How Internet Resources Are Providing a Collaborative Community for Chemistry

60 slides in 20 minutes

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Imagine a time when ….

- The internet is searchable by chemical structure and substructure (e.g.Wikipedia, Google Scholar)
- Chemistry articles are indexed and searchable by a free online service
- The web is linked together through the “language of chemistry”

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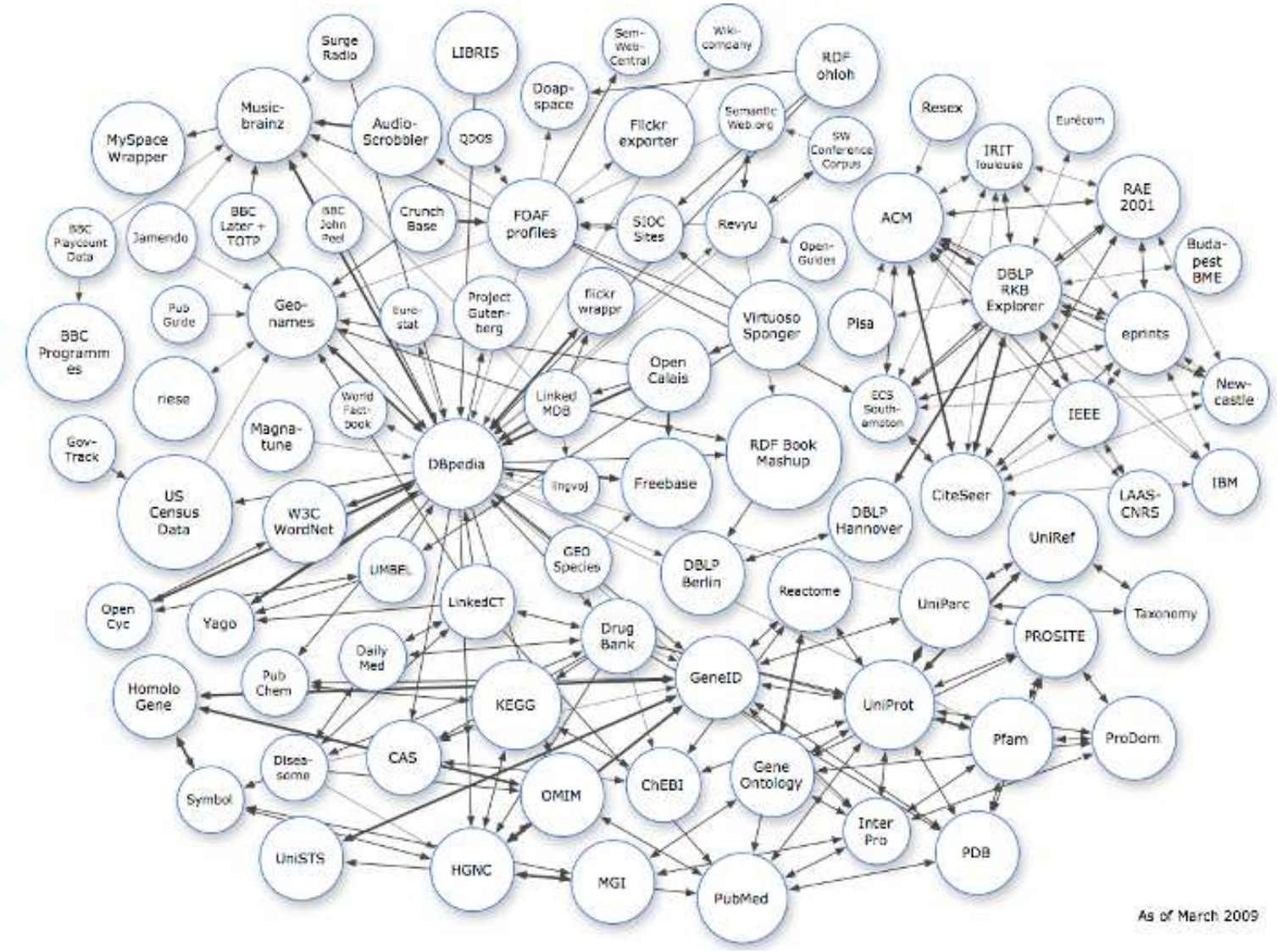
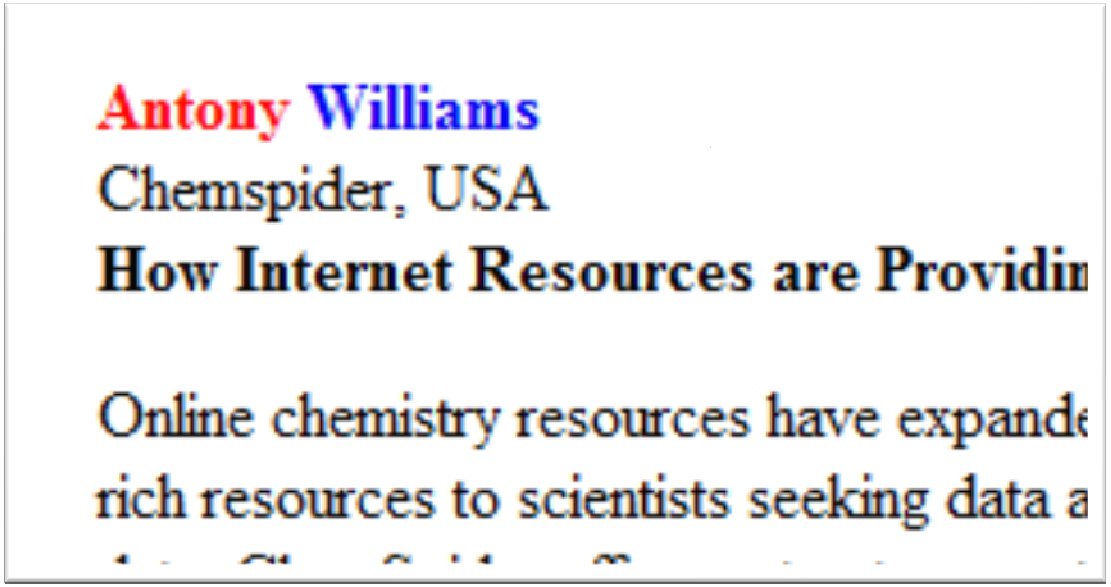
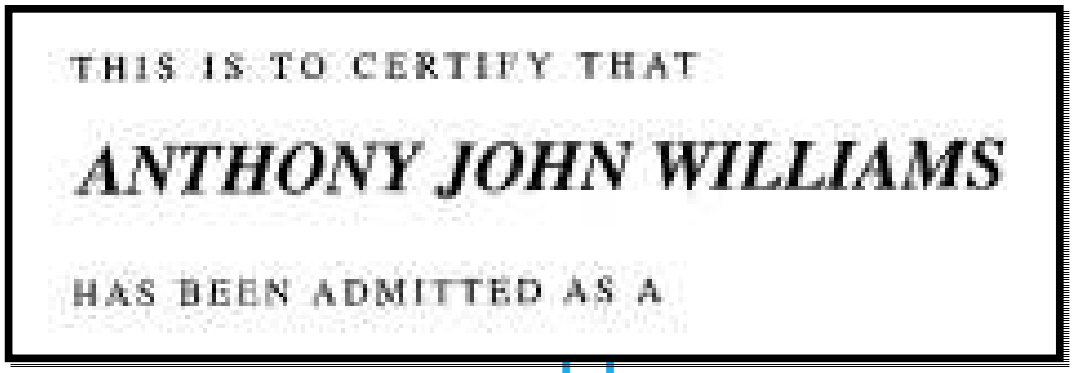
It's Coming…Linked Data Cloud



Thanks to the Organizers…





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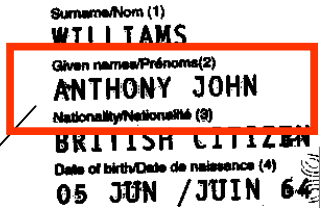
Antony Williams vs Identifiers

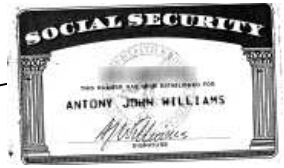
Dad, Tony, others

5 email addresses
ChemSpiderman (blog, Twitter account, Facebook, Friendfeed)
OpenID
….



Passport ID

License



SSN

Green Card

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Aspirin vs Chemical Identifiers

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
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Aspirin names and synonyms

Depositor-Supplied Synonyms: (Total: 335)

aspirin
Acylpyrin
Colfarit
Ecotrin
Acetylsalicylate
ACETYLSALICYLIC ACID
Enterosarein
Acenterine
Polopiryna
Micristin
Acetosal
Acetosalic acid
2-Acetoxybenzoic acid
Enterosarine
Acetophen
Acetosalin
Acetylsal
Aspirdrops
Bialpirina
Clariprin
Entericin
Enterophen

- Text searches depend on correct association
- **335** suggested identifiers for Aspirin just on PubChem!
- Disambiguation dictionaries are necessary

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CHEMISTRY SPECIAL ISSUE

INFORMATION RETRIEVAL FACILITY NEWSLETTER

The Science and Industry Platform for a Sustainable Innovation Cycle

Issue #2 | October 2009

CHEMICAL PATENT SEARCHES IN FREE ONLINE DATABASES

How reliable are free online tools for an exhaustive patent search?
A small case study illustrates the shortcomings faced by chemical patent searchers.

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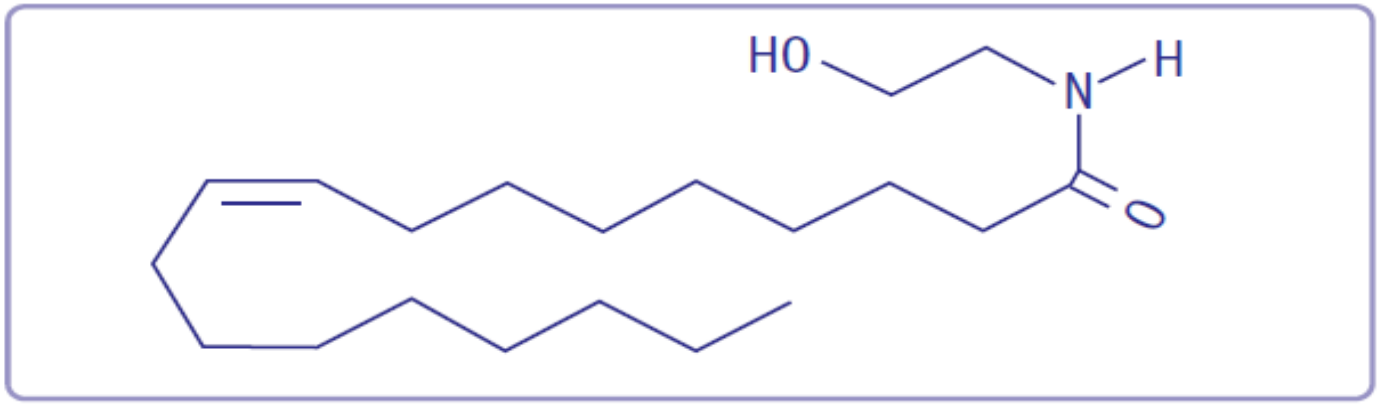
What is a good strategy to search for chemical compounds? We compared various free online databases and search engines for N-oleoylethanolamine (OEA, CAS Registry Number 111-58-0), a very interesting compound and the Nature "lipid of the month June 2009". OEA has been found to induce satiety and decrease 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.



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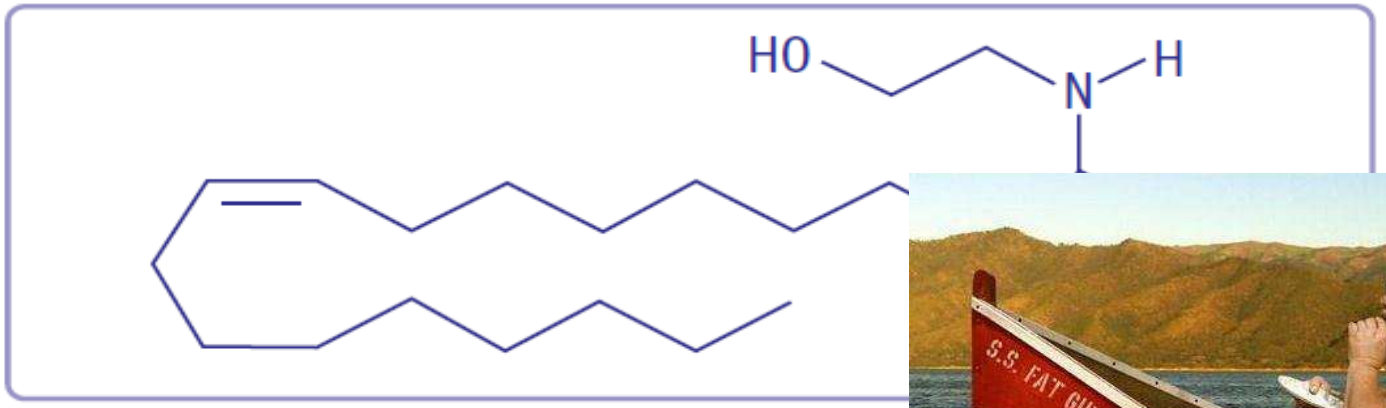

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The Final Search Strategy

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")

