

SciFinder Web

源于化学，超越化学的一站式检索平台

SciFinder Web 培训

CAS北京代表处
培训专员

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20131031

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提纲

- 介绍

- SciFinder Web内容

- **SciFinder Web中的检索**

- SciFinder中的文献检索
 - SciFinder中的结构面板使用技巧
 - SciFinder中的物质结果及物质检索方法
 - SciFinder中的反应检索技巧

- **SciFinder Web的注册和常见问题**

美国化学文摘社—Chemical Abstract Service

- ACS的分支机构，创立于1907年
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引文信息回溯到1997年之前，超过3亿条引文信息

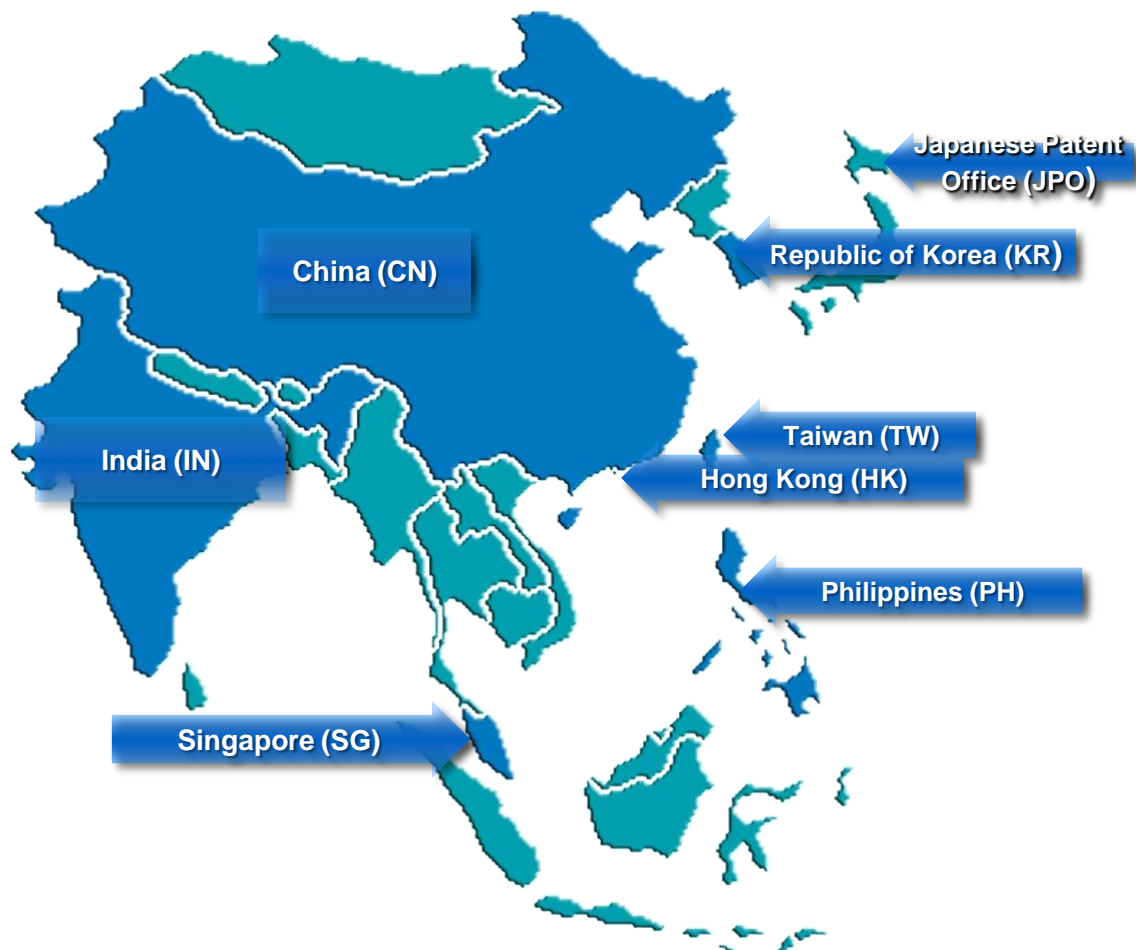
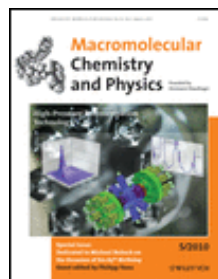
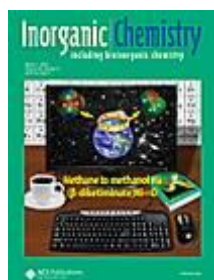
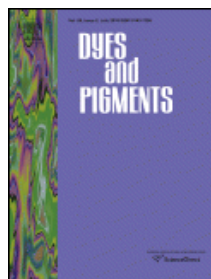
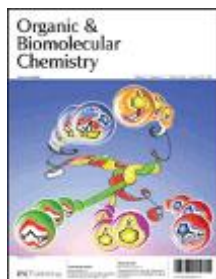
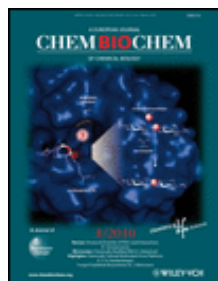
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>99.6万专利中的有机，有机金属结构

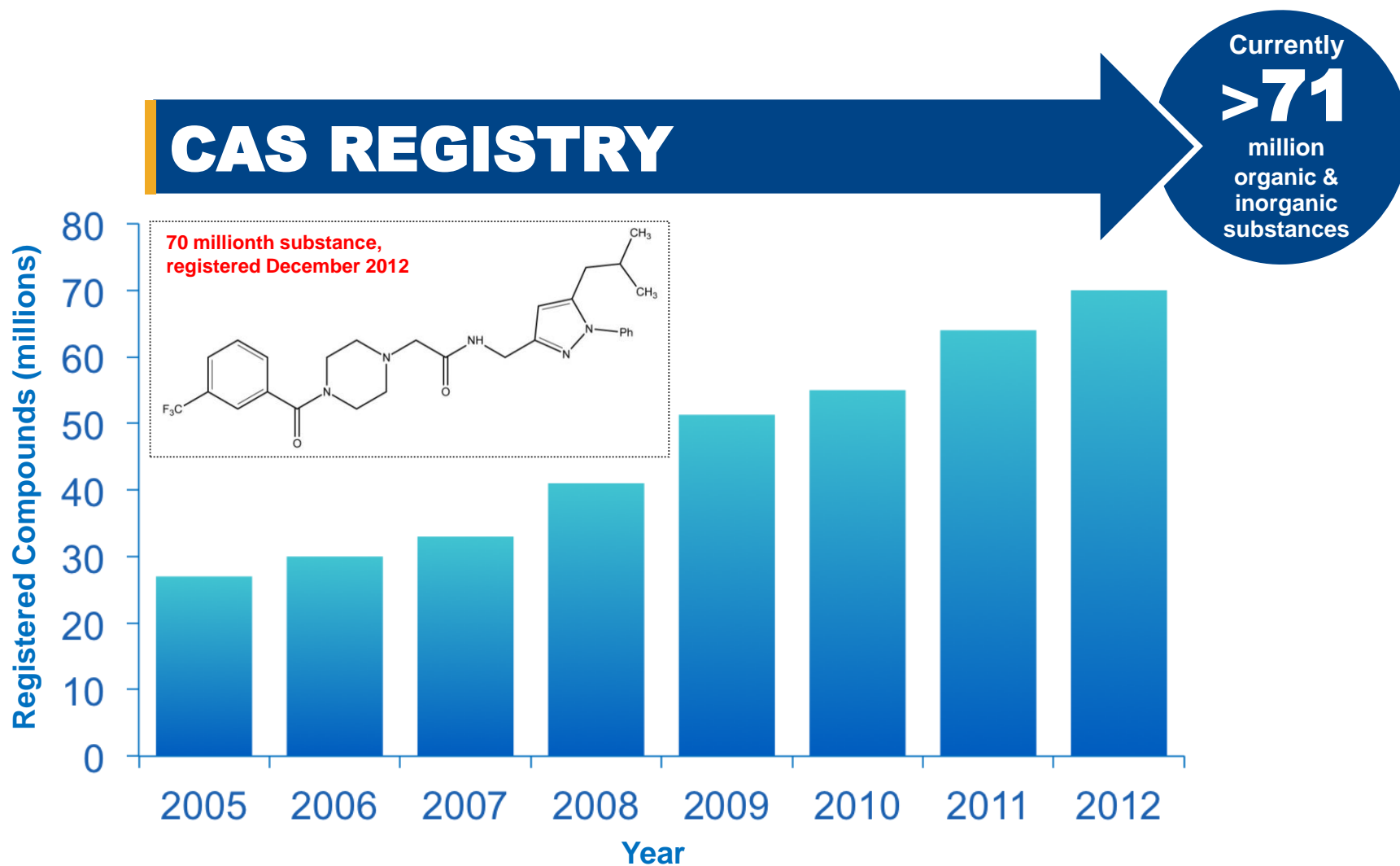
回溯至1961年

每天更新（60-75篇专利引文，以及150-200个Markush结构）

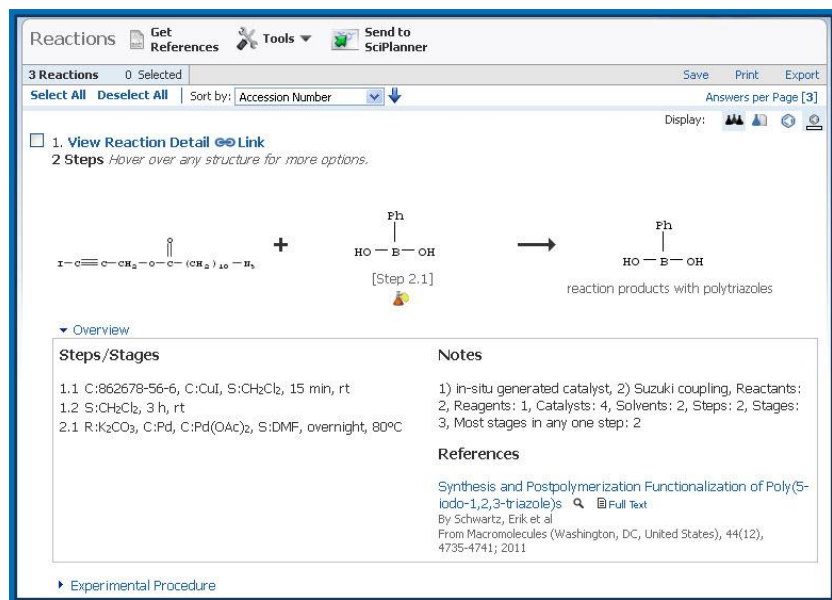
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SciFinder中的文献记录

REFERENCE DETAIL ⓘ
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Get Full Text
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Previous
Next

1. Selective oxidation of light alkanes: interaction between the catalyst and the gas phase on different classes of catalytic materials

By: Cavani, F.; Trifiro, F.

A review, with 202 refs., on the selective oxidn. of light (C₅6) alkanes to bulk and industrial chems., with emphasis on catalyst-gas phase interactions. Attention was given mainly to: (1) the role of the redox properties of transition metal oxide-based systems, and (2) the contribution of radical-type, homogeneous and heterogeneously-initiated homogeneous reactions over nonreducible metal oxide and noble metal catalysts. Other topics included: (1) key factors in selective oxidn. of light alkanes, (2) bulk and surface properties of catalysts, (3) oxidative dehydrogenation, (4) control of oxygen supply to the catalyst, (5) non-redox-type metal oxides (e.g., alk. earth oxides, rare earth oxides, boron oxides, tin oxides, and silica). Some research examples are: (1) oxidn. of propane to acrylic acid and isobutane to methacrylic acid over Keggin-type heteropolymolybdates, (2) oxidative dehydrogenation of alkanes to alkenes over vanadium oxide-based catalysts, and (3) oxidn. of butane and pentane over vanadyl pyrophosphate.

Indexing

Fossil Fuels, Derivatives, and Related Products (Section51-0)

Section cross-reference(s): 35, 45

Concepts

Redox reaction catalysts

catalyst-gas phase interactions in selective oxidn. of light alkanes to bulk and industrial chems.

Alkaline earth oxides Rare earth oxides

catalysts contg.; catalyst-gas phase interactions in selective oxidn. of light alkanes to bulk and industrial chems.

Catalyst use; Properties; Uses

Substances

12026-66-3 58834-75-6

catalyst-gas phase interactions in selective oxidn. of light alkanes to bulk and industrial chems.

Catalyst use; Uses

1303-86-2 Boron oxide, uses 1332-29-2 Tin oxide 7631-86-9 Silica, uses

QUICK LINKS

0 Tags, 0 Comments

SOURCE

Catalysis Today
Volume51
Issue3-4
Pages561-580
Journal; General Review
1999
CODEN:CATTEA
ISSN:0920-5861
DOI:10.1016/S0920-5861(99)00041-3

COMPANY/ORGANIZATION

Dipartimento di Chimica Industriale e dei Materiali
Bologna, Italy 40136

ACCESSION NUMBER

1999:340014
CAN131:159478
CAPLUS

PUBLISHER

Elsevier Science B.V.

