CWM Global Search: The internet search engine for chemists and biologists

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Hunting for information on the internet

Requirements:

- Information has to be up-to-date
- Information should not originate from databases containing data extracted from other sources on the internet (delay in up-dating data and indices)
- Information should be as comprehensive as possible and cover a wide area of interest

Solution:

- **Federated Searching** over publicly available major databases
- A federated search is 100% up-to-date in respect to the databases included
- A federated search is comprehensive; the domain of the search is a union of all databases in the search chain

.......CWM Global Search

August, 20, 2012

ACS Philadelphia
CWM Global Search

What is CWM Global Search?

CWM Global Search provides a single User Interface allowing for a true federated search over more than 60 major scientific databases and drug discovery data sources publicly available on the internet, using:

- Chemical Structure
- Chemical name
- CAS Registry numbers
This are the Results, not the quick search results. The quick search results are in the advanced search page. Tip: If you want to have a blue box around your text use "Formkontur"
Search for and comparison of two antifungal drugs – Balofloxacin and Prulifloxacin
Search results for Balofloxacin
CWM Global Search

Profile Search

Maslinic acid

The following data sources are defined in profile:
- CHEBI
- CHEMSPIDER
- GOOGLE
- PUBCHEM
- Quertle
- WIKIPEDIA
CWM Global Search

Results from Wikipedia hit

Clove
From Wikipedia, the free encyclopedia

This article needs additional citations for verification. Please help improve this article by adding citations to reliable sources. Unsourced material may be challenged and removed. (June 2009)

This article is about the spice. For other uses, see Clove (disambiguation).

Clove buds (Syzygium aromaticum) are the aromatic dried flower buds of a tree in the family Myrtaceae. Clove buds are native to the Maluku islands in Indonesia and used as a spice in cuisines all over the world. Cloves are harvested primarily in Indonesia, India, Madagascar, Zanzibar, Pakistan, and Sri Lanka. They have a numbing effect on mouth tissues.

The clove tree is an evergreen that grows to a height ranging from 6–12 m, having large leaves and sanguine flowers in numerous groups of terminal clusters. The flower buds are at first of a pale color and gradually become green, after which they develop into a bright red, when they are ready for collecting. Cloves are harvested when 1.5–2 cm long, and consist of a long calyx, terminating in four spreading sepals, and four unopened petals which form a small ball in the center.

Contents
1 Taxonomy and nomenclature
2 Uses
   1.1 Non-culinary uses
   2.2 Traditional medicinal uses
   2.3 Medicinal uses and Pharmaceutical preparations
3 Adulteration
4 History
5 Active compounds
6 See also
7 Notes and references

Active compounds

Eugenol comprises 72-80% of the essential oil extracted from cloves, and is the compound most responsible for the cloves' aroma. Other important essential oil constituents of clove oil include acetyl eugenol, beta-caryophyllene and vanillin, caryophyllene oxide, eugenol carboxylic acid, caryophyllene oxide, gallic acid, methyl salicylate (painkiller), the flavonoids eugenin, kaempferol, rhapontin, and eugenitin; terpenoids like oleanolic acid, stigmasterol and campessterol; and several sesquiterpenes.\(^{[20]}\)\(^{[21]}\)

Eugenol has pronounced antiseptic and anaesthetic properties. Of the dried buds, 15 - 20 percent is essential oils, and the majority of this is eugenol. A kilogram (2.2 lbs) of dried buds yields approximately 160 ml (1/4 of a pint) of eugenol.\(^{[22]}\)\(^{[unreliable source]}\)

Eugenol can be toxic in relatively small quantities—as low as 5 ml.\(^{[23]}\)

“Hidden treasure” find:
• No reference to original query term or CAS Registry Number
• CWM Global Search extended query to involve synonyms

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AKos Consulting & Solutions GmbH

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Search for derivatives of Oxytocin with unnatural amino acid in positions 3 or 8

3-Letter code for Oxytocin substructure generated with Proteax
Substructure search in ChEBI and result

24 ChEBI ID(s) found
Partial listings of the hits from ChEBI

<table>
<thead>
<tr>
<th>ID</th>
<th>Name</th>
<th>Formula</th>
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<td>oxytocin</td>
<td>(19-Amino-10-(2-carbamoyl-ethyl)-7-carbamoylmethyl-16-(4-hydroxy-benzyl)-18-(4-nitro-benzyl)-6,9,12,15,18-pentaoxo-1,2-dithia-6,8,11,14,17-pentaza-cyclooctane-4-carbonoyl-pyrrolidine-2-carbonyl-9-amino-5-guanido-pentanoylaminoo-acetic acid</td>
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</table>
Comparison: Oxytocin and derivative with different amino acid in position 3

Oxytocin derivative

Tyrosine

"Unusual" amino acid

Oxytocin
Requirements for CWM Global Search:

- Windows or Macintosh computer
- Silverlight Plugin and Java

Full version of CWM Global Search available for 30-day free trial at:

http://www.akosgmbh.de/globalsearch/licensekeyrequest.htm

For questions or further information:

- e-mail: globalsearch@akosgmbh.de
- website: http://www.akosgmbh.de

Please add that a free version is also available.