

朱传娴

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# 如何从SciFinder中获得科技信息



青岛大学

2022.4

# 提纲

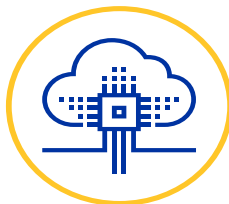
- 为什么需要美国化学文摘社
- SciFinder简介及检索方式
  - 文献检索
  - 物质检索
  - Markush检索
  - 反应检索
  - SciPlanner
- SciFinder常见问题及解决
- 上机练习

## 美国化学文摘社 (CAS) 隶属美国化学会 (ACS)，致力于追踪、收录、标引科学信息

- 拥有超过110年的经验；创立权威化学索引《化学文摘》(CA)
- 密切追踪、标引和提炼着全球化学相关的文献（包括专利）
- 提供各种科学信息和相关技术产品与服务
- 协助创新和保护创新, 助力于解决科研方面的难题与挑战



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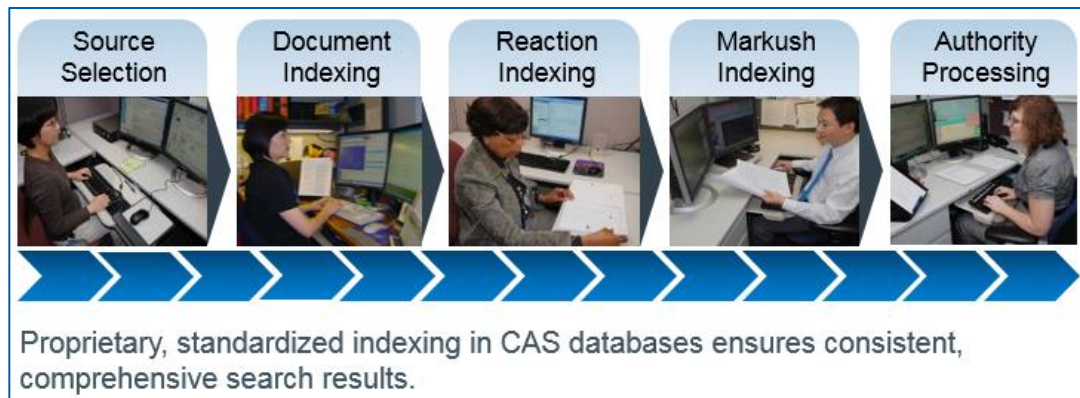
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- 生物化学：
  - 农化产品管控信息、生化遗传学、发酵、免疫化学、药理学
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- 大分子化学各领域：
  - 纤维素、木质素、造纸；涂料、墨水
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- 应用化学各领域：
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- 物理、无机、分析化学各领域：
  - 表面化学、催化剂、相平衡、核现象、电化学



## CAS科学家利用人类智慧对公开内容进行揭示，使相关信息更容易被挖掘



- 检索词的同义词拓展：解决不同科研人员由于教育背景、语言、表达习惯不同导致的对同一个技术术语描述的差异。
- 用名称、分子式等检索化合物，会导致检索不全、不准的问题。CAS RN很好地解决了该问题，帮助检索人员实现精准定位化合物的目标。
- 利用SciFinder中的标引信息（Index Term, CAS RN, CAS Role），提高效率，启发思路。

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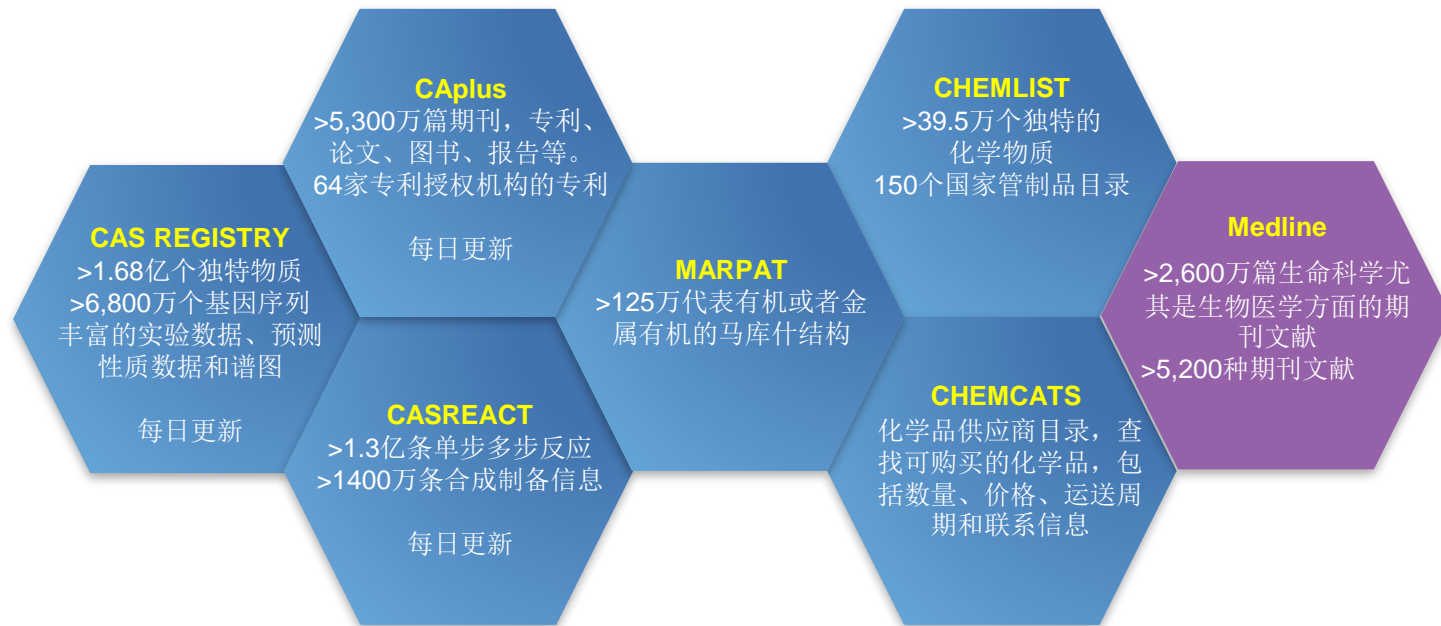
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# 提纲


- 美国化学文摘社简介
- SciFinder简介及检索方式
  - 文献检索
  - 物质检索
  - Markush检索
  - 反应检索
  - SciPlanner
- SciFinder常见问题及解决
- 上机练习



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# SciFinder主界面

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工具栏

Explore Saved Searches SciPlanner

REFERENCES: RESEARCH TOPIC

Research Topic  
Author Name  
Company Name  
Document Identifier  
Journal  
Patent  
Tags

Examples:  
The effect of antibiotic residues on dairy products  
Photocyanation of aromatic compounds

Search

Advanced Search

已保存的结果集

定题追踪

检索入口

SAVED ANSWER SETS

- CSF1R
- jmc
- EP 19870107847
- Dacatasvir-1
- SUB result
- EX result
- MF result
- polymer1
- polymer1
- structure search
- Autosaved Substance Set

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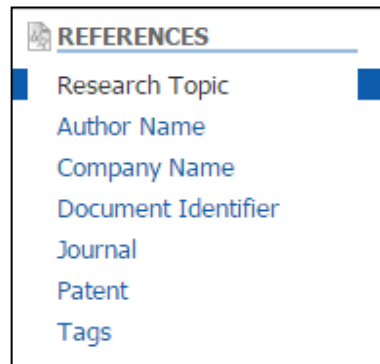


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# SciFinder检索——文献检索

## 文献检索方法

- 主题检索
- 作者名检索
- 机构名检索
- 文献标识符检索
- 期刊名称和专利信息（公开号，申请号等）
- 从物质，反应获得文献



## 检索策略推荐

- 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
- 关注某机构科研进展：机构名检索



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# 文献检索——主题

主题检索： 中药治疗新冠肺炎

检索式： Chinese Medicine in COVID-19

The screenshot displays the SciFinder web interface. At the top, there are three tabs: 'Explore', 'Saved Searches', and 'SciPlanner'. Below the tabs, the left sidebar is divided into two main sections: 'REFERENCES' and 'SUBSTANCES'. Under 'REFERENCES', there are several filter options: 'Research Topic', 'Author Name', 'Company Name', 'Document Identifier', 'Journal', 'Patent', and 'Tags'. Under 'SUBSTANCES', there are 'Chemical Structure' and 'Markush'. The main content area is titled 'REFERENCES: RESEARCH TOPIC' and features a search bar with the text 'chinese medicine in COVID-19'. Below the search bar, there are 'Examples:' such as 'The effect of antibiotic residues on dairy products' and 'Photocyanation of aromatic compounds'. A blue 'Search' button is prominently displayed. Below the button, there is a link for 'Advanced Search'.

关键词之间用介词连接：  
in, with, of...



# 主题检索的候选项

Explore ▾ Saved Searches ▾ SciPlanner

Research Topic "chinese medicine in COVID-19"

REFERENCES ?

Select All Deselect All

1 of 8 Research Topic Candidates Selected

	References
<input type="checkbox"/> 54 references were found containing "chinese medicine in COVID-19" as entered.	54
<input checked="" type="checkbox"/> 1096 references were found containing the two concepts "chinese medicine" and "COVID 19" closely associated with one another.	1096
<input type="checkbox"/> 1639 references were found where the two concepts "chinese medicine" and "COVID 19" were present anywhere in the reference.	1639
<input type="checkbox"/> 4176 references were found containing the concept "chinese medicine", and either the concept "COVID" or the concept "19". The concepts found were closely associated with one another.	4176
<input type="checkbox"/> 8396 references were found containing the concept "chinese medicine", and either the concept "COVID" or the concept "19". The concepts found were present anywhere (perhaps widely separated) within the reference.	8396
<input type="checkbox"/> 341298 references were found containing the concept "chinese medicine".	341298
<input type="checkbox"/> 106580 references were found containing the concept "COVID 19".	106580
<input type="checkbox"/> 1965032 references were found containing either the concept "COVID" or the concept "19".	1965032

Get References

- “Concepts”表示对主题词做了同义词的扩展
- “Closely associated with one another”表示同时出现在一个句子中
- “were present anywhere in the reference”表示同时出现在一篇文献中



# 按被引次数排序——Citing References

Explore ▾ Saved Searches ▾ SciPlanner

Research Topic "chinese medicine in COVID-19" > references (1022)

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REFERENCES ⓘ

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Analyze Refine Categorize

Sort by: Citing References Accession Number Author Name Citing References

1. Clinical features and therapeutic procedure for four cases with 2019 novel coronavirus pneumonia receiving combined Chinese and Western medicine treatment

By Wang, Zhenwei; Chen, Xiaorong; Lu, Yunfei; Chen, Feifei; Zhang, Wei  
From BioScience Trends (2020), 14(1), 64-68. | Language: English, Database: CAPLUS

Pneumonia assoc. with the 2019 novel coronavirus (2019-nCoV) is continuously and rapidly circulating at present. No effective antiviral treatment has been verified thus far. We report here the clin. characteristics and therapeutic procedure for four patients with mild or severe 2019-nCoV pneumonia admitted to Shanghai Public Health Clin. Center. All the patients were given antiviral treatment including lopinavir/ritonavir (Kaletra), arbidol, and Shufeng Jiedu Capsule (SFJDC, a traditional Chinese medicine) and other necessary support care. After treatment, three patients gained significant improvement.

2. Clinical features and treatment of COVID-19 patients in northeast Chongqing

By Wan, Suxin; Xiang, Yi; Fang, Wei; Zheng, Yu; Li, Boqun; Hu, Yanjun; Lang, Chunhui; Huang, Daoqiu; Sun, Qiuyan; Xiong, Yan; et al  
From Journal of Medical Virology (2020), 92(7), 797-806. | Language: English, Database: CAPLUS

The outbreak of the novel coronavirus in China (SARS-CoV-2) that began in Dec. 2019 presents a significant and urgent threat to global health. This study was conducted to provide the international community with a deeper understanding of this new infectious disease. Epidemiol., clin. features, lab. findings, radiol. characteristics, treatment, and clin. outcomes of 135 patients in northeast Chongqing were collected and analyzed in this study. A total of 135 hospitalized patients with COVID-19 were enrolled. The median age was 47 years (interquartile range, 36-55), and there was no significant difference in clinical features between the two groups.

3. COVID-19 infection and rheumatoid arthritis: Faraway, so close!

By Favalli, Ennio Giulio; Ingegnoli, Francesca; De Lucia, Orazio; Cincinelli, Gilberto; Cimaz, Rolando; Caporali, Roberto  
From Autoimmunity Reviews (2020), 19(5), 102523. | Language: English, Database: CAPLUS

A review. The outbreak of the new coronavirus infections COVID-19 in Dec. 2019 in China has quickly become a global health emergency. Given the lack of specific anti-viral therapies, the current management of severe acute respiratory syndrome coronavirus (SARS-CoV-2) is mainly supportive, even though several compounds are now under investigation for the treatment of this life-threatening disease. COVID-19 pandemic is certainly conditioning the treatment strategy of a complex disorder as rheumatoid arthritis (RA), whose infectious risk is increased compared to the general population because ...

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# 文献结果集

Explore ▾ Saved Searches ▾ SciPlanner Save Print Export

Research Topic "chinese medicine in COVID-19" > re

文献分析工具

REFERENCES ?

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Analyze Refine Categorize

Sort by: Accession Number ▾

0 of 1022 References Selected

Analyze by: Author Name

Anon	26
Zhang Wei	23
Liu Qingquan	11
Li Bin	10
Xie Chunguang	10
Li Jing	9
Miao Mingsan	9
Pang Bo	9
Zhang Jun Hua	9
Zhang Ying	9

Show More

1. **Traditional Chinese exercise for COVID-19: A protocol for systematic review and meta-analysis**  
Quick View Other Sources  
By Duan, Yuanxuan; Xiong, Mengran; Wang, Heping; Yao, Xiaoyan; Liu, Hanyuan; Li, Guangxi  
From Medicine (Philadelphia, PA, United States) (2020), 99(45), e23044. | Language: English, Database: CAPLUS  
Background: A new type of coronavirus (**COVID-19**), is spreading all over the world. Under the background of the comprehensive medical treatment and strict prevention and control in China, the no. of discharged patients increased substantially. By the end of July, more than 80,000 patients had been cured and discharged from hospital in China. In order to effectively promote the full recovery of the patient's phys. and mental functions and quality of life, gradually shift  
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2. **Anti-COVID-19 drug screening: Frontier concepts and core technologies**  
Quick View Other Sources  
By Luo, Hua; Zhao, Mingming; Tan, Dechao; Liu, Chang; Yang, Lin; Qiu, Ling; Gao, Yan; Yu, Hua  
From Chinese Medicine (London, United Kingdom) (2020), 15(1), 115. | Language: English, Database: CAPLUS  
Abstr.: The outbreak of **COVID-19** has recently evolved into a global pandemic. Up to July 2020, almost every country has confirmed **COVID-19** cases reported worldwide. Many leading experts have predicted that the epidemic will persist for relatively a long period of time. Thus far, there have been no remedies proven effective against the disease. As the nation where **COVID-19** broke out first, China has adopted a combination of traditional **Chinese medicine** and western **medicine** to fight against the disease, and has achieved significant clin. result. Up to now, the **COVID-19** pandemic has been eff...

3. **In-silico recognition of liquorice phytoconstituents specially glabranin B as a potential cathepsin L inhibitor to hinder 2019-NCOV host cell entry**  
Quick View Other Sources  
By Fathy, Hoda; Abdelhady, Walid; Ibrahim, Reham S.  
From International Journal of Pharmaceutical Sciences Review and Research (2020), 64(1), 197-202. | Language: English, Database: CAPLUS  
The pandemic caused by novel coronavirus disease 2019 infecting millions of populations worldwide and the lack of specific treatment necessitate the use of all resources to remedy this scourge. The chem.-diverse natural products have been valuable sources for drug leads for centuries. Traditional **Chinese Medicine** (TCM) has a long history and achieved remarkable therapeutic effect during the treatment period of **COVID-19** in China. This brief article discusses the therapeutic potential of some bioactive compds. from liquorice (*Glycyrrhiza glabra*) root for the treatment of **COVID-19** by binding t...

