Facilitating Scientific Discovery through Crowdsourcing and Distributed Participation

Antony Williams
NETTAB
October 17th 2013

If it was not just about me…

- Together we might:
  - build an encyclopedia
  - …and rate restaurants
  - …share book reviews
  - …and movie reviews
  - …and reviews of service providers
  - …organize sit-ins and social action
  - …and more data might just be Open

If it was not just about me…

- Together we might:
  - build an encyclopedia
  - …and rate restaurants
  - …share book reviews
  - …and movie reviews
  - …and reviews of service providers
  - …organize sit-ins and social action
  - …and more data might just be Open

amazon.com

NETFLIX

Angie's list

Crowdsource the galaxy

GALAXY ZOO

ZOONIVERSE
REAL SCIENCE ONLINE

Climate

Model Earth's climate using wartime ship logs

Help scientists recover worldwide weather observations made by Royal Navy ships.

oldWeather

Classify over 30 years of tropical cyclone data.

Scientists at NOAA's National Climatic Data Center need your help.

CycloneCenter

Humanities

Study the lives of ancient Greeks

The data gathered by Ancient Lives helps scholars study the Oxyrhynchus collection.

ANCIENT LIVES

Nature

Hear Whales communicate

You can help marine researchers understand what whales are saying

WHALE FM

Help explore the ocean floor

The HabCam team and the Woods Hole Oceanographic Institution need your help!

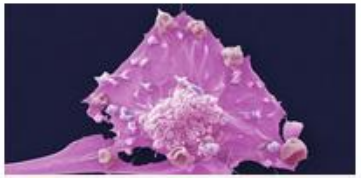
SEAFLOOR EXPLORER

You're hot on the trail of bats!

Help scientists characterise bat calls recorded by citizen scientists.

BAT DETECTIVE

Biology



Analyse real life cancer data.

You can help scientists from the world's largest cancer research institution find cures for cancer.

Cell Slider

Various ways to contribute

23andMe

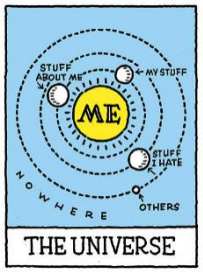
Have you ever been diagnosed or treated for any of the following conditions?

An autoimmune disease (a disease in which your immune system attacks part of your body)	○ Yes	○ No	○ I'm not sure
A mental health or psychiatric condition	○ Yes	● No	○ I'm not sure
Infertility or subfertility	○ Yes	● No	○ I'm not sure
Hepatitis or liver disease	○ Yes	● No	○ I'm not sure
A heart-related problem	○ Yes	● No	○ I'm not sure

CHOOSE ANSWER

Skip Question

Where Am I From?



Ancestry Composition tells you what percent of your DNA comes from each of 22 populations worldwide. The analysis includes DNA you received from all of your ancestors, on both sides of your family. The results reflect where your ancestors lived 500 years ago, before ocean-crossing ships and airplanes came on the scene.

99.4%	European
0.1%	Sub-Saharan African
0.6%	Unassigned
100%	**Antony Williams**

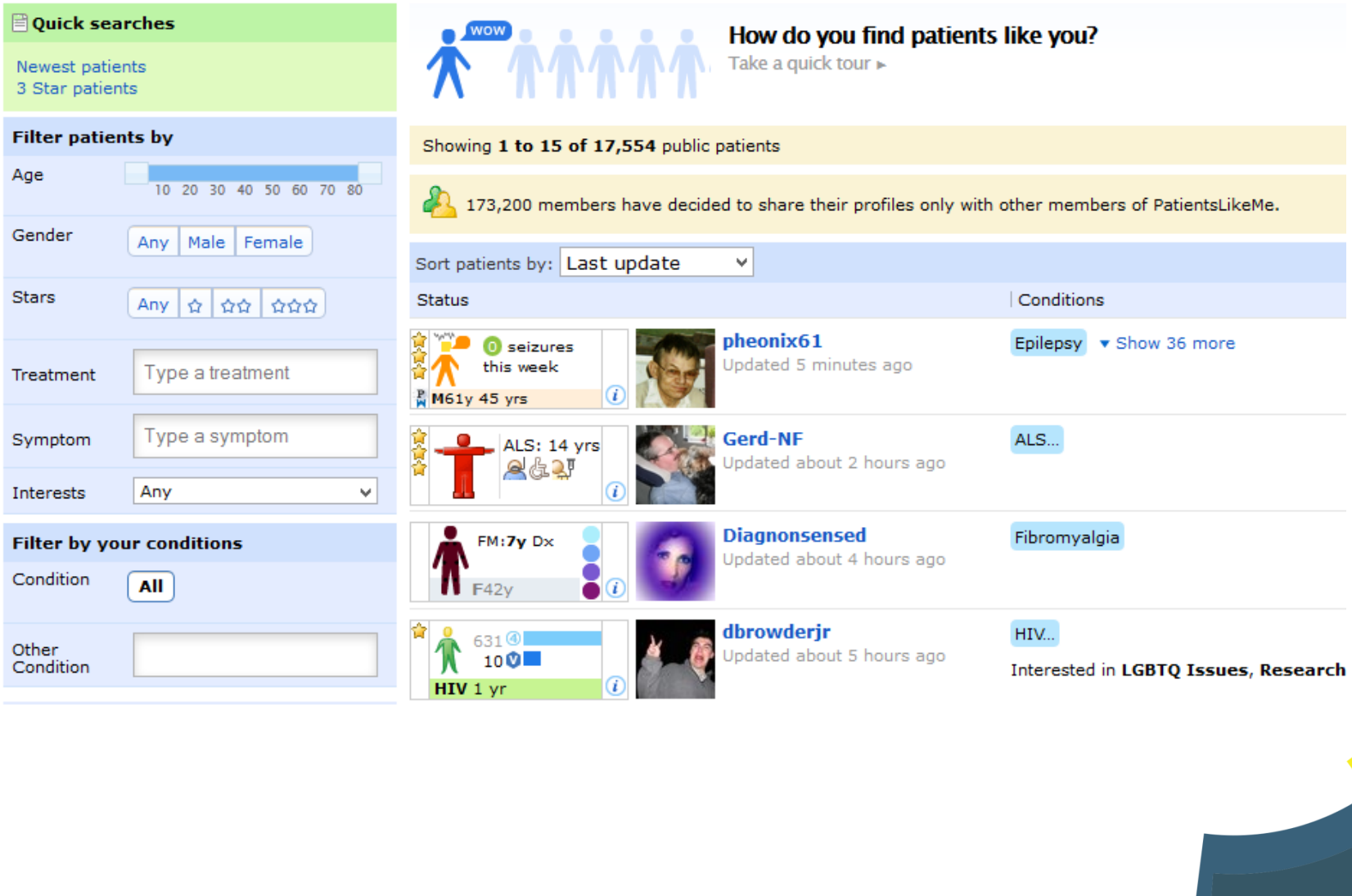
What can be done with Big Data

Decreased Risk

NAME	CONFIDENCE	YOUR RISK	AVG. RISK	COMPARED TO AVERAGE
Prostate Cancer ♂	★★★★	**9.2%**	17.8%	0.51x
Age-related Macular Degeneration	★★★★	**2.4%**	6.5%	0.37x
Melanoma	★★★★	**2.2%**	2.9%	0.75x
Rheumatoid Arthritis	★★★★	**1.3%**	2.4%	0.54x
Restless Legs Syndrome	★★★★	**0.86%**	1.96%	0.44x
Multiple Sclerosis	★★★★	**0.24%**	0.34%	0.69x
Exfoliation Glaucoma	★★★★	**0.16%**	0.75%	0.22x
Type 1 Diabetes	★★★★	**0.11%**	1.02%	0.11x
Celiac Disease	★★★★	**0.07%**	0.12%	0.58x
Primary Biliary Cirrhosis	★★★★	**0.05%**	0.08%	0.66x

Patients Like Me

Patients Like Me



Let’s Change the World

- Let’s map together all historical chemistry data and build systems to integrate new data
- Heck, let’s integrate chemistry and biology data and add in disease data too
- Lets model the data and see if we can extract new relationships – quantitative and qualitative
- Let’s make it all available on the web

That’s a BIG Request

What About Something Smaller?

- We're going to map the world
- We're going to take photos of as many places as we can and link them together
- We'll let people annotate and curate the map
- Then let's make it available free on the web
- We'll make it available for decision making
- Put it on Mobile Devices, Give it Away

I’m from here…

Afon-wen

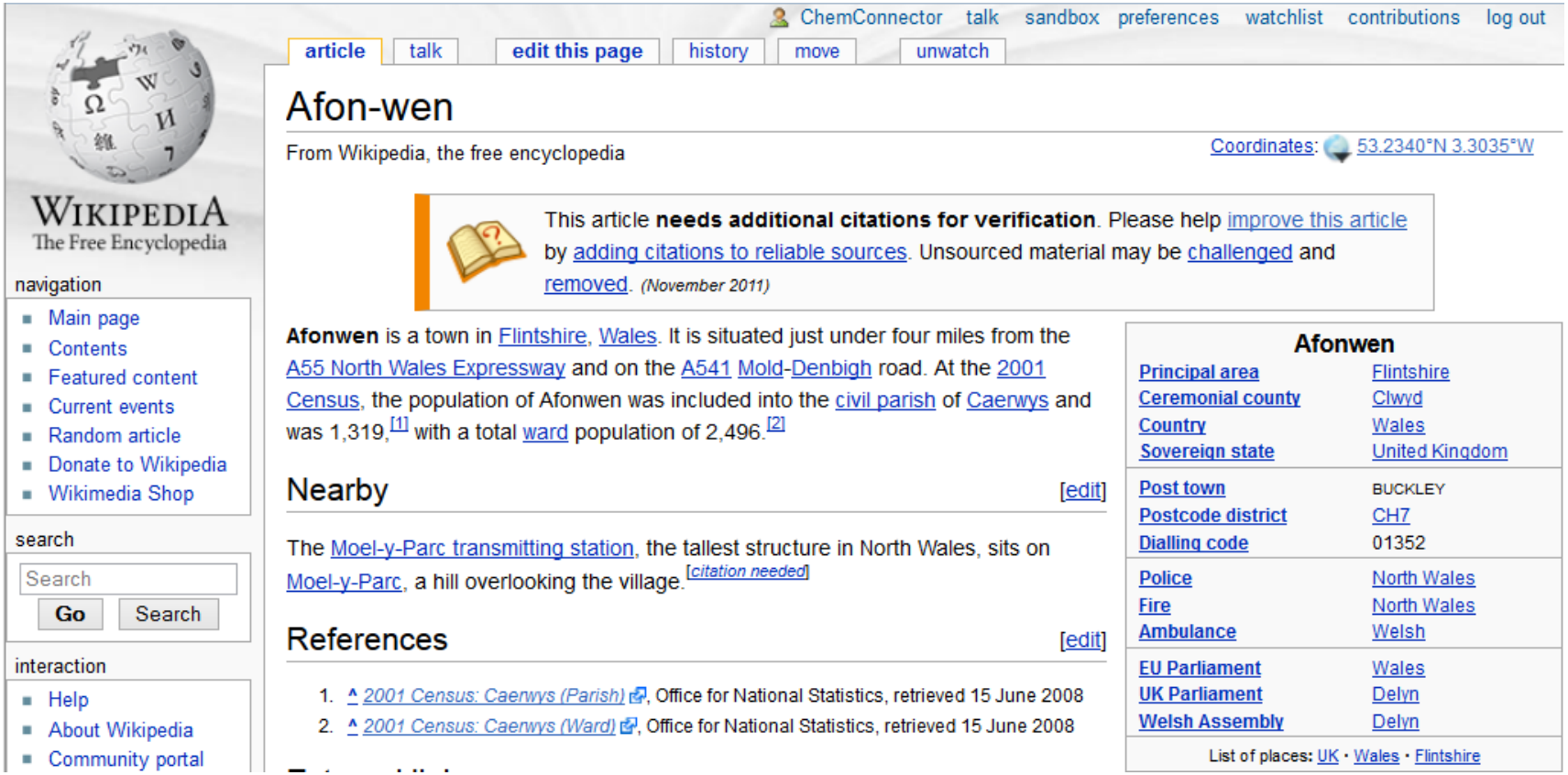
Town in United Kingdom

Afonwen is a town in Flintshire, Wales. It is situated just under four miles from the A55 North Wales Expressway and on the A541 Mold-Denbigh road. Wikipedia

Weather: 43°F (6°C), Wind SE at 8 mph (13 km/h), 93% Humidity

Local time: Thursday 5:36 PM

Wikipedia



ChemConnector talk sandbox preferences watchlist contributions log out

article | talk | edit this page | history | move | unwatch

WIKIPEDIA
The Free Encyclopedia

navigation
- Main page
- Contents
- Featured content
- Current events
- Random article
- Donate to Wikipedia
- Wikimedia Shop

search
Search
Go | Search

interaction
- Help
- About Wikipedia
- Community portal

Afon-wen

From Wikipedia, the free encyclopedia

Coordinates: 53.2340°N 3.3035°W

This article **needs additional citations for verification**. Please help improve this article by adding citations to reliable sources. Unsourced material may be challenged and removed. *(November 2011)*

Afonwen is a town in Flintshire, Wales. It is situated just under four miles from the A55 North Wales Expressway and on the A541 Mold-Denbigh road. At the 2001 Census, the population of Afonwen was included into the civil parish of Caerwys and was 1,319,[1] with a total ward population of 2,496.[2]

Nearby [edit]

The Moel-y-Parc transmitting station, the tallest structure in North Wales, sits on Moel-y-Parc, a hill overlooking the village.[citation needed]

References [edit]

1. ^ *2001 Census: Caerwys (Parish)*, Office for National Statistics, retrieved 15 June 2008
2. ^ *2001 Census: Caerwys (Ward)*, Office for National Statistics, retrieved 15 June 2008

Afonwen

Principal area	Flintshire
Ceremonial county	Clwyd
Country	Wales
Sovereign state	United Kingdom
Post town	BUCKLEY
Postcode district	CH7
Dialling code	01352
Police	North Wales
Fire	North Wales
Ambulance	Welsh
EU Parliament	Wales
UK Parliament	Delyn
Welsh Assembly	Delyn

List of places: UK · Wales · Flintshire

Wikipedia

ChemConnector talk sandbox preferences watchlist contributions log out

article | talk | edit this page | history | move | unwatch

WIKIPEDIA
The Free Encyclopedia

navigation
- Main page
- Contents
- Featured content
- Current events
- Random article
- Donate to Wikipedia
- Wikimedia Shop

search
Search
Go | Search

interaction
- Help
- About Wikipedia
- Community portal

Afon-wen

From Wikipedia, the free encyclopedia

Coordinates: 53.2340°N 3.3035°W

This article **needs additional citations for verification**. Please help improve this article by adding citations to reliable sources. Unsourced material may be challenged and removed. *(November 2011)*

Afonwen is a town in Flintshire, Wales. It is situated just under four miles from the A55 North Wales Expressway and on the A541 Mold-Denbigh road. At the 2001 Census, the population of Afonwen was included into the civil parish of Caerwys and was 1,319,[1] with a total ward population of 2,496.[2]

Nearby [edit]

The Moel-y-Parc transmitting station
Moel-y-Parc, a hill overlooking the vil
sits on Moel-y-Parc, a hill overlooking the village.[citation needed]

References [edit]

1. ^ *2001 Census: Caerwys (Parish)*, Office for National Statistics, retrieved 15 June 2008
2. ^ *2001 Census: Caerwys (Ward)*, Office for National Statistics, retrieved 15 June 2008

Afonwen	
Principal area	Flintshire
Ceremonial county	Clwyd
Country	Wales
Sovereign state	United Kingdom
Post town	BUCKLEY
	352
	th Wales
	th Wales
Ambulance	Welsh
EU Parliament	Wales
UK Parliament	Delyn
Welsh Assembly	Delyn

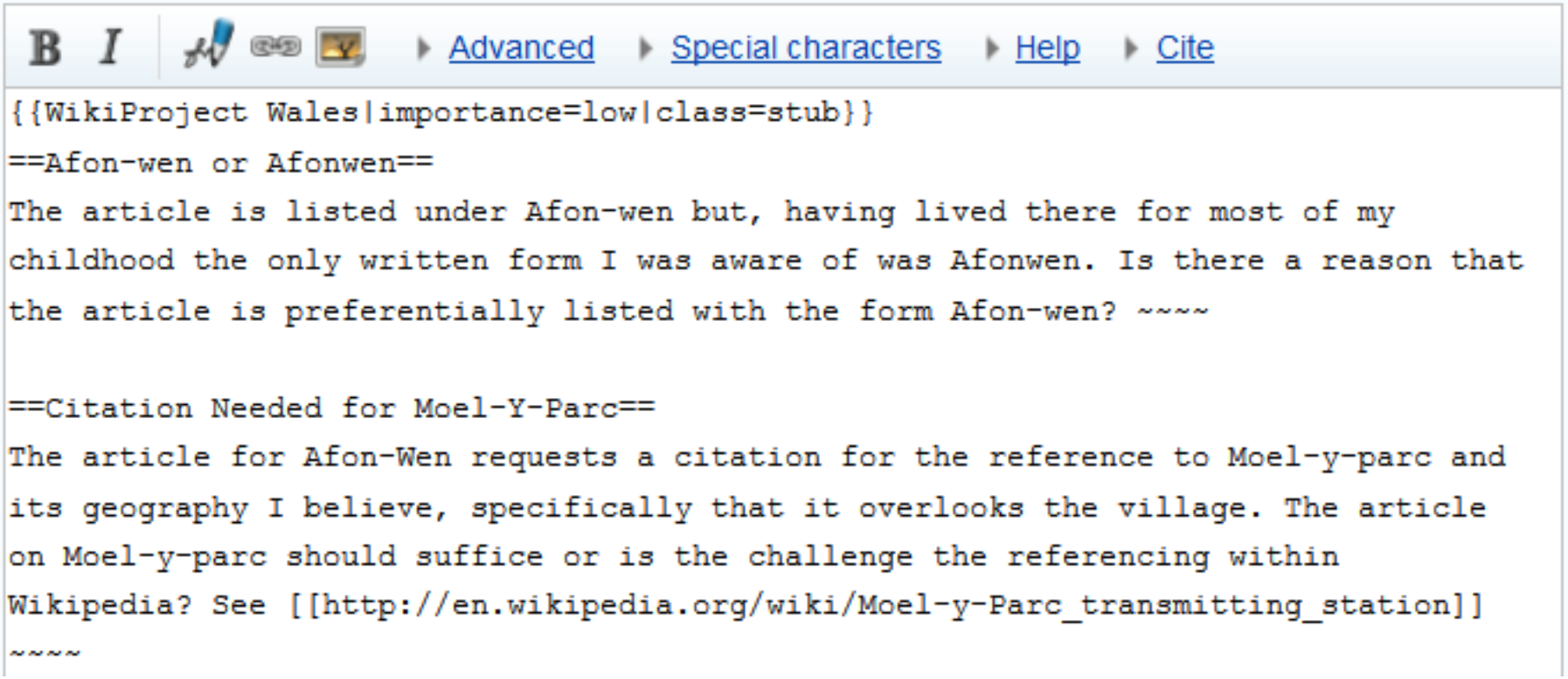
List of places: UK · Wales · Flintshire

Moel-Y-Parc


Map
Traffic
A541
A541
Llys-Y-Pentre
Llys-Y-Pentre
A


eptember 2009
Report a problem

I care…I want to contribute…



The Power of Contribution

Afon-wen or Afonwen [edit]

The article is listed under Afon-wen but, having lived there for most of my childhood the only written form I was aware of was Afonwen. Is there a reason that the article is preferentially listed with the form Afon-wen? ChemConnector (talk) 16:51, 11 April 2013 (UTC)

Citation Needed for Moel-Y-Parc [edit]

The article for Afon-Wen requests a citation for the reference to Moel-y-parc and its geography I believe, specifically that it overlooks the village. The article on Moel-y-parc should suffice or is the challenge the referencing within Wikipedia? See [[1]] ChemConnector (talk) 16:51, 11 April 2013 (UTC)

How do you spell Afonwen?

And the Welsh know!

WICIPEDIA
Y Gwyddoniadur Rhydd

Hafan
Porth y Gymuned
Y Caffi
Materion cyfoes
Newidiadau diweddar
Erthygl ar hap

Erthygl | Sgwrs

Afonwen

Gallai **Afonwen** gyfeirio at un o ddau bentref:

- Afon Wen (hefyd: Afonwen), Gwynedd
- Afon-wen (hefyd: Afonwen), Sir y Fflint

Tudalen wahaniaethu yw hon, sef cymorth c
Os cyrhaeddoch yma drwy glicio ar ddolen fewnol ,
honno a newid y ddolen.

Whoa…

- So the world can be mapped…
- We can enter a 3D environment within the map
- We can add annotations
- We can use the data, we can reference it, we can extract it, we can make decisions with it
- And we can do it on our lap, in our hands
- **Let's crowdsource chemistry**

Chemistry Data is Everywhere

Safety (MSDS) data for **DDT** - Physical and Theoretical **Chemistr**...
physchem.ox.ac.uk/**msds**/DD/**DDT**.html
Mar 29, 2005 - **Safety data** for **DDT**. Hazard: toxic Hazard: environmental hazard. Glossary of terms on this data sheet. The information on this web page is ...

[PDF] **Material Safety Data** Sheet EnviroGard。 **DDT** - Modern Water
www.modernwater.com/.../**MSDS**/9998093.4%20EG%20**DDT**%20**MSD**...
Material Safety Data Sheet. EnviroGard。 **DDT**. **MATERIAL** IDENTIFICATION. Manufacturer/Distributor: Modern Water Inc. 15 Read's Way, Suite 100. New Castle ...

[PDF] **DDT** Pesticide Handling, Application, and Bioassay Process
https://sib.illinois.edu/pittendrigh/documents/SOP_**DDT**_Pesticide.pdf
DDT (**Dichloro-Diphenyl-Trichloroethane**) pesticide and Acetone are combined ... Read the **Material Safety Data** Sheet (**MSDS**) prior to handling **DDT** Pesticide ...

DDT (dichlorodiphenyltrichloroethane)
pmep.cce.cornell.edu › ... › Carbaryl to Dicrotophos
DDT is no longer registered for use in the United States, although it is still used in ... fate and **chemistry data** presented here refer to the technical product **DDT**. ..... miscarriage: A hypothesis of correlation, Ecotoxicol Environ **Safety** 17:1-11.

