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2012 eScience Workshop
eScience in Action

The Possibilities and Pitfalls of Internet-Based Chemical Data

Antony Williams

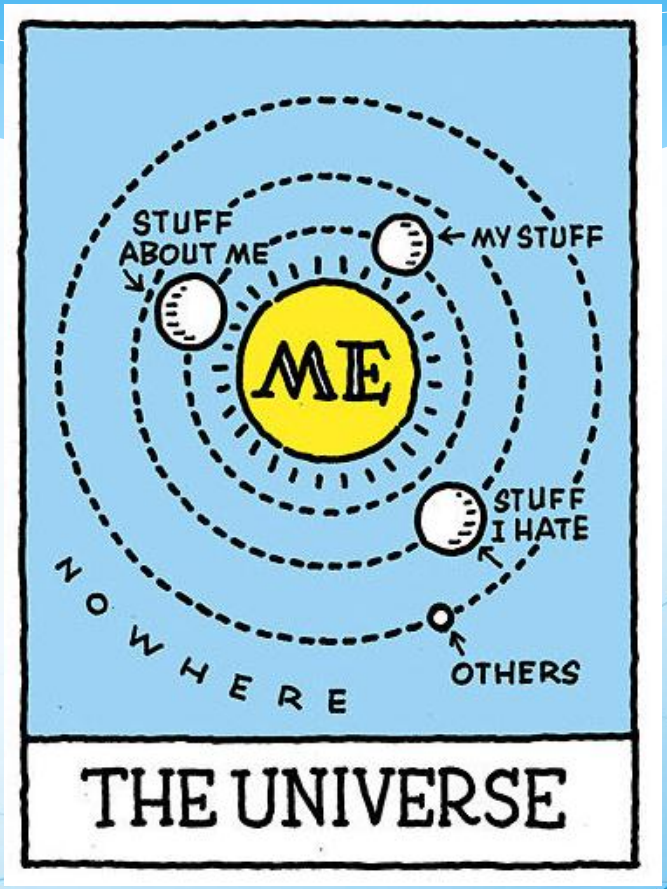
Royal Society of Chemistry

About Me… as a Chemist

* I've performed a few dozen chemical syntheses
* I've run thousands of analytical spectra
* I've generated thousands of NMR assignments
* I've probably published <5% of all work
* But things can be different today….

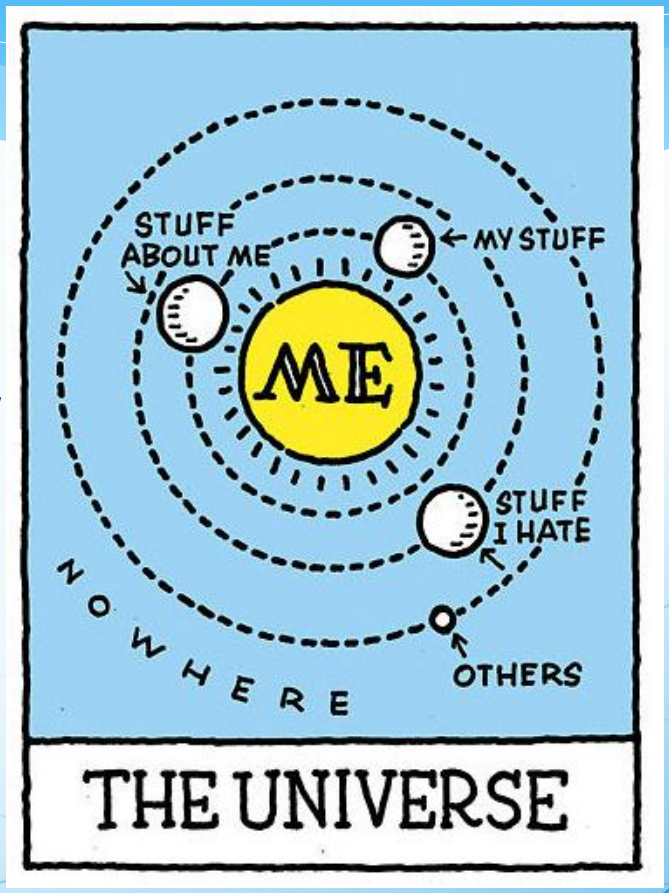
My Early Scientific Computing

If it was not just about me…



If it was not just about me…

* Together we might:
  * build an encyclopedia
  * …and rate restaurants
  * …provide book reviews to each other
  * …or movie reviews
  * …or 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:
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  * …or movie reviews
  * …or reviews of service providers
  * …organize sit-ins and social action
  * …and more data might just be Open
  * …**more Chemists might share rather than just take!**

amazon.com

NETFLIX

Angie's list

A story of a hobby gone wild… Years 1 and 2

* A hobby-project to connect chemistry data on the web
* Three servers – one purchased, two hand-built
* Software begged and borrowed – and thanks to Microsoft!
* Some late nights – 10pm to 2am for over a year
* Some survival of the naysayers in the community
* …and taking advantage of a changing world of data availability and the crowdsourcing of willing participants

* **NO formal funding. Simply passion and abilities lining up.**

ChemSpider (Year 2-present)

* ***Building a Free Chemical Database***

* A central hub for chemists to source information
  * >28 million unique chemical records
  * Aggregated from >400 data sources
  * Chemicals, analytical data, movies, images, podcasts, links to patents, publications, predictions
  * Web services for integration
  * Daily updates of data

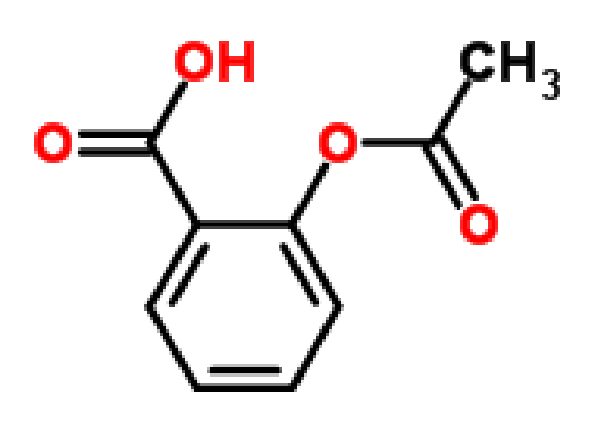
RSC | Advancing the Chemical Sciences

Answer Questions for Chemists

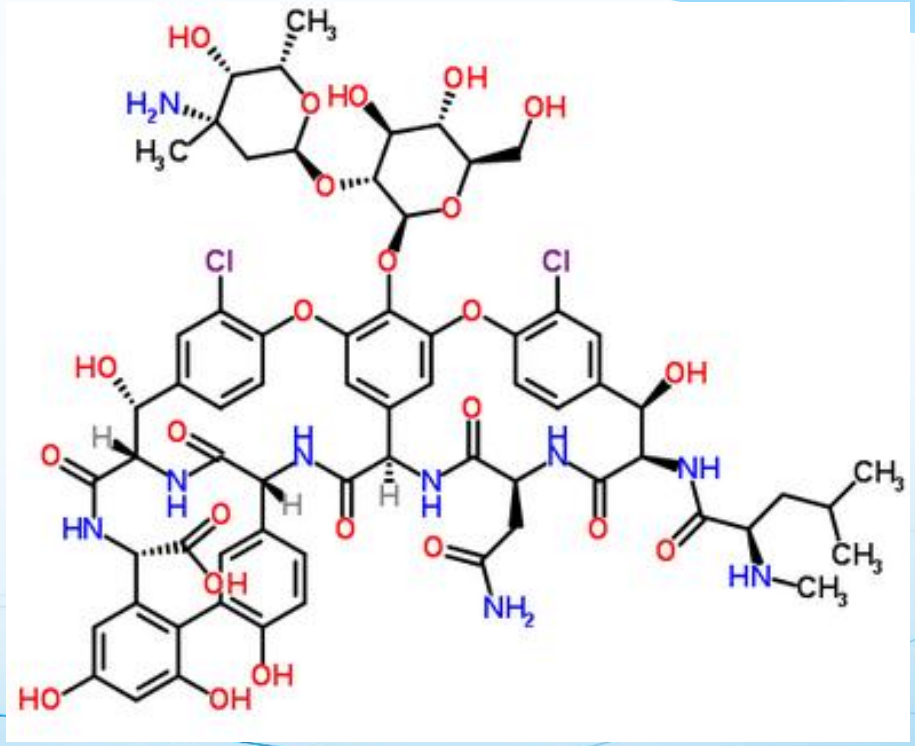
* Questions a chemist might ask…
  * What is the melting point of n-heptanol?
  * What is the chemical structure of Xanax?
  * Chemically, what is phenolphthalein?
  * What are the stereocenters of cholesterol?
  * Where can I find publications about xylene?
  * What are the different trade names for Ketoconazole?
  * What is the NMR spectrum of Aspirin?
  * What are the safety handling issues for Thymol Blue?

A LITTLE Chemistry First

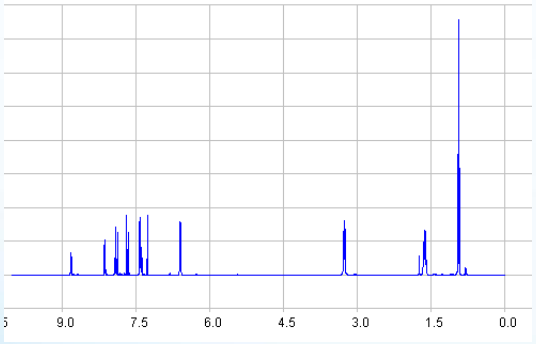
Structural Diagrams

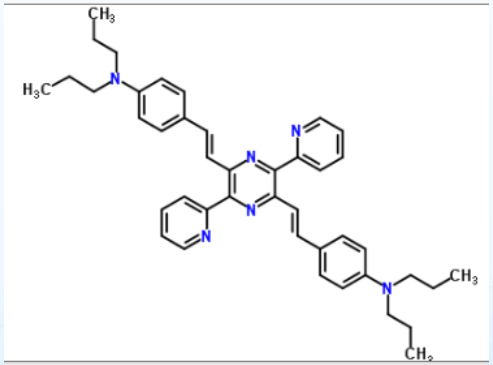


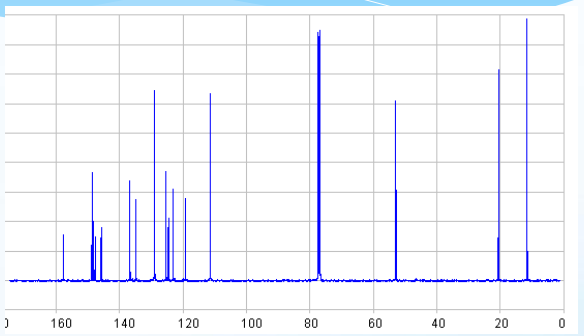
Structural Diagrams

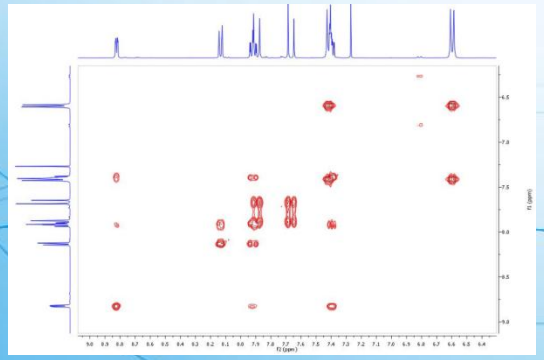


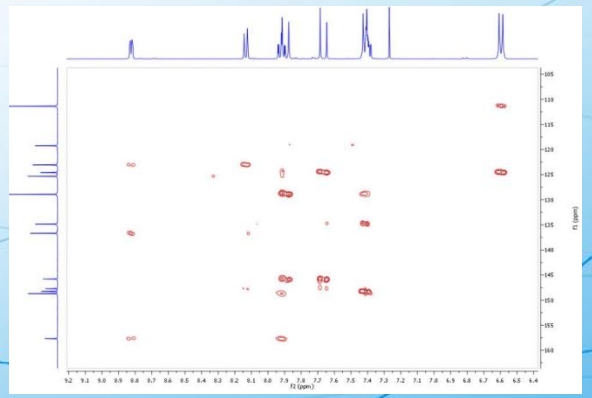
Analytical Data



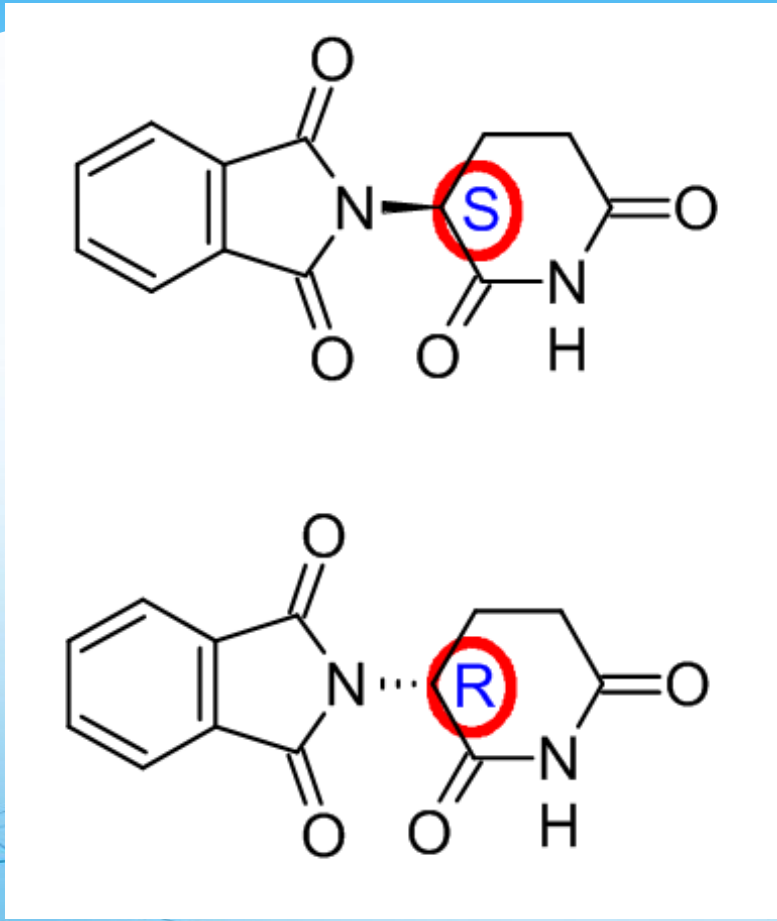




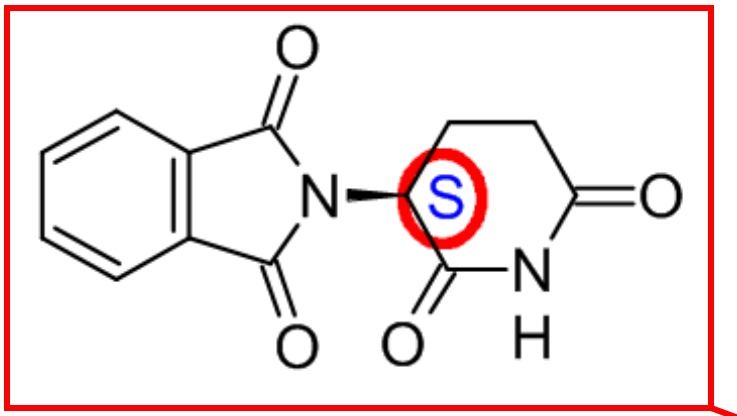


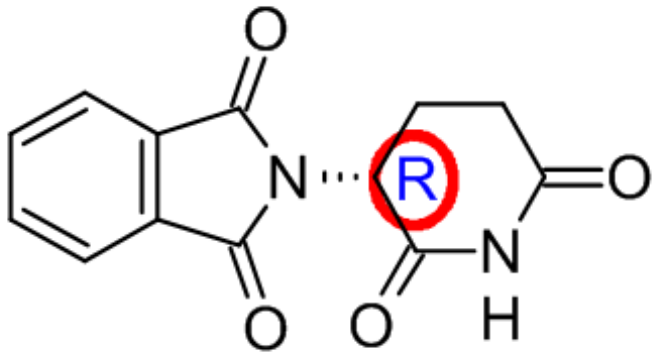


Does Stereochemistry Matter?



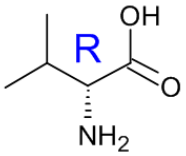
Does one stereocenter matter?



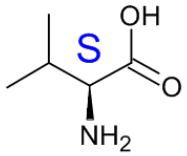


- Distaval, Talimol, Nibrol, Sedimide, Quietoplex, Contergan, Neurosedyn, Softenon, **Thalidomide**

Structural Representations



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



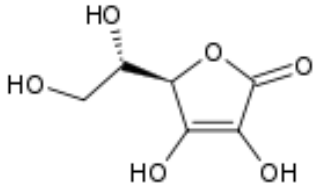
CC(C)[C@H](N)C(=O)O

```
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
```

CH_3CH_2OH

ethanol

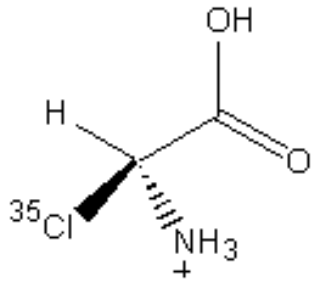
InChI=1/C2H6O/c1-2-3/h3H,2H2,1H3



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

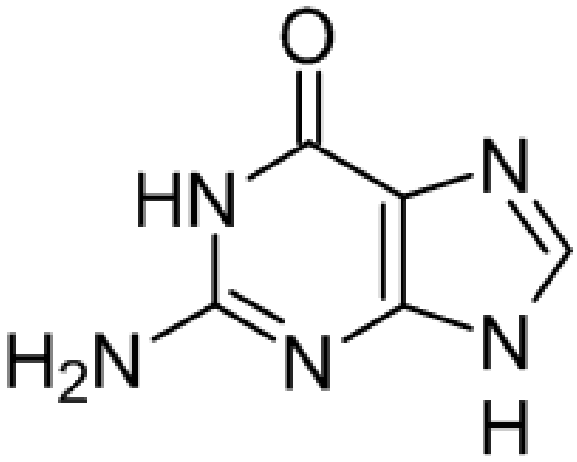
Charge layer

Stereochemical layer

Isotopic layer

Fixed-H layer

InChIKeys
Search the Web by Structure



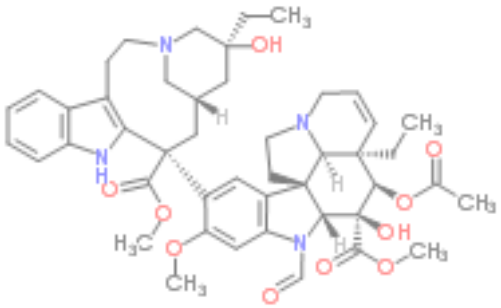
InChI=1/C5H5N5O/c6-5-9-3-2(4(11)10-5)7-1-8-3/h1H,(H4,6,7,8,9,10,11)

SHA-256 HASH Algorithm

Lookup

UYTPUPDQBNUYGX-UHFFFAOYAE

I want to know about “Vincristine”



2D 3D Save Zoom

- 9 of 9 defined stereocentres

Vincristine

ChemSpider ID: **5758**

Molecular Formula: $C_{46}H_{56}N_4O_{10}$

Monoisotopic mass: 824.399644 Da

▼ Systematic name

(2α,2'β,3α,4α,5β,19β)-22-oxovincaleukoblastine

▶ SMILES and InChIs

Wikibox

Embed

Deprecate

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Manage data slice

OGWKCGZFUXNPDA-XQKSVPLYSA-N

[Vincristine - Wikipedia, the free encyclopedia](#)
en.wikipedia.org/wiki/Marqibo
Mechanism · Uses · Side-effects · History · Suppliers
... c1-7-42(55)22-28-23-45(40(53)58-5,36-30(14-18-48(24-28)
Key:**OGWKCGZFUXNPDA-XQKSVPLYSA-N** ... Vincristine (brand name, Oncovin), ...

