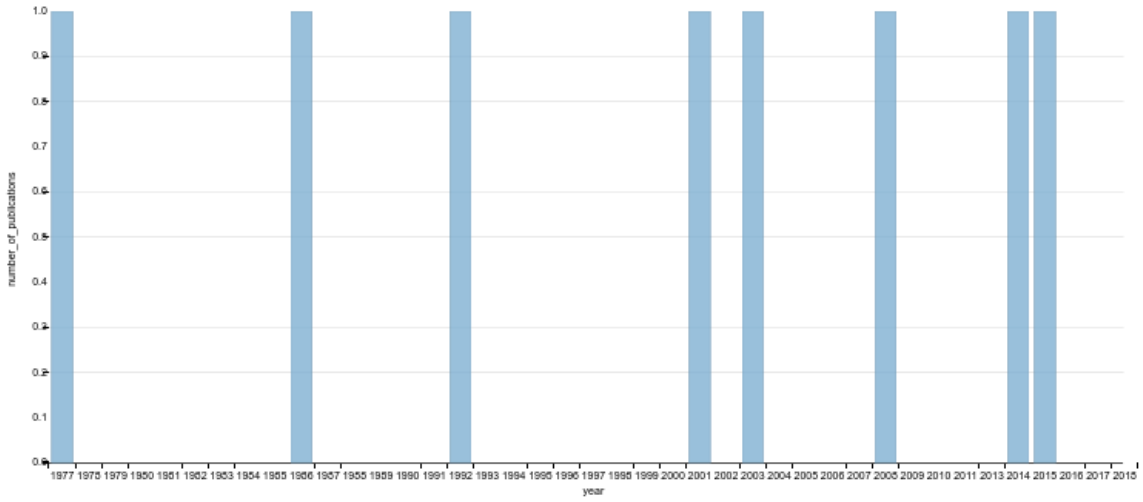
Search:

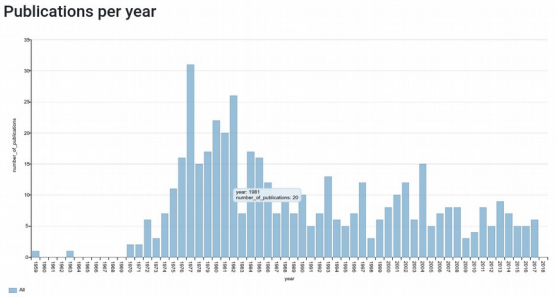
Date	Work	Type	Topics
2015-11-25	Metabolism and elimination of methyl, iso- and n-butyl paraben in human urine after single oral dosage.	scientific article	butylparaben // isobutylparaben // methylparaben // metabolism
2014-09-17	Overdosage of methylparaben induces cellular senescence in vitro and in vivo.	scientific article	drug overdose // methylparaben
2008-07-01	Paraben esters: review of recent studies of endocrine toxicity, absorption, esterase and human exposure, and discussion of potential human health risks.	scientific article	paraben // toxicity
2003-01-01	Propylparaben: physical characteristics.	scientific article	propylparaben
2001-06-01	Safety assessment of propyl paraben: a review of the published literature.	scientific article	propylparaben
1992-09-01	Methylparaben and propylparaben do not alter cerebral blood flow in humans.	scientific article	Homo sapiens // blood flow // propylparaben // methylparaben
1986-10-01	The toxicological implications of the interaction of butylated hydroxytoluene with other antioxidants and phenolic chemicals	scientific article	eugenol // ferulic acid // guaiacol // Butylated hydroxyanisole // arachidonic acid // methylparaben // butylated hydroxytoluene // hydrogen peroxide // vanillin
1977-05-01	Methylparaben--an overlooked cause of local anesthetic hypersensitivity.	scientific article	hypersensitivity // methylparaben

Edit on query.Wikidata.org

Showing 1 to 8 of 8 entries

Publications per year





Wikidata and Scholia as hub linking metabolite knowledge

Redirecting

If you know the identifier then Scholia can make a lookup based on the identifier:

cas/50-00-0
Lookup CAS 50-00-0. This will identify formaldehyde and redirect to its Scholia page.

inchikey/QTBSBXVTEAMEQO-UHFFFAOYSA-N
Redirect also works for InChIKeys, here for acetic acid.

Identifiers

Show 10 entries

IDpred	Id
ATC code	G01AD02
ATC code	S02AA10
Beilstein Registry Number	506007
CAS Registry Number	64-19-7
ChEBI ID	15366
ChEMBL ID	CHEMBL539
ChemSpider ID	171
CosIng number	31572
DSSTOX substance identifier	DTXSID5024394
Drugbank ID	03166

Edit on query.Wikidata.org

Showing 1 to 10 of 30 entries

Previous 1 2 3 Next

Conclusions

- Wikidata + WikiCite + Scholia

  - Largest open data set that link CAS numbers to chemical structures
  - Literature is central
  - Integrates ontological relations with data
  - Large community around it
    - Powerful query service
    - FAIR by design