Citations

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 Haber, J; ACS Symp Series 1996, 638, 20
 Oyama, S; ACS Symp Series 1996, 638, 2
 Lee, J; Catal Rev-Sci Eng 1988, 30, 249
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 Delmon, B; Catalysts in Petroleum Refining and Petrochemical Industries 1995 1996
 Burch, R; J Mol Catal A 1995, 100, 13
 Schmidt, L; Chem Eng Sci 1994, 49, 3981
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 Trifiro, F; Selective Partial Oxidation of Hydrocarbons and Related Oxidations 1994
 Trifiro, F; Oxidative dehydrogenation and alternative dehydrogenation processes 1993
 Cavani, F; Catal Today 1995, 24, 307

一篇完整的文献界面包括:

1. 题录信息
2. 摘要信息
3. 文献中重要的概念
4. 文献中重要的物质
5. 书目信息
6. 获得文献中的物质, 反应, 引文等
7. 文献中的引文信息

SciFinder中的文献检索方法

功能方面

- 主题检索
- 作者名检索
- 机构名检索
- 文献标示符检索
- 从物质，反应获得文献

检索方法推荐

- 关注某特定领域的文献——主题检索
- 关注物质有关的文献——先获得物质，再获得文献
- 关注某科研人员的文献——作者名检索

SciFinder中的主题检索

主题词: Traditional Chinese medicine with antitumor

The screenshot displays the SciFinder web interface. At the top, the SciFinder logo is on the left, and navigation links for 'Preferences', 'SciFinder Help', and 'Sign Out' are on the right. Below the header, a navigation bar includes 'Explore', 'Saved Searches', and 'SciPlanner'. The main content area shows a search for 'Research Topic "Traditional Chinese medicine w..." > references (1413)'. On the left sidebar, under the 'REFERENCES' section, 'Research Topic' is highlighted with a red box. Below it, a list of search criteria includes 'Author Name', 'Company Name', 'Document Identifier', 'Journal', 'Patent', and 'Tags'. The 'SUBSTANCES' section includes 'Chemical Structure', 'Markush', 'Molecular Formula', 'Property', and 'Substance Identifier'. The 'REACTIONS' section includes 'Reaction Structure'. In the center, the 'REFERENCES: RESEARCH TOPIC' section features a search input field containing 'traditional Chinese medicine with antitumor', which is also highlighted with a red box. Below the input field, there are examples: 'The effect of antibiotic residues on dairy products' and 'Photocyanation of aromatic compounds'. A blue arrow points to the 'Search' button. To the right of the search area, there is a 'SAVED ANSWER SETS' section with a list of sets including '20131022', '20131016-1', '20131016', '20131016 alloy molecule', '20131016 alloy molecule', '20131009', '20130923', '20130807', '丁苯橡胶', '20130806', 'Autosaved Reference Set', and 'View All | Import'. At the bottom right, there is a 'KEEP ME POSTED' section with '20130916 Sep 21, 2013(1)'.

术语之间最好用英文的介词如 of, with, beyond, in, on, as 等连接;
最多输入 5 个术语, 2~3个左右最好

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Research Topic "Traditional Chinese medicine w..."

REFERENCES ⓘ

Select All Deselect All

1 of 5 Research Topic Candidates Selected

	References
<input type="checkbox"/> 101 references were found containing "Traditional Chinese medicine with antitumor" as entered.	101
<input checked="" type="checkbox"/> 1413 references were found containing the two concepts "Traditional Chinese medicine" and "antitumor" closely associated with one another.	1413
<input type="checkbox"/> 3427 references were found where the two concepts "Traditional Chinese medicine" and "antitumor" were present anywhere in the reference.	3427
<input type="checkbox"/> 73337 references were found containing the concept "Traditional Chinese medicine".	73337
<input type="checkbox"/> 968439 references were found containing the concept "antitumor".	968439

Get References

关键词拼写上的变化及同义词都会被检索到
通常,第二项有“concept”和“closely associated with one another” 的选项是更好的选择

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Research Topic "Traditional Chinese medicine w..." > references (1413)

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Analyze Refine Categorize

Sort by: Citing References

Accession Number
Author Name
Citing References

Analyze by: Author Name

Kan Zhaoyun 39
Zhang Zongsheng 28
Liang Hong 17
Chen Zhen Feng 16
Cheng Yiyu 14
Efferth Thomas 14
Ge Zhiwei 14
Liu Li 13
Dou Jing 12

1. and phenolic compounds of 112 traditional Chinese medicinal plants associated with anticancer
By Cai, Yizhong; Luo, Qiong; Sun, Mei; Corke, Harold
From Life Sciences (2004), 74(17), 2157-2184. | Language: English, Database: CAPLUS
~510

2. Structure-radical scavenging activity relationships of phenolic compounds from traditional Chinese medicinal plants
By Cai, Yi-Zhong; Sun, Mei; Xing, Jie; Luo, Qiong; Corke, Harold
From Life Sciences (2006), 78(25), 2872-2888. | Language: English, Database: CAPLUS
~180


3. Arsenic Trioxide Controls the Fate of the PML-RARα Oncoprotein by Directly Binding PML
By Zhang, Xiao-Wei; Yan, Xiao-Jing; Zhou, Zi-Ren; Yang, Fei-Fei; Wu, Zi-Yu; Sun, Hong-Bin; Liang, Wen-Xue; Song, Ai-Xin; Lallemand-Breitenbach, Valerie; Jeanne, Marion; et al
From Science (Washington, DC, United States) (2010), 328(5975), 240-243. | Language: English, Database: CAPLUS
~132

选择sort by里的citing reference 可以获得被引用次数最多的文献

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Analyse-作者姓名分析

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Analyze by: 


Author Name ▼

Kan Zhaoyun	39
Zhang Zongsheng	28
Liang Hong	17
Chen Zhen Feng	16
Cheng Yiyu	14
Efferth Thomas	14
Ge Zhiwei	14
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Kan Zhaoyun在此领域发表了**39**篇文献

Analyze - Author Name

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3650 Items 1 Selected [Export](#)

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Select bars to view only those references within the current answer set.

<input checked="" type="checkbox"/> Kan Zhaoyun	39
<input type="checkbox"/> Zhang Zongsheng	28
<input type="checkbox"/> Liang Hong	17
<input type="checkbox"/> References not containing information for this analysis	16
<input type="checkbox"/> Chen Zhen Feng	16
<input type="checkbox"/> Cheng Yiyu	14
<input type="checkbox"/> Efferth Thomas	14
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<input type="checkbox"/> Liu Li	13
<input type="checkbox"/> Dou Jing	12

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Analyze by: ?

CA Section Title

Pharmaceuticals 551

Pharmacology 421

Pharmaceutical Analysis 21

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抗肿瘤中药主要应用的领域有：
制药，药理，药物分析，食品
和饲料化学等等

有551篇关于抗肿瘤中药在制药领域的文献报道

Sort by: Citing References 0 of 551 References Selected

Answers per Page [20] Display: 1 of 28

- 1. Antioxidant activity and phenolic compounds of 112 traditional Chinese medicinal plants associated with anticancer**

By Cai, Yizhong; Luo, Qiong; Sun, Mei; Corke, Harold
From Life Sciences (2004), 74(17), 2157-2184. | Language: English, Database: CAPLUS

A review and discussion. **Cancer prevention** and treatment using **traditional Chinese medicines** have attracted increasing interest. This study characterizes antioxidant activity and phenolic compds. of **traditional Chinese medicinal** plants assocd. with **anticancer**, comprising 112 species from 50 plant families. The improved ABTS.+ method was used to systematically assess the total antioxidant capacity (Trolox equiv. antioxidant capacity, TEAC) of the **medicinal** exts. The TEAC values and total phenolic content for methanolic exts. of herbs ranged from 46.7 to 17,323 µmol Trolox equiv./100 g dry w...
- 2. Identification of five hepatotoxic pyrrolizidine alkaloids in a commonly used traditional Chinese medicinal herb, herba senecionis scandentis (Qianliguang)**

By Li, Song-Lin; Lin, Ge; Fu, Peter P.; Chan, Chi-Leung; Li, Mi; Jiang, Zhi-Hong; Zhao, Zhong-Zhen
From Rapid Communications in Mass Spectrometry (2008), 22(4), 591-602. | Language: English, Database: CAPLUS

Senecio scandens Buch.-Ham is a plant source for a commonly used **traditional Chinese medicinal** (TCM) herb Qianliguang. A TCM herbal proprietary product contg. Qianliguang as the major herb for the treatment of sinusitis has been used in China for several decades, and has also been exported to other regions and countries worldwide. In the present study, the aq. ext. of *S. scandens* collected in the Shanxi Province of China was detd., for the first time, to contain hepatotoxic and **tumorigenic** pyrrolizidine alkaloids (PAs) by using high-performance liq. chromatog./mass spectrometric (HPLC/MS) an...
- 3. Potential new inorganic antitumor agents from combining the anticancer traditional Chinese medicine (TCM) liriodenine with metal ions, and DNA binding studies**

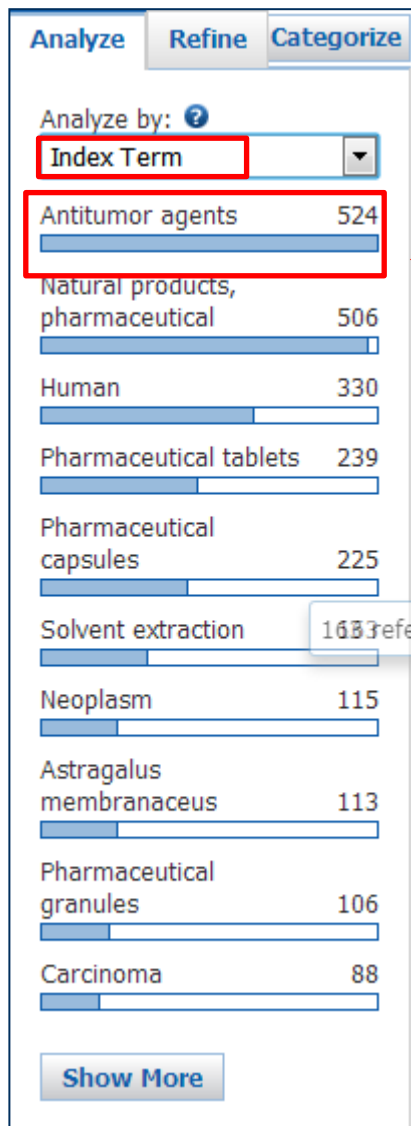
By Chen, Zhen-Feng; Liu, Yan-Cheng; Liu, Li-Min; Wang, Heng-Shan; Qin, San-Hai; Wang, Bo-Long; Bian, He-Dong; Yang, Bin; Fun, Hoong-Kun; Liu, Hua-Gang; et al
From Dalton Transactions (2009), (2), 262-272. | Language: English, Database: CAPLUS

Liriodenine (L), an active component of the **anticancer traditional Chinese medicine** (TCM), was isolated from *Zanthoxylum nitidum*. Its reactions with Pt(II) and Ru(II) afforded three metal complexes: cis-[PtCl₂(L)], cis-[PtCl₂(L)(DMSO)], and cis-[RuCl₂(L)(DMSO)₂]. 1.5H₂O, the crystal structures of L, 2 and 3 were detd. by single-crystal X-ray diffraction methods. These complexes were fully characterized by elemental anal., IR spectrophotometry, ¹H and ¹³C NMR spectroscopies, and ES mass spectrometry. The in vitro cytotoxicity of L and its complexes against 11 human **tumor** cell lines was assayed...
- 4. Divalent later transition metal complexes of the traditional Chinese medicine (TCM) liriodenine: coordination chemistry, cytotoxicity and DNA binding studies**

By Liu, Yan-Cheng; Chen, Zhen-Feng; Liu, Li-Min; Peng, Yan; Hong, Xue; Yang, Bin; Liu, Hua-Gang; Liang, Hong; Orvig, Chris
From Dalton Transactions (2009), (48), 10813-10823. | Language: English, Database: CAPLUS

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Analyse-索引词分析



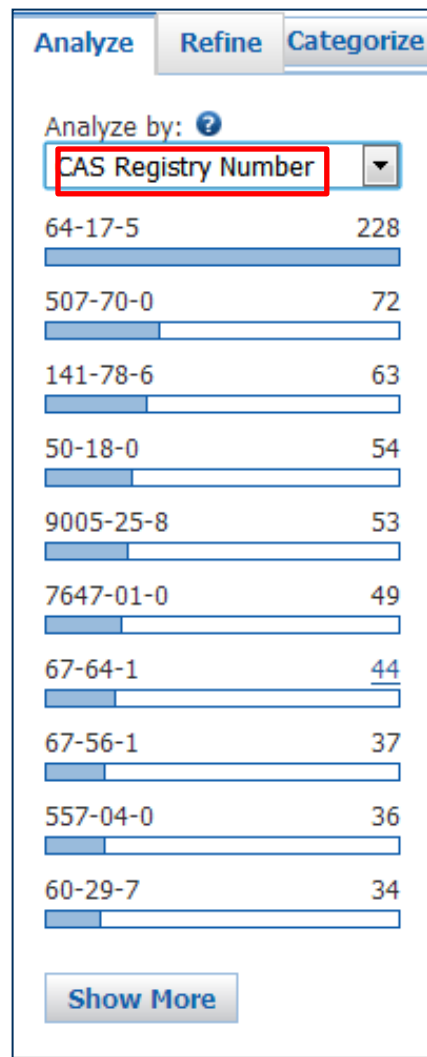
Index Term帮助分析文献中出现的重要内容

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0 of 551 References Selected **有524篇关于制药领域中抗肿瘤剂的文献报道** of 27

- 1. Antioxidant activity and phenolic compounds of 112 traditional Chinese medicinal plants associated with anticancer**
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By Chen, Zhen-Feng; Liu, Yan-Cheng; Liu, Li-Min; Wang, Heng-Shan; Qin, San-Hai; Wang, Bo-Long; Bian, He-Dong; Yang, Bin; Fun, Hoong-Kun; Liu, Hua-Gang; et al
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From Dalton Transactions (2009), (48), 10813-10823. | Language: English, Database: CAPLUS
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Analyse-机构名称, 期刊名称, CAS No分析



Refine-主题词限定

Analyze

Refine

Categorize

Refine by: ?

