

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

Guenter Grethe, Hans-Jürgen Himmeler, Alexander Kos

244th ACS National Meeting, Philadelphia, PA – August 19-23, 2012

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

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**

CWM Global Search



Home Page

CWM Global Search

Home Simple search Advanced search Results

QuickSearch Add/Remove custom profile Clear structure box Clear text box Find tautomers for structure Find structure for chemical name Find structures using name patterns Help

Simple search

☒ Search all datasources
☐ Search profiles

Chemical structure: CCOC(=O)C(C1CCCCC1)C2CCCCC2N

☐ Include isomers
☐ Include Substructures
☐ Include similar compounds
Similarity coefficient (1-100)
90.00

Search for CAS Registry number or synonym name or systematic name or free text
e.g. silver nitrate or tamiflu or 50-78-2 or antirheumatic

Search All Data Sources

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CWM Global Search



CWM Global Search

Quick Search Results

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"

CWM Global Search

Home Simple search Advanced search Results

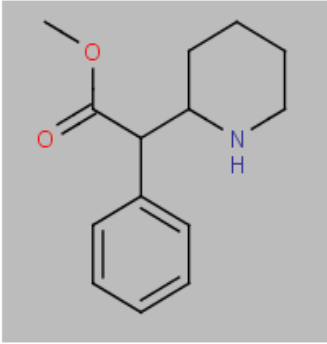
Export results Open selected links in Browser Cancel search Cancel Help

Results

7/20/2012 9:31:13
7/20/2012 9:32:32

Structure

Double click to zoom structure



Chemical structure: COC(=O)C(c1ccccc1)N2CCCC2

Globalsearch links Quicklinks

Remove all filter

Extreg	Number of hits
RECORD_1	79

1 2 3 4

Drag a column header and drop it here to group by that column

Rank		Datasource	Link	Category
11	<input checked="" type="checkbox"/>	ChEBI	1 ChEBI ID(s) found.	Bioactivity
7	<input type="checkbox"/>	ChemExper	Hit(s) found	Suppliers
6	<input type="checkbox"/>	Chemicalland21	8 Hit(s)	Chemistry
1	<input type="checkbox"/>	PubChem	Hit(s) found	Bioactivity
2	<input type="checkbox"/>	ChemSpider	Hit(s) found	Chemistrv

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Results from EBI and PubChem

EMBL-EBI

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ChEBI Home

Advanced Search

Browse

Submissions

Downloads

Documentation

Developer Resources

Preferences

Contact ChEBI

Printer Friendly View

EBI > Databases > Small Molecules > ChEBI > Main

methylphenidate (CHEBI:6887)

Main

ChEBI Ontology

Automatic Xrefs

ChEBI Name

methylphenidate

ChEBI ID

CHEBI:6887

Stars

☆☆☆

This entity has been manually annotated by the ChEBI Team.

Secondary ChEBI IDs

CHEBI:14

See structure as:

Image

App

Download Molfile

Find compounds which contain this structure

Find compounds which resemble this structure

Wikipedia

We are unable to retrieve the wikipedia information for this entry at this time

Read full article at Wikipedia

Formula

C₁₄H₁₉NO₂

Net Charge

0

Average Mass

233.30620

InChI

InChI=1S/C₁₄H₁₉NO₂/c1-17-14(16)13(11-7-3-2-4-8-1)

InChIKey

InChIKey=DUGOZIWWEXMGBE-UHFFFAOYSA-N

SMILES

COC(=O)C(C1CCCCN1)c1ccccc1

ChEBI Ontology

Outgoing

methylphenidate (CHEBI:6887) is a carboxylic ester (CHEBI:33308)

methylphenidate (CHEBI:6887) is conjugate base of methylphenidate(1+) (CHEBI:51856)

NCBI

PubChem Compound

Search

Methylphenidate - Compound Summary (CID 4158)

Also known as: Daytrana, Methylphenidan, Phenidylate, Calocain, Methylin, Plimasine, Meridil, Ritalin-SR, Centedrin

Molecular Formula: C₁₄H₁₉NO₂ Molecular Weight: 233.30616 InChIKey: DUGOZIWWEXMGBE-UHFFFAOYSA-N

A central nervous system stimulant used most commonly in the treatment of attention-deficit disorders in children and for narcolepsy. Its mechanisms appear to be similar to those of DEXTROAMPHETAMINE. From: MeSH

