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)

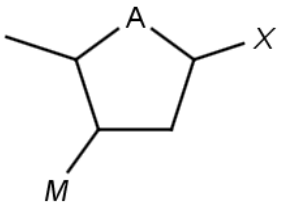
Predictor – (training)

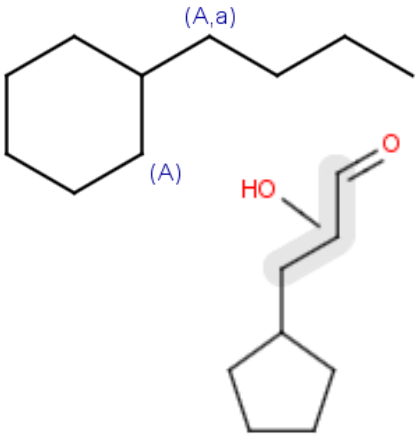
…and of course

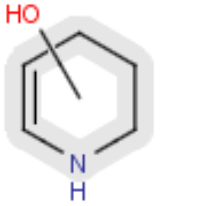
chemicalize.org

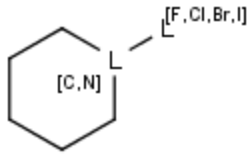
What's hot for this room

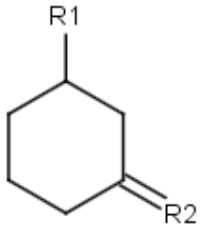
Markush search and enumeration

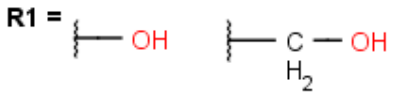


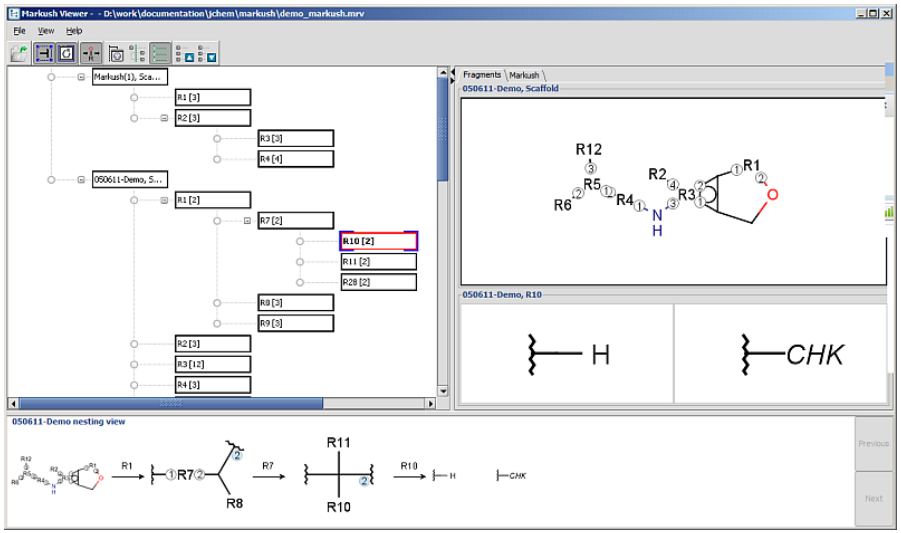


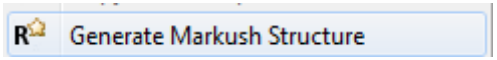


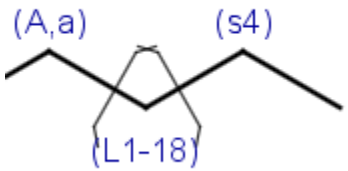


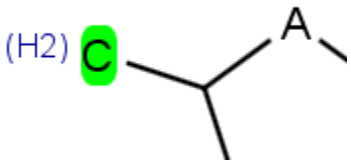












What's hot for this room

Markush search and enumeration

Marvin JavaScript – beta v soon

Document > DB (Documentum) – v soon

SharePoint (D>S)

Metabolizer

NMR prediction (solubility soon)