Research Topic

Author

Company Name

Document Type

Publication Year

Language

Database

Research Topic

active constituent

Examples:

The effect of antibiotic residues on dairy products

Photocyanation of aromatic compounds

Refine

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Sort by: Citing References

0 of 4 References Selected

有4篇是关于抗肿瘤剂活性成分方面的报导

1. Cytotoxic cycloartane triterpenes of the traditional Chinese medicine "Shengma" (Cimicifuga dahurica)

By Nian, Yin; Wang, Hai-Yan; Zhou, Lin; Su, Jia; Li, Yan; Qiu, Ming-Hua

From Planta Medica (2013), 79(1), 60-69. | Language: English, Database: CAPLUS

2. Research progress of traditional Chinese medicine Wikstroemia indica (L.) C.A.Mey

By Chen, Yang; Sun, Li-xin

From Shenyang Yaoke Daxue Xuebao (2009), 26(7), 587-590. | Language: Chinese, Database: CAPLUS

3. Application of organic concept chart to extraction and dosage form design of traditional Chinese medicine

By Ma, Jun-gang; Zhang, Ye-wang; Qu, Bei-bei; Xu, Zhi-long; Zhang, Dai-jia; Yuan, Lu-bing

From Dalian Ligong Daxue Xuebao (2001), 41(6), 671-675. | Language: Chinese, Database: CAPLUS

快速浏览

Quick View

Research progress of traditional Chinese medicine Wikstroemia indica (L.) C.A.Mey

Full Text

By Chen, Yang; Sun, Li-xin

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Substance Images

91-64-5 Coumarin

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20

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0 of 4 References Selected

其中4篇均是期刊文献

1. Cytotoxic cycloartane triterpenes of the traditional Chinese medicine "Shengma" (Cimicifuga dahurica)

By Nian, Yin; Wang, Hai-Yan; Zhou, Lin; Su, Jia; Li, Yan; Qiu, Ming-Hua

From Planta Medica (2013), 79(1), 60-69. | Language: English, Database: CAPLUS

Twelve new 9,19-cycloartane triterpenes (1-12), together with fourteen known compds. (13-26), were isolated from the roots of Cimicifuga dahurica. Their structures were detd. by application of spectroscopic analyses and chem. methods. Biol. evaluation of the compds. against human HL-60, SMMC-7721, A549, MCF-7, and SW-480 cell lines indicated that cimigenol-type glycosides (1-3, 19, and 20) showed broad-spectrum and moderate cytotoxicities, with IC50 values ranging from 4.2 to 14.5 μM. Meanwhile, cimigenol-type aglycons (6-8, 15, 16, and 18) exhibited broad-spectrum and week cytotoxicities, ...

2. Research progress of traditional Chinese medicine Wikstroemia indica (L.) C.A.Mey

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From Dalian Ligong Daxue Xuebao (2001), 41(6), 671-675. | Language: Chinese, Database: CAPLUS

Org. concept chart was applied to traditional Chinese medicine. Org. character values and inorg. character values of the active constituents of traditional Chinese medicine were calcd., to ascertain the distribution of the active constituents of traditional Chinese medicine in org. concept chart. The relationship between the active constituents of traditional Chinese medicine and org. concept chart was analyzed, which can validate the properties of the active constituents of the most traditional Chinese medicine and explain the extrn. and sepn., pharmaceutical preps. and compd. mixing of sev...

4. ...

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2. Research progress of traditional Chinese medicine Wikstroemia indica (L.) C.A.Mey

By: Chen, Yang; Sun, Li-xin

A review. The objective of this work to overview the constituents and pharmacol. action and other aspects of Wikstroemia indica (L.) C.A. Mey. The constituents and pharmacol. action were summarized, based more than 30 literatures. The results showed that the main constituents of Wikstroemia indica (L.) C.A.Mey are coumarins, flavonoids, lignans. It had antibacterial, antiviral, anti-inflammatory and anticancer activities. Upper respiratory tract infection, hepatitis, mastitis can be cured by Wikstroemia indica (L.) C.A.Mey. It was concluded that this article provides a research direction for the further research on Wikstroemia indica (L.) C.A.Mey.

Indexing

Pharmaceuticals (Section63-0)

Concepts

Traditional and alternative medicine

Chinese medicine; research progress of traditional Chinese medicine Wikstroemia indica

Respiratory system disease

infection; research progress of traditional Chinese medicine Wikstroemia indica

Anti-inflammatory agents

Antibacterial agents

Antitumor agents

Antiviral agents

Hepatitis

Mastitis

Wikstroemia indica

research progress of traditional Chinese medicine Wikstroemia indica

Flavonoids

Lignans

research progress of traditional Chinese medicine Wikstroemia indica

Substances

91-64-5 Coumarin

research progress of traditional Chinese medicine Wikstroemia indica

Biological study, unclassified; Biological study

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10. Research progress of traditional Chinese medicine Wikstroemia indica (L.) C.A.Mey

By: Chen, Yang; Sun, Li-xin

A review. The objective of this work to overview the constituents and pharmacol. action and other aspects of Wikstroemia indica (L.) C.A. Mey. The constituents and pharmacol. action were summarized, based more than 30 literatures. The results showed that the main constituents of Wikstroemia indica (L.) C.A.Mey are coumarins, flavonoids, lignans. It had antibacterial, antiviral, anti-inflammatory and anticancer activities. Upper respiratory tract infection, hepatitis, mastitis can be cured by Wikstroemia indica (L.) C.A.Mey. It was concluded that this article provides a research direction for the further research on Wikstroemia indica (L.) C.A.Mey.

Indexing

Pharmaceuticals (Section63-0)

Concepts

Traditional and alternative medicine

Chinese medicine; research progress of traditional Chinese medicine Wikstroemia indica

Respiratory system disease

QUICK LINKS

0 Tags, 0 Comments

SOURCE

Shenyang Yaoke Daxue
Xuebao
Volume26
Issue7
Pages587-590
Journal; General Review
2009
CODEN:SYDXFF

Sort by: CAS Registry Number

0 of 1 Substance Selected

1. **Substance Detail**
91-64-5

~11908

O=C1C=CC2=CC=CC=C2O1

C9 H6 O2
2H-1-Benzopyran-2-one

Spectra
Experimental Properties

从文献可以直接
获得文献中的物
质，反应，引用
等信息

系统分类功能

Categorize ?

1. Select a heading and category.

Category Heading	Category
All	
Biology	
General chemistry	
Biotechnology	
Genetics & protein chemistry	
Technology	
Analytical chemistry	Analysis (62)
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Synthetic chemistry	Reagents & other substances (87)
Physical chemistry	
Environmental chemistry	
Catalysis	

2. Select index terms of interest.

Index Terms		
Select All	Deselect All	
<input type="checkbox"/>	Solvent extraction	179
<input checked="" type="checkbox"/>	Extraction	57
<input type="checkbox"/>	Liquid chromatography	36
<input checked="" type="checkbox"/>	HPLC	22
<input checked="" type="checkbox"/>	TLC (thin layer chromatography)	19
<input type="checkbox"/>	Blotting, Western	13
<input type="checkbox"/>	Xenograft Model Antitumor Assays	13
<input type="checkbox"/>	Concentration (process)	12
<input checked="" type="checkbox"/>	Mass spectrometry	12
<input type="checkbox"/>	Chromatography, High Pressure Liquid	11
<input type="checkbox"/>	Cytometry, flow	10
<input type="checkbox"/>	Dissolution	10
<input type="checkbox"/>	Pharmaceutical analysis	9

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Analytical chemistry > Analysis > 4 Index Term(s) Selected

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1. Advance research on anti-metastatic mechanism of traditional Chinese medicine
By Jia, Bing; Ye, Lihong
From Zhongguo Fangzhi Yanjiu (2013), 40(6), 620-623. | Language: Chinese, Database: CAPLUS
The advance research on anti-metastatic mechanism of traditional Chinese medicine was summarized with several subsections as follow: inducing apoptosis of tumor cells, changing junction of tumor cells, inhibiting degrdn. of extracellular matrix, inhibiting migration of tumor cells, blocking angiogenesis and lymphangiogenesis of tumor, enhancing immunosurveillance and immunomodulation, regulating tumor microenvironment, and conclusions and prospect in the future.

2. Effect of traditional Chinese medicine combined with CIK cell treatment on quality of life and immune function in patients with advanced cancer
By Chai, Xiao-shu; Li, Liu-ning; He, Chun-xia; Zhang, Li-wen; Liu, Bo; Chen, Zhi-jian; Lu, Min
From Xiandai Zhenduan Yu Zhiliao (2012), 23(4), 224-226. | Language: Chinese, Database: CAPLUS
Objective To observe the effects of traditional Chinese medicine (TCM) combined with cytokine-induced killer (CIK) cells on the quality of life and immune function in the patients with advanced malignant tumor. Method According to the inclusion criteria, 218 cases of clin. diagnosed patients with advanced malignant tumor were randomly assigned to two groups, the 110 patients in the treatment group received TCM combined with CIK cells treatment, and the other 108 patients in the control group received TCM alone.

3. Novel fu
By Qin, Qin
From Europ
Multidru

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Page: 1 of 71

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3. Novel function of N,N-bis(2-chloroethyl)docos-13-enamide for reversal of multidrug resistance in tongue cancer

By Qin, Qing; Ma, Peng-Fei; Kuang, Xiao-Cong; Gao, Ming-Xing; Mo, De-Juan; Xia, Shuang; Jin, Ning; Xia, Jun-Jie; Qi, Zhong-Quan; Lin, Cui-Wu

From European Journal of Pharmacology, Ahead of Print. | Language: English, Database: CAPLUS

Multidrug resistance (MDR) is a key element in the failure of chemotherapies, and development of agents to overcome MDR is crucial to improving cancer treatments. The

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提纲

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- SciFinder Web新界面

- **SciFinder Web中的检索**

- SciFinder中的文献检索
 - SciFinder中的结构面板使用技巧
 - SciFinder中的物质结果及物质检索方法
 - SciFinder中的反应检索技巧

- **SciFinder Web的注册和常见问题**

SciFinder结构绘制工具

The image shows the SciFinder Structure Editor interface with various tools labeled in Chinese. The labels are connected to the corresponding tools in the software interface by red lines.

Tools and Labels:

- 铅笔 (Pencil)
- 橡皮 (Eraser)
- 结构 and 反应切换功能 (Structure and Reaction Switching Function)
- 元素周期表 (Periodic Table)
- 常用基团 (Common Groups)
- 可变基团 (Variable Groups)
- R基团定义工具 (R-Group Definition Tool)
- 重复基团工具 (Repeat Group Tool)
- 可变位置连接工具 (Variable Position Connection Tool)
- 碳链工具 (Carbon Chain Tool)
- 模版工具 (Template Tool)
- 选择工具 (Selection Tool)
- 索套选择工具 (Lasso Selection Tool)
- 环锁定工具 (Ring Locking Tool)
- 原子锁定工具 (Atom Locking Tool)
- 旋转工具 (Rotation Tool)
- 镜面旋转工具 (Mirror Rotation Tool)
- 正电子 (Positron)
- C原子和单键恢复工具 (C-Atom and Single Bond Restoration Tool)
- 负电子 (Electron)
- 单双键, RS构型, 不确定键定义工具 (Single/Double Bond, RS Configuration, Uncertain Bond Definition Tool)
- 常见环, 多元环工具 (Common Rings, Polycyclic Rings Tool)
- 结构检索选择 (Structure Search Selection)

Structure Editor Interface Details:

- Structure Editor window title bar.
- Draw or change atoms or bonds. (Yellow bar)
- Shortcut Keys (Link)
- Drawing Editor: Structure (Selected), Reaction, Markush.
- Get substances that match your query using: Exact search, Substructure search (Selected), Similarity search.
- Scale 100.
- Buttons: 确定 (OK), 取消 (Cancel).
- Bottom bar: (query), C, H, O, S, N, P, Cl, Br, F, I, Si, and various ring/atom symbols.

SciFinder中的反应定义工具

The image shows the 'Reaction Editor' window in SciFinder. The interface includes a toolbar on the left with various drawing tools, a central workspace for drawing, and a right-hand panel with options for drawing and searching. Red boxes and lines highlight specific tools and their functions:

- 反应箭头** (Reaction Arrow): Points to the arrow icon in the toolbar.
- 反应原子标记工具** (Reaction Atom Labeling Tool): Points to the 'A' and 'B' atom labeling icons in the toolbar.
- 反应官能团列表** (Reaction Functional Group List): Points to the 'aldehyde', 'ketone', and 'aldol' icons in the toolbar.
- 反应角色工具** (Reaction Role Tool): Points to the 'A' and 'B' atom labeling icons in the toolbar.
- 反应位置标记工具** (Reaction Position Labeling Tool): Points to the '1' and '2' position labeling icons in the toolbar.

The right-hand panel includes the 'Drawing Editor' section with radio buttons for 'Structure', 'Reaction' (selected), and 'Markush'. Below this is a section titled 'Get reactions where the structure(s) are:' with options for 'Variable' (radio button) and 'Substructures' (radio button). At the bottom right are '确定' (OK) and '取消' (Cancel) buttons.

