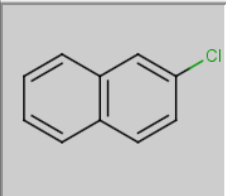


Structure ⓘ

View Help



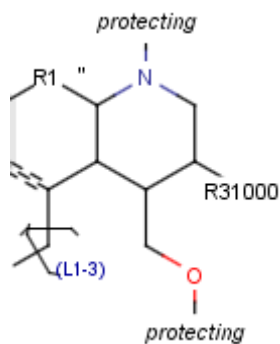
Powered by [ChemAxon Marvin](#)

Structure Search Options ⓘ

- Substructure Search
- Similarity Search %
- Exact (parent only)

ChemAxon relevance to:

Publishers, IP specialists, any chemist...



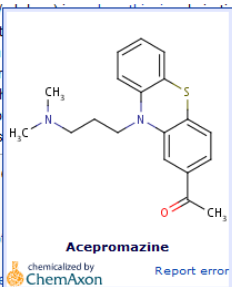
Alex Allardyce

Acepromazine

From Wikipedia, the free encyclopedia

Acepromazine or **acetylpromazine** (more commonly known depending on mg) is a first-generation antipsychotic used in humans (it is frequently used in pharmaceutical preparations in conjunction with other drugs and as such is not out of the prenasal cavity).

- 1 Administration
 - 1.1 Canine
 - 1.1.1 Potency
 - 1.2 Equine
 - 1.2.1 Prevalence
 - 1.3 Feline
- 2 References



What's in it for publishers

Content production, management and delivery

- Platform independent & web ready toolkits
- Industry leading performance and support
- Widest range of functionality (consolidate all your platforms to ChemAxon)
- Sexy and state of the art functionality for your portal/content
- Deployed throughout STM publishing
- Still called ChemAxon
- Friendly/flexible pricing models

Everything you need to completely integrate chemistry into your production and delivery platform

Visualization



Marvin

Structure, query & reaction editor, viewer & visualization

Property Prediction



Calculator Plugins

Structure property prediction & calculation

Selected calculations listing

- pKa, Major microspecies
- logP, logD
- Charge
- Tautomerization
- Stereoisomer
- Conformation and 3D alignment
- Topology Analysis
- Molecular Surface Area
- Markush Enumeration
- Hydrogen bond donor/ acceptor
- Structural Frameworks
- Structure to Name
- etc...

Add-ons



Markush Search

Store & search Markush structures



JChem Webservices

Web services integration interface

Chemical DB – toolkit



JChem Cartridge

JChem/Oracle integration



JChem Base

Structure searching & db access



Standardizer

Chemical business rules processing

Structure checker

Batch structure file validation and correction

Chemical DB – desktop



Instant JChem

Structure db management, search & prediction



JChem for Excel

Enabling chemistry in Excel

Nomenclature



Name to Structure

Import & search chemical names

Enumeration



Reactor

Enumeration via reaction modelling

Library analysis



JKluster

Clustering & diversity analysis



Fragmenter

Decomposition to fragments and R-groups



Screen

HT pharmacophore screening



Innovation for IP professionals - MMS structure storage and search

Toolkit and desktop application choices for storing and searching Markush structures (without enumeration).

Includes Markush enumeration and interactive visualization for advanced Markush manipulation.

Use cases:

- novelty search,
- idea generation,
- Markush creation,
- patent busting / white space identification

Thomson Reuters MMS/DWPI content implemented in ChemAxon's Instant JChem desktop application

Instant JChem 5.3.8

File Edit View Search Data Lists Tools Window Help

Projects [ijc-project-markush-demose...] Welcome Grid view for Inventions Grid view for chemaxon_sample Form view for Inventions

Design Query Browse Entity: vmns

ID: 219

Title: New spiro-heterocyclic chromans, thiochromans and dihydroquinolines useful for treating e.g. apoptosis in cancer cells, cardiovascular disease, Alzheimer disease, Parkinson disease, depression or chronic obstructive pulmonary disease

Description: Spiro-heterocyclic chromans, thiochromans and dihydroquinolines of formula (I), their stereoisomers and salts are new. X=O, S(O)n or NR; n=0 - 2; R1, R3, and R4=hydrogen, alkyl, cycloalkyl, halogen, nitro, cyano.