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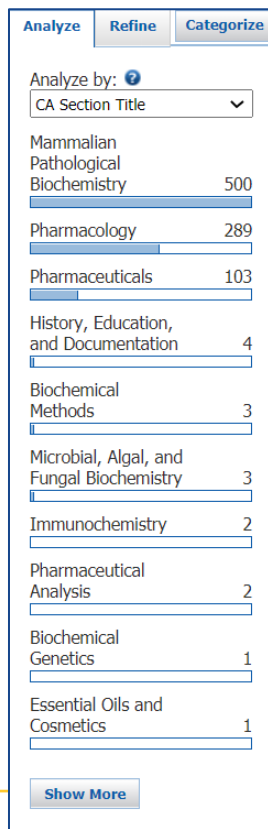


# 分析文献结果集——Analyze

期刊



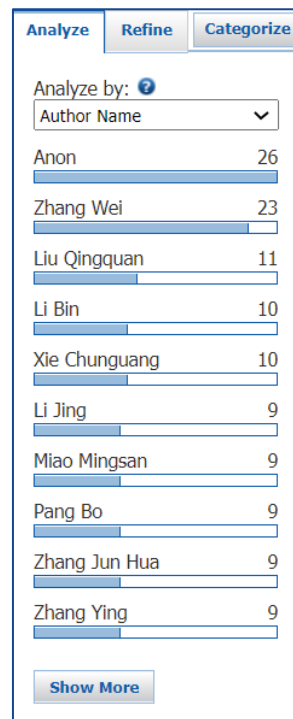
涉及学科领域



本领域研究机构、合作伙伴、竞争对手



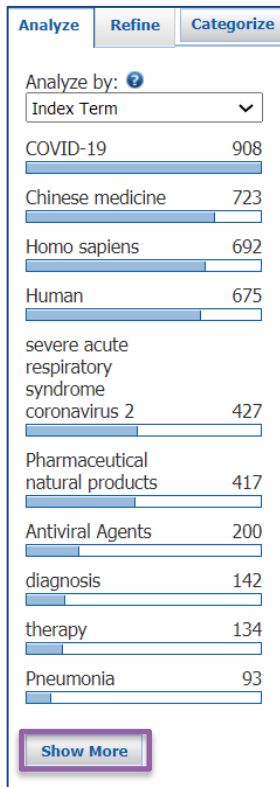
本领域研究人员



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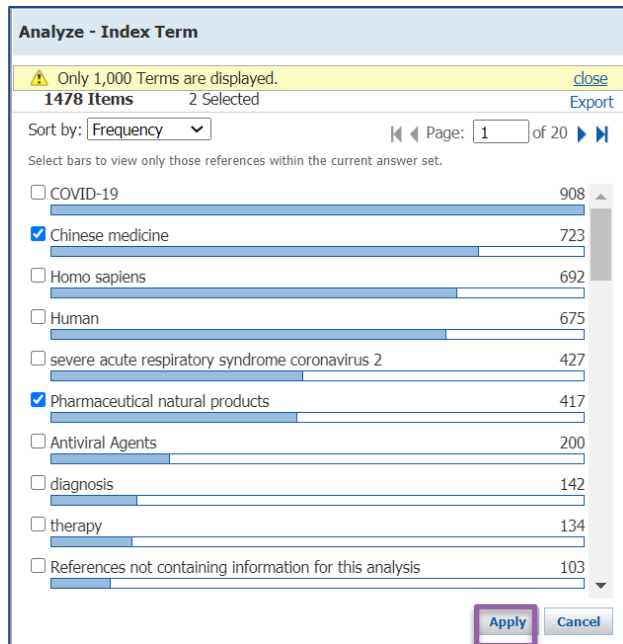
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# 分析文献结果集——Analyze



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# 筛选文献结果集——Refine

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Refine by: ?

☐ Research Topic

☐ Author

☐ Company Name

☒ Document Type

☐ Publication Year

☐ Language

☐ Database

Document Type(s)

☐ Biography

☐ Book

☐ Clinical Trial

☐ Commentary

☐ Conference

☐ Dissertation

☐ Editorial

☐ Historical

☐ Journal

☐ Letter

☐ Patent

☐ Preprint

☐ Report

☒ Review

Refine

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Send selected records to SciPlanner. Send to SciPlanner

Sort by: Accession Number

0 of 212 References Selected

Page: 1 of 11

Display Options

☐ 1. **Herbal immune-boosters: Substantial warriors of pandemic Covid-19 battle**  
Quick View Other Sources  
By Khanna, Kanika; Kohli, Sukhmeen Kaur; Kaur, Ravdeep; Bhardwaj, Abhay; Bhardwaj, Vinay; Ohri, Puja; Sharma, Anket; Ahmad, Ajaz; Bhardwaj, Renu; Ahmad, Parvaiz  
From Phytomedicine (2020), Ahead of Print. | Language: English, Database: CAPLUS  
A review. Current scenario depicts that world has been clenched by COVID-19 pandemic. Inevitably, public health and safety measures could be undertaken in order to dwindle the infection threat and mortality. Moreover, to overcome the global menace and drawing out world from moribund stage, there is an exigency for social distancing and quarantines. Since Dec., 2019, coronavirus, SARS-CoV-2 (COVID-19) have came into existence and up till now world is still in the state of shock. At this point of time, COVID-19 has entered perilous phase, creating havoc among individuals, and this has been ...

☐ 2. **The global registry of COVID-19 clinical trials: indicating the design of traditional Chinese medicine clinical trials**  
Quick View Other Sources  
By Wei, Xuxu; Zhao, Mengzhu; Zhao, Chen; Zhang, Xiaoyu; Qiu, Ruijin; Lin, Yiyi; Sun, Yang; Guan, Manke; Shang, Hongcai  
From TMR Modern Herbal Medicine (2020), 3(3), 140-146. | Language: English, Database: CAPLUS  
A review. Objective: To analyze the registration information of Corona Virus Disease 2019 (COVID-19) related clin. trials from all the clin. trial registry accepted by the International Committee of Medical Journal Editors (ICMJE). Methods: All the database of ICMJE-accepted clin. trial registry platform were searched for COVID-19 related clin. trials that registered from Dec. 8, 2019 to Feb. 19, 2020. Results: All the database totally contained data of 209 COVID-19 related clin. trials, including 66(31.6%) traditional Chinese medicine (TCM) related studies and 143(68.4%) non-TCM related st...

☐ 3. **Discuss about the application of Artemisia annua prescriptions in the treatment of COVID-19**  
Quick View Other Sources  
By Dong, Ruolan; Xiong, Xinyu; Chen, Guang  
From TMR Modern Herbal Medicine (2020), 3(3), 158-164. | Language: English, Database: CAPLUS  
A review and discussion. The applications of traditional Chinese medicine (TCM) have been playing an important role in treating the epidemics of Coronavirus Disease 2019 (COVID-19), which is now prevalent all over the world. Exploring the mechanisms of TCM compd. prescriptions might be difficult though, pharmacol. studies on elucidating the effective components of TCM could serve as the exptl. basis in the application of TCM compd. prescription in treating COVID-19. As the crit. active ingredients of Qinghao (Artemisia annua), artemisinin was initially used as antimalaria drug. Artemisia a...

☐ 4. **A review and comment on the current situation of 2019 novel coronavirus prevention by traditional Chinese medicine**  
Quick View Other Sources  
By Li, Mi; Jiang, Zixiang; Wang, Xian; Li, Kai; Xie, Yiqiang  
From TMR Modern Herbal Medicine (2020), 3(3), 147-157. | Language: English, Database: CAPLUS  
A review. Objective: To provide some valuable research ideas for the prevention of 2019-nCoV through reviewing and commenting the Chinese herbs in existing prevention programs of TCM. Methods: Firstly, searching the prevention and treatment programs for 2019-nCoV issued before Jan. 29, 2020. There are only three sources that can be selected in, including national and provincial health commissions, research and clin. institutes of TCM and national famous TCM doctors. Secondly, from the collections of all prevention and treatment programs, we sorted out prevention parts within Chinese herbs ...

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# 分类文献结果集——Categorize

学科领域  
主分类

学科领域  
副分类

Index Term

选中的Index Term

Categorize

1. Select a heading and category.

Category Heading	Category
All	Miscellaneous substances (321)
General chemistry	Substances in property studies (208)
Genetics & protein chemistry	
<b>Physical chemistry</b>	<b>Gas, liquid, &amp; solid phenomena (22)</b>
Polymer chemistry	Substances in processes (28)
Biotechnology	Mechanics (4)
Biology	Particle phenomena (3)
Technology	Thermodynamics (3)
Analytical chemistry	Spectra & spectroscopy (3)
Environmental chemistry	Electric & magnetic phenomena (2)
Synthetic chemistry	Subatomics (1)
Catalysis	

2. Select index terms of interest.

Index Terms	
Select All	Deselect All
<input checked="" type="checkbox"/> Pharmaceutical decoctions	60
<input checked="" type="checkbox"/> Pharmaceutical injections	20
<input type="checkbox"/> Sputum	9
<input type="checkbox"/> Blood plasma	5
<input type="checkbox"/> Convalescent plasma	5
<input type="checkbox"/> Binding energy	2
<input type="checkbox"/> Blood serum	2
<input type="checkbox"/> Body fluid	2
<input type="checkbox"/> Disorder	2
<input type="checkbox"/> Air	1
<input type="checkbox"/> Blood	1
<input type="checkbox"/> Crystallization	1
<input type="checkbox"/> Drops	1
<input type="checkbox"/> Exudate	1

Selected Terms

Click 'x' to remove the category from 'Selected Terms'

☒ Physical chemistry > Gas, liquid, & solid phenomena (2 Terms)

Physical chemistry > Gas, liquid, & solid phenomena > 2 Index Term(s) Selected

OK

Cancel

Categorize学科分类功能，基于Index Term，根据大学科方向对文献进行自动分类。



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# 文献结果集的保存——Save, Print, Export

Searches ▾ SciPlanner Save Print Export

ally removed.

COVID-19 > references (1022) > refine by categories

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Sort by: Accession Number ▾

0 of 80 References Selected

Page: 1 of 4

**1. Chemical composition and pharmacological mechanism of shenfu decoction in the treatment of novel coronavirus pneumonia (COVID-19)**

By Li, Xiaoling; Lin, Haowen; Wang, Qic; Cui, Liao; Luo, Hui; Luo, Lianjiang  
From Drug Development and Industrial Pharmacy (2020), Ahead of Print. | Language: English, Database: CAPLUS

Purpose Shenfu decoction has outstanding curative effects in the treatment of COVID-19. This study aimed to explore the material basis and mol. mechanism of Shenfu Decoction through network pharmacol. and mol. mechanisms, to provide a research basis for clin. medication and clues for subsequent research. Methods The active components and targets of Shenfu decoction were searched in the Traditional Chinese Medicine Systems Pharmacol. Database and Anal. Platform (TCMSP), and the COVID-19-assoc. genes were collected using the GeneCards platform.

**2. Traditional Chinese medicine Lianhua Qingwen treating corona virus disease 2019 (COVID-19): Meta-analysis of randomized controlled trials**

Quick View [Other Sources]  
By Zeng, Mengjie; Li, Lijun; Wu, Zheqian  
From Frontiers in Immunology (2020), 11(9), e593828. | Language: English, Database: CAPLUS

As the global epidemic continues to spread, countries have tapped effective drugs to treat new coronavirus pneumonia. The therapeutic effect of the traditional Chinese medicine Lianhua Qingwen in this new coronary pneumonia epidemic has attracted attention from all walks of life, and relevant research reports continue to appear. Therefore, we conducted a systematic review of the clin. efficacy and safety of the traditional Chinese medicine Lianhua Qingwen in the treatment of new coronavirus pneumonia (COVID-19) (referred to as "new coronary pneumonia"), and evaluated the overall level of res...

**3. Chemoprophylaxis, diagnosis, treatments, and discharge management of COVID-19: An evidence-based clinical practice guideline (updated version)**

Quick View [Other Sources]  
By Jin, Ying-Hui; Zhan, Qing-Yuan; Peng, Zhi-Yong; Ren, Xue-Qun; Yin, Xun-Tao; Cai, Lin; Yuan, Yu-Feng; Yue, Ji-Rong; Zhang, Xiao-Chun; Yang, Qi-Wei; et al  
From Military Medical Research (2020), 7(1), 41. | Language: English, Database: CAPLUS

The novel severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) is the cause of a rapidly spreading illness, coronavirus disease 2019 (COVID-19), affecting more than seventeen million people worldwide. Diagnosis and treatment guidelines for clinicians caring for patients are needed. In the early stage, we have issued "A rapid advice guideline for the diagnosis and treatment of 2019 novel coronavirus (nCoV) infected pneumonia (std. version)"; now there are many direct evidences emerged and may change some of previous recommendations and it is ripe for develop an evidence-based...

**4. A case of treatment of a new coronavirus pneumonia patient with consistent fever using Fenghuolun theory by professor Du Shaohui**

Quick View [Other Sources]  
By Yang, Hai; Du, Shaohui; Liu, Min; Guo, Rui-sheng; Cao, Jiao-jiao; He, Zhen-yu; Zhang, Ping; Li, Ling; Yue, Ting-ting; Zhu, Yan-xian  
From Open Access (OA) Online-First Publishing of Research Papers on COVID-19 (2020), 1-4. | Language: Chinese, Database: CAPLUS

A COVID-19 patient with consistent fever was treated by professor Du Shaohui using Chinese traditional medicine theory, Fenghuolun. The patient was treated with pharmaceutical natural products Xiaocaihu decoction and Mahuangshengma decoction.

文献详细信息

Save: 保存在服务器上, 方便以后登陆查看, 每次可存2万条记录。

Export: 导出至本地电脑。

Print: 打印成PDF格式

Export ▾

Export:

- ☐ All
- ☐ Selected
- ☐ Range

Example: 2-20

For:

Citation Manager

- ☐ Citation export format (\*.ris)
- ☐ Quoted Format (\*.bt)
- ☐ Tagged Format (\*.bt)

Offline review

- ☒ Portable Document Format (\*.pdf)
- ☐ Rich Text Format (\*.rtf)
- ☐ Answer Keys (\*.bt)

Saving locally

- ☐ Answer Key eXchange (\*.alox)

Details:

File Name: \*

Reference\_06\_19\_2012\_100848

Format:

- ☐ Summary without abstracts
- ☐ Summary with partial abstracts
- ☐ Summary with full abstracts
- ☐ Detail (full record)

Include:

- ☐ Task History
- ☐ Tags
- ☐ Comments

Export Cancel

Citation manager: 保存成RIS等格式, 可导入EndNote 等文献管理工具

Offline Review: 保存成PDF, RTF等格式, 用于脱机浏览



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# 文献信息——题录、摘要、索引

REFERENCE DETAIL

Get Substances

Get Related Citations

Link to Other Sources

Send to SciPlanner

Return

Previous | Next

## 1. Chemical composition and pharmacological mechanism of shenfu decoction in the treatment of novel coronavirus pneumonia (COVID-19)

By: Li, Xiaoling; Lin, Haowen; Wang, Qu; Cui, Liao; Luo, Hui; Luo, Lianxiang

Purpose Shenfu decoction has outstanding curative effects in the treatment of COVID-19. This study aimed to explore the material basis and mol. mechanism of Shenfu Decoction through network pharmacol. and mol. mechanisms, to provide a research basis for clin. medication and clues for subsequent research. Methods The active components and targets of Shenfu decoction were searched in the Traditional Chinese Medicine Systems Pharmacol. Database and Anal. platform (TCMSP), and the COVID-19 associated genes were collected using the Gene Cards platform. The target protein-protein interaction network map was constructed by mapping two genes, and the 'drug-active ingredient-target' network was constructed using Cytoscape software. The Gene Ontol. (GO) function and Kyoto Encyclopedia of Genes and Genomes (KEGG) pathway enrichment of the mapping targets were analyzed. Result Based on Traditional Chinese medicine, Shenfu Decoction can take effect in the lung, spleen, kidney and heart. Considering oral bioavailability (OB)  $\geq 30\%$  and drug-like (DL)  $\geq 0.18$  as the std., 43 active compds. were screened and 114 Shenfu decoction action targets were collected. The key targets were CASP3, MAPK8, PTGS2, IL1B, PPARG, ICAM1, IFNG, RELA, NOS2, NOS3, HMOX1, CASP8, STAT1, and TGFBI. According to the std. of  $p < .05$ , GO function was enriched in 108 biol. processes, 16 cell processes and 21 mol. processes. Sixty-three signaling pathways were enriched by KEGG, which can be divided into four types: viral infection pathways, signal pathways, biol. process pathways and different disease pathways. The combination of neg. and pos. prescriptions further reflects the pos. effect of Shenfu decoction against COVID-19. Finally, the effective ingredients with the high degree were mol. docked with Mpro, RdRp and Spro protein. Conclusion Shenfu decoction played an important role in regulating the anti-virus process, regulating immunity, inhibiting inflammation and the mechanism of multi-components and multi-targets, to treat patients with severe COVID-19.

### Indexing

Pharmacol.