提纲

- 介绍

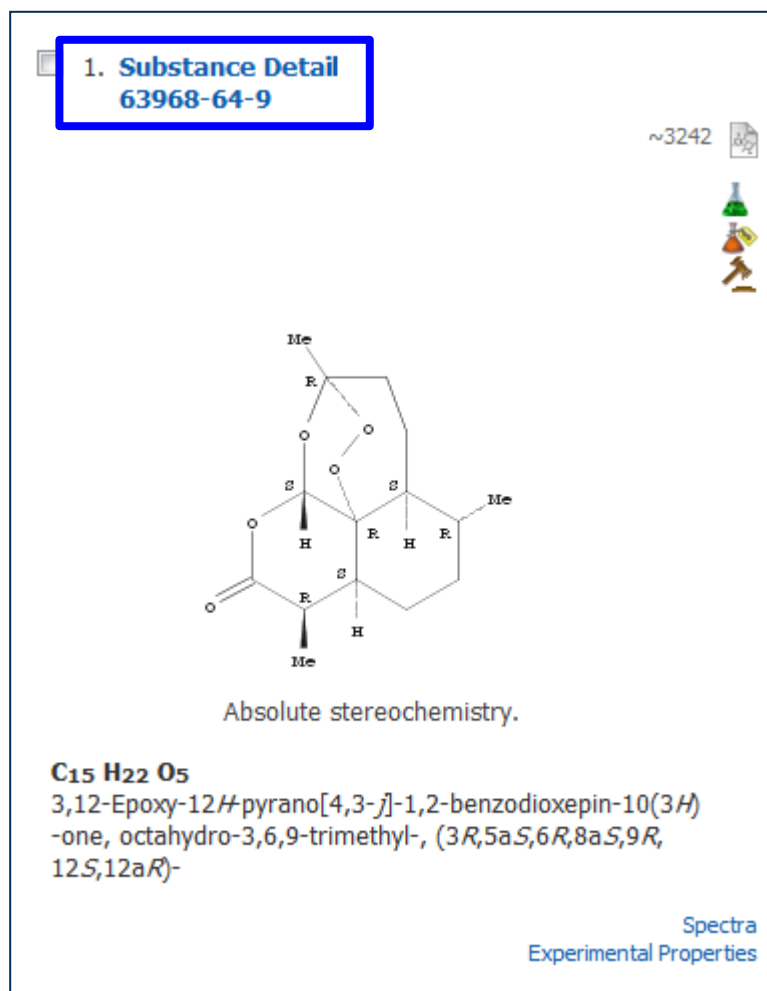
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SciFinder中的物质结果界面



一个完整的物质结果界面包含：

- 物质详情连接
- 文献连接
- 反应连接
- 商品信息连接
- 管制品信息连接
- 谱图连接
- 实验性质连接

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Substance Identifier "qinghaosu" > substances (1) > 63968-64-9

SUBSTANCE DETAIL ⓘ

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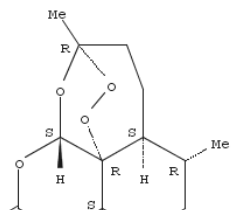
CAS Registry Number: 63968-64-9

C₁₅ H₂₂ O₅

3,12-Epoxy-12H-pyrano[4,3-*j*]-1,2-benzodioxepin-10(3*H*)-one, octahydro-3,6,9-trimethyl-, (3*R*,5*a*,5,6*R*,8*a*,5,9*R*,12*S*,12*a**R*)-

3,12-Epoxy-12H-pyrano[4,3-*j*]-1,2-benzodioxepin-10(3*H*)-one, octahydro-3,6,9-trimethyl-, [3*R*-(3*a*,5*a*β,6β,8*a*β,9*a*,12β,12*a**R**)]-; (+)-Arteannuin; (+)-Artemisinin; (+)-Qinghaosu; Arteannuin; Artemef; Artemisine; Artemisinin; Artemisinine; Huanghuahaosu; NSC 369397; QHS; Qing Hau Sau; Qing Hau Su; Qinghaosu; Qinghosu

Deleted CAS Registry Numbers: 91487-93-3



物质的CAS号、分子式、结构式、化学名、别名

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Analytical Study	✓	✓	✓	✓
Biological Study	✓	✓	✓	✓
Formation, Nonpreparative		✓	✓	✓
Miscellaneous	✓	✓		
Occurrence	✓	✓		✓
Preparation	✓	✓	✓	✓
Process	✓	✓	✓	✓
Properties	✓	✓	✓	✓
Prophetic in Patents	✓			
Reactant or Reagent	✓	✓	✓	✓
Uses	✓	✓	✓	✓

查看物质的衍生物信息

CAS Role	Patents	Nonpatents	Nonspecific Derivatives from Patents	Nonspecific Derivatives from Nonpatents
Analytical Study	✓	✓	✓	✓
Biological Study	✓	✓	✓	✓
Formation, Nonpreparative		✓	✓	✓
Miscellaneous	✓	✓		
Occurrence	✓	✓		✓
Preparation	✓	✓	✓	✓
Process	✓	✓	✓	✓
Properties	✓	✓	✓	✓
Prophetic in Patents	✓			
Reactant or Reagent				
Uses				

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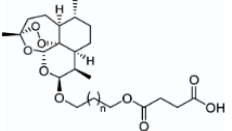
0 of 88 References Selected

1. **Studies on Molecular Mechanism and Action and Synthesis of New Derivatives of the Antimalarial Drug Artemisinin** [Full Text](#)
By Ho, Wing Yan
No Corporate Source data available | (2002), No pp.. | Language: English, Database: CAPLUS

2. **The Diels-Alder Reaction in the Synthesis of Qinghaosu Analogues** [Full Text](#)
By Wu, Kit Ying Kitty
No Corporate Source data available | (2002), No pp.. | Language: English, Database: CAPLUS

3. **Simple Analogues of Qinghaosu (Artemisinin)** [Full Text](#)
By Li, Yun; Hao, Hong-Dong; Wittlin, Sergio; Wu, Yikang
From Chemistry - An Asian Journal (2012), 7(8), 1881-1886, S1881/1-S1881/183. | Language: English, Database: CAPLUS
A series of 1,2,4-trioxanes, e.g., I [R1 = Me, Pr-i, Bu-i], II [R2 = α - & β -OCH₂Ph, α - & β -OOSiMe₂CM₂], III & IV, were synthesized in which the key peroxy bonds were installed through a molybdenum-catalyzed perhydrolysis of the epoxy rings. A core structure was identified that may serve as a promising lead structure for further investigations because of its high antimalarial activity (comparable to that of artesunate and chloroquine), apparent potential for scale-up and derivatization, and facile monitoring/tracing by using UV light.

4. **Linker-Based Hemisuccinate Derivatives of Artemisinin: Synthesis and Antimalarial Assessment against Multidrug-Resistant Plasmodium yoelii nigeriensis in Mice** [Full Text](#)
By Singh, Chandan; Kanchan, Rani; Chaudhary, Sandeep; Puri, Sunil K.
From Journal of Medicinal Chemistry (2012), 55(3), 1117-1126. | Language: English, Database: CAPLUS


12f n = 6
12i n = 10

Artesunic acid (I), the hemisuccinate deriv. of dihydroartemisinin, is the only clin. useful water-sol. deriv. of artemisinin (II). However, being a lactol ester, it is rapidly hydrolyzed back to dihydroartemisinin in aq. alk. soln., a reaction that seriously limits its utility. A new series of potentially more stable linker-based hemisuccinate derivs. III (n = 0 - 4, 6 - 8 and 10) and IV (n = 1, 2, 3) have been prepd. The process involved acid-catalyzed reaction of dihydroartemisinin with various diols and polyethylene glycols to give hydroxy-functionalized ethers V [n = 0 - 4, 6 - 8 and 1...]

Substance Detail—查看生物活性信息

▼ Bioactivity Indicators <small>NEW</small>		References
Anti-infective agents (all) >>> Antimalarials		805
Anti-infective agents (all) >>> Antiviral agents		34
Anti-infective agents (all) >> Parasitocides		43
Anti-inflammatory agents (all) > Anti-inflammatory agents		41
Antitumor agents (all) > Antitumor agents		169
Natural products MD pharmaceutical		108

▼ Target Indicators <small>NEW</small>		References
Cytokines (all) >> Chemokines		13
Cytokines (all) >> Tumor necrosis factors		11
DNA-binding proteins (all) >>> Transcription factor NF- κ B		21
Enzymes (all) >>>> Adenosine triphosphatase		15
Enzymes (all) >>>> 26S proteasome		15
Enzymes (all) >>>>>> Src kinase		13
Glycoproteins (all) >> P-glycoproteins		15
Hemoproteins (all) >>> Cytochrome P 450		12
Hemoproteins (all) >>> Cytochrome P 450 3A4		12
Phosphoproteins (all) >> P-glycoproteins		15
Proteins		19
Receptors (all) > Toll-like receptors		13
RNA formation factors (all) >>> Transcription factor NF- κ B		21
Transport proteins (all) >> P-glycoproteins		15
Transport proteins (all) >> P-glycoproteins		15

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0 of 24 References Selected

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Author Name ▼

Hyde Roderick A 13

Malaska Stephen L 13

Sweeney Elizabeth A 13

Wood Lowell L Jr 12

Paris Daniel 3

Bakshi Pancham 2

Mullan Michael J 2

Ait Ghezala Ghania 1

...

1. Enhanced IL-12p40 production in LPS-stimulated macrophages by inhibiting JNK activation by artemisinin ⓘ Full Text

By Cho, Young-Chang; Lee, Sung Ho; Lee, Mina; Kim, Hyun Jung; Oak, Min-ho; Lee, Ik-Soo; Kang, Bok Yun
From Archives of Pharmacol Research (2012), 35(11), 1961-1968. | Language: English, Database: CAPLUS
Artemisinin can be isolated from *Artemisia annua* L. In addn. to its well-known anti-malarial activity, artemisinin has antitumor and anti-microbial effects. In this study, we investigated the effect of artemisinin on the prodn. of IL-12p40, which is important in the generation of T helper 1 responses. Artemisinin significantly induced IL-12p40 prodn. in LPS-stimulated RAW264.7 macrophage cells. To elucidate the signaling mols. regulated by artemisinin in induced IL-12p40 prodn., the DNA-binding activity of several transcription factors and activation of mitogen-activated protein kinase (MA...

2. Artemisinin attenuates post-infarct myocardial remodeling by down-regulating the NF- κ B pathway ⓘ Full Text

By Gu, Yongwei; Wang, Xi; Wang, Xin; Yuan, Mingjie; Wu, Gang; Hu, Juan; Tang, Yanhong; Huang, Congxin
From Tohoku Journal of Experimental Medicine (2012), 227(3), 161-170. | Language: English, Database: CAPLUS
Myocardial infarction (MI) leads to progressive left ventricular (LV) dilatation and is assoc. with interstitial fibrosis in the non-infarcted myocardium. The NF- κ B signaling pathway plays an important role in ventricular remodeling after MI. Recent studies have indicated that the anti-malarial agent artemisinin can inhibit NF- κ B activation, which may attenuate post-infarct myocardial remodeling. In this study, we investigated the effect of artemisinin on post-infarct myocardial remodeling using a rat model of MI. Adult male Sprague Dawley rats were divided into a sham group (n = 10) and ...

Substance Detail—物质预测性质信息

Predicted Properties: Biological Chemical Density Lipinski and Related Spectra Structure-related Thermal

[Top](#)

Biological Properties	Value	Condition	Note
Bioconcentration Factor	38.6	pH 1 Temp: 25 °C	(27)
Bioconcentration Factor	38.6	pH 2 Temp: 25 °C	(27)
Bioconcentration Factor	38.6	pH 3 Temp: 25 °C	(27)
Bioconcentration Factor	38.6	pH 4 Temp: 25 °C	(27)
Bioconcentration Factor	38.6	pH 5 Temp: 25 °C	(27)
Bioconcentration Factor	38.6	pH 6 Temp: 25 °C	(27)
Bioconcentration Factor	38.6	pH 7 Temp: 25 °C	(27)
Bioconcentration Factor	38.6	pH 8 Temp: 25 °C	(27)
Bioconcentration Factor	38.6	pH 9 Temp: 25 °C	(27)
Bioconcentration Factor	38.6	pH 10 Temp: 25 °C	(27)

Chemical Properties	Value	Condition	Note
Koc	476	pH 1 Temp: 25 °C	(27)
Koc	476	pH 2 Temp: 25 °C	(27)
Koc	476	pH 3 Temp: 25 °C	(27)
Koc	476	pH 4 Temp: 25 °C	(27)
Koc	476	pH 5 Temp: 25 °C	(27)
Koc	476	pH 6 Temp: 25 °C	(27)
Koc	476	pH 7 Temp: 25 °C	(27)
Koc	476	pH 8 Temp: 25 °C	(27)
Koc	476	pH 9 Temp: 25 °C	(27)
Koc	476	pH 10 Temp: 25 °C	(27)
logD	2.39	pH 1 Temp: 25 °C	(27)
logD	2.39	pH 2 Temp: 25 °C	(27)
logD	2.39	pH 3 Temp: 25 °C	(27)
logD	2.39	pH 4 Temp: 25 °C	(27)
logD	2.39	pH 5 Temp: 25 °C	(27)
logD	2.39	pH 6 Temp: 25 °C	(27)
logD	2.39	pH 7 Temp: 25 °C	(27)
logD	2.39	pH 8 Temp: 25 °C	(27)
logD	2.39	pH 9 Temp: 25 °C	(27)
logD	2.39	pH 10 Temp: 25 °C	(27)
logP	2.391±0.772	Temp: 25 °C	(27)
Mass Intrinsic Solubility	Sparsingly Soluble (0.16 g/L)	Temp: 25 °C	(27)
Mass Solubility	Sparsingly Soluble (0.16 g/L)	pH 1 Temp: 25 °C	(27)
Mass Solubility	Sparsingly Soluble (0.16 g/L)	pH 2 Temp: 25 °C	(27)
Mass Solubility	Sparsingly Soluble (0.16 g/L)	pH 3 Temp: 25 °C	(27)
Mass Solubility	Sparsingly Soluble (0.16 g/L)	pH 4 Temp: 25 °C	(27)