Table of Contents

Show subcontent titles

Identification

Related Records

Use and Manufacturing

Pharmacology

Biomedical Effects and Toxicity

Safety and Handling

Exposure Standards and Regulations

Monitoring and Analysis Methods

Literature

Patents

Biomolecular Interactions and Pathways

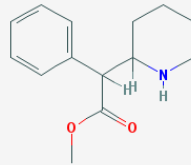
Biological Test Results

Classification

Chemical and Physical Properties

2D Structure

3D Conformer



Links and Related Information

Properties

Compound ID: 4158

Molecular Weight: 233.30616 [g/mol]

Molecular Formula: C₁₄H₁₉NO₂

XLogP3: 0.2

H-Bond Donor: 1

H-Bond Acceptor: 3

BioActivity Data Links

This Compound

with Similar Compounds

with Similar Conformers

Related Compounds

Same, Connectivity (18)

Same, Stereochemistry (4)

Same, Isotopes (8)

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Search for and comparison of two antifungal drugs – Balofloxacin and Prulifloxacin

Search results for Prulifloxacin

Search for CAS Registry number or synonym name or systematic name or free text.

Query

Balofloxacin
Prulifloxacin

Results

7/21/2012 7:04:52
7/21/2012 7:06:09
Query : Prulifloxacin
7/21/2012 7:06:09
Query : Balofloxacin

Structure

Double click to zoom structure

Chemical structure of Prulifloxacin

Globalsearch links

Remove all filter

RECORD_1 70

Drag a column header and drop it here to group by that column

Rank	Datasource	Link	Category	Keywords	Searchtype	Query
7	ChemExper	Hit(s) found	Suppliers		CASNUMBER	123447-62
6	Chemicaland21	3 Hit(s)	Chemistry		CASNUMBER	123447-62
1	PubChem	Hit(s) found	Bioactivity		CASNUMBER	123447-62
9	eMolecules	Results 1-1 of 1	Suppliers		CASNUMBER	123447-62
2	ChemSpider	Hit(s) found	Chemistry		CASNUMBER	123447-62
14	Google	About 56,200 results	Search engine		CASNUMBER	123447-62

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Search results for Balofloxacin

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Home Simple search Advanced search Results

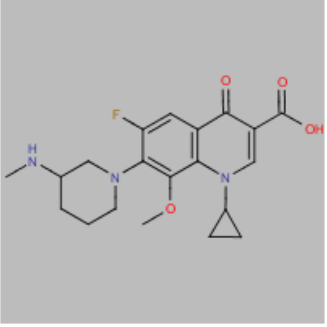
Export results Open selected links in Browser Cancel search Session manager Help

Results

7/21/2012 7:04:52
7/21/2012 7:06:09
Query : Prulifloxacin
7/21/2012 7:06:09
Query : Balofloxacin

Structure

Double click to zoom structure



Globalsearch links Quicklinks

Remove all filter

Count	Source	Results	Category	Database
6	Chemicaland21	4 Hit(s)	Chemistry	CAS
1	PubChem	Results: 2	Bioactivity	CAS
7	ChemExper	Hit(s) found	Suppliers	CAS
9	eMolecules	Results 1-1 of 1	Suppliers	CAS
18	CHEMICALDATABASE	Documents 1 - 1 of 1 matches.	Chemistry	CAS
4	ChemicalBook	Results 1 - 1 of 1	Suppliers	CAS
22	Wikipedia	Result 1 of 1	Dictionary	CAS
41	PubMedCentral	Results: 7	Literature	CAS
27	ChemIDPlus	Hit(s) found	Toxicity	CAS
1	PubChem	Results: 4	Bioactivity	SYN
2	ChemSpider	2 hits found	Chemistry	SYN

CWM Global Search



NCBI PubChem Compound

Search

prulifloxacin - Compound Summary (CID 65947)

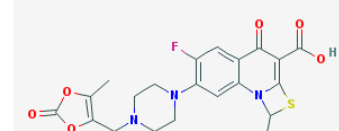
Also known as: Pruvex, NM 441, CCRIS 7686, 123447-62-1
Molecular Formula: $C_{21}H_{29}FN_3O_5S$ Molecular Weight: 461.463403 InChIKey: PWNMXPKBYZCOO-UHFFFAOYSA-N

Table of Contents

- Identification
- Related Records
- Literature
- Patents
- Biological Test Results
- Classification
- Chemical and Physical Properties

