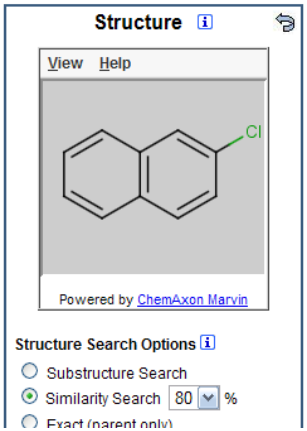
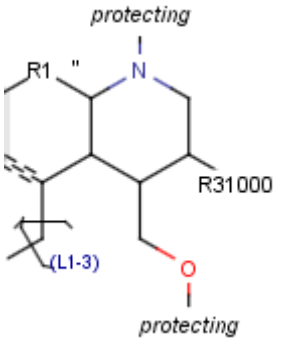
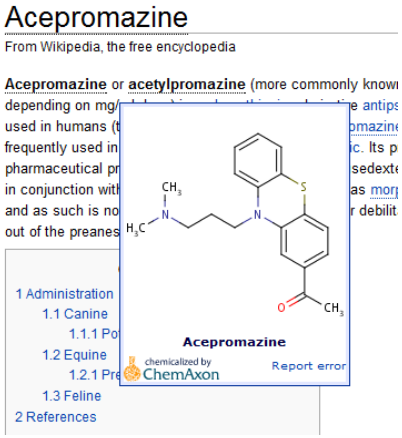






ChemAxon relevance to:

Publishers, IP specialists, any chemist…

Alex Allardyce

ChemAxon
Solutions for Cheminformatics

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...

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

JKlustor
Clustering & diversity analysis

Fragmenter