Molar Solubility	Sparsingly Soluble (5.7E-4 mol/L)	Unbuffered Water pH 7.00 Temp: 25 °C	(27)
Molecular Weight	282.33		(27)
Vapor Pressure	2.76E-6 Torr	Temp: 25 °C	(27)
Top			
Density Properties	Value	Condition	Note
Density	1.24±0.1 g/cm3	Temp: 20 °C Press: 760 Torr	(27)
Molar Volume	226.4±5.0 cm3/mol	Temp: 20 °C Press: 760 Torr	(27)
Top			
Lipinski and Related Properties	Value	Condition	Note
Freely Rotatable Bonds	0		(27)
H Acceptors	5		(27)
H Donors	0		(27)
H Donor/Acceptor Sum	5		(27)
logP	2.391±0.772	Temp: 25 °C	(27)
Molecular Weight	282.33		(27)
Top			
Spectra Properties	Value	Condition	Note
Carbon-13 NMR Spectrum	See spectrum		(28)
Proton NMR Spectrum	See spectrum		(28)
Top			
Structure-related Properties	Value	Condition	Note
Polar Surface Area	54.0 Å2		(27)
Top			
Thermal Properties	Value	Condition	Note
Boiling Point	389.9±42.0 °C	Press: 760 Torr	(27)
Enthalpy of Vaporization	63.93±3.0 kJ/mol	Press: 760 Torr	(27)
Flash Point	172.0±27.9 °C		(27)

Substance Detail—物质实验性质信息

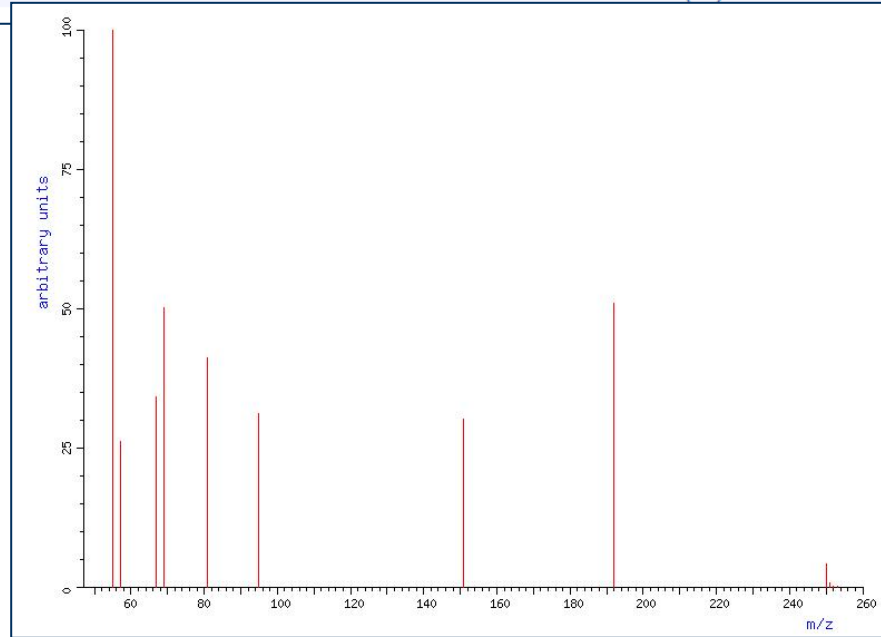
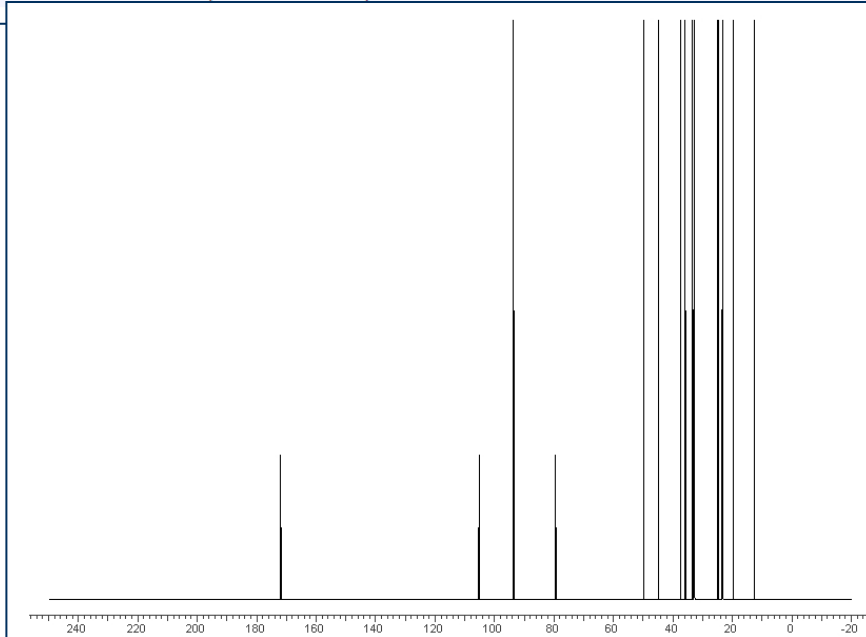
Experimental Properties: Biological Chemical Density Flow and Diffusion Lipinski and Related Optical and Scattering Spectra Structure-related Thermal				Top
Biological Properties	Value	Condition	Note	
ADME (Absorption, Distribution, Metabolism, Excretion)	See full text		(1)CAS	
Half-Life (Biological)	See full text	1 of 2	(1)CAS	
Median Lethal Dose(LD50)	5576 mg/kg	Organism: rat Route: oral	(15)APC	
Median Lethal Dose(LD50)	5105 mg/kg	Organism: mouse Route: oral	(15)APC	
Median Lethal Dose(LD50)	2800 mg/kg	Organism: mouse Route: intramuscular	(15)APC	
Median Lethal Dose(LD50)	2571 mg/kg	Organism: rat Route: intramuscular	(15)APC	
Median Lethal Dose(LD50)	1558 mg/kg	Organism: mouse Route: intraperitoneal	(15)APC	
Minimum Inhibitory Concentration	See full text	1 of 2	(20)CAS	
Chemical Properties	Value	Condition	Note	Top
Ionization Potential	See full text		(2)CAS	
logP	See full text	1 of 2	(12)CAS	
Molecular Electric Dipole Moment	See full text		(21)CAS	
Solubility	See full text	1 of 9	(7)CAS	
Density Properties	Value	Condition	Note	Top
Density	1.300 g/cm3		(7)CAS	
Flow and Diffusion Properties	Value	Condition	Note	Top
Diffusion Coefficient	See full text		(8)CAS	

Density Properties	Value	Condition	Note	Top
Density	1.300 g/cm3		(7)CAS	
Flow and Diffusion Properties	Value	Condition	Note	Top
Diffusion Coefficient	See full text		(8)CAS	
Lipinski and Related Properties	Value	Condition	Note	Top
logP	See full text	1 of 2	(12)CAS	
Optical and Scattering Properties	Value	Condition	Note	Top
Optical Rotatory Power	+87.9 °	Solv: 1,4-dioxane (123-91-1); Wavlen: 589.3 nm	(22)CAS	
Optical Rotatory Power	+75-+78 °	Conc: 1.0 g/100mL; Solv: ethanol (64-17-5); Wavlen: 589.3 nm; Temp: 20 °C	(16)CAS	
Optical Rotatory Power	+68.2 °	Conc: 0.97 g/100mL; Solv: chloroform (67-66-3); Temp: 25 °C	(18)IC	
Optical Rotatory Power	+67.6 °	Conc: 1.75 g/100mL; Solv: chloroform (67-66-3); Wavlen: 589.3 nm; Temp: 25 °C	(17)CAS	
Optical Rotatory Power	+66.6 °	Conc: 1.57 g/100mL; Solv: chloroform (67-66-3); Wavlen: 589.3 nm; Temp: 24 °C	(17)CAS	
Optical Rotatory Power	+66.3 °	Conc: 1.64 g/100mL; Solv: chloroform (67-66-3); Wavlen: 589.3 nm; Temp: 17 °C	(15)APC	
Optical Rotatory Power	+61 °	Conc: 0.2 g/100mL; Solv: chloroform (67-66-3); Wavlen: 589.3 nm; Temp: 24 °C; Len: 1 dm	(5)CAS	

Substance Detail—查看实验谱图信息

Spectra Properties	Value	Condition	Note
Carbon-13 NMR Spectrum	See spectrum		(3)ACD
Carbon-13 NMR Spectrum	See spectrum		(4)ACD
Carbon-13 NMR Spectrum	See full text	1 of 8	(5)CAS
Circular Dichroism Spectrum	See full text	1 of 2	(6)CAS
IR Absorption Spectrum	See full text	1 of 11	(2)CAS
Mass Spectrum	See spectrum		(13)WSS
Mass Spectrum	See spectrum		(13)WSS
Mass Spectrum	See full text	1 of 10	(14)CAS
Proton NMR Spectrum	See full text	1 of 10	(17)CAS
Raman Spectrum	See full text	1 of 2	(24)CAS
Two-Dimensional NMR Spectrum	See full text	1 of 2	(8)CAS
UV and Visible Absorption Spectrum	See full text		(6)CAS
UV and Visible Emission/Luminescence Spectrum	See full text		(26)CAS

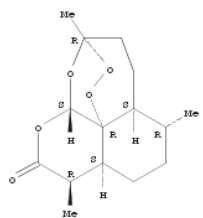
直接点击高亮的数字链接到该文献



物质有关的反应

1. Substance Detail
63968-64-9

~3242



Absolute stereochemistry.

C₁₅ H₂₂ O₅
3,12-Epoxy-12H-pyrano[4,3-j]-1,2-benzodioxepin-10(3H)-one, octahydro-3,6,9-trimethyl-, (3R,5aS,6R,8a,S,9R,12S,12aR)-

Get Reactions

Limit results by reaction role:

☒ Product

☐ Reactant

☐ Reagent

☐ Reactant or reagent

☐ Catalyst

☐ Solvent

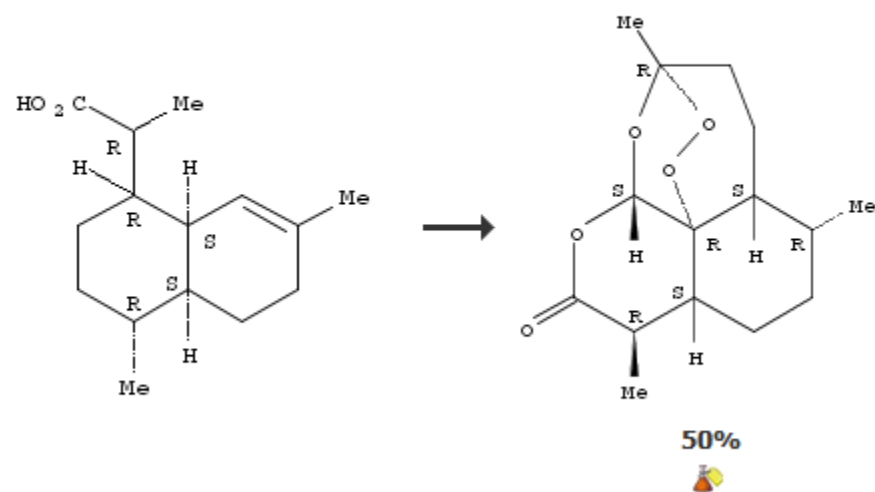
☐ Any role

Get

Cancel

1. View Reaction Detail Link Similar Reactions

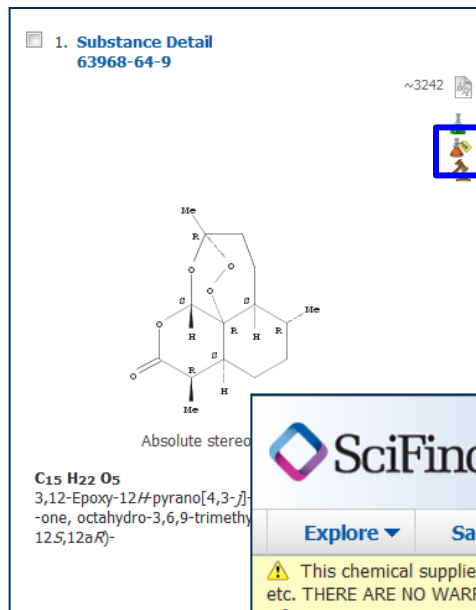
Single Step *Hover over any structure for more options.*



► Overview

物质有关的商业来源

可以直接**Export**到**Excel**中，又或者使用分析工具，对商业信息进行处理



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Substance Identifier "qinghaosu" > substances (1) > 63968-64-9 > commercial sources (91)

COMMERCIAL SOURCES ?

Analyze

Sort by: Catalog Name ↑

Answers per Page [20]

0 of 91 Commercial Sources Selected

Analyze by: ?

Catalog Name ▼

Accel Pharmtech
Product List 2

AK Scientific Product
Catalog 2

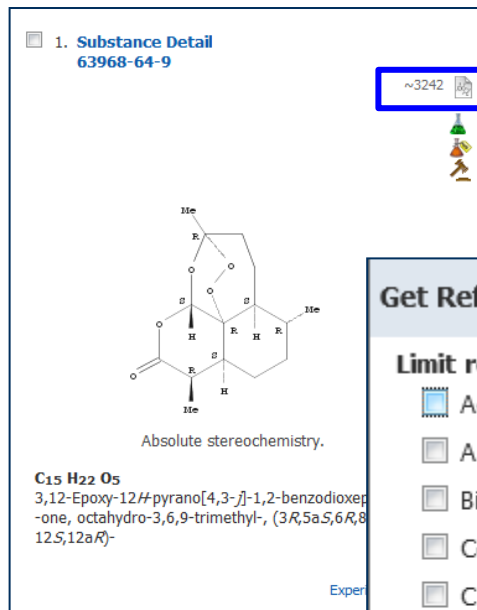
Chemieliva
Pharmaceutical
Product List 2

ChemPacific Product

1. **3B Scientific Corporation Product List**
Supplier Name: 3B Scientific Corporation, Catalog Publication Date: 12 Jul 2012
Order Number: 382-3802
Quantity: 1g
63968-64-9 Artemisinin
[Link](#)

2. **A Chemtek Product List**
Supplier Name: A Chemtek, Catalog Publication Date: 13 Mar 2013
Order Number: 031-18967
Quantity: N/A
63968-64-9 Artemisinin

物质有关的文献信息



一键获得文献，可以获得全部，也可以勾选特别感兴趣的内容，不勾选，默认获得全部

Get References

Limit results to:

<input checked="" type="checkbox"/> Adverse Effect, including toxicity	<input type="checkbox"/> Prophetics in Patents
<input type="checkbox"/> Analytical Study	<input type="checkbox"/> Preparation
<input type="checkbox"/> Biological Study	<input type="checkbox"/> Process
<input type="checkbox"/> Combinatorial Study	<input type="checkbox"/> Properties
<input type="checkbox"/> Crystal Structure	<input type="checkbox"/> Reactant or Reagent
<input type="checkbox"/> Formation, nonpreparative	<input type="checkbox"/> Spectral Properties
<input type="checkbox"/> Miscellaneous	<input type="checkbox"/> Uses
<input type="checkbox"/> Occurrence	

For each sequence, retrieve:

☐ Additional related references, e.g., activity studies, disease studies.