[Vincristine - PubChem](#)
pubchem.ncbi.nlm.nih.gov/summary/summary.cgi?cid=5978
Also known as: Leurocristine, 22-Oxovincaleukoblastine, Vincrystine ... Molecular Formula: C 46 H 56 N 4 O 10 Molecular Weight: 824.95764 InChIKey: **OGWKCGZFUXNPDA-XQKSVPLYSA-N**

[Vincristine CAS 57-22-7 - Chemical Industries Manufacturer ...](#)
www.chemicalregister.com/Vincristine/Suppliers/pid34508.htm
LGM Pharma www.lgmpharma.com/product/vincristine | SEND INQUIRY | Profile ...
OGWKCGZFUXNPDA-XQKSVPLYSA-N

[VINCRISTINE - PULP-PEDIA, THE BITCH CHEAP ENCYCLOPEDIA](#)
lohere.net/kulkapedia/samuel/Vincristine
... c1-7-42(55)22-28-23-45(40(53)58-5,36-30(14-18-48(24-28) key:**ogwkcgzfuxnpda-xqksvplysa-n** ... vincristine (brand name, oncovin), formally ...

[وینکریستین - ویکی‌پدیا](#)
fa.wikipedia.org/wiki/وینکریستین
... متابولیسم · ... مکانیسم اثر · موارد مصرف
... c1-7-42(55)22-28-23-45(40(53)58-5,36-30(14-18-48(24-28) key:**ogwkcgzfuxnpda-xqksvplysa-n** ... وین کریستین (به انگلیسی): vincristine ...

[长春新碱 - 维基百科，自由的百科全书](#)
zh.wikipedia.org/wiki/长春新碱 Translate this page
机理 · 用途 · 副作用 · 历史 · 另见 · 参考资料
维基百科，自由的百科全书 ...
c1-7-42(55)22-28-23-45(40(53)58-5,36-30(14-18-48(24-28) key: **ogwkcgzfuxnpda-xqksvplysa-n**

[vincristine CAS 57-22-7 Reference,buy vincristine at guidechem](#)
www.guidechem.com/reference/dic-179.html
ogwkcgzfuxnpda-xqksvplysa-n【canonical smiles】
ccc1(cc2cc(c3=c(ccn(c2)c1)c4=cc=cc=c4n3)(c5=c(c=c6c(=c5)c78ccn9c7c(c=cc9)(c(c(c8n6c=o)(c(=o)oc)o)oc(=o)c)cc)oc)c(=o)oc)o

[Learn and talk about Vincristine, Acetate esters, Alkaloids ...](#)
www.digplanet.com/wiki/Vincristine
... c1-7-42(55)22-28-23-45(40(53)58-5,36-30(14-18-48(24-28)
Key:**OGWKCGZFUXNPDA-XQKSVPLYSA-N** ... Vincristine (brand name, Oncovin), ...

[Vincristine Information, Videos, Pictures and News](#)
www.rtbot.net/Vincristine
Lucas' Port Access for Chemotherapy (Vincristine) 6 yr old having port ...
c1-7-42(55)22-28-23-45(40(53)58-5,36-30(14-18-48(24-28)
Key:**OGWKCGZFUXNPDA-XQKSVPLYSA-N** ...

[Vincristineとは - goo Wikipedia (ウィキペディア)](#)
wpedia.goo.ne.jp/enwiki/Vincristine Translate this page
... c1-7-42(55)22-28-23-45(40(53)58-5,36-30(14-18-48(24-28)
Key:**OGWKCGZFUXNPDA-XQKSVPLYSA-N** ... Vincristine (brand name, Oncovin), ...

[About: Vincristine](#)
dbpedia.org/resource/Vincristine Translate this page
OGWKCGZFUXNPDA-XQKSVPLYSA-N; dbpprop:unii: 5 (xsd:integer)
dbpprop:verifiedfields: changed; dbpprop:verifiedrevid: 461759697 (xsd:integer) ...

[vincristine: Definition from Answers.com](#)
www.answers.com/topic/vincristine
Jul 01, 2002 · Microtubles. Definition. Vincristine is a drug used to treat certain ...
c1-7-42(55)22-28-23-45(40(53)58-5,36-30(14-18-48(24-28)
Key:**OGWKCGZFUXNPDA-XQKSVPLYSA-N** ...

[Vincristine Details - The People's Medicine Community](#)
www.prescriptiondrug-info.com/drug_details.asp?title=Vincristine&...
... c1-7-42(55)22-28-23-45(40(53)58-5,36-30(14-18-48(24-28)
Key:**OGWKCGZFUXNPDA-XQKSVPLYSA-N** ... Vincristine (brand name, Oncovin), ...

Vincristine: Identifiers and Properties

Names and Identifiers

Names and Synonyms | Database ID(s)

Validated by Experts, Validated by Users, Non-Validated,

(2'β)-22-Oxovincaleukoblastine

200-318-1 *[EINECS/ELINCS]*

22-Oxovincaleukoblastine

57-22-7 *[RN]*

vincaleukoblastine, 22-oxo-

vincaleukoblastine, 22-oxo-, (2'β)-

vincaleukoblastine, 22-oxo-, (3β,4'β)-

Vincristine *[Wiki]*

Vincristinum *[Latin]*

VIN

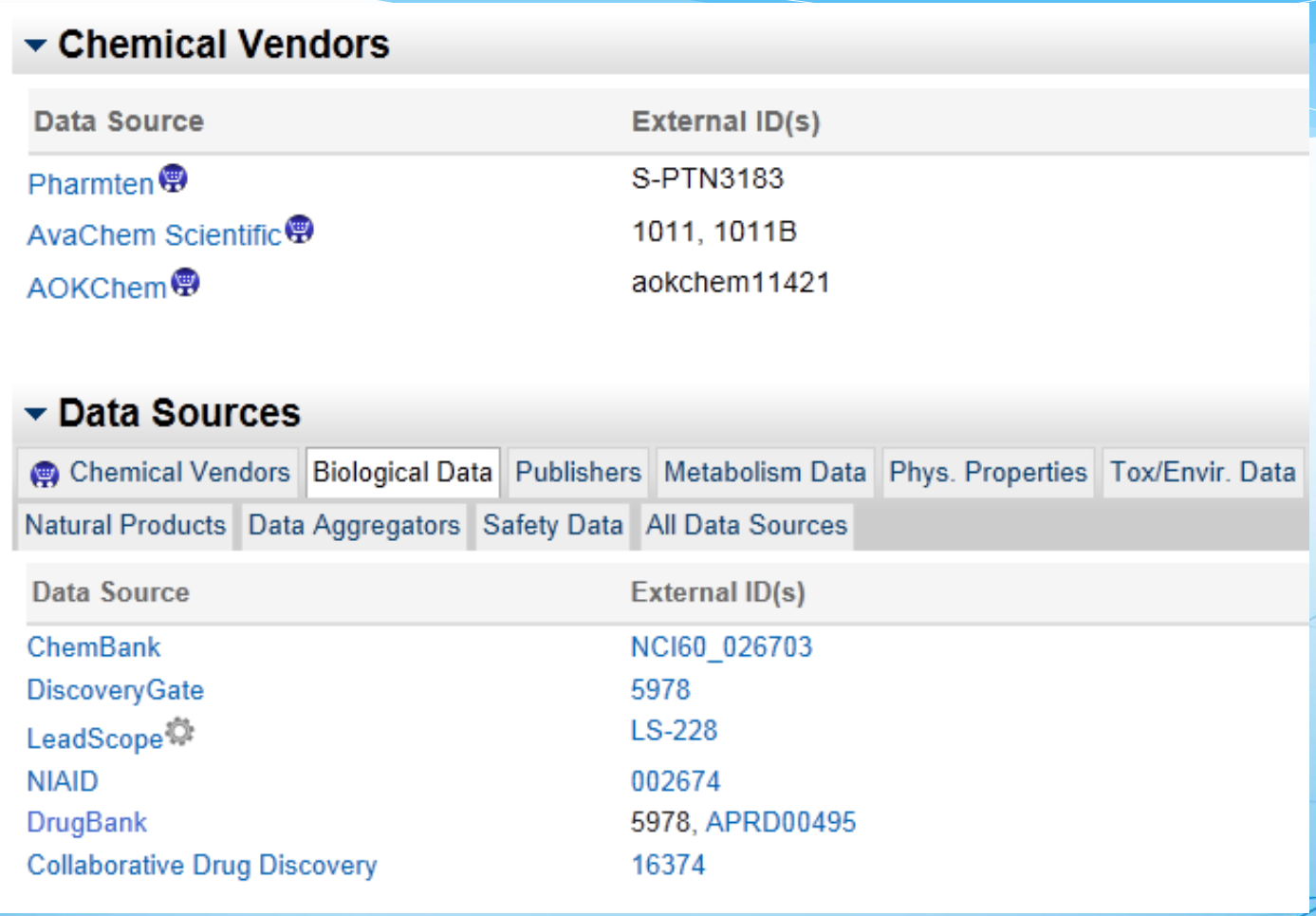
Properties

Experimental data | Predicted - ACD/Labs | Predicted - ChemAxon

Data supplied by datasources and users.

- Experimental Physchem Properties
  - **Melting Point:** 218 - 220 C
- Miscellaneous
  - **Appearance:** solid
  - **Stability:** Stable, but may be heat sensitive. Incompatible with strongoxidizing agents.
  - **Toxicity:** IVN-RAT LD50 1300 mg kg-1, IPR-MUS LD50 5.2 mg kg-1
  - **Safety:** Safety glasses, gloves, good ventilation.

Vincristine: Vendors and Sources



Chemical Vendors

Data Source	External ID(s)
Pharmten	S-PTN3183
AvaChem Scientific	1011, 1011B
AOKChem	aokchem11421

Data Sources

Chemical Vendors | Biological Data | Publishers | Metabolism Data | Phys. Properties | Tox/Envir. Data | Natural Products | Data Aggregators | Safety Data | All Data Sources

Data Source	External ID(s)
ChemBank	NCI60_026703
DiscoveryGate	5978
LeadScope	LS-228
NIAID	002674
DrugBank	5978, APRD00495
Collaborative Drug Discovery	16374

Vincristine: Patents

Patents

Google Patents | USPTO Granted | USPTO Applications | European Granted | European Applications | WO/PCT | Japanese Abstracts

powered by Google™

[Vincristine-containing product]

US Pat. 5055449 - Nov 07, 1988 - Akzo N.V.

Vincristine is a mitosis-retarding Vinca alkaloid which is fairly effective in combating various types of cancer, particularly Hodgkins disease and other ...

[Method of preparing vincristine]

US Pat. 4375432 - Nov 16, 1981 - Eli Lilly and Company

METHOD OF PREPARING **VINCRISTINE** CROSS-REFERENCE This application is a continuation-in-part of my copending application Ser. No. 262836 filed May 12, 1981, ...

[Process for the preparation of vincristine]

US Pat. 4767855 - Jun 02, 1986 - P. F. Medicament

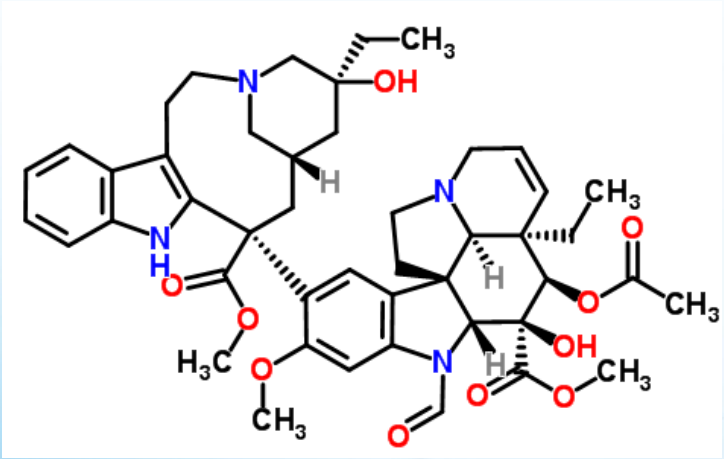
4767855 25 PROCESS FOR THE PREPARATION OF **VINCRISTINE** The present invention relates to a particularly effi- 5 cient process for the preparation of ...

[Method of preparing vincristine]

US Pat. 4303584 - Apr 02, 1980 - Eli Lilly and Company

Primary Examiner — Donald G. Daus Assistant Examiner — Diana G. Rivers Attorney, Agent, or Firm — James L. Rowe; Arthur R. Whale [57] ABSTRACT **Vincristine** ...