Decomposition to fragments and R-groups

Screen
HT pharmacophore screening

Add-ons

Markush Search
Store & search Markush structures

JChem Webservices
Web services integration interface

Innovation for IP professionals - MMS structure storage and search

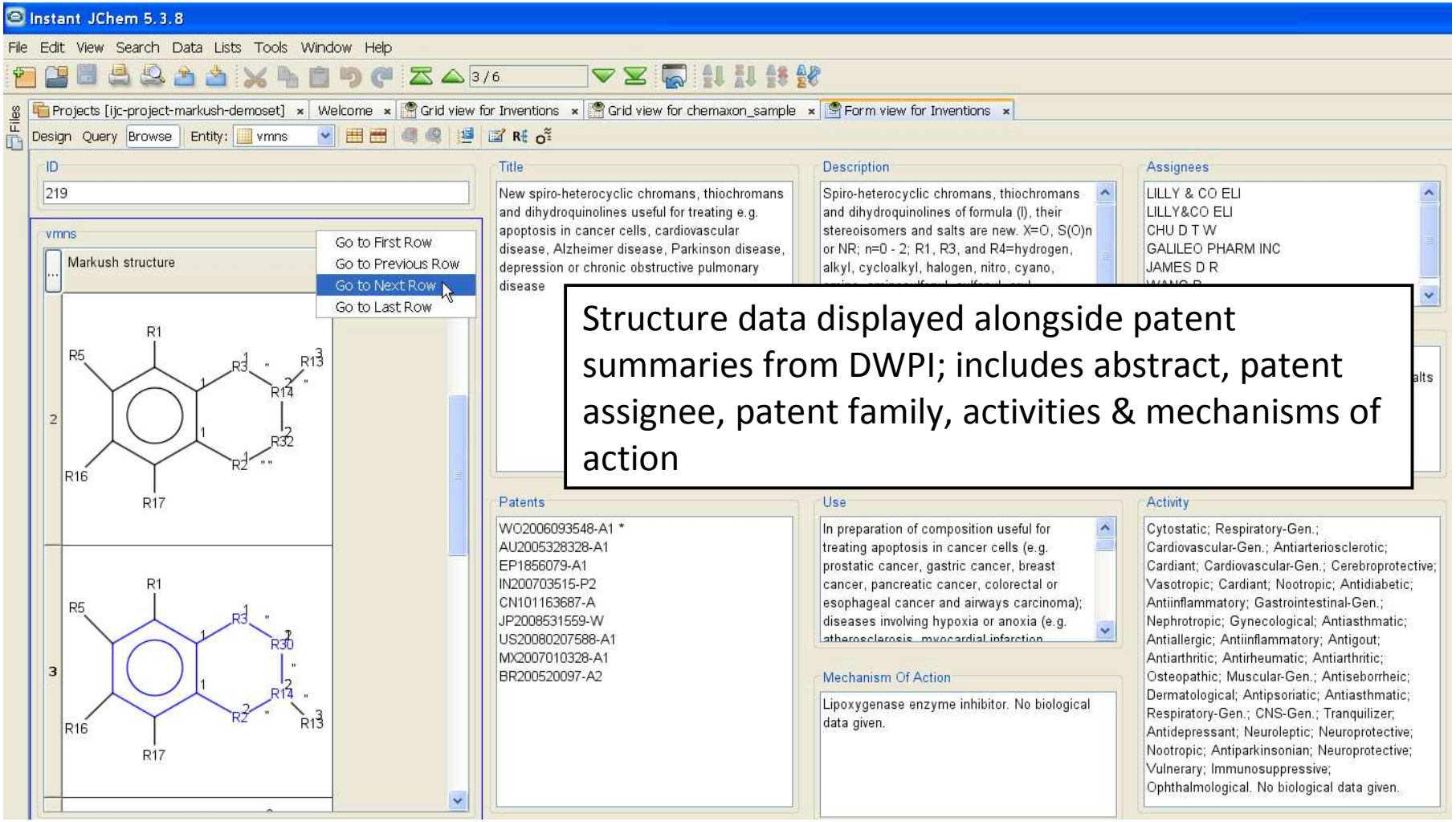
Toolkit and desktop application choices for storing and searching Markush structures (without enumeration).