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SciFinder中的物质检索方法

■ 功能方面

- 物质名称, CAS No
- 分子式
- 结构式
- 理化性质

■ 推荐的物质检索功能

- 有机物, 天然产物及衍生物
- 无机物
- 高分子化合物

---结构比较方便

---分子式比较方便


---首先分子式, 其次结构

物质名称检索

The screenshot displays the SciFinder homepage. At the top, the SciFinder logo is visible. Below the logo, there are navigation tabs: 'Explore', 'Saved Searches', and 'SciPlanner'. A breadcrumb trail indicates the current search path: 'Substance Identifier "qinghaosu" > substances (1) > 63968-64-9 > commercial sources (91)'. On the left side, there is a sidebar menu with categories: 'REFERENCES' (with sub-items: Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, Tags), 'SUBSTANCES' (with sub-items: Chemical Structure, Markush, Molecular Formula, Property, Substance Identifier), and 'REACTIONS' (with sub-item: Reaction Structure). The 'Substance Identifier' option is highlighted. The main content area is titled 'SUBSTANCES: SUBSTANCE IDENTIFIER'. It features a large text input field containing 'qinghaosu'. Below the input field, there is a note: 'Enter one per line. Examples: 50-00-0, 999815, Acetaminophen'. A blue 'Search' button is positioned below the input field. A black arrow points from the bottom right towards the input field.


直接输入物质的名称，**CAS No**，俗名，都能检索，一次最多检索**25**个物质，用换行换开

理化性质检索


Preferences

Explore ▾ Saved Searches ▾ SciPlanner


Reaction Structure structure variable only at spe... > reactions (1122) > keep analysis "Reagent" (242)

 REFERENCES

[Research Topic](#)
[Author Name](#)
[Company Name](#)
[Document Identifier](#)
[Journal](#)
[Patent](#)
[Tags](#)

 SUBSTANCES

[Chemical Structure](#)
[Markush](#)
[Molecular Formula](#)
[Property](#)
[Substance Identifier](#)

 REACTIONS

[Reaction Structure](#)

SUBSTANCES: PROPERTY ?

Select the category and enter an appropriate value or range.

☒ Experimental

Value or Range

Select Property... ▾

Select Property...
Boiling Point (°C)
Density (g/cm³)
Electric Conductance (S)
Electric Conductivity (S/cm)
Electric Resistance (ohm)
Electric Resistivity (ohm*cm)
Glass Transition Temp. (°C)
Magnetic Moment (μB)
Median Lethal Dose (LD50) (mg/kg)
Melting Point (°C)
Optical Rotatory Power (degrees)
Refractive Index
Tensile Strength (MPa)

Value or Range

Examples: Individual value as 44,
range as 25-35, or open ended
range as >125 or <125

Value or Range

Examples: Individual value as 44,
range as 25-35, or open ended
range as >125 or <125

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42

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分子式检索

SciFinder®

Explore ▾ Saved Searches ▾ SciPlanner

Substance Identifier "qinghaosu" > substances (1) > 63968-64-9 > commercial sources (91)

REFERENCES

- Research Topic
- Author Name
- Company Name
- Document Identifier
- Journal
- Patent
- Tags

SUBSTANCES

- Chemical Structure
- Markush
- Molecular Formula**
- Property
- Substance Identifier

REACTIONS

- Reaction Structure

SUBSTANCES: MOLECULAR FORMULA

(C3 H6 O. C2 H4 O)x

Examples:
H4SiO4
(C3H6O.C2H4O)x

Search

分子式的检索，根据hill排序规则书写，**C,H**写在前面，其他元素按照字母顺序写

分子式检索

■ 多组分物质

- 包含盐，水合物，合金，混合物等
- 用 “.” 将不同组分点开

■ Hill排序

— 单一组分物质

- 对于不含**C**的物质，按照字母顺序排序
- 对于含**C**的物质，**CH**写在前面，其他的按照字母顺序排列
- 相邻的两个元素之间必须有区分号，即数字或者空格，倘若数字为1，那么可以用空格来区分
- 区分大小写

— 多组分物质

- 每一组分必须遵照单一组分物质的分子式来书写。
- 不同组分之间的排序按照各组分的首元素的字母顺序排序，但是含**C**组分的一定排在不含**C**的组分前面。
- 倘若不同组分的首元素相同，则看元素数量多少，数量多的排在前面，若元素数量一样，则按次元素的顺序排列。

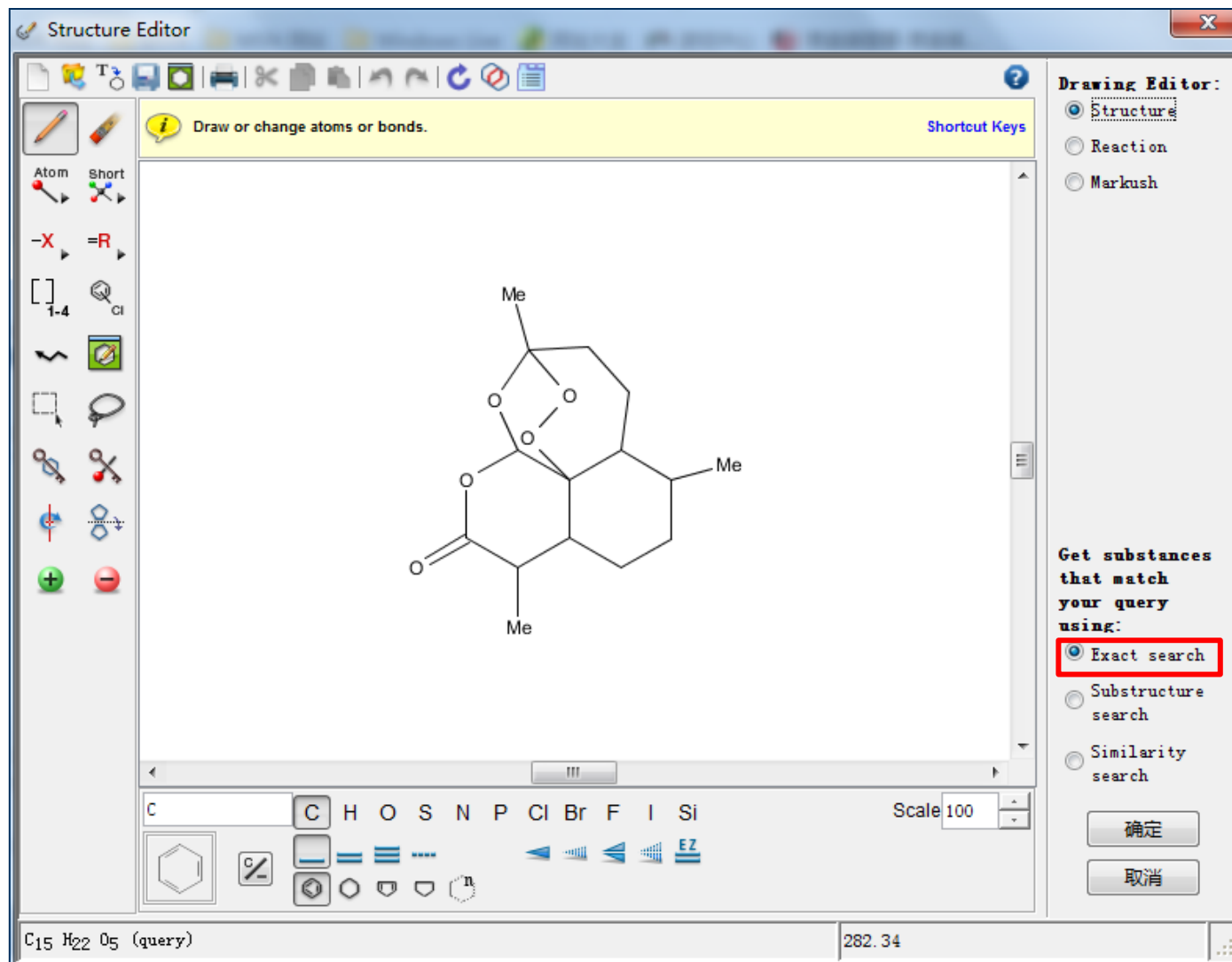
结构式检索—精确检索

The screenshot displays the SciFinder web application interface. At the top, the SciFinder logo is visible on the left, and a 'Pref' link is on the right. Below the logo, there are three main navigation tabs: 'Explore', 'Saved Searches', and 'SciPlanner'. The 'Explore' tab is currently active.

Below the navigation tabs, a breadcrumb trail indicates the current search path: 'Substance Identifier "qinghaosu" > substances (1) > 63968-64-9 > commercial sources (91)'. On the left side, there is a sidebar menu with three main categories: 'REFERENCES', 'SUBSTANCES', and 'REACTIONS'. Under 'REFERENCES', options include Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, and Tags. Under 'SUBSTANCES', options include Chemical Structure (which is highlighted with a blue bar), Markush, Molecular Formula, Property, and Substance Identifier. Under 'REACTIONS', the option is Reaction Structure.

The main content area is titled 'SUBSTANCES: CHEMICAL STRUCTURE'. It features a central workspace with a chemical structure editor window that says 'Click to Edit'. To the right of this workspace, there are search type options: 'Exact Structure' (selected with a radio button), 'Substructure', and 'Similarity'. Below these options is a checkbox for 'Show precision analysis'. At the bottom of the workspace, there is an 'Import CXF' button and a 'Search' button. A link for 'Advanced Search' is also present at the bottom.

青蒿素结构检索



精确结构结构检索

结构检索界面

SciFinder®

Explore ▾ Saved Searches ▾ SciPlanner

Chemical Structure exact > substances (62)

REFERENCES

- Research Topic
- Author Name
- Company Name
- Document Identifier
- Journal
- Patent
- Tags

SUBSTANCES

- Chemical Structure
- Markush
- Molecular Formula
- Property
- Substance Identifier

REACTIONS

- Reaction Structure

SUBSTANCES: CHEMICAL STRUCTURE ?

Structure Editor:

Java Non-Java

Click image to change structure or view detail.

Import CXF

Search

Advanced Search

Search Type:

- ☒ Exact Structure
- ☐ Substructure
- ☐ Similarity

☐ Show precision analysis

与已绘制的结构完全相同的物质：同位素化合物，配位化合物，单体组成的聚合物，离子化合物，异构体，互变异构体

检索结果页面

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Welcome Della Li

Explore | Saved Searches | SciPlanner

Save | Print | Export

Chemical Structure exact > substances (62)

SUBSTANCES

Get References | Get Reactions | Get Commercial Sources | Tools

Create Keep Me Posted Alert | Send to SciPlanner

Analyze | Refine

Sort by: Relevance

0 of 62 Substances Selected

Answers per Page [15] View: |||

Page: 1 of 5

1. Substance Detail 63968-64-9

2. Substance Detail 113472-97-2

3. Substance Detail 1061342-74-2

Quick View

CAS Registry Number: 63968-64-9

Formula: C₁₅H₂₂O₅

CA Index Name: 3,12-Epoxy-12H-pyrano[4,3-*j*]-1,2-benzodioxepin-10(3*H*)-one, octahydro-3,6,9-trimethyl-, (3*R*,5*a*,6*R*,8*a*,9*R*,12*S*,12*aR*)-

Other Names

3,12-Epoxy-12H-pyrano[4,3-*j*]-1,2-benzodioxepin-10(3*H*)-one, octahydro-3,6,9-trimethyl-, [3*R*-(3*a*,5*a*,6*β*,8*a*,9*a*,12*β*,12*aR*)]-; (+)-Arteannuin; (+)-Artemisinin; (+)-Qinghaosu; Arteannuin; Artemef; Artemisine; Artemisinin; Artemisinine; Huanghuahaosu; NSC 369397; QHS; Qing Hau Sau; Qing Hau Su; Qinghaosu; Qinghosu