Concepts

Substances

QUICK LINKS

SOURCE

COMPANY/ORGANIZATION

重要概念

重要物质

Antiviral agents  
Chinese medicine  
Homo sapiens  
Molecular docking  
Severe acute respiratory syndrome coronavirus 2

COVID-19  
Genome  
Human  
Pharmaceutical decoctions

Chem. compn. and pharmacol. mechanism of shenfu decoction in the treatment of novel coronavirus pneumonia (COVID-19)

Interleukin 1β  
Peroxisome proliferator-activated receptor γ  
Transcription factor STAT1  
Type II interferons

Transcription factor RelA  
Transforming growth factor β1

Chem. compn. and pharmacol. mechanism of shenfu decoction in the treatment of novel coronavirus pneumonia (COVID-19)

Biological study, unclassified; Biological study

9026-28-2 RdRp  
169592-56-7 CASP3  
179241-78-2 CASP8  
218925-73-6 Mpro protease  
289898-51-7 MAPK8  
329900-75-6 PTGS2  
501433-35-8 NOS2  
503473-02-7 NOS3  
1355645-85-0 HMOX1

Chem. compn. and pharmacol. mechanism of shenfu decoction in the treatment of novel coronavirus pneumonia (COVID-19)

Biological study, unclassified; Biological study

83-46-5 β-Sitosterol  
83-48-7 Stigmasterol  
117-52-2 Fumarin  
520-18-3 Kaempferol

QUICK LINKS

SOURCE

COMPANY/ORGANIZATION

0 Tags, 0 Comments

Drug Development and Industrial Pharmacy  
PagesAhead of Print  
Journal  
2020  
CODEN:DDIPD8  
ISSN:0363-9045  
DOI:10.1080/03639045.2020.1826510

Animal Experiment Center  
Guangdong Medical

文献详情界面包括：

- 标题
- 摘要
- 文献中重要的技术术语
- 文献中重要的物质
- 书目信息
- 获得文献中的物质、反应
- 参考文献
- 链接原文



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# 文献检索小结

1. 使用介词 in, with, of 等作为连接词
2. 根据检索要求选择合适的候选项
3. 通过Analyze/Refine/Categorize功能来筛选结果
4. 从Related Citations拓展检索，获得更多灵感

# 提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
  - 文献检索
  - 物质检索
  - Markush检索
  - 反应检索
  - SciPlanner
- SciFinder常见问题及解决
- 上机练习

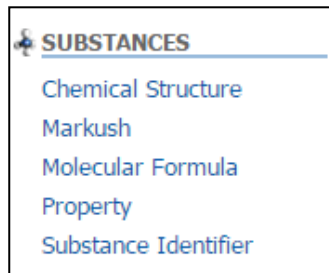




# SciFinder检索——物质检索

## ■ 物质检索方法

- 结构式检索
- 分子式检索
- 理化性质检索
- 物质标识符检索：化学名称，CAS RN



## ■ 物质检索策略推荐

- 有机化合物，天然产物：结构检索
- 无机物，合金：分子式检索
- 高分子化合物：分子式检索和结构检索



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# 物质检索——标识符检索

检索Argireline，类肉毒杆菌、六胜肽

Explore ▼ Saved Searches ▼ SciPlanner

Research Topic "chinese medicine in COVID-19" > references (1022) > refine by categories > Chemical composition and pharm

**REFERENCES**

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

**SUBSTANCES**

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

**SUBSTANCES: SUBSTANCE IDENTIFIER**

Argireline

Enter one per line.  
Examples:  
50-00-0  
999815  
Acetaminophen

Search

物质标识符包括CAS RN  
和化学名称，化学名称  
可以是通用名称、商品  
名、俗名。

提示：

- 一次最多可输入25个物质。
- 每行一个物质标识符。






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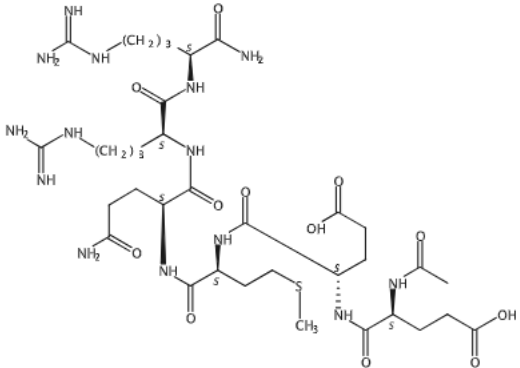
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# SciFinder中的物质记录

点击CAS RN 获得物质详细信息

☐ 1. **616204-22-9**

~695   ~62 



Absolute stereochemistry.

**C<sub>34</sub> H<sub>60</sub> N<sub>14</sub> O<sub>12</sub> S**  
L-Argininamide, *N*-acetyl-L-α-glutamyl-L-α-glutamyl-L-methionyl-L-glutamyl-L-arginyl-  
Protein Sequence  
Sequence Length: 6  
**▶ Key Physical Properties**  
Regulatory Information

**CAS Registry Number: 616204-22-9**

- » View Substance Detail
- 🔍 Explore by Structure ▶
- Synthesize this...
- Get Reactions where Substance is a ▶
- Get Commercial Sources
- Get Regulatory Information
- Get References
- Export as Image
- Export as molfile
- Send to SciPlanner

在SciFinder中，鼠标滑过物质，即可打开物质标准菜单，获得与物质相关的所有内容

## SciFinder中的物质记录

## SUBSTANCE DETAIL ?



## Get References



## Get Reactions



## Get Commercial Sources

Return

CAS Registry Number 616204-22-9

~695


$$\text{C}_{34} \text{H}_{60} \text{N}_{14} \text{O}_{12} \text{S}$$

L-Argininamide, *N*-acetyl-L- $\alpha$ -glutamyl-L- $\alpha$ -glutamyl-L-methionyl-L-glutaminy-L-arginyl-

### Molecular Weight

888.99

## Density (Predicted)

Value: 1.54±0.1 g/cm<sup>3</sup> | Condition: Temp: 20 °C Press: 760 Torr

pKa (Predicted)

Value: 4.43±0.10 | Condition: Most Acidic Temp: 25 °C

### Other Names

*N*-Acetyl-L- $\alpha$ -glutamyl-L- $\alpha$ -glutamyl-L-methionyl-L-glutaminyl-L-arginyl-L-argininamide

Acetyl hexapeptide 8

Acetyl hexapeptide-3

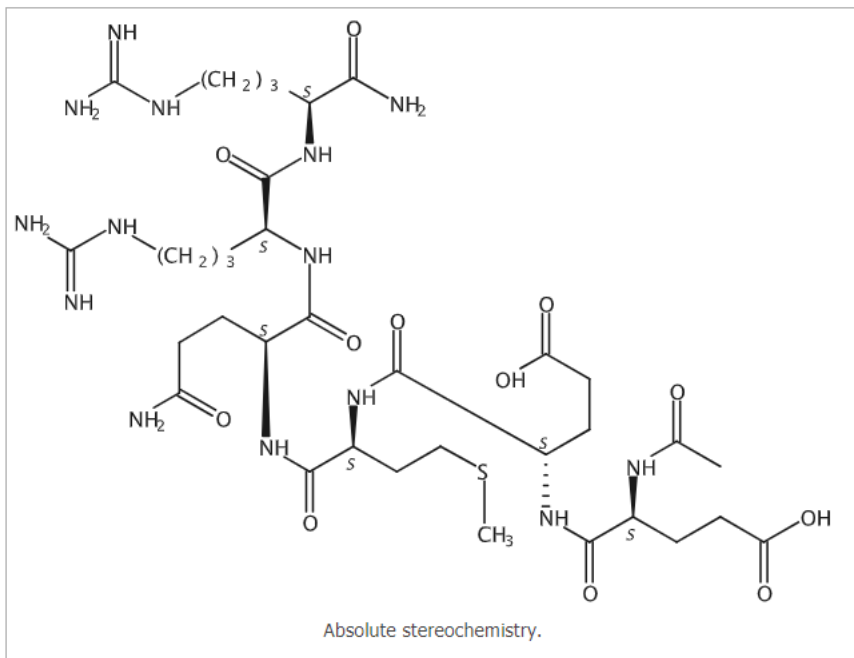
Argireline

Argireline NP

### Protein Sequence

Sequence Length: 6  
modified

由物质获得文献, 反应, 供应商等信息



## 物质详情

# SciFinder中的物质记录

▼ **SEQUENCE DETAILS**

Sequence:

1 EEMQRR

蛋白序列

Sequence Modifications

Type	Location	Description
terminal mod.	Glu-1	N-acetyl
terminal mod.	Arg-6	C-terminal amide

► **PREDICTED PROPERTIES**

► **PREDICTED SPECTRA**

<sup>1</sup>H NMR <sup>13</sup>C NMR

<sup>1</sup>H NMR Properties

Value	Condition	Note
Proton NMR Spectrum	See spectrum	(2)

Notes

(2) Predicted NMR data calculated using Advanced Chemistry Development, Inc. (ACD/Labs) Software V11.01 (© 1994-2020 ACD/Labs)

► **REGULATORY INFORMATION**

► **TARGET INDICATORS**

► **CAS REFERENCE ROLES**

► **ADDITIONAL DETAILS**



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# 物质检索——Property explore

https://scifinder.cas

CAS Solutions

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A CAS SOLUTION

Explore ▾ Saved Searches ▾

**REFERENCES**

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

**SUBSTANCES**

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

Select Property...

- Bioconcentration Factor
- Boiling Point (°C)
- Density (g/cm<sup>3</sup>)
- Enthalpy of Vaporization (kJ/mol)
- Flash Point (°C)
- Freely Rotatable Bonds
- H Donor/Acceptor sum
- H Acceptors
- H Donors
- Koc
- logD
- logP
- Mass Intrinsic Solubility (g/L)
- Mass Solubility (g/L)
- Molar Intrinsic Solubility (mol/L)
- Molar Solubility (mol/L)
- Molar Volume (cm<sup>3</sup>/mol)
- Molecular Weight**
- pKa

Molecular Weight

Examples: 44, 25-35, >125

250-400

Examples: 44, 25-35, >125

Search

寻找分子量在250-400之间的物质



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# 物质结果集的筛选——Refine

SUBSTANCES ?

Get References Get Reactions Get Commercial Sources Tools

Analyze Refine

Sort by: CAS Registry Number

0 of 45142315 Substances Selected

Refine by:

- Chemical Structure
- Isotope-Containing
- Metal-Containing
- Commercial Availability
- Property Availability
- Property Value
- Reference Availability
- Atom Attachment

Structure Editor:

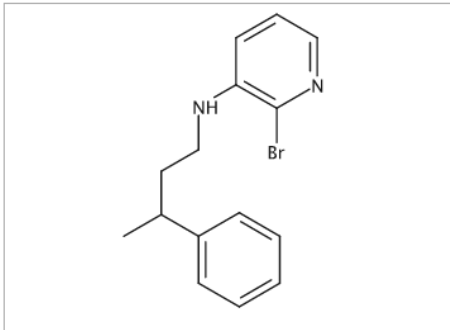
Java Non-Java

Click to Edit

Search type: Exact Structure

Only retrieve substances

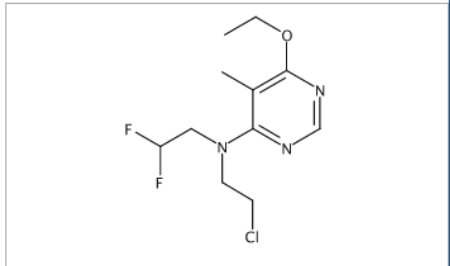
1. 1986293-22-4



$C_{15}H_{17}BrN_2$   
3-Pyridinamine, 2-bromo-N-(3-phenylbutyl)-

Key Physical Properties

2. 1986293-21-3



$C_{11}H_{16}ClF_2N_3O$   
4-Pyrimidinamine, N-(2-chloroethyl)-N-(2,2-difluoroethyl)-6-ethoxy-5-methyl-

Key Physical Properties

4. 1986293-16-6

5. 1986293-14-4

4500多万个结构,  
如何筛选黄酮类物质?



# 物质结果集的筛选——Refine

**SUBSTANCES**

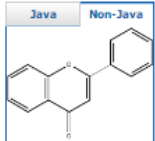
Analyze Refine

Refine by:

- ☒ Chemical Structure
- ☐ Isotope-Containing
- ☐ Metal-Containing
- ☐ Commercial Availability
- ☐ Property Availability
- ☐ Property Value
- ☐ Reference Availability
- ☐ Atom Attachment

Structure Editor:

Java Non-Java



Click image to change structure or view detail.  
Search type: **Substructure**

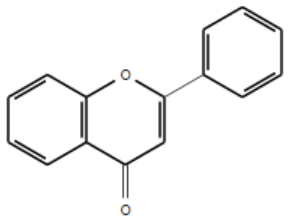
Only retrieve substances that:

- ☐ Have references
- ☐ Are commercially available
- ☒ Are a single component
- ☐ Are in specific substance classes
- ☐ Are in specific types of studies

Refine

**Structure Editor**

Draw or change atoms or bonds. Shortcut Keys



Get substances that match your query using:

- ☐ Exact search
- ☒ Substructure search

OK Cancel

C15H10O2 222.24

锁环工具：避免在被锁定的环结构上出现新的环结构



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# 物质检索结果集

Explore ▼ Saved Searches ▼ SciPlanner

Property "Predicted - Molecular Weight, ..." > substances (45142315) > refine "substructure" (16901)

**SUBSTANCES**

Get References Get Reactions Get Commercial Sources Tools ▼

Analyze Refine

Sort by: Relevance ▼

0 of 16901 substances Selected

Refine by:

- ☒ Chemical Structure
- ☐ Isotope-Containing
- ☐ Metal-Containing
- ☐ Commercial Availability
- ☐ Property Availability
- ☐ Property Value
- ☐ Reference Availability
- ☐ Atom Attachment

Structure Editor:

Java Non-Java

Click image to change structure or view detail.  
Search type: Substructure

1. 1373355-19-1

~3

$C_{17}H_{14}O_2$   
4H-1-Benzopyran-4-one, 2-(3,5-dimethylphenyl)-  
▶ Key Physical Properties

2. 912915-64-1

~6 ~3

$C_{15}H_{10}O_4$   
4H-1-Benzopyran-4-one, 2-(3,5-dihydroxyphenyl)-  
▶ Key Physical Properties

4. 6665-68-5

~38 ~7

5. 22395-22-8

~269 ~67

从4500多万个结构中

筛选出16901个黄酮类物质



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# 物质检索——分子式

**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**  
  
Examples:  
H4SiO4  
(C3H6O.C2H4O)x  
**Search**

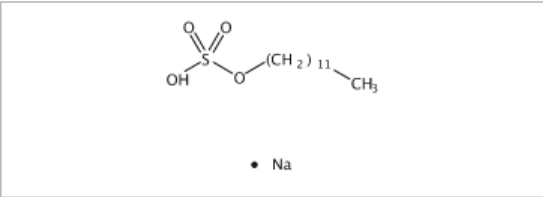
金属盐：金属离子和  
阴离子间用点 (.) 分  
开

分子式输入需要遵守Hill排序规则：不含碳化合物，按元素符号的字母顺序排列；分子式为含碳化合物时，则“C”在前；如有氢则紧随其后，其它元素符号按字母顺序排在氢的后面

1. 151-21-3

(Component: 151-41-7)

~84904 ~276



**C<sub>12</sub>H<sub>26</sub>O<sub>4</sub>S.Na**  
Sulfuric acid monododecyl ester sodium salt (1:1)

► **Key Physical Properties**  
Regulatory Information  
Spectra  
Experimental Properties



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# 物质检索——结构

**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 to Edit

Search Type:

- ☐ Exact Structure
- ☒ Substructure
- ☐ Similarity

☐ Show precision analysis

**ChemDraw**

Launch a SciFinder substance or reaction

Import CXF

**Search**

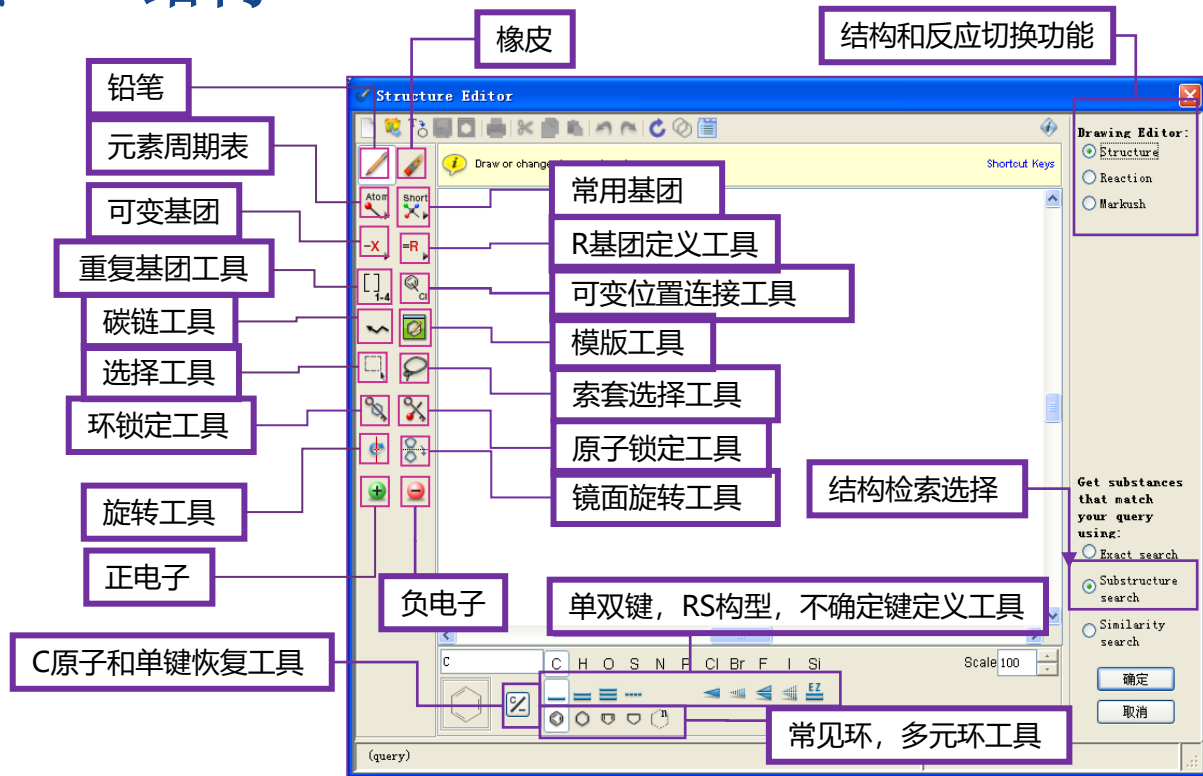
[Advanced Search](#) ☒ Always Show



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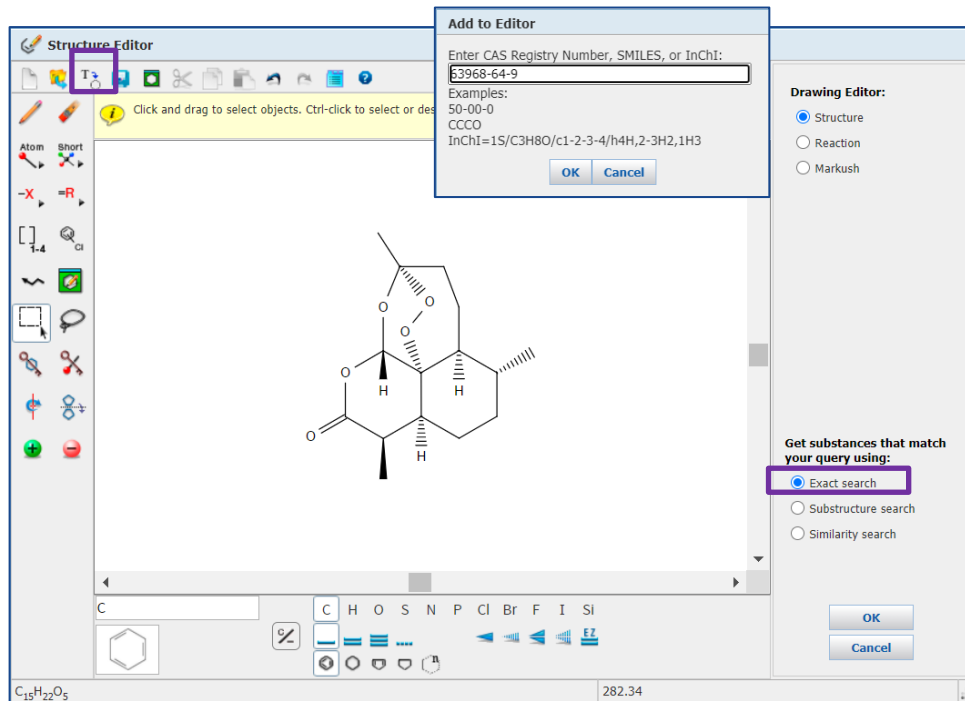
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# 物质检索——结构



# 物质检索——精确结构检索

## 检索青蒿素的组合物



Select All Deselect All

1 of 5 Stereo Candidates Selected

- ☒ Absolute stereo match
- ☐ Absolute stereo mirror image
- ☐ Relative stereo match
- ☐ Stereo that doesn't match query
- ☐ No stereo in answer structure

Get Substances

精确结构检索



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# 精确结构检索结果集

0 of 59 Substances Selected

1. 63968-64-9

~6058

Absolute stereochemistry.

**C<sub>15</sub> H<sub>22</sub> O<sub>5</sub>**  
3,12-Epoxy-12H-pyrano[4,3-f]-1,2-benzodioxepin-10(3H)-one, octahydro-3,6,9-trimethyl-, (3R,5aS,6R,8aS,9R,12S,12aR)-

Key Physical Properties  
Regulatory Information  
Spectra  
Experimental Properties

2. 1061342-74-2

~13

63968-64-9  
C<sub>15</sub> H<sub>22</sub> O<sub>5</sub>

Absolute stereochemistry.

4085-31-8  
C<sub>29</sub> H<sub>32</sub> Cl<sub>2</sub> N<sub>6</sub>

90-34-6  
C<sub>15</sub> H<sub>21</sub> N<sub>3</sub> O

**C<sub>29</sub> H<sub>32</sub> Cl<sub>2</sub> N<sub>6</sub> · C<sub>15</sub> H<sub>22</sub> O<sub>5</sub> · C<sub>15</sub> H<sub>21</sub> N<sub>3</sub> O**  
3,12-Epoxy-12H-pyrano[4,3-f]-1,2-benzodioxepin-10(3H)-one, octahydro-3,6,9-trimethyl-, (3R,5aS,6R,8aS,9R,12S,12aR)-, mixt. with N,N'-(6-methoxy-8-quinolyl)-1,4-pentanediamine and 4,4'-(1,3-propanediyl)di-4,1-piperazinediyl]bis[7-chloroquinoline]

3. 1201556-23-1

~10

63968-64-9  
C<sub>15</sub> H<sub>22</sub> O<sub>5</sub>

Absolute stereochemistry.

173531-58-3  
C<sub>24</sub> H<sub>26</sub> Cl N<sub>3</sub> O · 2 H<sub>3</sub> O<sub>4</sub> P

173531-57-2  
C<sub>24</sub> H<sub>26</sub> Cl N<sub>3</sub> O

7664-38-2  
H<sub>3</sub> O<sub>4</sub> P

**C<sub>24</sub> H<sub>26</sub> Cl N<sub>3</sub> O · C<sub>15</sub> H<sub>22</sub> O<sub>5</sub> · 2 H<sub>3</sub> O<sub>4</sub> P**  
3,12-Epoxy-12H-pyrano[4,3-f]-1,2-benzodioxepin-10(3H)-one, octahydro-3,6,9-trimethyl-, (3R,5aS,6R,8aS,9R,12S,12aR)-, mixt. with naphthoquinone phosphate

4. 436149-07-4

~6

63968-64-9  
C<sub>15</sub> H<sub>22</sub> O<sub>5</sub>

Absolute stereochemistry.

7585-39-9  
C<sub>42</sub> H<sub>70</sub> O<sub>35</sub>

Absolute stereochemistry.

**C<sub>42</sub> H<sub>70</sub> O<sub>35</sub> · C<sub>15</sub> H<sub>22</sub> O<sub>5</sub>**  
β-Cyclodextrin, compd. with (3R,5aS,6R,8aS,9R,12S,12aR)-octahydro-3,6,9-trimethyl-3,12-epoxy-12H-pyrano[4,3-f]-1,2-benzodioxepin-10(3H)-one (1:1)

**CAS**

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38

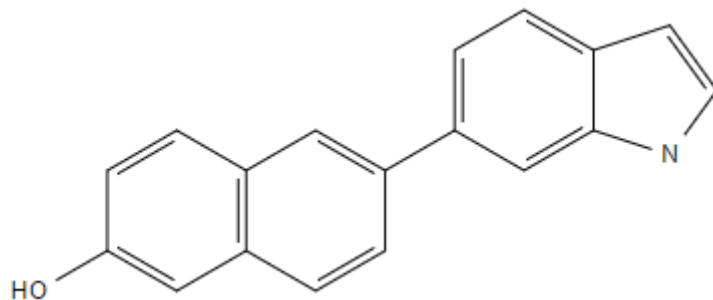
# 物质检索——精确结构检索

- 精确结构检索：

获得被检索结构的盐、混合物、配合物、聚合物等，被检结构不能被取代

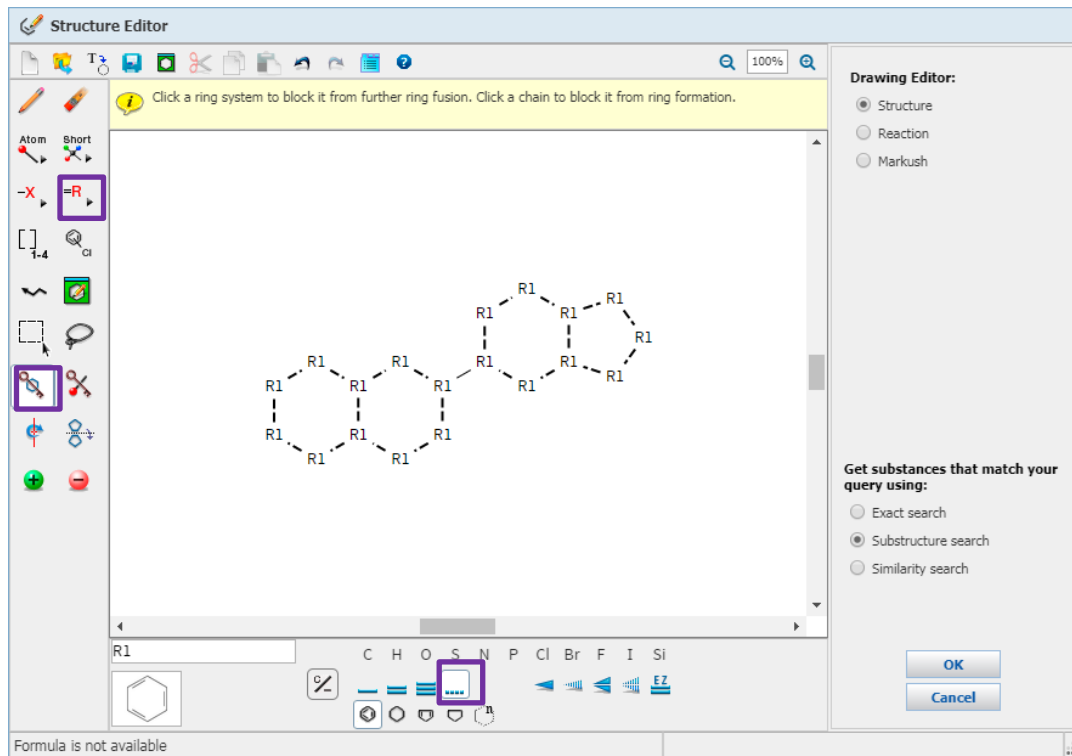
# 物质检索——亚结构检索

确定具有下图母核结构环骨架的新颖性





# 物质检索——亚结构检索



R = C、N、O

- |                 |   |
|-----------------|---|
| Characteristics | <input checked="" type="checkbox"/> Single component                |
|                 | <input type="checkbox"/> Commercially available                     |
|                 | <input type="checkbox"/> Included in references                     |
| Classes         | <input type="checkbox"/> Alloys                                     |
|                 | <input type="checkbox"/> Coordination compounds                     |
|                 | <input type="checkbox"/> Incompletely defined                       |
|                 | <input type="checkbox"/> Mixtures                                   |
|                 | <input type="checkbox"/> Polymers                                   |
|                 | <input checked="" type="checkbox"/> Organics, and others not listed |
| Studies         | <input type="checkbox"/> Analytical                                 |
|                 | <input type="checkbox"/> Biological                                 |
|                 | <input type="checkbox"/> Preparation                                |
|                 | <input type="checkbox"/> Reactant or reagent                        |



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# 物质检索——亚结构检索

Explore ▾ Saved Searches ▾ SciPlanner Save Print Export

Chemical Structure substructure with limiters > substances (24054)

SUBSTANCES Get References Get Reactions Get Commercial Sources Tools ▾

Create Keep Me Posted Alert Send to SciPlanner

Analyze Refine

Sort by: CAS Registry Number ▾

0 of 24054 Substances Selected

Page: 1 of 482

Sample Analysis: Substance Role ▾

Preparation  $\geq 11433$

Biological Study  $\geq 8965$

Uses  $\geq 4424$

Reactant or Reagent  $\geq 3106$

Properties  $\geq 675$

Prophetic in Patents  $\geq 544$

Analytical Study  $\geq 253$

Process  $\geq 186$

Occurrence  $\geq 147$

Formation, Nonpreparative  $\geq 19$

Show More

<input type="checkbox"/> 1. <a href="#">2538777-33-0</a>  $C_{15}H_9ClN_4O$ INDEX NAME NOT YET ASSIGNED	<input type="checkbox"/> 2. <a href="#">2538703-55-6</a>  $C_{16}H_{13}N_5O_2$ INDEX NAME NOT YET ASSIGNED	<input type="checkbox"/> 3. <a href="#">2538679-57-9</a>  $C_{18}H_{13}ClN_4$ INDEX NAME NOT YET ASSIGNED	<input type="checkbox"/> 4. <a href="#">2538640-01-4</a>  $C_{15}H_{10}N_4O_2$ INDEX NAME NOT YET ASSIGNED
<input type="checkbox"/> 5. <a href="#">2538632-82-3</a>  $C_{18}H_{13}ClN_2$ INDEX NAME NOT YET ASSIGNED	<input type="checkbox"/> 6. <a href="#">2538625-37-3</a>  $C_{15}H_{11}N_5$ INDEX NAME NOT YET ASSIGNED	<input type="checkbox"/> 7. <a href="#">2538584-52-8</a>  $C_{17}H_{12}FN_4O$ INDEX NAME NOT YET ASSIGNED	<input type="checkbox"/> 8. <a href="#">2538583-61-6</a>  $C_{15}H_{11}N_6$ INDEX NAME NOT YET ASSIGNED
<input type="checkbox"/> 9. <a href="#">2538582-78-2</a>  $C_{17}H_{12}F_2N_2$ INDEX NAME NOT YET ASSIGNED	<input type="checkbox"/> 10. <a href="#">2538581-14-3</a>  $C_{15}H_{14}N_6$ INDEX NAME NOT YET ASSIGNED	<input type="checkbox"/> 11. <a href="#">2538578-13-9</a>  $C_{14}H_8N_6O_2$ INDEX NAME NOT YET ASSIGNED	<input type="checkbox"/> 12. <a href="#">2538577-28-3</a>  $C_{15}H_{15}F_2N$ INDEX NAME NOT YET ASSIGNED
<input type="checkbox"/> 13. <a href="#">2538532-43-1</a>	<input type="checkbox"/> 14. <a href="#">2538476-63-8</a>	<input type="checkbox"/> 15. <a href="#">2538429-31-9</a>	<input type="checkbox"/> 16. <a href="#">2538429-21-7</a>

如何判断哪些物质是从植物中提取出来的呢？



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# 物质结果集的筛选——亚结构检索

Analyze Refine

Refine by:

☒ Chemical Structure

☐ Isotope-Containing

☐ Metal-Containing

☐ Commercial Availability

☐ Property Availability

☐ Property Value

☐ Reference Availability

☐ Atom Attachment

Structure Editor:

Java Non-Java

Click image to change structure or view detail.  
Search type: **Substructure**

Only retrieve substances that:

☒ Have references

☐ Are commercially available

☐ Are a single component

☐ Are in specific substance classes

☒ Are in specific types of studies

☐ Analytical

☒ Biological

☐ Preparation

☐ Reactant or reagent

Refine

SUBSTANCES

Get References

Get Reactions

Get Commercial Sources

Tools

Analyze Refine

Sort by: CAS Registry Number

0 of 10690 Substances Selected

Page: 1 of 214

Analyze by:

Substance Role

Biological Study 10663

Preparation 9766

Uses 4692

Reactant or Reagent 985

Properties 531

Prophetic in Patents 438

Analytical Study 230

Process 163

Occurrence 160

Formation, Nonpreparative 7

Show More

1. 2538149-73-2

$C_{28}H_{30}BrN_5O_3$   
INDEX NAME NOT YET ASSIGNED

2. 2538149-72-1

$C_{28}H_{30}BrN_5O_3$   
INDEX NAME NOT YET ASSIGNED

3. 2538149-71-0

$C_{28}H_{30}BrN_5O_3$   
INDEX NAME NOT YET ASSIGNED

4. 2538149-70-9

$C_{28}H_{30}BrN_5O_3$   
INDEX NAME NOT YET ASSIGNED

5. 2538149-69-6

$C_{22}H_{16}BrN_5O_3$   
INDEX NAME NOT YET ASSIGNED

6. 2538149-64-1

$C_{22}H_{16}BrN_5O_3$   
INDEX NAME NOT YET ASSIGNED

7. 2538149-62-9

$C_{22}H_{16}BrN_5O_3$   
INDEX NAME NOT YET ASSIGNED

8. 2538149-58-3

$C_{22}H_{16}BrN_5O_3$   
INDEX NAME NOT YET ASSIGNED

9. 2538149-57-2

$C_{21}H_{14}BrN_5O_3$   
INDEX NAME NOT YET ASSIGNED

10. 2538149-56-1

$C_{20}H_{13}N_5O_3$   
INDEX NAME NOT YET ASSIGNED

11. 2538149-54-9

$C_{20}H_{13}N_5O_3$   
INDEX NAME NOT YET ASSIGNED

12. 2538149-50-5

$C_{24}H_{21}N_5O_3$   
INDEX NAME NOT YET ASSIGNED

先用Refine缩小范围，再通过Occurrence筛选



CAS

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# 物质结果集的筛选——亚结构检索

0 of 160 Substances Selected

1. 2411630-35-6

2. 2411630-34-5

3. 2411630-33-4

4. 2304924-40-9

5. 2303538-03-4

6. 2259292-41-4

7. 2259292-41-4

8. 2253378-11-5

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## Silychristin derivatives conjugated with coniferylalcohols from silymarin and their pancreatic $\alpha$ -amylase inhibitory activity

By: Kato, Eisuke; Kushibiki, Natsuka; Satoh, Hiroshi; Kawabata, Jun

Silymarin is a mixt. of flavonolignans extd. from the fruit of *Silybum marianum* (milk thistle). The latter is used as a medicinal plant to treat liver and gallbladder disorders. Recently, silymarin has been investigated for its effects against diabetes mellitus, and shown to reduce serum levels of glucose in model animals and in clin. trials. This effect can be explained mainly by the protective effect of silymarin against pancreatic beta-cells, but the involvement of other mechanisms is possible. We demonstrated the  $\alpha$ -amylase inhibitory activity of silymarin and investigated the components responsible for this effect. Two major flavonolignans, silibinin and silychristin, did not show inhibition against  $\alpha$ -amylase, but two novel silychristin derivs. conjugated with dehydroconiferyl alc. were isolated as the mildly inhibiting components of silymarin. Further analyses indicated the presence of various silychristin derivs. in silymarin that may act synergistically to show  $\alpha$ -amylase inhibitory activity.

### Indexing

Pharmacology (Section1-10)

### Concepts

Antidiabetic agents  
New natural products  
Silybum marianum

Diabetes mellitus  
Pharmaceutical natural products

silychristin derivs. conjugated with coniferylalcs. from silymarin and their pancreatic  $\alpha$ -amylase inhibitory activity

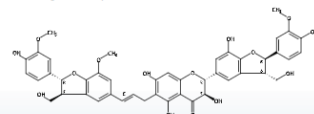
### Flavonolignans

silychristin derivs. conjugated with coniferylalcs. from silymarin and their pancreatic  $\alpha$ -amylase inhibitory activity

Natural product occurrence; Pharmacological activity; Therapeutic use; Biological study; Occurrence; Uses

### Substances

2411630-35-6 6-Dehydroconiferylsilychristin  
Absolute stereochemistry. Double bond geometry as shown.



6-Dehydroconiferylsilychristin; silychristin derivs. conjugated with coniferylalcs. from silymarin and their pancreatic  $\alpha$ -amylase inhibitory activity

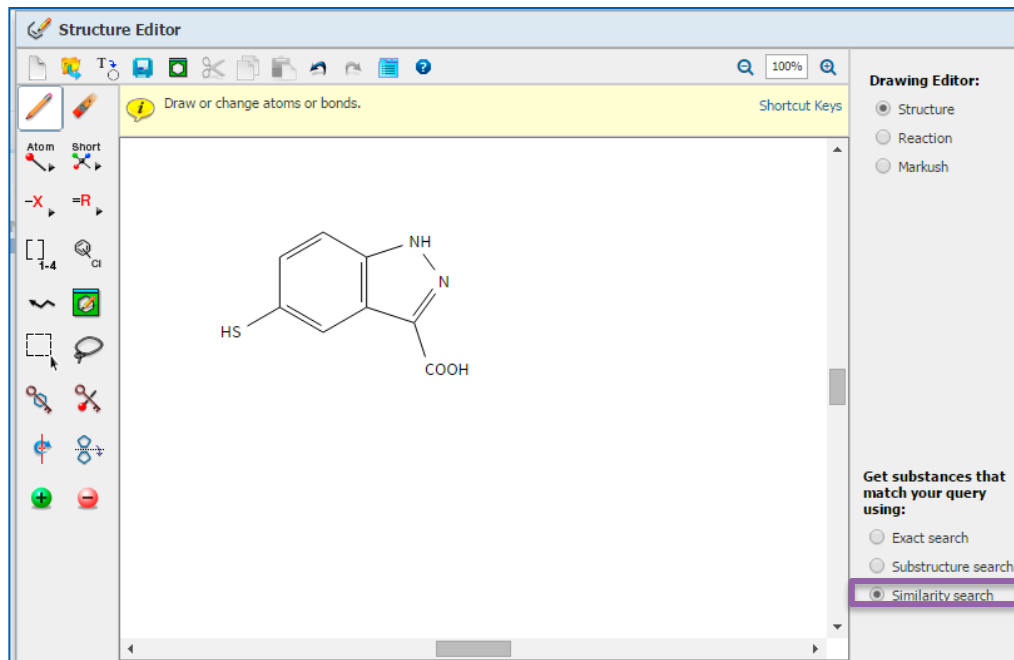
Natural product occurrence; Pharmacological activity; Therapeutic use; Biological study; Occurrence; Uses

# 物质检索——亚结构检索

- 亚结构检索：

包括精确结构检索结果，及被检索结构的修饰结构

# 物质检索——相似结构检索



# 相似结构检索结果

Select All Deselect All

0 of 6 Similarity Candidates Selected

	Substances
<input type="checkbox"/> ≥ 99 (most similar)	0
<input type="checkbox"/> 95-98	0
<input type="checkbox"/> 90-94	0
<input type="checkbox"/> 85-89	11
<input type="checkbox"/> 80-84	34
<input type="checkbox"/> 75-79	84
<input type="checkbox"/> 70-74	267
<input type="checkbox"/> 65-69	696
<input type="checkbox"/> 0-64 (least similar)	1818

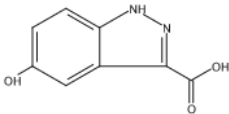
Get Substances

评分越高，相似度越高，结构越相似

Score: 88

☐ 1. 885518-94-5

~1 ~35



**C<sub>8</sub>H<sub>6</sub>N<sub>2</sub>O<sub>3</sub>**  
1H-Indazole-3-carboxylic acid, 5-hydroxy-

▶ Key Physical Properties

取代基变化

Score: 86

☐ 5. 858227-12-0

~7 ~41



**C<sub>9</sub>H<sub>8</sub>N<sub>2</sub>O<sub>2</sub>**  
1H-Indazole-3-carboxylic acid, 6-methyl-

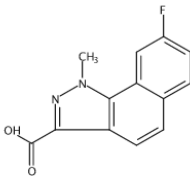
▶ Key Physical Properties

取代基位置变化

Score: 65

☐ 541. 1100422-

~1



**C<sub>13</sub>H<sub>8</sub>FN<sub>2</sub>O<sub>2</sub>**  
1H-Benz[ghi]indazole-3-carboxylic acid, 8-fluoro-1-methyl-

▶ Key Physical Properties

母体结构变化



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# 相似结构检索结果

**SUBSTANCES**

Get References Get Reactions Get Commercial Sources Tools

Create Keep Me Posted Alert Send to SciPlanner

Display Options

Analyze Refine

Analyze by:

Substance Role

Reactant or Reagent 25

Preparation 17

Uses 6

Biological Study 3

Proprietary in Patents 2

Analytical Study 1

Combinatorial Study 1

Process 1

Properties 1

Show More

Sort by: Similarity Score

0 of 49 Substances Selected

Score: 88  
1. **885518-94-5**

C8H6N2O3  
1H-Indazole-3-carboxylic acid, 5-hydroxy-  
Key Physical Properties

Score: 87  
2. **1201-24-7**

C9H6N2O2  
1H-Indazole-3-carboxylic acid, 5-methyl-  
Key Physical Properties  
Experimental Properties

Score: 87  
3. **108259-82-1**

1201-24-7  
C9H6N2O2

113-00-8  
C4H5N3

N#NC(=N)N

C9H6N2O2, C4H5N3  
1H-Indazole-3-carboxylic acid, 5-methyl-, compd. with guanidine (1:1)

Score: 87  
4. **1638221-34-7**

(Component: 1201-24-7)

C9H6N2O2, H2O  
1H-Indazole-3-carboxylic acid, 5-methyl-, hydrate (1:1)

Score: 86  
5. **858227-12-0**

C9H6N2O2  
1H-Indazole-3-carboxylic acid, 6-methyl-  
Key Physical Properties

Score: 85  
6. **4498-67-3**

C8H6N2O2  
1H-Indazole-3-carboxylic acid  
Regulatory Information  
Spectra

Score: 85  
7. **108259-78-5**

4498-67-3  
C9H6N2O2

113-00-8  
C4H5N3

Score: 85  
8. **108259-86-5**

4498-67-3  
C9H6N2O2

4271-95-8  
C10H8N4

查看结果集，根据适应症或靶点信息选取分子，或通过Substance Role筛选物质



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# 物质检索——相似结构检索

- 相似结构检索：

获得片段或整体结构与被检索结构相似的结果，母体结构可以被取代，也可以被改变

# 提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
  - 文献检索
  - 物质检索
  - Markush检索
  - 反应检索
  - SciPlanner
- SciFinder常见问题及解决
- 上机练习



# Markush检索

(19) 中华人民共和国国家知识产权局



(12) 发明专利申请



(10) 申请公布号 CN 104945470 A

(43) 申请公布日 2015.09.30

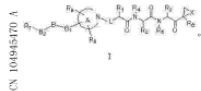
(21) 申请号 201410122313.4  
(22) 申请日 2014.03.30  
(71) 申请人 浙江大学  
地址 310027 浙江省杭州市西湖区浙大路38号  
申请人 中国科学院上海药物研究所  
(72) 发明人 胡永洲 李佳 刘洁 张建康 周宇波 杨波 何伟军 许磊 胡小蓓  
(74) 专利代理机构 杭州求是专利事务所有限公司 33200  
代理人 张法高 赵杭丽  
(51) Int. Cl.  
C07K 5/087(2006.01)  
C07K 5/063(2006.01)

权利要求书3页 说明书24页 附图4张

(54) 发明名称  
杂环构建的三肽环氧酮类化合物及制备和应用

(57) 摘要

本发明提供一种杂环构建的三肽环氧酮类化合物,以Carfilizomib为先导化合物,经缩合、酸性条件下脱去Boc保护基、碱性条件下反应得氨基酸甲酯异氰酸酯、水解、在缩合剂作用下获得。本发明是小分子短肽类蛋白酶抑制剂。本发明化合物具有极强的蛋白酶抑制活性及细胞增殖抑制活性,是有前景的蛋白酶抑制剂。为癌症治疗药物的研究提供了新的思路。本发明化合物的合成所需原料易得,路线设计合理,反应条件温和,各步产率高,操作简便,适合工业化生产。具有下述式1的结构通式:



## 具体实施方式

[0026] 本发明结合附图和实施例作进一步的说明,以下实施例仅是说明本发明,而不是以任何方式限制本发明。

[0027] 制备实施例1、4-(吡嗪-2-基氨甲酰基)哌啶-1-甲酸叔丁酯(1a,1b)

将1-(叔丁氧羰基)哌啶-4-甲酸(2.75g,12mmol)置于50mL三颈瓶中,在N<sub>2</sub>保护下加入25mL无水CH<sub>2</sub>Cl<sub>2</sub>,然后缓缓滴入吡啶(2.5mL,30mmol)和二氯亚砷(1.1mL,14mmol),该反应液置于室温反应半小时。随后,2-氨基吡嗪(0.95g,10mmol)和三乙胺(5.7mL,40mmol)溶于15mL CH<sub>2</sub>Cl<sub>2</sub>后缓缓滴入上述反应液,室温反应6小时。反应液加30mL饱和食盐水稀释,分出有机层,水层CH<sub>2</sub>Cl<sub>2</sub>提取(15mL×3),合并有机层,无水硫酸钠干燥后减压除去溶剂,柱层析分离得白色固体2.3g,收率74%。m.p.: 134-136°C; <sup>1</sup>H NMR (500MHz, CDCl<sub>3</sub>): δ = 9.55 (s, 1H, pyrazine-H), 8.35 (d, 1H, J=2.0Hz, pyrazine-H), 8.23 (s, 1H, pyrazine-H), 7.97 (s, 1H, NH), 4.20 (m, 2H, CH<sub>2</sub>), 2.81 (m, 2H, CH<sub>2</sub>), 2.48 (m, 1H, CH), 1.93 (d, 2H, J=12.5Hz, CH<sub>2</sub>), 1.76 (m, 2H, CH<sub>2</sub>), 1.47 (s, 9H, CH<sub>3</sub>) ppm; ESI-MS: m/z = 307 [M+H]<sup>+</sup>。

[0028] 制备实施例2、4-(吡嗪-2-酰基)哌啶-1-甲酸叔丁酯(1c,1d)

吡嗪-2-羧酸(1.5g,12mmol)置于50mL反应瓶中,加入35mL无水CH<sub>2</sub>Cl<sub>2</sub>溶解,随即加入1-羟基苯并三氮唑(1.6g,12mmol)和N-(3-二甲氨基丙基)-N'-乙基碳二亚胺盐酸盐(3.5g,18mmol),室温反应半小时。随后,哌啶-1-甲酸叔丁酯(1.9g,10mmol)加入反应液中,室温反应3小时。反应液加入30mL饱和碳酸氢钠水溶液稀释,分出有机层,饱和食盐水

具体物质[Specific Substance]:

以具体化学结构陈述的特定物质, 会被分配CAS RN



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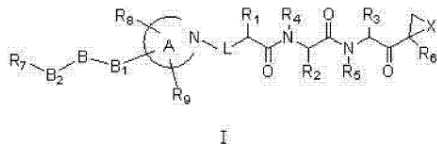
# Markush检索

CN 104945470 A

权 利 要 求 书

1/3 页

1. 一种杂环构建的三肽环氧酮类化合物,具有下述结构通式 I:



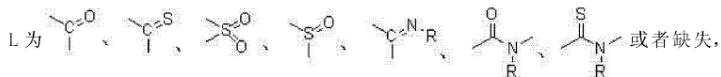
其中:

$R_1, R_2, R_3$  各自独立选自 H、 $C_{1-6}$  烷基 -D、卤代的  $C_{1-6}$  烷基 -D、 $C_{1-6}$  羟基烷基、 $C_{1-6}$  巯基烷基、 $C_{1-6}$  烷氧基烷基、芳基、芳烷基、杂芳基或杂芳烷基;其中:D 为 N( $R_0$ ) ( $R_0$ ) 或缺失, $R_0, R_6$  各自独立选自 H、OH、 $C_{1-6}$  烷基、卤代的  $C_{1-6}$  烷基或 N 末端保护基;

$R_4, R_5$  各自独立选自 H、OH、 $C_{1-6}$  烷基、卤代的  $C_{1-6}$  烷基或芳烷基;

$R_6$  选自 H、 $C_{1-6}$  烷基、卤代的  $C_{1-6}$  烷基、 $C_{1-6}$  羟基烷基、 $C_{1-6}$  烷氧基、卤代的  $C_{1-6}$  烷氧基、C(O)- $C_{1-6}$  烷基、C(O)NH- $C_{1-6}$  烷基、芳烷基;

X 为 O、S、NH、N- $C_{1-6}$  烷基或 N- 卤代的  $C_{1-6}$  烷基;



其中 R 选自 H、 $C_{1-6}$  烷基或卤代的  $C_{1-6}$  烷基;

环 A 选自 5 ~ 7 元的饱和脂肪杂环、不饱和杂环、或者有取代的 5 ~ 7 元的饱和脂肪杂环、不饱和杂环,所述的杂环包含 0 ~ 3 个选自 O、N 和 S 的杂原子并任选地被  $R_8, R_9$  和  $B_1$  基团取代;

