

Screen chemical  
Naming Stereoisomer workflow  
ChemAxon Plugins Geometry analysis  
Resonance virtual  
Spotfire Metabolizer Isomers  
Molecular-Surface-Area libraries Partitioning  
chemicalize.org  
Customizable Elemental-Analysis  
Polarizability MetabolizerCalculator-Plugins Desktop  
HBDA Marvin Enumeration Pipeline  
Instant-JChem MarvinSketch  
JChem-Cartridge Microspecies  
Molecular-Dynamics Flexible-3D-Alignment performance Pilot  
Markush-Search Charge Fragmenter logP  
to enterprise  
SharePoint Name Structure-Checker analyze systems  
pKa Orbital-Electronegativity  
Discovery and  
JKlustor Standardizer Web-Services  
Predictor  
NMR Workflow-integration Conformer Topology-Analysis  
Refractivity Markush-Enumeration management  
InforSense Reactor platform Huckel-Analysis Isoelectric-Point Conformation  
Structural-Framework architecture NMR-Predictor database Structure  
JChem-for-Excel JChem-Base  
IUPAC Tautomerization Polar-Surface-Area  
JChemforExcel  
JChem-search  
Markush



ChemAxon  
cheminformatics solved

# Why ChemAxon:

*Industry leader for enterprise & web based structure content management & delivery*

- Platform independent & web ready
- Industry leading performance and support
- Covers the functionality of most platform competitors
- Widest / deepest file format support
- Various ways to work with functionality (API/services...)
- Deployed widely throughout STM publishing
- Major inertia and adoption in pharma and biotech
- Still called JChem and we are still called ChemAxon
- Friendly commercial terms, pragmatic approach

## Commercial

- Aureus Pharma
- Cengage
- Council of Europe
- CCDC
- Elsevier
- EPO
- GVK Bio
- IBM
- Informa/T&F/CRC Press
- Pearson
- RSC
- Nature / SureChem
- Thomson Reuters
- Wiley

## Public/free

- Binding DB
- EPA (ACToR, +)
- EMBL EP
- IUCr
- KAIST
- Ligand Depot
- NIH NLM
- NIH NIAID
- OECD
- RCSB PDB
- U. New Mex. (Wombat)
- U. Alberta (DrugBank)
- ZINC

• ...

# What's hot for this room

Markush search and enumeration

Marvin JavaScript – beta v soon

Document > DB (Documentum) – v soon

SharePoint (D>S)

Metabolizer

NMR prediction (solubility soon)

Predictor – (training)

...and of course

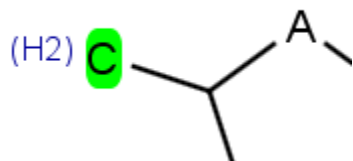
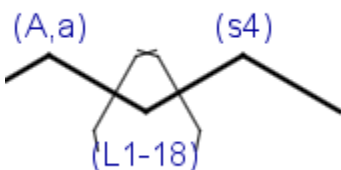
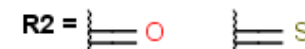
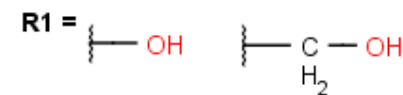
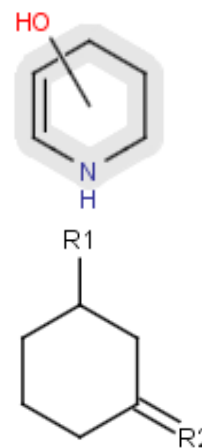
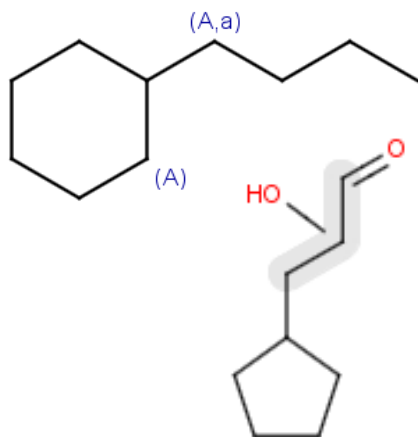
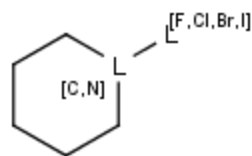
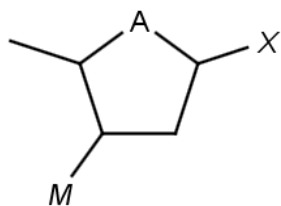
chemicalize.org

Sold  
&  
Deployed

]

# What's hot for this room

## Markush search and enumeration



050611-Demo, Scaffolds

- Markush(1), Scaffold
  - R1 [3]
  - R2 [3]
  - R3 [3]
  - R4 [4]
- 050611-Demo, Scaffolds
  - R1 [2]
  - R7 [2]
  - R10 [2]
  - R11 [2]
  - R20 [2]
  - R8 [3]
  - R9 [3]
  - R2 [3]
  - R3 [4]
  - R4 [3]