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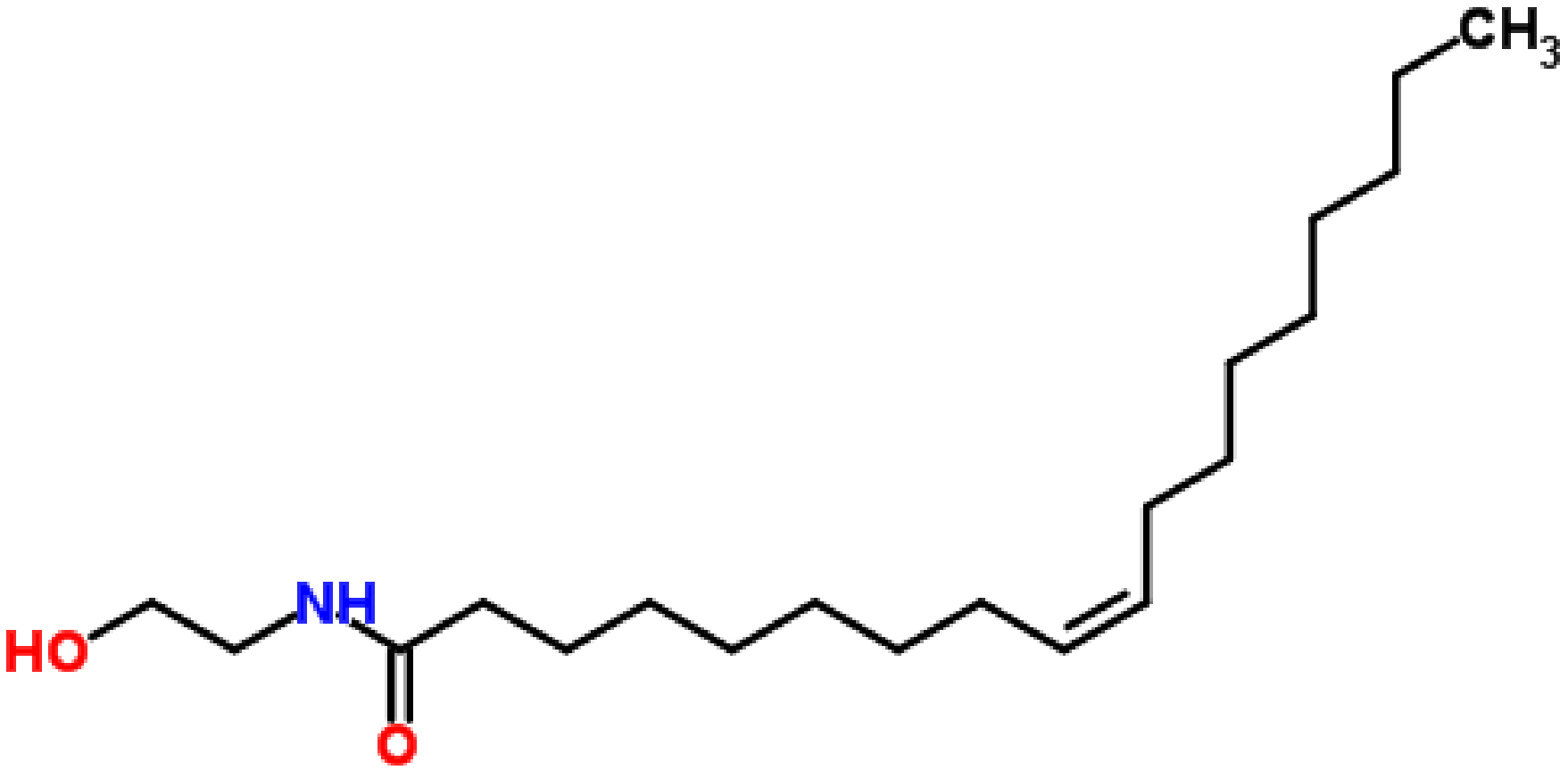
All Those Names, One Structure



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Searching Chemistry on the **Internet**

- How complete a result set will we get if we search for “chemicals” by name?
- Is there a better way to link chemistry databases? Linking by “names” is dangerous
- Chemists want structure and SUBstructure searching

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The InChI Identifier

International Chemical Identifier

From Wikipedia, the free encyclopedia

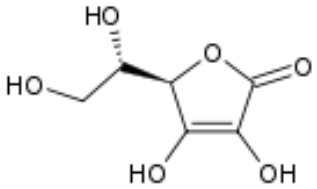
(Redirected from InChI)

The **IUPAC International Chemical Identifier** (**InChI**, pronounced "INchee") is a textual identifier for chemical substances, designed to provide a standard and human-readable way to encode molecular information and to facilitate the search for such information in databases and on the web. Developed by IUPAC and NIST during 2000-2005, the format and algorithms are non-proprietary and the software is freely available under the open source LGPL license (though the term "InChI" is a trademark of IUPAC).[1]

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

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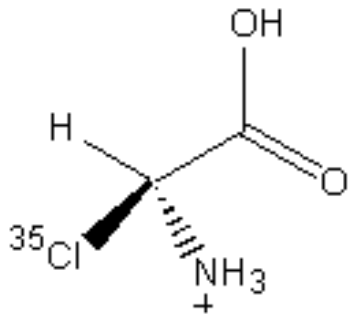
Multiple Layers



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

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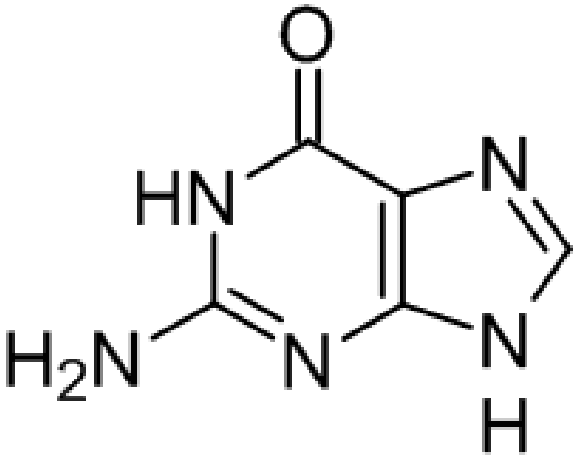
InChIStrings Hash to InChIKeys



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

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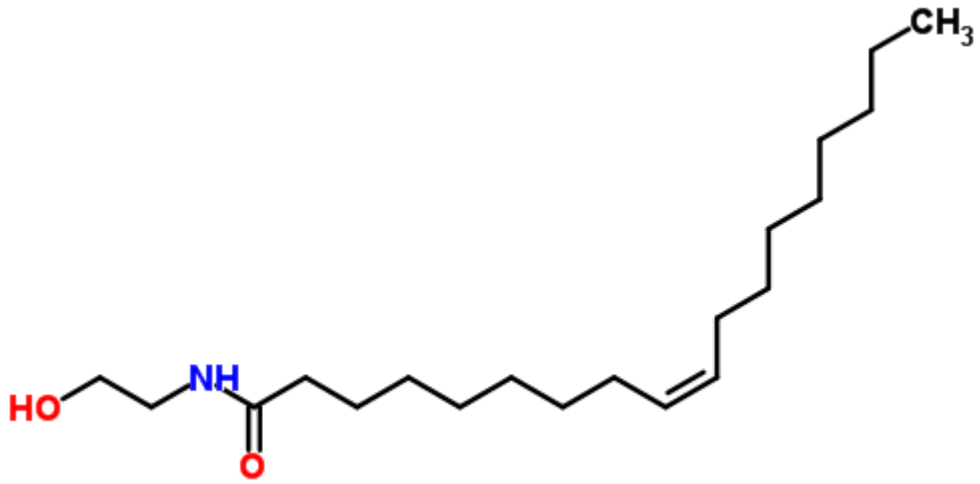
Oleoylethanolamine



InChI=1S/C20H39NO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20(23)21-18-19-22/h9-10,22H,2-8,11-19H2,1H3,(H,21,23)/b10-9-

BOWVQLFMWHZBEF-KTKRTIGZSA-N

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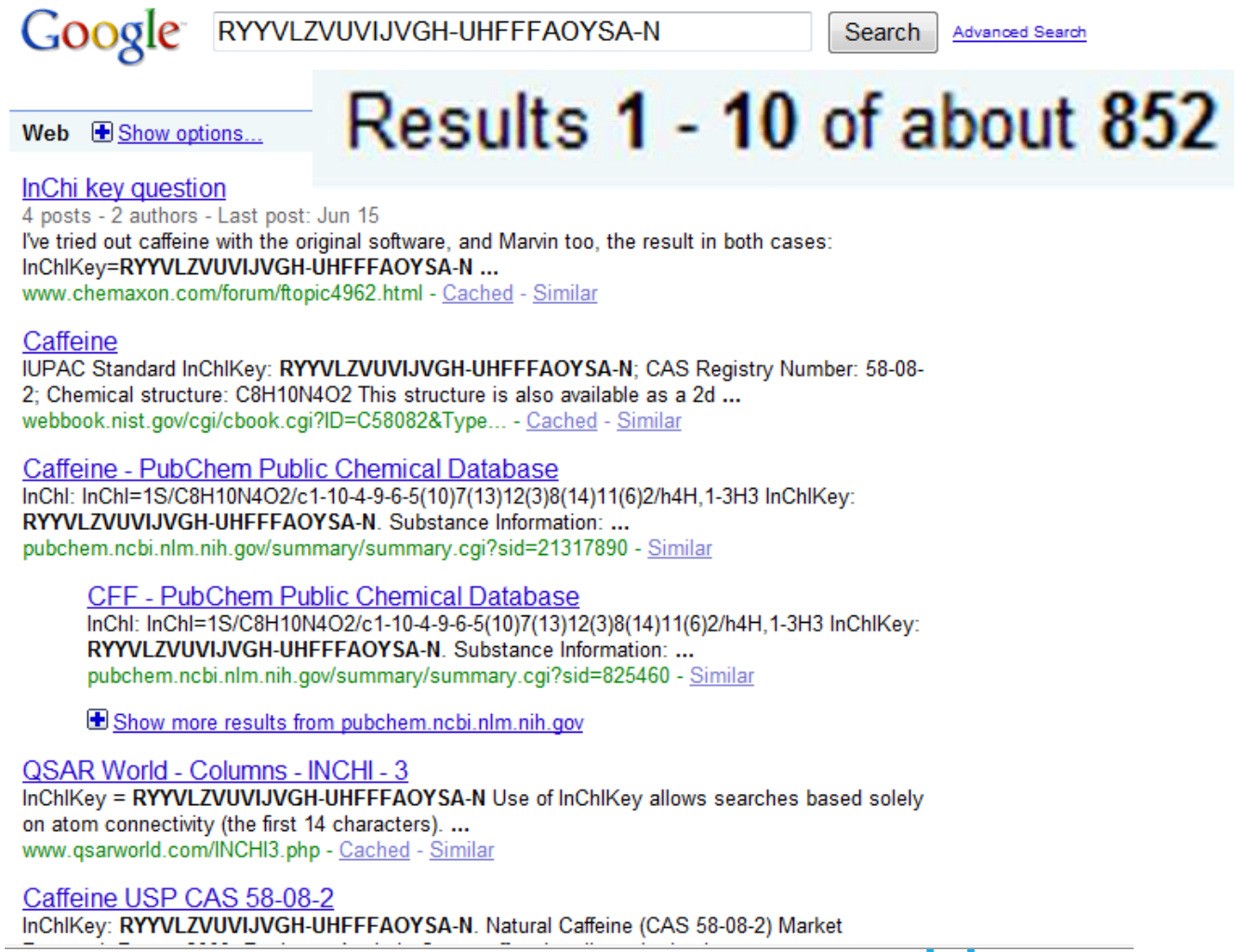
Search Engine Dependencies



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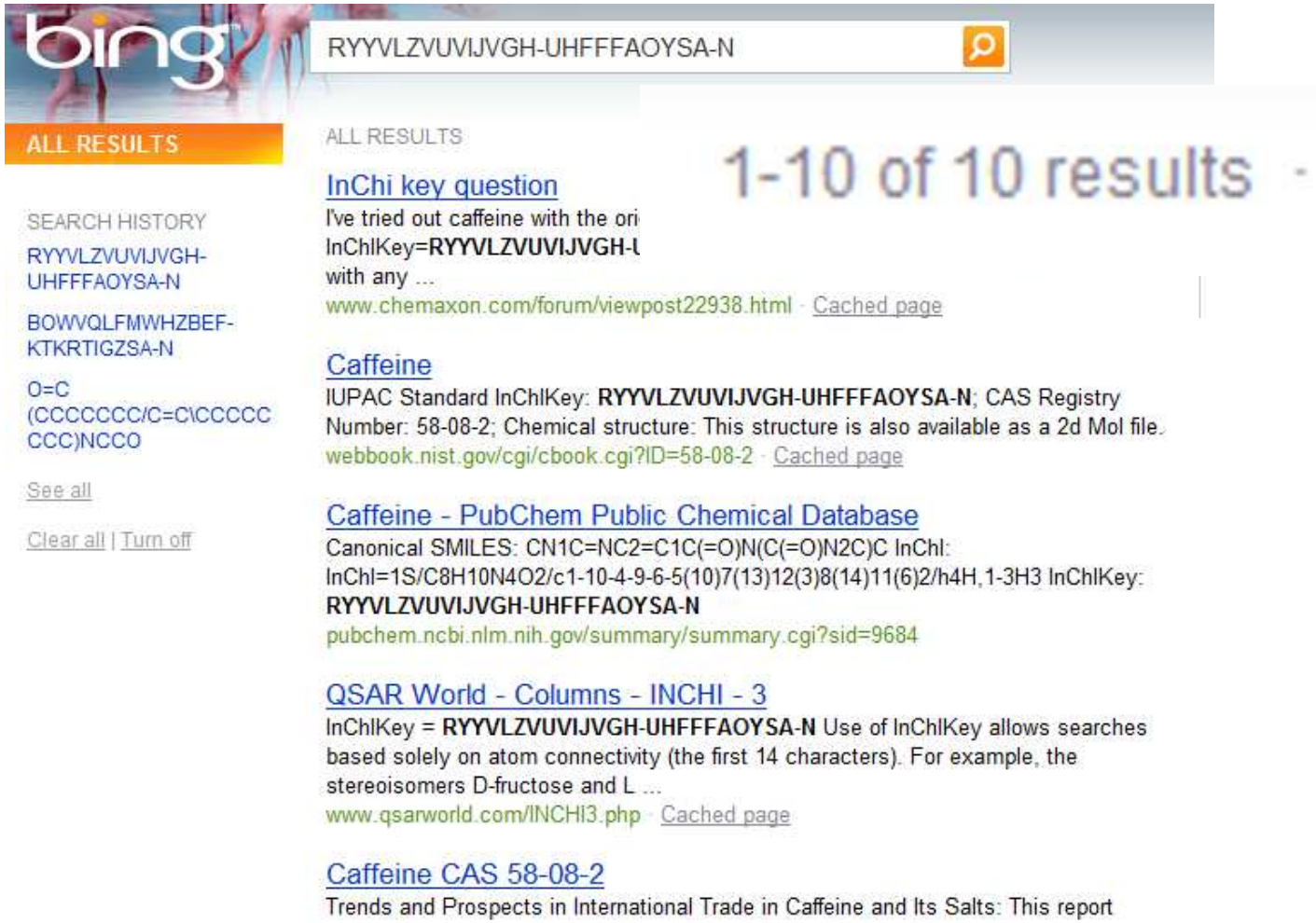
Search Engine Dependencies