Expand all sub-sections

2D Structure 3D Conformer



Links and Related Information

Properties

Compound ID: 65947
Molecular Weight: 461.463403 [g/mol]
Molecular Formula: $C_{21}H_{29}FN_3O_5S$
XLogP3-AA: 1
H-Bond Donor: 1
H-Bond Acceptor: 11

BioActivity Data Links

- This Compound
- with Similar Compounds
- with Similar Conformers

Information about
Prulifloxacin in PubChem

Information about
Balofloxacin in
PubMedCentral

NCBI Resources How To

PMC US National Library of Medicine National Institutes of Health

Search 127294-70-6[EC/RN Number]

Save search Limits Advanced Journal List

Display Settings: Summary, 20 per page, Sorted by Default order

Send to: Filter your results:

All (7)
NIH grants (0)

Manage Filters

Find related data

Database: Select

Find items

Search details

"127294-70-6"[EC/RN Number]

Search

See more...

Results: 7

- Comparative study of pharmacokinetics of two new fluoroquinolones, balofloxacin and grepafloxacin, in elderly subjects.
1. O Kozawa, T Uematsu, H Matsuno, M Niwa, S Nagashima, M Kanamaru
Antimicrob Agents Chemother. 1996 December; 40(12): 2824-2828.
PMCID: PMC163630
[Summary](#) [PDF-209K](#)
- Reduced phototoxicity of a fluoroquinolone antibacterial agent with a methoxy group at the 8 position in mice irradiated with long-wavelength UV light.
K Marutani, M Matsumoto, Y Otabe, M Nagamuta, K Tanaka, A Miyoshi, T Hasegawa, H Nagano, S Matsubara, R Kamide, et al.
Antimicrob Agents Chemother. 1993 October; 37(10): 2217-2223.
PMCID: PMC192253
[Summary](#) [Page Browse](#) [PDF-1.3M](#)
- Photostability and biological activity of fluoroquinolones substituted at the 8 position after UV irradiation.
M Matsumoto, K Kojima, H Nagano, S Matsubara, T Yokota
Antimicrob Agents Chemother. 1992 August; 36(8): 1715-1719.
PMCID: PMC192036
[Summary](#) [Page Browse](#) [PDF-890K](#)

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Profile Search

CWM Global Search

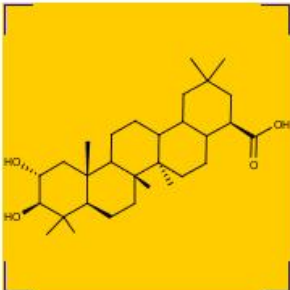
Home Simple search Advanced search Results

QuickSearch Add/Remove custom profile Clear structure box Clear text box Find tautomers for structure Find structure for chemical name Find structures using name patterns Help

Simple search

☐ Search all datasources
☒ Search profiles

Maslinic acid



☒ Include isomers
☐ Include Substructures
☐ Include similar compounds
Similarity coefficient (1-100)
90.00

Search for CAS Registry number or synonym name or systematic name or free text

e.g. silver nitrate or tamiflu or 50-78-2 or antirheumatic

Search Free Data Sources Search for General Information Search in Chemistry Databases Search for Drug Information Search for Suppliers Search for Toxicity Information Search for Chemical Safety Search in Literature

Search in open access journals Search in Patents Sub Structure Search

The following data sources are defined in profile

- CHEBI
- CHEMSPIDER
- GOOGLE
- PUBCHEM
- Quertle
- WIKIPEDIA

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Search results from Profile Search