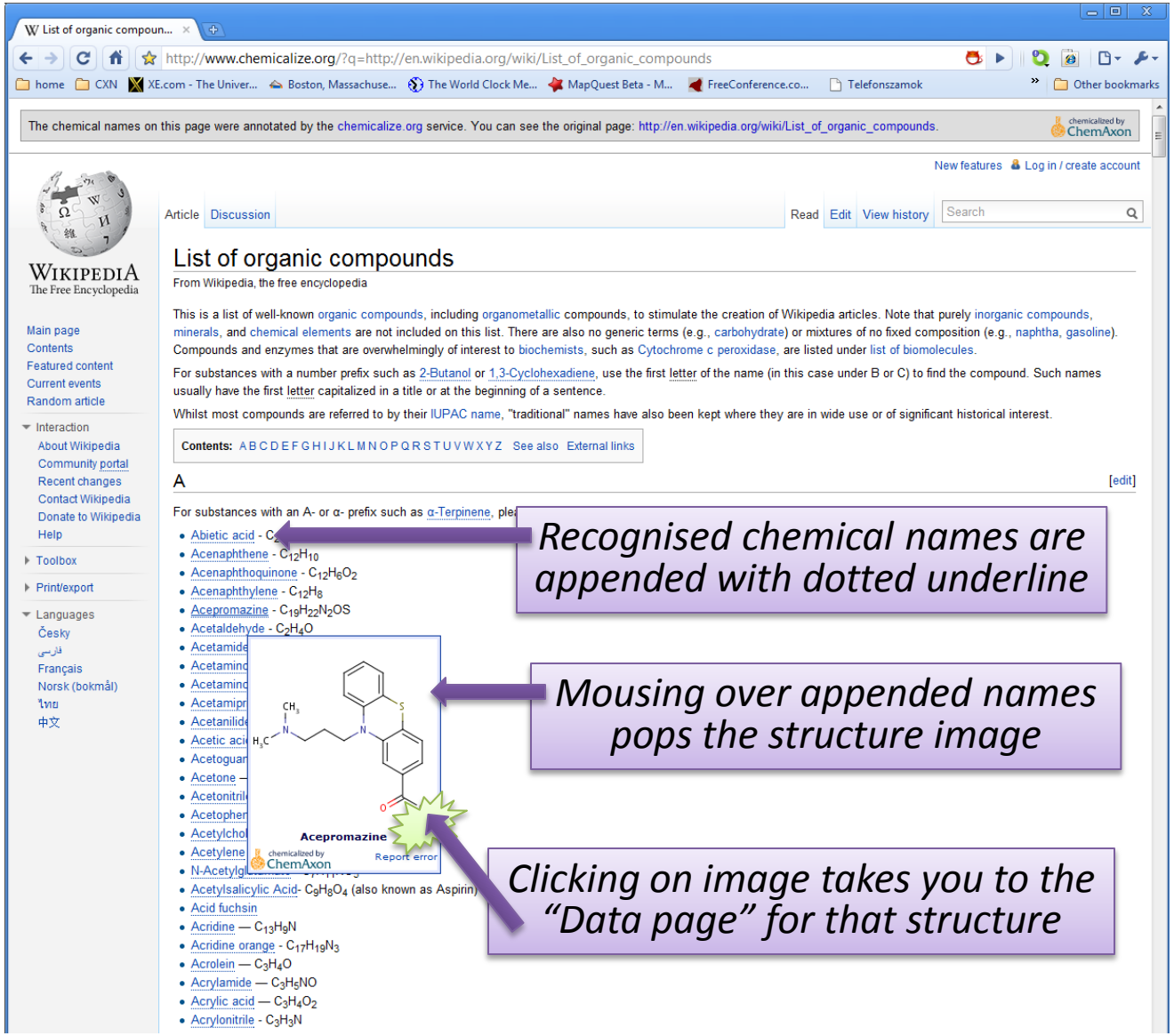
Predictor – (training)

…and of course

chemicalize.org

Webpage Viewer

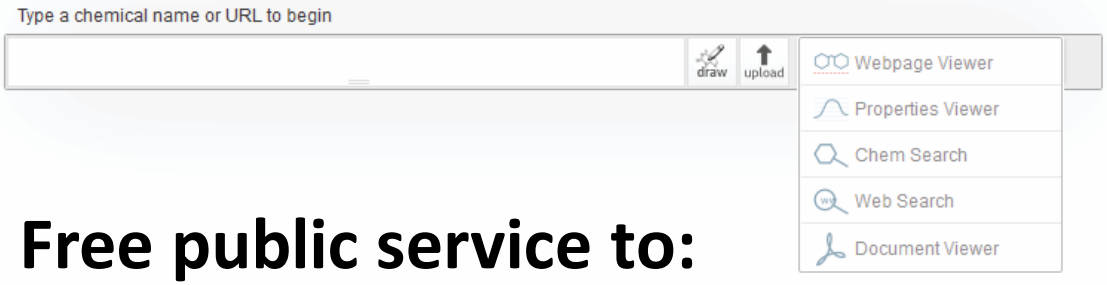
Wikipedia: List of Organic compounds – chemicalized



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)

Thanks



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 ›