Includes Markush enumeration and interactive visualization for advanced Markush manipulation.

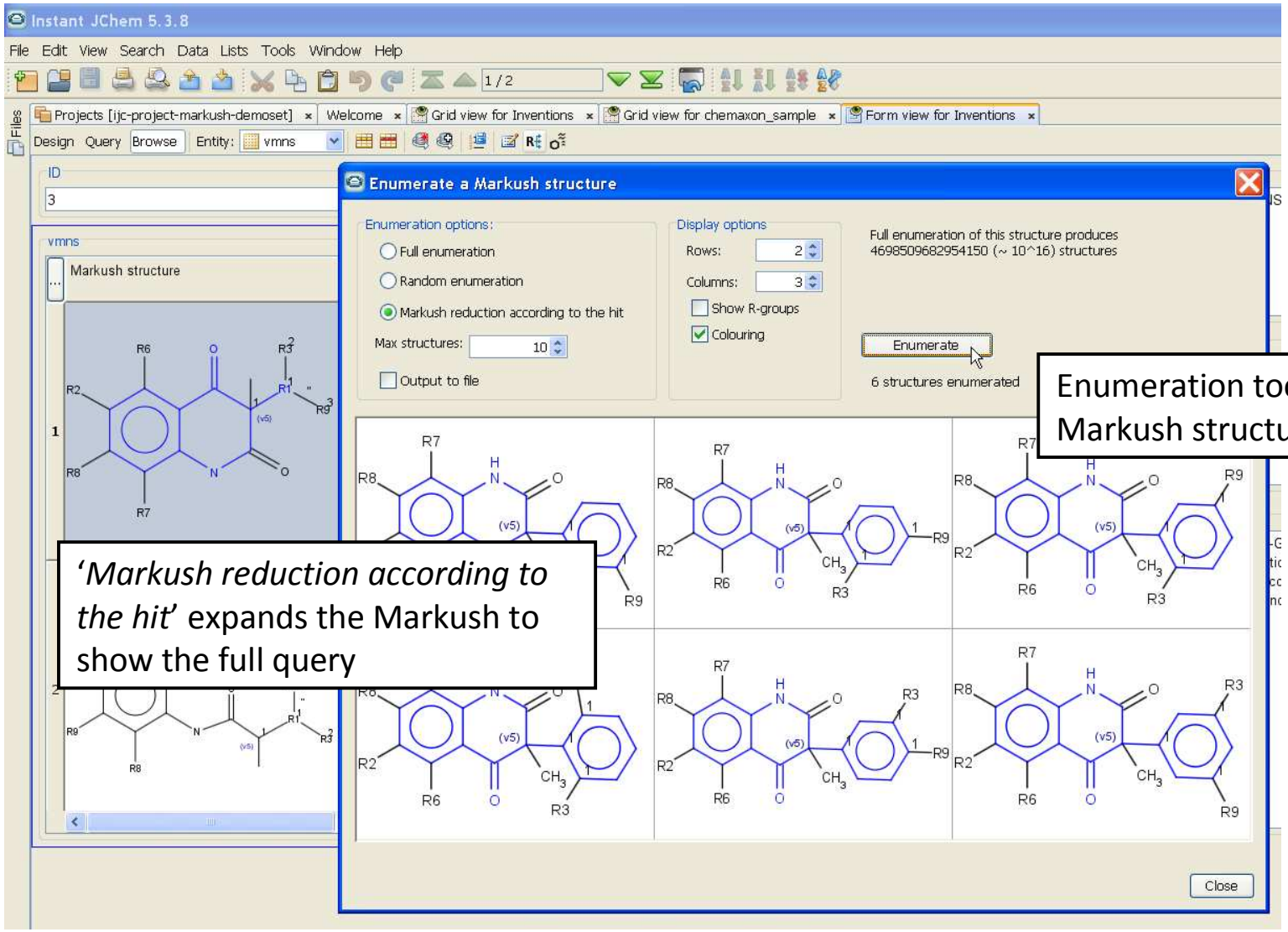
Use cases:

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

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



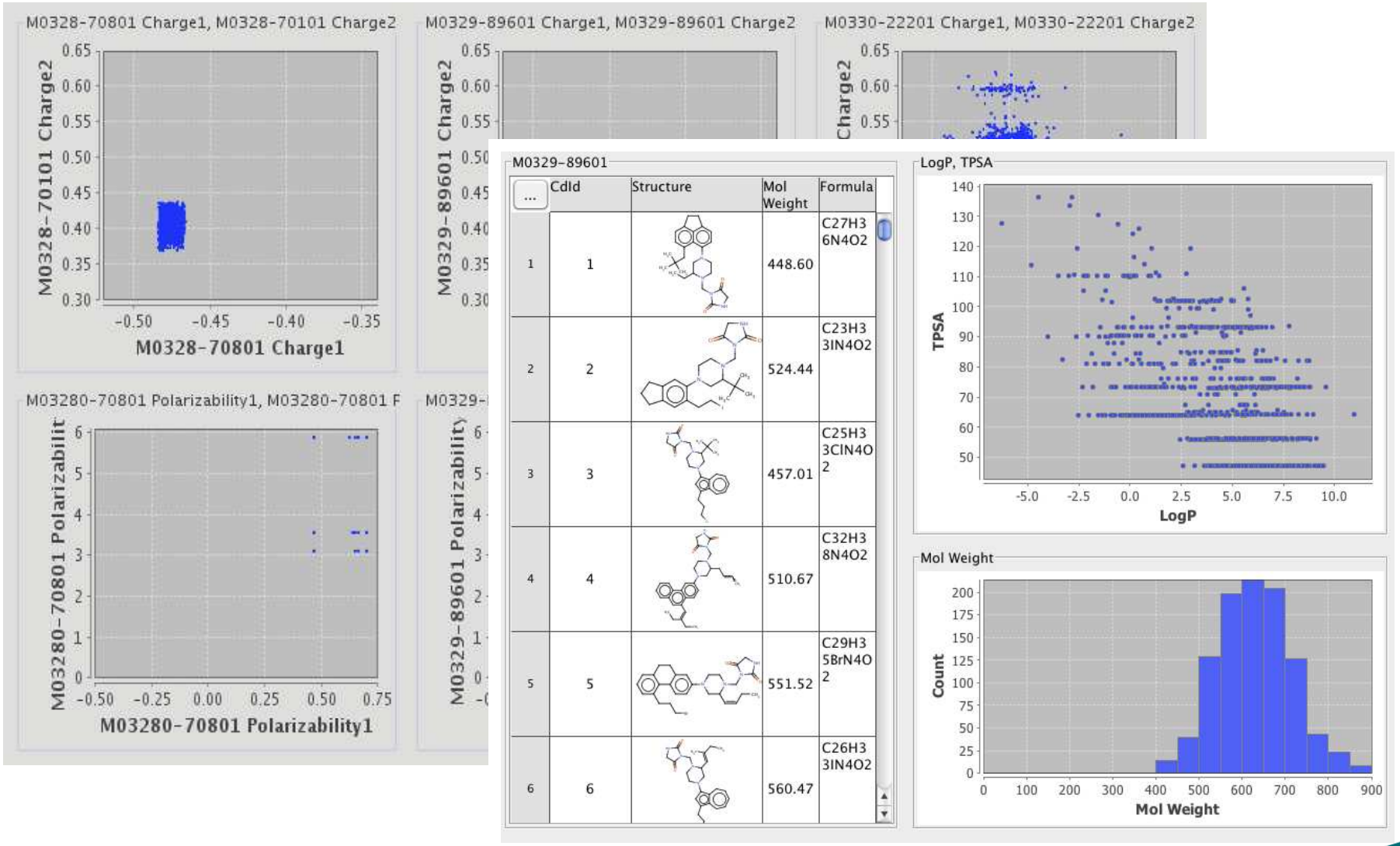
Highlighted search results, ‘reduced’ Markush hits & selective enumeration