CWM Global Search v_6.6.3.0 - Windows Internet Explorer

http://cwmglobalsearch.com/gswdev/gswdevnewdesign.html

Home Simple search Advanced search Results

Export results Grid operations Cancel search Cancel Help

Results

6/5/2012 7:56:50 PM
6/5/2012 8:04:47 PM
6/5/2012 8:30:12 PM
6/5/2012 8:32:46 PM

Structure

Double click to zoom structure

Chemical structure image: CC(C)(C)C1C(C(C(C1)O)C(C)C)C(C(C)C)C(C)C

Globalsearch links Quicklinks

Remove all filter

05.06.2012 20:32:46

Extreg	Number of hits
RECORD_1	28

Drag a column header and drop it here to group by that column

Rank	Dataset	Link	Category	Keywords	Searchtype	Query
14	Google	About 48,100 results	Search engine		CASNUMBER	4373-41-5
22	Wikipedia	Result 1 of 1	Dictionary		CASNUMBER	4373-41-5
1	PubChem	Results: 2	Bioactivity		CASNUMBER	4373-41-5
11	ChEBI	100 ChEBI ID(s) found. Top 78 IDs are retrieved	Bioactivity		SYNONYMNAME	"maslinic acid"
11	ChEBI	100 ChEBI ID(s) found. Top 78 IDs are retrieved	Bioactivity		SYNONYMNAME	maslinic acid
11	ChEBI	100 ChEBI ID(s) found. Top 78 IDs are retrieved	Bioactivity		SYNONYMNAME	"Crategolic acid"
14	Google	About 127,000 results	Search engine		SYNONYMNAME	"maslinic acid"
14	Google	About 122,000 results	Search engine		SYNONYMNAME	maslinic acid
14	Google	About 6,090 results	Search engine		SYNONYMNAME	"Crategolic acid"
1	PubChem	Hit(s) found	Bioactivity		FULLSTRUCTURE	
22	Wikipedia	Results 1-5 of 5	Dictionary		SYNONYMNAME	"maslinic acid"
22	Wikipedia	Results 1-5 of 5	Dictionary		SYNONYMNAME	maslinic acid
22	Wikipedia	Result 1 of 1	Dictionary		SYNONYMNAME	"Crategolic acid"
14	Google	About 573 results	Search engine		FULLSTRUCTURE	

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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 \(disambiguation\)](#).

Cloves (*Syzygium aromaticum*) are the aromatic dried [flower buds](#) of a tree in the family [Myrtaceae](#). Cloves 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 8–12 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 [\[hide\]](#)

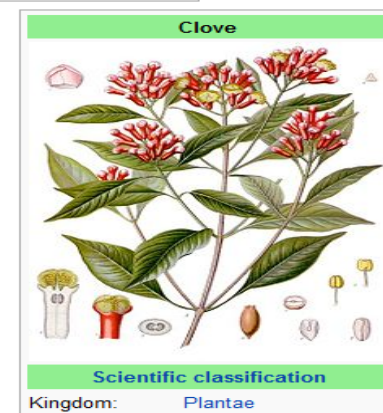
- [Taxonomy and nomenclature](#)
- [Uses](#)
 - [2.1 Non-culinary uses](#)
 - [2.2 Traditional medicinal uses](#)
 - [2.3 Medicinal uses and Pharmaceutical preparations](#)
- [Adulteration](#)
- [History](#)
- [Active compounds](#)
- [See also](#)
- [Notes and references](#)

Active compounds

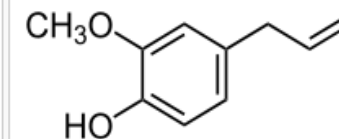
Eugenol comprises 72-90% of the [essential oil](#) extracted from cloves, and is the compound most responsible for the cloves' aroma. Other important essential oil constituents of clove oil include [acetyl eugenol](#), [beta-caryophyllene](#) and [vanillin](#), [categoric acid](#), [tannins](#), [gallotannic acid](#), [methyl salicylate](#) (painkiller); the [flavonoids](#) [eugenin](#), [kaempferol](#), [rhamnetin](#), and [eugenitin](#); [triterpenoids](#) like [oleanolic acid](#), [stigmasterol](#) and [campesterol](#); 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 150 ml (1/4 of pint) of [eugenol](#).^{[22][unreliable source?]}

Eugenol can be toxic in relatively small quantities—as low as 5 ml.^[23]



[\[edit\]](#)