Assignees: LILLY & CO ELI, LILLY&CO ELI, CHU D T W, GALILEO PHARM INC, JAMES D R, WANG P

Patents: WO2006093548-A1, AU2005328328-A1, EP1856079-A1, IN200703515-P2, CN101163687-A, JP2008531559-W, US20080207588-A1, MX2007010328-A1, BR200520097-A2

Use: In preparation of composition useful for treating apoptosis in cancer cells (e.g. prostatic cancer, gastric cancer, breast cancer, pancreatic cancer, colorectal or esophageal cancer and airways carcinoma); diseases involving hypoxia or anoxia (e.g. atherosclerosis, myocardial infarction)

Mechanism Of Action: Lipoxigenase enzyme inhibitor. No biological data given.

Activity: Cytostatic; Respiratory-Gen.; Cardiovascular-Gen.; Antiarteriosclerotic; Cardiant; Cardiovascular-Gen.; Cerebroprotective; Vasotropic; Cardiant; Nootropic; Antidiabetic; Antiinflammatory; Gastrointestinal-Gen.; Nephrotropic; Gynecological; Antiasthmatic; Antiallergic; Antiinflammatory; Antigout; Antiarthritic; Antirheumatic; Antiarthritic; Osteopathic; Muscular-Gen.; Antiseborrheic; Dermatological; Antipsoriatic; Antiasthmatic; Respiratory-Gen.; CNS-Gen.; Tranquillizer; Antidepressant; Neuroleptic; Neuroprotective; Nootropic; Antiparkinsonian; Neuroprotective; Vulnerary; Immunosuppressive; Ophthalmological. No biological data given.

Structure data displayed alongside patent summaries from DWPI; includes abstract, patent assignee, patent family, activities & mechanisms of action

Highlighted search results, 'reduced' Markush hits & selective enumeration

Instant JChem 5.3.8

File Edit View Search Data Lists Tools Window Help

Projects [jic-project-markush-demoset] x Welcome x Grid view for Inventions x Grid view for chemaxon_sample x Form view for Inventions x

Design Query Browse Entity: vmns

ID: 3

vmns

Markush structure

1

2

Enumerate a Markush structure

Enumeration options:

- Full enumeration
- Random enumeration
- Markush reduction according to the hit

Max structures: 10

Output to file

Display options

Rows: 2

Columns: 3

Show R-groups

Colouring

Enumerate

6 structures enumerated

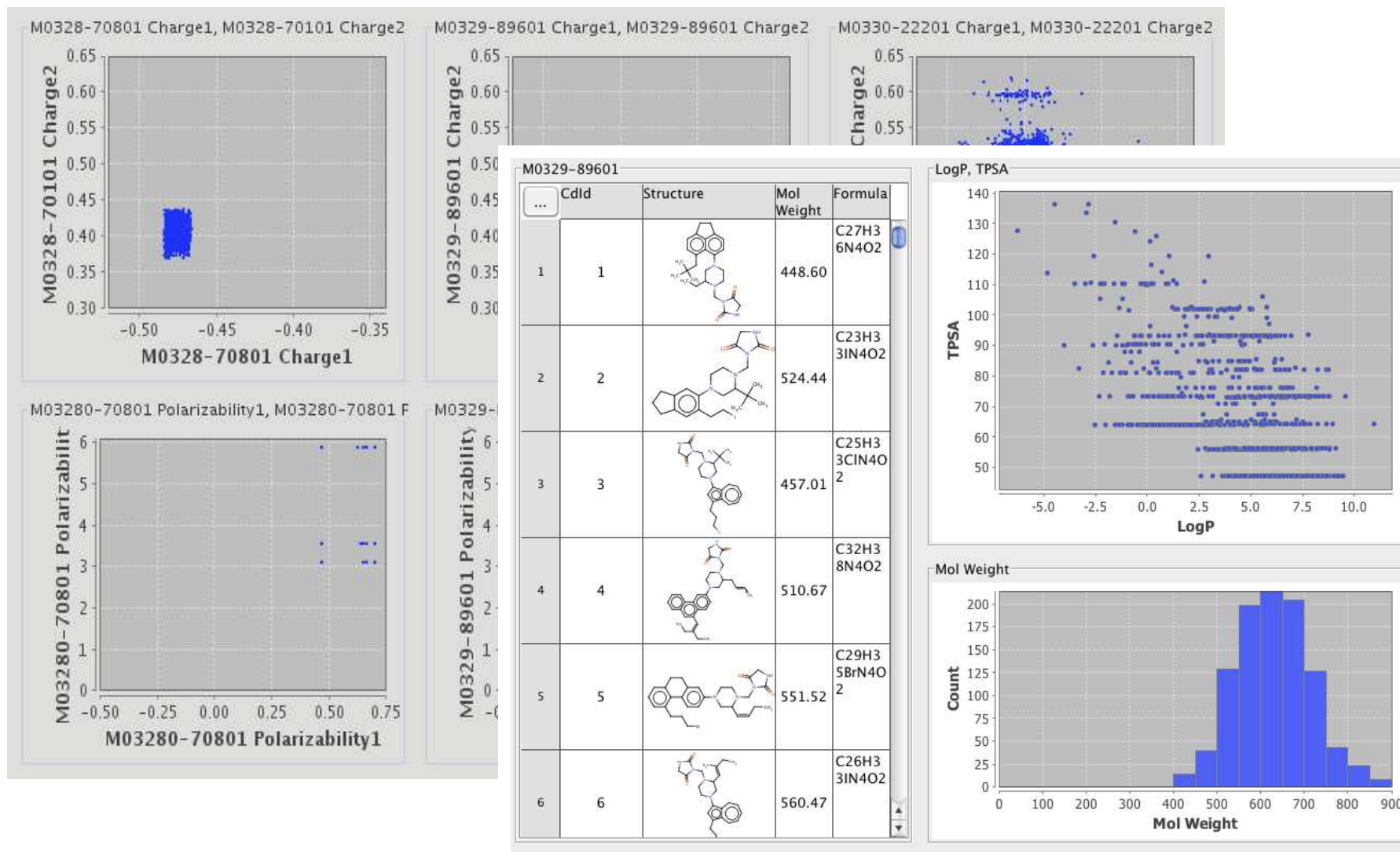
Full enumeration of this structure produces 4698509682954150 (~10¹⁶) structures

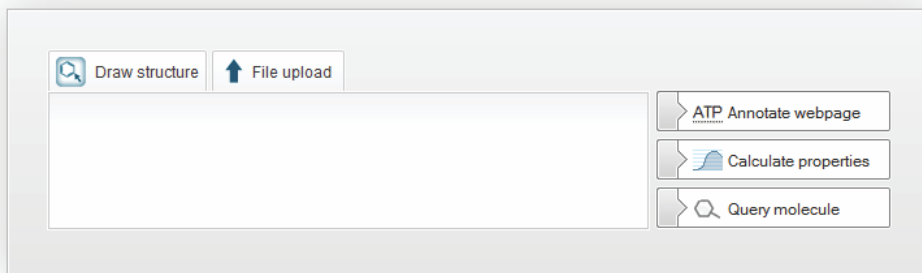
Close

Enumeration tool enables Markush structure mining

'Markush reduction according to the hit' expands the Markush to show the full query

Enumerated structure properties can be generated automatically and displayed in Instant JChem





chemicalize.org

Free public service to:

- Add chemical structures to web pages in real time
- Search all structures (and URL's) already chemicalized (structure search the web!)
- See predicted properties for discrete chemical structures
- Gather links of interest to chemists for post processing (search, analysis, reporting, fun...)

chemicalize >

Wikipedia: List of Organic compounds – chemicalized

The chemical names on this page were annotated by the [chemicalize.org](http://www.chemicalize.org) service. You can see the original page: http://en.wikipedia.org/wiki/List_of_organic_compounds.