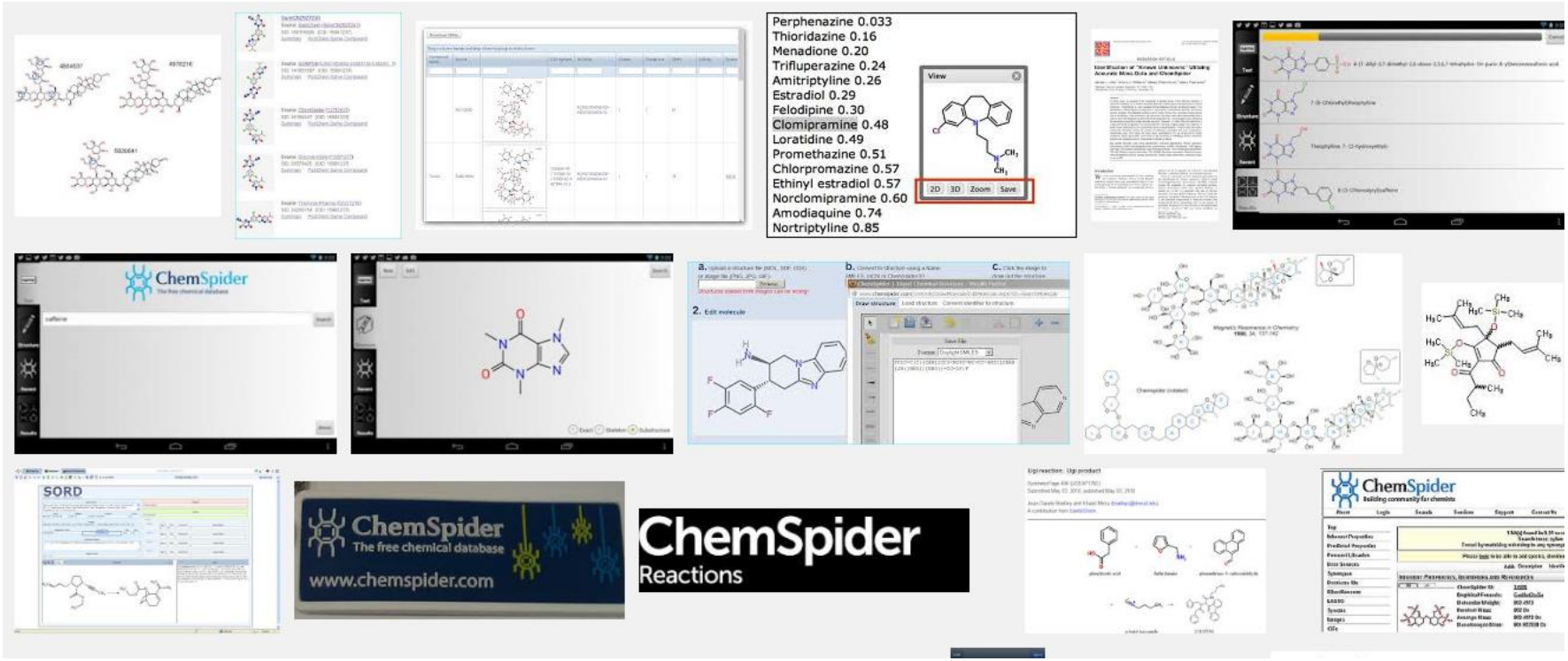
4,4'-**DDT** 98% | Sigma-Aldrich
www.sigmaaldrich.com/catalog/product/aldrich/386340?lang=en...
Sigma-Aldrich offers Aldrich-386340, 4,4'-DDT for your research needs. Find product specific information including CAS, **MSDS**, protocols and references. ... QSAR study to predict endocrine-disrupting effects of environmental **chemicals**.

About 200,000 results (0.30 seconds)

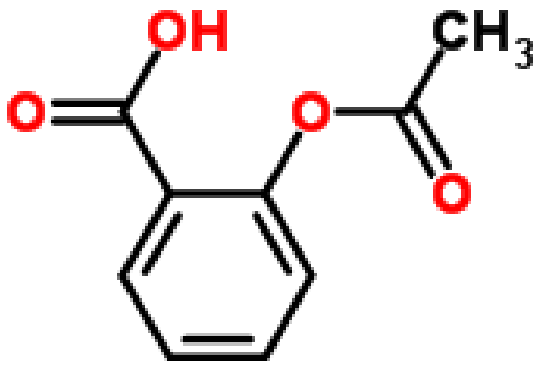
In a Galaxy far, far away…

- Build a structure-centric hub
- Aggregate structure-based data and integrate
- Link to additional data sources
  - Patents
  - Publications
  - Vendors
  - Models

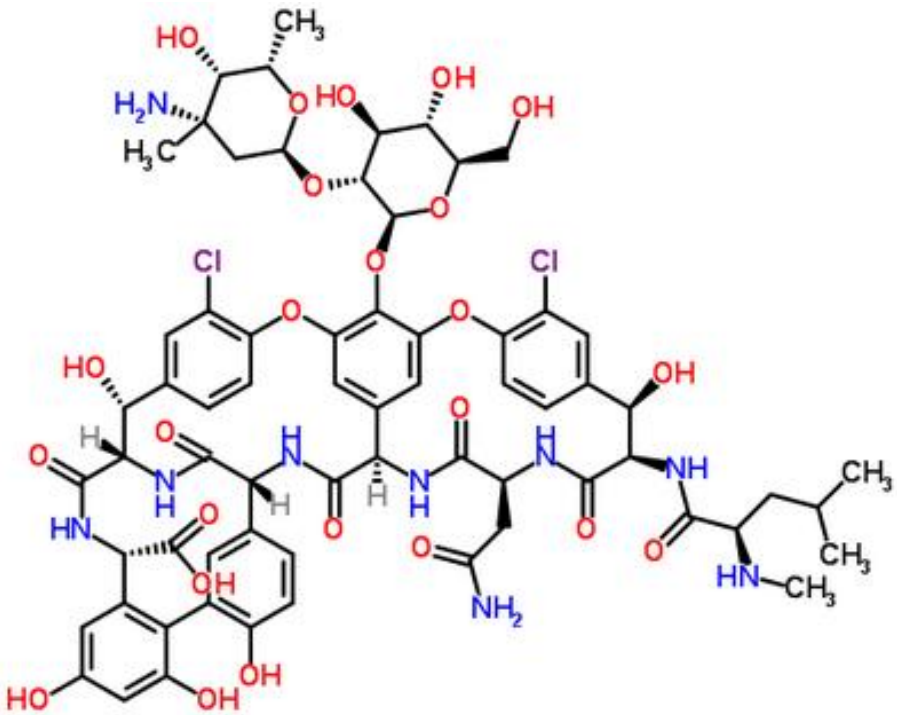
A LITTLE Chemistry First



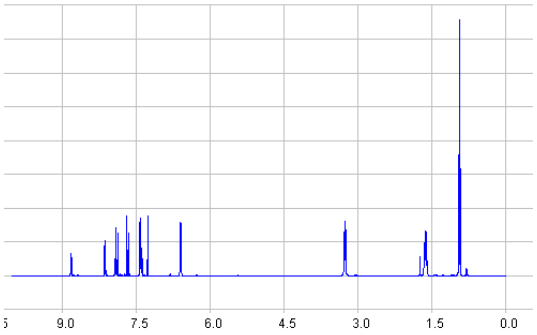
Structural Diagrams

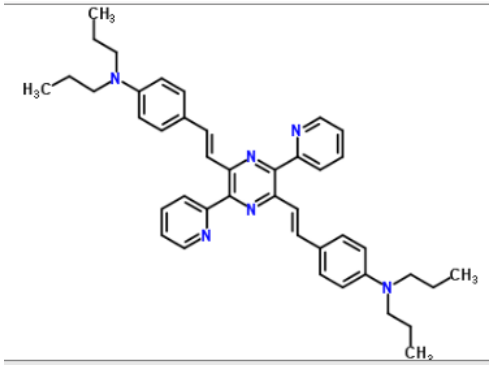


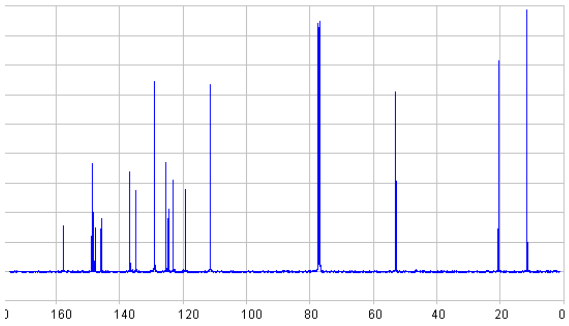
Structural Diagrams

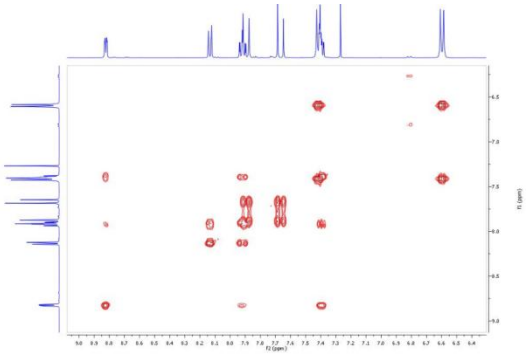


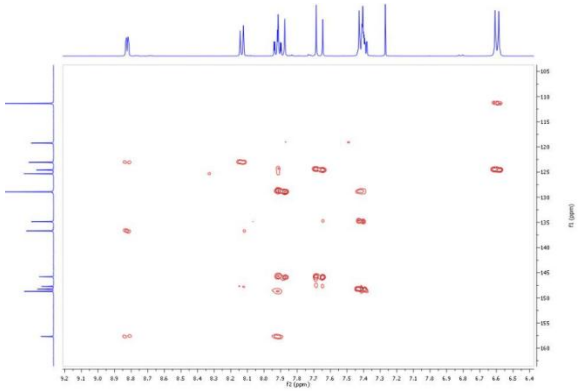
Analytical Data



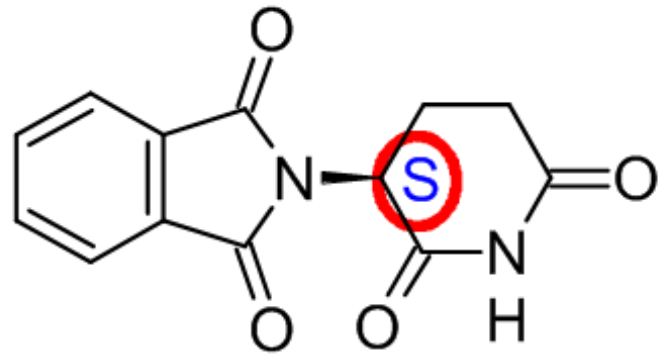


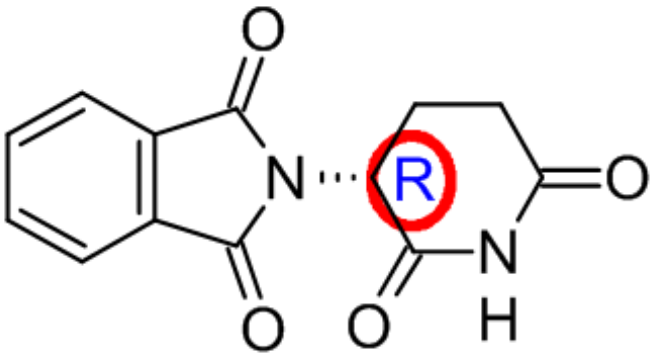




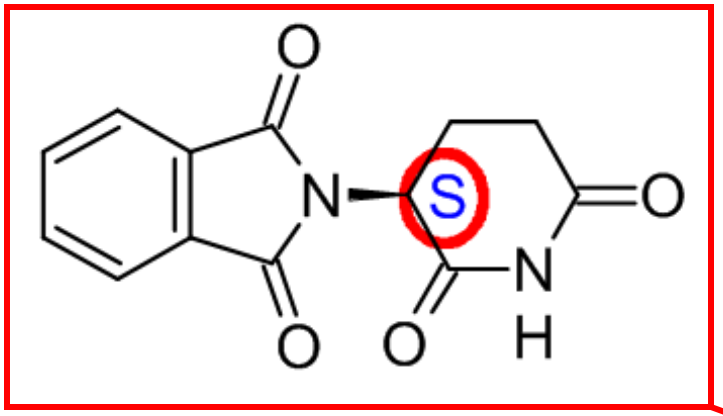


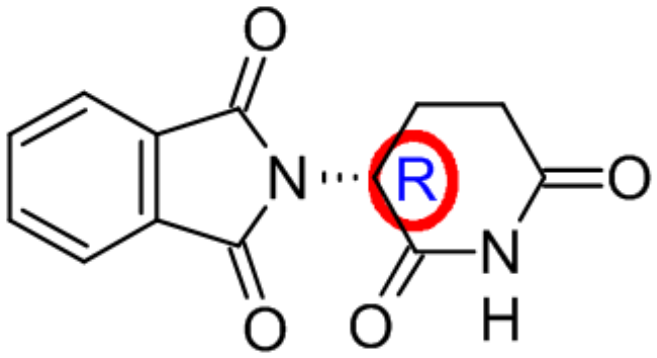
Does Stereochemistry Matter?





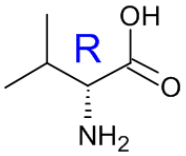
Does one stereocenter matter?



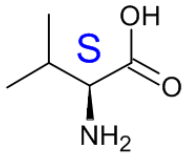


- Distaval, Talimol, Nibrol, Sedimide, Quietoplex, Contergan, Neurosedyn, Softenon, **Thalidomide**

Structural Representations

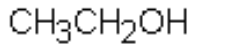


CC(C)[C@@H](N)C(=O)O



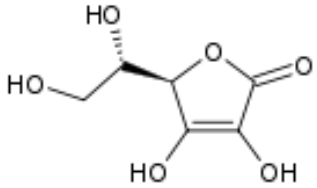
CC(C)[C@H](N)C(=O)O

```
26 29  0  0  0  0  0  0  0  0  1 V2000
   28.5814  -10.1773   -1.9118 C   0  0  0
   28.7872  -11.2789   -2.8314 O   0  0  0
   27.9434  -12.3121   -2.5033 C   0  0  0
   27.3170  -10.6017   -1.1805 C   0  0  0
   28.4273   -8.8528   -2.6723 C   0  0  0
   29.7808  -10.0933   -0.9842 C   0  0  0
   26.9692  -11.8613   -1.5539 C   0  0  0
   30.6602  -11.1619   -0.9380 C   0  0  0
   29.5196   -8.3328   -3.3521 C   0  0  0
   29.4154   -7.1290   -4.0289 C   0  0  0
   31.7788  -11.1097   -0.1230 C   0  0  0
   28.0403  -13.4475   -2.9129 O   0  0  0
   30.0202   -8.9710   -0.2039 C   0  0  0
   27.2235   -8.1591   -2.6831 C   0  0  0
   32.0229   -9.9838    0.6457 C   0  0  0
   28.2149   -6.4358   -4.0315 C   0  0  0
```



ethanol

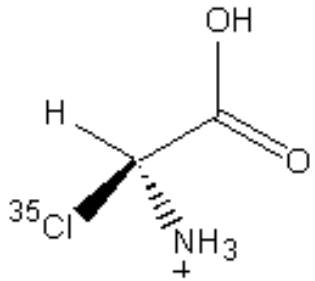
```
InChI=1/C2H6O/c1-2-3/h3H,2H2,1H3
```



L-ascorbic acid

```
InChI=1/C6H8O6/c7-1-2(8)5-3(9)4(10)6(11)12-5/h2,5,7-10H,1H2/t2-
,5+/m0/s1
```

The InChI Standard



InChI=1/C2H4ClNO2/c3-1(4)2(5)6/h1H,4H2,(H,5,6)/p+1/t1-/m1/s1/i3+0/fC2H5ClNO2/h4-5H/q+1

Main layer

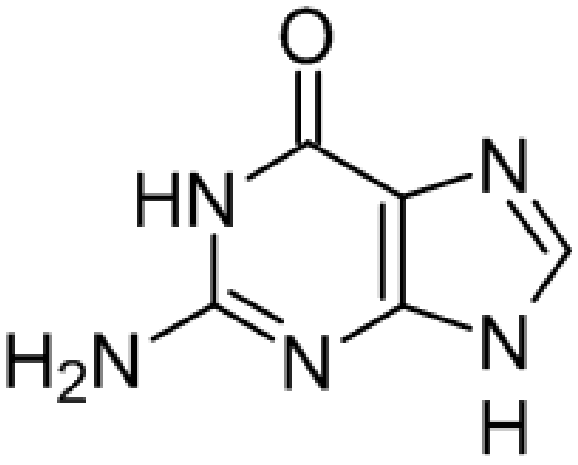
Charge layer

Stereochemical layer

Isotopic layer

Fixed-H layer

InChIKeys
Search the Web by Structure



InChI=1/C5H5N5O/c6-5-9-3-2(4(11)10-5)7-1-8-3/h1H,(H4,6,7,8,9,10,11)

SHA-256 HASH Algorithm

Lookup

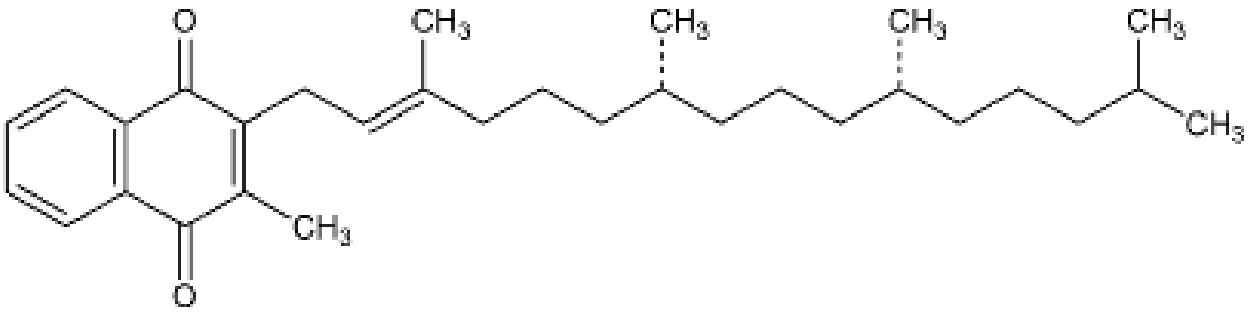
UYTPUPDQBNUYGX-UHFFFAOYAE

The Quality of Chemical Data Online
What is the Structure of Vitamin K?

A lipid cofactor that is required for normal blood clotting. Several forms of vitamin K have been identified: **VITAMIN K1 (phytomenadione) derived from plants**, VITAMIN K2 (menaquinone) from bacteria & synthetic naphthoquinone provitamins, VITAMIN K3 (menadione).

What is the Structure of Vitamin K1?

7380. Phylloquinone.

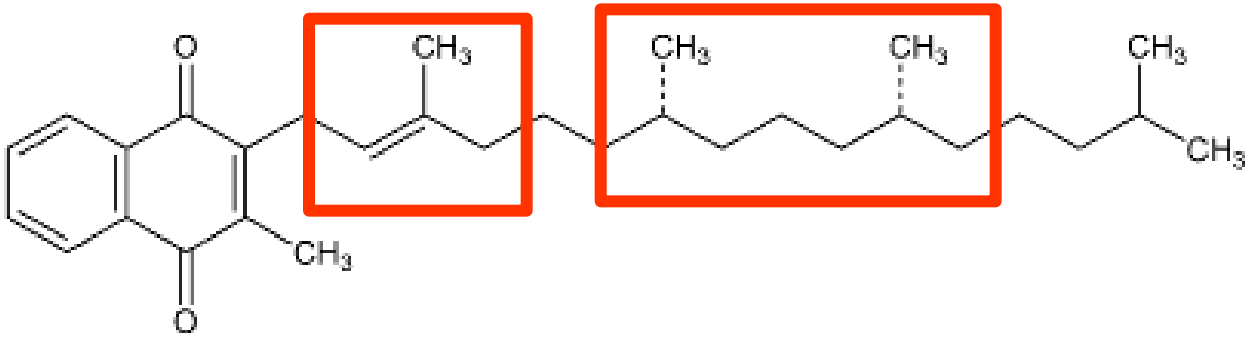


Vitamin K_1

The Merck Index, 14th Edition

What is the Structure of Vitamin K1?

7380. Phylloquinone.



Vitamin K_1

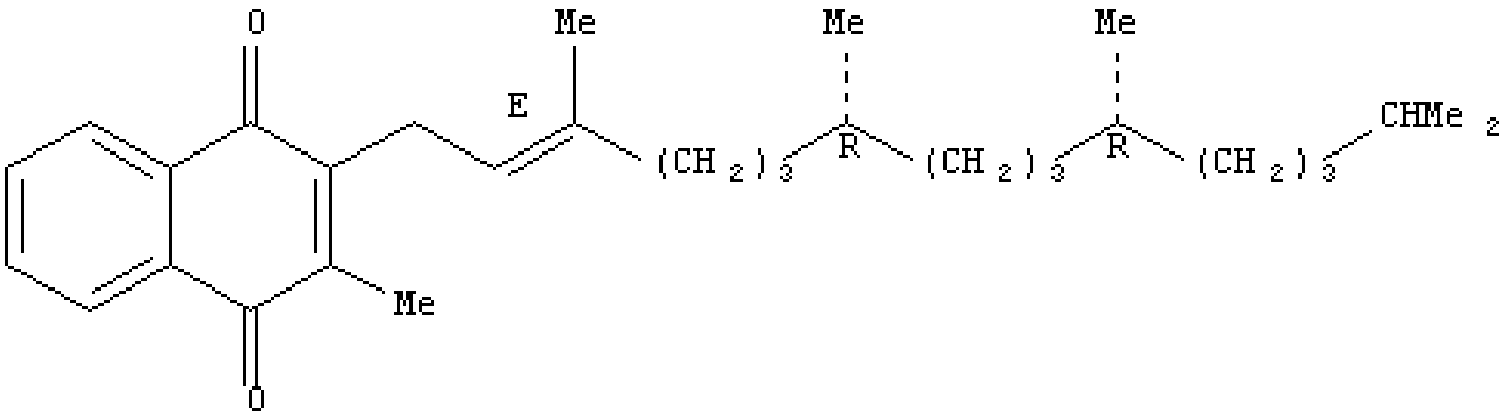
The Merck Index, 14th Edition

Chemical Abstracts Service

Registry Number: 84-80-0

Formula: $C_{31}H_{48}O_2$

ABSOLUTE STEREOCHEMISTRY.



Wikipedia

Phylloquinone

From Wikipedia, the free encyclopedia
(Redirected from Vitamin K1)

Phylloquinone is a polycyclic aromatic ketone, based on 2-methyl-1,4-naphthoquinone, with a 3-phytyl substituent.

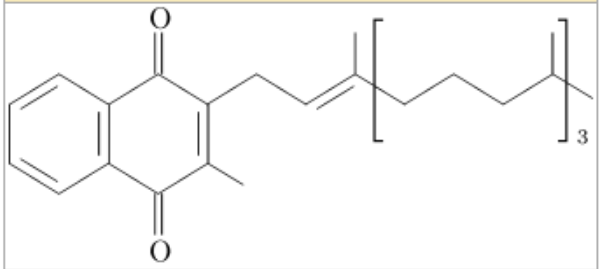
It is a fat-soluble vitamin that is stable to air and moisture but decomposes in sunlight. It is found naturally in a wide variety of green plants.

Terminology [edit]

It is often called **vitamin K_1**[1] or **phytonadione**. Sometimes a distinction is made with phylloquinone considered natural and phytonadione considered synthetic.[2]

A stereoisomer of phylloquinone is called vitamin k_1 (note the difference in capitalization).

Phylloquinone



IUPAC name [hide]
2-methyl-3-[(2*E*)-3,7,11,15-tetramethylhexadec-2-en-1-yl] naphthoquinone

Identifiers	
CAS number	84-80-0
PubChem	4812
SMILES	[show]
Properties	
Molecular formula	$C_{31}H_{46}O_2$

Wolfram Alpha

WolframAlpha computational knowledge engine

vitamin K1

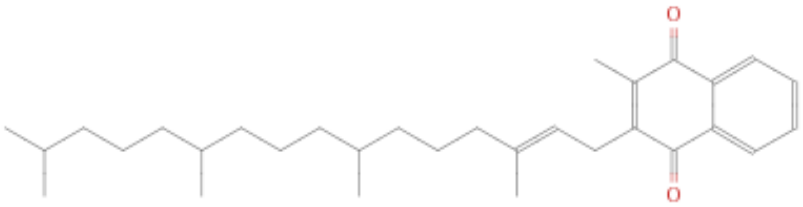
Input interpretation: *Mathematica* form

phytonadione

Chemical names and formulas: More

formula	$C_{31}H_{46}O_2$
name	phytonadione
IUPAC name	3–methyl–2–[(E)–3,7,11,15–tetramethylhexadec–2–enyl]naphthalene–1,4–dione

Structure diagram: Show all atoms | Show bond information



DailyMed

Download the FDA official PDF of this label

Search By Drug Name or NDC Code:

GO

Vitamin K1 (phytonadione) Injection, Emulsion
[Hospira, Inc.]