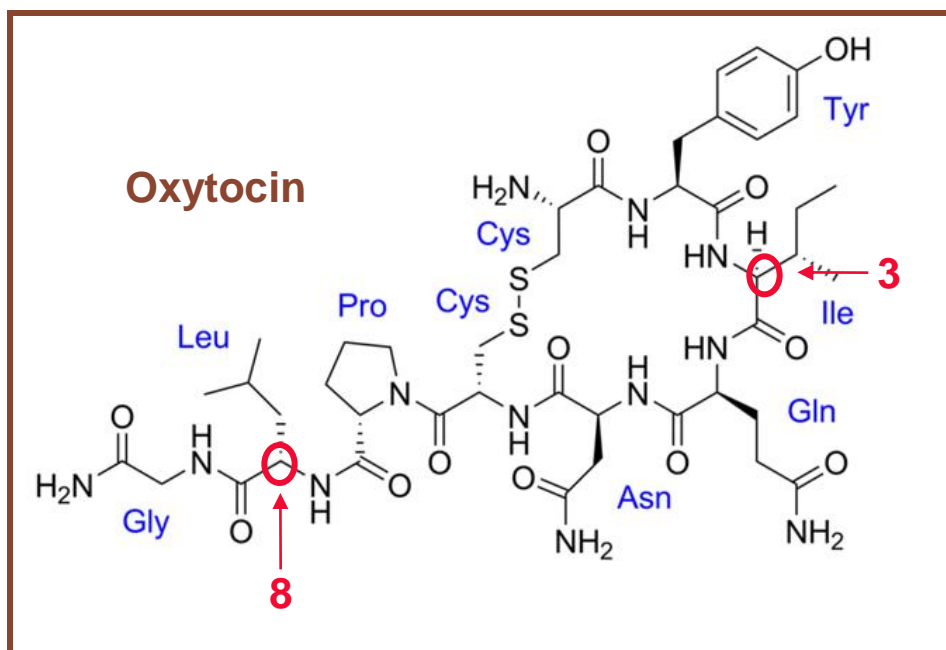
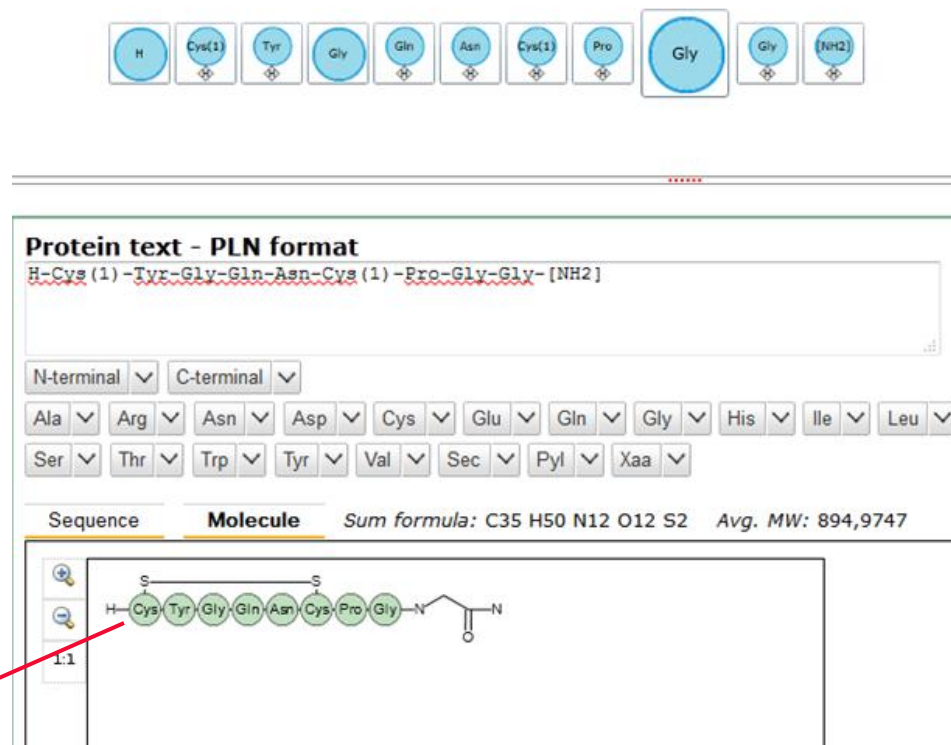


The compound [eugenol](#) is responsible for most of the characteristic aroma of cloves.