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InChIs have traction…

At Last! URIs for InChI

The info registry has now added in the InChI namespace (see registry entry here) which now means that chemical compounds identified by InChIs (IUPAC's International Chemical Identifiers) are expressible in URI form and thus amenable to many Web-based description technologies that use URI as the means to identify objects, e.g. XLink, RDF, etc. As an example, the InChI identifier for naphthalene is

InChI=1/C10H8/c1-2-6-10-8-4-3-7-9(10)5-1/h1-8H

and can now be legitimately expressed in URI form as

info:inchi/InChI=1/C10H8/c1-2-6-10-8-4-3-7-9(10)5-1/h1-8H

info:inchi/

info-namespace	inchi
namespace-title	Namespace for IUPAC International Chemical Identifiers (InChI)
registration-date	2007-02-19
namespace-authority	

organisation-name	IUPAC
organisation-address	IUPAC Secretariat, P.O. Box 13757, Research Triangle Park, NC 27709

RDF Linking of Structures

OpenMolecules RDF

About http://cb.openmolecules.net/rdf/?InChI=1/CH4/h1H4

Identifier info:inchi/InChI=1/CH4/h1H4
InChI InChI=1/CH4/h1H4

Source Chemical blogspace
Blog Discussion http://chem-bla-ics.blogspot.com/2008/09/ubiquity-fun-entering-semantic-markup.html
Blog Discussion http://chem-bla-ics.blogspot.com/2007/09/tagging-molecules-mashup-of-connotea.html
PubChem CID 297
Name methane

Source ChEBI
Identifier CHEBI:17620

Bookmark this on del.icio.us

RDF Powered

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PubChem

PubChem

From Wikipedia, the free encyclopedia

PubChem is a database of chemical molecules. The system is maintained by the National Center for Biotechnology Information (NCBI), a component of the National Library of Medicine, which is part of the United States National Institutes of Health (NIH). PubChem can be accessed for free through a web user interface. Millions of compound structures and descriptive datasets can be freely downloaded via FTP. PubChem contains substance descriptions and small molecules with fewer than 1000 atoms and 1000 bonds. The American Chemical Society tried to get the U.S. Congress to

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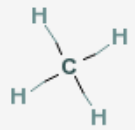
The Simplest Organic Molecule

Charcoal - Compound Summary (CID: 297)

An amorphous form of carbon prepared from the incomplete combustion of animal or vegetable matter, e.g., wood. The activated form of charcoal is used in the treatment of poisoning. (Grant & Hackh's Chemical Dictionary, 5th ed)

Table of Contents

- Drug and Chemical Information
  - Pharmacological Action
  - Pharmacological Classification
  - Chemical Classification
  - Safety and Toxicology
  - Literature Links
  - Literature Mining
- Synonyms
- Properties
- Descriptors
- Compound Information
- Substance Information
  - Category
- Exports



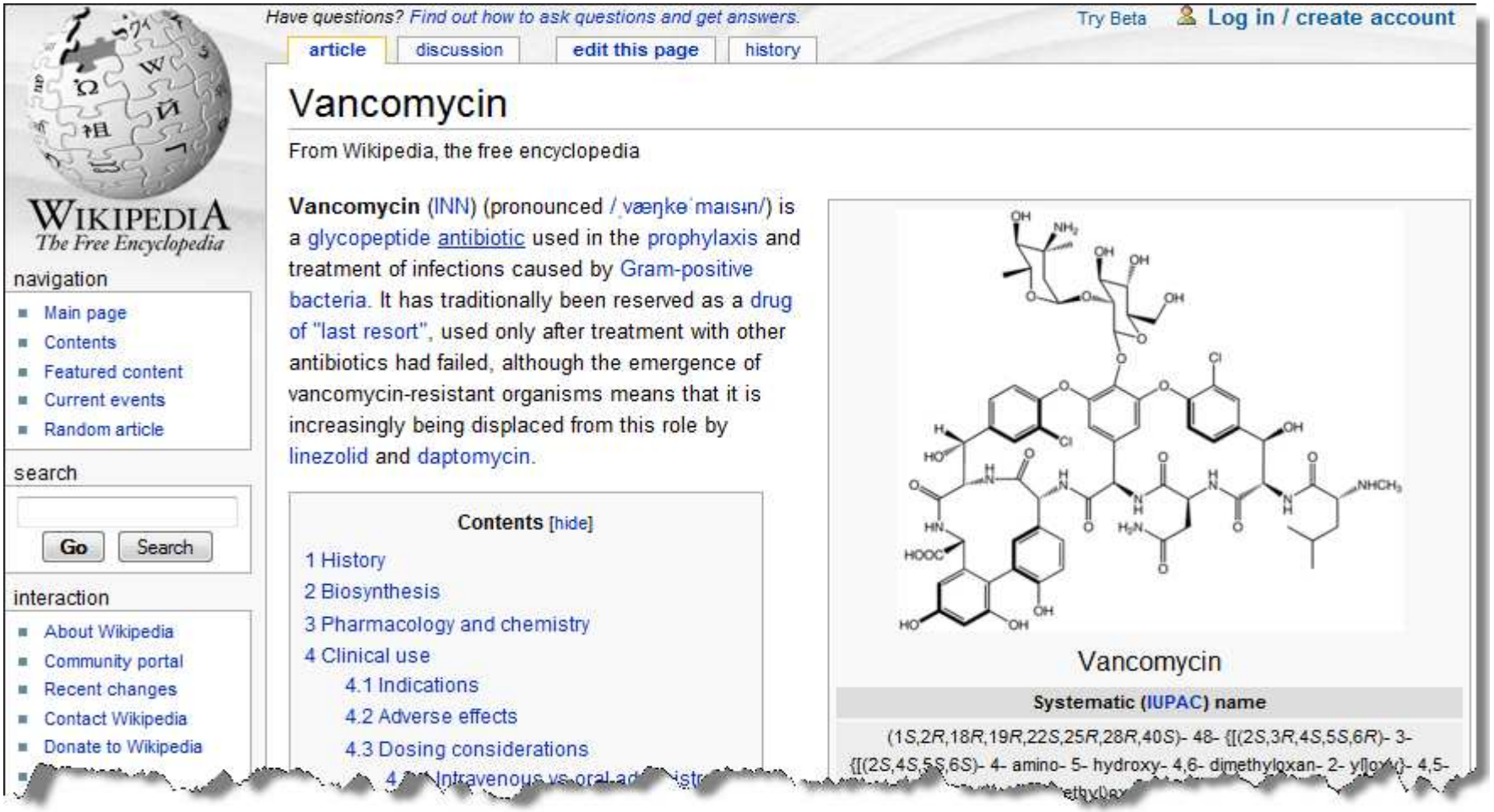
Compound ID	**297**
Molecular Weight	16.04246 [g/mol]
Molecular Formula	CH_4
H-Bond Donor	0
H-Bond Acceptor	0

Plumbago (graphite)
Carbon-12
Philblack N 550
Philblack N 765
DIAMOND
Monarch 700
Witcarb 940
Graphite (synthetic)
Irgalite 1104

METHANAL, OXOMETHANE, OXYMETHYLENE, METHYLENE OXIDE, FORMIC ALDEHYDE, METHYL ALDEHYDE

1-Chlorobenzylethyl-3,5,7,9,11,13,15-heptaisobutylpentacyclo[9.5.1.1(3,9).1(5,15).1(7,13)]octasiloxane, mixture of isomers

Vancomycin



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From Wikipedia, the free encyclopedia
< Wikipedia:Wikipedia Signpost | 2009-05-18

The Wikipedia Signpost

← CURRENT ISSUE Chemistry data

WikiChemists and Chemical Abstracts announce collaboration

By Physchim62, 16 May 2009

Chemicals – love 'em or hate 'em, but you couldn't live without 'em. Water, glucose and sodium chloride are pretty essential for all of us. Other chemicals make our clothes, or colour them, or provide jobs for millions of workers. Still more chemicals (sometimes the same ones as before) can do us some pretty nasty harm if we're not careful, or degrade the environment for our children and grandchildren. Some chemicals are only really of interest to a professional chemist, or to someone who is easily amused by silly names – arsole, moronic acid and vomitoxin all have Wikipedia articles, after all. But information about chemical compounds is big business, worth several billions of U.S. dollars annually worldwide, and the Chemical Abstracts Service (CAS, a division of the American Chemical Society) is a leading player, "the global leader" as they prefer to put it!

Vinegar like most people have never seen it – crystals of pure acetic acid.

But if there's *something* interesting that can be said about a chemical, then sooner or later *someone* is going to write an article about it... That's why the Chemicals WikiProject slaves away at over five thousand articles about individual chemical compounds (nearly

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Vancomycin

1: CID: 441141

Vancocin; VANCOMYCIN; Vancomycin HCL ...
MW: 1449.253600 g/mol | MF: $C_{66}H_{75}Cl_2N_9O_{24}$
Anti-Bacterial Agents... more

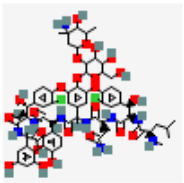
2: CID: 14969

Vancocin; VANCOMYCIN; Vancomycin [USAN] ...
MW: 1449.253600 g/mol | MF: $C_{66}H_{75}Cl_2N_9O_{24}$
Anti-Bacterial Agents... more

3: CID: 14970

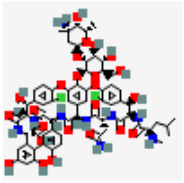
Vancoled; Vancomycin HCL; Vancocin HCL ...
MW: 1485.714540 g/mol | MF: $C_{66}H_{76}Cl_3N_9O_{24}$
Anti-Bacterial Agents... more

4: CID: 6426898



VANCOMYCIN
MW: 1449.253600 g/mol | MF: $C_{66}H_{75}Cl_2N_9O_{24}$
Anti-Bacterial Agents... more

5: CID: 5311496



VANCOMYCIN
MW: 1449.253600 g/mol | MF: $C_{66}H_{75}Cl_2N_9O_{24}$
Anti-Bacterial Agents... more

- Who will curate?
- How would you clean such a large dataset?

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Vancomycin on ChemSpider

Description

Edit

ChEBI article: Vancomycin [CHEBI:28001], a glycopeptide isolated from *Streptomyces orientalis*, inhibits a specific step in the synthesis of the peptidoglycan layer in *Staphylococcus aureus* and *Clostridium difficile*. For over 40 years it has been used to kill bacteria when no other drug works and has become known as the "antibiotic of last resort". However, in recent years vancomycin-resistant enterococci (VRE) have emerged, prompting restrictions in the drug's use. A 3-D representation of the molecule is available here.

The structure elucidation of vancomycin has a long history and this structure on ChemSpider has been confirmed by collaborative efforts between ChemSpider and ChEBI staff (Kirill Degtyarenko).

The crystal structure of vancomycin was determined by Sheldrick et al. (1). Fig. 1 from that paper has been reproduced in the literature a number of times. That diagram shows deprotonated COO- group and two positive charges on nitrogens elsewhere, so that the overall charge is +1. We are interested in an uncharged version of vancomycin. Note the R configuration of the carbamoyl group in the lower central part of Sheldrick's diagram: it is going DOWN. That was corrected in work by Harris et al. (2), diagram 7, where the carbamoyl group is going UP (thus making it part of the L-asparagine residue).