Number of References

~3,342

Document Types

Book, Conference, Dissertation, Journal, Patent, Preprint, Report

Properties

Experimental
Spectra
Predicted

Commercial Sources

Available

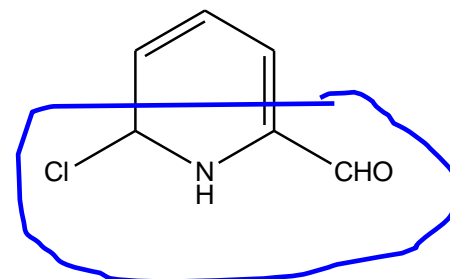
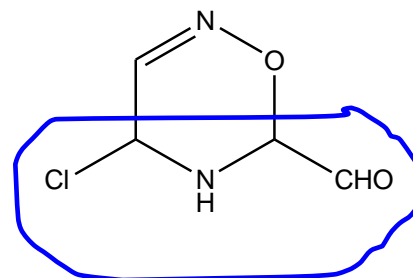
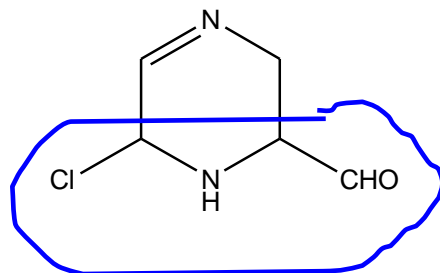
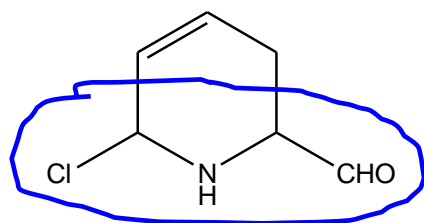
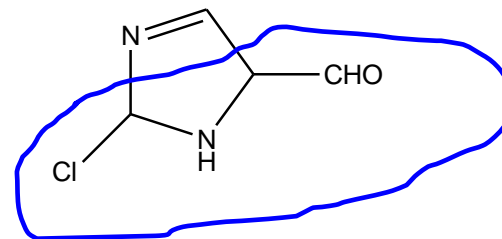
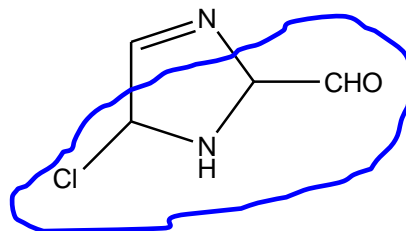
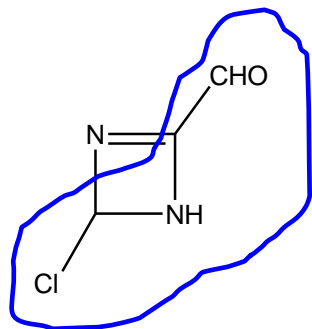
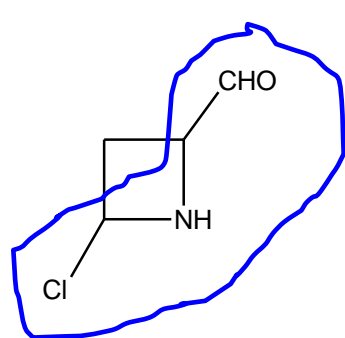
Absolute stereochemistry.

Absolute stereochemistry.

Absolute stereochemistry.

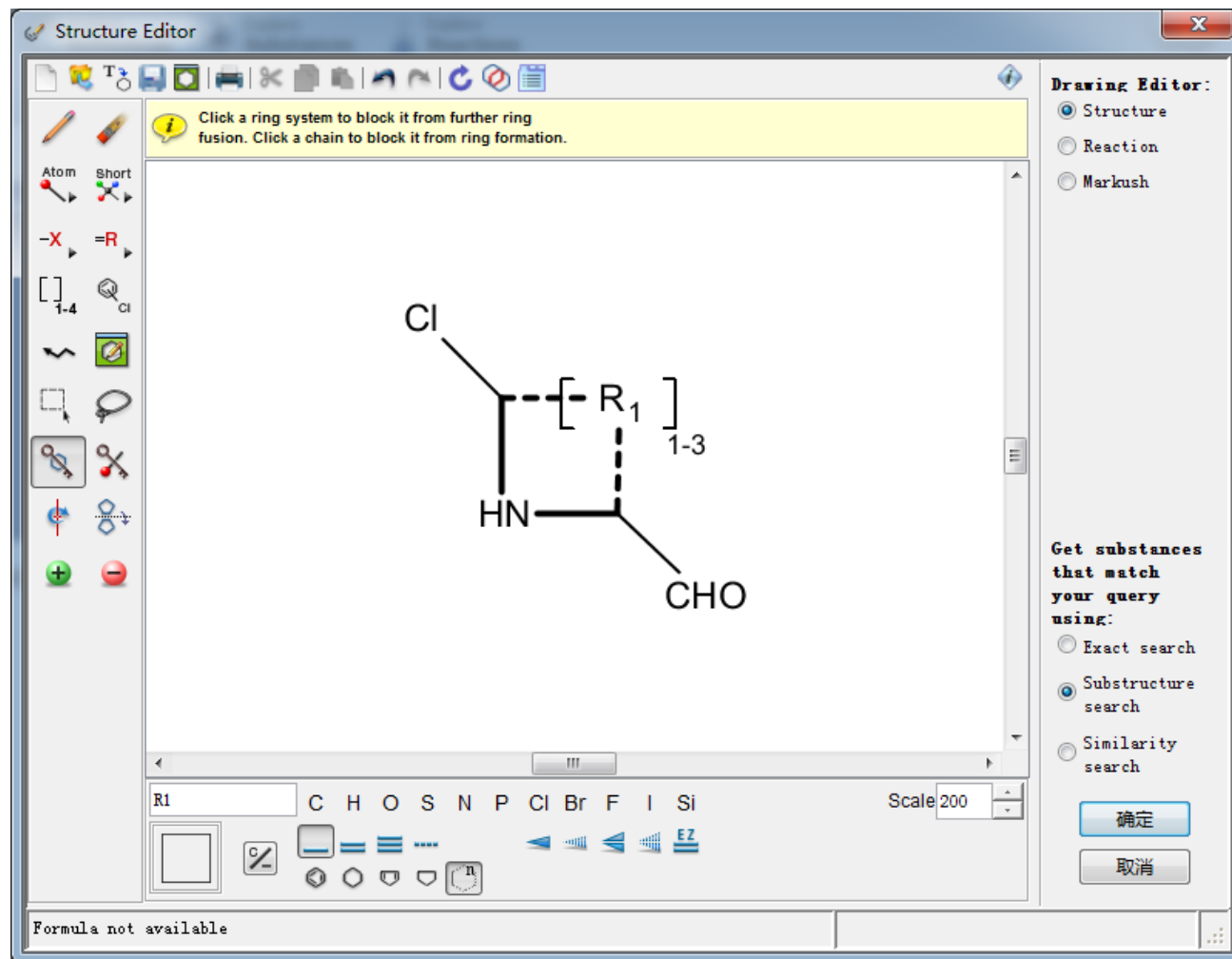
Absolute stereochemistry.

我想获得以下的一系列物质



.....

结构定义



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亚结构检索结果

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Chemical Structure substructure > substances (469)

SUBSTANCES ? Get References Get Reactions Get Commercial Sources Tools ▾ Create Keep Me Posted Alert Send to SciPlanner

Analyze Refine

Sort by: Number of References ▾

Answers per Page [50] View: ||| ||| |||

0 of 469 Substances Selected

Page: 1 of 10

Analyze by: ?

Substance Role ▾

Preparation 155

Reactant or Reagent 123

Biological Study 15

Uses 11

Prophetic in Patents 8

Properties 6

Formation, Nonpreparative 2

Analytical Study 1

1. Substance Detail 54087-03-5 ~33

Clc1cccc(C=O)n1

C6H4ClNO

2. Substance Detail 1757-28-4 ~19

O=Cc1cc(Cl)c[nH]1

C5H4ClNO
1H-Pyrrole-2-carboxaldehyde, 5-chloro-

Experimental Properties

3. Substance Detail 81293-97-2 ~11

O=Cc1c(Cl)c[nH]c1Cl

C4H2Cl2N2O
1H-Imidazole-2-carboxaldehyde, 4,5-dichloro-

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从物质获得反应

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SUBSTANCE DETAIL ⓘ

Get References

Get Reactions

Get Commercial Sources

Get Regulatory Information

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Return

CAS Registry Number: 63968-64-9

C15 H22 O5

3,12-Epoxy-12H-pyrano[4,3-j]-1,2-benzodioxepin-10(3H)-one, octahydro-3,6,9-trimethyl-, (3*R*,5*a*,5*b*,6*R*,8*a*,9*R*,12*S*,12*a**R*)-

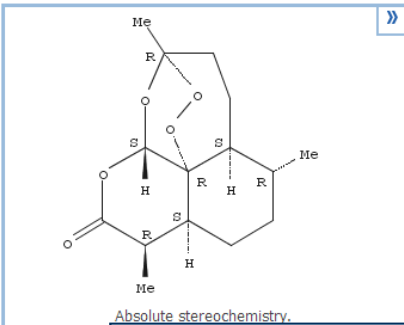
3,12-Epoxy-12H-pyrano[4,3-j]-1,2-benzodioxepin-10(3H)-one, octahydro-3,6,9-trimethyl-, [3*R*-(3*a*,5*a*β,6β,8*a*β,9*a*,12β,12*a**R**)]-; (+)-Artemannuin; (+)-Artemisinin; (+)-Qinghaosu; Artemannuin; Artemef; Artemisine; Artemisinin; Artemisinine; Huanghuahaosu; NSC 369397; QHS; Qing Hau Sau; Qing Hau Su; Qinghaosu; Qinghosu

Deleted CAS Registry Numbers: 91487-93-3

Source of Registration: CA

~3,342 References

Document Types: Book, Conference, Dissertation, Journal, Patent, Preprint, R



Absolute stereochemistry.

Get Reactions

Limit results by reaction role:

- ☒ Product
- ☐ Reactant
- ☐ Reagent
- ☐ Reactant or reagent
- ☐ Catalyst
- ☐ Solvent
- ☐ Any role

Get Cancel

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REACTIONS

Get References | Tools

Send to SciPlanner

Analyze | Refine

Analyze by: Reagent (New)

O ₂	192
H ₂ O ₂	101
HCl	72
NaHCO ₃	61
NaOH	59
H ₂ SO ₄	54
K ₂ CO ₃	53
F ₃ CCO ₂ H	52
Et ₃ N	48

Group by: Document | Sort by: Accession Number

No Grouping
Document Selected
Transformation

1. View Reaction Detail Link

3 Steps Hover over any structure for more options.

我们获得275条反应

反应筛选的第一步是Group By Document，让一篇文献出现一条反应

Group by: Document | Sort by: Accession Number

Answers per Page [15] Display: [icon]

0 of 275 Reactions Selected

1. High-level semi-synthetic production of the potent antimalarial artemisinin Full Text

4 Reactions

3 Steps Hover over any structure for more options.

Overview

按照反应类型分类显示

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REACTIONS

Get References | Tools

Analyze | Refine

Analyze by: Reagent (New)

O₂ 192
H₂O₂ 101
HCl 72
NaHCO₃ 61
NaOH 59
H₂SO₄ 54
K₂CO₃ 53
F₃CCO₂H 52
Et₃N 48

Group by: Transformation | Sort by: Accession Number

No Grouping
Document
Transformation

1. View Reaction Detail | Link

3 Steps Hover over any structure for more options.

Transformation 帮助我们判断大部分的研究人员采用哪种合成方法

1. Reduction of the Double or Triple Bonds Conjugated to Carbonyl or Cyano Groups
12 Reactions

$$\begin{array}{c} R^1 \\ | \\ R^2-C=C-R^4 \\ | \\ R^3 \end{array} \xrightarrow{\quad} \begin{array}{c} R^1 \\ | \\ R^2-CH-CH-R^4 \\ | \\ R^3 \end{array}$$

$$\begin{array}{c} R^1 \\ | \\ R^2-C \equiv N \\ | \\ R^3 \end{array} \xrightarrow{\quad} \begin{array}{c} R^1 \\ | \\ R^2-CH_2-CH_2-NH_2 \\ | \\ R^3 \end{array}$$

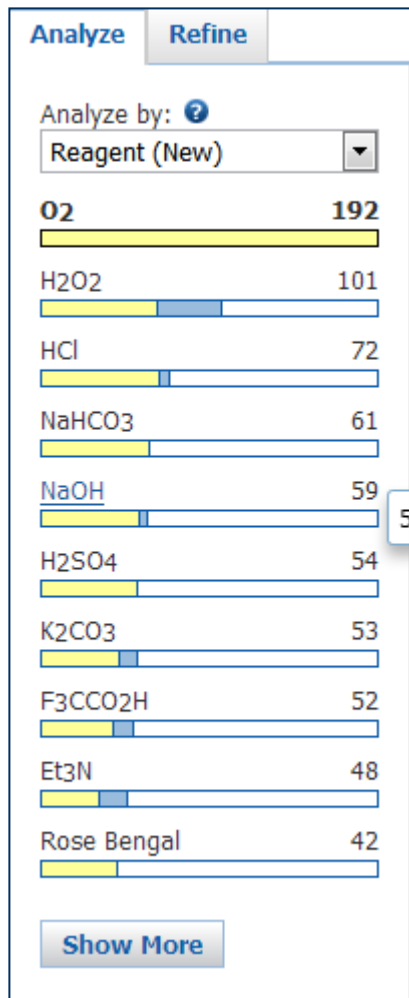
2. Hydrolysis of Acetals/ Orthoesters/ Enol Ethers and Similar Compounds
2 Reactions

$$\begin{array}{c} R^2O \\ | \\ R-C-OR^2 \\ | \\ R^1 \end{array} \xrightarrow{H^+} \begin{array}{c} O \\ || \\ R-C-R^1 \end{array} + R^2-OH$$