RxNorm Names

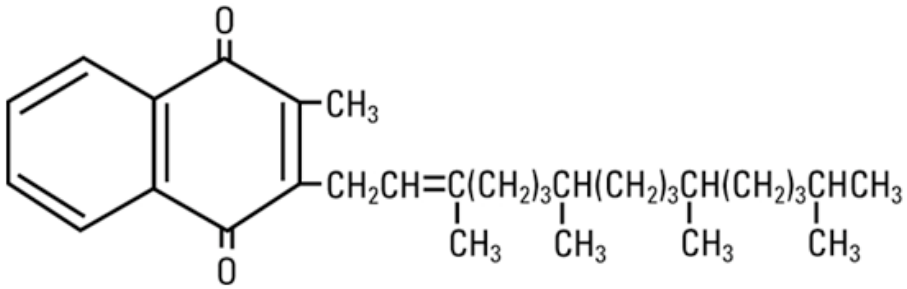
Review RxNorm Normal Forms

Category	DEA Schedule	Marketing Status
HUMAN PRESCRIPTION DRUG LABEL		

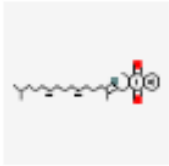
DESCRIPTION

Phytonadione is a vitamin, which is a clear, yellow to amber, viscous, odorless or nearly odorless liquid. It is insoluble in water, soluble in chloroform and slightly soluble in ethanol. It has a molecular weight of 450.70.

Phytonadione is 2-methyl-3-phytyl-1, 4-naphthoquinone. Its empirical formula is $C_{31}H_{46}O_2$ and its structural formula is:

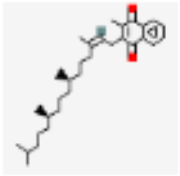


CID: 5284607



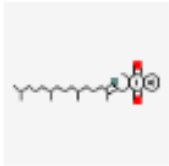
Phylloquinone; phytonadione; 3-Phytylmenadione ...
IUPAC: 2-methyl-3-[(E,7R,11R)-3,7,11,15-tetramethylhex
2-enyl]naphthalene-1,4-dione
MW: 450.695740 g/mol | MF: $C_{31}H_{46}O_2$
Tested in BioAssays: All: 104, Active: 1; BioActivity Ans
Vitamins... more

CID: 9846607



Vitamin K 1; CID9846607
IUPAC: 2-methyl-3-[(Z,7R,11R)-3,7,11,15-tetramethylhexadeo
2-enyl]naphthalene-1,4-dione
MW: 450.695740 g/mol | MF: $C_{31}H_{46}O_2$
Vitamins... more

CID: 5280483

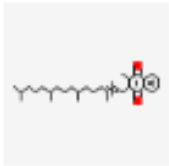


phytonadione; Phylloquinone; Phytomenadione ...
IUPAC: 2-methyl-3-[(E)-3,7,11,15-tetramethylhexadeo-2-
1,4-dione
MW: 450.695740 g/mol | MF: $C_{31}H_{46}O_2$
Tested in BioAssays: All: 118, Active: 0; BioActivity Ans
Vitamins... more

CID: 7048755

Vitamin K 1; ZINC03831331; CID7048755
IUPAC: 2-methyl-3-[(E,7S,11R)-3,7,11,15-tetramethylhexadeo
2-enyl]naphthalene-1,4-dione
MW: 450.695740 g/mol | MF: $C_{31}H_{46}O_2$
Vitamins... more

CID: 4812

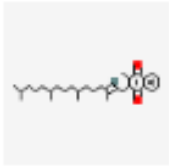


phytonadione; Phylloquinone; Phytomenadione ...
IUPAC: 2-methyl-3-(3,7,11,15-tetramethylhexadeo-2-enyl
1,4-dione
MW: 450.695740 g/mol | MF: $C_{31}H_{46}O_2$
Vitamins... more

CID: 7048754

Vitamin K 1; ZINC03831330; CID7048754
IUPAC: 2-methyl-3-[(E,7R,11S)-3,7,11,15-tetramethylhexadeo
2-enyl]naphthalene-1,4-dione
MW: 450.695740 g/mol | MF: $C_{31}H_{46}O_2$
Vitamins... more

CID: 10863350

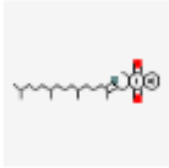


Vitamin K 1; CID10863350
IUPAC: 2-methyl-3-[(E)-3,7,11,15-tetramethylhexadeo-2-
1,4-dione
MW: 452.695500 g/mol | MF: $C_{31}H_{46}O_2$
Vitamins... more

CID: 7048753

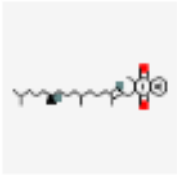
Vitamin K 1; ZINC03831329; CID7048753
IUPAC: 2-methyl-3-[(E,7S,11S)-3,7,11,15-tetramethylhexadeo
2-enyl]naphthalene-1,4-dione
MW: 450.695740 g/mol | MF: $C_{31}H_{46}O_2$
Vitamins... more

CID: 10961411



Vitamin K 1; CID10961411
IUPAC: 2-methyl-3-[(E)-3,7,11,15-tetramethylhexadeo-2-
1,4-dione
MW: 452.695500 g/mol | MF: $C_{31}H_{46}O_2$
Vitamins... more

CID: 5315258



Vitamin K 1; CID5315258
IUPAC: 2-methyl-3-[(E,11S)-3,7,11,15-tetramethylhexadeo-2-
enyl]naphthalene-1,4-dione
MW: 450.695740 g/mol | MF: $C_{31}H_{46}O_2$
Vitamins... more

People Use Trusted Resources…

In the Pipeline: Don't miss Derek Lowe's excellent commentary on drug discove

In the Pipeline

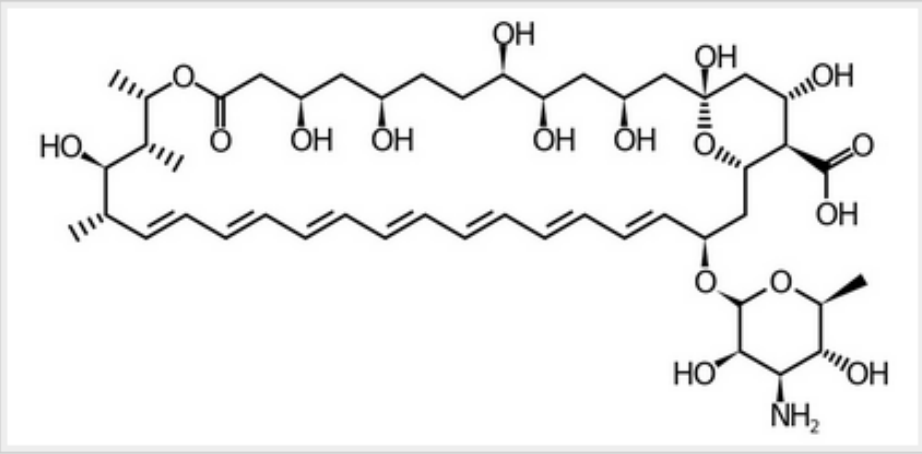
« Arsenic Life No More | Main | Targacep

October 8, 2012

Nasty Drug Molecules: Amphotericin B

Posted by **Derek**

You've probably seen the headlines about fungal meningitis showing up, ca
supplies. As soon as I heard these stories, I wondered what you treat this c
B, most likely". And so it appears.



ABOUT THIS AUTHOR

Derek Lowe, an Arkansan by birth, got his BA from Hendrix College and his PhD in organic chemistry from Duke before spending time in Germany on a Humboldt Fellowship on his post-doc. He's worked for several major pharmaceutical companies since 1989 on drug discovery projects against schizophrenia, Alzheimer's, diabetes, osteoporosis and other diseases. To contact Derek email him directly: derekb.lowe@gmail.com
Twitter: Dereklowe

Search Amazon:

GO!

We can all help clean it up…

6. Dave on October 8, 2012 9:25 AM writes…

I'd just point out that the structure from Wikipedia is a little deceptive as the stereobond at the anomeric carbon of the mannose is very ambiguous (due to the way that the wedge is used). The structure should have a beta-D-mannopyranose (see http://www.chemspider.com/Chemical-Structure.10237579, for a clearer depiction).

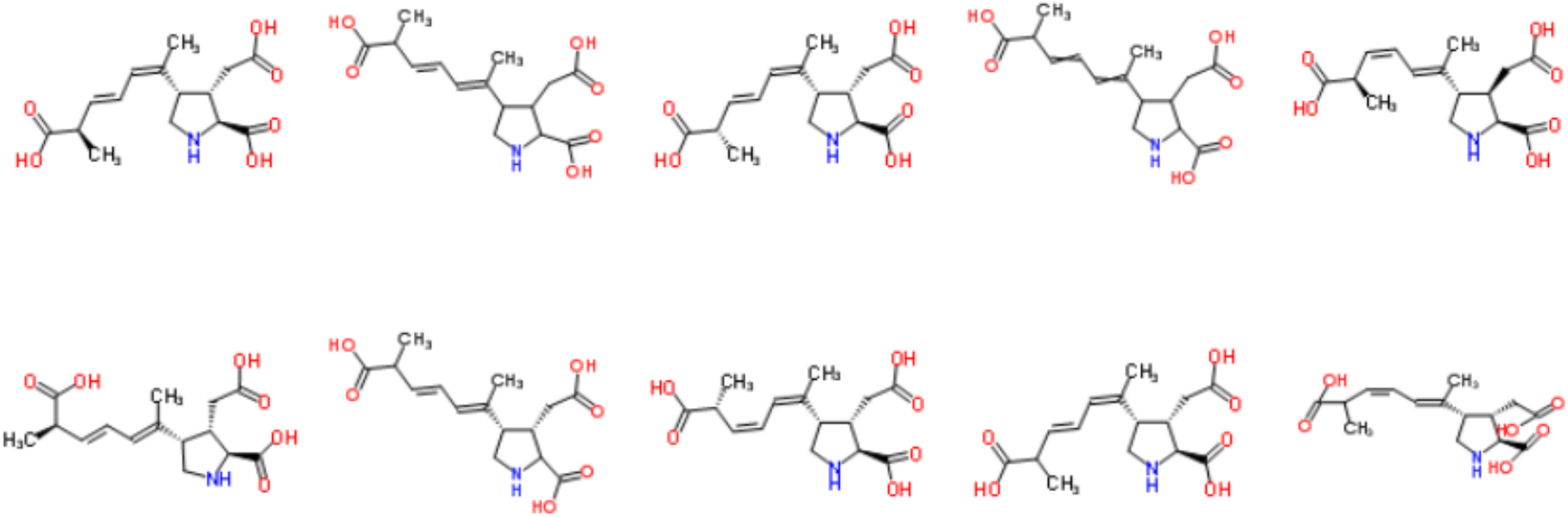
How will it improve?

Participation

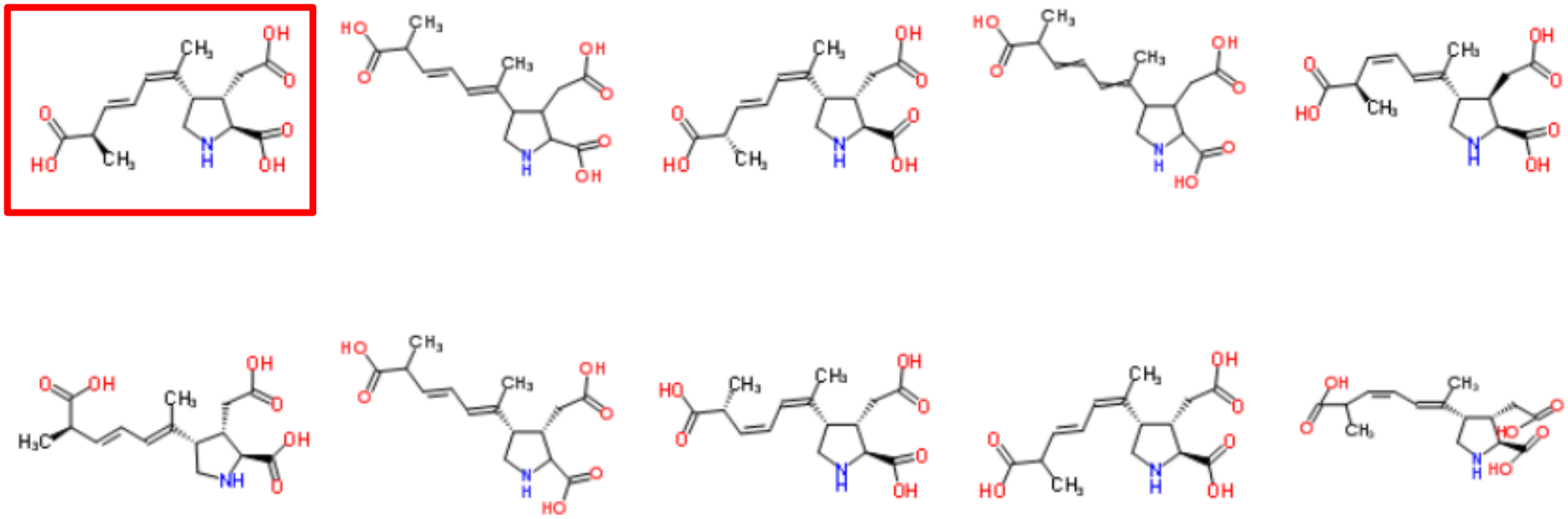
and

contribution

Building a chemistry hub ..issues
ALL Different, ALL “Domoic Acids”



ONE is “correct”



The EXPERTS must get it right?!

Northwest Fisheries Science Center
Harmful Algal Blooms

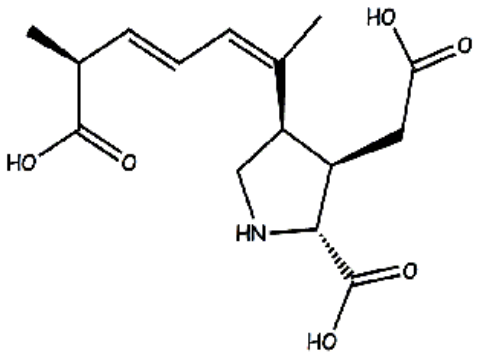
Home • HABs & Biotoxins • Research • Outreach • Links • Search

Domoic Acid Poisoning

Domoic acid has been responsible for several deaths and both permanent and transitory illness in over a hundred people. The toxin is produced by marine diatoms which are members of the genus *Pseudo-nitzschia*. Both shellfish and fish can accumulate this toxin without apparent ill effects; however, in humans the toxin crosses into the brain and interferes with nerve signal transmission. People poisoned with very high doses of the toxin can die, while lower doses can cause permanent brain damage (short term memory loss). When this toxin was discovered in certain West coast fish and shellfish, both recreational and commercial fisheries were briefly closed. This closure, though relatively short, had serious economic impacts on those communities dependent on these fisheries.

Harmful effects of Domoic Acid

The first reported outbreak of domoic acid poisoning occurred in 1987 when shellfish from Prince Edward Island Canada were consumed. In that outbreak, 3 people died and over 100 people developed various toxic symptoms. Domoic acid was found to be produced by the diatom Pseudo-nitzschia multiseries. The most unusual, and most serious toxic symptom, was a loss of short term memory--hence the initial designation of the syndrome in humans as amnesiac shellfish poisoning (ASP). However, since the toxin has been found in fin-fish and the chemical structure of the toxin is now known, a more accurate term is Domoic Acid Poisoning. In 1991, along the beaches of Monterey Bay, CA, dead and dying seabirds



Domoic Acid

HABs & Biotoxins

- Overview
- Phytoplankton
- Marine Biotoxins
  - Detection & Analyses
  - **Domoic Acid Poisoning**
  - Paralytic Shellfish Poisoning
  - Diarrhetic Shellfish Poisoning
- West Coast HABs

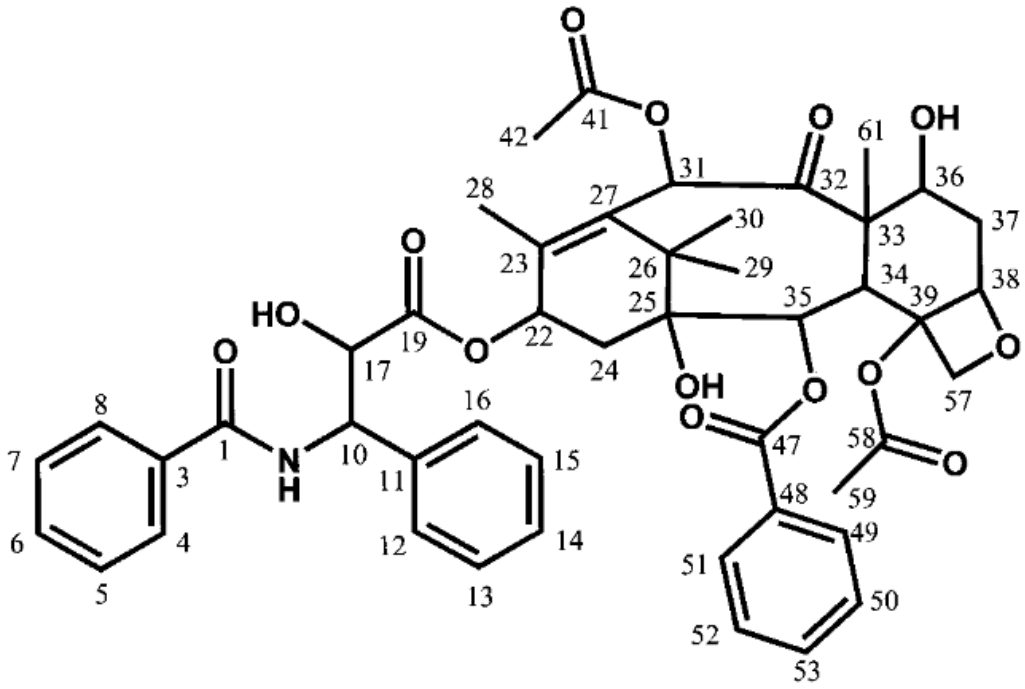
Web 2.0 Contribution

- We have been contributing to the web for a along time already – but how much in chemistry?
- A few blogs, an increasing amount of tweeting but what about data sharing in chemistry?

Challenging a Publication
This story is only 11 years ago!

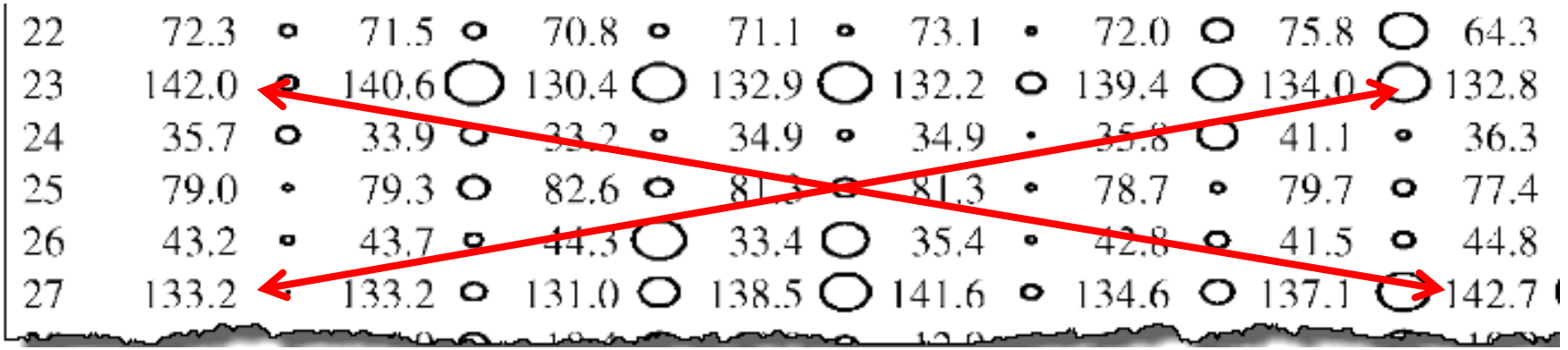
Using Neural Networks for ^{13}C NMR Chemical Shift Prediction–Comparison with Traditional Methods

Received January 29, 2002; revised June 10, 2002



ID	Exp.	*(new)*	*(old)*	*DRAW PRO*	*SPECTOOL*	*SPECINFO*	*NMR 1.3*	*CNMR 6.0*	*4.5*	*98*
1	167.0	166.1	167.2	167.9	167.6	166.8	167.6	166.6	157.7	190.6
3	138.0	*136.0*	*133.9*	*133.5*	*133.5*	*133.2*	*134.2*	*136.3*	*121.7*	*135.7*
4	127.0	127.8	127.4	127.3	127.3	127.6	127.7	127.2	126.8	133.6
5	129.0	128.6	129.0	128.6	128.6	128.1	128.4	128.1	130.8	124.5
6	128.3	*131.9*	*132.3*	*131.9*	*131.9*	*131.6*	*132.0*	*131.7*	*129.6*	*132.9*
7	129.0	128.6	129.0	128.6	128.6	128.1	128.4	128.1	131.3	125.6
8	127.0	127.8	127.4	127.3	127.3	127.6	127.7	127.2	128.1	133.6
10	55.0	55.0	59.9	52.4	51.6	54.6	54.9	55.8	54.6	59.1
11	133.6	*136.7*	*138.1*	*142.4*	*138.8*	*136.7*	*140.7*	*136.1*	*135.8*	*138.7*
12	127.0	126.8	128.0	127.1	128.3	127.2	126.9	128.3	128.0	130.1
13	128.7	128.3	130.0	128.3	128.6	128.6	128.4	129.2	130.1	127.8
14	131.9	*127.9*	*127.7*	*126.5*	*125.8*	*127.7*	*127.4*	*126.2*	*130.6*	*128.2*
15	128.7	128.3	130.0	128.3	128.6	128.6	128.4	129.2	129.4	127.6
16	127.0	126.8	128.0	127.1	128.3	127.2	126.9	128.3	129.9	130.7
17	73.2	73.3	70.8	85.2	85.2	72.9	74.0	74.0	75.4	76.0
19	172.7	171.4	171.7	172.0	172.0	172.8	172.1	172.3	163.8	178.6
22	72.3	71.5	70.8	71.1	73.1	72.0	75.8	64.3	70.5	69.2
23	142.0	140.6	130.4	132.9	132.2	139.4	134.0	132.8	142.3	137.0
24	35.7	33.9	33.2	34.9	34.9	35.8	41.1	36.3	35.8	38.6
25	79.0	79.3	82.6	81.3	81.3	78.7	79.7	77.4	77.4	73.1
26	43.2	43.7	44.3	33.4	35.4	42.8	41.5	44.8	47.2	41.0
27	133.2	133.2	131.0	138.5	141.6	134.6	137.1	142.7	118.7	133.8

Oops…



22	72.3	71.5	70.8	71.1	73.1	72.0	75.8	64.3
23	142.0	140.6	130.4	132.9	132.2	139.4	134.0	132.8
24	35.7	33.9	[illegible]	34.9	34.9	[illegible]	41.1	36.3
25	79.0	79.3	82.6	[illegible]	81.3	78.7	79.7	77.4
26	43.2	43.7	44.3	33.4	35.4	42.8	41.5	44.8
27	133.2	133.2	131.0	138.5	141.6	134.6	137.1	142.7