Chemical Names and Synonyms
VALIDATION OF NAMES



(2'β)-22-Oxovincaleukoblastine

200-318-1 *[EINECS]*

22-Oxovincaleukoblastine

57-22-7 *[RN]*

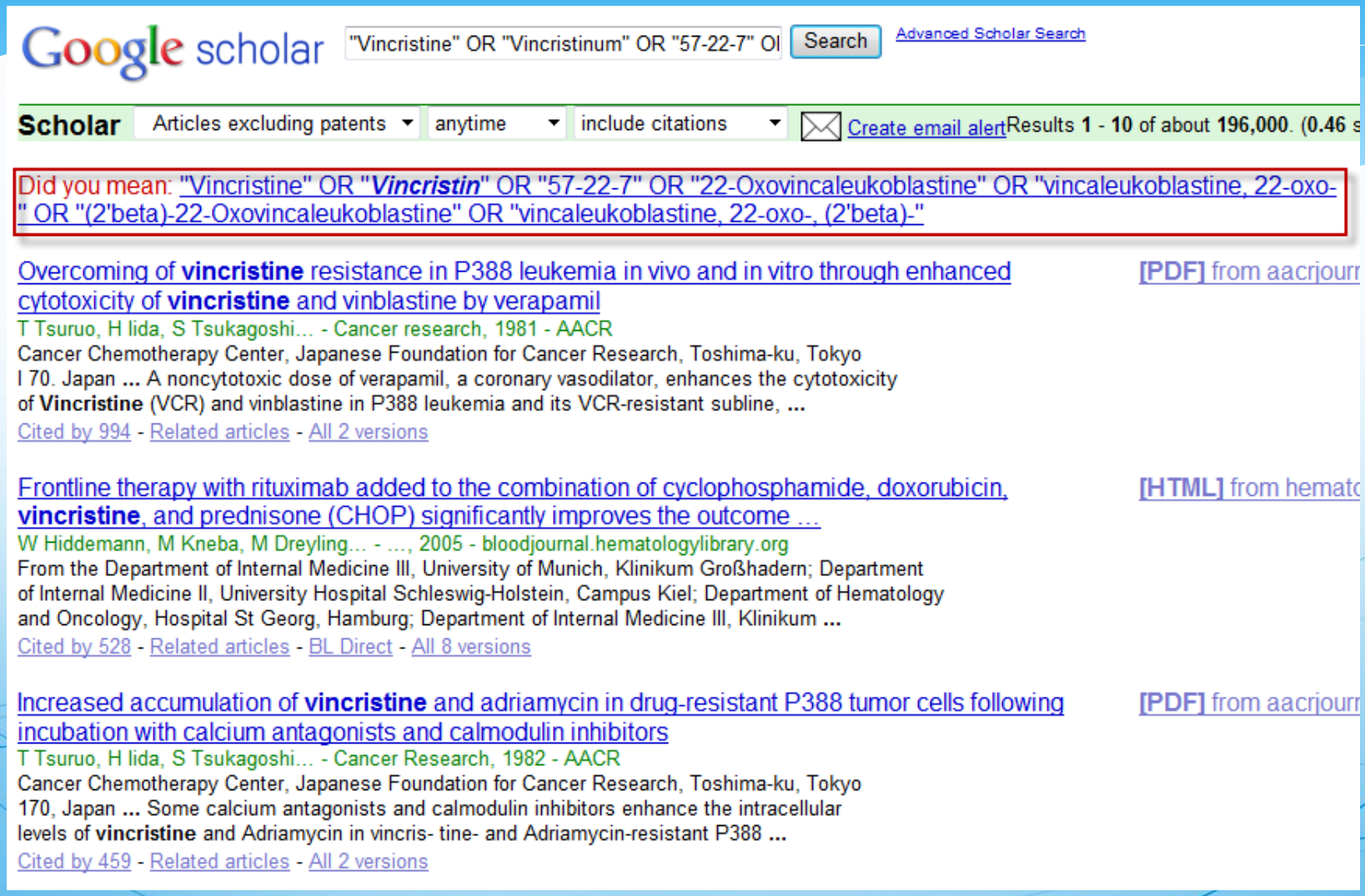
vincaleukoblastine, 22-oxo-

vincaleukoblastine, 22-oxo-, (2'β)-

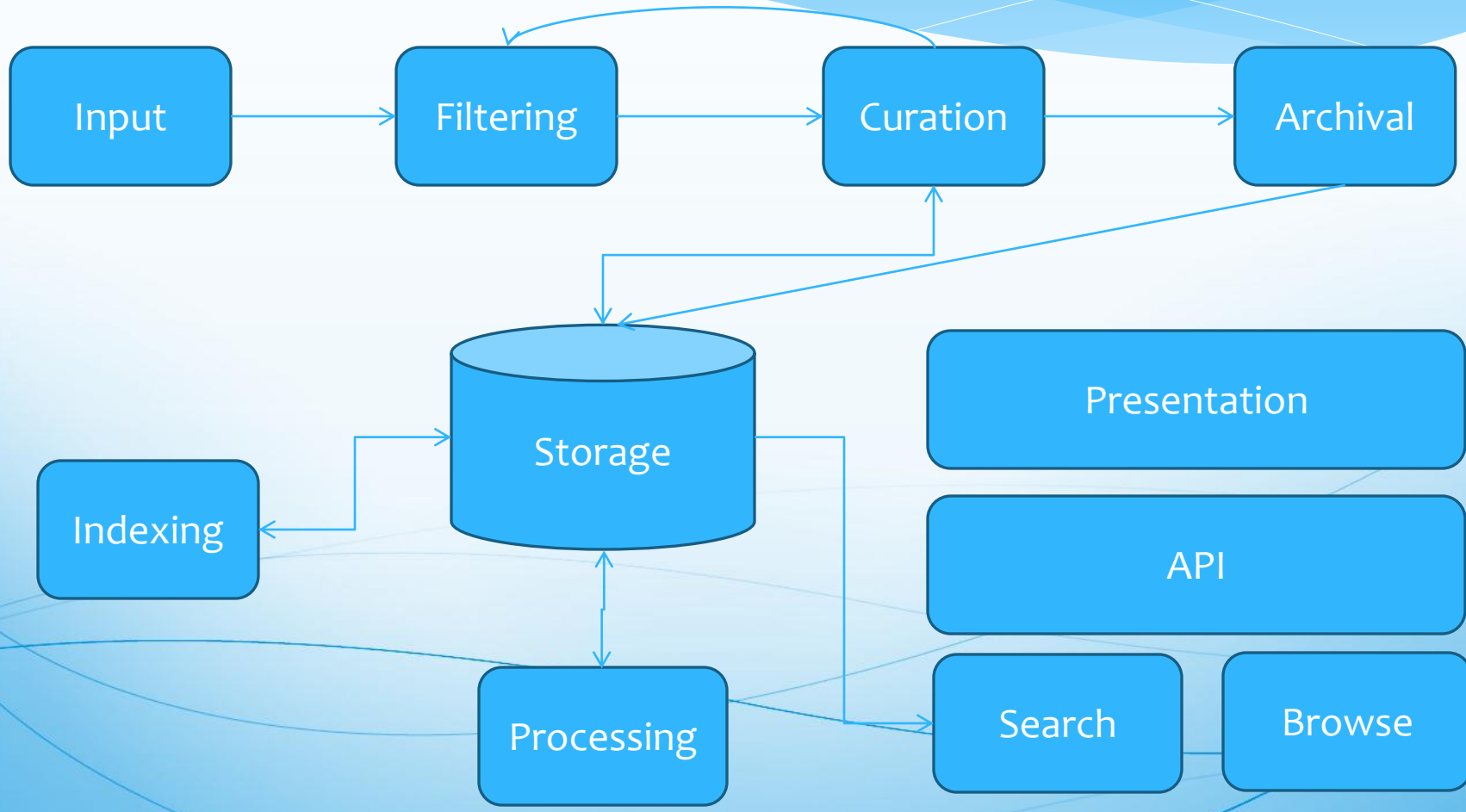
vincaleukoblastine, 22-oxo-, (3β,4'β)-

Vincristine *[Wiki]*

Validated Names for Searching…



Information System Architecture

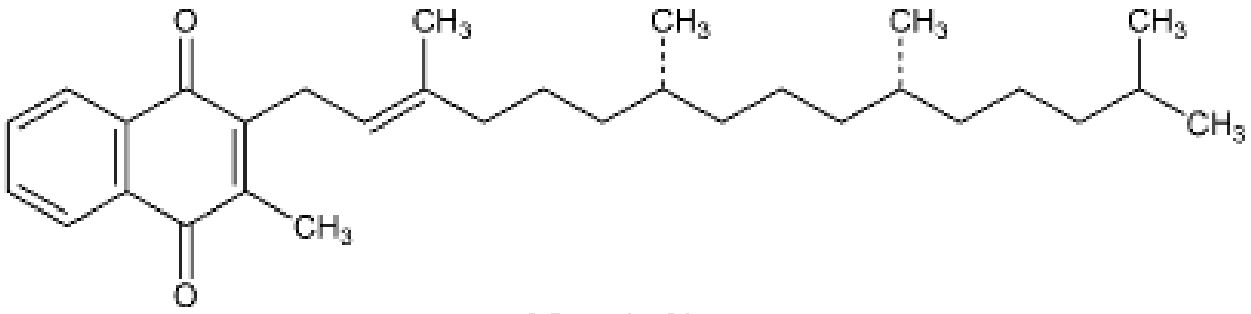


The Quality of Chemical Data Online What is the Structure of Vitamin K?

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.

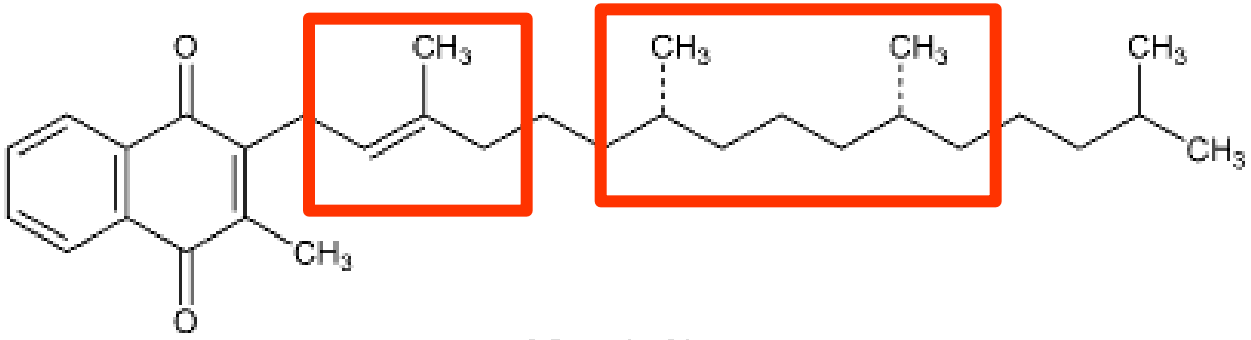


Vitamin K_1

The Merck Index, 14th Edition

What is the Structure of Vitamin K1?

7380. Phylloquinone.



Vitamin K_1

The Merck Index, 14th Edition

CAS's Common Chemistry

CAS Presents "COMMON CHEMISTRY"

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Substance Details

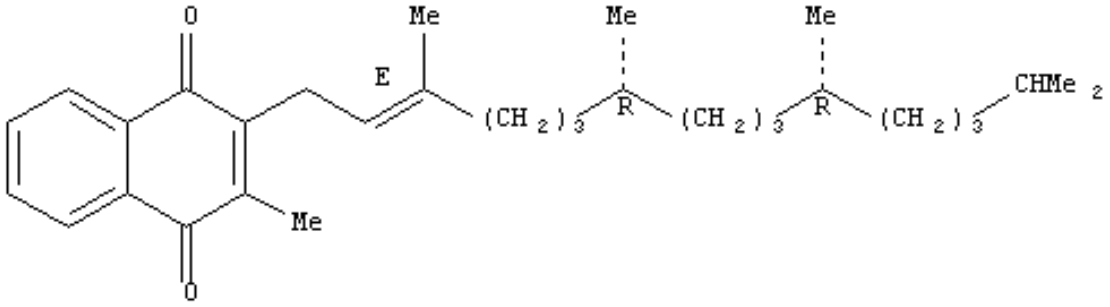
CAS Registry Number: 84-80-0

CA Index Name: 1,4-Naphthalenedione, 2-methyl-3-[(2E,7R,11R)-3,7,11,15-tetramethyl-2-hexadecenyl]-

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)

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Nederlands

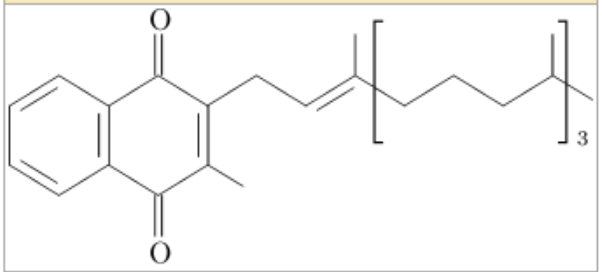
Phylloquinone is a polycyclic aromatic ketone, based on 2-methyl-1,4-naphthoquinone, with a 3-phytyl substituent.

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

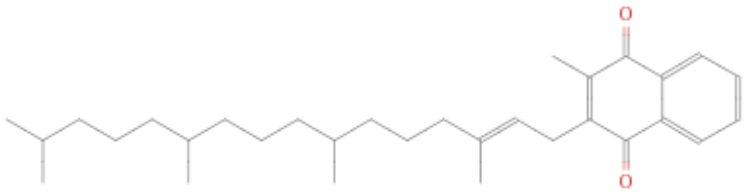
Input interpretation: *Mathematica* form

phytonadione

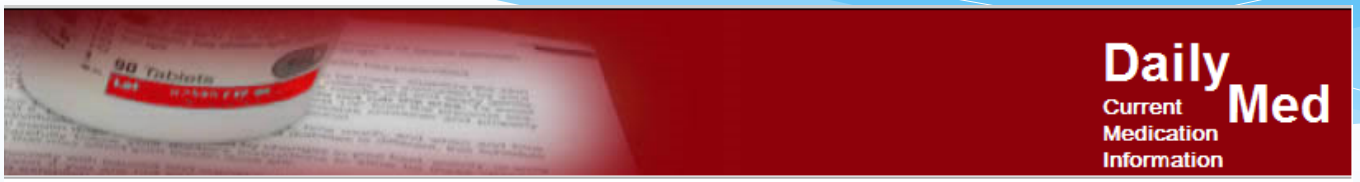
Chemical names and formulas: More

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

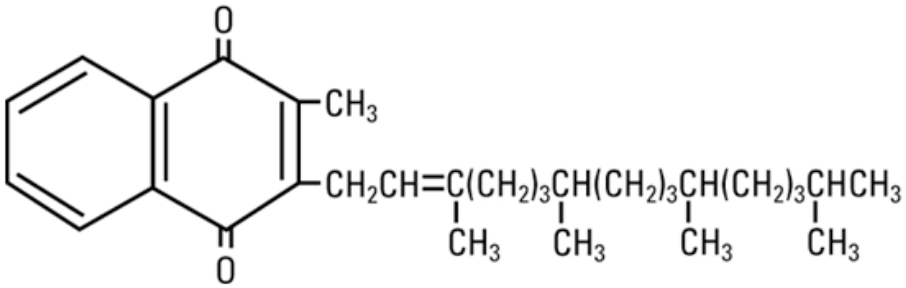
Review RxNorm Normal Forms

Category	DEA Schedule	Marketing Status
HUMAN PRESCRIPTION DRUG LABEL		

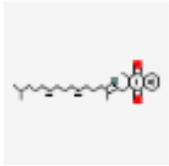
DESCRIPTION

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:

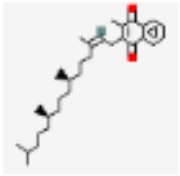


CID: 5284607



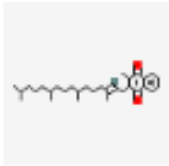
Phylloquinone; phytonadione; 3-Phytylmenadione ...
IUPAC: 2-methyl-3-[(E,7R,11R)-3,7,11,15-tetramethylhex
2-enyl]naphthalene-1,4-dione
MW: 450.695740 g/mol | MF: $C_{31}H_{46}O_2$
Tested in BioAssays: All: 104, Active: 1; BioActivity Ans
Vitamins... more

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

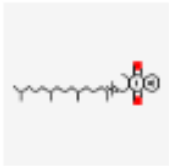


phytonadione; Phylloquinone; Phytomenadione ...
IUPAC: 2-methyl-3-[(E)-3,7,11,15-tetramethylhexadeo-2-
1,4-dione
MW: 450.695740 g/mol | MF: $C_{31}H_{46}O_2$
Tested in BioAssays: All: 118, Active: 0; BioActivity Ans
Vitamins... more

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

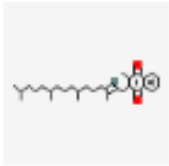


phytonadione; Phylloquinone; Phytomenadione ...
IUPAC: 2-methyl-3-(3,7,11,15-tetramethylhexadeo-2-enyl
1,4-dione
MW: 450.695740 g/mol | MF: $C_{31}H_{46}O_2$
Vitamins... more

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

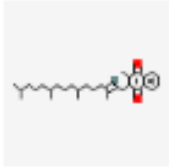


Vitamin K 1; CID10863350
IUPAC: 2-methyl-3-[(E)-3,7,11,15-tetramethylhexadeo-2-
1,4-dione
MW: 452.695500 g/mol | MF: $C_{31}H_{46}O_2$
Vitamins... more

CID: 7048753

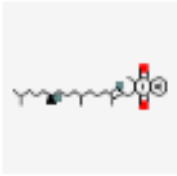
Vitamin K 1; ZINC03831329; CID7048753
IUPAC: 2-methyl-3-[(E,7S,11S)-3,7,11,15-tetramethylhexadeo
2-enyl]naphthalene-1,4-dione
MW: 450.695740 g/mol | MF: $C_{31}H_{46}O_2$
Vitamins... more

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

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

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In the Pipeline

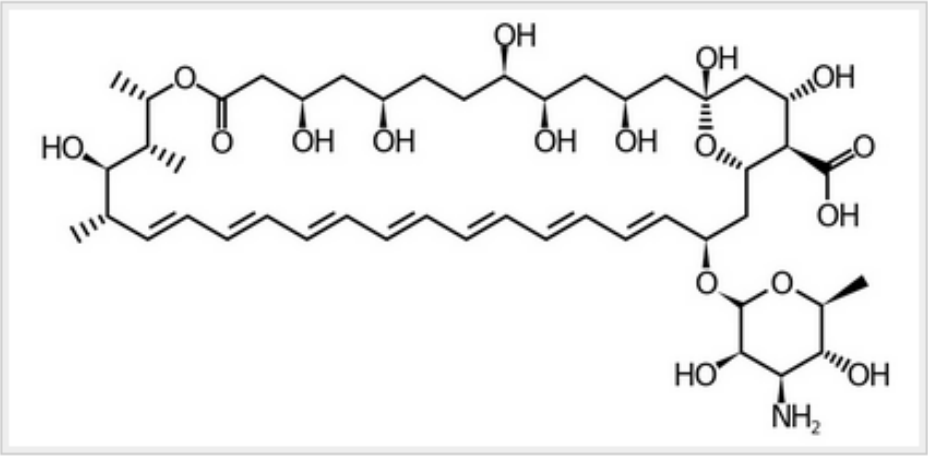
« Arsenic Life No More | Main | Targacep

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.



Just Yesterday…

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).

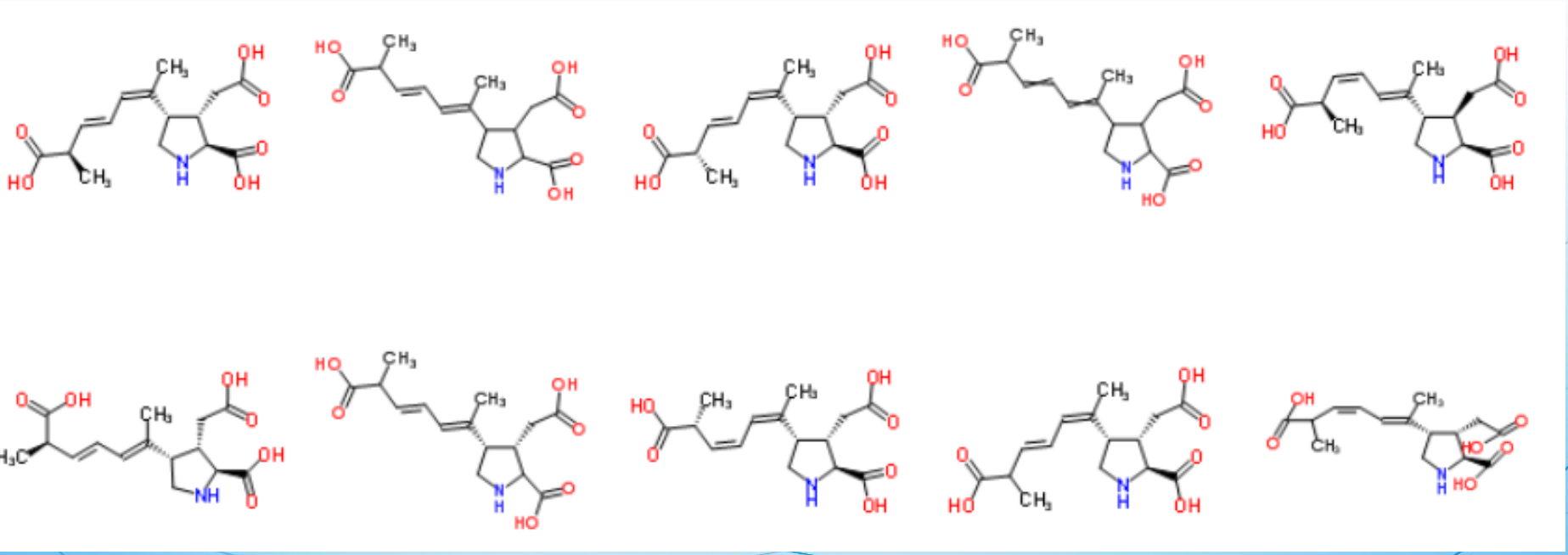
How will it improve?

Participation

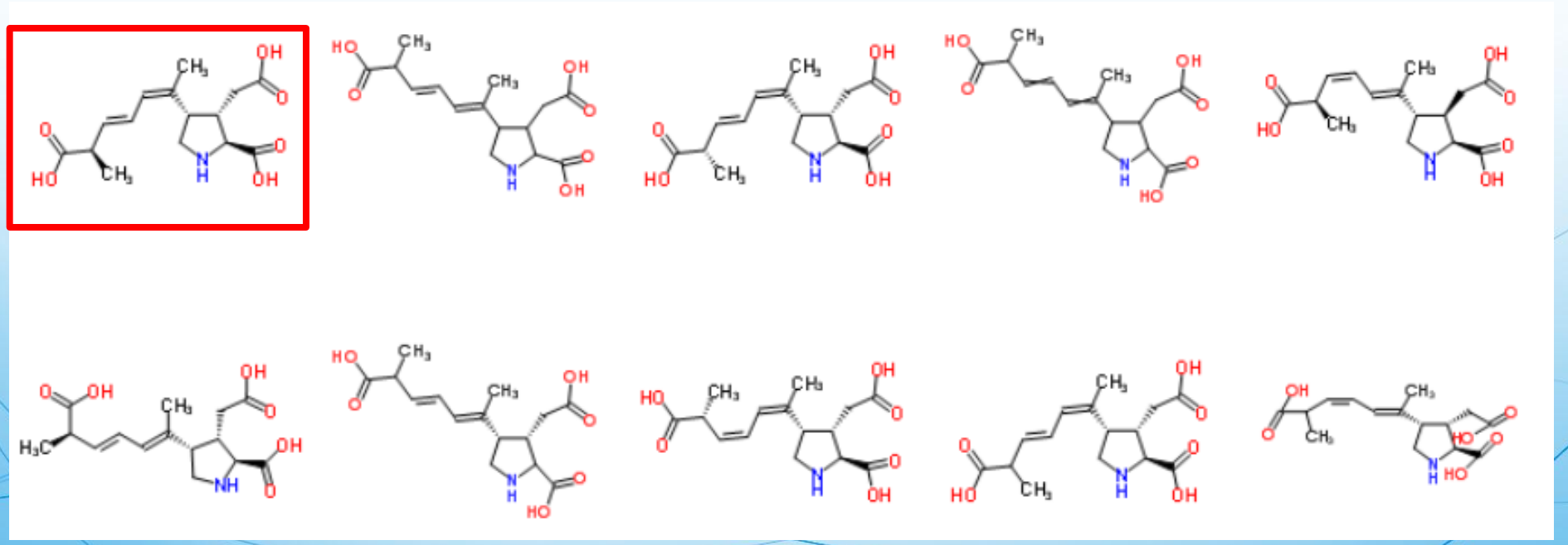
and

contribution

ALL Different, ALL "Domoic Acids"



ALL Different, ALL "Domoic Acids"



The EXPERTS must get it right?!