WIKIPEDIA
The Free Encyclopedia

Article Discussion Read Edit View history Search

List of organic compounds

From Wikipedia, the free encyclopedia

This is a list of well-known organic compounds, including organometallic compounds, to stimulate the creation of Wikipedia articles. Note that purely inorganic compounds, minerals, and chemical elements are not included on this list. There are also no generic terms (e.g., carbohydrate) or mixtures of no fixed composition (e.g., naphtha, gasoline). Compounds and enzymes that are overwhelmingly of interest to biochemists, such as Cytochrome c peroxidase, are listed under list of biomolecules.

For substances with a number prefix such as 2-Butanol or 1,3-Cyclohexadiene, use the first letter of the name (in this case under B or C) to find the compound. Such names usually have the first letter capitalized in a title or at the beginning of a sentence.

Whilst most compounds are referred to by their IUPAC name, "traditional" names have also been kept where they are in wide use or of significant historical interest.

Contents: ABCDEFGHIJKLMNOPQRSTUVWXYZ See also External links

A

For substances with an A- or α - prefix such as α -Terpinene, please see the parent page (in this case Terpinene).

- Abietic acid - C₂₀H₃₀O₂
- Acenaphthene - C₁₀H₈
- Acenaphthoquinone - C₁₂H₆O₂
- Acenaphthylene - C₁₂H₈
- Acepromazine - C₁₉H₂₂N₂OS
- Acetaldehyde - C₂H₄O
- Acetamide
- Acetaminophen
- Acetaminophenol
- Acetamidophenol
- Acetanilide
- Acetic acid
- Acetoguanidine
- Acetone
- Acetonitrile
- Acetophenone
- Acetylcholine
- Acetylene
- N-Acetylglucosamine
- Acetylsalicylic Acid - C₉H₈O₄ (also known as Aspirin)
- Acid fuchsin
- Acridine - C₁₃H₉N
- Acridine orange - C₁₇H₁₉N₃
- Acrotoxin - C₃H₄O
- Acrylamide - C₃H₅NO
- Acrylic acid - C₃H₄O₂
- Acrylonitrile - C₃H₃N

Recognised chemical names are appended with dotted underline

Mousing over appended names pops the structure image

Clicking on image takes you to the "Data page" for that structure

Acepromazine

CN(C)CCCN(C1=CC=C2C(=C1)S(=O)(=O)C=C2)C(=O)O

Links are respected (chemicalized) – so building the chemicalized proportion of the www

The chemical names on this page were annotated by the [chemicalize.org](http://www.chemicalize.org) service. You can see the original page: <http://en.wikipedia.org/wiki/Acepromazine>.

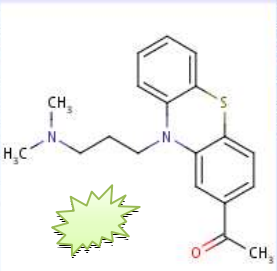
WIKIPEDIA
The Free Encyclopedia

Article Discussion Read Edit View history Search

Acepromazine

From Wikipedia, the free encyclopedia

Acepromazine or **acetylpromazine** (more commonly known as **ACP**, **Ace**, or by the trade names **Atravet** or **Acezine 2**, number depending on mg) is a **phenothiazine** antipsychotic drug. It was first used in humans in the 1950s,^[1] but is now little used in humans (it is frequently used in pharmaceutical preparations in conjunction with other drugs and as such is not out of the preanes). **Acepromazine** is still used as an antipsychotic in humans). **Acepromazine** is its principal value is in quietening and calming anxious animals. The standard sedextensively in horses, dogs, and cats; especially as a preanesthetic agent often as **morphine** or **buprenorphine**. Its potential for cardiac effects can be profound or debilitated animals in these cases it is often substituted with **midazolam** or left



Acepromazine
chemicalized by ChemAxon Report error

1 Administration
1.1 Canine
1.1.1 Pre
1.2 Equine
1.2.1 Pre
1.3 Feline
2 References

Administration

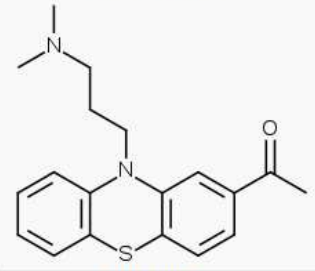
[edit]

Canine

[edit]

When used as a **premedication** it is commonly administered via the subcutaneous route.