$R_8, R_9$  分别独立选自 H、OH、 $C_{1-6}$  烷基、 $C_{1-6}$  烷氧基、 $C_{1-6}$  羟基烷基、 $C_{1-6}$  巯基烷基、 $C_{1-6}$  烷基 -D、芳基、杂芳基、环烷基和杂环基,这些基团可以被卤素、硝基、氨基、CN、 $C_{1-6}$  烷基、卤代的  $C_{1-6}$  烷基、 $C_{1-6}$  烷氧基或卤代的  $C_{1-6}$  烷氧基取代,每个基团可与一个或多个芳基或杂环

预测性物质[Prophetic Substance]:

— 使用Markush结构陈述的预测物质, 一个Markush可以陈述上百或上千个化学物质

— 被Markush结构包含, 但未被实施或呈现在表格、权利要求书或说明书中的结构, 不会被CAS分配CAS Registry Number

— Markush检索, 能检索到通过结构检索检不到的专利

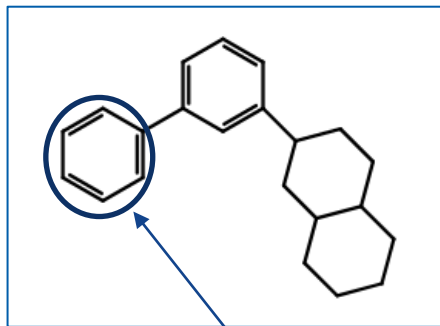


CAS®

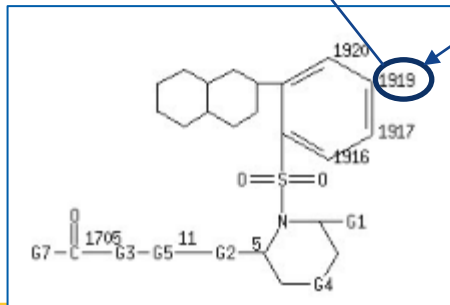
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# Markush检索

## 检索式



## 专利文献中匹配的Markush结构



1916, 1917, 1919, 1920: opt. substd. by Ph

Patent location:

claim 1

Note:

or pharmaceutically acceptable salts, prodrugs, or metabolites

Note:

additional oxo-substitution also disclosed

Note:

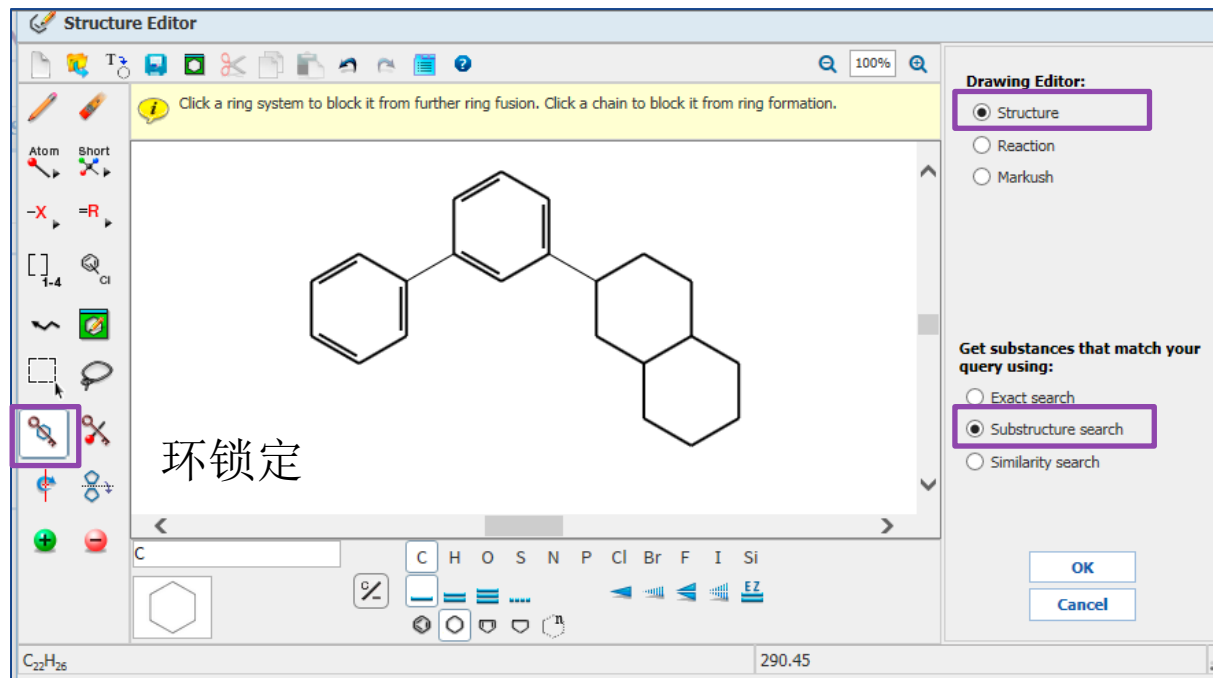
also incorporates claim 35



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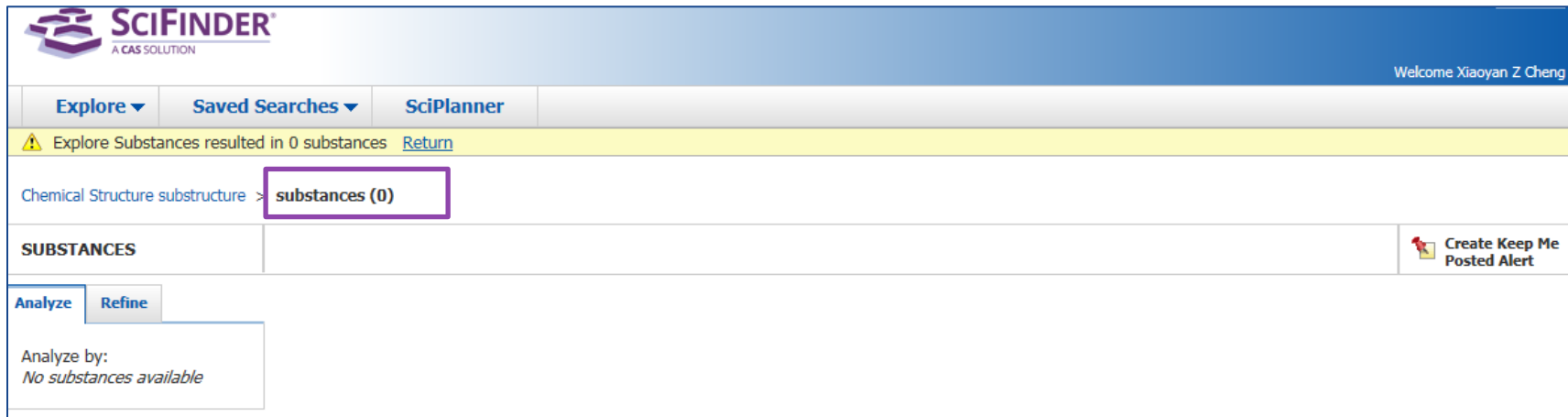
# Markush检索



结构检索

亚结构检索

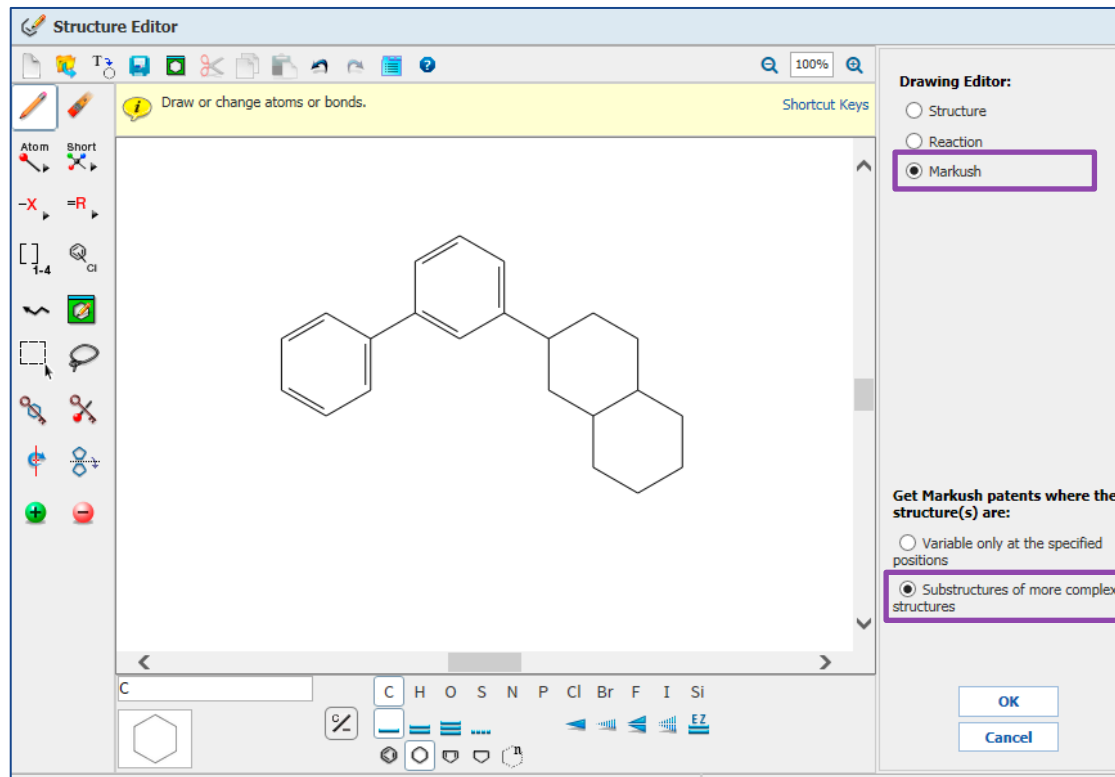
# Markush检索



The screenshot displays the SciFinder web interface. At the top, the SciFinder logo is visible, along with the text "A CAS SOLUTION" and a user greeting "Welcome Xiaoyan Z. Cheng". Below the header, there are navigation tabs: "Explore", "Saved Searches", and "SciPlanner". A yellow warning banner states: "Explore Substances resulted in 0 substances" with a "Return" link. The search input field shows "Chemical Structure substructure" followed by a dropdown menu currently displaying "substances (0)". Below the search bar, the "SUBSTANCES" section is visible, featuring "Analyze" and "Refine" buttons. A message box indicates "Analyze by: No substances available". On the right side of the interface, there is a button labeled "Create Keep Me Posted Alert".

物质亚结构检索结果集：零！

# Markush检索



Markush检索

亚结构检索



# Markush检索

Get Substances
 Get Reactions
 Get Related Citations
 Tools

Create Keep Me Posted Alert
 Send SciP

Sort by: Accession Number

0 of 23 References Selected

☐ 1. **Preparation of hole transport material for OLED**  
[Quick View](#) **PATENTPAK**  
 By Wang, Yalong; Li, Hongyan; Xue, Zhen; Wang, Jinping; Chen, Zhiwei; Li, Lingang; Yan, Shan; Wang, Weijun; Ren, Zenggang  
 From Faming Zhuanli Shenqing (2019), CN 110156746 A 20190823. | Language: Chinese, Database: CAPLUS  

The title hole transport material with general formula of  $R^1Ar^1-N(Ar^2R^3)-Ar^3R^2$ , wherein,  $Ar^1-Ar^3$  are independently selected from substituted or unsubstituted C6-30 arylene, including phenylene, bis-phenylene, heteroarylene, etc.;  $R^1-R^3$  are independently selected from H, substituted or unsubstituted C8-30 alkyl, substituted or unsubstituted C8-30 alkenyl, substituted or unsubstituted C8-30 alkynyl, etc. The inventive hole transport material is not only suitable for solar cells, but also suitable for org. semiconductor and other photoelec. fields.

☐ 2. **Process for the reduction of the NOx emissions with combustion engines by fuel additives.**  
[Quick View](#) **PATENTPAK**  
 By Kantlehner, Willi  
 From Ger. Offen. (2019), DE 102018001260 A1 20190822. | Language: German, Database: CAPLUS  

Processes are claimed, with which the nitrogen oxide contents in the exhaust gas of fuel-powered piston engines can be reduced, as additives - fed together or sep. - are supplied to the combustion chamber, in addn. to fuel, and the additives are preferably nitriles or org., nitrogen-contg. nitrile precursors, from which thermolysis products develop in the combustion chamber, which react with nitrogen oxides to form carbon dioxide and nitrogen.

☐ 3. **Polymerizable compound with good storage stability for optically anisotropic article**  
[Quick View](#) **PATENTPAK**  
 By Horiguchi, Masahiro; Aoki, Yoshio; Hayashi, Takuo; Tsuruta, Toru  
 From Jpn. Kokai Tokkyo Koho (2017), JP 2017218391 A 20171214. | Language: Japanese, Database: CAPLUS  

$$P^1-(Sp^1-X^1)_{k1}-A^1-Z^1-B^1-Z^2-A^2-R^2 \quad (I)$$
 The present invention relates to a monomer of  $P^1-(Sp^1-X^1)_{k1}-A^1-Z^1-B^1-Z^2-A^2-R^2$ , wherein  $P^1$  = radical, cationic, or anionic polymerizable group;  $Sp^1$  = independently spacer or direct bond;  $X^1$  = independently O, S,  $OCH_2$ ,  $CH_2O$ , CO, COO, etc.;  $k1$  = 1-10 integer;  $A^1$ ,  $A^2$ ,  $B^1$  = independently aliph. or arom.-aliph. fused ring optionally contg. O in the ring;  $Z^1$ ,  $Z^2$  = independently O, S,  $OCH_2$ ,  $CH_2O$ , etc.; and  $R^2$  = H, F, Cl, Br, I, etc.

## Markush检索结果集：23项专利！



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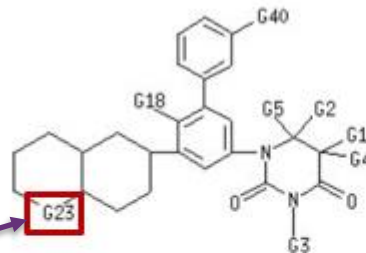
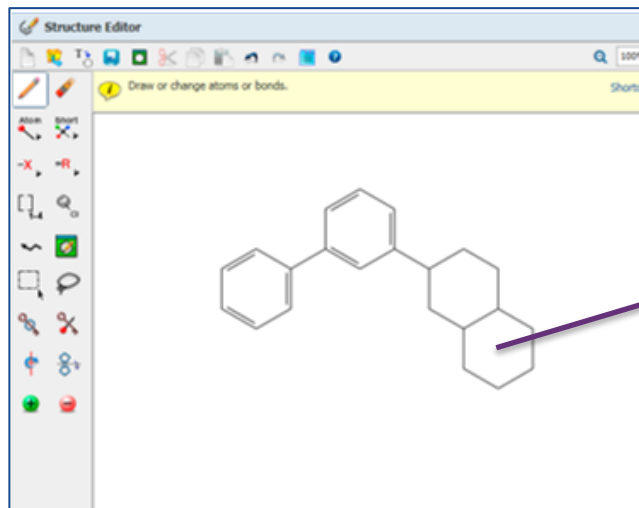
# Markush检索

## 1. Preparation of anti-infective pyrimidines for treating hepatitis C

[Quick View](#) **PATENTPAK**

By Flentge, Charles A.; Hutchinson, Douglas K.; Betebenner, David A.; DeGoey, David A.; Donner, Pamela L.; Kati, Warren M.; Krueger, Allan C.; Liu, Dachun; Liu, Yaya; Longenecker, Kenton L.; et al  
From PCT Int. Appl. (2009), **WO 2009039134 A1** 20090326. | Language: English, Database: CAPLUS

This invention relates to: (a) compds. and salts thereof that, inter alia, inhibit HCV; (b) intermediates useful for the prepn. of such compds. and salts; (c) compns. comprising such compds. and salts; (d) methods for prepg. such intermediates, compds., salts, and compns.; (e) methods of use of such compds., salts, and compns.; and (f) kits comprising such compds., salts, and compns. The compds. of the invention have general formula I (wherein the dotted bond is either a single or double bond; R<sup>1</sup> is H, Me, and nitrogen-protecting group; R<sup>2</sup> is H, halo, OH, Me, cyclopropyl, and cyclobutyl; R<sup>3</sup> i...