Northwest Fisheries Science Center
Harmful Algal Blooms

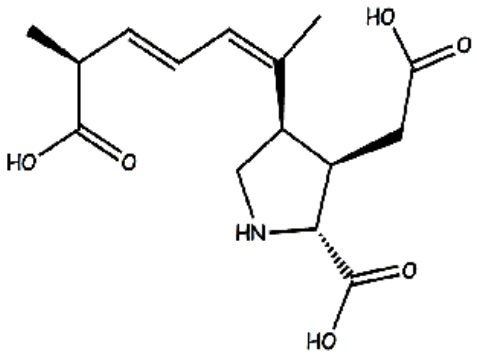
Home • HABs & Biotoxins • Research • Outreach • Links • Search

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

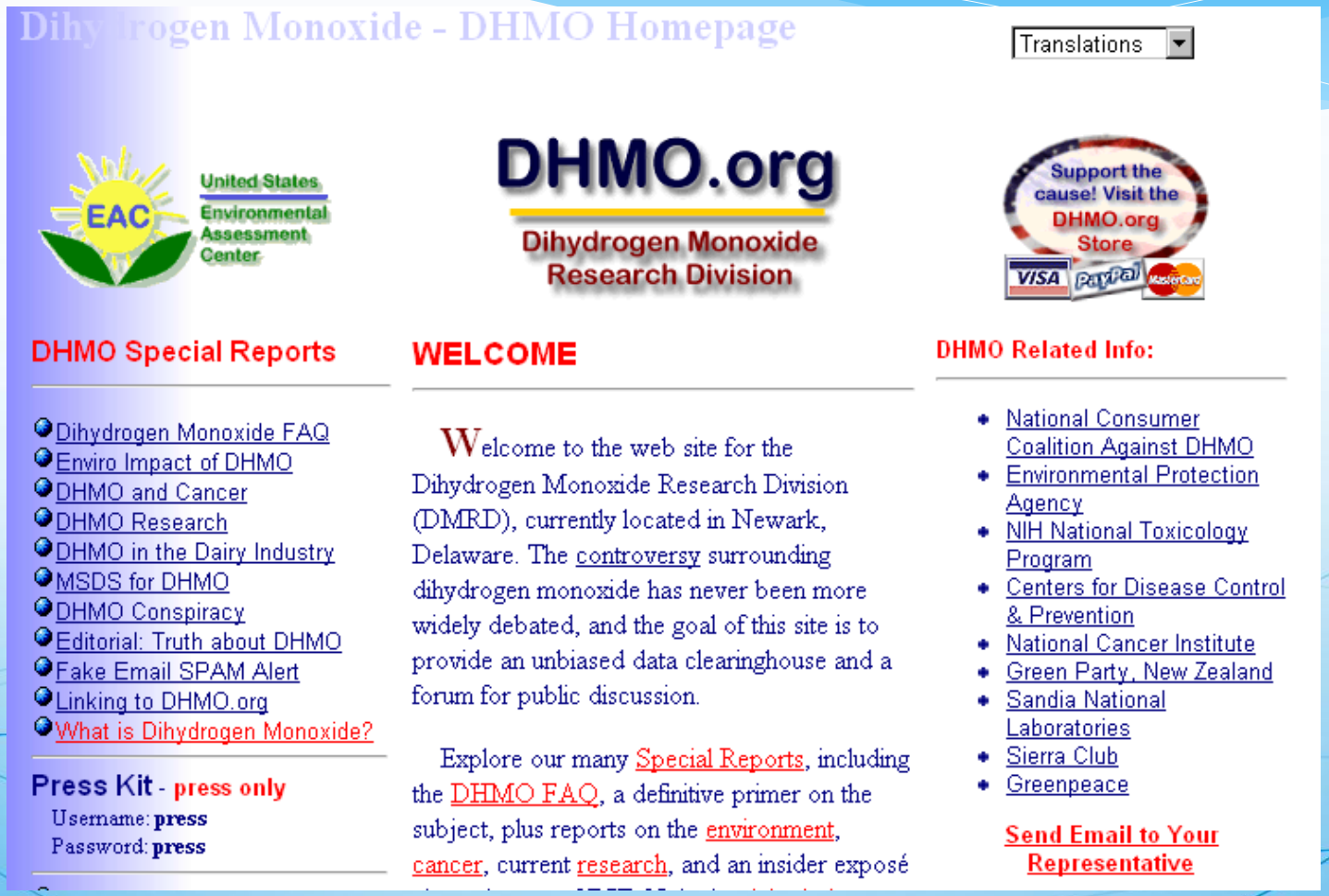


Domoic Acid

HABs & Biotoxins

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

Question Everything Online: www.dhmo.org



Deposition, Annotation and Validation

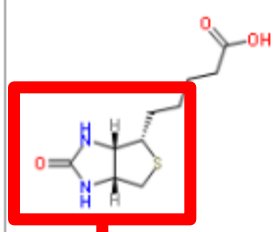
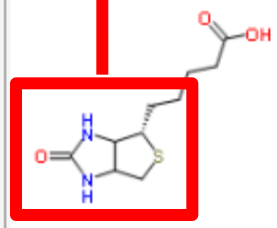
* **ANYBODY** can annotate a record on ChemSpider
* Registered users can deposit new data
* Registered users can validate existing data

CURATION Search "Vitamin H"

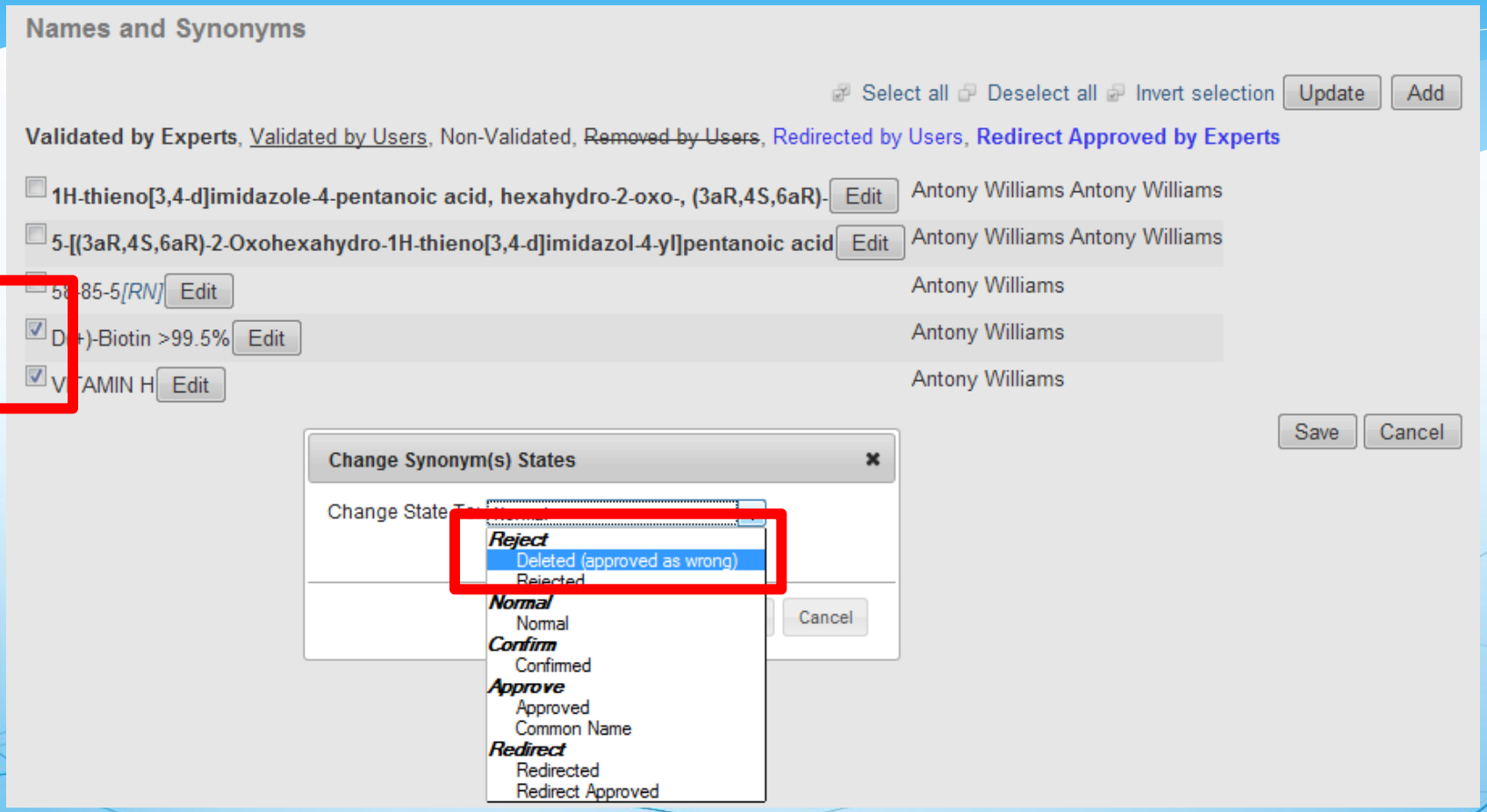
Search

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

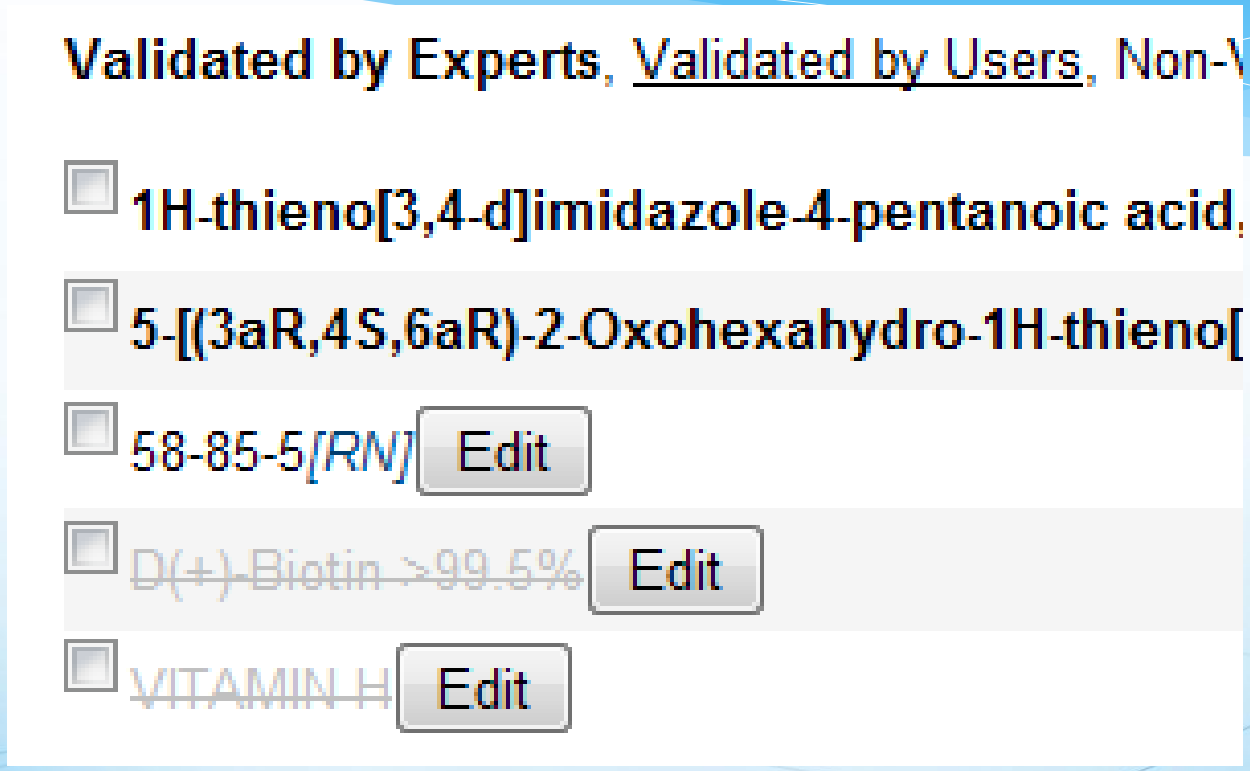
Grid Tile Table Record ChemRefer Entrez PubChem

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



ChemSpider Web Services

- **AsyncSimpleSearch**
  Search by Name, SMILES, InChI, InChIKey, etc. Returns transaction ID which can be used to access search status and result. Security token is required.
- **CSID2ExtRefs**
  Return a list of external references (data sources). Security token with Service Subscriber role is required.
- **GetAsyncSearchResult**
  Returns the list of CSIDs found by AsynchSearch operation. Security token is required.
- **GetAsyncSearchResultPart**
  Return a slice of the list of CSIDs found by AsynchSearch operation. Returns full list if start = 0 and count = -1. If (start + count) > (# of results) all results starting at start position are returned. Security token is required.
- **GetAsyncSearchStatus**
  Query asynchronous operation status. Requires transaction ID returned by AsynchSearch operation. Security token is required.
- **GetCompoundInfo**
  Get record details (CSID, InChIKey, InChI, SMILES) by CSID. Security token is required.

Open APIs for Science

* ChemSpider via web service access
  * For structure identification for mass spectrometry
  * For name and structure resolution
  * For structure and substructure searching
  * For an “innovative medicines initiative” semantic web project…

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
* 36 months project – first public release version is imminent

Guiding principle is open access, open usage, open source

- **Key to standards adoption** -

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

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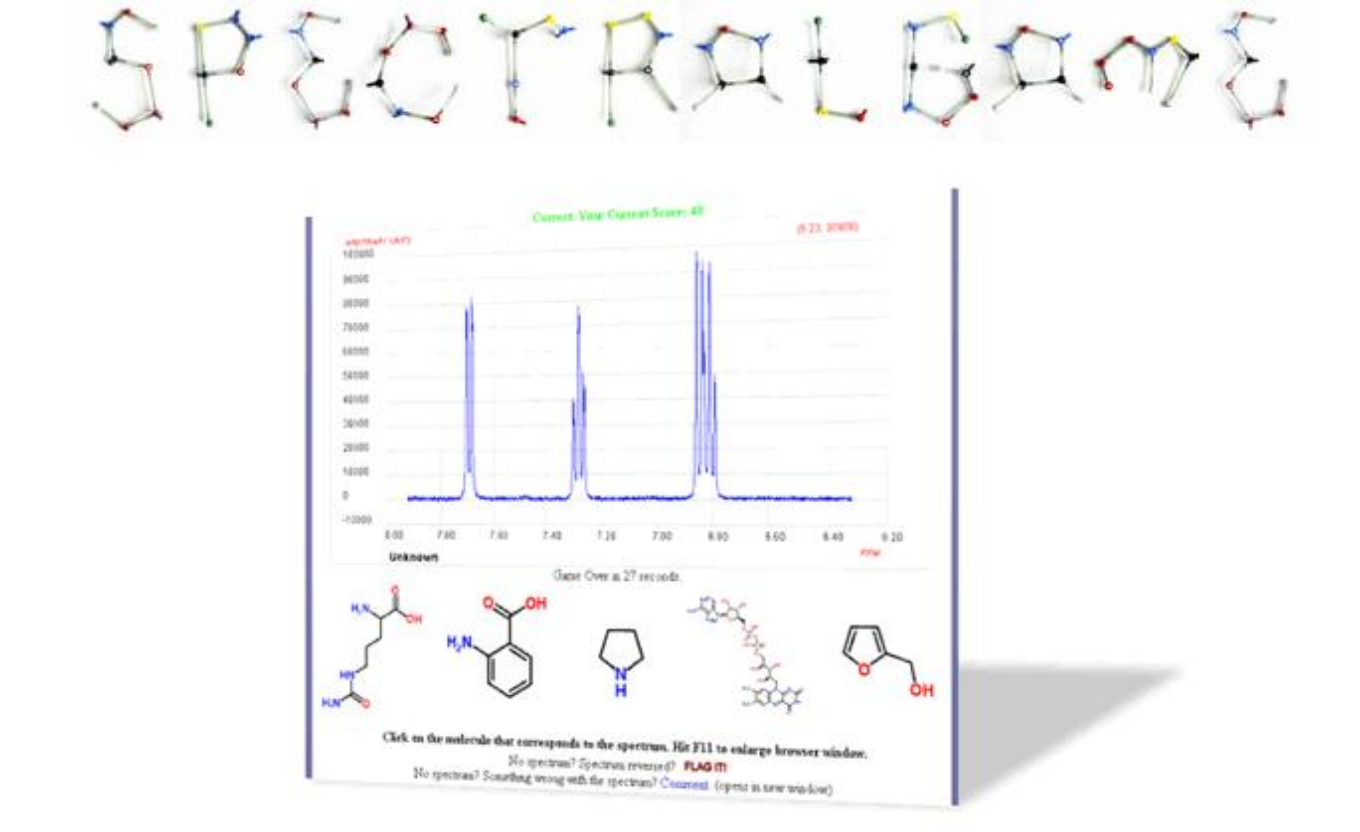
www.SpectralGame.com

http://www.jcheminf.com/content/1/1/9



The World of Contribution

* Times have changed
  * Immediacy of social networks
  * Commenting on articles/data is here
  * The “participating scientist” has high profile
  * And who can be a scientist now???

A Ten Year Old Scientist

Computational and Theoretical Chemistry

Volume 979, 1 January 2012, Pages 33–37

A computational study of novel nitratoxycarbon, nitritocarbonyl, and nitrate compounds and their potential as high energy materials

Robert W. Zoellner[a], Clara L. Lazen[b], Kenneth M. Boehr[b]

[a] Department of Chemistry, Humboldt State University, One Harpst Street, Arcata, CA 95521-8299, USA

[b] Border Star Montessori School, 6321 Wornall Road, Kansas City, MO 64113-1792, USA

'A 13-year-old American student named Aristides Poehlman, known as 'Cheese' online, is ranked in Foldit's Top Ten protein folders and has become a celebrity in his own right'

Gamers Unravel the Secret Life of Protein

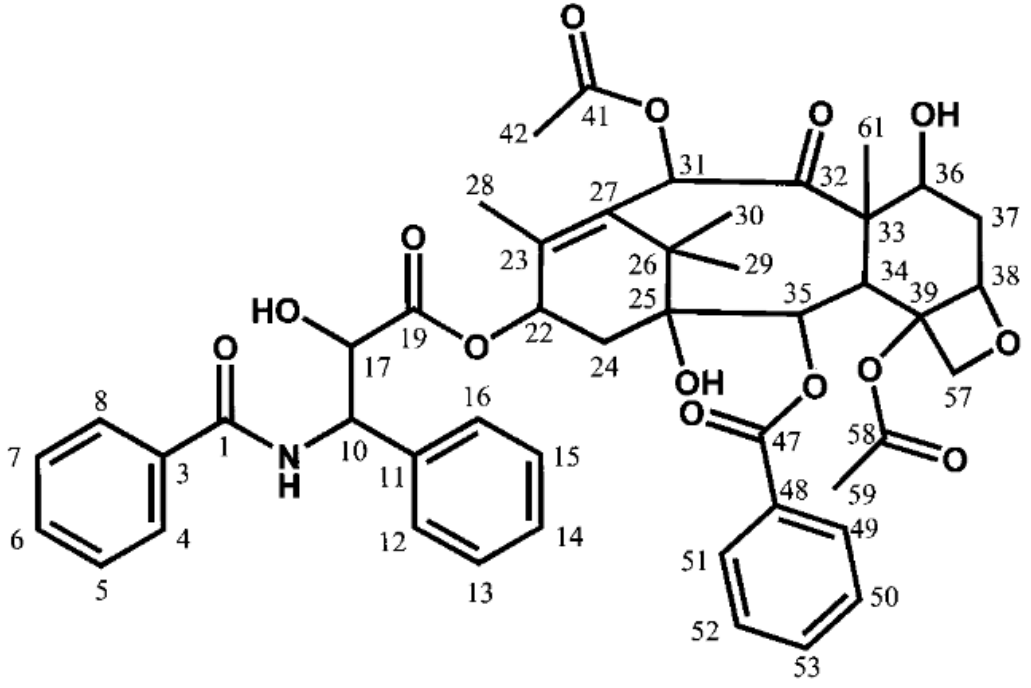
By John Bohannon 04.20.09

A model of a protein from *Streptomyces avermitilis*, a source of antibiotics.
Origami/photo: Robert J. Lang / Talia Chetrit