>2 Years to Resolution

Journal of Magnetic Resonance

Volume 157, Issue 2, August 2002, Pages 242–252

Journal of Magnetic Resonance

Volume 171, Issue 1, November 2004, Pages 1–3

The New Way of Challenging

Published Online December 2 2010
Science 3 June 2011:
Vol. 332 no. 6034 pp. 1163-1166
DOI: 10.1126/science.1197258

RESEARCH ARTICLE

A Bacterium That Can Grow by Using Arsenic Instead of Phosphorus

Challenging Science…

TECHNICAL COMMENTS

Comment on "A Bacterium That Can Grow by Using Arsenic Instead of Phosphorus"

James B. Cotner and Edward K. Hall

Science 3 June 2011: 1149.Published online 27 May 2011

»Abstract »Full Text »Full Text (PDF)

TECHNICAL COMMENTS

Response to Comments on "A Bacterium That Can Grow Using Arsenic Instead of Phosphorus"

Felisa Wolfe-Simon, Jodi Switzer Blum, Thomas R. Kulp, Gwyneth W. Gordon, Shelley E. Hoeft, Jennifer Pett-Ridge, John F. Stolz, Samuel M. Webb, Peter K. Weber, Paul C. W. Davies, Ariel D. Anbar, and Ronald S. Oremland

Science 3 June 2011: 1149.Published online 27 May 2011

»Abstract »Full Text »Full Text (PDF)

TECHNICAL COMMENTS

Comment on "A Bacterium That Can Grow by Using Arsenic Instead of Phosphorus"

Steven A. Benner

Science 3 June 2011: 1149.Published online 27 May 2011

»Abstract »Full Text »Full Text (PDF)

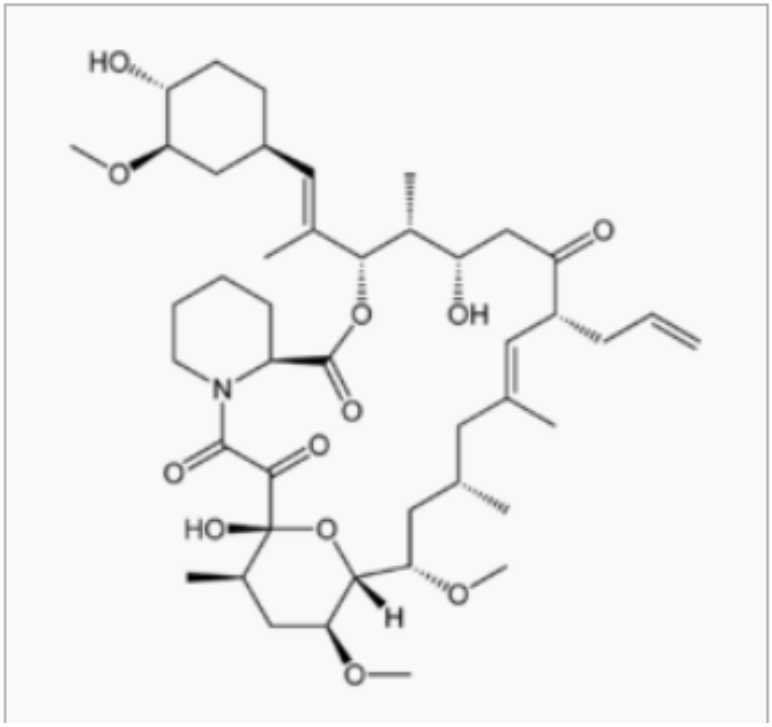
Collaboration towards completion

Tacrolimus (also **FK-506** or **fujimycin**, trade names **Prograf**, **Advagraf**, **Protopic**) is an immunosuppressive drug that is mainly used after allogeneic organ transplant to reduce the activity of the patient's immune system and so lower the risk of organ rejection. It is also used in a topical preparation in the treatment of atopic dermatitis (eczema), severe refractory uveitis after bone marrow transplants, exacerbations of minimal change disease, and the skin condition vitiligo.

It is a 23-membered macrolide lactone discovered in 1984 from the fermentation broth of a Japanese soil sample that contained the bacteria *Streptomyces tsukubaensis*. It reduces interleukin-2 (IL-2) production by T-cells.

Contents [hide]

Tacrolimus



Detailed constructive dialog

Ben (talk) 00:04, 31 May 2008 (UTC)

I put the systematic name you provided above into ChemDraw and compared it with the structure in my Image:Tacrolimus-2D-sk stereochemistry at one particular carbon. I've made a comparison here. I believe my structure is correct (and therefore the nar on the x-ray crystal structure of tacrolimus complexed to a protein in PDB file 1bkf - compare the skeletal structures of the disp structure of the fragment from 1bkf.

I may, however, have made a mistake in interpreting the information here, so it'd be great if several people could check.

Cheers again

Ben (talk) 01:11, 31 May 2008 (UTC)

Ben, take a look at the image shown on [this DailyMed page http://dailymed.nlm.nih.gov/dailymed/drugInfo.cfm?id=2958]. I ChemSpiderMan (talk) 06:06, 31 May 2008 (UTC)

I've found the same structure but from a more reliable source: *Acta Cryst.* (1995). D**51**, 522-528.

Both of these structures are have the same stereochemistry same as my image at the fragment in question, i.e. the R group and in the same direction, while the OH group is pointing in the opposite direction.

Looking at the ChemSpider structure again, now that we've identified the part we think if different, the Chemspider structure is al the name given above.

How did you come to the conclusion that the image in this article was wrong? Was it due to the name? If so, there might not be a

Ben (talk) 10:16, 31 May 2008 (UTC)

Oxidation by Sodium Hydride?

Reductive and Transition-Metal-Free: Oxidation of Secondary Alcohols by Sodium Hydride

Xinbo Wang , Bo Zhang , and David Zhigang Wang *

J. Am. Chem. Soc., 2011, *133* (13), pp 5160-5160
DOI: 10.1021/ja904224y
Publication Date (Web): July 21, 2009

This manuscript has been withdrawn for scientific reasons.

friendfeed

Search

Advanced search
Tools

Search: **nah jacs**

Save search - Share / embed search - Pop out

Michael Nielsen

TotallySynthetic.com » Blog Archive » **NaH** as an Oxidant - Liveblogging! - http://totallysynthetic.com/blog...

August 4 from delicious - Comment - Like - Share

Liveblogging a chemistry experiment to refute a paper: "an intriguing paper has been published in **JACS** by Xinbo Wang, Bo Zhang and David Zhigang Wang. In this, they suggest it is possible to oxidise benzylic alcohols to the corresponding ketones using sodium hydride (amongst other chemistry). Given that sodium hydride is, well, a hydride - this is quite something. Does it work? Hard to say without giving it a go, so I am." - Michael Nielsen

Jiahao Chen

jacs paper reports using **NaH** as an oxidant. wait, WHAT?! http://pubs.acs.org/doi... http://www.thechemblog.com/...

August 3 from Twitter - Comment - Like - Share

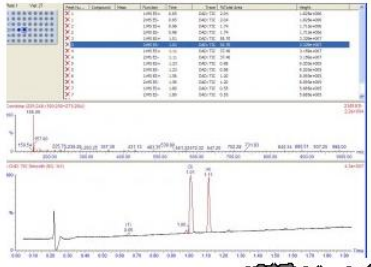
The Blogosphere Analyzes…

totally synthetic

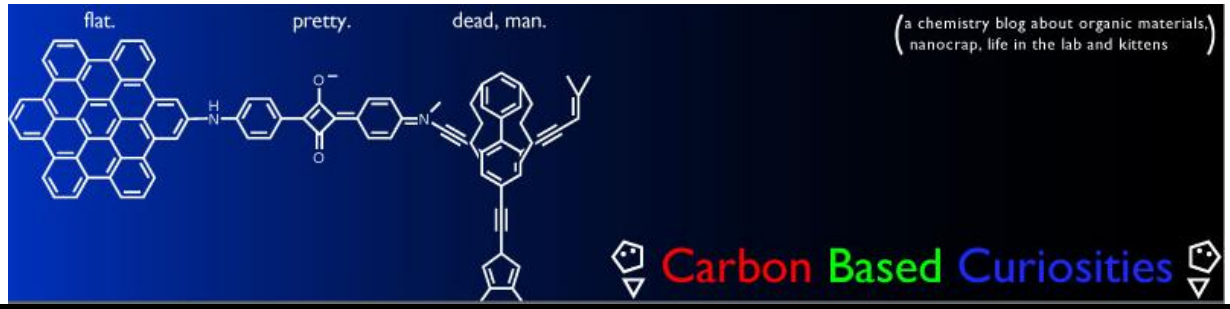
NaH as an Oxidant – Liveblogging! +1 1

22 JULY 2009 135,162 VIEWS 211 COMMENTS

13.20 – Okay, I couldn't wait any longer, so I LCMSed the reaction mixture. This is what I got:



How much is in the archives?



EDIT: Here's a paper from 1946 on how sodium hydride can reduce benzophenone in refluxing xylene, and also demonstrates that benzaldehyde can self-condense to form benzyl benzoate with catalytic NaH. Another, more relevant paper from a commenter on Tot. Syn.

The Action of Sodium Hydride on Certain Carbonyl Compounds. Condensations[1] and Reductions

Frederic W. Swamer , Charles R. Hauser

J. Am. Chem. Soc., **1946**, *68* (12), pp 2647-2649
DOI: 10.1021/ja01216a067
Publication Date: December 1946

First Page

Hi-Res PDF [394 KB]

Data Mine the Archives

- Imagine the power of data-mining the archives of the publishers
- Generate nanopublications from the articles and make available to the reasoning engines
- Now imagine extracting all the “data” and freeing it up to the semantic web.

- MORE LATER ON THAT!

Open Notebook Science Analysis

Useful Chemistry XML UsefulChem wiki

OPEN Notebook Science AC I

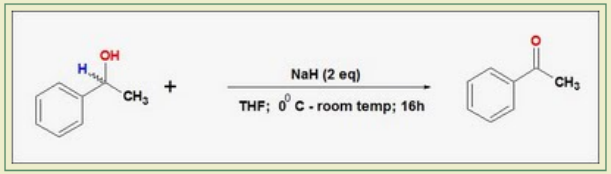
WEDNESDAY, AUGUST 05, 2009

Our attempt to reproduce an oxidation by NaH

Yesterday I was discussing with my students the controversy over the claim that NaH can act as an oxidant for secondary alcohols (Wang, JACS09). There has been a lot of discussion and an attempt to reproduce one of the experiments has appeared on Totally Synthetic.

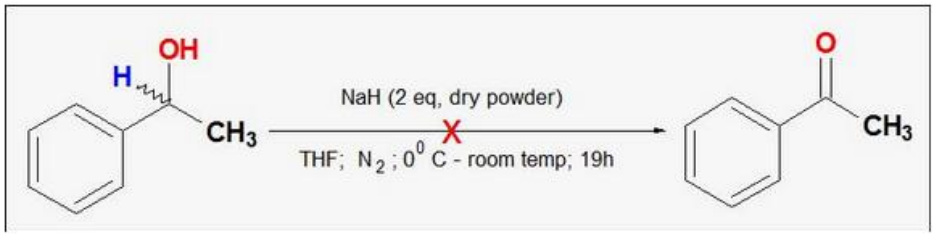
Khalid Mirza and Marshall Moritz thought it would be worthwhile to see if we can shed any light on the situation. I was also curious to see what the reaction did over time, before quenching.

We had 1-phenylethanol on hand, for which the Wang paper claims a 75% conversion (by GC) to acetophenone. All the details can be found on the notebook page UC243.



The reaction was monitored by taking aliquots of the solution then

Researchers - Khalid Mirza & Marshall Moritz



Objective

To convert DL-α-methylbenzyl alcohol to acetophenone using NaH, following a recently published JACS protocol

Procedure

Sodium hydride is added to a stirred THF solution of α-methylbenzyl alcohol at 0 C. After stirring for 12min the bath was removed and the mixture was allowed to warm to room temperature. Aliquots were removed over the course of the reaction, and NMRs were taken after adding benzene-d6 without quenching.

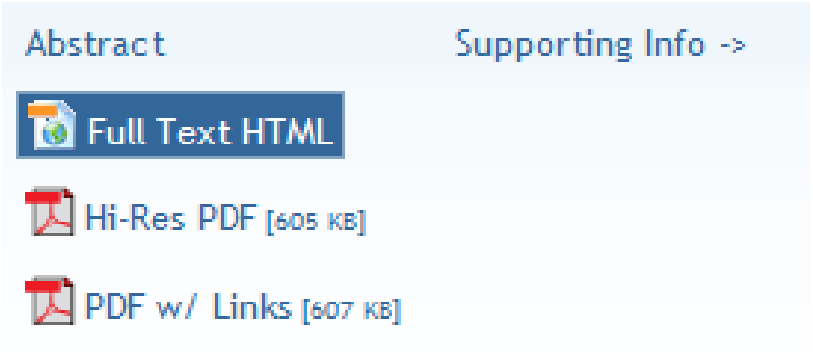
The glassware set up:

Oxidation by Sodium Hydride?

Reductive and Transition-Metal-Free: Oxidation of Secondary Alcohols by Sodium Hydride

Xinbo Wang , Bo Zhang , and David Zhigang Wang *

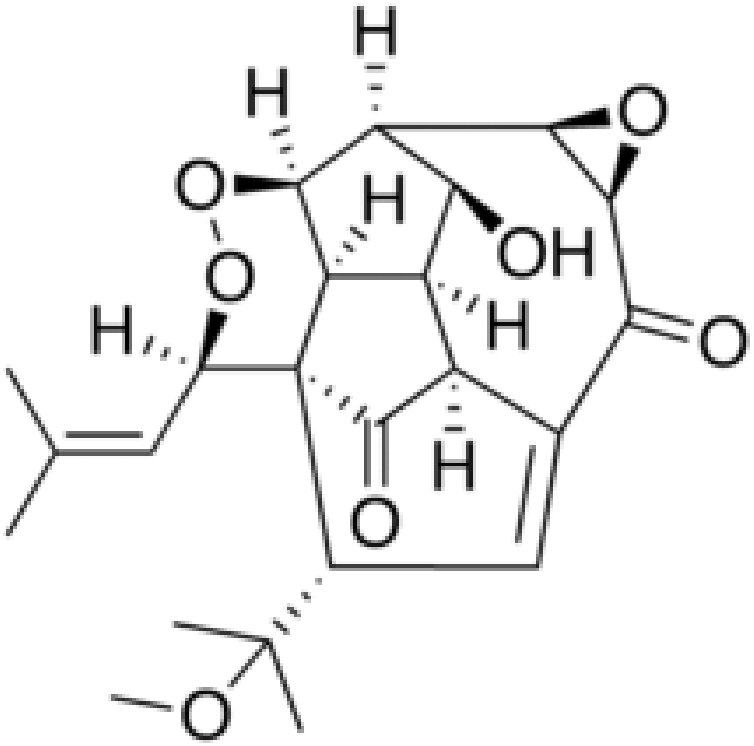
J. Am. Chem. Soc., 2011, *133* (13), pp 5160-5160
DOI: 10.1021/ja904224y
Publication Date (Web): July 21, 2009

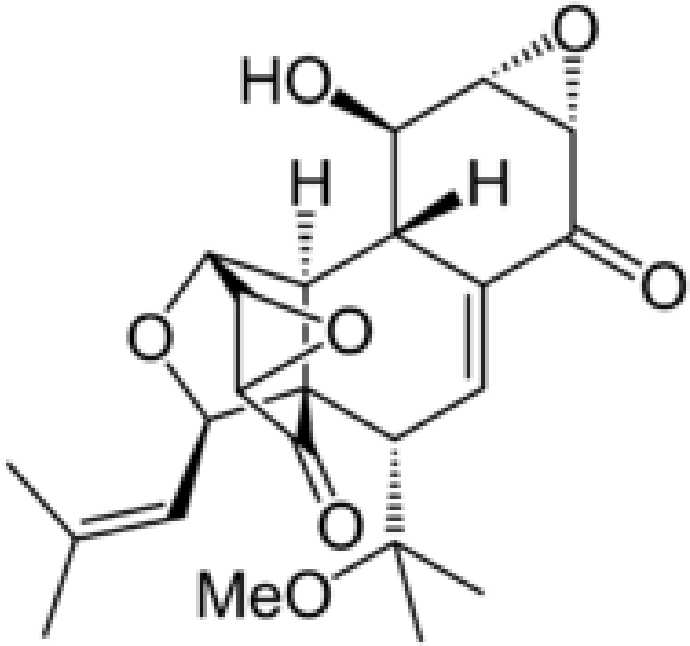


This manuscript has been withdrawn for scientific reasons.

THIS IS A COP OUT!!!

What is Hexacyclinol?





The Blogosphere “Discusses”…

Structure Revision of **Hexacyclinol** / Total Synthesis pt. I
totallysynthetic.com/blog/?p=110
Additionally, one spectrum was duplicated and a copy of the spectra for natural 5-epi-**hexacyclinol** was not provided.” Intriguing stuff. So how closely to the data …

Chemistry Blog » **Hexacyclinol** - Buy Viagra Online No Prescription
www.chemistry-blog.com/tag/**hexacyclinol**
Some stories never seem to end. The **hexacyclinol** story is one of them. Is it over now? I assume most readers will be familiar with the controversy about the two …

Hexacyclinol: A Forensic Case. In the Pipeline:
pipeline.corante.com/archives/2009/02/19/**hexacyclinol**_a_forensic...
About this Author Derek Lowe, an Arkansan by birth, got his BA from Hendrix College and his PhD in organic chemistry from Duke before spending time in Germany on a …

Hexacyclinol? Or Not?. In the Pipeline:
pipeline.corante.com/archives/2006/06/05/**hexacyclinol**_or_not.php
There's an interesting scandal brewing in synthetic organic chemistry - well, actually, more than one, but I haven't covered the Sames matter at all. This is a new …

sanfrancisco_2006: **Hexacyclinol** Showdown: The Biggest …
cenonline.blogs.com/sanfrancisco_2006/2006/09/**hexacyclinol**_sh.html
By Bethany Halford Like almost every other chemistry journalist and blogger at the ACS meeting, I spent Wednesday afternoon at the "Total Synthesis of Complex …

What is real, what is fake?

http://www.youtube.com/watch?v=hMpAoC-h5SA

Question Everything Online: www.dhmo.org

Chemistry is Dangerous!

LEE COUNTY
SOUTHWEST FLORIDA
Information Release
Board of County Commissioners

FOR IMMEDIATE RELEASE
Contact: Patty DiPiero
239-533-8534

Lee County Utilities Water Safe To Drink

FORT MYERS, FL (April 1, 2013) – Lee County Utilities (LCU) is receiving reports that a local radio station is reporting that the water is not safe to use for any reason.

LCU is not having any issues with the water supply and the water is safe to use.

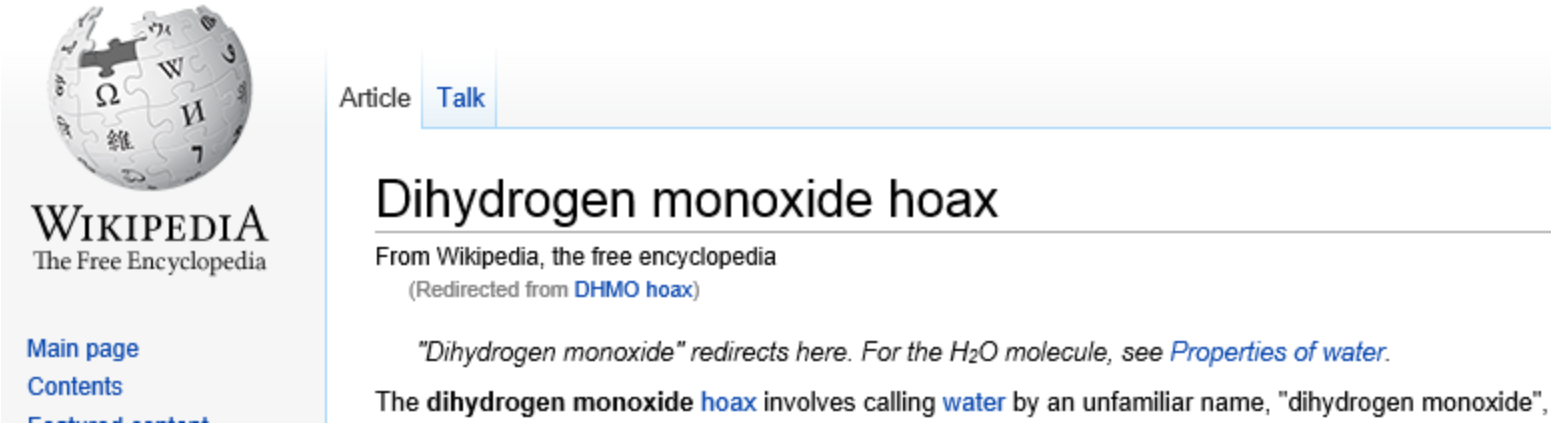
Lee County Utilities believes this is an April Fool's Day prank.

http://tinyurl.com/cl2awnj

Chemistry is Dangerous

Florida DJs May Face Felony for April Fools' Water Joke

"… told their listeners that "dihydrogen monoxide" was coming out of the taps throughout the Fort Myers area."



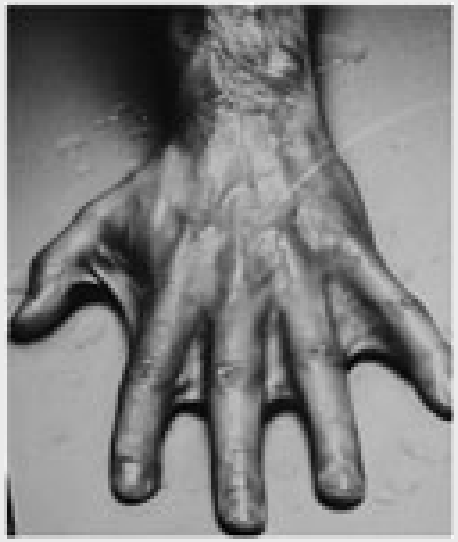
How do you recognize good vs bad?

Letter to the Editor

Cell Death and Differentiation (2005) **12,** 410. doi:10.1038/sj.cdd.4401614

Apoptotic gene therapy in the interdigital web

Is this real?



Re-creation of the interdigital web after WSD gene gun in a nonprofessional swimmer, now regional champion (Ohmy God Ih Svimfast). We thank Arena Italia spa thanks to Enzo Guida, Brand Manager Arena Italia spa; www.arenaitalia.it; the photo was made by LSD, Lowe Pirella Agency, and Umberto Casagrande, Art Direction and Creativity Director

Full figure and legend (120K)

Junk vs Real

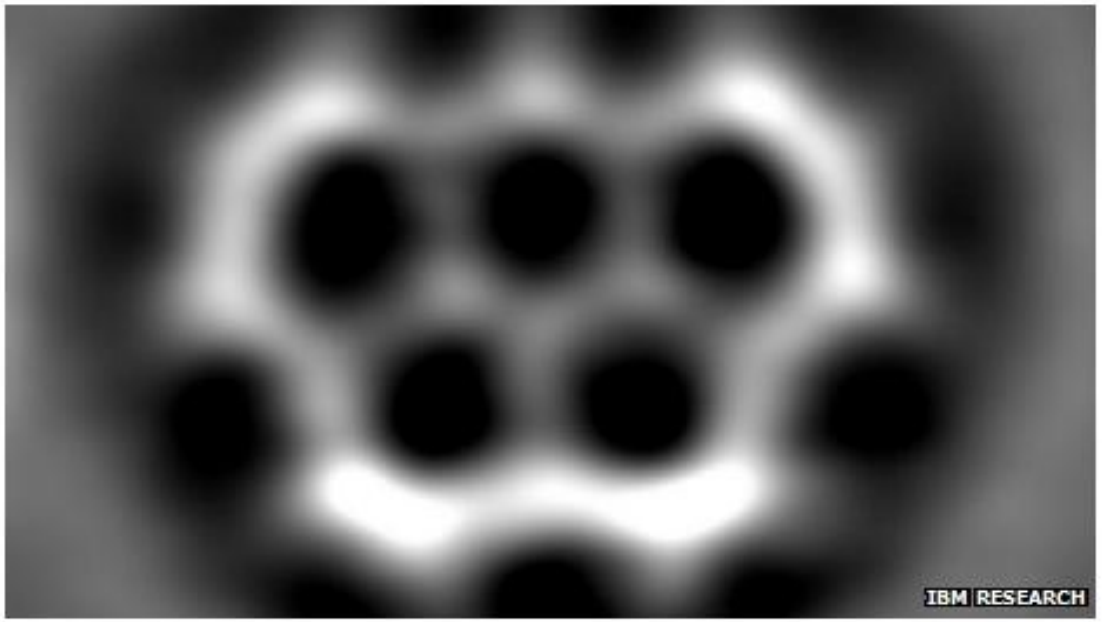
- “We then established a collaboration with professor Sum Ting Wong, a fugitive from the North Korean University Hu Yu Hai Ding”

- “..identified as the new protein Wai So Dim”

What is real, what is fake?