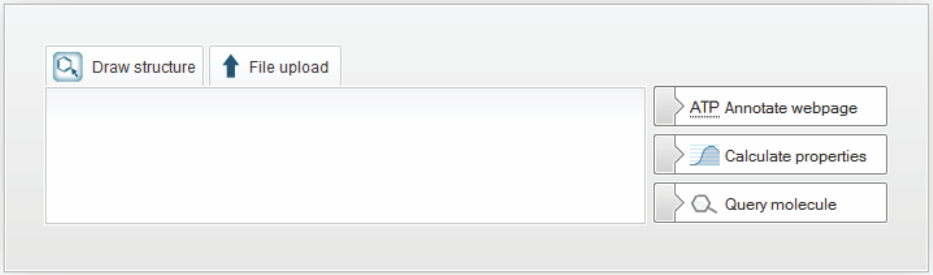


Enumeration tool enables Markush structure mining

‘*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



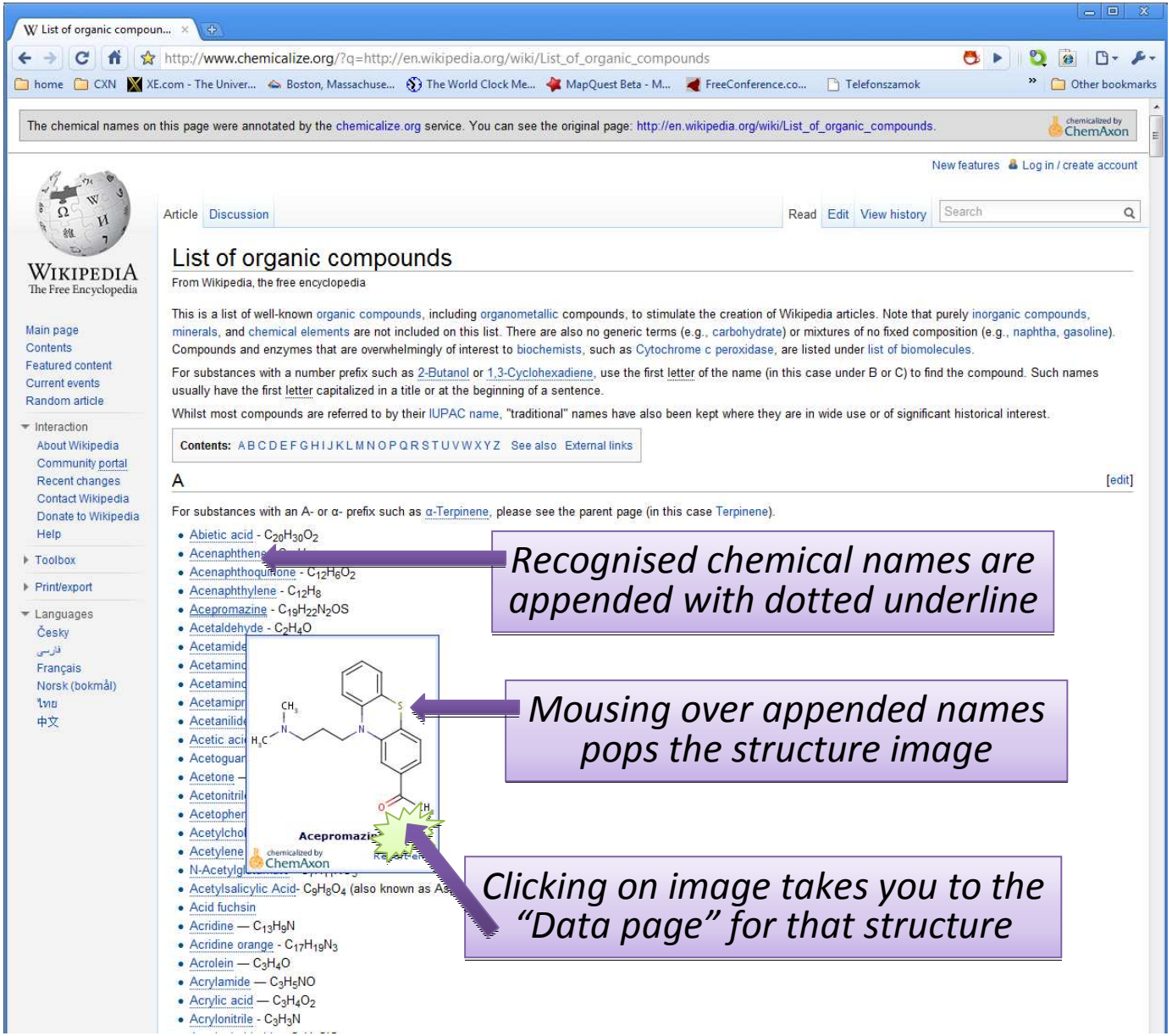


chemicalize.org

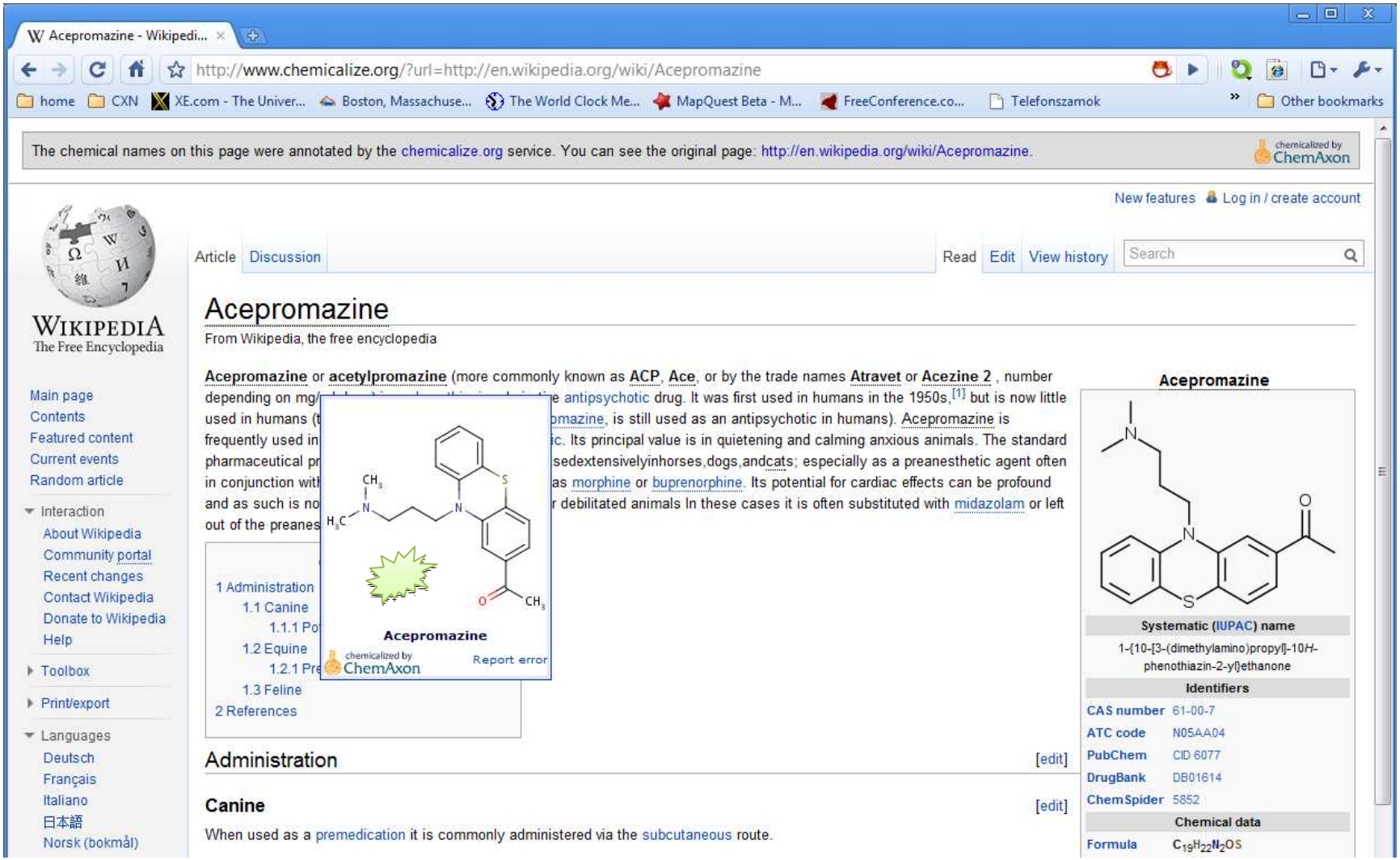
Free public service to:

- 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…)