050611-Demo, R10

Enumerate a Markush structure

Generate Markush Structure

050611-Demo nesting view

R11

R10

R7

R8

R1

R2

R3

R4

R5

R6

R9

H

CHK

Enumerate a Markush structure

Generate Markush Structure

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[chemicalize.org](http://chemicalize.org)

## List of Organic compounds – chemicalized

W List of organic compoun... x

http://www.chemicalize.org/?q=http://en.wikipedia.org/wiki/List\_of\_organic\_compounds

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

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Article Discussion

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## 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: [A](#) [B](#) [C](#) [D](#) [E](#) [F](#) [G](#) [H](#) [I](#) [J](#) [K](#) [L](#) [M](#) [N](#) [O](#) [P](#) [Q](#) [R](#) [S](#) [T](#) [U](#) [V](#) [W](#) [X](#) [Y](#) [Z](#) See also [External links](#)

**A** [edit]

For substances with an A- or α- prefix such as [α-Terpinene](#), please

- [Abietic acid](#) - C<sub>20</sub>H<sub>30</sub>O<sub>2</sub>
- [Acenaphthene](#) - C<sub>12</sub>H<sub>10</sub>
- [Acenaphthoquinone](#) - C<sub>12</sub>H<sub>6</sub>O<sub>2</sub>
- [Acenaphthylene](#) - C<sub>12</sub>H<sub>8</sub>
- [Acetpromazine](#) - C<sub>19</sub>H<sub>22</sub>N<sub>2</sub>O<sub>2</sub>S
- [Acetaldehyde](#) - C<sub>2</sub>H<sub>4</sub>O
- [Acetamide](#)
- [Acetaminophen](#)
- [Acetaminophenol](#)
- [Acetamidophenol](#)
- [Acetanilide](#)
- [Acetic acid](#)
- [Acetoguanine](#)
- [Acetone](#)
- [Acetonitrile](#)
- [Acetophenone](#)
- [Acetylcholine](#)
- [Acetylene](#)
- [N-Acetylglucosamine](#)
- [Acetylsalicylic Acid](#) - C<sub>9</sub>H<sub>8</sub>O<sub>4</sub> (also known as Aspirin)
- [Acid fuchsin](#)
- [Acridine](#) — C<sub>13</sub>H<sub>9</sub>N
- [Acridine orange](#) - C<sub>17</sub>H<sub>13</sub>N<sub>3</sub>
- [Acrolein](#) — C<sub>3</sub>H<sub>4</sub>O
- [Acrylamide](#) — C<sub>3</sub>H<sub>5</sub>NO
- [Acrylic acid](#) — C<sub>3</sub>H<sub>4</sub>O<sub>2</sub>
- [Acrylonitrile](#) - C<sub>3</sub>H<sub>3</sub>N

**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**

**Acetpromazine** chemicalized by ChemAxon

Report error

# Old news but not to be forgotten

- We are interested in the topic (no exit strategy)
- Major and increasing adoption of back end platform by large pharma (and others)
- Free
  - for academic teaching and research
  - for free websites
  - eval - incl. Markush search against full TR content
- What are the users doing with us:
  - UGM archives (7 years) all slides available, many with videos
- Public forum (see how we support real users)
- Most enterprise functionality available through desktop applications (...4XL and IJC)

Sold  
&  
Deployed



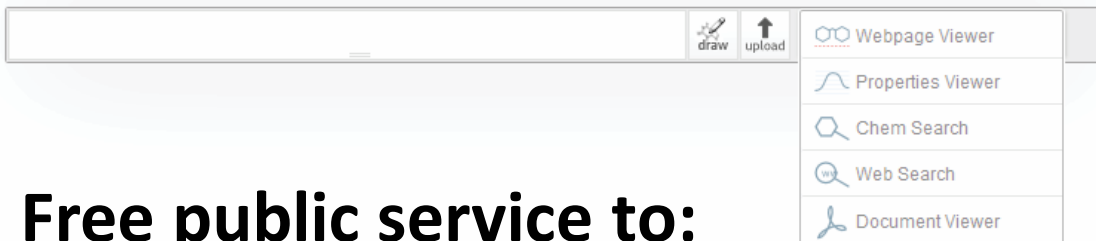
Thanks



 chemicalize.org<sup>beta</sup>

The logo for chemicalize.org consists of two blue-outlined hexagons connected at one side, followed by the text "chemicalize.org" in a dark grey, sans-serif font. The word "beta" is written in a smaller, orange font as a superscript to the right of ".org".

Type a chemical name or URL to begin



**chemicalize.org**

## Free public service to:

- Identify and add chemical structures to web pages and pdf documents on demand
- Search all structures (and URL's) already chemicalized (structure search the web!)
- See predicted properties for discrete chemical structures
- Add chemistry to search engine searches
- Gather links of interest to chemists for post processing (search, analysis, reporting, fun...)

chemicalize >