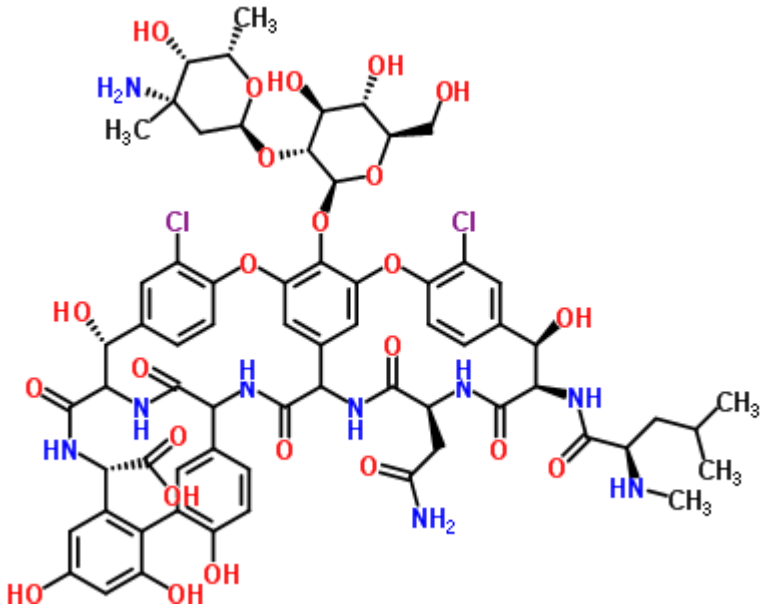
Williamson & Williams (3) looked at the configuration of carboxylate I. See diagram 6 in Williamson & Williams, where it is connected by a wavy bond, and discussed in that paper "These conclusions are summarized in 6, and leave only the stereochemistry at the carbon bearing s1 undetermined in this region. Neither coupling constants (Table II) nor nOe's allow us to distinguish between R and S configurations at the carbon bearing s1. However, the R configuration would require first-order broadening of H, (see 6) in the 1H spectrum of the europium salt of vancomycin; this is not observed, but the data are in good accord with the S configuration."

1) Sheldrick, G.M., Jones, P.G., Kennard, O., Williams, D.H. and Smith, G.A. (1978) Structure of vancomycin and its complex with acetyl-D-alanyl-D-alanine. Nature 271, 223-225. http://dx.doi.org/10.1038/271223a0

2) Harris, C.M., Kopecka, H. and Harris, T.M. (1983) Vancomycin: structure and transformation to CDP-I. J. Am.Chem. Soc. 105, 6915-6922. http://dx.doi.org/10.1021/ja00361a029

3) Williamson, M.P. and Williams, D.H. (1981) Structure revision of the antibiotic vancomycin. Use of nuclear Overhauser effect difference spectroscopy. J. Am.Chem. Soc. 103, 6580-6585. http://dx.doi.org/10.1021/ja00412a008

Vancomycin



Std. InChIKey: MYPYJXKWCTUITO-LYRMYLQWSA-N

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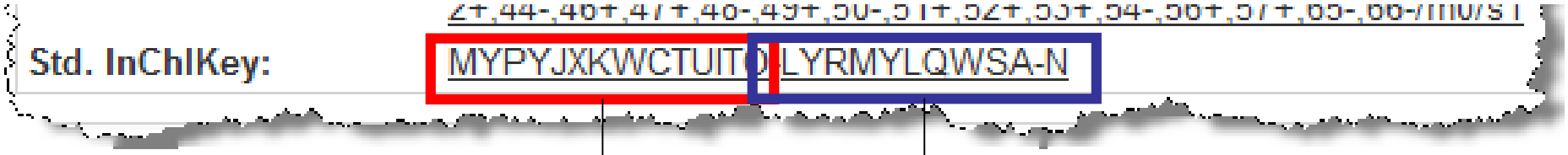
Vancomycin



Search Molecular SKELETON

Search Full Molecule

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Full **Skeleton** Search: 104 Hits

vancomycin (CHEBI 28001)
Jul 24, 2008 ... InChIKey. InChIKey=**MYPYJXKWCTUITO**-GOYUGWFFDN. InChIKey=**MYPYJXKWCTUITO**-GOYUGWFFDN. SMILES ...
www.ebi.ac.uk/chebi/searchId.do?chebiId=28001 - Cached - Similar -

DrugBank: Showing Vancomycin (DB00512)
Feb 19, 2009 ... InChI Key, **MYPYJXKWCTUITO**-RBHQQIGCDM. KEGG Drug, D00212 Link Image. KEGG Compound, C06689 Link Image. PubChem Compound, 441141 Link Image ...
www.drugbank.ca/drugs/DB00512 - Cached - Similar -

Vancomycin - PubChem Public Chemical Database
...,48+,49?,50-,51+,52+,53+,54-,56+,57+,65-, 66-/m0/s1 InChIKey: **MYPYJXKWCTUITO**-UTHKAUQRSA-N. Substance Information: ...
pubchem.ncbi.nlm.nih.gov/summary/summary.cgi?sid=8914 - Similar -

Vancomycin CAS 1404-90-6
InChIKey: **MYPYJXKWCTUITO**-LYRMYLQWSA-N. Sterile Vancomycin HCL (CAS 1404-93-9) Market Research Report 2009: Business Analytic Center offers its clients ...
www.chemicalregister.com/Vancomycin/.../pid35484.htm - Cached - Similar -

Ligand Depot Graph Search Summary
InChIKey descriptor, **MYPYJXKWCTUITO**-JIUMHQLRDL. Status Information. Last modified, 2008-10-15. Created, 1999-07-08. Release status, REL ...
ligand-expo.rcsb.org/reports/V/VAN/index.html - Cached - Similar -

Prestwick0_000497
InChIKey: InChIKey=**MYPYJXKWCTUITO**-GOYUGWFFDN ... Registries: ChemSpider: InChIKey=**MYPYJXKWCTUITO**-GOYUGWFFDN · PubChem CID 14969 · PubChem ID 11466525 ...
sci-toys.com/scichem/jqp060/14969.html - Cached - Similar -

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Full **Molecule** Search: 4 Hits

Web Show options... Results **1** - **4** of **4** for **MYPYJXKWCTUITO-LYRMYLQWSA-N**. (**0.32** seconds)

Vancomycin CAS 1404-90-6
InChIKey: **MYPYJXKWCTUITO-LYRMYLQWSA-N**. Sterile Vancomycin HCL (CAS 1404-93-9) Market Research Report 2009: Business Analytic Center offers its clients **...**
www.chemicalregister.com/Vancomycin/.../pid35484.htm - Cached - Similar -

InChI=1/C66H75Cl2N9O24/c1-23(2)12-34(71-5)58(88)76-49-51(83)26-7 **...**
Empirical Formula: C66H75Cl2**N**9O24. Molecular Weight: 1449.2536. Nominal Mass: 1447 Da **....** Std. InChIKey: **MYPYJXKWCTUITO-LYRMYLQWSA-N ...**
www.chemspider.com/Chemical-Structure.14253.html - Cached - Similar -

InChI=1/C66H75Cl2N9O24/c1-23(2)12-34(71-5)58(88)76-49-51(83)26-7 **...**
Std. InChIKey: **MYPYJXKWCTUITO-LYRMYLQWSA-N ....** Kinases, PDGFrb, platelet derived growth factor receptor kinase, **N**/A, 0.00. Nuclear Hormone Receptors, RXRa, **...**
www.chemspider.com/14253 - Similar -

Vancomycin - PubChem Public Chemical Database
34+,35-,42+,44-,46+,47+,48-,49+,50-,51+,52+,53+,54-,56+,57+,65-, 66-/m0/s1 InChIKey: **MYPYJXKWCTUITO-LYRMYLQWSA-N**. Compound Information: **...**
pubchem.ncbi.nlm.nih.gov/summary/summary.cgi?cid=14969 - Similar -

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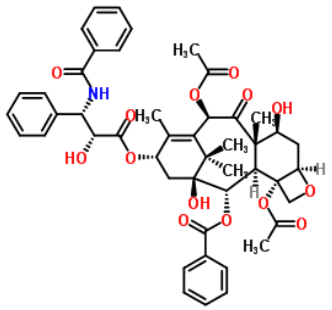
The InChI "Resolver"

InChIs Version: 0.0.0.0

Home Resolver Generator Web Service Configurations



Download MOL Download SDF

ChemSpider ID:	10368587
SMILES:	O=C(N[C@@H](c1ccccc1)[C@@H](O)C(=O)O[C@H]5C[C@@]6(O)[C@@H](OC(=O)c2ccccc2)[C@H]3[C@@](C)([C@@H](O)C[C@H]4OC[C@@]34OC(C)=O)C(=O)[C@H](OC(C)=O)\C(=C5/C)[C@]6(C)C)c7ccccc7
Molecular Formula:	$C_{47}H_{51}NO_{14}$
Molecular Weight:	853.9061
InChI (v1.02b):	InChI=1/C47H51NO14/c1-25-31(60-43(56)36(52)35(28-16-10-7-11-17-28)48-41(54)29-18-12-8-13-19-29)23-47(57)40(61-42(55)30-20-14-9-15-21-30)38-45(6,32(51)22-33-46(38,24-58-33)62-27(3)50)39(53)37(59-26(2)49)34(25)44(47,4)5/h7-21,31-33,35-38,40,51-52,57H,22-24H2,1-6H3,(H,48,54)/t31-,32-,33+,35-,36+,37+,38-,40-,45+,46-,47+/m0/s1
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InChI Key (v1.02s):	RCINICONZNJXQF-MZXODVADSA-N

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Content is King and **Quality** Costs

- Curated Chemistry “content” is expensive to create
  - Patent searching
  - Structures and properties
  - Drug databases
  - Literature databases

- **Chemical Abstracts Service** (CAS), the “Gold Standard” in Chemistry related information
  - 102 years of content
  - >50 million substances
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The EXPERTS must get it right?!

Northwest Fisheries Science Center
Harmful Algal Blooms

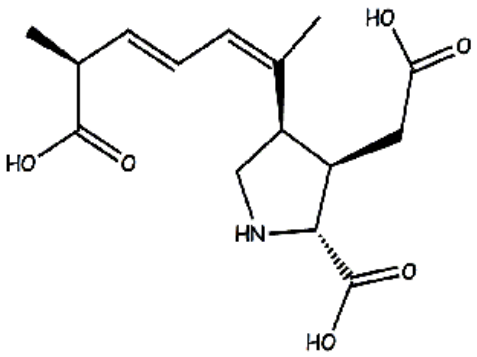
Home • HABs & Biotoxins • Research • Outreach • Links • Search

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

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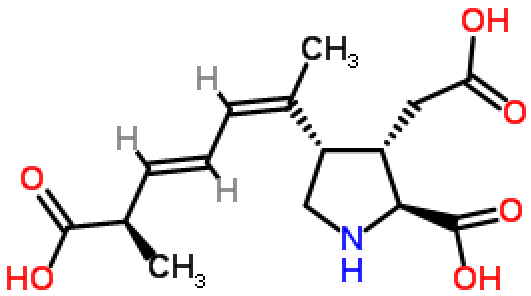
Wikipedia, C&E News, PubChem

C&E News (from ACS)



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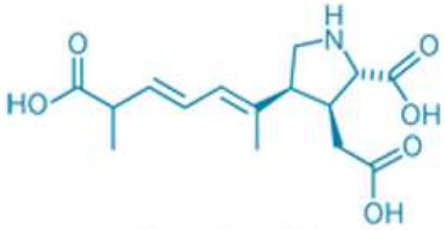
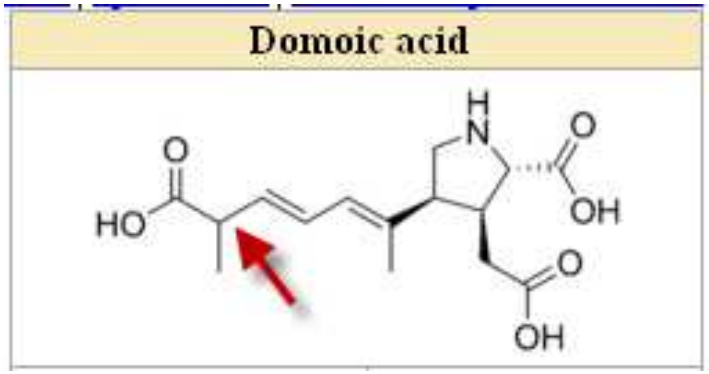


Domoic acid

arge amounts of domoic acid, which can cause
short-term memory loss in people who ingest it in



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Feedback from Steve Ritter

- "Although CAS and C&EN are both part of the ACS Publications Division, **we at C&EN still have to pay for our SciFinder access, strangely enough."**

- "It would be **nice to have an authoritative web-based source of standard, well-drawn structures** for chemists to go to so they can freely cut and paste structures into their papers, PowerPoint presentations, and anything else they might need. **Maybe Wikipedia will be that source one day**."

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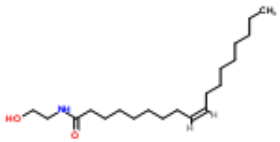
Maybe it will be ChemSpider?

- What is ChemSpider?
  - A database of almost 23 million compounds, >200 data sources
  - A deposition and curation platform
  - A publishing platform for the community
  - Grows daily – more depositions, more links, more data sources

Search OEA

Inherent Properties, Identifiers and References

2D 3D



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Quick Links: Permalink Similar Isomers Wikibox

ChemSpider ID:	4446574
Empirical Formula:	$C_{20}H_{39}NO_2$
Molecular Weight:	325.5292
Nominal Mass:	325 Da
Average Mass:	325.5292 Da
Monoisotopic Mass:	325.298079 Da
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SMILES:	O=C(NCCO)CCCCCCC\C=C/CCCCCCCC
InChI:	InChI=1/C20H39NO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20(23)21-18-19-22/h9-10,22H,2-8,11-19H2,1H3,(H,21,23)/b10-9-
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Std. InChIKey:	BOWVQLFMWHZBEF-KTKRTIGZSA-N

Wikipedia Article(s)

License

Oleoylethanolamide (OEA) is an endogenous peroxisome proliferator-activated receptor alpha (PPAR-α) agonist. It is a naturally-occurring lipid derivative that regulates feeding and body weight in vertebrates ranging from mice to pythons. OEA is the monounsaturated analogue of the endocannabinoid anandamide, but unlike anandamide it acts independently of the cannabinoid pathway, regulating PPAR-α activity to stimulate lipolysis. OEA is produced by the small intestine following feeding in two steps. First an N-acyl transferase (NAT) activity joins the free amino terminus of phosphatidylethanolamine (PE) to the oleoyl group (one variety of acyl group) derived from *sn*-1-oleoyl-phosphatidylcholine, which contains the fatty acid oleic acid at the sn-1 position. (illustration). This produces an N-acylphosphatidylethanolamine, which is then split (hydrolyzed) by N-acyl phosphatidylethanolamine-specific phospholipase D (NAPE-PLD) into phosphatidic acid and OEA. OEA has recently been demonstrated to bind to the novel cannabinoid receptor GPR119. OEA has been suggested to be the receptor's endogenous ligand.
Read more... or Edit at Wikipedia...