'Olympic rings' molecule olympicene striking image

By Jason Palmer
Science and technology reporter, BBC News



The technique showcases details well under a billionth of a metre in size

Helping to change science

- Participation and contribution
- Immediacy of action
- Platforms for contribution
- Openness…whatever that is

Getting Called Out in Public… Rules for Licensing Data

PERSPECTIVE OPEN ACCESS

Why Open Drug Discovery Needs Four Simple Rules for Licensing Data and Models

Article | Metrics | Related Content | Comments: 1

Antony J. Williams[1*], **John Wilbanks**[2], **Sean Ekins**[3]

1 Royal Society of Chemistry, Wake Forest, North Carolina, United States of America, **2** Consent to Research, Oakland, California, United States of America, **3** Collaborations in Chemistry, Fuquay-Varina, North Carolina, United States of America

To **add a note**, highlight some text. Hide notes

Make a general comment

Challenged in the Twittersphere

Egon Willighagen @egonwillighagen 1 Oct

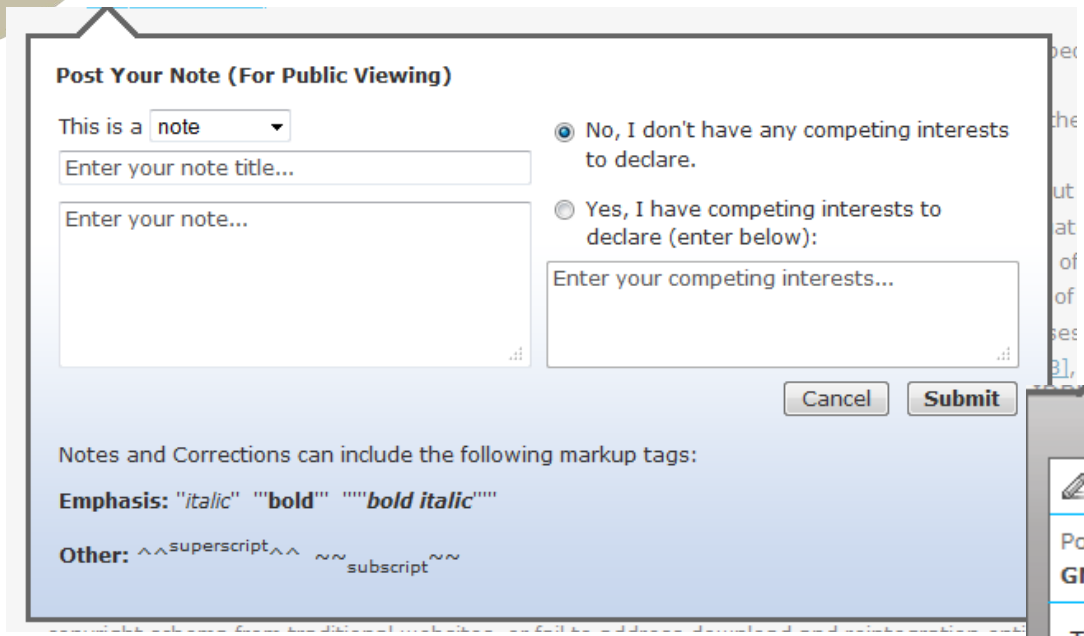
@ChemConnector maybe the text was meant differently, but that is how it reads to me...

Expand

Egon Willighagen @egonwillighagen 1 Oct

@ChemConnector where can I download those public domain parts of @ChemSpider then? ploscompbiol.org/article/info%3...

Annotating Articles Today…



Attribution to me…

PERSPECTIVE OPEN ACCESS

Why Open Drug Discovery Needs Four Simple Rules for Licensing Data and Models

Article | Metrics | Related Content | Comments: 1

Make a new comment on this article

0 responses	Change public domain to "public"	Posted by ChemConnector on 01 Oct 2012 at 16:56 GMT

Most recent response on **01 Oct 2012** at **16:56 GMT**

Back to Chemistry….

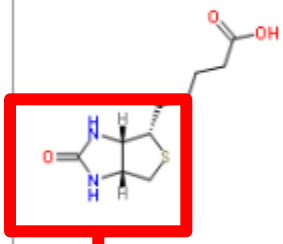
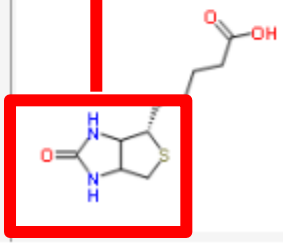
- **ANYBODY** can annotate a record on ChemSpider
- Registered users can deposit new data
  - Compounds
  - Reactions
  - Links
  - Analytical Data
  - Images
  - Movies,
  - Data sets
- Registered users can validate existing data

CURATION Search “Vitamin H”

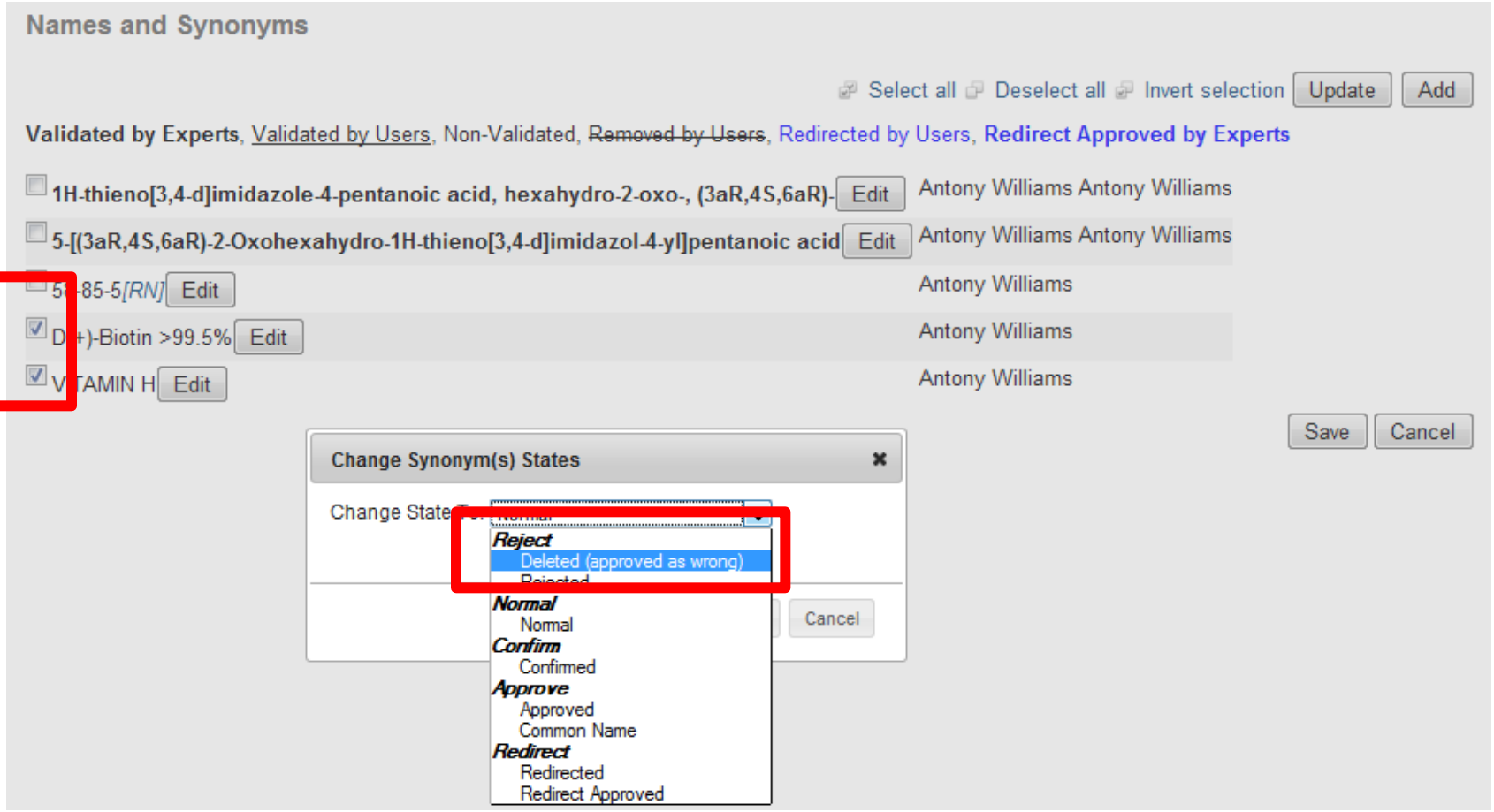
Search

2 hits found in 0.16 seconds.
Search terms: vitamin H
Found by synonym

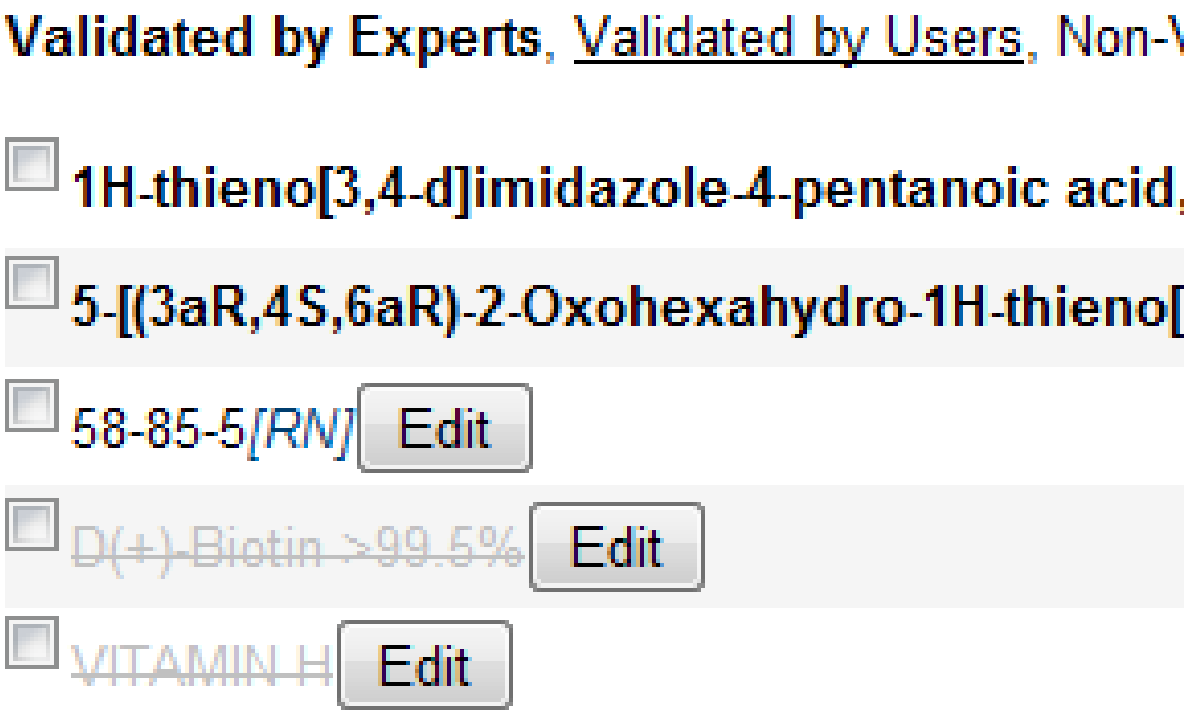
Grid Tile Table Record ChemRefer Entrez PubChem

ID	Structure	Empirical Formula	Molecular Weight	# of Data Sources	# of References
149962		$C_{10}H_{16}N_2O_3S$	244.3106	55	256
5408838		$C_{10}H_{16}N_2O_3S$	244.3106	3	3

“Curate” Identifiers



“Curate” Identifiers



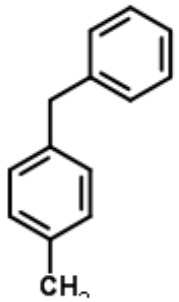
Data Validation is Exacting Work

name	mp °C	source	SMILES
4-methyldiphenylmethane	5.00	American Petroleum Institute	Cc2ccc(Cc1ccccc1)cc2
benzene, 1-methyl-4-(phenylmethyl)-[1]	-30.00	PHYSPROP	Cc2ccc(Cc1ccccc1)cc2
p-tolyltoluene[2]	125.00	PHYSPROP	Cc2ccc(Cc1ccccc1)cc2
4-benzyltoluene[3]	97.50	peer reviewed journal	c1c(cccc1)Cc2ccc(cc2)C
4-benzyltoluene	5.00	open notebook	c1c(cccc1)Cc2ccc(cc2)C
4-benzyltoluene[4]	-30.00	government database	c1c(cccc1)Cc2ccc(cc2)C
4-benzyltoluene	4.58	government database	c1c(cccc1)Cc2ccc(cc2)C

compound: 4-benzyltoluene - melting point: 4.86 °C

Entries highlighted in red are not used in calculating the average value:

1. freezes at -15C after 16 days http://usefulchem.wikispaces.com/Exp266 JCB
2. clearly a liquid at rt http://usefulchem.wikispaces.com/Exp266 JCB
3. clearly a liquid at rt http://usefulchem.wikispaces.com/Exp266 JCB
4. freezes at -15C after 16 days http://usefulchem.wikispaces.com/Exp266 JCB



It is so difficult to navigate…

LETTERS NATURE CHEMICAL BIOLOGY VOLUME 3 NUMBER 5 MAY 2007 nature chemical biology

Chemical genetics reveals a complex functional ground state of neural stem cells

Phedias Diamandis[1–4], Jan Wildenhain[4], Ian D Clarke[1,2], Adrian G Sacher[1,2], Jeremy Graham[1,2], David S Bellows[3], Erick K M Ling[1,2,5], Ryan J Ward[1,2,5], Leanne G Jamieson[1,2,5], Mike Tyers[3,4] & Peter B Dirks[1,2,5,6]

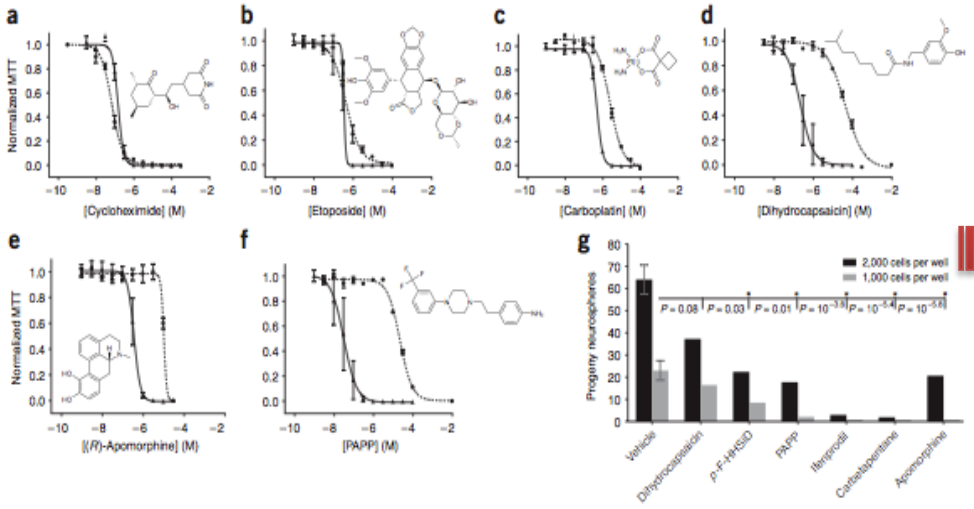


Figure 2 Identification of potent NPC-specific compounds. (a–f) Dose-response curves and chemical structures of controls: cycloheximide (a), etoposide (b) and carboplatin (c), and of selected newly identified compounds: dihydrocapsaicin (d), apomorphine (e) and PAPP (f). Each plot shows the fitted sigmoidal logistic curve to MTT proliferation assay readings of both astrocytes (- -●- -) and neurosphere cultures (–▲–). Values represent the mean and

- **Open PHACTS Project**
- Develop a set of robust standards
- Integrate Chemistry and Biology data by implementing the standards in a *semantic integration hub*
- Deliver services to support drug discovery programs in pharma and public domain
- **INITIALLY** 22 partners, 8 pharmaceutical companies, 3 biotechs

Guiding principle is open access, open usage, open source

- **Key to standards adoption** -

ChemSpider serving RDF and the semantic web

- Using RDF permalinks
- http://www.chemspider.com/Chemical-Structure.7787.rdf

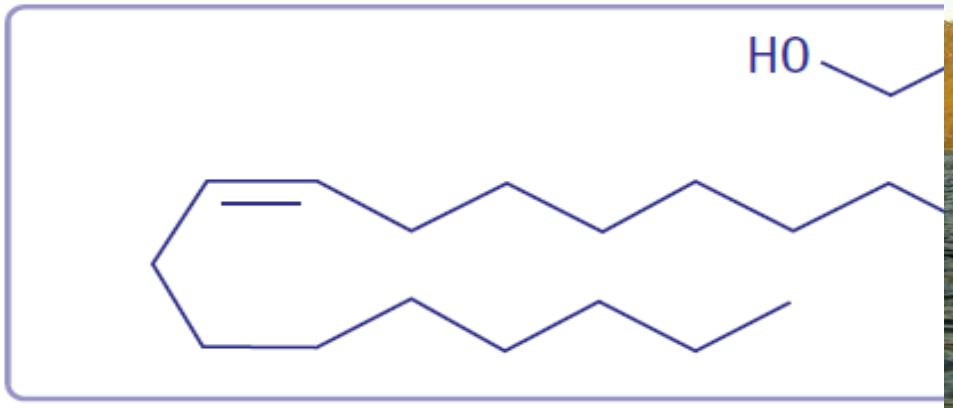
- Using a Search Term
- http://www.chemspider.com/rdf.ashx?q=cyclohexane
- http://rdf.chemspider.com/cyclohexane

RDF and the semantic web

```
- <rdf:RDF xml:base="http://www.chemspider.com/Chemical-Structure.5758.rdf">
  - <rdf:Description rdf:about="http://www.chemspider.com/">
      <rdfs:label>ChemSpider</rdfs:label>
      <rdfs:seeAlso rdf:resource="http://www.rsc.org/"/>
    </rdf:Description>
  - <rdf:Description rdf:about="http://www.chemspider.com/Chemical-Structure.5758.html">
      <dc:format>text/html</dc:format>
      <dc:rights rdf:resource="http://www.chemspider.com/Disclaimer.aspx"/>
      <dcterms:creator rdf:resource="http://www.chemspider.com/"/>
      <dcterms:modified rdf:datatype="http://www.w3.org/2001/XMLSchema#dateTime">2012-10-02</dcterms:modified>
      <ore:aggregatedBy rdf:resource="#Aggregation"/>
      <rdf:type rdf:resource="http://xmlns.com/foaf/0.1/Document"/>
    </rdf:Description>
  - <rdf:Description rdf:about="">
      <dc:format>application/rdf+xml</dc:format>
      <dc:rights rdf:resource="http://www.chemspider.com/Disclaimer.aspx"/>
      <dcterms:creator rdf:resource="http://www.chemspider.com/"/>
      <dcterms:modified rdf:datatype="http://www.w3.org/2001/XMLSchema#dateTime">2012-10-02</dcterms:modified>
      <ore:aggregatedBy rdf:resource="#Aggregation"/>
      <rdf:type rdf:resource="http://xmlns.com/foaf/0.1/Document"/>
      <foaf:primaryTopic rdf:resource="#Compound"/>
      <foaf:primaryTopic rdf:resource="#ResourceMap"/>
    </rdf:Description>
```

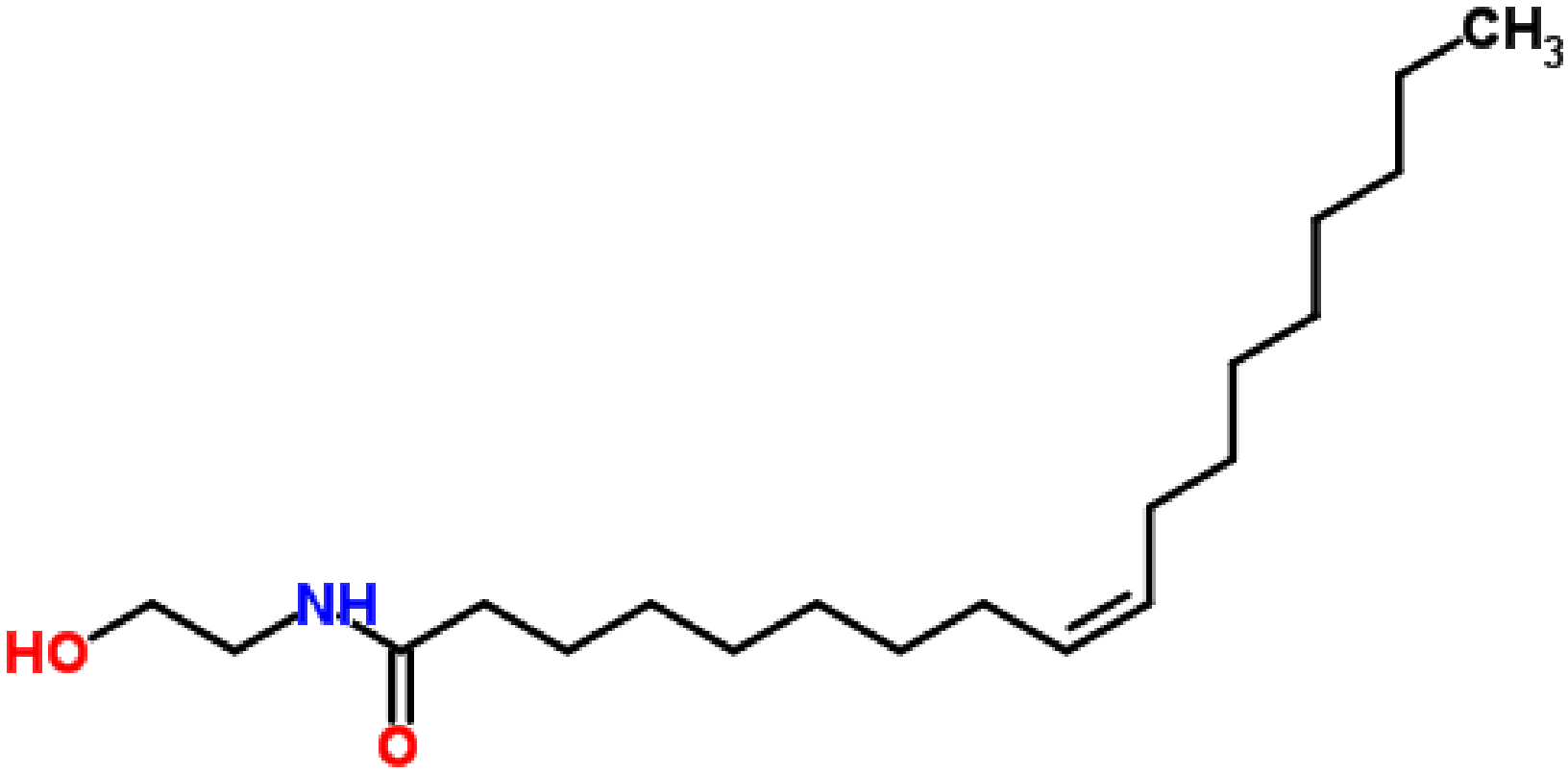
The issue of identifiers

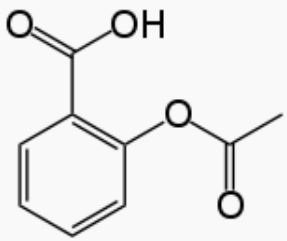
What is a good strategy to search for chemical compounds? We compared various free online databases and search engines for N-oleoylethanolamine (OEA, CAS Registry Number 111-58-0), a very interesting compound and the Nature "lipid of the month June 2009". OEA has been found to induce satiety and decrease meal frequency, and is therefore a potential therapeutic target for treatment of obesity, diabetes and eating disorders. OEA is also used in the treatment of psoriasis, due to its ceramidase inhibiting effects.