Challenging a Publication

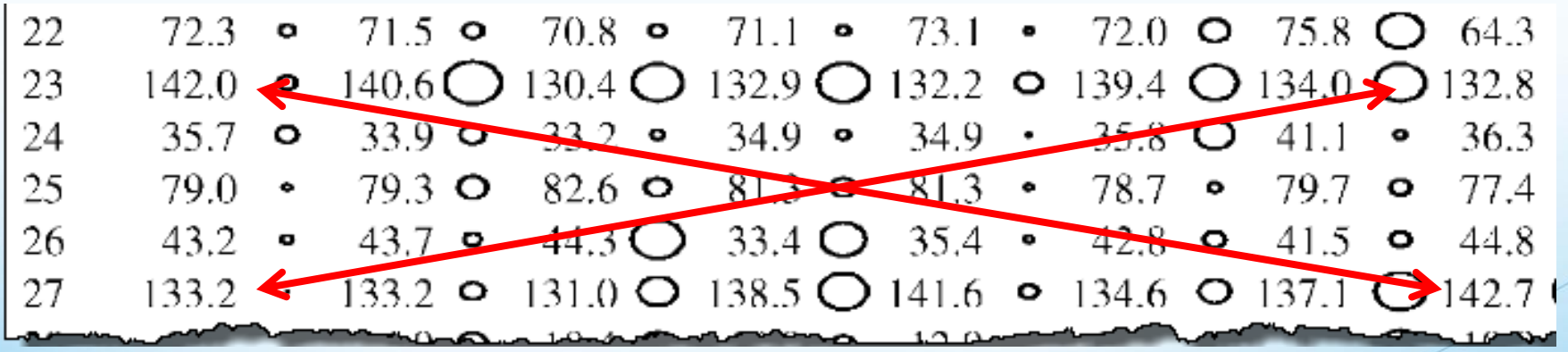
Using Neural Networks for ^{13}C NMR Chemical Shift Prediction–Comparison with Traditional Methods

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 34.9 34.9 41.1 36.3
25 79.0 79.3 82.6 78.7 79.7 77.4
26 43.2 43.7 33.4 35.4 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

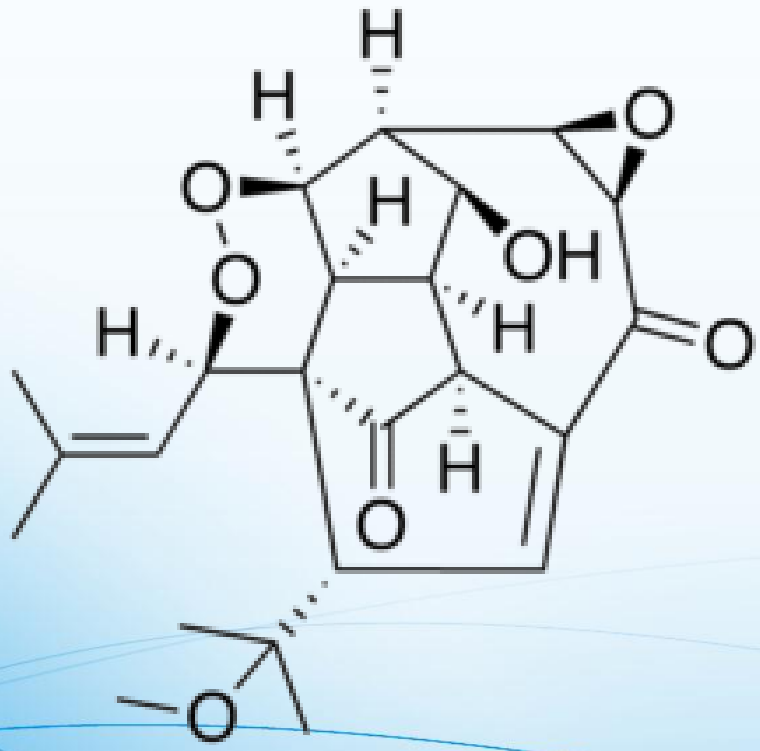
Journal of Magnetic Resonance

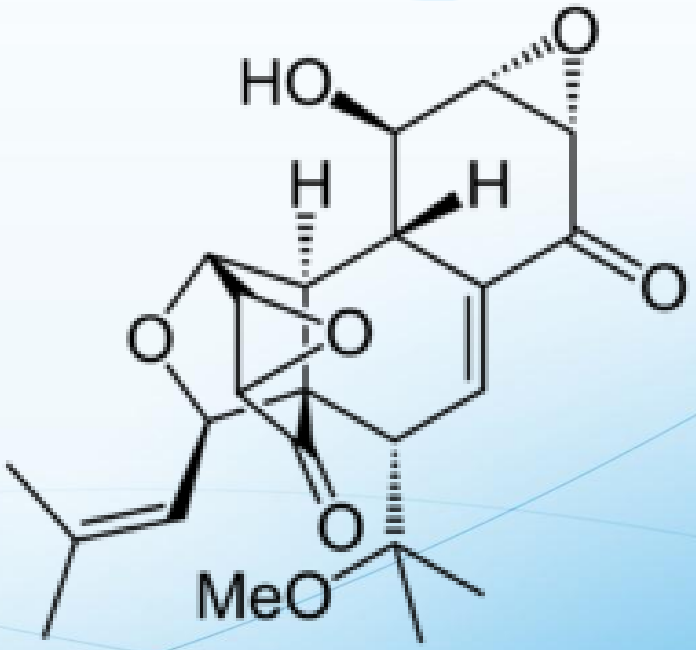
Volume 157, Issue 2, August 2002, Pages 242–252

Journal of Magnetic Resonance

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

What of 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 …

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.

The Blogosphere Analyzes…

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Search: **nah jacs**

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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…

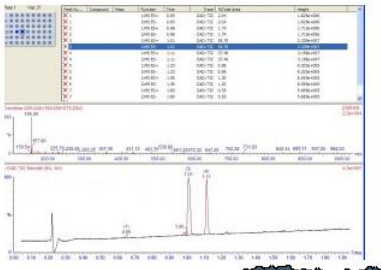
totally synthetic

NaH as an Oxidant – Liveblogging!

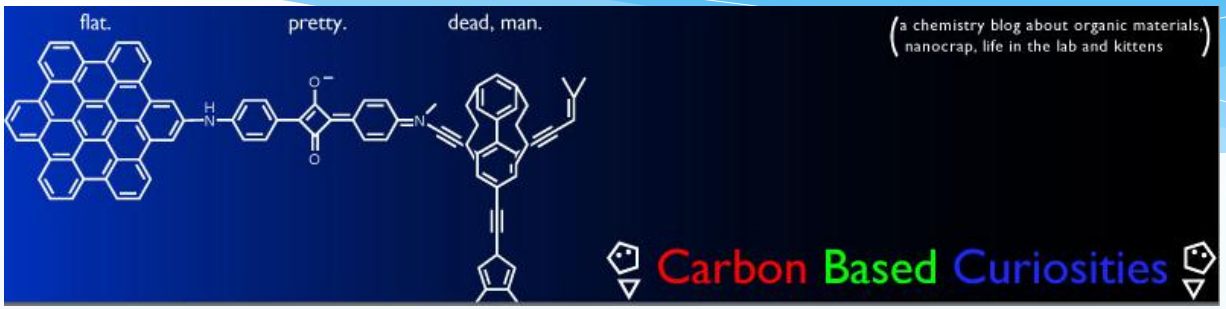
+1 1

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]

Open Notebook Science Analysis

Useful Chemistry XML UsefulChem wiki

OPEN Notebook Science

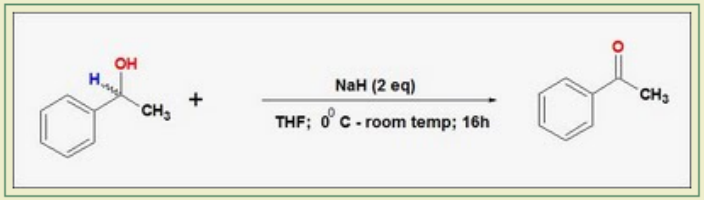
WEDNESDAY, AUGUST 05, 2009

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.

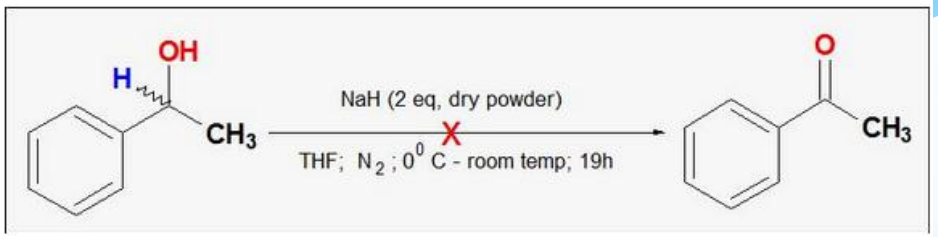
Khalid Mirza and Marshall Moritz thought it would be worthwhile to see if we can shed any light on the situation. I was also curious to see what the reaction did over time, before quenching.

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

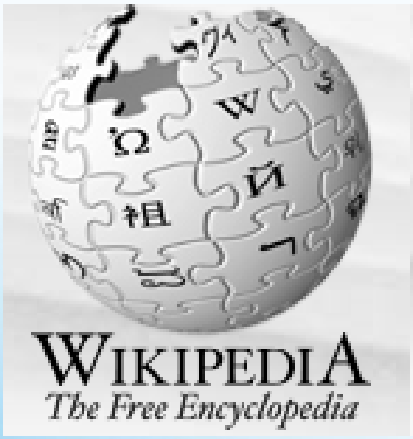
To convert DL-α-methylbenzyl alcohol to acetophenone using NaH, following a recently published JACS protocol

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:

Motivation
Faster Science, Better Science



Open Notebook Science

From Wikipedia, the free encyclopedia

Open Notebook Science is the practice of making the entire primary record of a research project publicly available online as it is recorded. This involves placing the personal, or laboratory, notebook of the researcher online along with all raw and processed data, and any associated material, as this material is generated. The

Openness – Still Carries Licensing

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Attribution		
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* Open Source licenses
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* Open Notebook Science

We Suggest Rules for Licensing Data

* License data based on GOALS: scientific, commercial, or mixed
* Explore the benefits of open licensing and drawbacks of enclosure
* Provide simple explanations terms of use
* If you can't make the data public domain, make the metadata **public domain.**

We Suggest 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...

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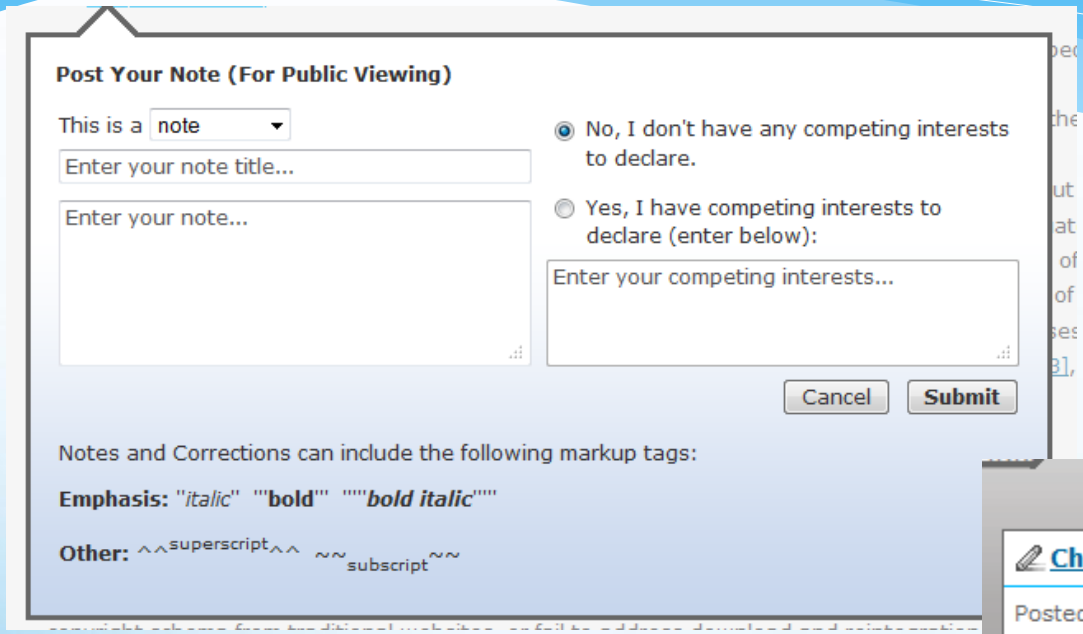
Egon Willighagen @egonwillighagen 1 Oct

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

Annotating Articles Today…



Attribution to me…

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

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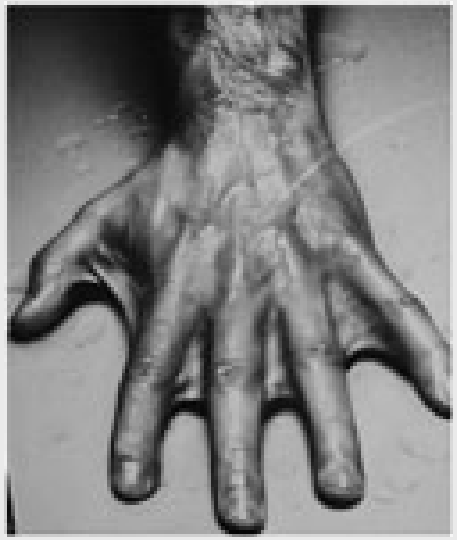
0 responses	Change public domain to "public"	Posted by ChemConnector on 01 Oct 2012 at 16:56 GMT

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

Other Publications to Annotate…

Other Publications to Annotate…



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)

Publications to Annotate…

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

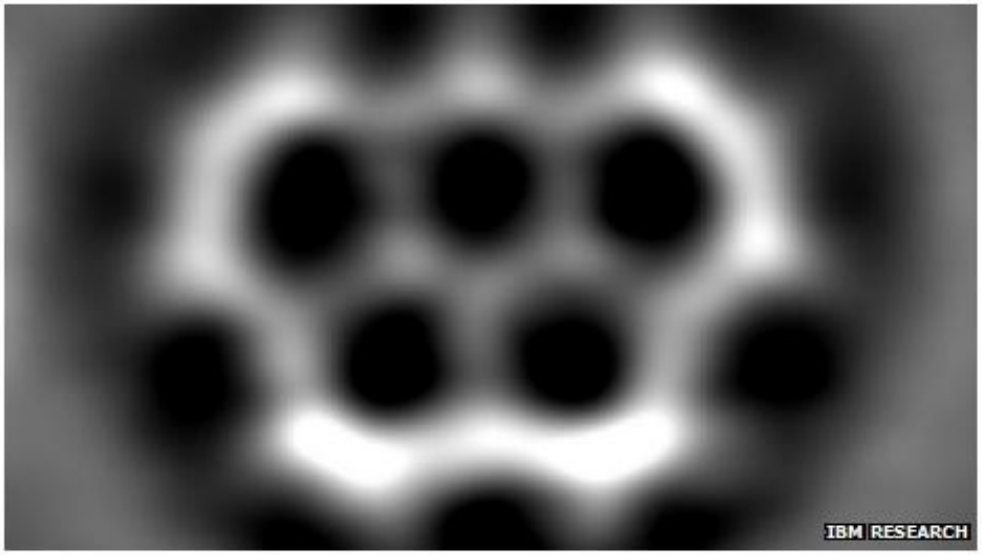
"..identified as the new protein Wai So Dim"

A New World for Publishing?

An Adventure into the World of **Small** but significant contribution..

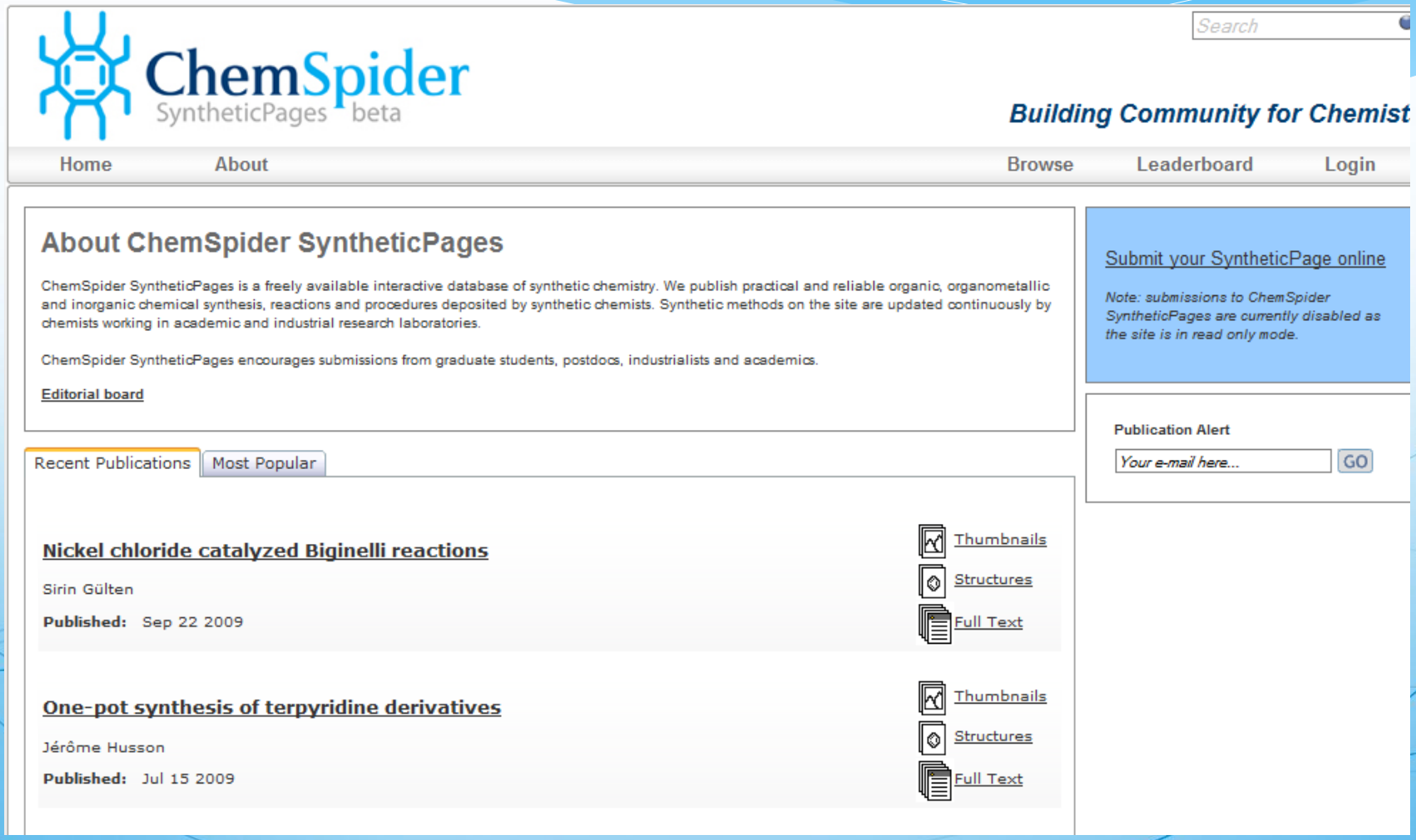
'Olympic rings' molecule olympicene striking image

By Jason Palmer
Science and technology reporter, BBC News



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

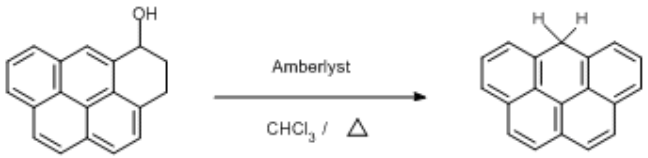
ChemSpider SyntheticPages



Micropublishing with Peer Review (a chemical synthesis blog?)