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Associated Data Sources and Commercial Suppliers

Data Source	External ID(s)
Calbiochem	495417
Cayman Chemical	90265
ChemIDplus	000111580
ChemZoo	1137
DiscoveryGate	5283454
EINECS	N/A
eMolecules	25691684
Emory University Molecular Libraries Screening Center	EU-0100942
Human Metabolome Database	HMDB02088
LeadScope	LS-97729
LipidMAPS	LMFA08040015
MeSH	N-oleoylethanolamine
Nature Chemical Biology	nchembio.86-comp11
NCGC	NCGC00015761-01, NCGC00025182-01
PubChem	5283454
Sigma-Aldrich	O0383_SIGMA
Single Depositions	N-Oleoylethanolamine
Thomson Pharma	00025080, 00047619
Tocris Bioscience	1484
Wikipedia	Oleoylethanolamine

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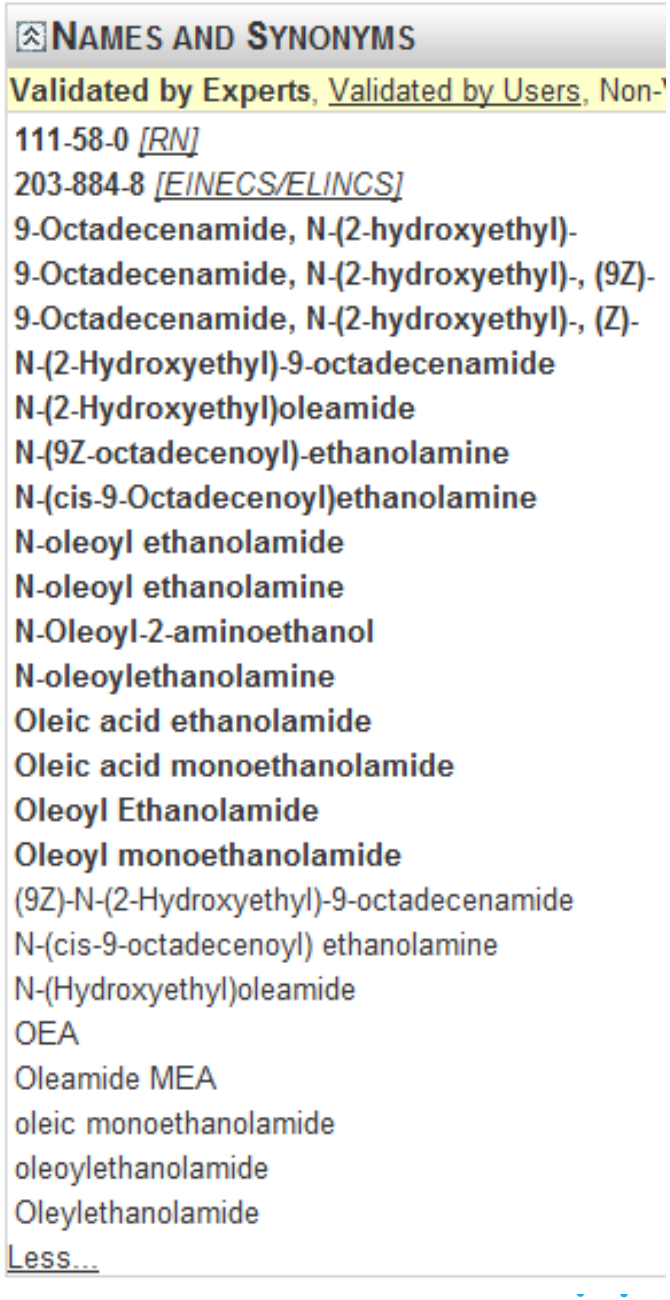

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Welcome to PubMed

The PubMed database comprises more than 19 million citations for biomedical articles from MEDLINE and life science journals. Citations may include links to full-text articles from PubMed Central or publisher web sites.

PubMed Articles

- Sun Y, Alexander SP, Garle MJ, Gibson CL, Hewitt K, Murphy SP, Kendall DA, Bennett AJ. Cannabinoid activation of PPARα: a novel neuroprotective mechanism, Br J Pharmacol, Volume 152, Issue 5, 2007 Nov, Pages: 734-743.
- Lee JT, Xu J, Lee JM, Ku G, Han X, Yang DI, Chen S, Hsu CY. Amyloid-β peptide induces oligodendrocyte death by activating the neutral sphingomyelinase–ceramide pathway, J Cell Biol, Volume 164, Issue 1, 2004 Jan 5, Pages: 123-131.
- Moise AM, Eisenstein SA, Astarita G, Piomelli D, Hohmann AG. An Endocannabinoid Signaling System Modulates Anxiety-like Behavior in Male Syrian Hamsters, Psychopharmacology (Berl), Volume 200, Issue 3, 2008 Oct, Pages: 333-346.
- Tripathy S, Kleppinger-Sparace K, Dixon RA, Chapman KD. N-Acylethanolamine Signaling in Tobacco Is Mediated by a Membrane-Associated, High-Affinity Binding Protein, Plant Physiol, Volume 131, Issue 4, 2003 Apr, Pages: 1781-1791.
- Wise LE, Cannavacciulo R, Cravatt BF, Martin BF, Lichtman AH. Evaluation of fatty acid amides in the carrageenan-induced paw edema model, Neuropharmacology, Volume 54, Issue 1, 2008 Jan, Pages: 181-188.
- Ligresti A, Morera E, Van Der Stelt M, Monory K, Lutz B, Ortar G, Di Marzo V. Further evidence for the existence of a specific process for the membrane transport of anandamide., Biochem J, Volume 380, Issue Pt 1, 2004 May 15, Pages: 265-272.
- Edmunds NJ, Lal H, Woodward B. Effects of tumour necrosis factor-α on left ventricular function in the rat isolated perfused heart: possible mechanisms for a decline in cardiac function, Br J Pharmacol, Volume 126, Issue 1, 1999 Jan, Pages: 189-196.
- Edmunds NJ, Woodward B. Effects of tumour necrosis factor-α on the coronary circulation of the rat isolated perfused heart: a potential role for thromboxane A2 and sphingosine, Br J Pharmacol, Volume 124, Issue 3, 1998 Jun, Pages: 493-498.
- Strelow A, Bernardo K, Adam-Klages S, Linke T, Sandhoff K, Krönke M, Adam D. Overexpression of Acid Ceramidase Protects from Tumor Necrosis Factor–Induced Cell Death, J Exp Med, Volume 192, Issue 5, 2000 Sep 5, Pages: 601-612.

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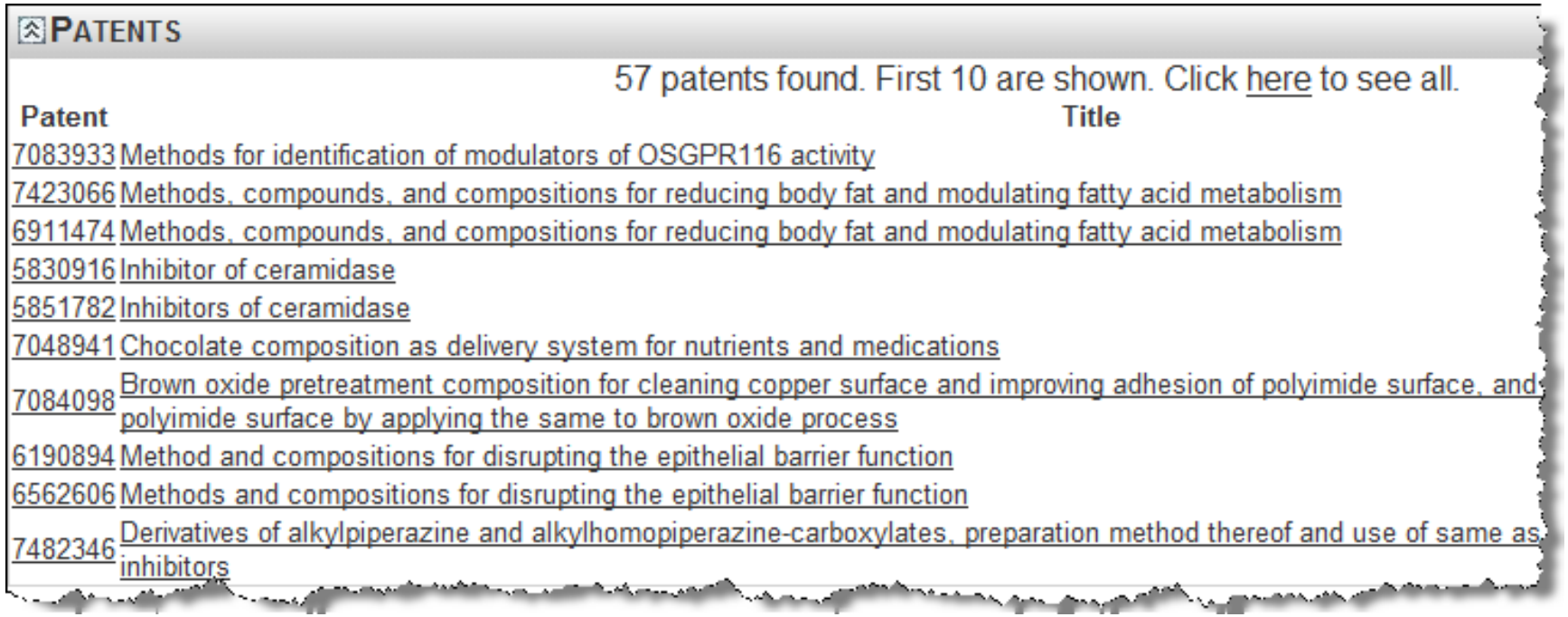
Linked Patents for OEA



PATENTS

57 patents found. First 10 are shown. Click here to see all.

Patent	Title
7083933	Methods for identification of modulators of OSGPR116 activity
7423066	Methods, compounds, and compositions for reducing body fat and modulating fatty acid metabolism
6911474	Methods, compounds, and compositions for reducing body fat and modulating fatty acid metabolism
5830916	Inhibitor of ceramidase
5851782	Inhibitors of ceramidase
7048941	Chocolate composition as delivery system for nutrients and medications
7084098	Brown oxide pretreatment composition for cleaning copper surface and improving adhesion of polyimide surface, and polyimide surface by applying the same to brown oxide process
6190894	Method and compositions for disrupting the epithelial barrier function
6562606	Methods and compositions for disrupting the epithelial barrier function
7482346	Derivatives of alkylpiperazine and alkylhomopiperazine-carboxylates, preparation method thereof and use of same as inhibitors

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57 patents found in USPTO.

Patent No.	Title
7083933	Methods for identification of modulators of OSGPR116 activity
7423066	Methods, compounds, and compositions for reducing body fat and modulating fatty acid metabolism
6911474	Methods, compounds, and compositions for reducing body fat and modulating fatty acid metabolism
5830916	Inhibitor of ceramidase
5851782	Inhibitors of ceramidase
7048941	Chocolate composition as delivery system for nutrients and medications
7084098	Brown oxide pretreatment composition for cleaning copper surface and improving adhesion of polyimide surface, and method for improving adhesion of polyimide surface by applying the same to brown oxide process
6190894	Method and compositions for disrupting the epithelial barrier function
6562606	Methods and compositions for disrupting the epithelial barrier function
7482346	Derivatives of alkylpiperazine and alkylhomopiperazine-carboxylates, preparation method thereof and use of same as fatty acid amido hydrolase enzyme inhibitors

139 patents found in USPTOA.

Patent No.	Title
20060199229	Methods for identification of modulators of OSGPR116 activity, and their use in the treatment of disease
20030018081	Methods, compounds, and compositions for reducing body fat and modulating fatty acid metabolism
20050187254	Methods, compounds, and compositions for reducing body fat and modulating fatty acid metabolism
20090005447	METHODS, COMPOUNDS, AND COMPOSITIONS FOR REDUCING BODY FAT AND MODULATING FATTY ACID METABOLISM
20050054730	Compounds, compositions and treatment of oleoylethanolamide-like modulators of PPARalpha
20050101542	Combination therapy for controlling appetites
20050154064	Dietary and other compositions, compounds, and methods for reducing body fat, controlling appetite, and modulating fatty acid metabolism
20080089845	METHODS FOR DETERMINING EFFECTIVE DOSES OF FATTY ACID AMIDE HYDROLASE INHIBITORS IN VIVO
20090054526	INHIBITORS OF ANOREXIC LIPID HYDROLYSIS FOR THE TREATMENT OF EATING DISORDERS
20090099240	METHODS FOR TREATING ENERGY METABOLISM DISORDERS BY INHIBITING FATTY ACID AMIDE HYDROLASE ACTIVITY

17 patents found in EPA.