G23 = (0-1) CH2

Patent location:

Note:

Note:

claim 1

or salts

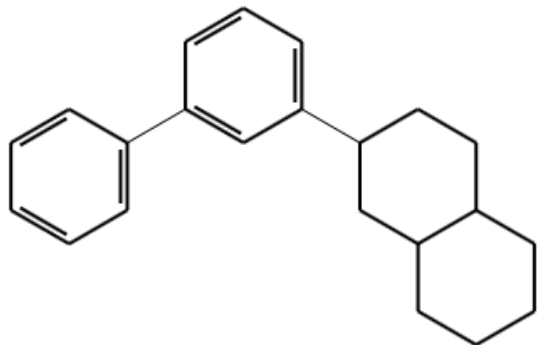
also incorporates claim 15



**CAS**

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## Markush检索



亚结构检索结果集：0

Markush检索结果集：23项专利

确定设计的物质新不新，有必要同时进行结构检索和Markush检索

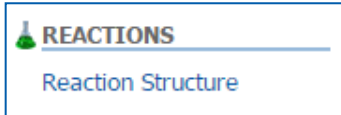
# 提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
  - 文献检索
  - 物质检索
  - Markush检索
  - 反应检索
  - SciPlanner
- SciFinder常见问题及解决
- 上机练习

# SciFinder检索——反应检索

## ■ 反应检索方法

结构式



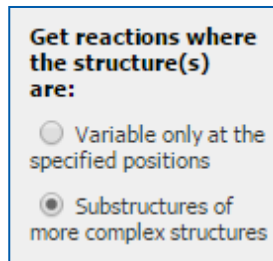
## ■ 常用获取方法

已知物质：由物质获取反应

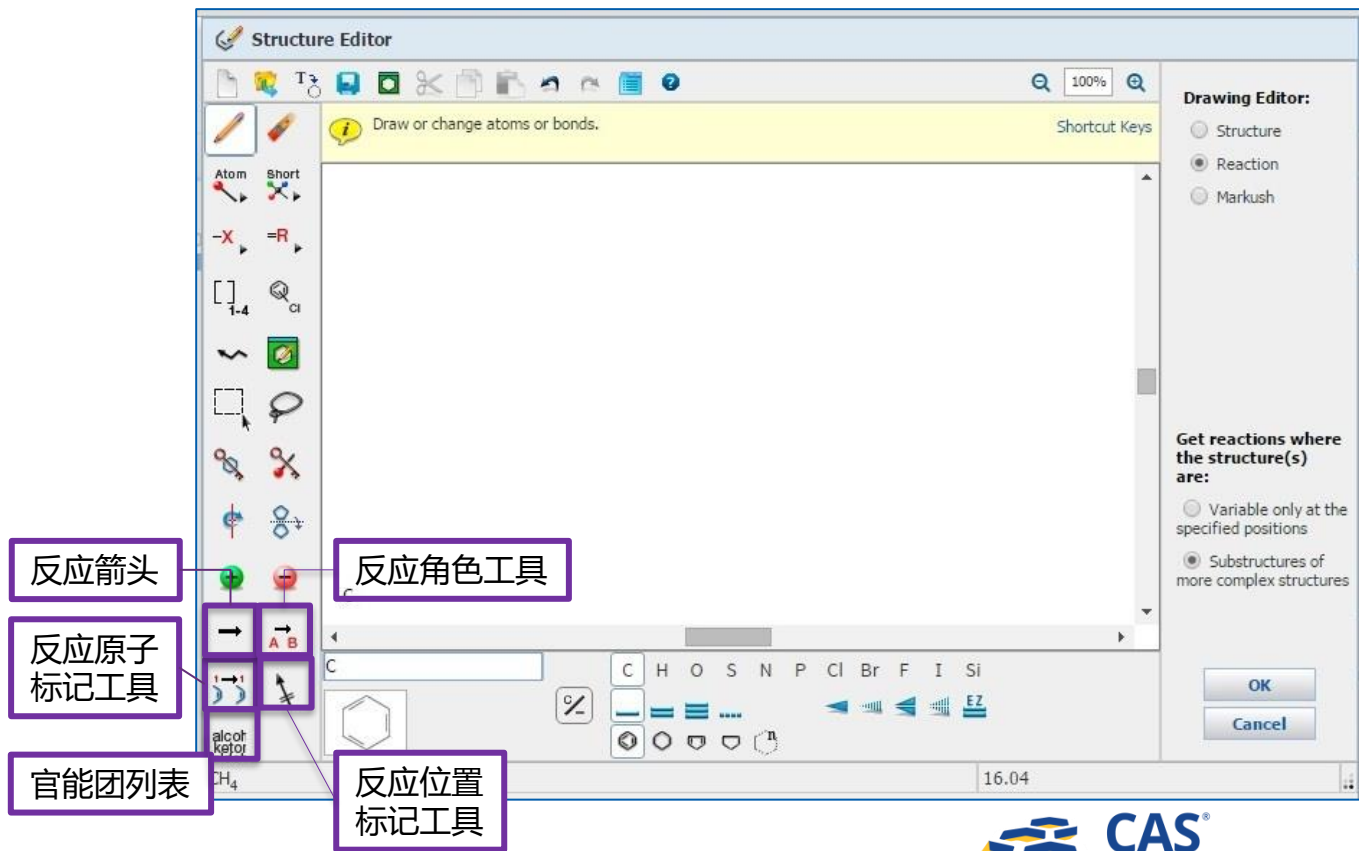
已知文献：从文献中获取反应

精确结构反应检索

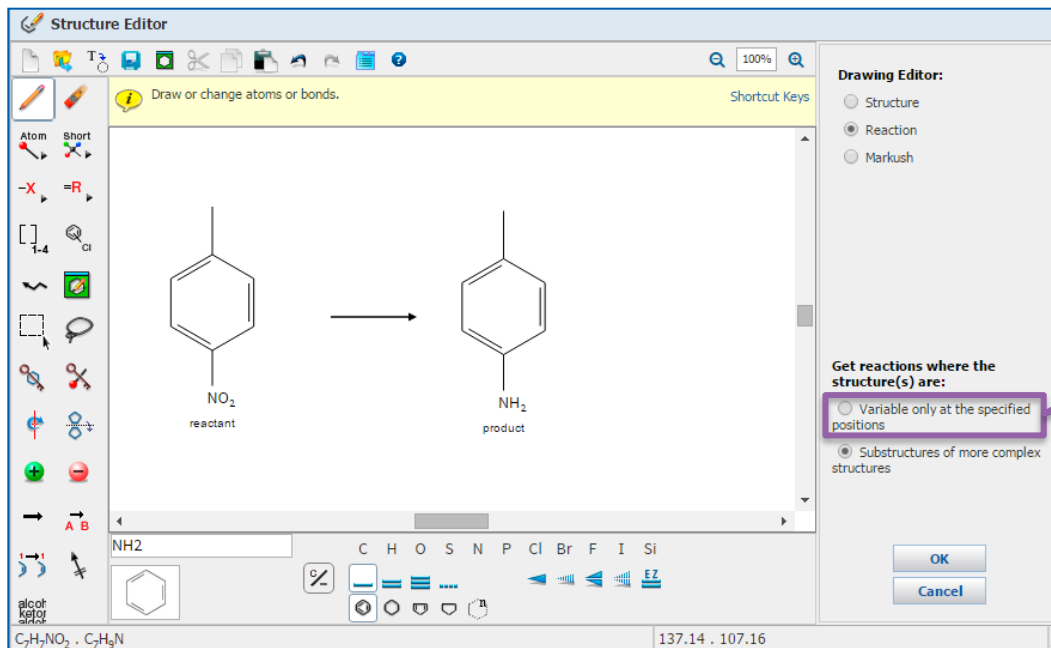
亚结构反应检索



# 反应绘制工具



# SciFinder反应检索——原子和环被锁定



原子和环被锁定



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# 反应检索结果

浏览记录，发现很多反应来自同一篇文献，通过Group by Document合并。

获取相似反应

Get References Tools

Group by: No Grouping No Grouping Document Transformation Selected

Sort by: Relevance

Display Options

Page: 1 of 11

1. View Reaction Detail Similar Reactions

Single Step Hover over any structure for more options.

Cc1ccc([N+](=O)[O-])cc1 → Cc1ccc(N)cc1

~102 ~122

100%

Overview

Steps/Stages

1.1 R:NaBH<sub>4</sub>, C:1832616-28-0, C:Ru, S:H<sub>2</sub>O, S:THF, 45 min, 25°C

Notes

solid-supported catalyst, ruthenium supported on porous organic polymer used, reusable catalyst, sealed tube used, scalable, Reactants: 1, Reagents: 1, Catalysts: 2, Solvents: 2, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Fabrication of Ruthenium Nanoparticles in Porous Organic Polymers: Towards Advanced Heterogeneous Catalytic Nanoreactors



# 获取相似反应

选择相似反应的相似限制：

Broad：仅反应中心相似

Medium：反应中心及附属原子和键

Narrow：反应中心及扩展的原子和键

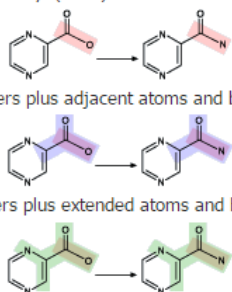
**Get Similar Reactions ?**

**Retrieve similar reactions from:**

- ☒ All reactions
- ☐ Current answer set

**Include this level of similarity:**

- ☒ Broad - Reaction centers only (2934)
- ☐ Medium - Reaction centers plus adjacent atoms and bonds (109)
- ☐ Narrow - Reaction centers plus extended atoms and bonds (95)



The diagram illustrates three levels of similarity for a chemical reaction. Each level shows a reaction between a pyridine-2-carboxamide derivative and a pyridine-2-carboxamide derivative. The reaction is represented by an arrow pointing from the reactant to the product. The reactant is a pyridine ring with a carboxamide group (-CONH2) at the 2-position. The product is a pyridine ring with a carboxamide group (-CONH2) at the 2-position. The similarity levels are defined by the extent of the highlighted atoms and bonds in the reactant and product structures.

- Broad - Reaction centers only (2934):** The reaction centers (the carbonyl carbon and the nitrogen atom) are highlighted in red.
- Medium - Reaction centers plus adjacent atoms and bonds (109):** The reaction centers and the adjacent atoms (the oxygen and nitrogen atoms) are highlighted in purple.
- Narrow - Reaction centers plus extended atoms and bonds (95):** The reaction centers and the extended atoms and bonds (the entire carboxamide group) are highlighted in green.



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# 按照反应类型排序

Group by: Transformation ▼ Sort by: Frequency ▼

☐ 0 of 560 Reactions Selected

☐ 1. Reduction of Nitro Compounds to Amines  
538 Reactions

$$\text{R-NO}_2 \longrightarrow \text{R-NH}_2$$

☐ 2. Reduction of Nitro to Azo Compounds  
11 Reactions

$$\text{Ar-NO}_2 \longrightarrow \text{Ar-N=N-Ar}$$

☐ 3. Reduction of Nitro to Azoxy Compounds  
11 Reactions

$$\text{Ar-NO}_2 \longrightarrow \text{Ar-N}^+=\text{N-Ar-O}^-$$

更精确的查找需要的反应



# 反应检索结果的筛选

获得特定物质做还原剂的反应

The screenshot displays a chemical reaction search interface. On the left, a sidebar titled 'REAGENTS' lists various reagents with their respective counts. A purple box highlights 'NaBH<sub>4</sub>' with a count of 51. An arrow points from this box to the main reaction area. The main area shows a reaction scheme: 4-nitrotoluene (SMILES: Cc1ccc([N+](=O)[O-])cc1) is reduced to 4-aminotoluene (SMILES: Cc1ccc(N)cc1) using NaBH<sub>4</sub> as the reagent. The reaction is labeled '100%' and '~122'. Below the reaction scheme, the 'Overview' section lists the steps/stages: '1.1 R:NaBH<sub>4</sub>, C:1832616-28-0, C:Ru, S:H<sub>2</sub>O, S:THF, 45 min, 25°C'. A purple box highlights the 'References' section, which contains the text: 'Fabrication of Ruthenium Nanoparticles in Porous Organic Polymers: Towards Advanced Heterogeneous Catalytic Nanoreactors'. An arrow points from this box to the text '获得文献详情' (Obtain literature details).

REAGENTS

Reagent	Count
H <sub>2</sub>	158
NaBH <sub>4</sub>	51
N <sub>2</sub> H <sub>4</sub> ·H <sub>2</sub> O	43
KOH	17
CO	16
HCO <sub>2</sub> H	16
NH <sub>4</sub> <sup>+</sup> ·HCO <sub>3</sub> <sup>-</sup>	16
H <sub>2</sub> O	14
N <sub>2</sub> H <sub>4</sub>	14
NaOH	14

1. View Reaction Detail [Link](#) [Similar Reactions](#)

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

Overview  
Steps/Stages

1.1 R:NaBH<sub>4</sub>, C:1832616-28-0, C:Ru, S:H<sub>2</sub>O, S:THF, 45 min, 25°C

Notes

solid-supported catalyst, ruthenium supported on porous organic polymer used, reusable catalyst, sealed tube used, scalable, Reactants: 1, Reagents: 1, Catalysts: 2, Solvents: 2, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Fabrication of Ruthenium Nanoparticles in Porous Organic Polymers: Towards Advanced Heterogeneous Catalytic Nanoreactors

获得文献详情




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# SciFinder囊括全球最大的反应实验过程合集

Single Step Hover over any structure for more options.



**Overview**

**Steps/Stages**

1.1 R:H<sub>2</sub>, R:Cs<sub>2</sub>CO<sub>3</sub>, C:1610424-70-8, C:1034343-98-0 (oxide), S:PhMe, 2 h, 100°C, 1 atm


**Notes**

solid-supported catalyst, palladium catalyst supported on graphene oxide prepared and used, reusable catalyst, Reactants: 1, Reagents: 2, Catalysts: 2, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

**References**

Catalyst Enhancement and Recyclability by Immobilization of Metal Complexes onto Graphene Surface by Noncovalent Interactions  
Q Quick View    Other Sources  
By Sabater, Sara et al  
From ACS Catalysis, 4(6), 2038-2047; 2014

**Experimental Procedure**

 **Catalysis** General/Typical Procedure: **General Procedure for Nitroarene Reductions.** Molecular hydrogen was added with a balloon filled with 1 atm of H<sub>2</sub> to a mixture of nitroarene (0.3 mmol), Cs<sub>2</sub>CO<sub>3</sub> (0.3 mmol), anisole as internal standard (0.3 mmol), and NHC-Pd-rGO (6 × 10<sup>-3</sup> mmol, based on metal) in toluene (5 mL). The system was then evacuated and backfilled with H<sub>2</sub> in cycles for three times before putting the reaction vessel in an oil bath at 100°C for 2h. Yields were determined by GC analyses using anisole (0.3 mmol) as internal standard. Products were identified according to spectroscopic data of the commercially available compounds. Entry: 4; Yield 100%.

不用阅读全文，直接获得包含实验过程的反应记录



# 亚结构反应检索

寻找底物中的伯醇氧化为醛，而仲醇不参与反应的选择性氧化条件

The screenshot displays the CAS Structure Editor interface. The main workspace shows a chemical reaction: a primary alcohol (labeled 'reactant') with a substituent 'A' and a hydroxyl group, reacting to form an aldehyde (labeled 'product'). Atoms are numbered: the carbon of the hydroxyl group is '2' and the oxygen is '1'. A purple arrow points from the 'alcohol ketone aldehyde' icon in the left toolbar to the reaction arrow. The 'Drawing Editor' panel on the right has 'Reaction' selected. Below it, the 'Get reactions where the structure(s) are:' section has 'Substructures of more complex structures' selected. The 'Non-participating Functional Groups' panel on the far right shows a list of functional groups with 'Secondary Alcohol' checked. The 'Number of Steps' is set to 1. The bottom status bar indicates 'Formula is not available'.