Dehydration of 3,4-dihydro-5H-Benzo[cd]pyren-5-ol; 6H-Benzo[cd]pyrene

SyntheticPage 542
DOI: 10.1039/SP542
Submitted Mar 15, 2012, published May 31, 2012
Anish Mistry (a.mistry@warwick.ac.uk)
A contribution from Fox Group, Warwick University



Chemicals Used

3,4-dihydro-5H-Benzo[cd]pyren-5-ol (prepared)
Amberlyst 15 (Sigma-Aldrich)
Chloroform

Procedure

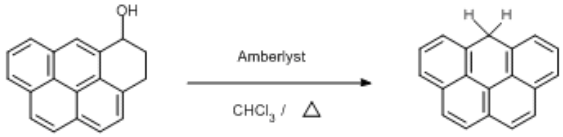
3,4-dihydro-5H-Benzo[cd]pyren-5-ol (0.1 g, 0.39 mmol) was dissolved in chloroform (30 ml) and Aberlyst 15 (0.1 g) added under a dinitrogen atmosphere. The reaction was heated to 30°C and left overnight under the inert atmosphere. The solution was then filtered to seperate the Amberlyst and washed with chloroform. The combined solvents were removed under vacuum using a Rotary evaporator. The crude product was column chromatographed under a dinitrogen atmosphere eluting with 1:1 chloroform:petroleum ether 40-60°C. A white solid was obtained using this method (50 mg, 54%).

Multi-Step Synthesis

Dehydration of 3,4-dihydro-5H-Benzo[cd]pyren-5-ol

Anish Mistry

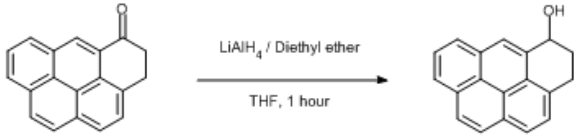
Published: May 31 2012



Reduction of 3,4-dihydro-5H-benzo[cd]pyren-5-one.

Anish Mistry

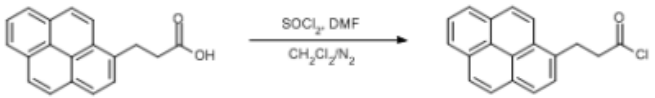
Published: Mar 12 2012



Chlorination of a carboxylic acid

Anish Mistry

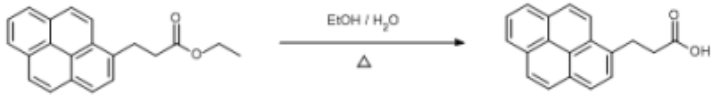
Published: Nov 27 2011



Hydrolysis of Ethyl 3-(1-pyrenyl)propanoate

Anish Mistry

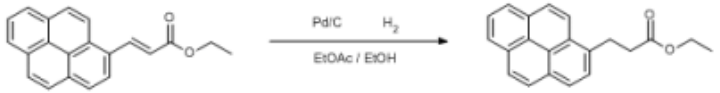
Published: Oct 11 2011



Hydrogenation of Ethyl 3-(1-pyrenyl)acrylate

Anish Mistry

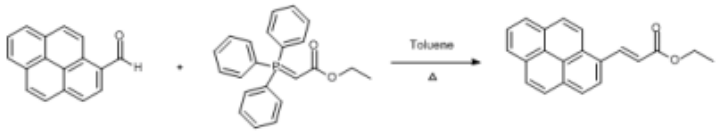
Published: Oct 06 2011



Wittig Reaction

Anish Mistry

Published: Sep 14 2011

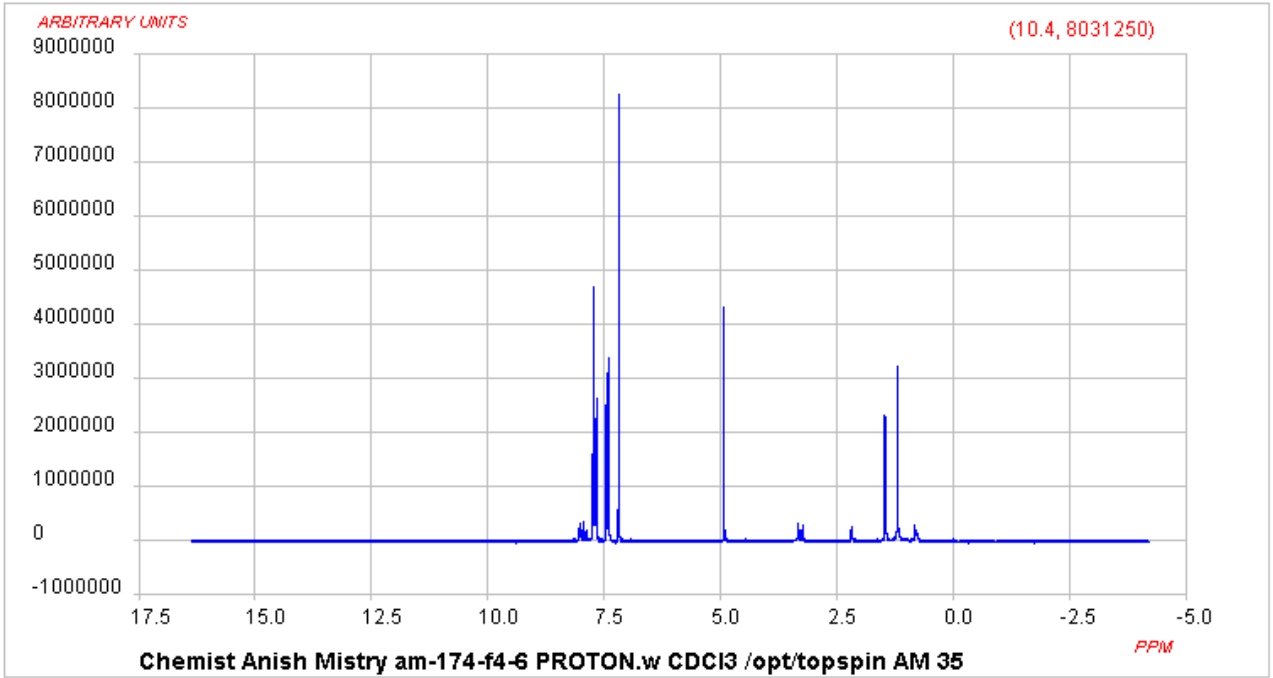


Interactive Data

Supplementary Information

Proton NMR shows the symmetric dihydrogen species as the major product, the small peaks which can be observed in the spectrum (around 2, 3.5 ppm and aromatic region) are presumably other isomers of the compound.

1H NMR spectrum of Olympicene - Click to view



1H NMR (Jan11-2012.dx)

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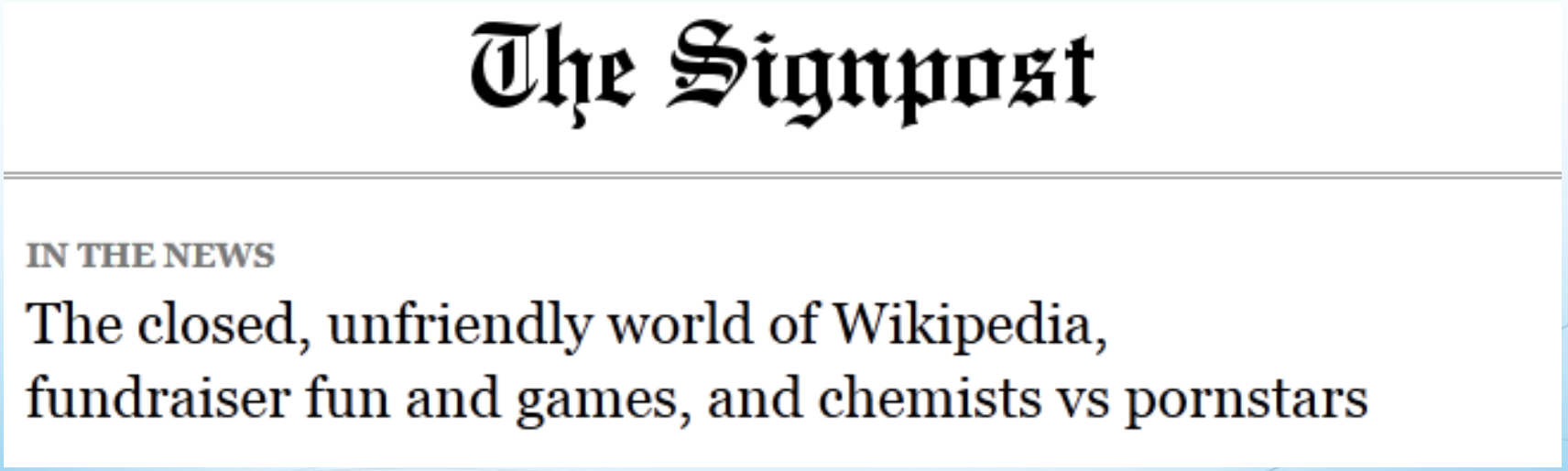
Get structure file (.cdx, .sk2, .mol)

A New Route for Scientific Recognition?

The Measure of a Scientist?

* How do “we” measure a scientist?
* The funding bodies, department heads etc. use
  * Publication profile
  * Impact factors
  * An index – h, m, g, i10, c, s …
  * Grants brought in
* Scientists are notable in different ways – technology can help measure different types of “impact”

What makes a Scientist Notable?


The Signpost

IN THE NEWS

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

Public Profiles of Scientists

* Online tools track activities of scientists
* Some are totally opt-in, an increasing number are *about* you and need checking!
* Take responsibility for your profile online
* Actively BUILD your online profile

Microsoft Academic Search

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antony J. williams

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Navigate geographically through organizations and authors in a specified domain.

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Antony J. Williams Royal Society of Chemistry

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Publications: 154 | Citations: 445 | G-Index: 14 | H-Index: 11

Interests: Computational Chemistry, Applied Chemistry, Pharmacology

Collaborated with 244 co-authors from 1974 to 2011; Cited by 925 authors

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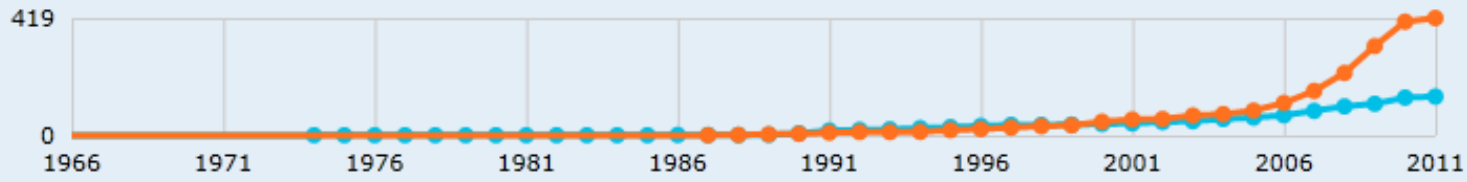

Publications (154) Export

Order by: Year

A quality alert and call for improved curation of public chemistry databases (Citations: 1)

Antony J. Williams, Sean Ekins

Journal: Drug Discovery Today - DRUG DISCOV TODAY, vol. 16, no. 17, pp. 747-750, 2011

In silico repositioning of approved drugs for rare and neglected diseases (Citations: 1)

Sean Ekins, **Antony J. Williams**, Matthew D. Krasowski, Joel S. Freundlich

Journal: Drug Discovery Today - DRUG DISCOV TODAY, vol. 16, no. 7, pp. 298-310, 2011

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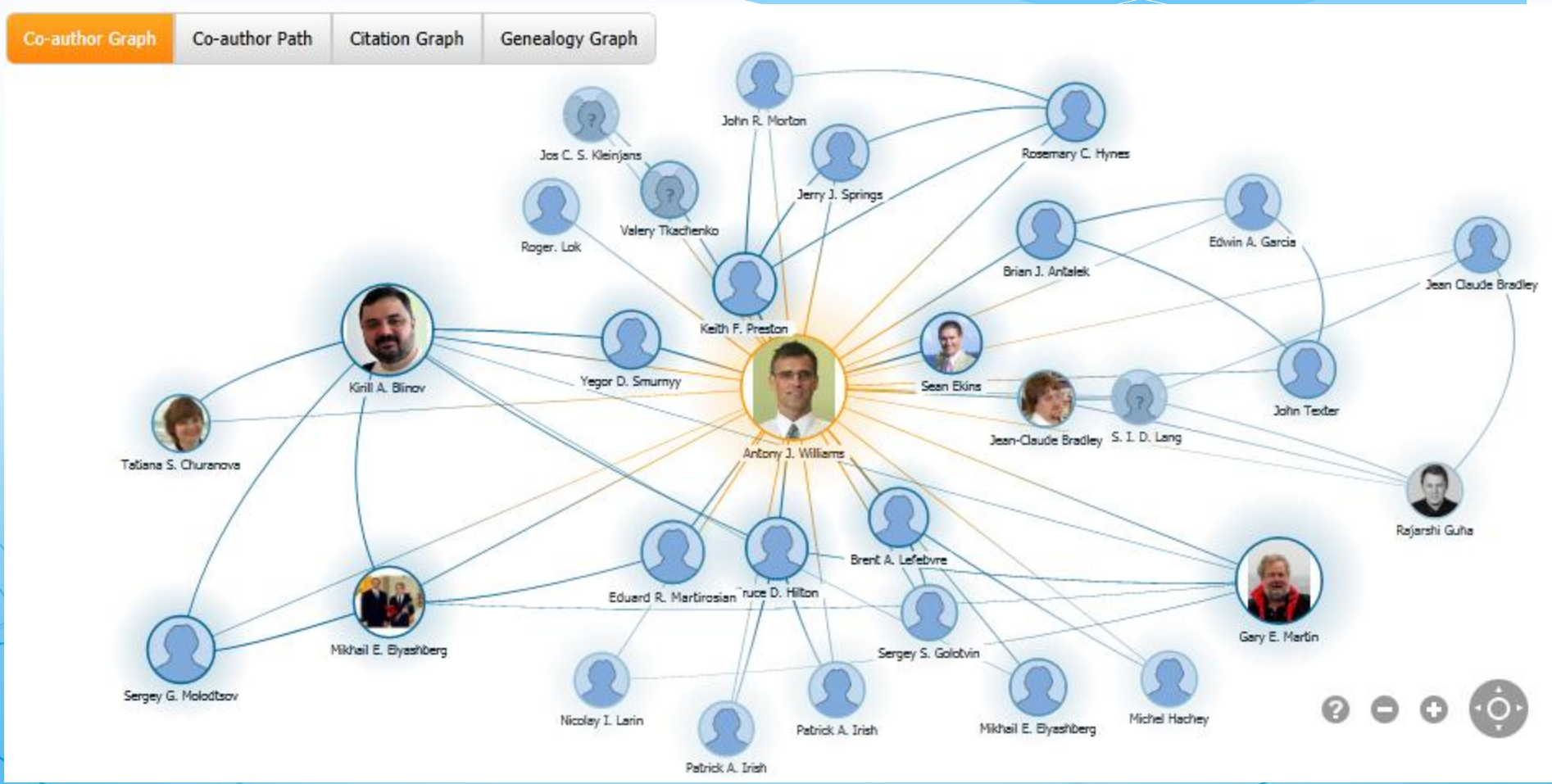

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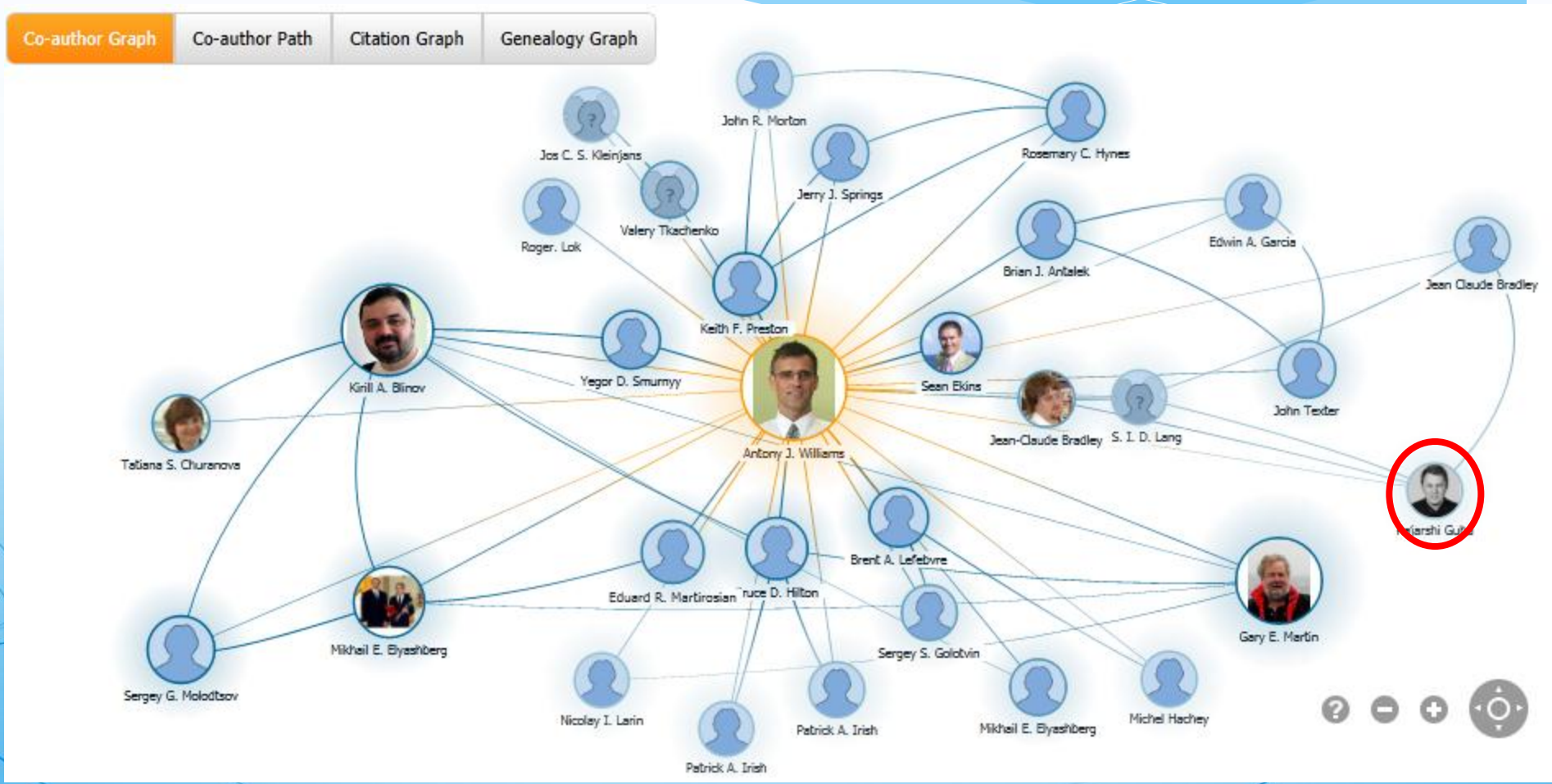