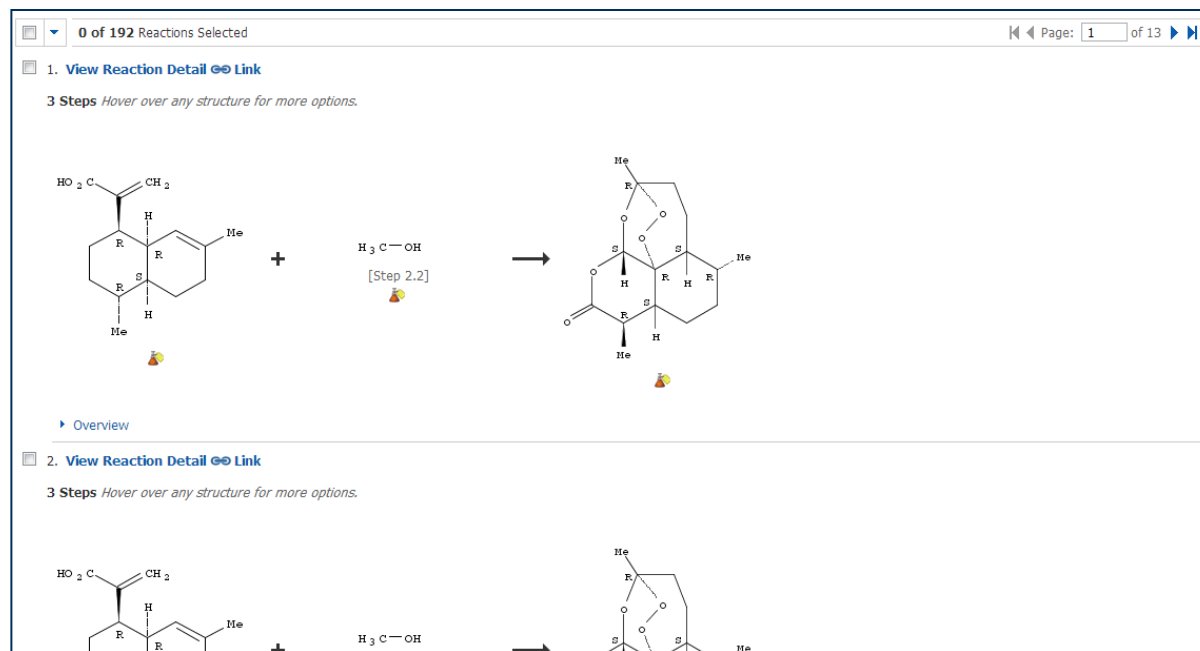
$$\begin{array}{c} R \\ | \\ R-C=C-R \\ | \\ OR^1 \end{array} \xrightarrow{H^+} \begin{array}{c} R \\ | \\ R-C-C-R \\ | \\ OR^1 \end{array} + R^1-OH$$

3. Formation of N/O/S Heterocycles
1 Reaction

按照试剂进行分析



有192篇文献都用的是O₂这个试剂



按照实验过程进行排序

REACTIONS ? Get References Tools Send to SciPlanner

Analyze Refine

Analyze by: Reagent (New)

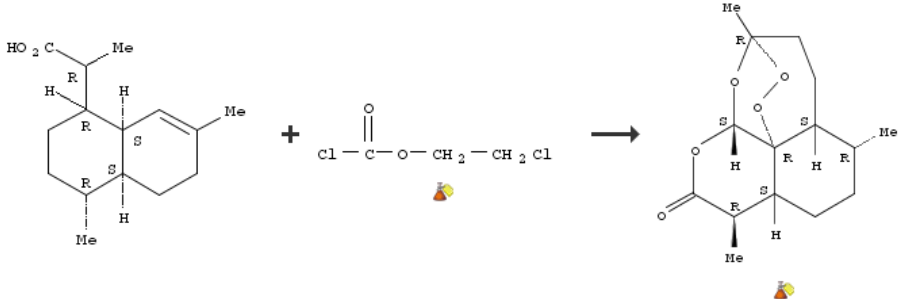
O2	192
HCl	67
H2O2	66
NaHCO3	61
NaOH	55
H2SO4	54
K2CO3	45
Rose Bengal	42
F3CCO2H	40
HgCl2	39

Group by: No Grouping Sort by: Experimental Procedure ↑

0 of 192 Reactions Selected Experimental Procedure Accession Number Number of Steps Product Yield Publication Year

☐ 1. [View Reaction Detail](#) Link

2 Steps *Hover over any structure for more options.*



[Overview](#)

[Experimental Procedure](#)

Step 1

Example 10: synthesis of (3*R*)-dihydroarteannuin B acid, 2-chloroethyl mixed carbonate 3.04 g (0.021 mol) of 2-chloroethyl chloroformate are added dropwise within 5 min. to a stirred solution of 5.01 g (0.021 mol) of DHAA and 4.04 g (0.029 mol) of K2CO3 in 25 mL of dichloromethane in an ice bath. After addition, stirring is continued for 20-30 min. The mixture is then washed twice with water (2 x 100 mL) and dried over MgSO4. The solution is then concentrated to dryness at reduced pressure and 6.78 g of an oily residue are obtained (crude yield = 93.5 %). The product can be used as such.

Step 2

General/Typical Procedure: Example 11: synthesis of artemisinin An amount of 4 g of the dihydroartemisinic acid (DHAA) derivative of formula (I) or (Ia) prepared in examples 1 to 10 above (1 eq.), 0.01 eq. of tetraphenylporphyrin and 80 mL of methylene chloride are introduced at 20°C in a clean 0.2 liter reactor. The mixture is then cooled down to -10°C and air or oxygen is bubbled through the mixture (40-50 mL/min.) under stirring at 300-400 rpm. After 30 min., trifluoroacetic acid (TFA, 0.5 eq.) is added and a halogen lamp is switched on. The mixture is stirred overnight (~19h) at -10°C and then warmed up to 10°C (60 min.) and stirred at 10°C during 60 min. The mixture is then warmed up to 20°C in about 60 min. and then the air introduction is stopped, the lamp switched off and the mixture stirred at 20°C during 2h. Then, the reaction mixture is treated by addition of 20 mL of water then 20 mL of a solution of aqueous saturated NaHCO3. The resulting mixture was then left for decantation and the two layers were separated. The organic layer is then loaded back in the vessel and washed again by addition of 20 mL of water then 20 mL of a solution of aqueous saturated NaHCO3. After decantation and layers separation, the organic layer is washed with 20 mL of water. After decantation, the organic layer is then concentrated under progressive vacuum at 30°C using a rotary evaporator. The dry product crystallizes at room temperature. Then 12 mL of n-heptane are added and the mixture is stirred during 1 h at 20°C. The reaction mixture is then filtrated under Buchner funnel (n°3). The wet solid is then washed first with 8 mL and then with 12 mL of n-heptane. The wet solid is then dried under vacuum at 40°C overnight (~15h). Crude artemisinin is obtained with good titrated yield (62% ti/ti). If desired, an additional recrystallization step in an ethanol/water mixture (70/30) can be performed on the solid product precipitated in n-heptane. Product name: artemisinin Yield: 54.9%

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REACTIONS ⓘ Get References Tools ▾ Send to SciPlanner

Analyze Refine

Analyze by: ⓘ
Reagent (New) ▾

O2	192
HCl	67
H2O2	66
NaHCO3	61
NaOH	55
H2SO4	54
K2CO3	45
Rose Bengal	42
F3CCO2H	40

Group by: No Grouping ▾ Sort by: Experimental Procedure ▾ ↑

0 of 192 Reactions Selected

Answers per Page [15] Display: ⓘ ⓘ

Page: 1 of 13

1. View Reaction Detail ⓘ Link

2 Steps Hover over any structure for more options.

Chemical reaction scheme showing the synthesis of a complex polycyclic ether. The reactant is a bicyclic structure with a carboxylic acid group (HO₂C) and a methyl group (Me). It reacts with 1,2-dichloroethane (Cl-CH₂-CH₂-Cl) to form a complex polycyclic ether product with multiple methyl groups and a fused ring system.

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SciFinder Web的注册和登陆

SciFinder Web的系统要求

Windows用户支持IE 7.x或者FireFox 2.x

Mac 用户支持 Firefox 和 Safari

Java 安装（初次使用结构时自动安装，建议安装Java 6）

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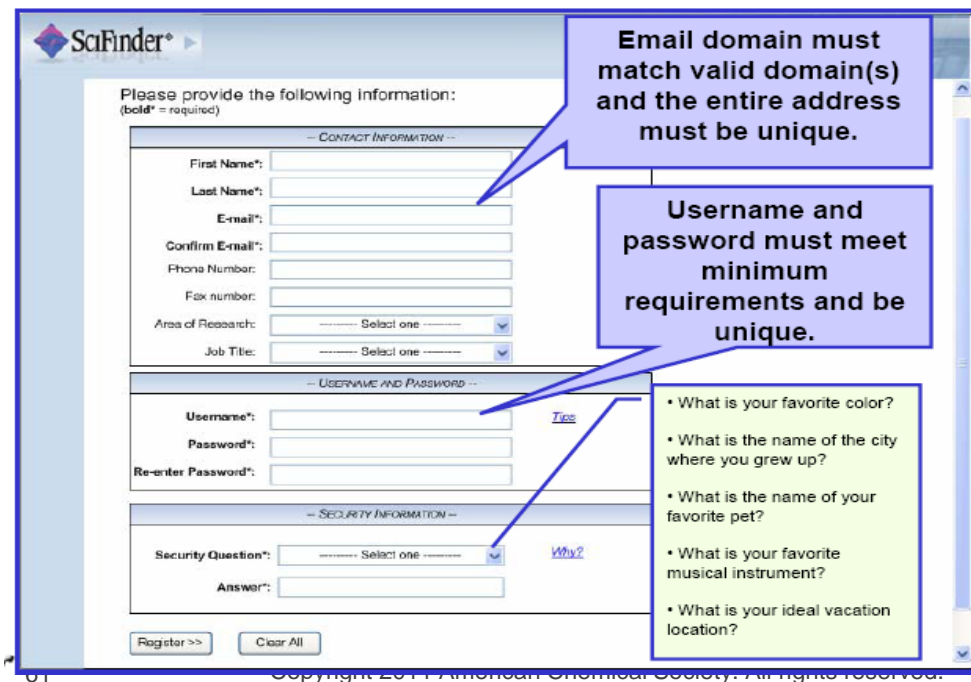
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(bold* = required)

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Last Name*:

E-mail*:

Confirm E-mail*:

Phone Number:

Fax number:

Area of Research: Select one

Job Title: Select one

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Password*:

Re-enter Password*:

— SECURITY INFORMATION —

Security Question*: Select one

Answer:

[Why?](#)

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Username and password must meet minimum requirements and be unique.

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- What is the name of the city where you grew up?
- What is the name of your favorite pet?
- What is your favorite musical instrument?
- What is your ideal vacation location?

设置用户名及密码注意事项

用户名：

必须是唯一的，且包含 **5-15** 个字符。它可以只包含字母或字母组合、数字和/或以下特殊字符：

- （破折号）
- _（下划线）
- .（句点）
- @（表示“at”的符号）

密码：

必须包含 **7-15** 个字符，并且至少包含三个以下字符：

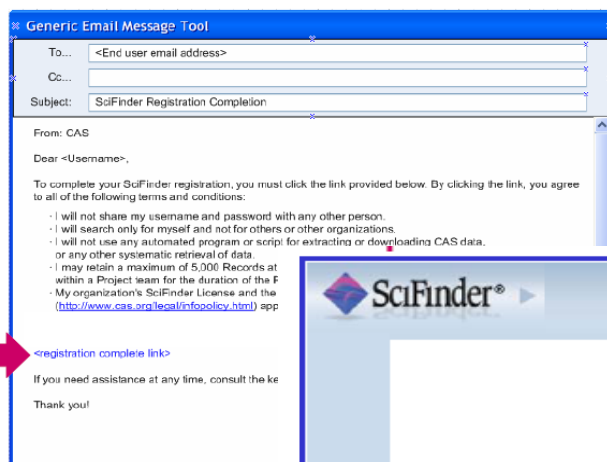
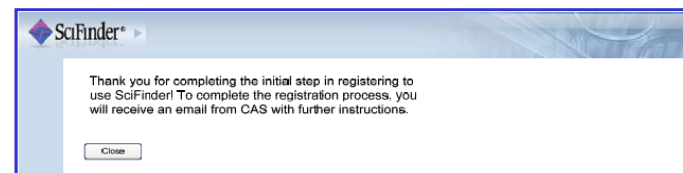
- 字母
- 混合的大小写字母
- 数字
- 非字母数字的字符（例如 @、#、%、&、*）

密码设置小技巧：

- 1：不要和账号中有重复的字符**
- 2：密码格式最好是abc@123**

对新ID的Email确认

需要点击邮件中的确认链接



SciFinder Web 常见问题



The screenshot shows the SciFinder web interface. At the top left is the SciFinder logo with the tagline "The choice for chemistry research.™". Below the logo, a red error message states: "Username and/or password is invalid. Try again, or contact CAS for assistance." To the left of the main content area is a "Sign In" section with input fields for "Username" and "Password", a "Remember me for two weeks unless I sign out" checkbox, and a "Sign In" button. Below the button is a link for "Forgot Username or Password?" and a note: "Your SciFinder username and password are assigned to you alone and may not be shared with anyone else." To the right of the login section is a "News & Updates" section with three articles: "Welcome to SciFinder", "The New SciFinder is Here!", "Collaboration Helps Integrate SciFinder to Streamline Research Workflows", "Expanded Coverage of Chemical Reaction Information in SciFinder", and "CAS is Collaborating with Springer to Help You Identify Preferred Synthetic Methods Faster". A 3D molecular model is positioned between the login and news sections.

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Collaboration Helps Integrate SciFinder to Streamline Research Workflows

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CAS is Collaborating with Springer to Help You Identify Preferred Synthetic Methods Faster

Thousands of new experimental procedures are [being added to SciFinder for chemical reactions](#).

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<http://www.cas.org/cgi-bin/casip>



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Sophisticated Analysis

Unprecedented Results



Thank You

李虹

SciFinder 培训专员

Mail: Della@igroup.com.cn

Tel: 010-82335058-807