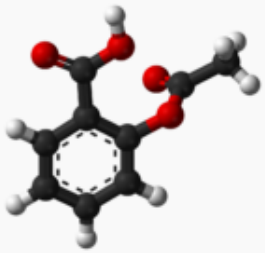


The final strategy for FreePatentsOnline:

TTL/(Oleoylethanolamine OR Oleoylethanolamide OR "Oleoyl ethanolamine" OR "N-oleoyl-ethanolamine" OR "oleoyl ethanolamide" OR "N-oleoyl ethanolamide" OR "N-oleoyl ethanolamine" OR "N-Oleoyl-2-aminoethanol" OR "N-Oleoylethanolamine" OR Oleylethanolamide OR "Oleyl ethanolamide" OR "oleic acid ethanolamide" OR Oleylethanolamine OR "N-Oleylethanolamine" OR "Oleyl ethanolamine" OR "N-oleyolethanolamine" OR "oleic acid ethanolamine") OR **ABST/**(Oleoylethanolamine OR Oleoylethanolamide OR "Oleoyl ethanolamine" OR "N-oleoyl-ethanolamine" OR "oleoyl ethanolamide" OR "N-oleoyl ethanolamide" OR "N-oleoyl ethanolamine" OR "N-Oleoyl-2-aminoethanol" OR "N-Oleoylethanolamine" OR Oleylethanolamide OR "Oleyl ethanolamide" OR "oleic acid ethanolamide" OR Oleylethanolamine OR "N-Oleylethanolamine" OR "Oleyl ethanolamine" OR "N-oleyolethanolamine" OR "oleic acid ethanolamine") OR **ACLM/**(Oleoylethanolamine OR Oleoylethanolamide OR "Oleoyl ethanolamine" OR "N-oleoyl-ethanolamine" OR "oleoyl ethanolamide" OR "N-oleoyl ethanolamide" OR "N-oleoyl ethanolamine" OR "N-Oleoyl-2-aminoethanol" OR "N-Oleoylethanolamine" OR Oleylethanolamide OR "Oleyl ethanolamide" OR "oleic acid ethanolamide" OR Oleylethanolamine OR "N-Oleylethanolamine" OR "Oleyl ethanolamine" OR "N-oleyolethanolamine" OR "oleic acid ethanolamine")


CH3
NH
HO
O





Aspirin

Systematic (IUPAC) name	
2-acetoxybenzoic acid	
Identifiers	
CAS number	50-78-2
ATC code	A01AD05 B01AC06, N02BA01
PubChem	2244
DrugBank	APRD00264
ChemSpider	2157

Identifiers

CAS number	50-78-2
ATC code	A01AD05 B01AC06, N02BA01
PubChem	2244
DrugBank	APRD00264
ChemSpider	2157

Aspirin on ChemSpider

2-(Acetyloxy)benzoic acid

2-(Acetyloxy)benzolcarbonsäure *[German] [ACD/IUPAC Name]*

200-064-1 *[EINECS]*

2-Acetoxybenzenecarboxylic acid

2-Acetoxybenzoesäure *[German] [ACD/IUPAC Name]*

2-Acetoxybenzoic acid *[ACD/IUPAC Name]*

2-Acetyloxybenzoic acid

50-78-2 *[RN]*

A.S.A.

Acesan

Acetard

Acetoxybenzoic acid

acetyl salicylic acid

Acetyl-SAL

ACETYLSALICYLIC ACID

Acetyonyl

Acetysalicylic acid

Acide 2-(acétyloxy)benzoïque *[French]*

Acide 2-acétoxybenzoïque *[French] [ACD/IUPAC Name]*

Ácido acetilsalicílico *[Portuguese]* *[Wiki]*

acidum acetylsalicylicum *[Latin]* *[INN]*

Asatard

Asetilsalisilik asit *[Turkish]* *[Wiki]*

Aspirin *[Wiki]* *[USP]* *[BAN]* *[JAN]* *[JP15]*

aspirina *[Basque]*

Aspropharm

Benzoic acid, 2-(acetyloxy)- *[ACD/Index Name]*

ECM

Kyselina 2-acetoxybenzoova *[Czech]*

Kyselina acetylsalicylova *[Czech]*

Melhoral

Miniasal

o-(Acetyloxy)benzoic Acid

o-Acetylsalicylic acid

QVR BOV1 *[WLN]*

Rhodine NC RP

Salicylic acid, acetyl-

Salospir

Tasprin

Toldex

Triaminicin

Ασπιρίνη *[Modern Greek (1453-)]* *[Wiki]*

Ацетилсалициловая кислота *[Russian]*

Ацетилсаліцилова кислота *[Ukrainian]*

アセチルサリチル酸 *[Japanese]* *[Wiki]*

אספירין *[Hebrew]* *[Wiki]*

एस्पिरिन *[Hindi]* *[Wiki]*

阿司匹林 *[Chinese]*

2-(acetoyloxy)benzoic acid

2-(acetyloxy)-benzoic acid

2-Carboxyphenyl acetate *[Spanish]*

2-O-Acetylsalicylic acid

4-10-00-00138 *[Beilstein]*

779271 *[Beilstein]*

Acenterine

Acesal

Aceticyl

Acetilsalicilico

Acenterine

Acesal

Aceticyl

Acetilsalicilico

Acetilum acidulatum

Acetisal

acetol

Acetophen

Acetosal

Acetosalic acid

Acetosalin

ACETYL SALYCYLIC ACID

Acetylin

Acetylsal

acetylsalicylicacid

Acetylsalicylsaeure

Acetylsalicylsaure *[German]*

acetyl-salicylsyra

acetylsalicylzuur

Acetylsaliycilic acid

Acetylsalycilic acid

Acetysal

acide 2-(acetyloxy)benzoique

acido acetilsalicilico *[Italian]*

Acido O-acetil-benzoico *[Italian]*

acidum acetylsalicylicum

Acimetten

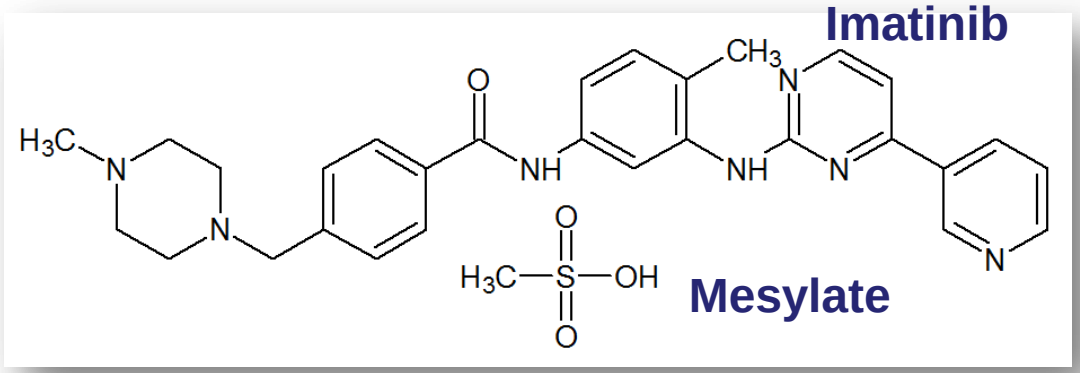
Acisal

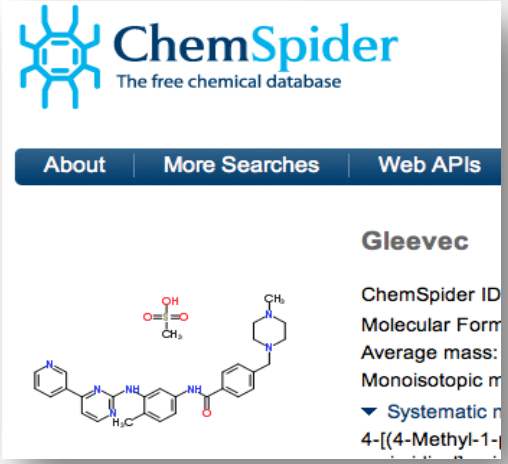
Acylpyrin

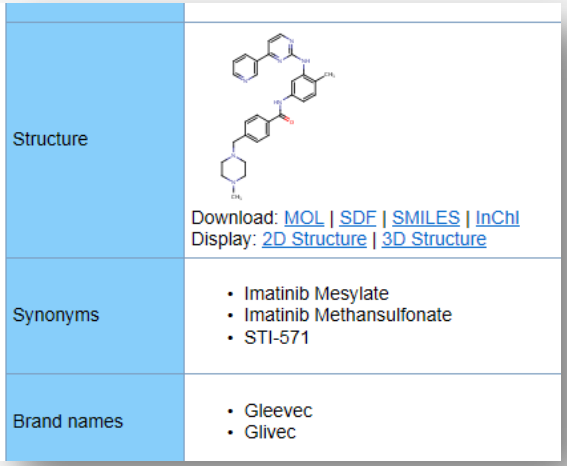
Adiro

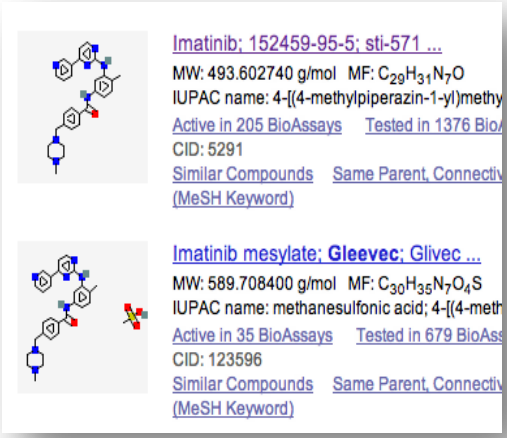
AIN

What is Gleevec









ChemSpider **Drugbank** **PubChem**

Dynamic Equality

chemspider:gleevec

drugbank:gleevec

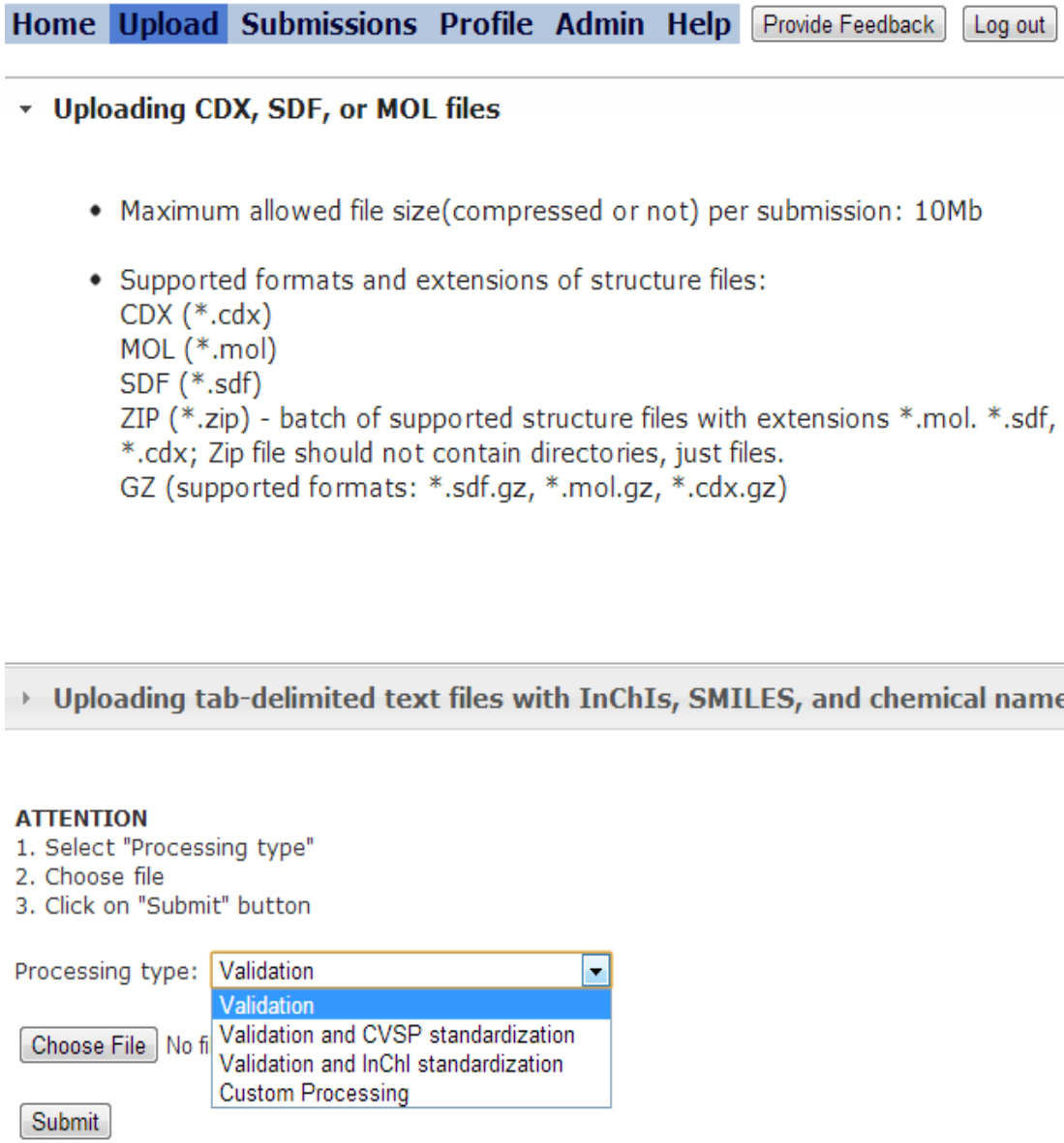
```
LinkSet#1 {
  chemspider:gleevec hasParent imatinib  ...
  drugbank:gleevec exactMatch imatinib  ...
}
```

But what about Data Quality???
CVSP : chemical validation

Free chemistry validation platform that performs:

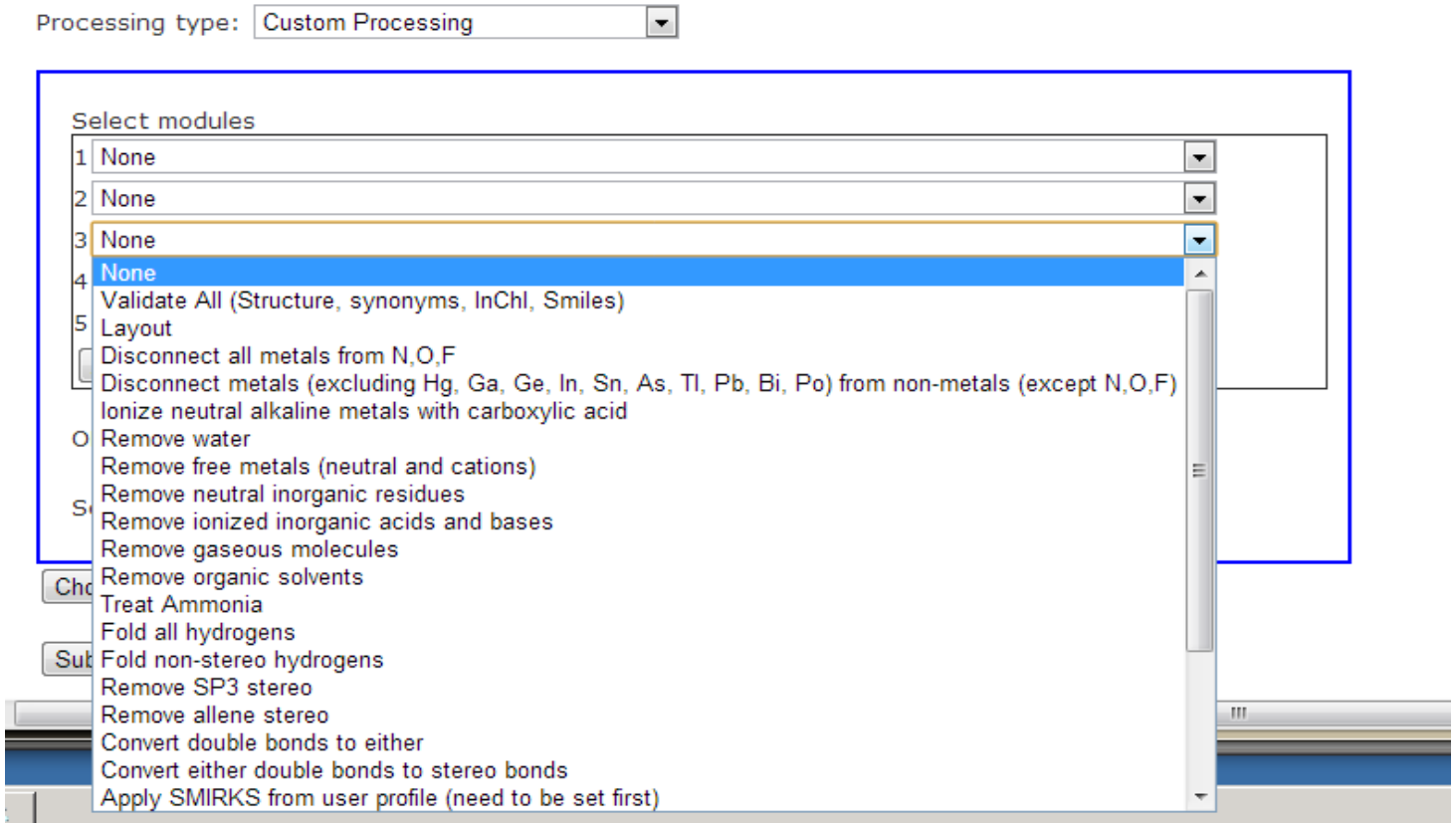
- Structure validation
  - Atoms
  - Bonds
  - Valence
  - Stereo
  - If aromatic - check that uniquely dearomatized
  - Strongest acid not ionized first in partially-ionized system
- Cross-matching of SDF fields
  - synonyms
  - InChIs
  - Smiles

Validation


Home Upload Submissions Profile Admin Help
Provide Feedback
Log out
Uploading CDX, SDF, or MOL files
Maximum allowed file size(compressed or not) per submission: 10Mb
Supported formats and extensions of structure files:
CDX (*.cdx)
MOL (*.mol)
SDF (*.sdf)
ZIP (*.zip) - batch of supported structure files with extensions *.mol. *.sdf, or *.cdx; Zip file should not contain directories, just files.
GZ (supported formats: *.sdf.gz, *.mol.gz, *.cdx.gz)
Uploading tab-delimited text files with InChIs, SMILES, and chemical names
ATTENTION
1. Select "Processing type"
2. Choose file
3. Click on "Submit" button
Processing type:
Validation
Validation
Validation and CVSP standardization
Validation and InChI standardization
Custom Processing
Choose File
No fi
Submit

Standardization

- Custom processing let's user to put together workflow from pre-defined standardization modules list



Data Review

Home Upload Submissions Profile Admin Help [Provide Feedback] [Log out]

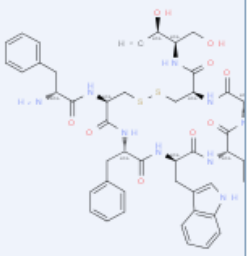
Status: Processed
File: DrugBank_Total.sdf.zip (6516 records)
Standardization Type: Validate and Standardize
Validation errors: 73 records
Validation warnings: 1079 records
Submission Actions: **Reprocess** **Delete**

Record Actions: **Download using filter settings**
Download standardized
Download selected

☐ Enable Auto Refresh
☐ Mark File as Demo

Filter records by issue type: Warning AND by Issue All ☐ AND Show standardized records only

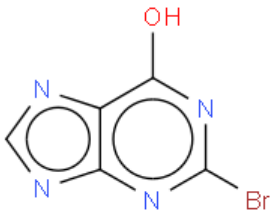
All
contains non-metal–transition metal bond
contains aluminium–non-metal bond
contains pentavalent nitro nitrogen
contains covalent metal--nitrogen bond
contains covalent metal--oxygen bond
nitrogenous base in acid form
contains ethane molecule(s)
not an overall neutral system
consists of more than one neutral molecule
contains unknown stereo bond
completely undefined stereo – enantiomers
completely undefined stereo – mixtures
partially undefined stereo – epimers
partially undefined stereo – mixtures
contains stereobond in six-membered ring
contains L-pyranose: intentional?
contains enol function
contains N=C-OH tautomer of a carbonyl compound
contains nitroso form of oxime

#ID	ChemSpider ID	Original	Standardized
4 ☐	**10482007**	 **Download**	No change

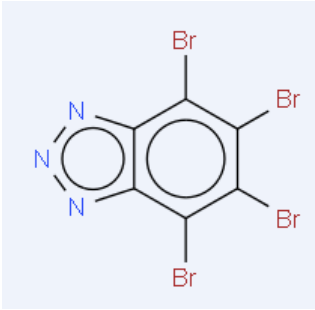
DrugBank

DrugBank dataset (6516 records)

~60 records that can’t be dearomatized unambiguously



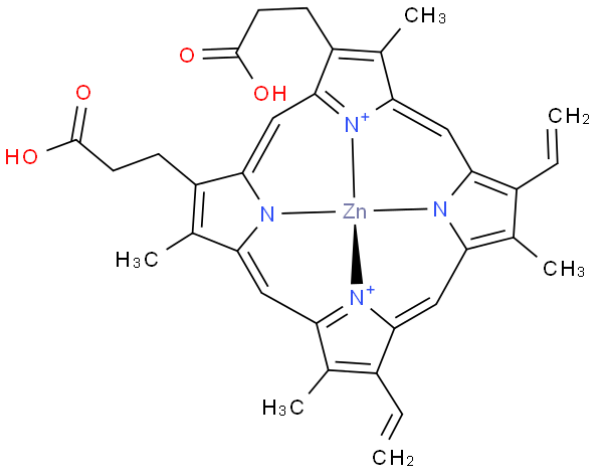
DB04283



DB04462

Nonsensical bonds

~30 records with bonds that do not make sense



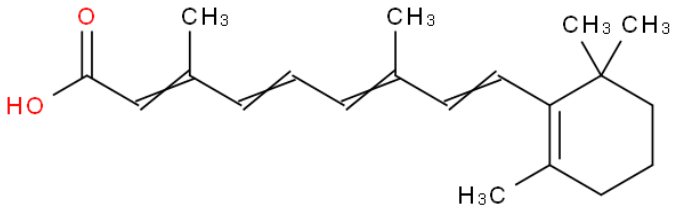
DDB04009

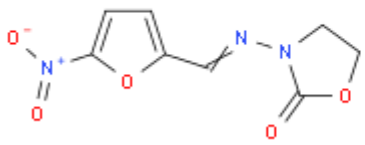
Mismatches – which is correct?