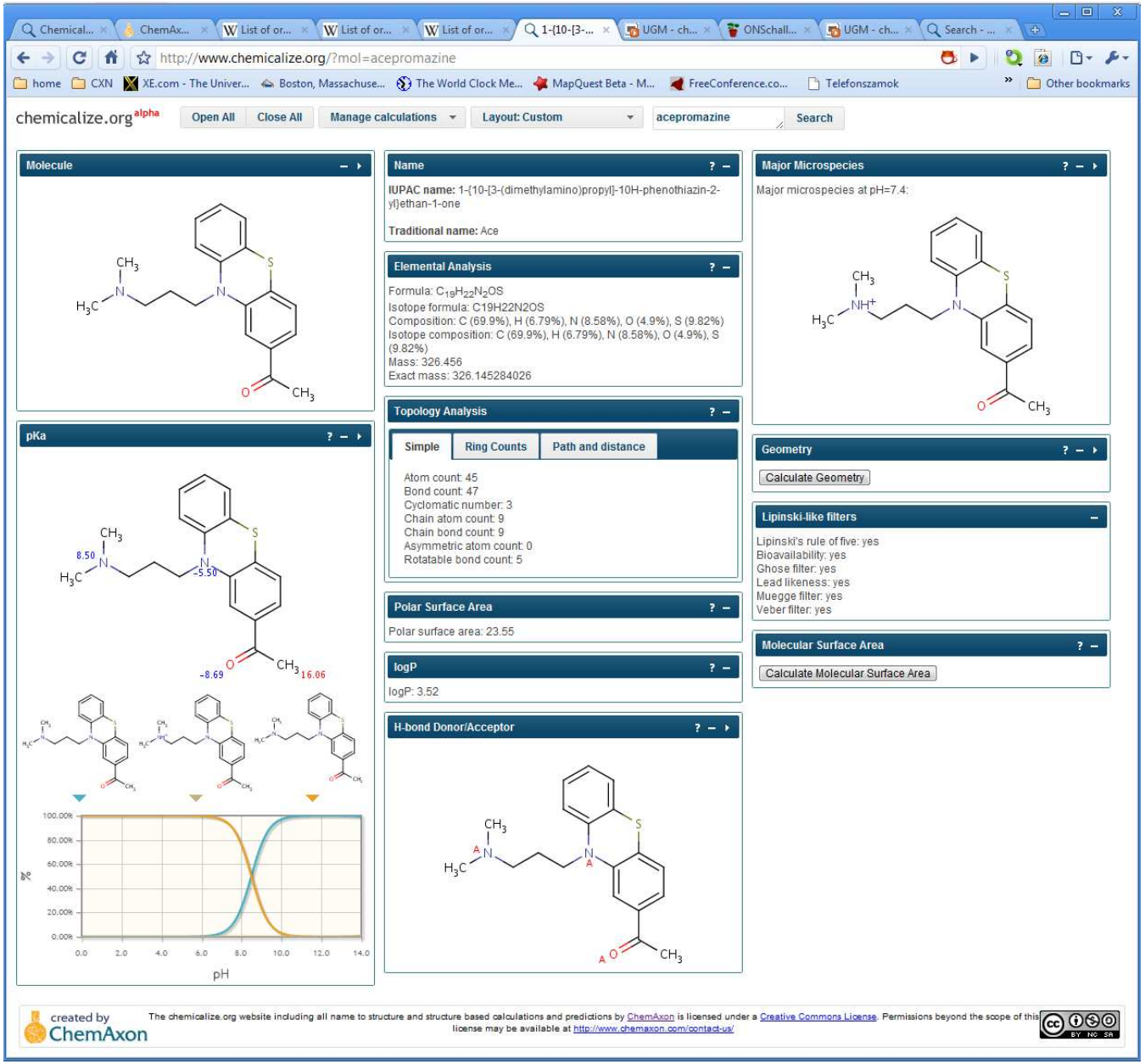
Wikipedia: List of Organic compounds – chemicalized



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



Datapage for “ace”: extensive predicted properties



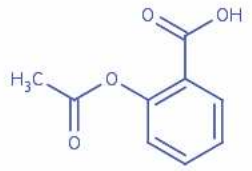
Customizable report layout for calculation results.