Acepromazine



Systematic (IUPAC) name
1-([3-(dimethylamino)propyl]-10H-phenothiazin-2-yl)ethanone

Identifiers

CAS number	61-00-7
ATC code	N05AA04
PubChem	CID 6077
DrugBank	DB01614
ChemSpider	5852

Chemical data

Formula	C ₁₉ H ₂₂ N ₂ OS
----------------	---

Datapage for "ace": extensive predicted properties

Chemicalize.org **alpha** Open All Close All Manage calculations Layout: Custom acepromazine Search

Molecule

Name

IUPAC name: 1-[10-[3-(dimethylamino)propyl]-10H-phenothiazin-2-yl]ethan-1-one
Traditional name: Ace

Elemental Analysis

Formula: C₁₉H₂₂N₂O
Isotope formula: C₁₉H₂₂N₂O
Composition: C (69.9%), H (6.79%), N (8.58%), O (4.9%), S (9.82%)
Isotope composition: C (69.9%), H (6.79%), N (8.58%), O (4.9%), S (9.82%)
Mass: 326.456
Exact mass: 326.145284026

Topology Analysis

Simple Ring Counts Path and distance

Atom count: 45
Bond count: 47
Cyclomatic number: 3
Chain atom count: 9
Chain bond count: 9
Asymmetric atom count: 0
Rotatable bond count: 5

Polar Surface Area

Polar surface area: 23.55

logP

logP: 3.52

H-bond Donor/Acceptor

Major Microspecies

Major microspecies at pH=7.4:

Geometry

Calculate Geometry

Lipinski-like filters

Lipinski's rule of five: yes
Bioavailability: yes
Ghose filter: yes
Lead likeness: yes
Muegge filter: yes
Veber filter: yes

Molecular Surface Area

Calculate Molecular Surface Area

pKa

8.50
-8.69
16.06

100.00%
80.00%
60.00%
40.00%
20.00%
0.00%

0.0 2.0 4.0 6.0 8.0 10.0 12.0 14.0

pH

created by ChemAxon

The chemicalize.org website including all name to structure and structure based calculations and predictions by ChemAxon is licensed under a Creative Commons License. Permissions beyond the scope of this license may be available at <http://www.chemaxon.com/contact-us/>

CC BY NC SA

Customizable report layout for calculation results.

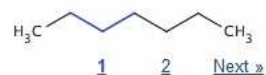
Users can move, open, close, expand calculation boxes and this is remembered on the next visit

Searching the web: Aspirin; searching chemicalize.org - query highlighted in results

Aspirin Draw Structure - Search type - ? Search Advanced input

16 structures found:

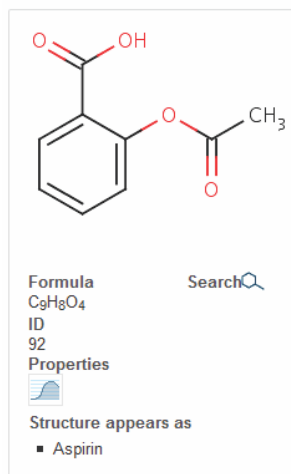
<p>Formula C₉H₈O₄ ID 92 Properties</p>	<p>Formula C₁₄H₁₀O₅ ID 2245 Properties</p>	<p>Formula C₁₀H₇F₃O₄ ID 7037 Properties</p>	<p>Formula C₁₆H₁₈FNO₄ ID 7814 Properties</p>	<p>Formula C₂₄H₃₃NO₄ ID 7903 Properties</p>
<p>Formula C₉H₇O₄ ID 8629 Properties</p>	<p>Formula C₉H₈AlO₅ ID 9371 Properties</p>	<p>Formula C₁₁H₁₀O₆ ID 10324 Properties</p>	<p>Formula C₁₇H₁₅NO₅ ID 10626 Properties</p>	<p>Formula C₉H₇Cu₂O₄ ID 13263 Properties</p>



searching chemicalize.org: Aspirin; web page hits

No structures shown

« [Back to search](#) | Structure found on 7457 pages:



[show all related structures >](#)

[show all related links >](#)

Diverse

[Eicosanoid - Wikipedia, the free encyclopedia](#)

1 Apr 2010 - original page
en.wikipedia.org/wiki/Eicosanoid_metabolism
[+ show structures on this page](#) [+ show pages from en.wikipedia.org](#)

[Excedrin - Wikipedia, the free encyclopedia](#)

1 Apr 2010 - original page
en.wikipedia.org/wiki/Excedrin
[+ show structures on this page](#) [+ show pages from en.wikipedia.org](#)

[File:Aspirin-skeletal.svg - Wikipedia, the free encyclopedia](#)

1 Apr 2010 - original page
en.wikipedia.org/wiki/File:Aspirin-skeletal.svg
[+ show structures on this page](#) [+ show pages from en.wikipedia.org](#)

[Changes related to "PTGS1" - Wikipedia, the free encyclopedia](#)

2 Apr 2010 - original page
en.wikipedia.org/wiki/Special:RecentChangesLinked/PTGS1
[+ show structures on this page](#) [+ show pages from en.wikipedia.org](#)

[Talk:Salicylic acid - Wikipedia, the free encyclopedia](#)

2 Apr 2010 - original page
en.wikipedia.org/wiki/Talk:Salicylic_acid
[+ show structures on this page](#) [+ show pages from en.wikipedia.org](#)

[Unplanned reoperation for bleeding. \[Am Surg. 1996\] - PubMed result](#)

2 Apr 2010 - original page
ncbi.nlm.nih.gov/pubmed/8540646
[+ show structures on this page](#) [+ show pages from www.ncbi.nlm.nih.gov](#)

[Kwas acetylosalicylowy - Wikipedia, wolna encyklopedia](#)

7 Apr 2010 - original page
pl.wikipedia.org/wiki/Kwas_acetylosalicylowy
[+ show structures on this page](#) [+ show pages from pl.wikipedia.org](#)

[United States Patent Application: 0100076056](#)

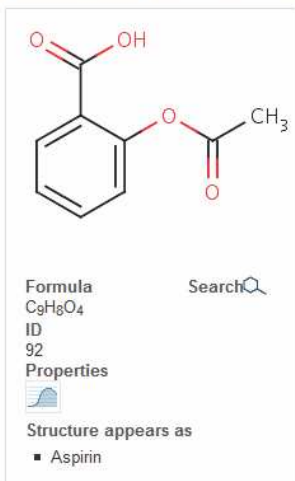
30 Mar 2010 - original page
appft.uspto.gov/netacgi/nph-Parser?Sect1=PTO2&Sect2=HITOFF&p=1&u=/netahtml/PT...
[+ show structures on this page](#) [+ show pages from appft.uspto.gov](#)

[Ibuprofen - Wikipedia](#)

30 Mar 2010 - original page
bs.wikipedia.org/wiki/Ibuprofen
[+ show structures on this page](#) [+ show pages from bs.wikipedia.org](#)

searching chemicalize.org: Aspirin; web page hits - "show" related structures

« Back to search | Structure found on 7457 pages:



hide all related structures <

show all related links >

Diverse

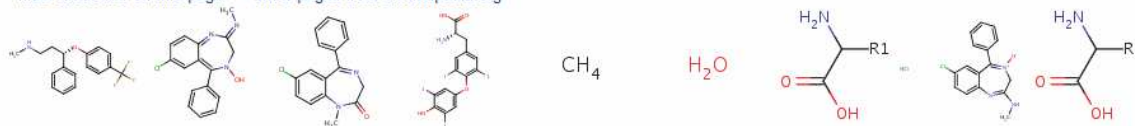
Select to show a diverse selection of the structures on linked web pages