Patent No.	Title
2107097	Oleoylethanolamide based functional mesophases
1287815	Use of a sphingoid base for inhibiting ceramidase activity
1707211	CERAMIDASE INHIBITOR
1840125	Derivatives of dioxane-2-alkyl carbamates, preparation thereof and application thereof in therapeutics
0606590	Pharmaceutical or cosmetic composition containing N-acylalcanolamines and N-acylphospho- or lysophospholipids
1972616	Derivatives of arylalkylcarbamates, process for their preparation and therapeutic application thereof
1923388	BRAIN/NEURONAL CELL-PROTECTING AGENT, AND THERAPEUTIC AGENT FOR SLEEP DISORDER
0213885	Grease compositions containing borated catechol compounds and hydroxy-containing soap thickeners
1561461	Adhesive mixture for transdermal delivery of highly plasticizing drugs
0887075	Adhesive mixture for transdermal delivery of highly plasticizing drugs

12 patents found in EPB.

Patent No.	Title
1305016	USE OF N-OLEOYLETHANOLAMINE FOR TREATING PSORIASIS
1250119	REDUCTION OF HAIR GROWTH
1411781	ADDITIVE FOR USE IN FEEDING STUFF OR DRINKING WATER
1383537	NOVEL CHOCOLATE COMPOSITION AS DELIVERY SYSTEM FOR NUTRIENTS AND MEDICATIONS
0971710	USE OF CHELERYTHRINE AND RADIATION FOR TUMOR THERAPY
1720848	DERIVATIVES OF ALKYLPIPERAZINE- AND ALKYLHOMOPIPERAZINE- CARBOXYLATES, PREPARATION METHOD THEREOF AND USE OF SAME AS FAAH ENZYME INHIBITORS
1701946	DERIVATIVES OF 1-PIPERAZINE- AND 1-HOMOPIPERAZINE-CARBOXYLATES, PREPARATION METHOD THEREOF AND USE OF SAME AS INHIBITORS OF THE FAAH ENZYME
1482920	COMPOSITIONS CONTAINING N-ACYL-PHOSPHATIDYL-ETHANOLAMINES AND/OR MIXTURES OF N-ACYL-ETHANOLAMINES WITH PHOSPHATIDIC ACIDS OR LYSOPHOSPHATIDIC ACIDS
1720550	DERIVATIVES OF PIPERIDINYLALKYLCARBAMATES, PREPARATION METHOD THEREOF AND USE OF SAME AS FAAH ENZYME INHIBITORS
1720829	DERIVATIVES OF HETEROARYL-ALKYLCARBAMATES, PREPARATION METHOD THEREOF AND USE OF SAME AS FAAH ENZYME INHIBITORS

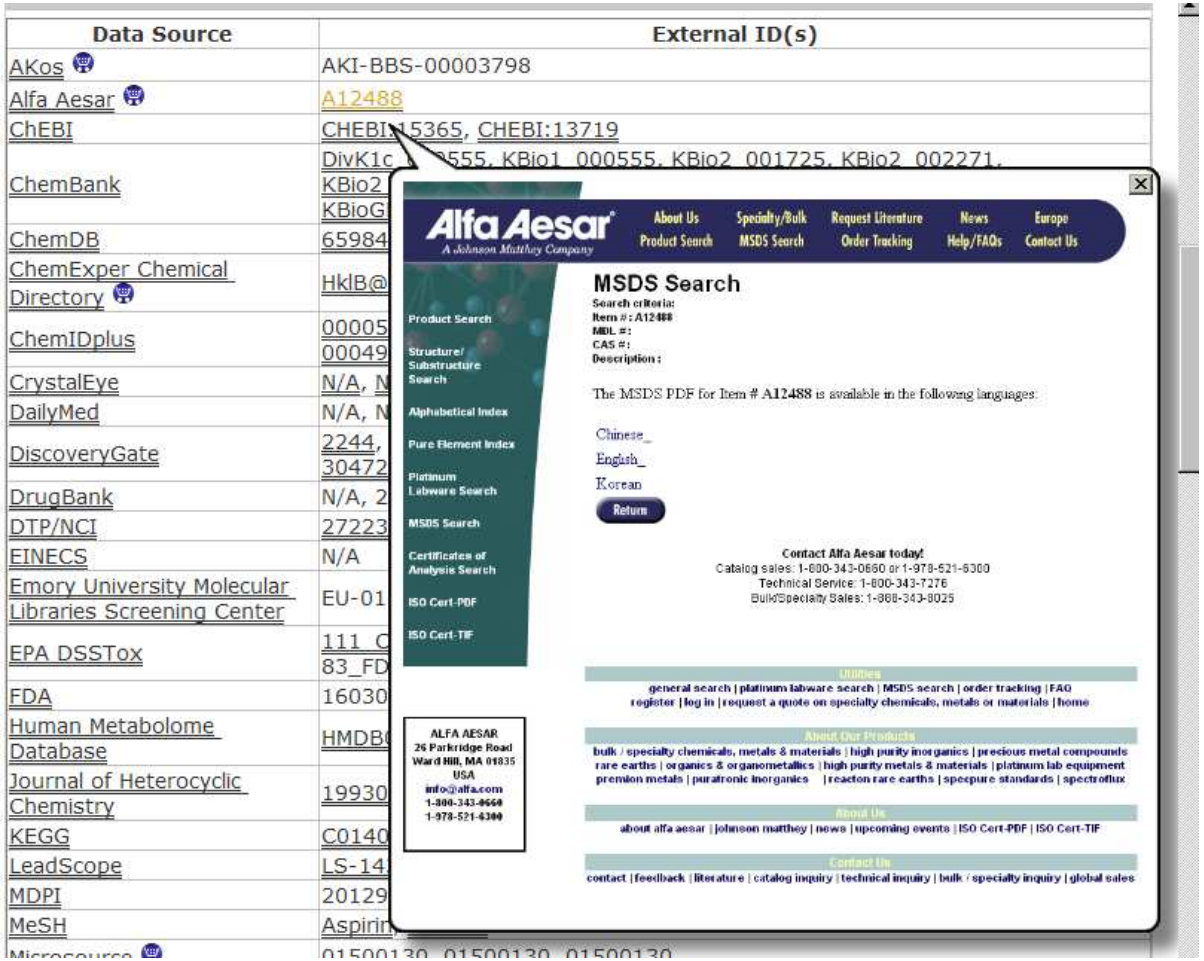
155 patents found in WOPCT.

Patent No.	Title
2002009687	USE OF N-OLEOYLETHANOLAMINE FOR TREATING PSORIASIS

Linked resources

- Vendor sites – Aldrich, Alfa Aesar, TCI and 100s of others
- Government databases – PubChem, DSSTox, FDA databases, ChemIDPlus,…
- Biological Databases – Protein Database, Stitch, KEGG, ChEBI,…
- Analytical databases –NMRShiftDB,…

Linked across the internet



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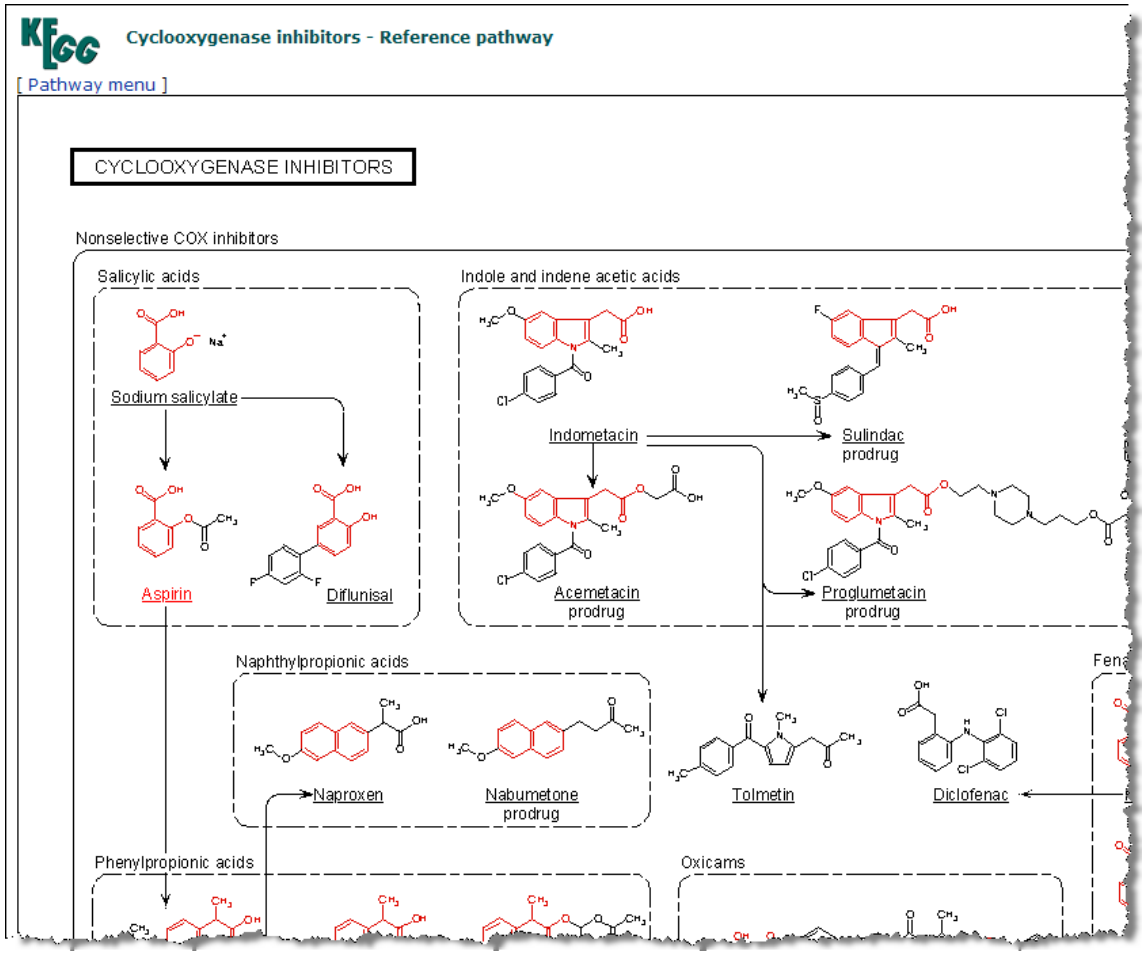
Kyoto Encyclopedia of Genes and Genomes



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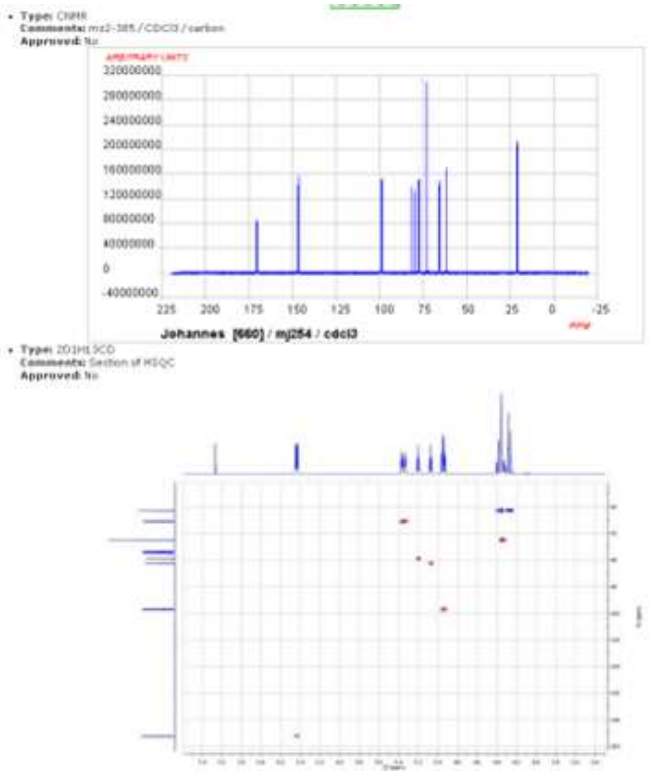
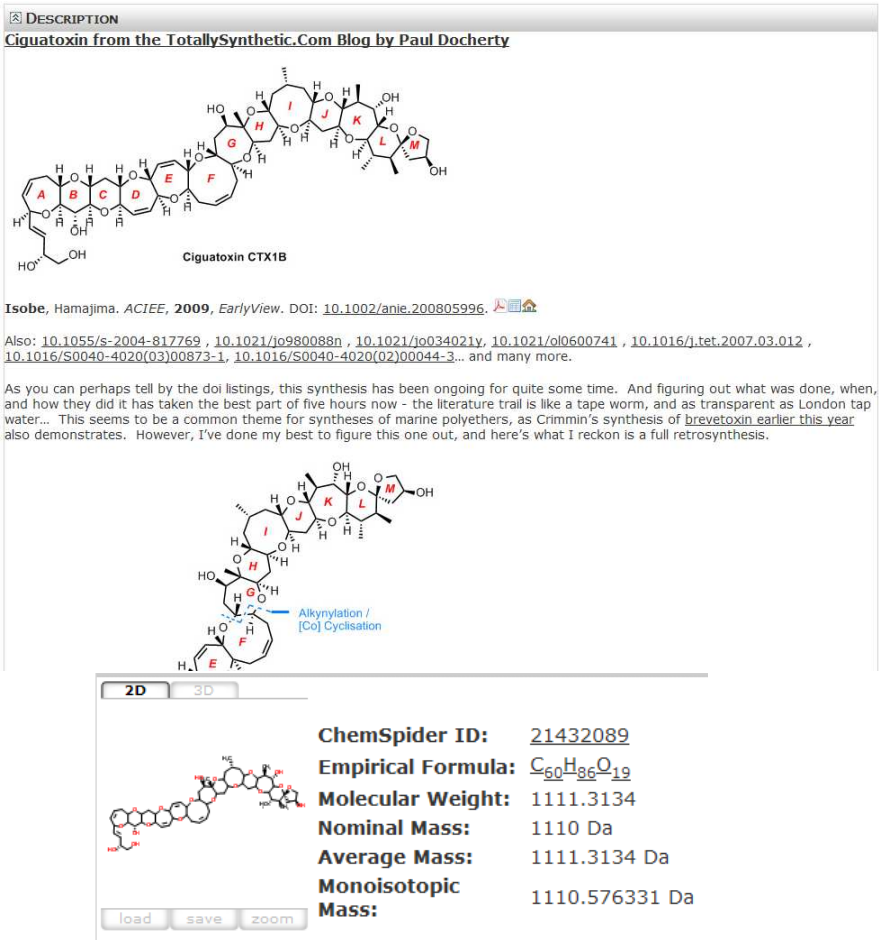
Complex Data and Information