“Hidden treasure” find:

- No reference to original query term or CAS Registry Number
- CWM Global Search extended query to involve synonyms

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

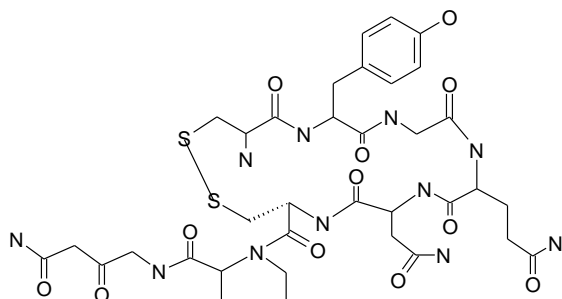
Protein text - PLN format
H-Cys(1)-Tyr-Gly-Gln-Asn-Cys(1)-Pro-Gly-Gly-[NH2]

N-terminal ▼ C-terminal ▼

Ala ▼ Arg ▼ Asn ▼ Asp ▼ Cys ▼ Glu ▼ Gln ▼ Gly ▼ His ▼ Ile ▼ Leu ▼
 Ser ▼ Thr ▼ Trp ▼ Tyr ▼ Val ▼ Sec ▼ Pyl ▼ Xaa ▼

Sequence **Molecule** Sum formula: C35 H50 N12 O12 S2 Avg. MW: 894,9747

1:1



Query substructure

3-Letter code for Oxytocin substructure generated with Proteax

CWM Global Search

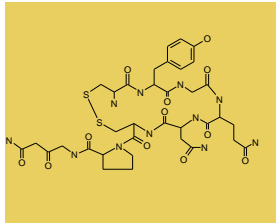


Substructure search in ChEBI and result

Search

6/5/2012 8:49:06 PM

Double click to edit structure



Structure Search

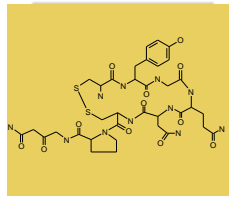
- ☐ Include isomers
- ☒ Include Substructures
- ☐ Include similar compounds

Similarity coefficient (1-100) 90,00

Result

6/5/2012 8:49:06 PM

Double click to zoom structure



Global search links

Remove all filter

05.06.2012 20:49:06

Extreg Number of hits:

RECORD_1 1

Page 1 of 1

Drag a column header and drop it here to group by that column

Rank	Name	Category
40	ACS Publications	Li
5	AKOSSAMPLES	S
40	Bielefeld Academic Search Engine	O
42	BindingDB	Pr
25	BioMed Central	O
61	BMRB	S
15	Buyersguide	S
26	CCRIS	Tr
11	<input checked="" type="checkbox"/> ChEBI	B
24	ChemAxon Chemicalize Search	S
60	ChemBank	B
47	ChEMBL	B
62	Chemo	C

11 ChEBI 24 ChEBI ID(s) found. Bioactivity SUBSTRUCTURE

24 ChEBI ID(s) found

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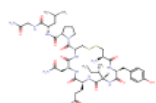
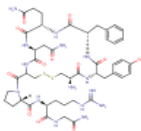
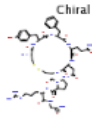
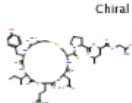
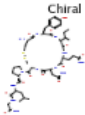
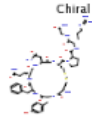

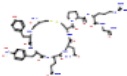
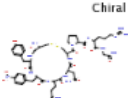
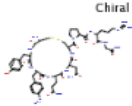
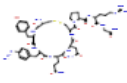

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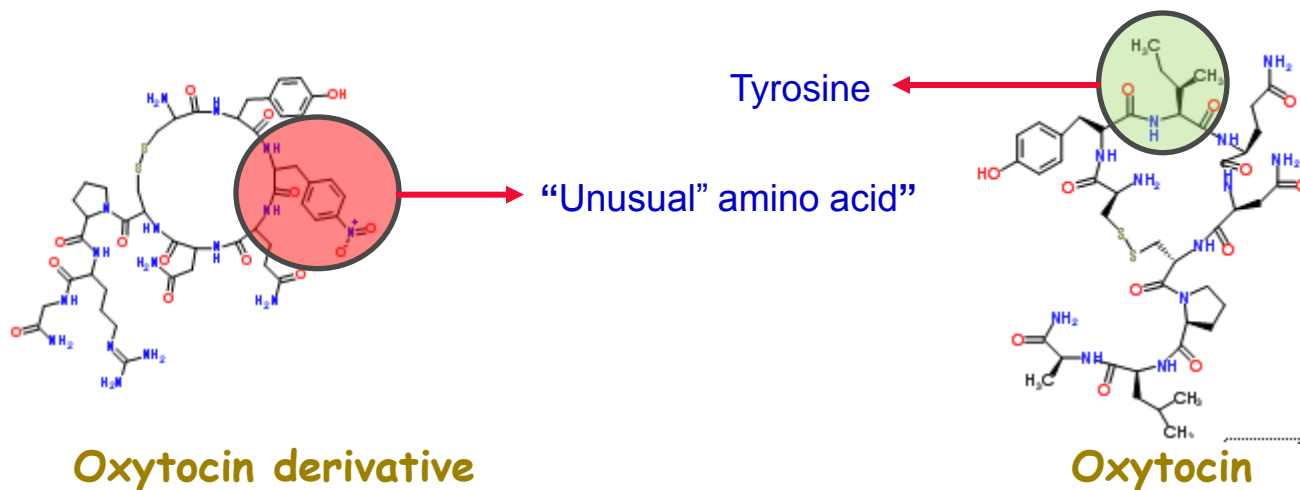
Partial listings of the hits from ChEBI