~40 records where InChIs did not match the structure

DrugBank ID: DB00755

InChI=1S/C20H28O2/c1-15(8-6-9-16(2)14-19(21)22)11-12-18-17(3)10-7-13-20(18,4)5H3,(H,21,22)/b9-6+,12-1



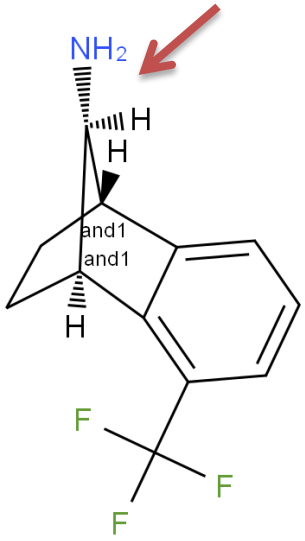


Warn	contains unknown stereo bond
Warn	depositor-specified name(s) do not match the structure : furazolidone
Warn	depositor-specified InChIs do not match the structure : InChI=1S/C8H7N3O5/c12-8-10(3-4-15-8)9-5-6-1-2-7(16-6)11(13)14/h1-2,5H,3-4H2/b9-5+

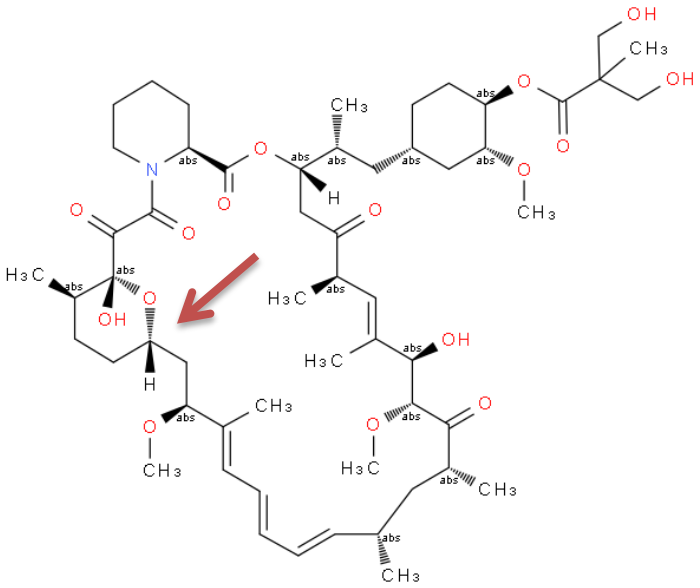
DruGBank ID: DB00614

Stereobond issues

7 records with 2 stereo bonds at chiral atoms

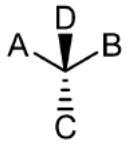


DB08128



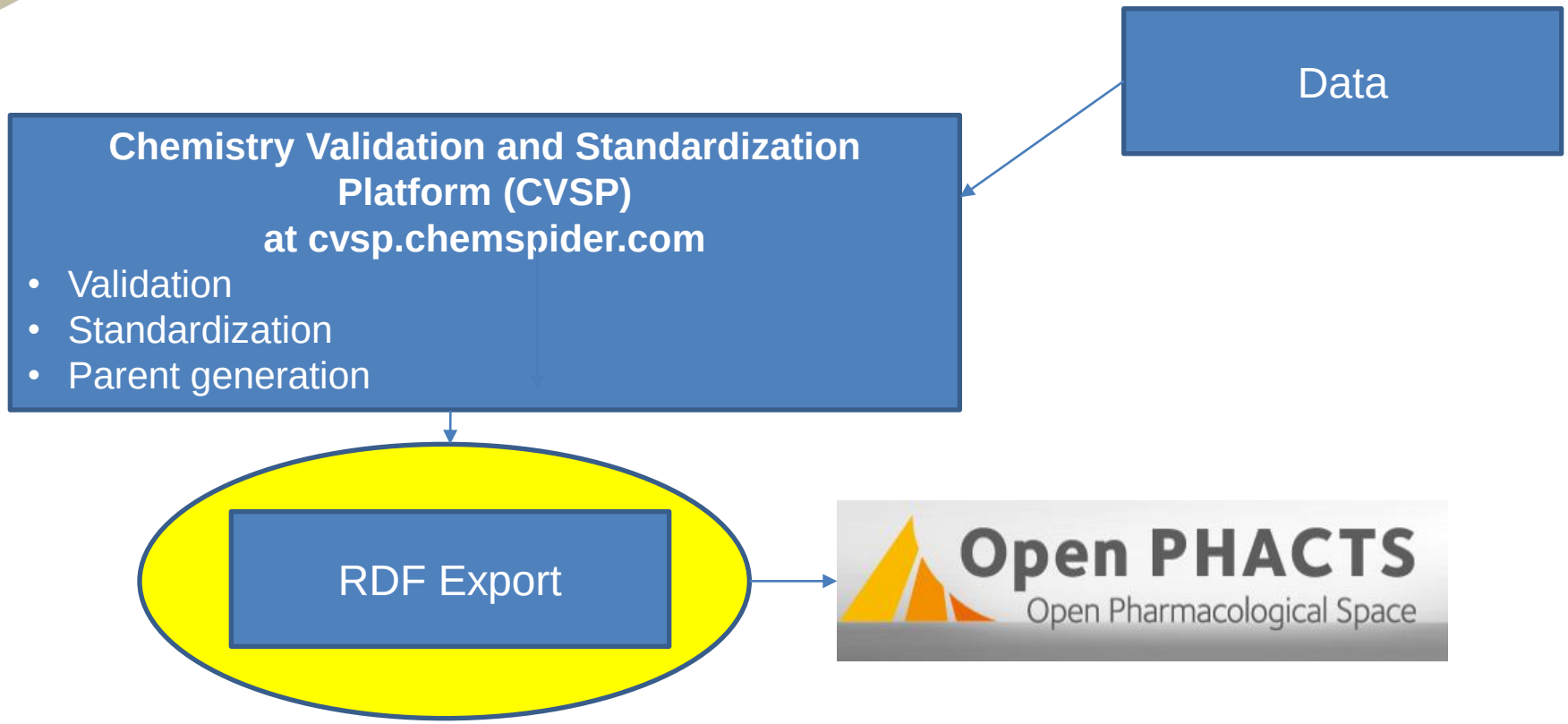
DB06287

J. Brechner, IUPAC Graphical Representation of stereochem. configurations Section: ST-1.1.10

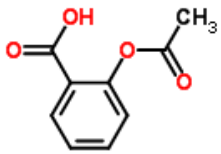


Not acceptable

Chemistry Data out to OPS



Data is being imported from ChemSpider to Open PHACTS in RDF/turtle



ALogP:
1.4

H-Bond Acceptors:
4

H-Bond Donors:
1

Mol Weight:
180.157

MW Freebase:
180.157

Polar Surface Area (Å²):
63.6

Rotatable Bonds:
3

Aspirin

Pharmacology Data | Structure Search | ChemSpider Info

The prototypical analgesic used in the treatment of mild to moderate pain. It has anti-inflammatory and antipyretic properties and acts as an inhibitor of cyclooxygenase which results in the inhibition of the biosynthesis of prostaglandins. Aspirin also inhibits platelet aggregation and is used in the prevention of arterial and venous thrombosis. (From Martindale, The Extra Pharmacopoeia, 30th ed, p5)

Aspirin is rapidly hydrolyzed primarily in the liver to salicylic acid, which is conjugated with glycine (forming salicyluric acid) and glucuronic acid and excreted largely in the urine.

ChemSpider ID:	2157
Molecular Formula:	$C_9H_8O_4$
SMILES:	CC(=O)Oc1ccccc1C(=O)O
Standard InChI:	InChI=1S/C9H8O4/c1-6(10)13-8-5-3-2-4-7(8)9(11)12/h2-5H,1H3,(H,11,12)
Standard InChIKey:	BSYNRYMUTXBXSQ-UHFFFAOYSA-N
Protein Binding:	High (99.5%) to albumin. Decreases as plasma salicylate concentration increases, with reduced plasma albumin concentration or renal dysfunction, and during pregnancy.
Toxicity:	Oral, mouse: LD_{50} = 250 mg/kg; Oral, rabbit: LD_{50} = 1010 mg/kg; Oral, rat: LD_{50} = 200 mg/kg. Effects of overdose include: tinnitus, abdominal pain, hypokalemia, hypoglycemia, pyrexia, hyperventilation, dysrhythmia, hypotension, hallucination, renal failure, confusion, seizure, coma, and death.
Melting Point:	135 °C (boiling point 140 °C)

RDF/VOID

- VoID is an RDF Schema vocabulary for expressing metadata about RDF datasets.
  - **skos:exactMatch** (Simple Knowledge Organisation System)

  e.g. To link compounds in OPS with compounds in ChEBI.
  - **skos:closeMatch**

  e.g. To link Stereo Insensitive Parents to their Children within OPS.
  - **skos:relatedMatch**

  e.g. To link Parent compounds that contain others as Fragments.

- Recommendations on VoID specified by Manchester Uni. here: http://www.cs.man.ac.uk/~graya/ops/2012/ED-datadesc/

RDF Export

```
@prefix rdf: <http://www.w3.org/1999/02/22-rdf-syntax-ns#> .
@prefix rdfs: <http://www.w3.org/2000/01/rdf-schema#> .
@prefix xsd: <http://www.w3.org/2001/XMLSchema#> .
@prefix void: <http://rdfs.org/ns/void#> .
@prefix skos: <http://www.w3.org/2004/02/skos/core#> .
@prefix cheminf: <http://semanticscience.org/resource/> .
@prefix obo2: <http://purl.obolibrary.org/obo#> .
@prefix ops: <http://ops.rsc.org/> .
@prefix : <ftp://ftp.rsc-
us.org/OPS_TEST/20130904/HMDB/LINKSET_CLOSE_PARENT_CHILD_STEREO_
UNSENSITIVE_PARENT_HMDB20130904.ttl#> .
<ftp://ftp.rsc-
us.org/OPS_TEST/20130904/HMDB/LINKSET_CLOSE_PARENT_CHILD_STEREO_
UNSENSITIVE_PARENT_HMDB20130904.ttl> void:inDataset
<ftp://ftp.rsc-us.org/OPS_TEST/20130904/void_2013-09-
04.ttl#hmdb_parent_child_stereo_unsensitive_parent_closeMatch> .
ops:OPS14 skos:closeMatch ops:OPS16 .
ops:OPS22 skos:closeMatch ops:OPS24 .
ops:OPS26 skos:closeMatch ops:OPS27 .
ops:OPS30 skos:closeMatch ops:OPS32 .
ops:OPS47 skos:closeMatch ops:OPS51 .
ops:OPS56 skos:closeMatch ops:OPS57 .
ops:OPS59 skos:closeMatch ops:OPS62 .
ops:OPS68 skos:closeMatch ops:OPS70 .
ops:OPS73 skos:closeMatch ops:OPS75 .
ops:OPS76 skos:closeMatch ops:OPS78 .
ops:OPS86 skos:closeMatch ops:OPS88 .
ops:OPS90 skos:closeMatch ops:OPS92 .
ops:OPS95 skos:closeMatch ops:OPS97 .
ops:OPS100 skos:closeMatch ops:OPS102 .
ops:OPS105 skos:closeMatch ops:OPS107 .
ops:OPS1721900 skos:closeMatch ops:OPS107 .
```

Ongoing Updates to Linksets

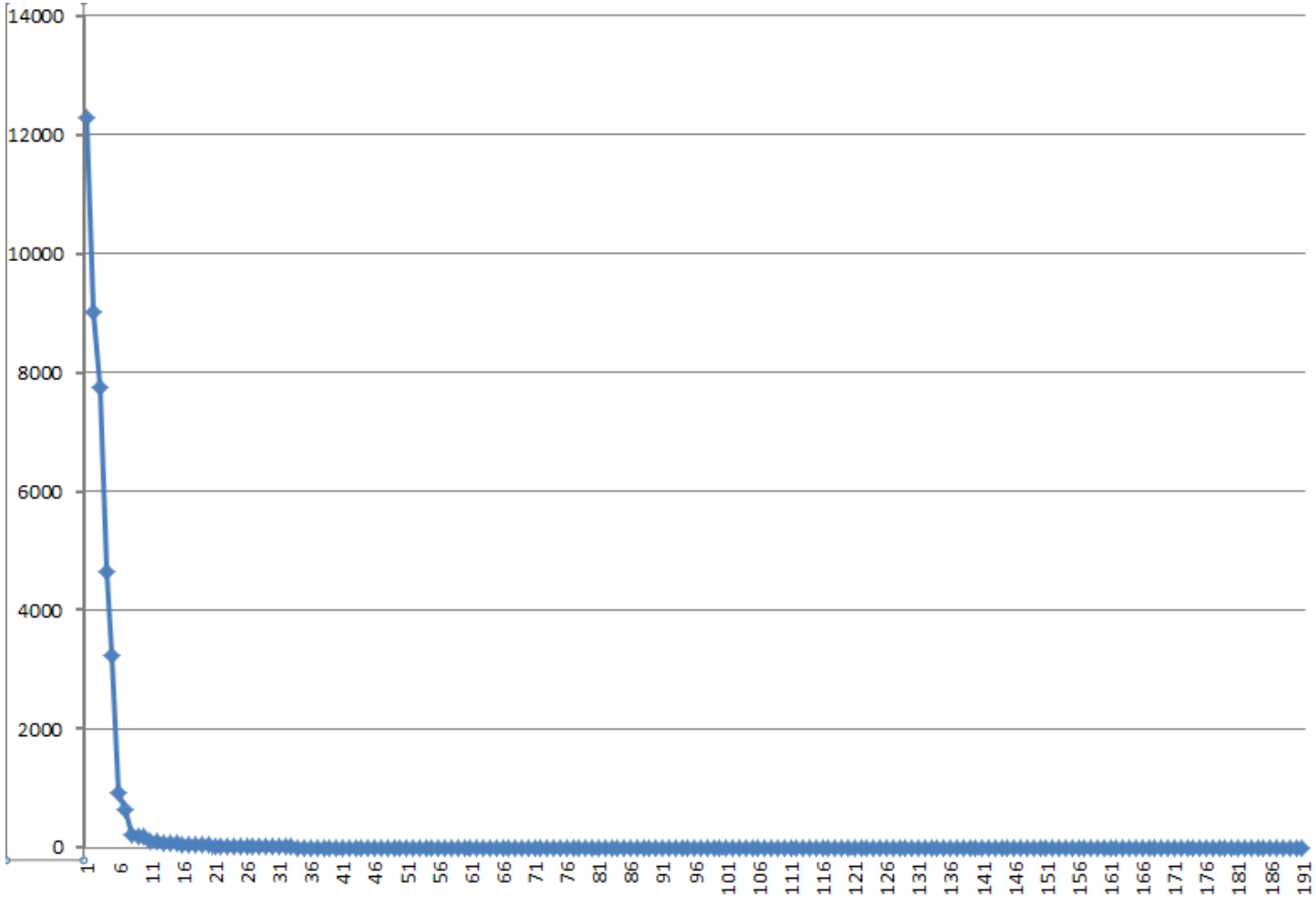
- Ongoing data checking activities on ChemSpider
- Does Crowdsourcing work?
- But WHY would people validate ChemSpider?
- What can be done to encourage participation?

- How will we deliver on Barend's Million Minds approach – he has ideas…see later

Crowdsourcing – does it work?

- >200 people EVER have deposited or curated data
- Database hosts make the **largest** contributions
- ChemSpider staff do the most curation

Contributions



Curation Activities

- 2009 – 8255 curations by 43 people
- 2010 – 10014 curations by 66 people
- 2011 – 16025 curations by 116 people
- 2012 – 13127 curations by 74 people

Depositors

- 2009 91 unique depositors
- 2010 120 unique depositors
- 2011 99 unique depositors
- 2012 120 unique depositors

- “The crowd is small – very small”

Rewards and Recognition

- The badgesonomy culture of recognition is growing.
- Badges are commonplace
  - FourSquare
  - Klout

Rewards and Recognition

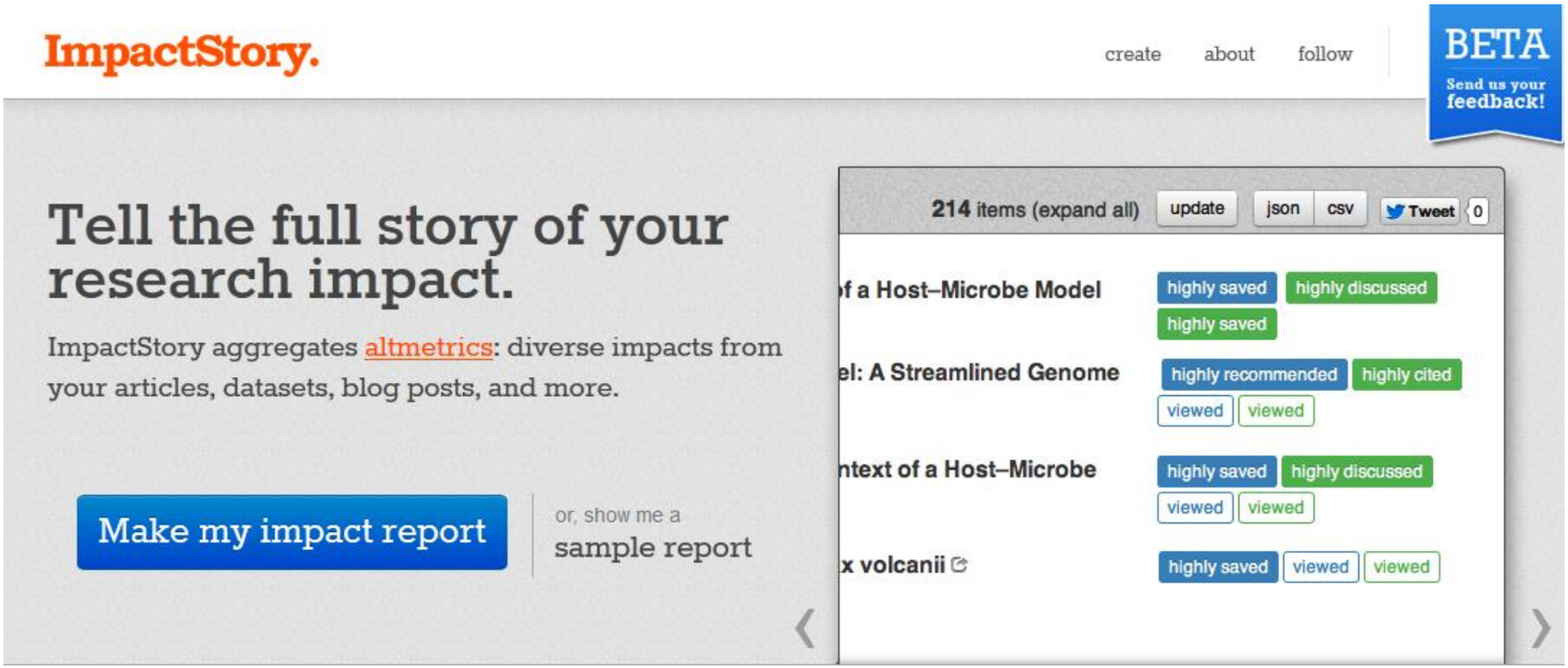
- Rewards and Recognition integrated across all ChemSpider related projects
- Including paths to expose such recognition on **AltMetrics platforms**

- MAY work for young scientists

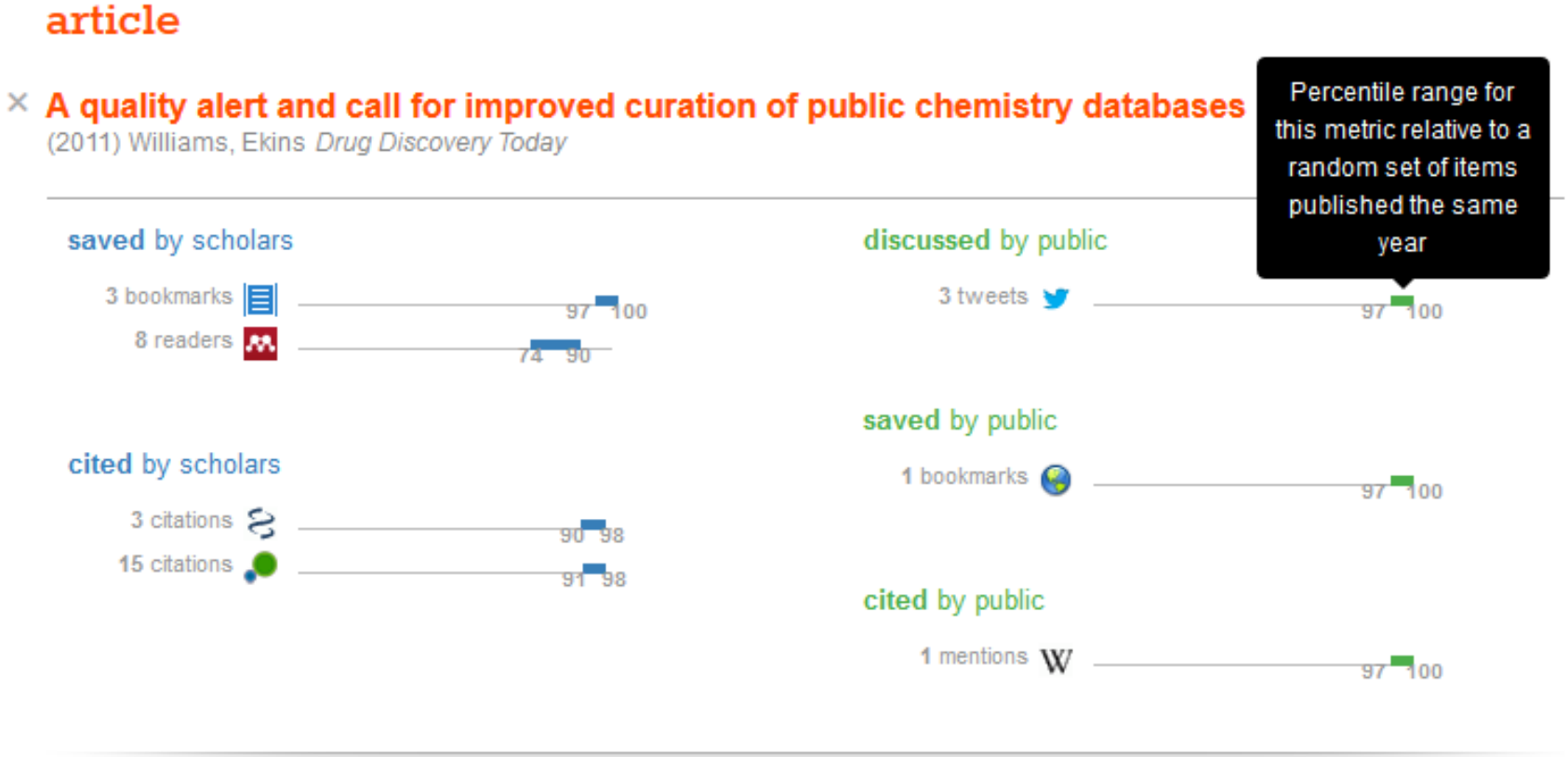
The Alt-Metrics Manifesto

http://altmetrics.org/manifesto/

ImpactStory



Future Recognition on ImpactStory.