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

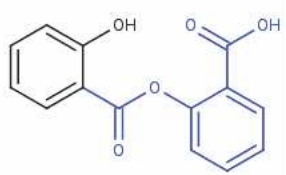
Searching the web: Aspirin; searching chemicalize.org - query highlighted in results

Aspirin | Draw Structure | - Search type - | ? | Search | Advanced input

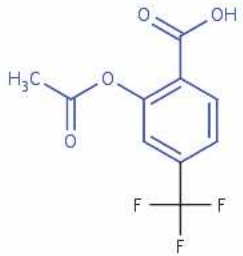
16 structures found:



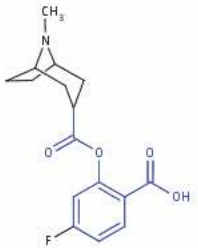
Formula $C_9H_8O_4$ Refine
ID 92
Properties



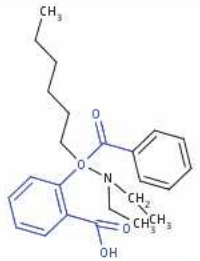
Formula $C_{14}H_{10}O_5$ Refine
ID 2245
Properties



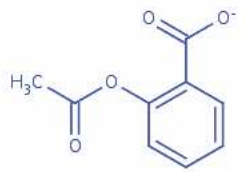
Formula $C_{10}H_7F_3O_4$ Refine
ID 7037
Properties



Formula $C_{16}H_{18}FNO_4$ Refine
ID 7814
Properties

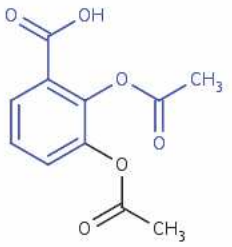


Formula $C_{24}H_{33}NO_4$ Refine
ID 7903
Properties

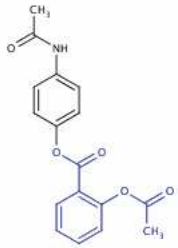


Formula $C_9H_7O_4$ Refine
ID 8629
Properties

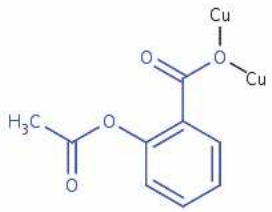
Formula $C_9H_8AlO_5$ Refine
ID 9371
Properties



Formula $C_{11}H_{10}O_6$ Refine
ID 10324
Properties



Formula $C_{17}H_{15}NO_5$ Refine
ID 10626
Properties

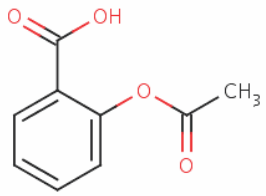


Formula $C_9H_7Cu_2O_4$ Refine
ID 13263
Properties

1 2 Next »

searching chemicalize.org: Aspirin; web page hits
No structures shown

« Back to search | Structure found on 7457 pages:



Formula Search
$C_9H_8O_4$
ID
92
Properties

Structure appears as
- Aspirin

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:

Formula
$C_9H_8O_4$
ID
92
Properties

Search

Structure appears as
- Aspirin

hide all related structures ‹

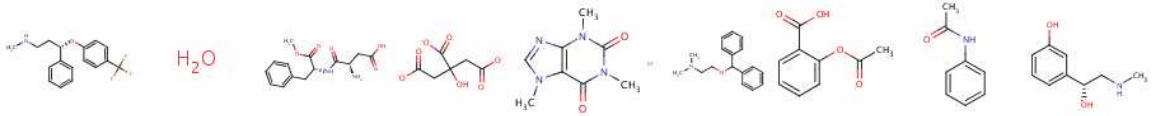
show all related links ›

Diverse

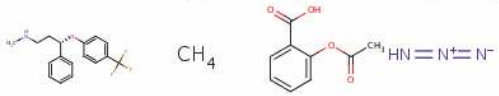
Select to show a diverse selection of the structures on linked web pages

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

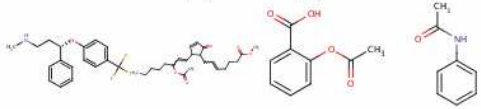
Excedrin - Wikipedia, the free encyclopedia
1 Apr 2010 - original page
en.wikipedia.org/wiki/Excedrin
- hide structures on this page + show pages from en.wikipedia.org



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