Eicosanoid - Wikipedia, the free encyclopedia

1 Apr 2010 - original page

en.wikipedia.org/wiki/Eicosanoid_metabolism

- hide structures on this page + show pages from en.wikipedia.org

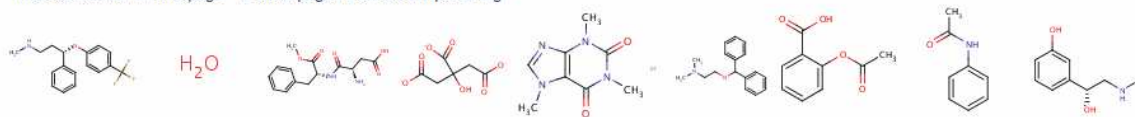


Excedrin - Wikipedia, the free encyclopedia

1 Apr 2010 - original page

en.wikipedia.org/wiki/Excedrin

- hide structures on this page + show pages from en.wikipedia.org

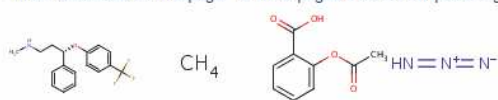


File:Aspirin-skeletal.svg - Wikipedia, the free encyclopedia

1 Apr 2010 - original page

en.wikipedia.org/wiki/File:Aspirin-skeletal.svg

- hide structures on this page + show pages from en.wikipedia.org

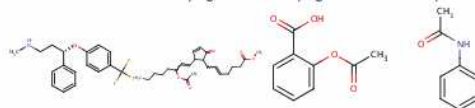


Changes related to "PTGS1" - Wikipedia, the free encyclopedia

2 Apr 2010 - original page

en.wikipedia.org/wiki/Special:RecentChangesLinked/PTGS1

- hide structures on this page + show pages from en.wikipedia.org



Talk:Salicylic acid - Wikipedia, the free encyclopedia

More cool bits: autosuggest, queries as URL's, display diverse structure selection, more structures and search short cuts

Draw structure

pen

ATP Annotate webpage

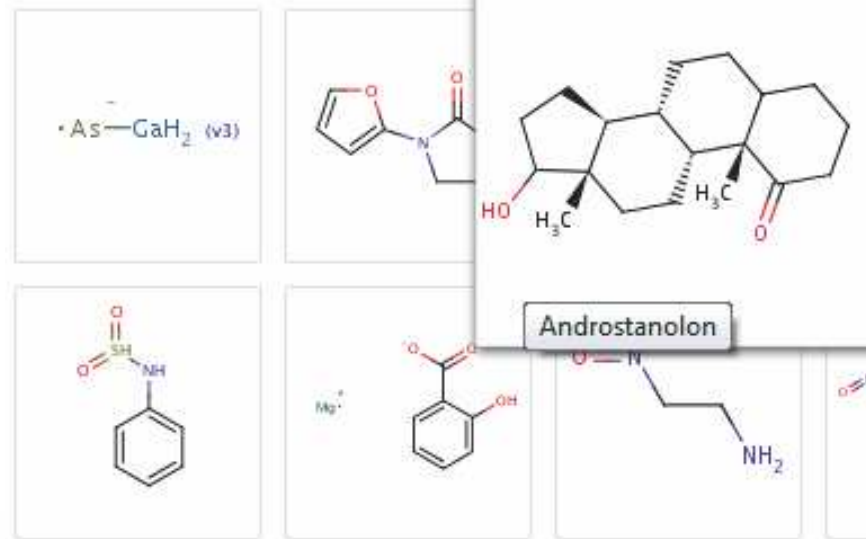
Calculate properties

Query molecule

-  Pentazocine
-  penicillin
-  Pentobarbital
-  Pentolinium
-  Pentamine
-  Pentane
-  Penfluridol

<http://www.chemicalize.org/search.php#m=penicillin/t=s/h=0>


Recently chemicalized mo



•As—GaH₂ (v3)

Androstanolon

Diverse

Refine 

SUB FULL

S