24 entries found, displaying 1 to 15.

<< < 1 2 > >>

 <p>CHEBI:7872 oxytocin</p> <p>Stars: ★★☆☆</p>	 <p>CHEBI:34543 argipressin</p> <p>Stars: ★★☆☆</p>	 <p>CHEBI:466860 (ChEMBL) CHEBI:466860</p>
 <p>CHEBI:1198609 (ChEMBL) CHEBI:1198609</p>	 <p>CHEBI:148705 (ChEMBL) OXYTOCIN</p>	 <p>CHEBI:155330 (ChEMBL) ARGENINE VASOPRESSIN</p>
 <p>CHEBI:155364 (ChEMBL) VASOTOCIN</p>	 <p>CHEBI:159013 (ChEMBL) [2-({1-[19-Amino-10-(2-carbamoyl-ethyl)-7-carbamoylmethyl-16-(4-hydroxy-benzyl)-13-(4-nitro-benzyl)-6,9,12,15,18-pentaoxo-1,2-dithia-5,8,11,14,17-pentaaza-cycloicosane-4-carbonyl]-pyrrolidine-2-carbonyl}-amino)-5-guanidino-pentanoylamino]-acetic acid</p>	 <p>CHEBI:159080 (ChEMBL) [2-({1-[19-Amino-10-(2-carbamoyl-ethyl)-7-carbamoylmethyl-16-(4-hydroxy-benzyl)-13-(4-nitro-benzyl)-6,9,12,15,18-pentaoxo-1,2-dithia-5,8,11,14,17-pentaaza-cycloicosane-4-carbonyl]-pyrrolidine-2-carbonyl}-amino)-5-guanidino-pentanoylamino]-acetic acid</p>
 <p>CHEBI:159337 (ChEMBL) [2-({1-[19-Amino-13-(4-azido-benzyl)-10-(2-carbamoyl-ethyl)-7-carbamoylmethyl-16-(4-hydroxy-benzyl)-6,9,12,15,18-pentaoxo-1,2-dithia-5,8,11,14,17-pentaaza-cycloicosane-4-carbonyl]-pyrrolidine-2-carbonyl}-amino)-5-guanidino-pentanoylamino]-acetic acid</p>	 <p>CHEBI:159338 (ChEMBL) [2-({1-[19-Amino-13-(4-azido-benzyl)-10-(2-carbamoyl-ethyl)-7-carbamoylmethyl-16-(4-hydroxy-benzyl)-6,9,12,15,18-pentaoxo-1,2-dithia-5,8,11,14,17-pentaaza-cycloicosane-4-carbonyl]-pyrrolidine-2-carbonyl}-amino)-5-guanidino-pentanoylamino]-acetic acid</p>	 <p>CHEBI:175563 (ChEMBL) cyclo[Cys-Tyr-Phe-Gln-Asn-D-Cys]-Pro-Arg-Gly-NH2</p>

Comparison: Oxytocin and derivative with different amino acid in position 3



[CHEBI:148705](#) (ChEMBL) OXYTOCIN

[CHEBI:159013](#) (ChEMBL) [2-({[19-Amino-10-(2-carbamoyl-ethyl)-7-carbamoylmethyl-16-(4-hydroxy-benzyl)-13-(4-nitro-benzyl)-6,9,12,15,18-pentaoxo-1,2-dithia-5,8,11,14,17-pentaaza-cycloicosane-4-carbonyl]-pyrrolidine-2-carbonyl]-amino)-5-guanidino-pentanoylamino]-acetic acid

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>

Please add that a free version is also available

For questions or further information.

e-mail: globalsearch@akosgmbh.de

website: <http://www.akosgmbh.de>