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Rajarshi Guha

National Institutes of Health, United States

Publications: 65 | Citations: 495 | G-Index: 21 | H-Index: 11

Interests: Computational Chemistry, Applied Chemistry, Polymer Chemistry

Homepage

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Rajarshi Guha

National Institutes of Health, United States

Publications: 65 | Citations: 495 | G-Index: 21 | H-Inde

Interests: Computational Chemistry, Applied Chemistry, Poly

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* First Name	Rajarshi
Middle Name	
* Last Name	Guha
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	e.g. Your name in your native language.
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i10-index	66	52

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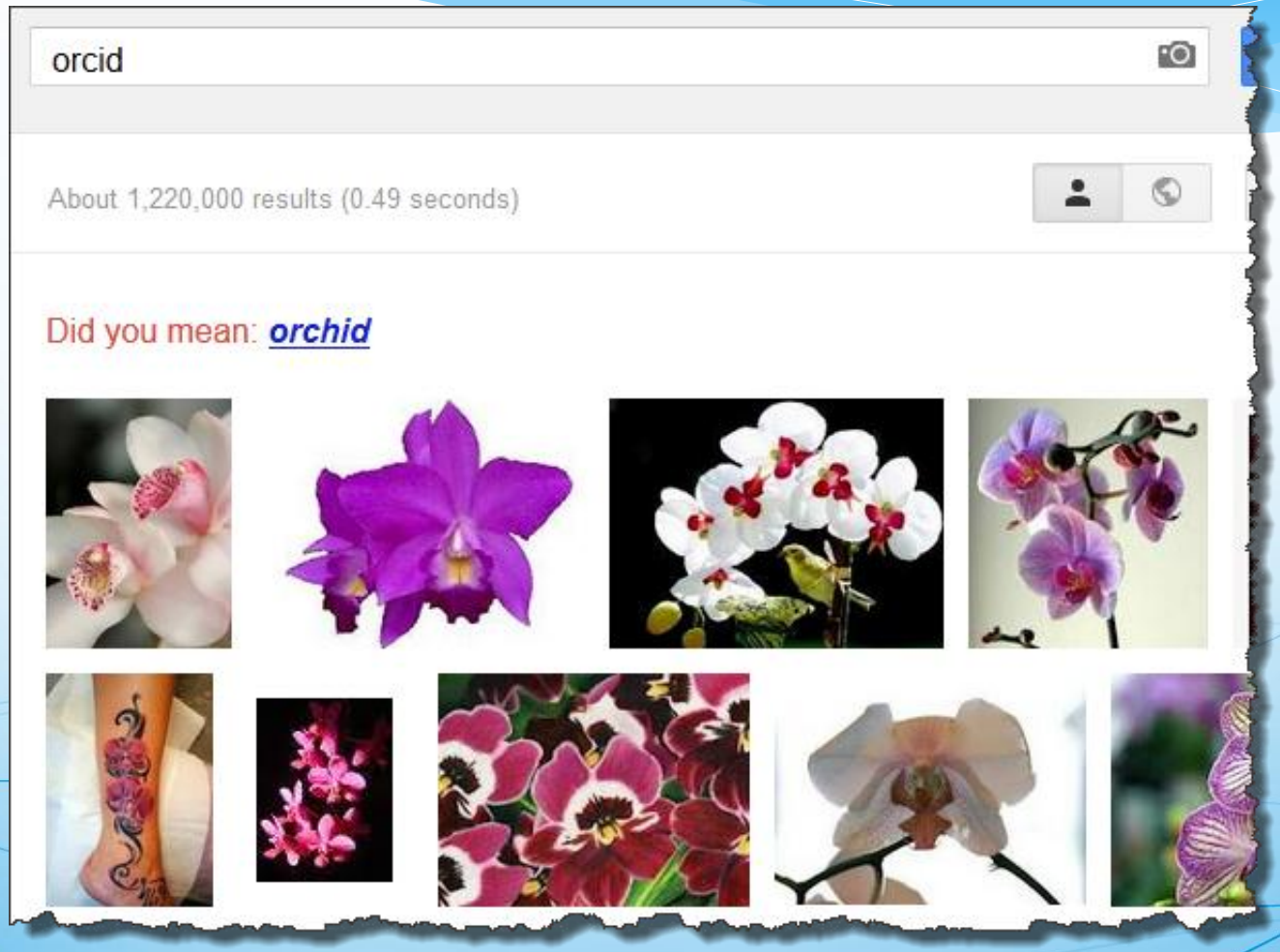
Title / Author	Cited by	Year
The use of NMR to study sodium dodecyl sulfate-gelatin interactions DD Miller, W Lenhart, BJ Antalek, AJ Williams, JM Hewitt Langmuir 10 (1), 68-71	56	1994
X-Ray Crystallographic, Single-Crystal EPR, and Theoretical Study of Metal-Centred Radicals of the Type [5C5R5Cr(CO)2L] (R = H, Me; L = CO, tertiary phosphine) S Fortier, MC Baird, KF Preston, JR Morton, T Ziegler, TC Jaeger, WC Watkins ... Journal of American Chemical Society 113 (2), 542–551	52 *	1991
Internet-based tools for communication and collaboration in chemistry AJ Williams Drug discovery today 13 (11), 502-506	49	2008

Scientists and Orcids?



ORCID Open Researcher & Contributor ID

* A unique identifier for a scientist – a Scientists InChI !
* Will enable aggregation of a scientists activities
* ORCIDs associated with publications, data, blog comments, other contributions (Wikipedia, reviews etc.) will be a way to measure their **impact**

The Alt-Metrics Manifesto

* http://altmetrics.org/manifesto/

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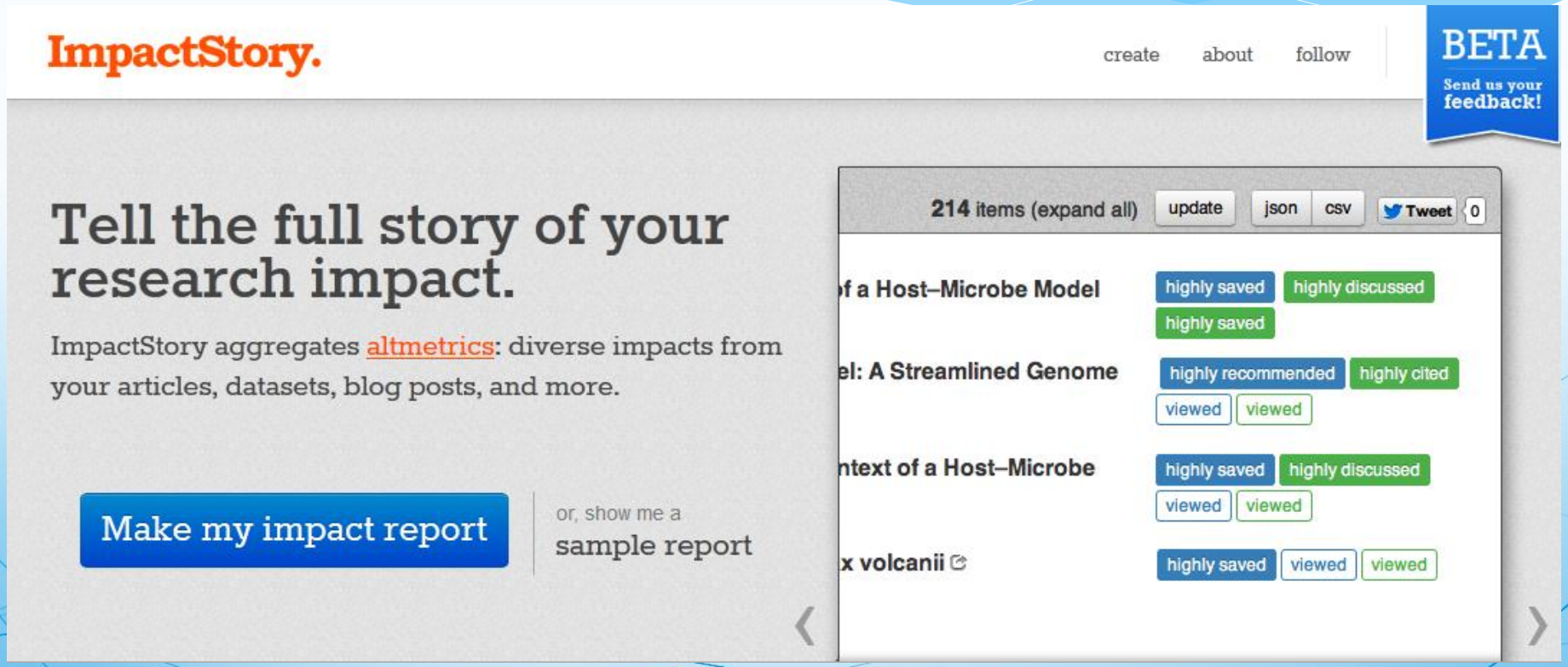

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Analysis and elimination of artifacts in indirect covariance NMR spectra via unsymmetrical processing

(2005) Blinov, Larin, Kvasha et al. *Magn. Reson. Chem.*

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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

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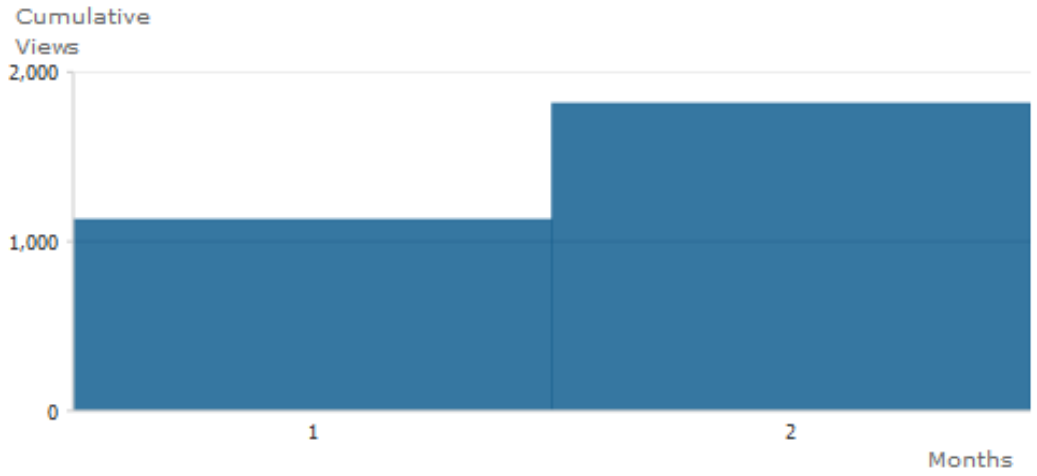
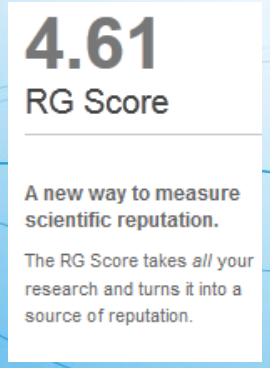
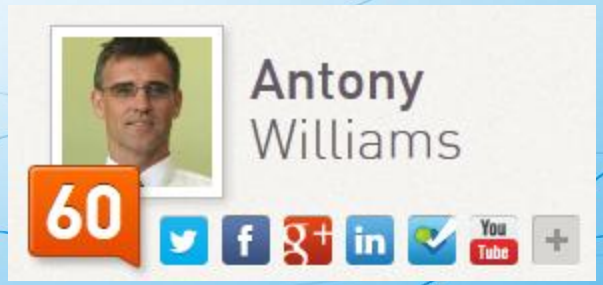


New Measures of Impact

* Impact will be an aggregate measure of
  * Publications – classic measures and article level metrics
  * Data, algorithms and code – and its distribution and reuse
  * Contributions as comments, annotation and curation activities

* New "impact factors" will develop with time





The Challenges

* Some challenges are technology based
  * The growth in data – storage and compute speed
  * Ontologies, dictionaries and trusted sources
* Many challenges are “about us”
  * Licenses and rights
  * Rewards and recognition
  * Participation, contribution and **collaboration**

Tear Down Walls between Government Labs

* There are many government institutions building public compound databases that should collaborate more:
  * National Cancer Institute (NCI)
  * National Institutes of Health (NIH)
  * Environmental Protection Agency (EPA)
  * Food and Drug Administration (FDA)
  * National Library of Medicine (NLM)

NCATS National Center for Advancing Translational Sciences

Discovering New Therapeutic Uses for Existing Molecules

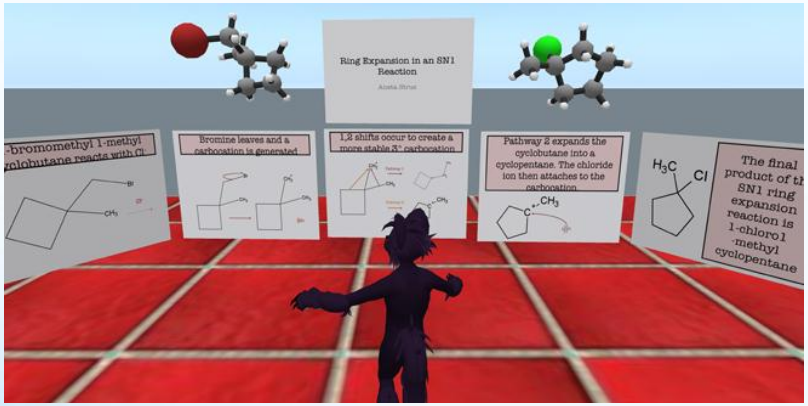
Discovering New Therapeutic Uses for Existing Molecules is a collaborative pilot program designed to develop partnerships between pharmaceutical companies and the biomedical research community to advance therapeutic development.

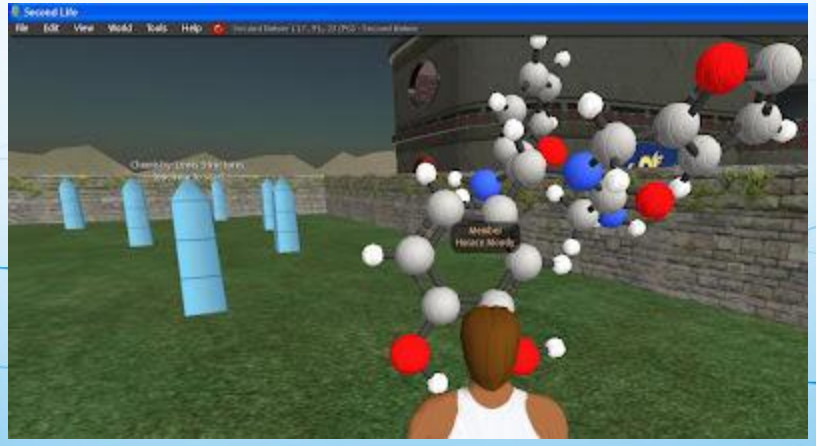
Collectively, these companies have agreed to make 58 of these compounds available for the pilot program. The compounds have undergone significant research and development by industry, including safety testing in humans, providing a strong starting point for scientists and permitting the process to move more rapidly.

Release STRUCTURES Please!

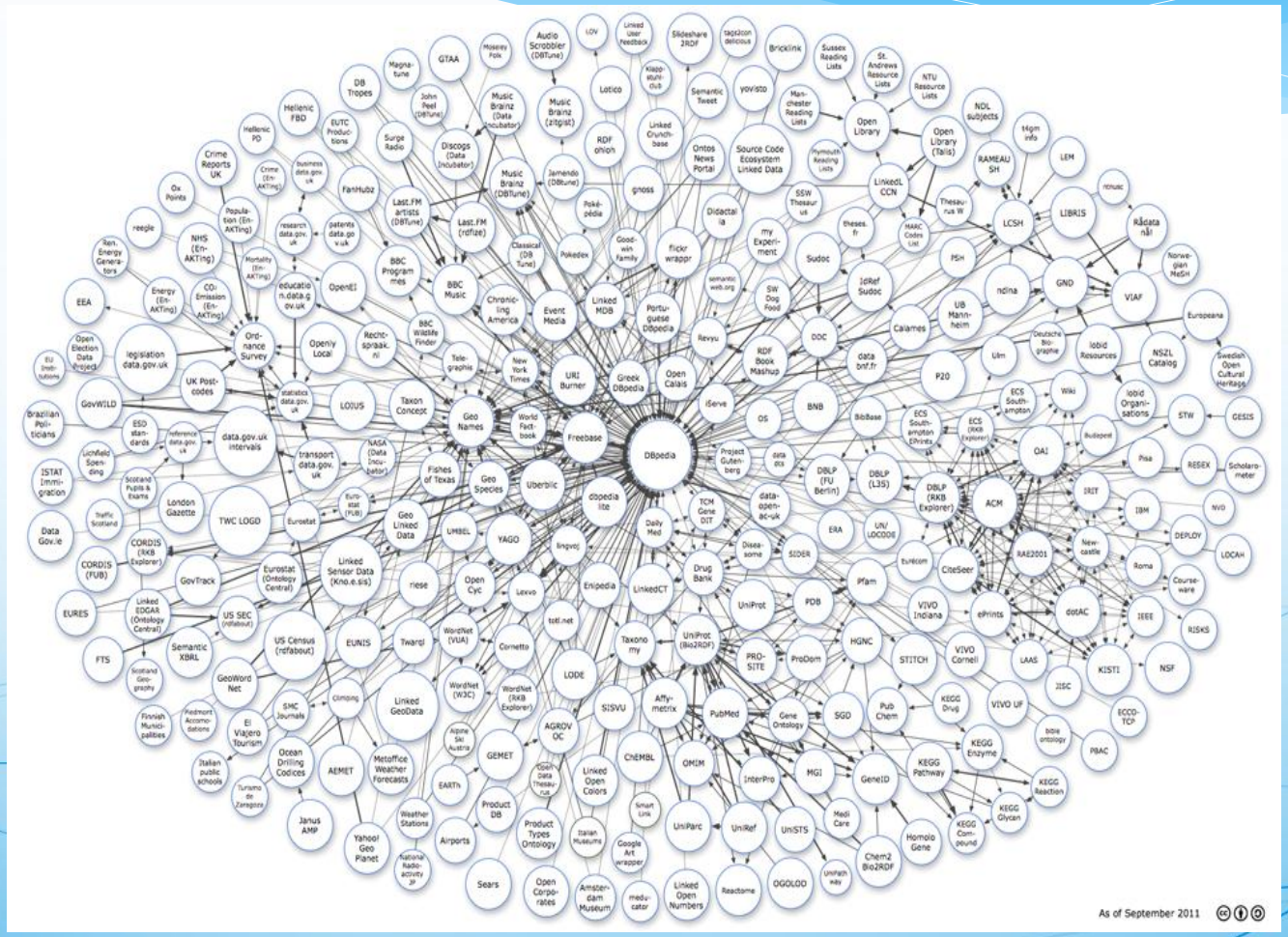
Code Number & Link to More Information	Mechanism of Action	Original Development Indication(s)
AVE5530 canosimibe	Acyl-coenzyme A:cholesterol O-acyltransferase (ACAT) inhibitor Cholesterol absorption inhibitor	Hypercholesterolemia
SSR149744C celivarone	Anti-arrhythmic, Vaughan Williams Class I to IV	Maintenance of sinus rhythm in atrial fibrillation patients Prevention of shocks and major clinical outcomes in patients with implanted cardiac defibrillator
PF-05416266 senicapoc (ICA-17043)	Calcium-activated potassium channel blocker (KCa3.1), intermediate-conductance	Sickle cell disease Asthma
ABT-639	Calcium channel, voltage-gated (Cav3.2, T-type) blocker	Pain

What Does the Future Hold?