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Remember – **QUALITY ISSUES**

ASN.1 XML SDF

Charcoal - Compound Summary (CID: 297)

An amorphous form of carbon prepared from the incomplete combustion of animal or vegetable matter, e.g., wood. The activated form of charcoal is used in the treatment of poisoning. (Grant & Hackh's Chemical Dictionary, 5th ed)

Table of Contents

- Drug and Chemical Information
  - Pharmacological Action
  - Pharmacological Classification
  - Chemical Classification
  - Safety and Toxicology
  - Literature Links
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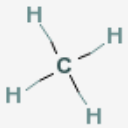
- Properties
- Descriptors
- Compound Information
- Substance Information
  - Category
- Exports



Compound ID	**297**
Molecular Weight	16.04246 [g/mol]
Molecular Formula	CH_4
H-Bond Donor	0
H-Bond Acceptor	0

Plumbago (graphite)
Carbon-12
Philblack N 550
Philblack N 765
DIAMOND
Monarch 700
Witcarb 940
Graphite (synthetic)
Irgalite 1104

METHANAL, OXOMETHANE, OXYMETHYLENE, METHYLENE OXIDE, FORMIC ALDEHYDE, METHYL ALDEHYDE

1-Chlorobenzylethyl-3,5,7,9,11,13,15-heptaisobutylpentacyclo[9.5.1.1(3,9).1(5,15).1(7,13)]octasiloxane, mixture of isomers

The FDA's DailyMed

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Merriam-Webster Turn Dictionary On

Download the FDA official PDF of this label Search By Drug Name: GO

Tolinase (tolazamide) Tablet
[Pharmacia and Upjohn Company]

RxNorm Names
Review RxNorm Normal Forms

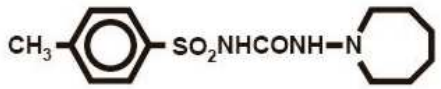
Drug Label Sections

Description | Clinical Pharmacology | Indications & Usage | Contraindications | Warnings | Precautions
Adverse Reactions | Overdosage | Dosage & Administration | How Supplied | Patient Counseling Information
Supplemental Patient Material | Boxed Warning | Patient Package Insert | Highlights | Full Table of Contents

DESCRIPTION

TOLINASE Tablets contain tolazamide, an oral blood glucose lowering drug of the sulfonylurea class. Tolazamide is a white or creamy-white powder with a melting point of 165° to 173° C. The solubility of tolazamide at pH 6.0 (mean urinary pH) is 27.8 mg per 100 mL.

The chemical names for tolazamide are (1) Benzenesulfonamide, *N*-[[(hexahydro-1*H*-azepin-1-yl) amino] carbonyl]-4-methyl-; (2) 1-(Hexahydro-1*H*-azepin-1-yl)-3-(*p*-tolylsulfonyl)urea and its molecular weight is 311.40. The structural formula is represented below:



TOLINASE Tablets for oral administration are available as scored, white tablets containing 100 mg, 250 mg or 500 mg tolazamide. Inactive ingredients: calcium sulfate, docusate sodium, magnesium stearate, methylcellulose, sodium alginate.

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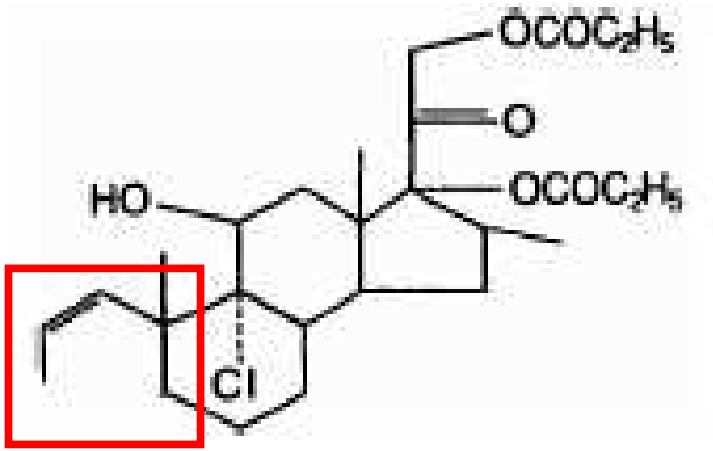
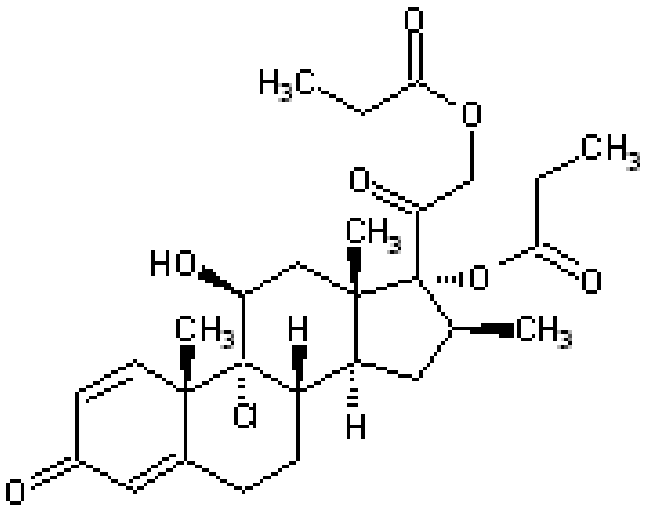
Incorrect Structures





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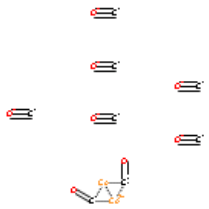
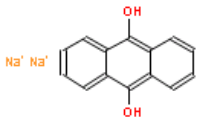
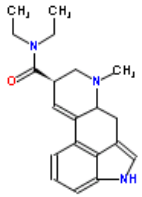
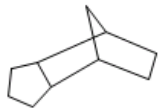
Crowd-sourcing Chemistry Curation

23412		5/1/2008 1:02:27 PM	Extreme	New	This structure should be deprecated. The structure is abysmal	Antony Williams antony.williams@chemspider.com
16352795		4/29/2008 3:42:04 PM	Normal	New	disodium salt or anthracene-9,10-diol ???	kolshorn@uni-mainz.de
5558		4/24/2008 2:52:04 AM	High	New	I look for 2-Butenedioic acid (2Z)-, homopolymer (RN 26099-09-2), but I get 50-37-3. It does not seem alright. Searching with key word of 26099-0902, no results can be found. But in ChemIDplus, it does exist.	alxu@sina.com
16815		4/9/2008 4:31:48 AM	Normal	New	Missing stereo bonds ?	Heinz Kolshorn kolshorn@uni-mainz.de

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The Currency of Recognition

- We need to build a platform for recognition ….

4588649		16/10/2009 00:17:00	Normal	Fixed	Strcuture is that of the quinone imine and not pyronardine! see: A Pulse radiolysis study of free radicals formed by one electron oxidation of the antimalarial drug pyronaridine. Fyaz M. D. Ismail, Michael G.B.Drew, Suppiah Navaratnam and Roger H. Bisby. Research on Chemical Intermediates, (2008) 35:4,363-377. Special PULS2008 conference issue, Accepted 5 December;Online publication date: 1-May-2009 Pdf avaialble upon request, Dr Fyaz M. D.ismail Schhol of Pharmacy & Chemistry Liverpool John Moores University *Verdict: Both tautomers have been approved, linked to WIkipedia and associated via DOI to the article: 10.1007/s11164-009-0051-7*
61574		13/10/2009 01:20:16	Normal	Fixed	These are not two tautomeric forms. I think that both forms are useful since they represent partially the probable charge distribution. (hko) *Verdict: I have done a redorect between the two records to link them*
		13/10/2009			This appears to be a tautomeric form of 16735691 I suggest that all data from this record be copied/migrated into that record and this record deprecated

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Chemistry – A Deposition Platform

- CAS indexes published literature, patents and chemical vendors
- CAS indexes ChemSpider – >303,000 records
- “Lost Chemistry” – syntheses in theses, lab notebooks? Compounds in private collections?
- ChemSpider accepts public depositions, linking to websites, hosting of details etc. Accepts structures, text, spectra, images.

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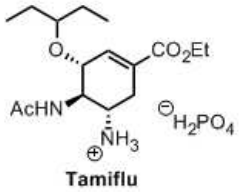
Blogs should be searchable too…

totallysynthetic*

home about index aup faq

Oseltamivir phosphate (Tamiflu) Pt. 5



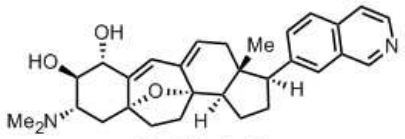
Tamiflu

Shibasaki, Yamatsugu, Yin, Kamijo, Kimura and Kanai. *ACIEE*, **2008**, *EarlyView*. DOI: 10.1002/anie.200804777.

A fifth appearance for my favourite drug 'interloper' in to this natural-product space; alarm bells shouldn't be ringing – just cause I work in pharma doesn't mean I've turned my back on natural products! Tamiflu is of course based on a natural product, shikimic acid – the starting point for the original synthesis. But as natural sources go, it's rather hard to get hold of, and thus damned pricey (£248 for 5g on SA just now). Other routes used involved chemistry that was perhaps a mite 'tetchy' on scale, such as azides and aziridines. A few years

Posted at 2pm on 29/11/08 | 33 comments | Filed Under: Still In The RBF
read on

Cortistatin Pt. III



Cortistatin A

Shair, Lee, and Nieto-Oberhuber, *JACS*, **2008**, *ASAP*. DOI: 10.1021/ja8071918.

A third showing for everybodies favourite androstane, this offering from Matt Shair adds to the quantity of inovative chemistry used in it's contruction. As a quick reminder, first up was Phil Baran, back in May; then came Nicolaou and Chen in August – along with several 'studies towards papers'. However, rather than my going through it all again, have a look at this excellent review by Stefan Bräse which was in ACIEE last month.

If you read it through, you'll notice Nicolaou's use of the Hajos-Parrish ketone (the synthesis of which I discussed in my post on that work); Shair

Posted at 12am on 24/11/08 | 39 comments | Filed Under: Still In The RBF
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TB Shikimic acid is made ver..(Go)
Jose milkshake- chemspider mig..(Go)
sjb Re facelift. Whilst I ..(Go)
anon milkshake - we're stuck w..(Go)
milkshake Now that we are in full-b..(Go)
Flower Thank you but in this App..(Go)
cvengo yeah, but then there are ..(Go)
anniechem cvengo - you're looking a..(Go)
cvengo one thing that is annoyin..(Go)

In Other News...

K. A. Woerpel *et al.* Mechanisms for nucleophilic substitutions of cyclic acetals: nucleophile strength versus stereoselectivity. 10.1021/ol8019956

P. A. Evans *et al.* Intermolecular rhodium-catalyzed [3+2+2] cyclization of

Blogs

Carbon-Based Curiosities
Curly Arrow
Dylan's Tenderblog
In The Pipeline
KinasePro
Lamentations on Chemistry
Liquid Carbon
Molecule Of The Day
One In Ten-Thousand

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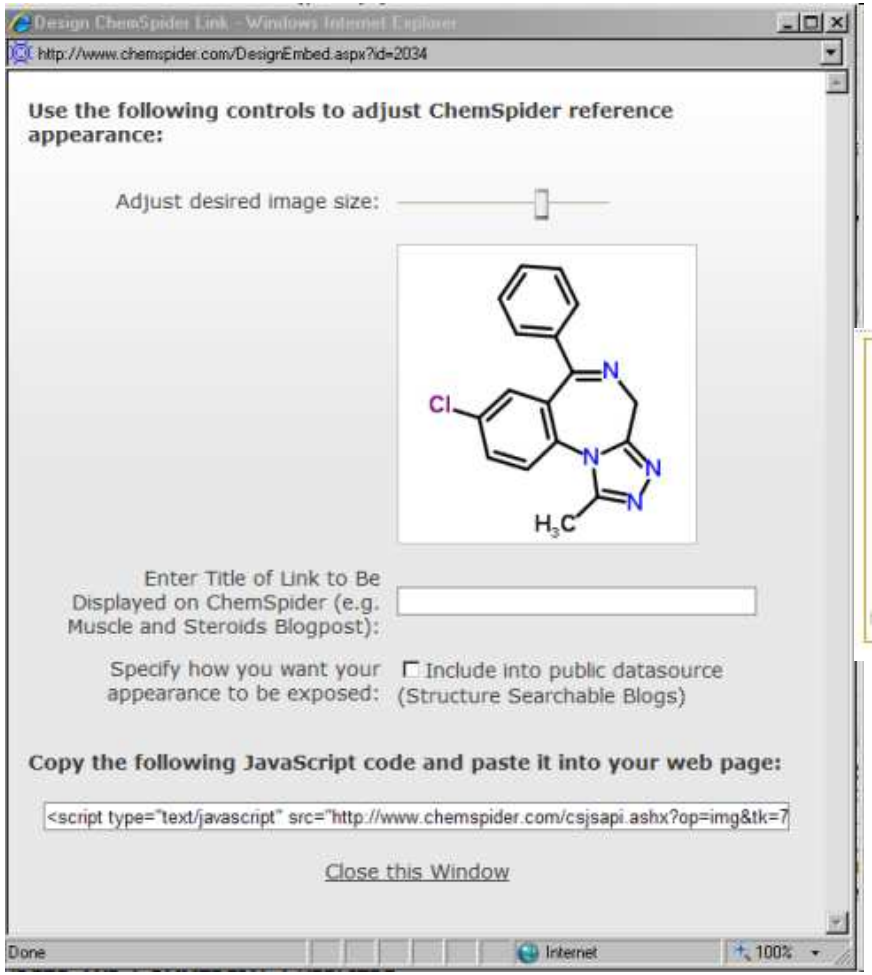
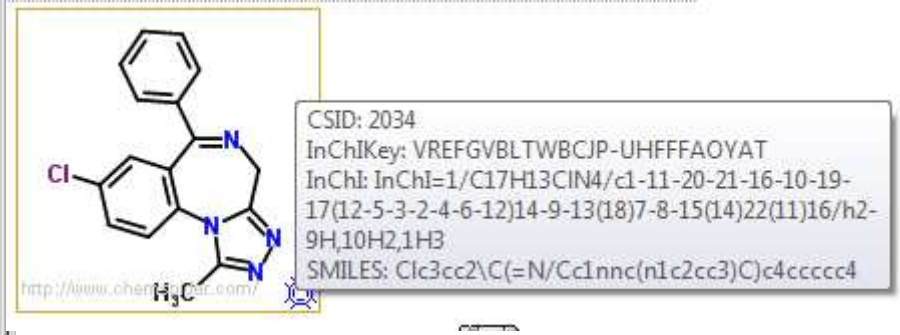
Use Intelligent Structures :
ChemSpider Embed Web Service