Structure Editor

Click an atom in the reactant and its corresponding atom in the product.

reactant

product

Drawing Editor:

- ☐ Structure
- ☒ Reaction
- ☐ Markush

Get reactions where the structure(s) are:

- ☐ Variable only at the specified positions
- ☒ Substructures of more complex structures

OK

Cancel

Non-participating Functional Groups

Select Solvents

Close

View: All 217

1 Selected Clear Selections

- ☐ Quaternary Ammonium
- ☐ o-Quinone
- ☐ p-Quinone
- ☐ S-O Group
- ☐ Se Group
- ☒ Secondary Alcohol
- ☐ Secondary Amine
- ☐ Selenide
- ☐ Selenol
- ☐ Silyl
- ☐ Silyl Enol Ether
- ☐ Sulfenyl Halide
- ☐ Sulfide
- ☐ Sulfinate

Reactions must have ☒ all selections ☐ any selection

Number of Steps 1

Examples: 1, 1-3, 1-, -3

alcohol ketone aldehyde

Formula is not available

# 亚结构反应检索

**REACTIONS**

Get References Tools

Analyze **Refine**

Analyze by:   
 Reagent

O <sub>2</sub>	388
MnO <sub>2</sub>	270
PhI(OAc) <sub>2</sub>	226
NaHCO <sub>3</sub>	223
Me <sub>4</sub> -piperidoxyl	222
NaOH	212
Na <sub>2</sub> S <sub>2</sub> O <sub>3</sub>	175
H <sub>2</sub>	131
Et <sub>3</sub> N	101
Martin's reagent	100

[Show More](#)

Group by: No Grouping Sort by: Accession Number

0 of 2735 Reactions Selected Display Options Page: 1 of 55

☐ 1. [View Reaction Detail](#) [Similar Reactions](#)

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

[Overview](#)

☐ 2. [View Reaction Detail](#) [Similar Reactions](#)

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

# 通过后处理工具筛选反应——Analyze

Analyze by: **Product Yield**

0 of 2735 Reactions Selected

5. View Reaction Detail [Link](#) [Similar Reactions](#)

通过反应收率筛选反应

Yield Range	Count
>=90%	303
80-89%	244
70-79%	229
<10%	225
10-19%	159
60-69%	157
40-49%	120
50-59%	117
20-29%	115
30-39%	91

Show More

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

95%

Overview

6. View Reaction Detail [Link](#) [Similar Reactions](#)

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

100%



# 提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
  - 文献检索
  - 物质检索
  - Markush检索
  - 反应检索
  - SciPlanner
- SciFinder常见问题及解决
- 上机练习



# SciPlanner使用简介

3. View Reaction Detail Link

3 Steps Hover over any structure for more options.

1. 勾选想要的反应

2. 点击Send to SciPlanner

3. 进入SciPlanner 新建文件

4. 将刚推送过来的反应拖至编辑面板

Send to SciPlanner

Play Options

Overview

Steps/Stages

1.1 R: NH<sub>3</sub>, R: t-BuOK, R: t-BuOOH, S: THF  
2.1 R: NaH, S: THF  
3.1 R: POCl<sub>3</sub>, reflux

Notes

Reactants: 2, Reagents: 5, Solvents: 1, Steps: 3, Stages: 3, Most stages in any one step: 1

References

Syntheses of 4- and 6-substituted thiazolo[4,5-c]pyridines

SciPlanner

SciPlanner\_11\_19\_201

Workspace

Edit View GoTo

New  
Open  
Save  
Duplicate  
Import  
Export  
Print  
Close

Your Workspace is empty.

Drag items from the reference, substance, and reaction libraries (on the right) to this area.

Clear Reactions



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# SciPlanner使用简介

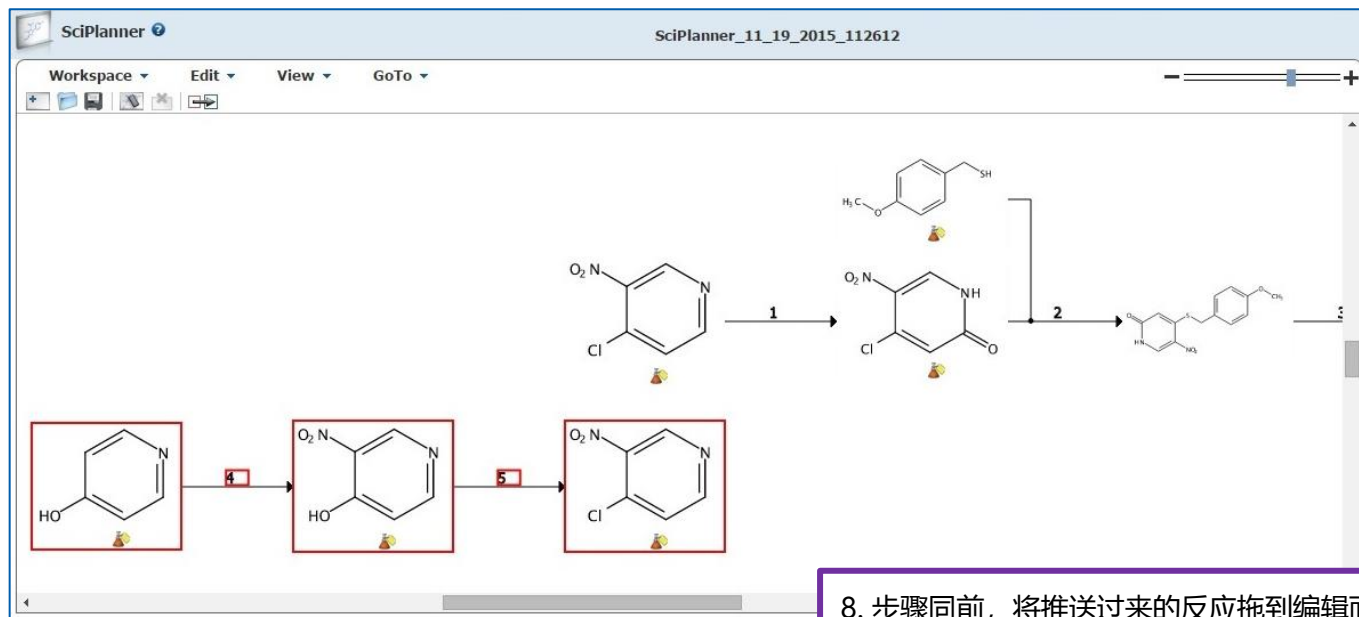
5. 打开中间产物的标准菜单选择Synthesis this

The screenshot displays the SciPlanner software interface. At the top, a workspace shows a chemical reaction sequence starting from a 2-chloro-4-nitrobenzaldehyde derivative, proceeding through an intermediate (a chloro-substituted enone), and finally to a product. A context menu is open over the intermediate structure, with the option 'Synthesize this...' highlighted. Below the workspace, a panel titled 'Get References' shows a list of reactions. The first reaction is selected, and its details are displayed below, showing the conversion of 3-hydroxypyridine to 3-chloro-5-nitropyridine. A 'Send to SciPlanner' button is visible in the top right of the reaction list panel.

6. 在检索到的反应中选择感兴趣的反应

7. 继续推送到SciPlanner

# SciPlanner使用简介



8. 步骤同前，将推送过来的反应拖到编辑面板中，可以看到两条反应中存在同样的结构

# SciPlanner使用简介

The screenshot displays the SciPlanner software interface with a chemical reaction workflow. The workflow consists of several chemical structures connected by numbered arrows (1, 2, 4, 5). A purple callout box labeled '9' points to two identical chemical structures, indicating they should be dragged to overlap to merge the reactions. Another purple callout box labeled '10' points to the 'Export' option in the 'Workspace' menu. A third purple callout box labeled '11' points to the 'Export' dialog box, which is open on the right side of the screen. The dialog box has sections for 'For:' (Offline Review, Saving Locally), 'Details:' (File Name, Title), and 'Include:' (SciPlanner Image, Reaction Details, Substance Details, Reference Details). The 'Export' button is highlighted at the bottom right of the dialog box.

10. 点击 Workspace, 选择Export 导出结果

9. 用鼠标将两个同样的结构拖至重叠, 两条反应合并

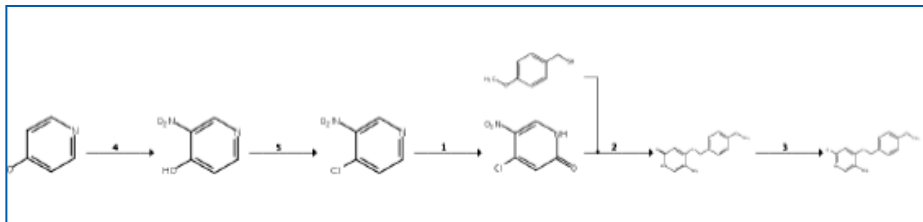
11. 选择适当的输出格式, 输出结果



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# SciPlanner导出结果



Reaction	Stages	Notes	Yield
5	<p>1.1 R:POCl<sub>3</sub>, S:PhMe, 0°C → rt; 16 h, rt → 110°C</p> <p>1.2 R:K<sub>2</sub>CO<sub>3</sub>, S:H<sub>2</sub>O, cooled, pH 10</p>	<p><b>Reactants:</b> 1, Reagents: 2, <b>Solvents:</b> 2, <b>Steps:</b> 1, <b>Stages:</b> 2</p> <p><b>Transformation:</b> 1. Formation of Alkyl Halides from Alcohols</p>	90%
<p><b>References</b> High color rendering index and color stable hybrid white efficient OLEDs with a double emitting layer structure using a single phosphorescence dopant of heteroleptic platinum complexes By Poleok, Anurach et al From Journal of Materials Chemistry C: Materials for Optical and Electronic Devices, 2(48), 10343-10356; 2014</p>			

Substance Information		
<p>1228150-22-8</p> <p>C<sub>13</sub>H<sub>12</sub>N<sub>2</sub>O<sub>3</sub>S 2-[1-(4-methoxyphenyl(methylthio)-5-nitro- Related Info: ~ 2 References Reactions</p>	<p>1228150-23-9</p> <p>C<sub>13</sub>H<sub>11</sub>ClN<sub>2</sub>O<sub>3</sub>S Pyridine, 2-chloro-4-[[4-( methoxyphenyl(methylthio)-5-nitro- Related Info: ~ 2 References Reactions</p>	<p>13091-23-1</p> <p>C<sub>5</sub>H<sub>3</sub>ClN<sub>2</sub>O<sub>2</sub> Pyridine, 4-nitro-3-nitro- Related Info: ~ 361 References Reactions ~ 100 Commercial Sources Regulatory Information</p>
<p>5435-54-1</p> <p>O<sub>2</sub>N HO C<sub>5</sub>H<sub>4</sub>N<sub>2</sub>O<sub>3</sub> 4-Pyridinol, 3-nitro- Related Info: ~ 113 References Reactions ~ 167 Commercial Sources Regulatory Information</p>	<p>6258-68-2</p> <p>H<sub>3</sub>C HO C<sub>8</sub>H<sub>10</sub>O S Benzenemethanethiol, 4-methoxy- Related Info: ~ 749 References Reactions ~ 71 Commercial Sources Regulatory Information</p>	<p>626-44-2</p> <p>HO C<sub>5</sub>H<sub>4</sub>N O 4-Pyridinol Related Info: ~ 151 References Reactions ~ 160 Commercial Sources Regulatory Information</p>
<p>850663-54-6</p> <p>O<sub>2</sub>N Cl C<sub>5</sub>H<sub>3</sub>ClN<sub>2</sub>O<sub>3</sub> 2-[1-(4-chloro-5-nitro- Related Info: ~ 22 References Reactions ~ 136 Commercial Sources</p>		



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# 提纲

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- 上机练习



## SciFinder浏览器选择建议

- Windows 7以上用户建议升级IE到10以上，不支持IE7、IE8
- Chrome和FireFox浏览器在所有系统上的表现都优于IE浏览器
- 不建议使用360浏览器检索SciFinder，会被自动拦截相关功能或插件

# 如何获取SciFinder账号

The screenshot displays the SciFinder registration interface, organized into three main sections:

- CONTACT INFORMATION--**: Includes input fields for First Name, Last Name, Email, Confirm Email, Phone Number, and Fax Number. It also features two dropdown menus for 'Area of Research' and 'Job Title', both currently set to 'Select one'.
- USERNAME AND PASSWORD--**: Contains fields for Username (with a 'Tips' link), Password, and Re-enter Password.
- SECURITY INFORMATION--**: Includes a dropdown menu for 'Security Question' (set to 'Select one') and an 'Answer' field (with a 'Why?' link).

At the bottom of the form are two buttons: 'Register>>' and 'Clear All'.

请注意:

1. 必须输入真实姓名和邮箱。  
2. 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)

3. 密码必须包含 7-15 个字符，并且至少包含三种以下字符：

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

例: abc@123

4. 从下拉列表选择一个密码提示问题并给出答案。

单击 Register (注册) 。

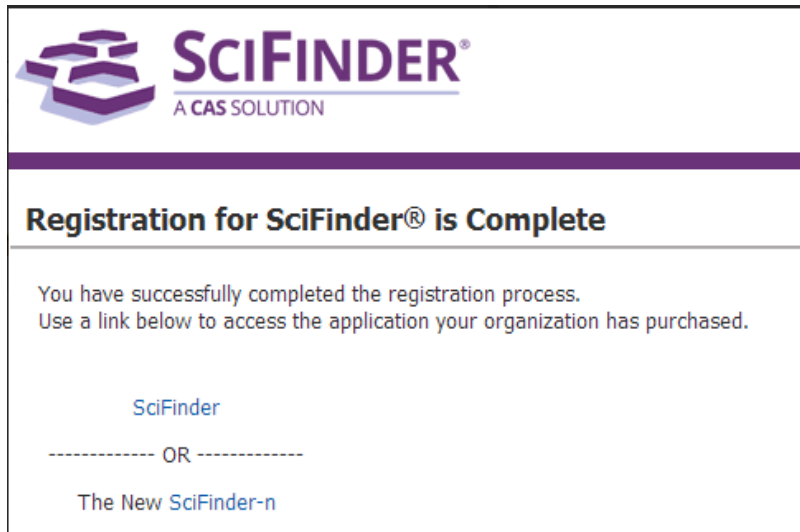


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# 如何获取SciFinder账号



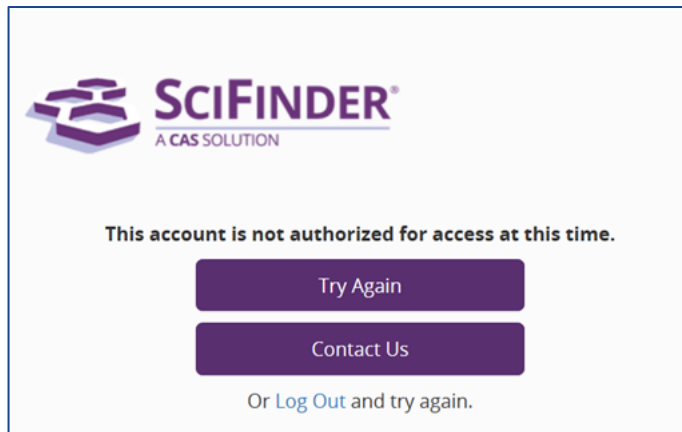
所有信息提交后注册成功。

之后直接点击<https://SciFinder.cas.org>即可访问SciFinder数据库

# SciFinder使用注意事项

- 一人注册一个帐号，在校内完成注册
- 实名注册，需提供真实姓名信息（中文名用汉语拼音全拼）
- 严禁过量下载（以电子形式存储不超过5,000条记录）
- 严禁账号分享
- 严禁将账号用于非学术研究

# SciFinder常见问题



- 确认账号密码是否正确
- 如果账号密码正确，请填好问题报告后联系图书馆或china@acs-i.org

# 提纲

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## 上机练习

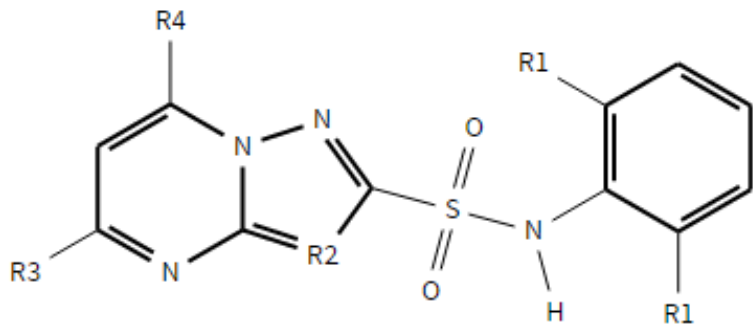
1. 检索“多功能载药蛋白纳米粒”的文献。有多少综述？被引次数最高的文献来自哪份期刊？该研究领域专利多还是期刊多？发文最多的研究机构是哪家？哪些文献是做分析研究的？研究紫杉醇（paclitaxel）的有多少文献？
2. 检索普克鲁胺（ [Proxalutamide](#) ）。原研公司是哪家？原研专利中披露了多少物质？该药物最早是用来治疗什么疾病？最新的研究中用于治疗什么疾病？
3. 检索Na<sub>2</sub>HPO<sub>4</sub>。

# 上机练习

4. 找到包含如下物质的所有合成制备的文献：

要求：

- R1 = X, H, -NO<sub>2</sub>, -CF<sub>3</sub>
- R2 = C 或 N
- R3 = 任意非氢原子
- R4 = 2-5个碳的碳链
- 结构中的环不发生稠环

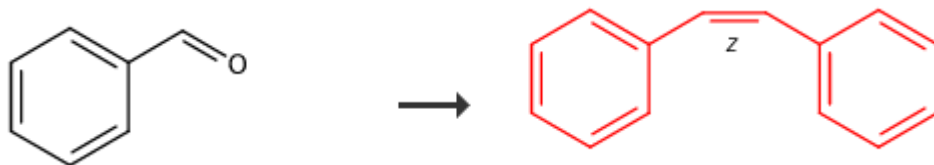


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## 上机练习

5. 查找合成格列卫（Glivec）的反应

6. 检索以下反应：



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# 谢 谢!

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