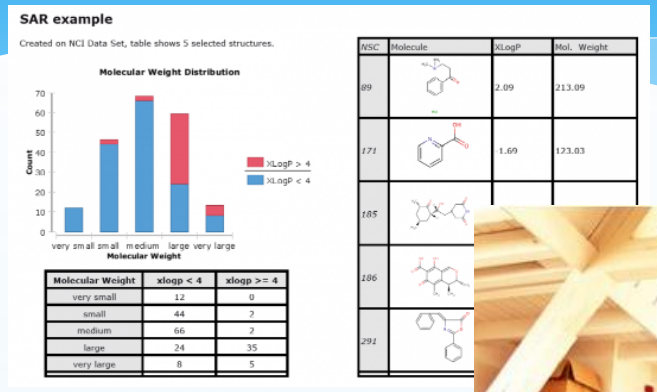


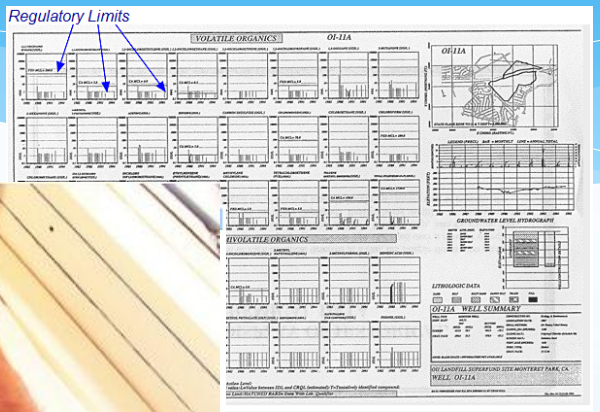


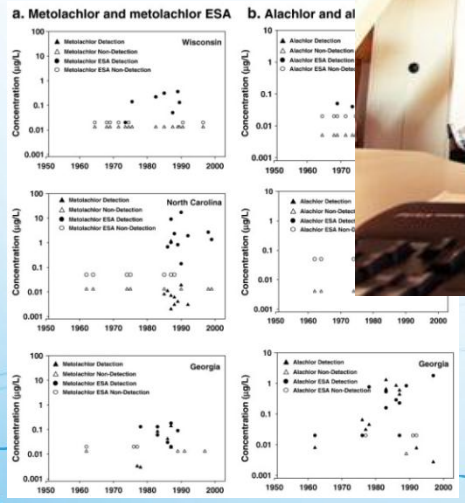
The Linked Network Will Grow

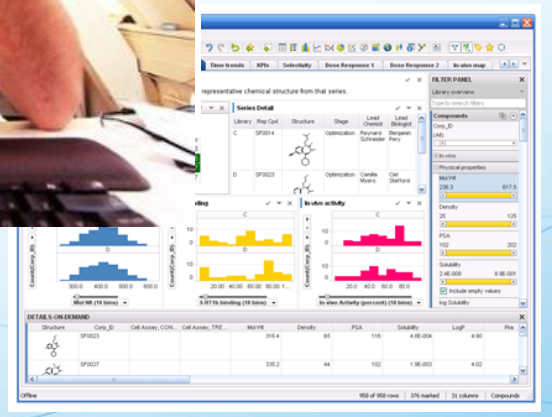


The Data Deluge Will Not Go Away





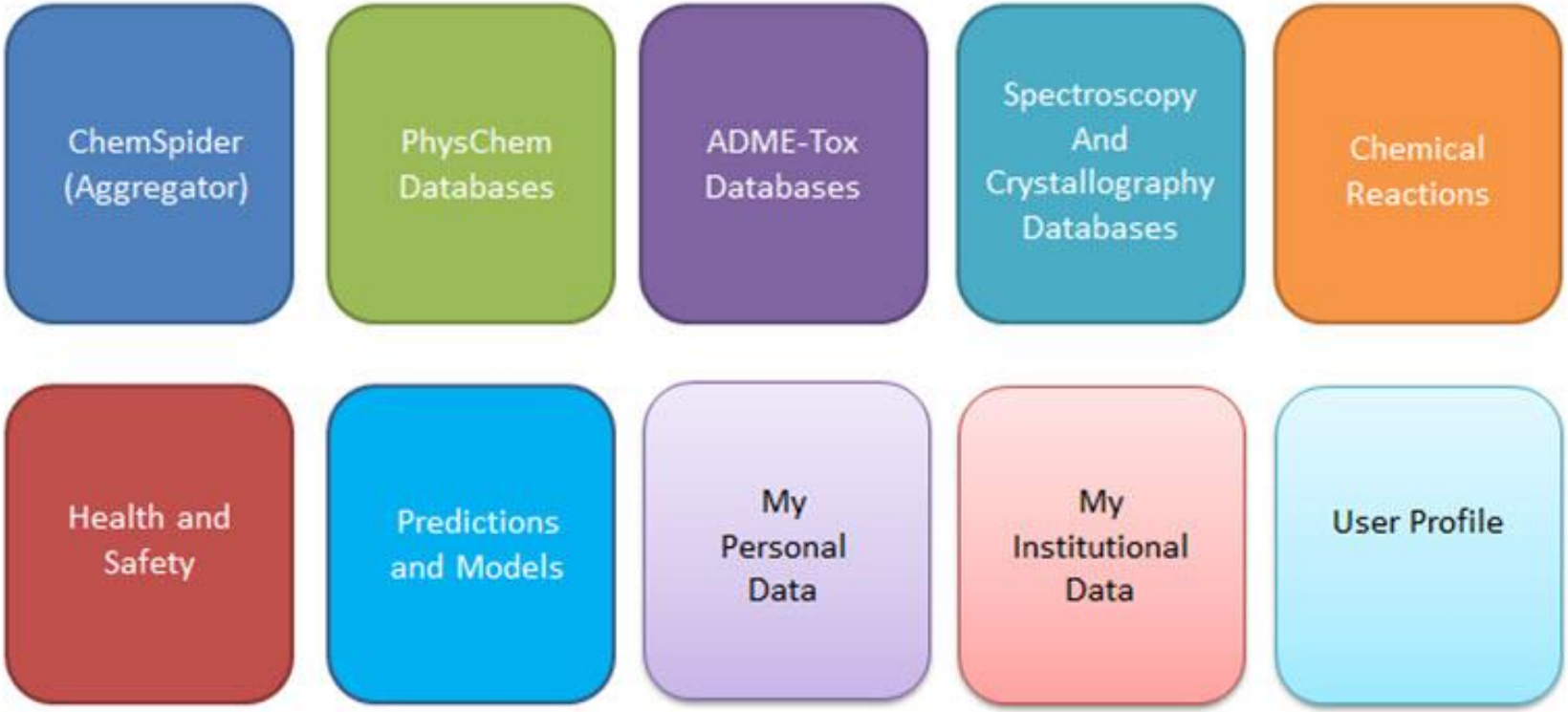




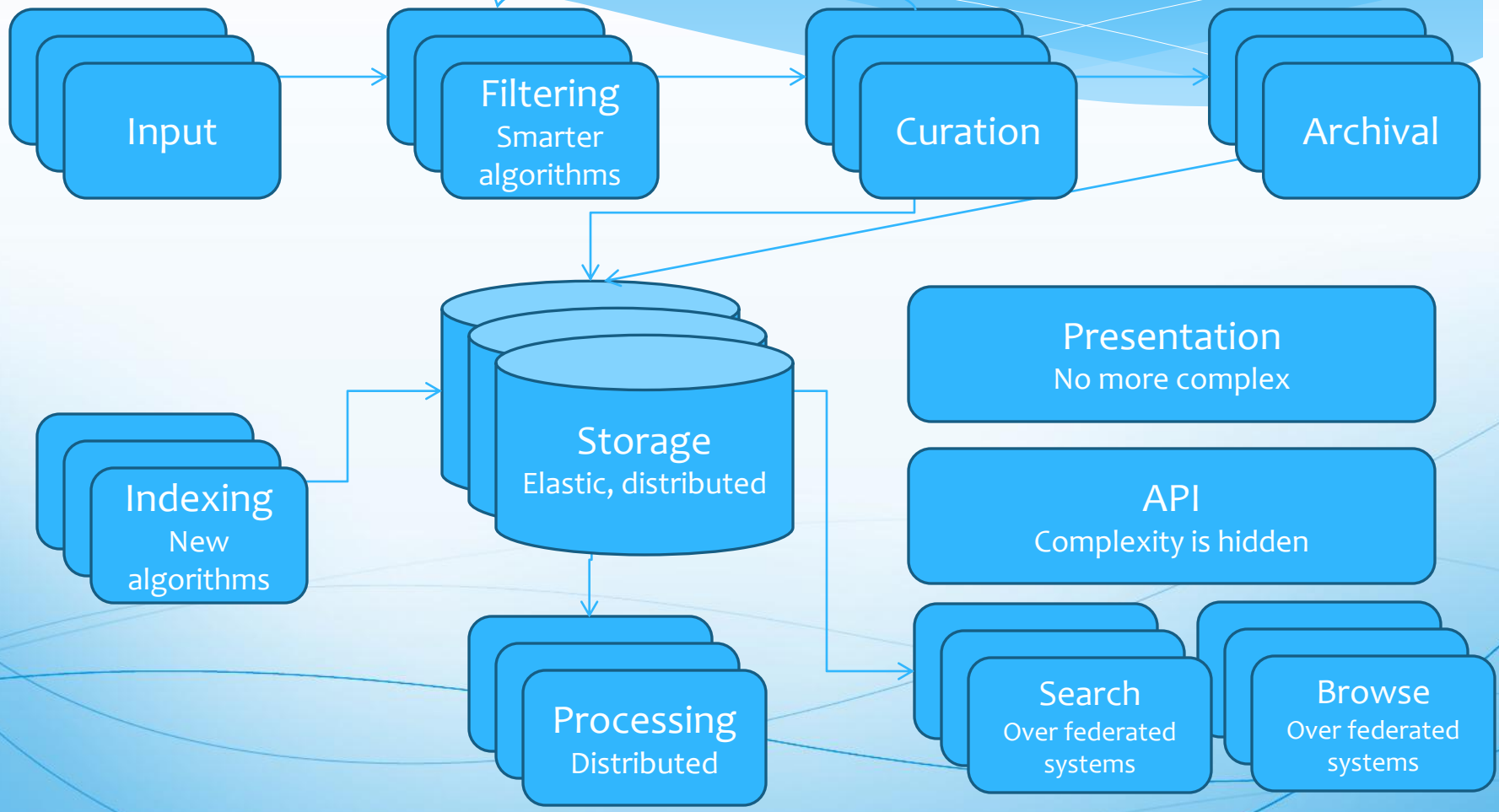
RSC Activities in Development

* Deliver a Global Chemistry Hub
* "Data enable" the RSC archive back to 1841:
  * Extract chemistry – chemicals, reactions, experimental data points, complex data
  * Enrich the articles for interactive viewing and crowdsourced annotation and curation
  * Enhance queries possible across the archive

Federated Data Segregation



Future System Architecture



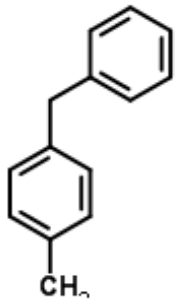
Data Validation is Exacting Work

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



“Challenge” the Community

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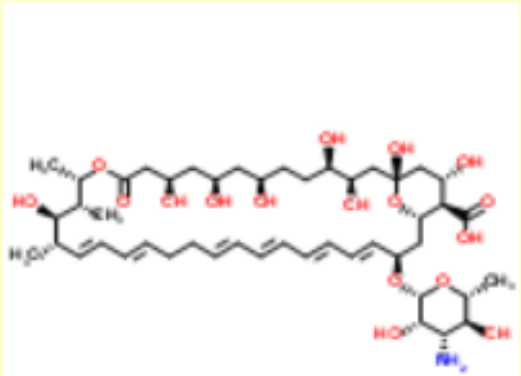

- 19/19 defined

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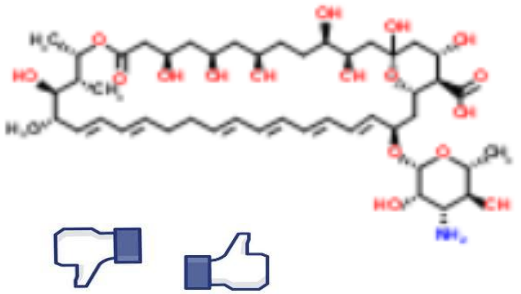


- 19/19 defined

Chemistry Data at RSC

* Chemistry is **NOT** just small molecules!
* Data in RSC publications will be "enabled"
* Data available for validation and curation
* The delivery of the "Datument"
* Data will be fed to models for validation, to retrain the models, full provenance retained
* Algorithms will be provided to the community

Enhanced Mark-Up?

Experimental

General comments

All extractions were carried out in a closed system consisting of a Soxhlet extractor equipped with a chilled condensor (-4°C). Benzene was determined to be an efficient extraction solvent and was easily recaptured and reused. The extraction apparatus was fitted into a large walk-in hood to ensure safe ventilation of any benzene vapor that might escape from the extraction unit. For the first flash chromatography separation, Fisher 70–230 mesh silica gel with a 60 Å pore size was used; the second chromatographic step employed J.T. Baker 40 μm silica gel flash chromatography packing with a 60 Å pore size. The progress of each separation was followed by TLC on 5 × 10 cm, 250 μm TLC plates (EMD Chemicals, Darmstadt, Germany) using EtOAc-isopropanol-NH_4OH, 80:14:1 (rf of cyclopamine 0.24). After develo… by staining with phosphomolybdic acid.

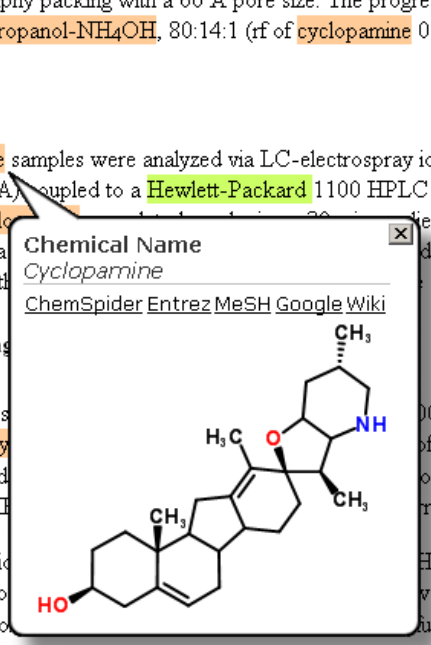
HPLC-MS

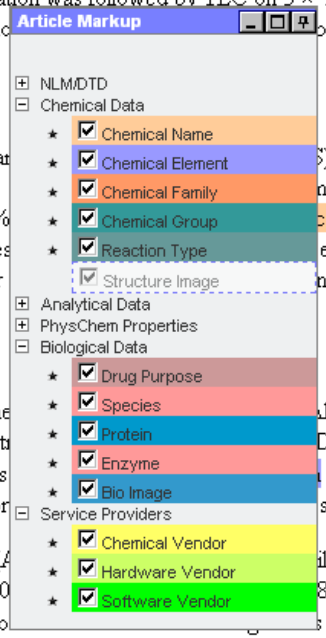
Cyclopamine samples were analyzed via LC-electrospray ionization (ESI)-tan… S) on a quadrupole ion trap mass spectrometer (LCQ Classic, Thermo-Finnigan, San Jose, CA) coupled to a Hewlett-Packard 1100 HPLC system. A 1.2 × … n C-18 reversed-phase LC column (Waters Corporation, Milford, MA) was utilized. Cyclo… ient starting at 10% … c acid to 70% acetonitrile, 0.2% aqueous formic acid with a flow rate of 100 μL/min and a… d between samples … ectra were also obtained either on a Waters Micromass ZQ Mass detector equipped with… array detector or … ntum equipped with an Agilent 1100 series HPLC system.

Nuclear mag…

Initial NMR s… 00 MHz spectrome… lto, CA) equipped with a 5 mm indirect detect z-gradient probe in 700 μL deuteromethy… of the proton spectr… DQCOSY experiment acquired in the phase-sensitive mode. The chemical shifts of unresolved… of the cross-peaks … resonances were made using gradient versions of multiplicity-edited HSQC, and gradient HM… relations. Some pr… stereochemical relationships were established by employing NOESY.

High-resolutio… Hz spectrometer (A… illerica, MA) equipped with a triple-resonance, z-gradient cryogenic probe (5 mm TCI Cryopro… was dissolved in 60… 8°K. In addition to standard proton and carbon spectra, a number of two-dimensio… ully assign the reso… s were aided by gradient phase-sensitive, DQCOSY spectra and gradient phase-sensitive NOESY spectra. Heteronuclear correlations were determined by using gradient multiplicity-edited, sensitivity-enhanced HSQC correlation spectroscopy, and long-range correlations were determined using gradient HMBC. Multiplicity (CH_n, n = 0–3) was confirmed through one-dimensional DEPT pulse sequences. Spectra were processed using the instrument software (TopSpin, Bruker Biospin, Inc.), and analysis was conducted using iNMR (Nucleomatica, Molfetta, Italy; http://www.inmr.net webcite), a computer program designed to aid in resonance assignments.





An Error in my Abstract?

An Error in my Abstract?

Chemists have embraced the web as a rich source of data and knowledge. However, all that glisters is not gold

Thanks Shakespeare

All that glitters is not gold

From Wikipedia, the free encyclopedia

For other uses, see All That Glitters (disambiguation).

All that glitters is not gold is a well-known saying, meaning t

The Merchant of Venice, which employs the word "glisters,"

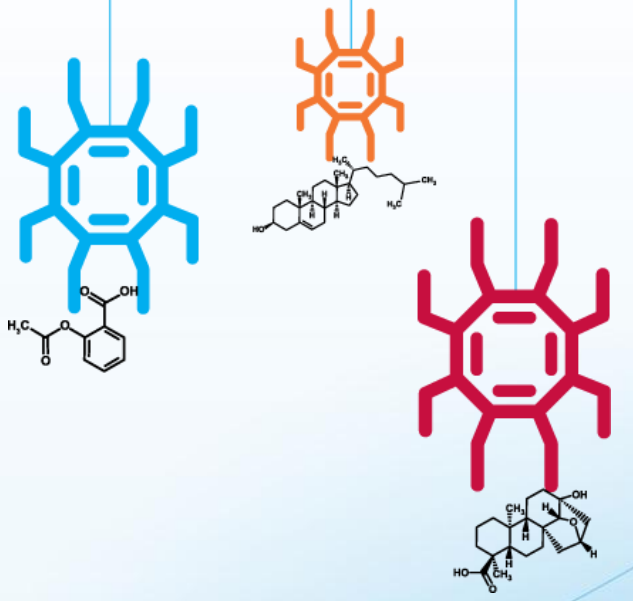
Acknowledgments

* RSC and RSC|Cheminformatics team
* All data source providers, curators and annotators
* All software providers: commercial and open source
* Contributors, curators, collaborators

* Trusted Advisors: Jean-Claude Bradley, Sean Ekins, Lee Harland, Gary Martin, Martin Walker and…

Meet Valery…
We'd love to chat…

Thank you



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