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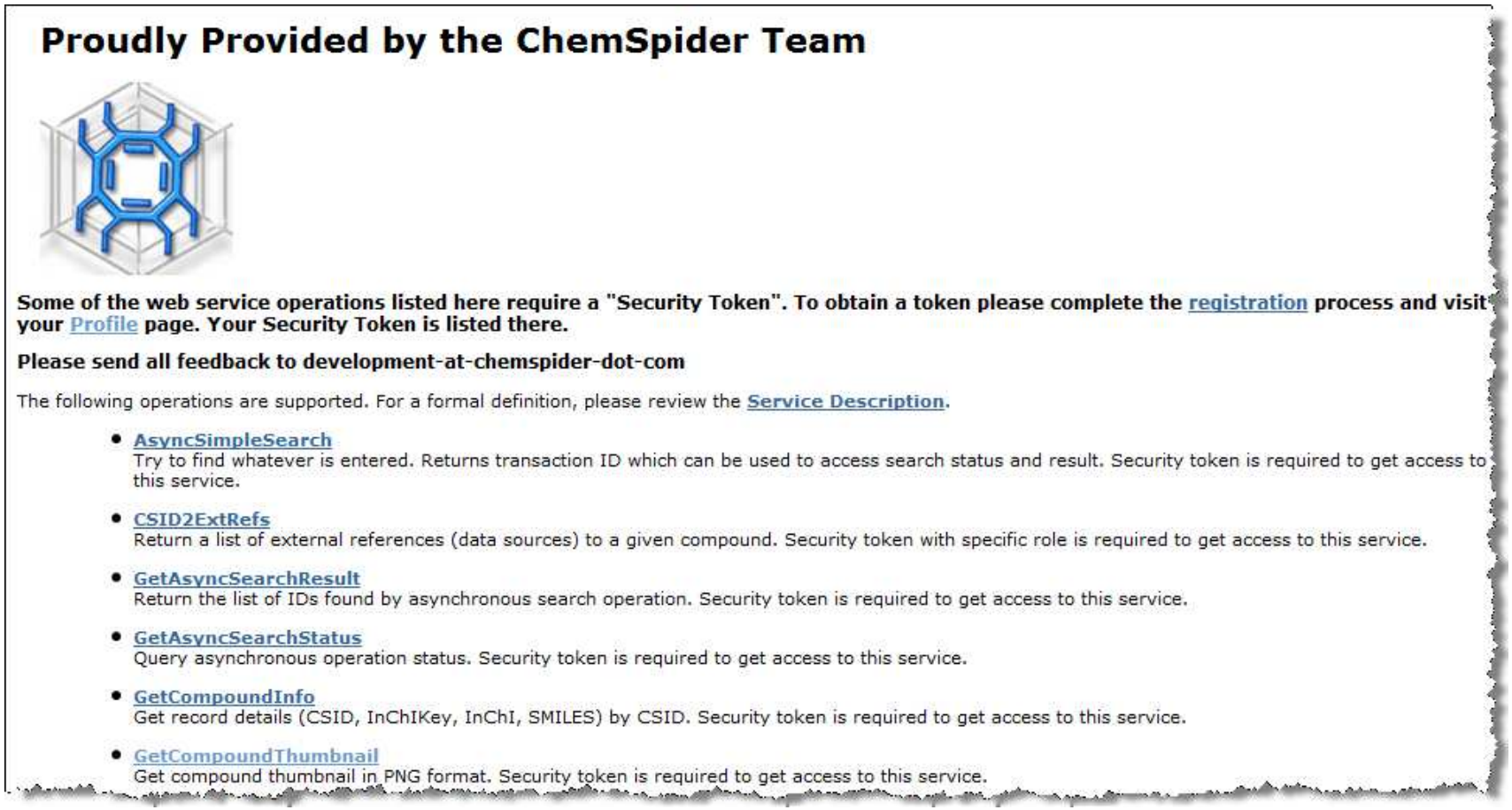
ChemSpider Web Services



Proudly Provided by the ChemSpider Team

Some of the web service operations listed here require a "Security Token". To obtain a token please complete the registration process and visit your Profile page. Your Security Token is listed there.

Please send all feedback to development-at-chemspider-dot-com

The following operations are supported. For a formal definition, please review the Service Description.

- **AsyncSimpleSearch**
  Try to find whatever is entered. Returns transaction ID which can be used to access search status and result. Security token is required to get access to this service.
- **CSID2ExtRefs**
  Return a list of external references (data sources) to a given compound. Security token with specific role is required to get access to this service.
- **GetAsyncSearchResult**
  Return the list of IDs found by asynchronous search operation. Security token is required to get access to this service.
- **GetAsyncSearchStatus**
  Query asynchronous operation status. Security token is required to get access to this service.
- **GetCompoundInfo**
  Get record details (CSID, InChIKey, InChI, SMILES) by CSID. Security token is required to get access to this service.
- **GetCompoundThumbnail**
  Get compound thumbnail in PNG format. Security token is required to get access to this service.

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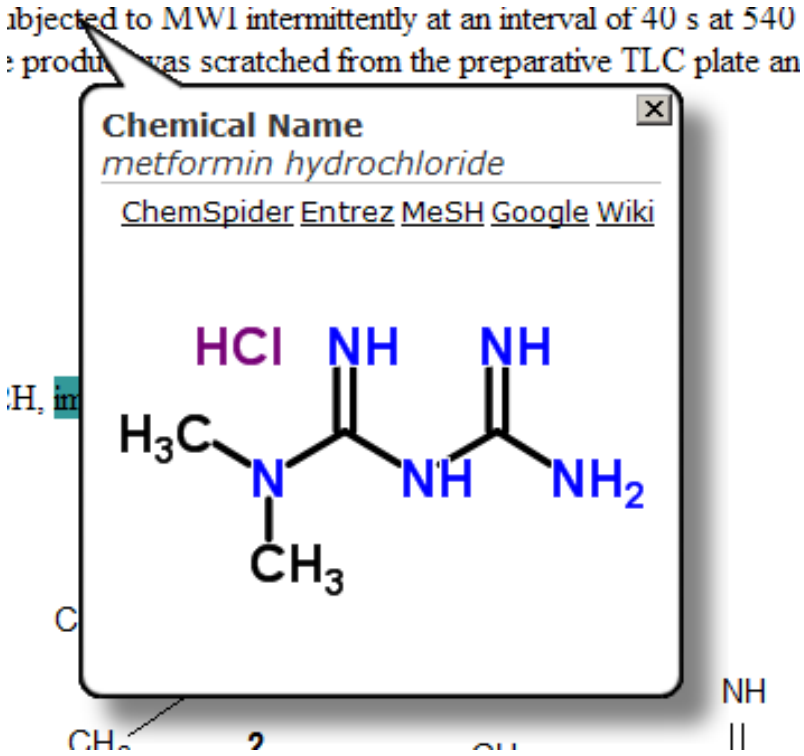
Semantic Linking of Structures

- What would you want to link off a structure?
  - Chemical suppliers
  - Other publications
  - Analytical Data
  - Related Reactions
  - Wikipedia
  - Patents
  - “Everything”



- See Richard Kidd’s Talk

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Conclusions

- Internet resources provide a collaborative community for chemistry
- Crowdsourcing to expand, curate and integrate to the benefit of chemists
- Searching the web for chemistry is arriving
- InChIs are enabling chemistry on the internet
- Question Quality!

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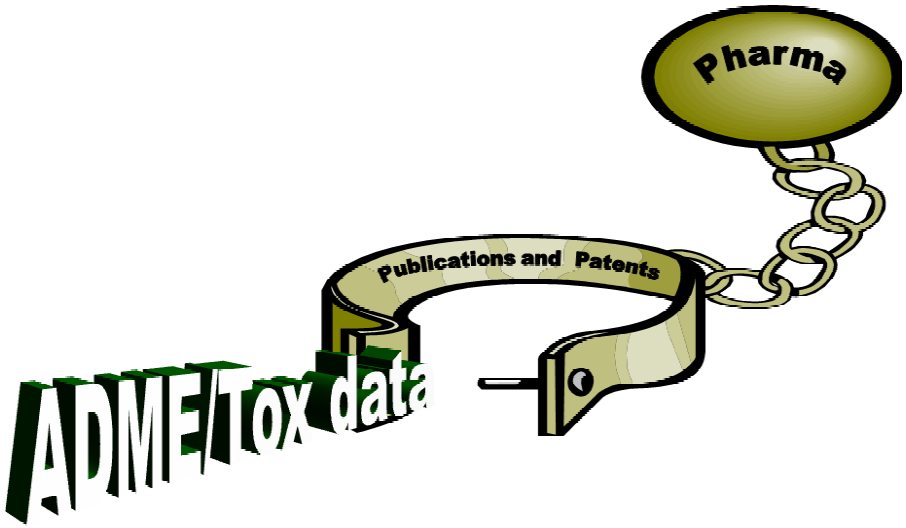
Lab on a Chip

Microfluidic & nanofluidic technologies for chemistry, physics, biology, and bioengineering

Precompetitive Preclinical ADME/Tox Data: Set It Free on the Web to Facilitate Computational Model Building and Assist Drug Development



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Acknowledgments

- Valery Tkachenko and Sergey Golotvin
- RSC infrastructure team
- The ChemSpider advisory group
- The Wikipedia Chemistry team

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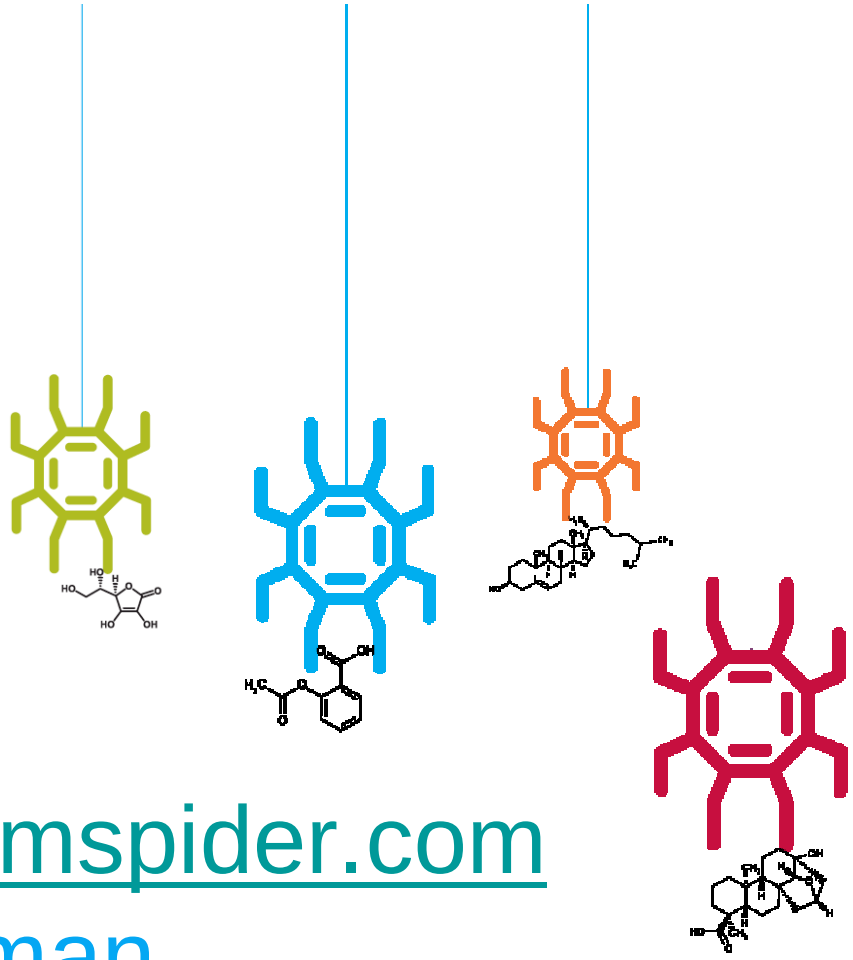

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