Scientists AltMetrics

Home / Antony Williams

Show Profile Data

Antony Williams

Connections in Chemistry

Links:

LinkedIn, ScientistDB, ChemConnector Blog, Twitter, about.me, Google Scholar, Microsoft Academic Search, Impact Story, Wikipedia, SlideShare, YouTube, Mendeley, PROskore, ResearchGate, amazon.com, Vizify, visualize.me, Pinterest, ORCID

Researcher from:

Sample Profiles

My passion is connecting people to chemistry. Over the past decade I ...

tony27587@gmail.com | 919-201-1516

All (452) | Presentation (201) | Article (114) | Other (54) | Paper (36) | Video (18) | Book (12) | Figure (11) | Data (4) | Poster (2)

CSV

Usage, Citations, Social Media, etc

Impact by Type: All

Year	Title	Type	All				
			Captures +	Citations +	Social Media +	Mentions +	Usage +
2013	Magnetism Inside the Human Body: Lessons for Ten Year Olds	Video			7		66
2013	Leading Scientists into Openness	Presentation			8		472
2013	Accessing the Inorganic Crystal Structure Database	Video			4		110
2013	Approaches for extraction and digital chromatography of chemical data	Presentation			2		273
2013	Four disruptive strategies for removing drug discovery bottlenecks.	Article		1	5		
2013	Chemical Database Projects Delivered by RSC eScience	Presentation			1		260
2013	RSC Databases in the CDS	Video			1		32
2013	Towards a gold standard and regarding quality in public domain chemistry databases and approaches to improving the situation	Paper			1		20
2013	13C-15N Connectivity networks via unsymmetrical indirect covariance processing of 1H-13C HSQC and 1H-15N IMPEACH spectra	Paper					3

Detailed Usage Statistics

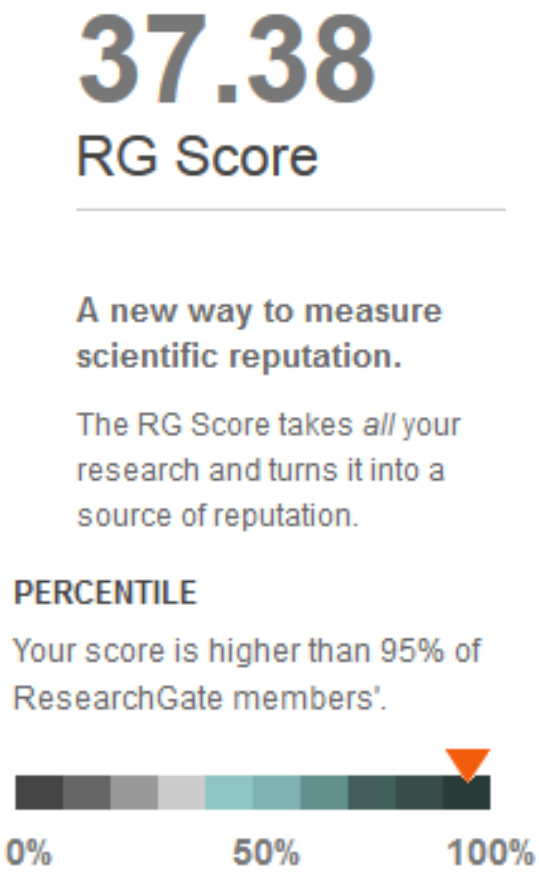
What makes a Scientist Notable? What will it be in the future???

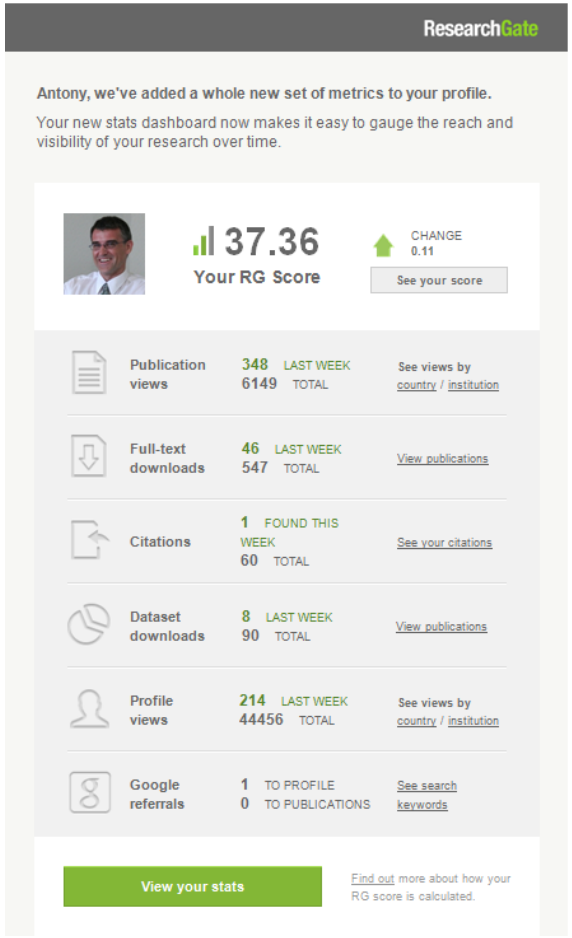
The Signpost

IN THE NEWS

The closed, unfriendly world of Wikipedia, fundraiser fun and games, and chemists vs pornstars

We Are All Being Quantified…





How I am Quantified…

Share your latest stats RG Share

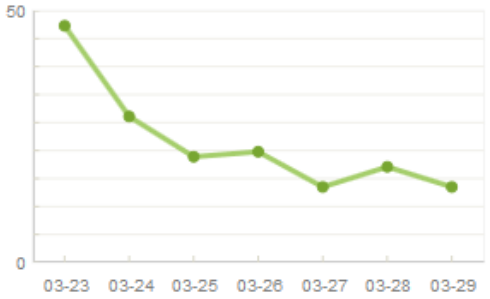
Publications

VIEWS LAST WEEK

283
Total views

Views by country
49 USA
4 Jamaica
2 Canada

PUBLICATION VIEWS daily / weekly



6,420
Total publication views

594
Total full-text downloads

105
Total dataset downloads

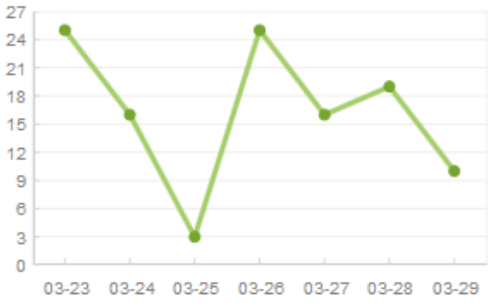
GOOGLE REFERRALS daily / weekly

VIEWS LAST WEEK

234
Total views

Views by country
106 USA
13 United Kingdom

PROFILE VIEWS daily / weekly



44,688 Total views

Profile views give you an insight into your visibility as a researcher.

Barend Mons

Professor in Biosemantics, Leiden universiteit medical center and NBIC
Computational Biology - e-Science - Biosemantics
Verified email at nbic.nl
Homepage

Citation indices

	All	Since 2008
Citations	2004	953
h-index	30	16
i10-index	53	26

Citations to my articles

Show: 20 **1-20** Next >

Title / Author	Cited by	Year
Calling on a million minds for community annotation in WikiProteins B Mons, M Ashburner, C Chichester, E van Mulligen, M Weeber, J den Dunnen ... Genome biology 9 (5), R89	125	2008
Distribution of information in biomedical abstracts and full-text publications MJ Schuemie, M Weeber, BJA Schijvenaars, EM van Mulligen, CC van der Eijk, R ... Bioinformatics 20 (16), 2597-2604	97	2004
Text mining for biology-the way forward: opinions from leading scientists RB Altman, CM Bergman, J Blake, C Blaschke, A Cohen, F Gannon, L Grivell, U ... Genome Biol 9 (Suppl 2), S7	73	2008
Online tools to support literature-based discovery in the life sciences M Weeber, JA Kors, B Mons Briefings in bioinformatics 6 (3), 277-286	67	2005
In vitro formation of ookinetes and functional maturity of Plasmodium berghei gametocytes CJ Janse, B Mons, RJ Rouwenhorst, PFJ Van der Klooster, JP Overdulve, HJ Van ... Parasitology 91 (01), 19-29	66	1985

Ross D. King

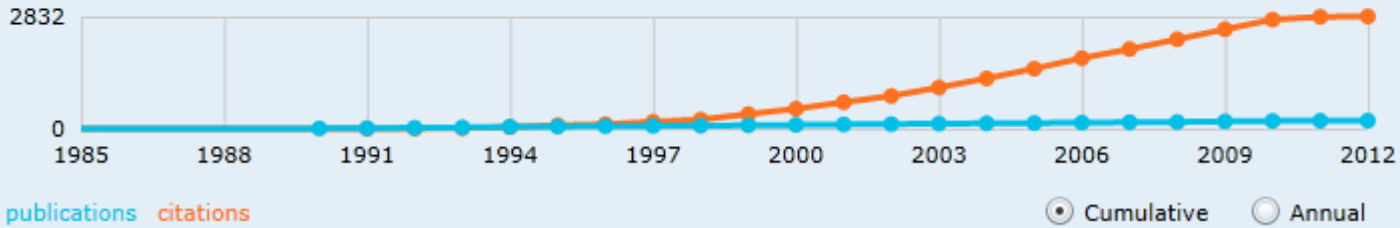
Technical University of Berlin

Publications: 214 | Citations: 3434

Fields: Artificial Intelligence, Bioinformatics & Computational Biology, Data Mining

Collaborated with 483 co-authors from 1990 to 2012 | Cited by 5061 authors

Edit



[Piezo-Polymer-Composite Unimorph Actuators for Active Cancellation of Flow Instabilities Across Airfoils]

D. Haller, A. Paetzold, N. Losse, S. Neiss, I. Peltzer, W. Nitsche, **R. King**, P. Woias

Journal: Journal of Intelligent Material Systems and Structures - J INTEL MAT SYST STRUCT, vol. 22, no. 5, pp. 461-474, 2011

[Cymbal type Piezo-Polymer-Composite actuators for active cancellation of flow instabilities on airfoils]

D. Haller, A. Paetzold, N. Goldin, S. Neiss, F. Goldschmidtboeing, W. Nitsche, **R. King**, P. Woias

Conference: International Conference on Solid State Sensors and Actuators - TRANSDUCERS, pp. 494-497, 2011

Likely Enabled by

ORCID
Connecting Research and Researchers

- Persistent unique digital identifier
- Integrates to workflows such as manuscript and grant submission
- Supports automated linkages with your professional activities

ChemConnector

0000-0002-2668-4821

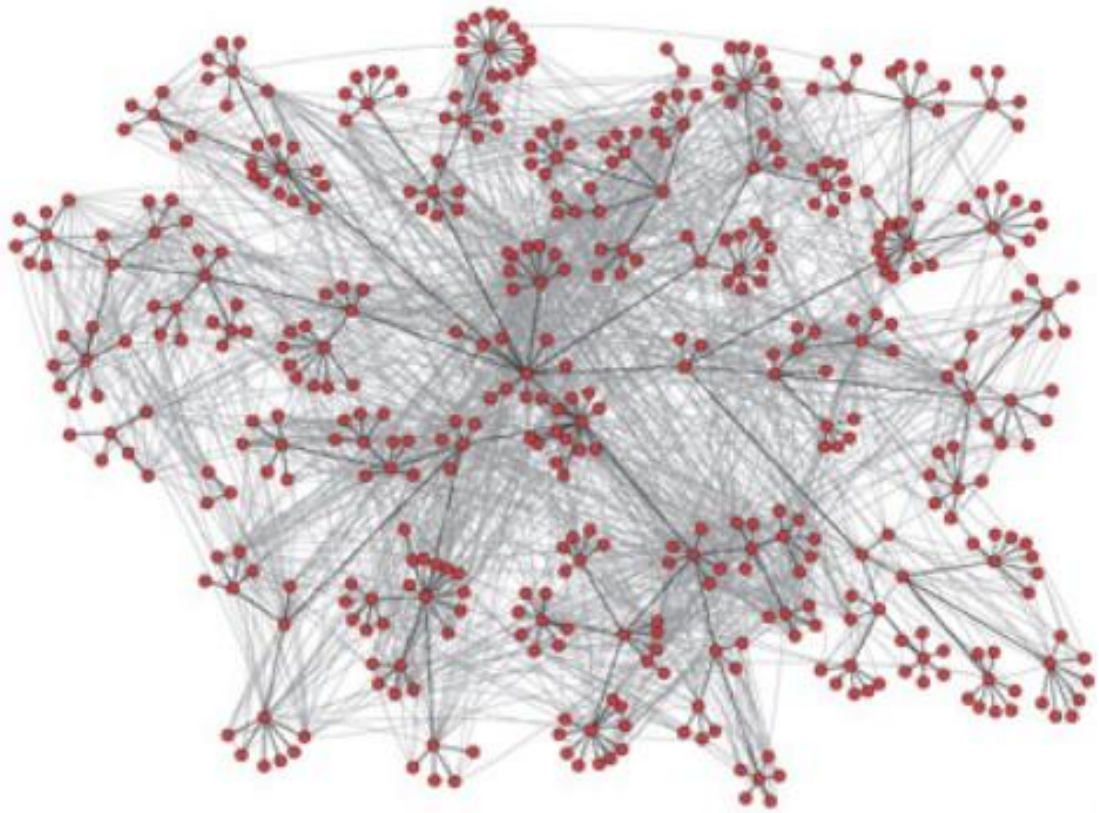
Summary

- A grand vision for semantic data linking is coming to fruition. We have a lot do.
- Data quality enhancements can come through crowdsourcing (and intelligent robots)
- Participation may be driven by new approaches to rewards and recognition
- Publishers are understanding the value of data, but still guard it, and generally don’t have systems to handle it. It’s changing.
- There is so much value in the historical data

Inside our Publication Archive

- How much **data** is in RSC archive, in the publications and in the supplementary info?

What if we could capture it all? Digitally Enhancing the RSC Archive



Start with data in publications

Chem. Sci., 2010, **1**, 561-566 | DOI: 10.1039/c0sc00351d | Edge Article

Total synthesis of all (−)-agelastatin alkaloids†

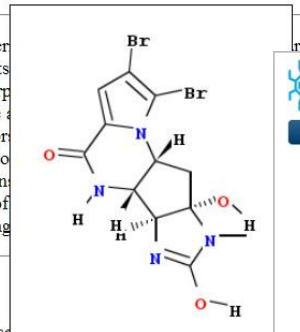
Mohammad Movassaghi *, Dustin S. Siegel and Sunkyu Han

Massachusetts Institute of Technology, Department of Chemistry, 77 Massachusetts Avenue 18-292, Cambridge, MA 02139-4307, USA. E-mail: movassag@mit.edu

Received 2nd July 2010 , Accepted 20th July 2010

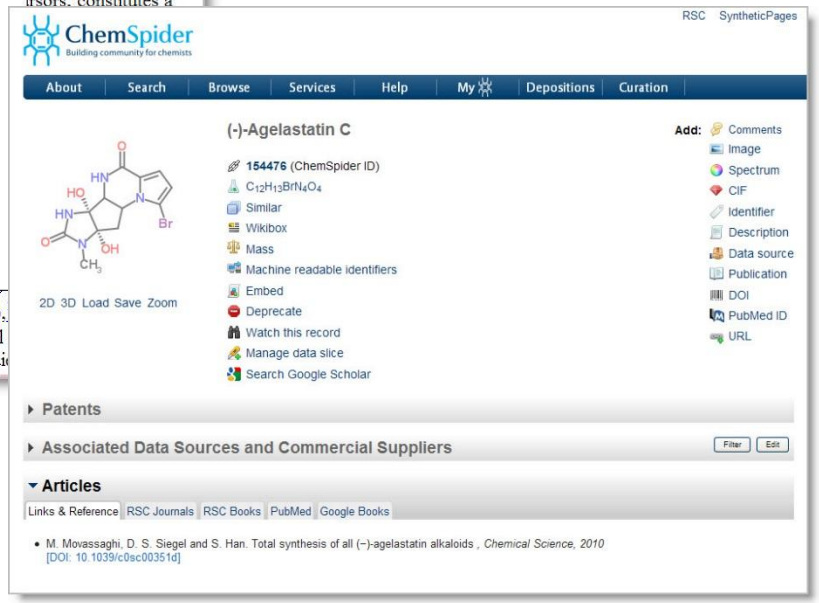
First published on the web 16th August 2010

The pyrrole-imidazole family of marine alkaloids, der…rsors, constitutes a diverse array of structurally complex natural products…that possess a tetracyclic molecular framework incorp…provide a hypothesis for the formation of the unique …intrinsic chemistry of plausible biosynthetic precursor…of all known agelastatin alkaloids including the first to…gram-scale chemical synthesis of agelastatin A was in…cyclopentane C-ring and required the development of…annulation reaction and a carbohydroxylative trapping…

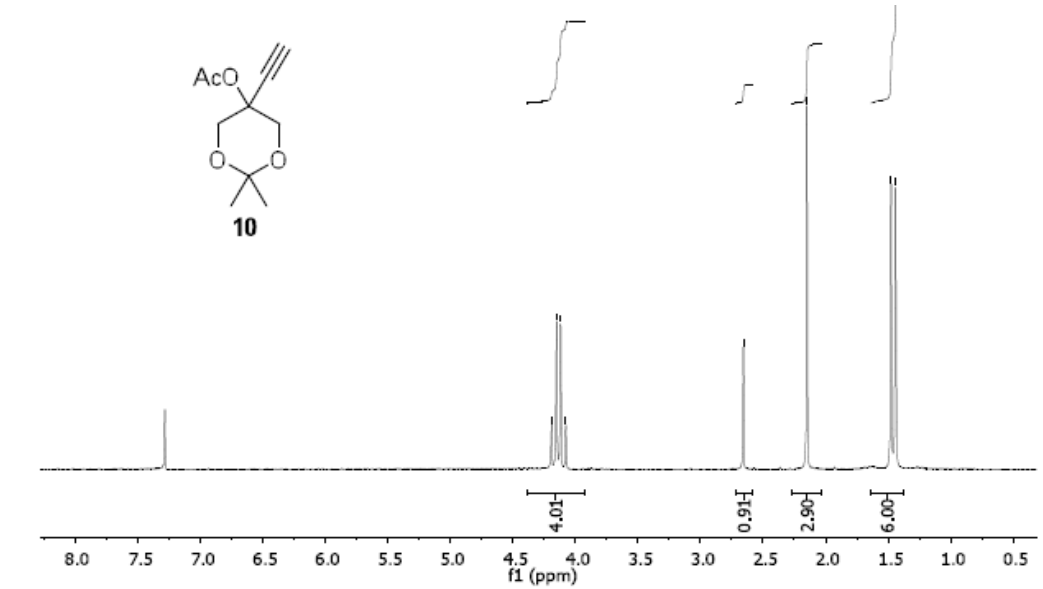


Introduction

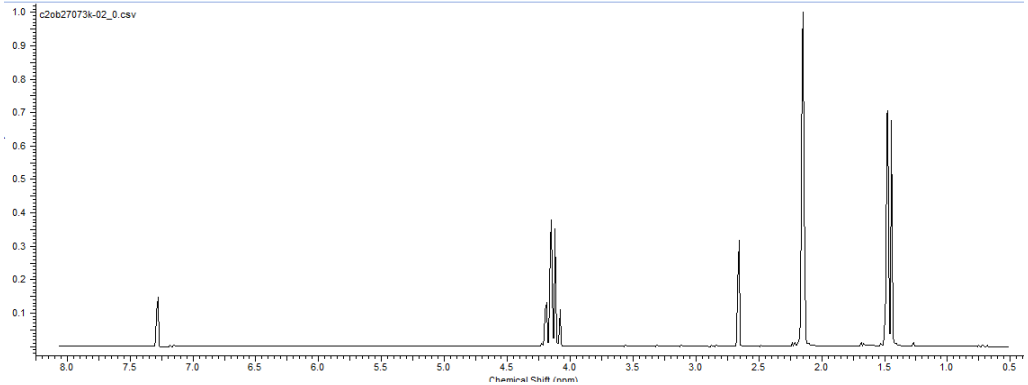
The agelastatin alkaloids constitute an intriguing subse…alkaloids that are likely derived from linear biogenetic precursors such as clathrodin (**7**), oroidin (**9**, Fig. 1).[3,4] (−)-Agelastatins A (**1**) and B (**2**) were first isolated from the Coral *dendromorpha* by Pietra *et al*. in 1993 who successfully identified and chemically studi…



Turn “Figures” Into Data



Spectral FIGURE



Extracted Spectrum

Text Mining

The N-(β-hydroxyethyl)-N-methyl-N'-(2-trifluoromethyl-1,3,4-thiadiazol-5-yl)urea prepared in Example 6 , thionyl chloride (5 ml) and benzene (50 ml) were charged into a glass reaction vessel equipped with a mechanical stirrer , thermometer and reflux condenser .

The reaction mixture was heated at reflux with stirring , for a period of about one-half hour .

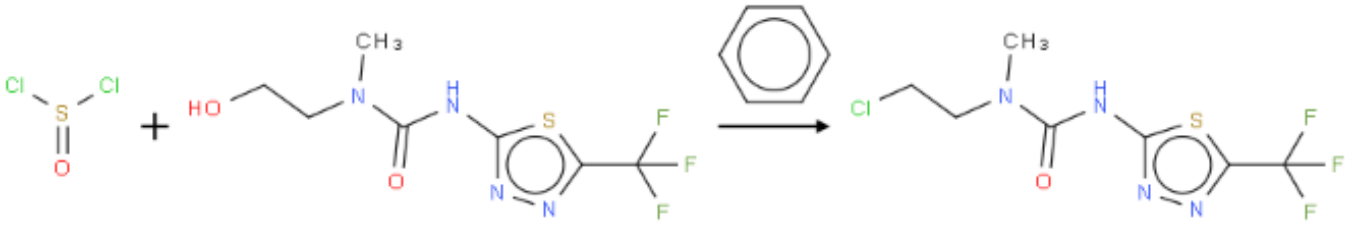
After this time the benzene and unreacted thionyl chloride were stripped from the reaction mixture under reduced pressure to yield the desired product N-(β-chloroethyl)-N-methyl-N'-(2-trifluoromethyl-1,3,4-thiaidazol-5-yl)urea as a solid residue

ChemSpider Reactions

ChemSpider
Reactions

ROYAL SOCIETY OF CHEMISTRY

About



RInChI: RInChI=0.02.1S////Cl2OS/c1-4(2)3///X/d-
RInChIKey-Long: bSA-BEANN---FYSNRJHAOHDILO-UHFFFAOY-N--X
RInChIKey-Short: bSA-BEANN-EANNATPGMB-IQKOBGSHGK-BIQAGPPMEE-NEANN-NEANN-NEANN
Type: 9.1.6 Hydroxy to chloro [9.1 Alcohol to halide]

ActionPhrase | NounPhrase | PrepPhrase | VerbPhrase | Chemical

The N-(β-hydroxyethyl)-N-methyl-N'-(2-trifluoromethyl-1,3,4-thiadiazol-5-yl)urea prepared in Example 6 , thionyl chloride (5 ml) and benzene (50 ml) were charged into a glass reaction vessel equipped with a mechanical stirrer , thermometer and reflux condenser .

The reaction mixture was heated at reflux with stirring , for a period of about one-half hour .

After this time the benzene and unreacted thionyl chloride were stripped from the reaction mixture under reduced pressure to yield the desired product N-(β-chloroethyl)-N-methyl-N'-(2-trifluoromethyl-1,3,4-thiaidazol-5-yl)urea as a solid residue .

Thank You

Email: williamsa@rsc.org

Twitter: ChemConnector

Personal Blog: www.chemconnector.com

SLIDES: www.slideshare.net/AntonyWilliams