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美国化学文摘社北京代表处

# SciFinder在医药学科中的应用

2021年3月

# 提纲

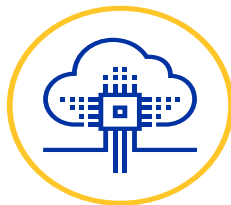
- 为什么需要美国化学文摘社
- SciFinder简介及检索方式
  - 文献检索 (PatentPak及MethodsNow-ANA的应用)
  - 物质检索
  - Markush检索
  - 反应检索 (MethodsNow-SYN的应用)
  - SciPlanner
- SciFinder常见问题及解决

## 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



**UNPARALLELED**  
SCIENTIFIC CONTENT



**SPECIALIZED**  
TECHNOLOGY



**UNMATCHED**  
HUMAN EXPERTISE



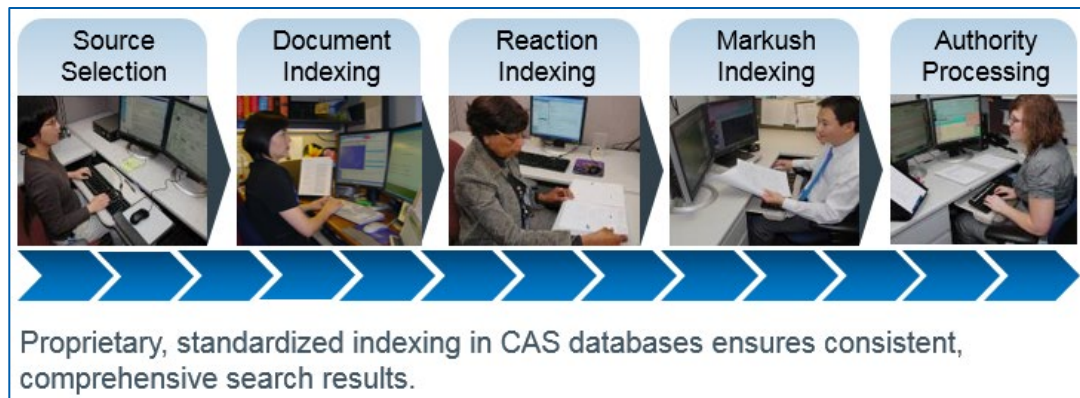
**CAS**<sup>®</sup>

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AMERICAN CHEMICAL SOCIETY

# CAS数据覆盖学科

- 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
- 有机化学各领域：
  - 氨基酸、生物分子、碳水化合物、有机金属化合物、类固醇
- 大分子化学各领域：
  - 纤维素、木质素、造纸；涂料、墨水
  - 染料、有机颜料；合成橡胶；纺织品、纤维
- 应用化学各领域：
  - 大气污染、陶瓷、精油、化妆品、化石燃料、黑色金属、合金
- 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。

# CAS各类科学信息研究工具

**STNext**

**SCIFINDER**  
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# LIMITLESS POSSIBILITIES 无限可能

定制服务应对挑战.



## CONTENT SERVICES 内容服务

- 定制数据集合  
Content licensing
- 数据结构  
Data structure
- 数据平台  
Data platforms



## TECHNOLOGY SERVICES 技术服务

- 数据架构  
Data architecture
- 平台整合  
Platform integration
- 检索引擎  
Search engines
- 定制解决方案  
Custom solutions



## KNOWLEDGE SERVICES 知识服务

- 外包IP检索  
Outsourced IP search
- 数据分析  
Analytics
- 机会分析  
Opportunity exploration
- 技术评估  
Technical Assessment



## PROFESSIONAL SERVICES 专业服务

- 人员派遣  
Talent augmentation
- 咨询  
Consulting
- Technical writing  
科技写作
- Scientific analysis  
科研分析

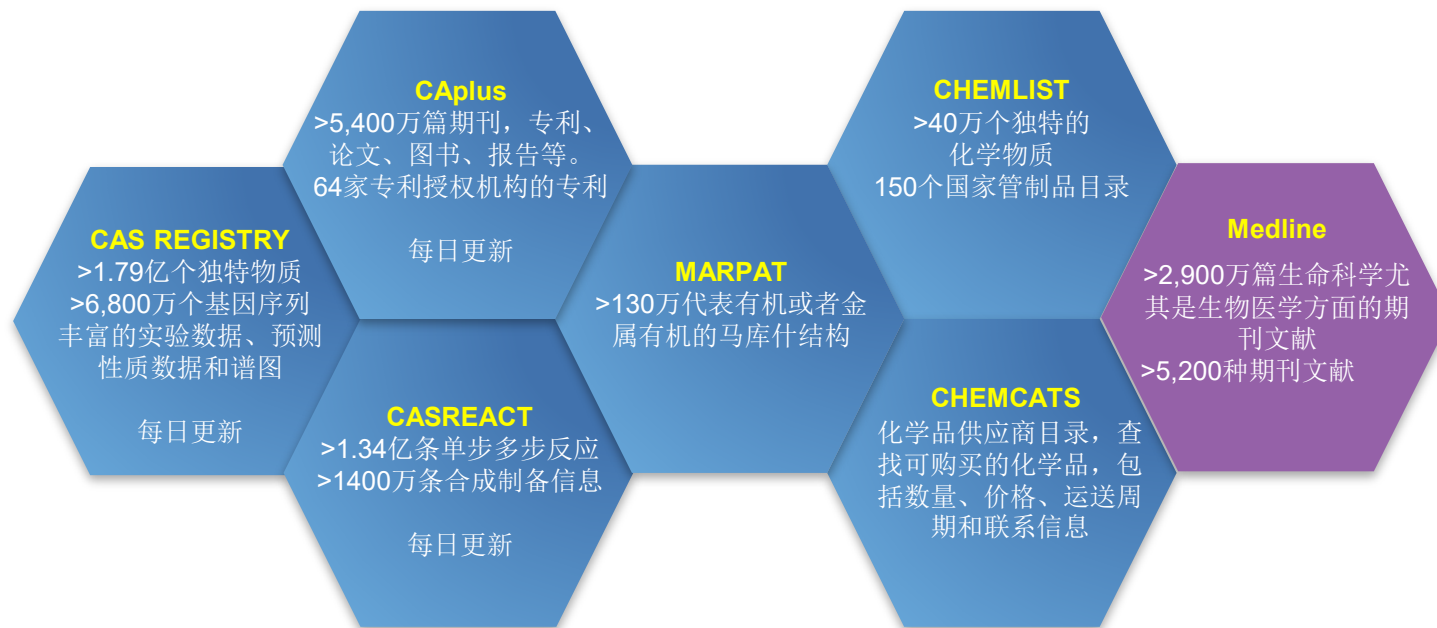


# 提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
  - 文献检索 (PatentPak及MethodsNow-ANA的应用)
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  - Markush检索
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  - SciPlanner
- SciFinder常见问题及解决



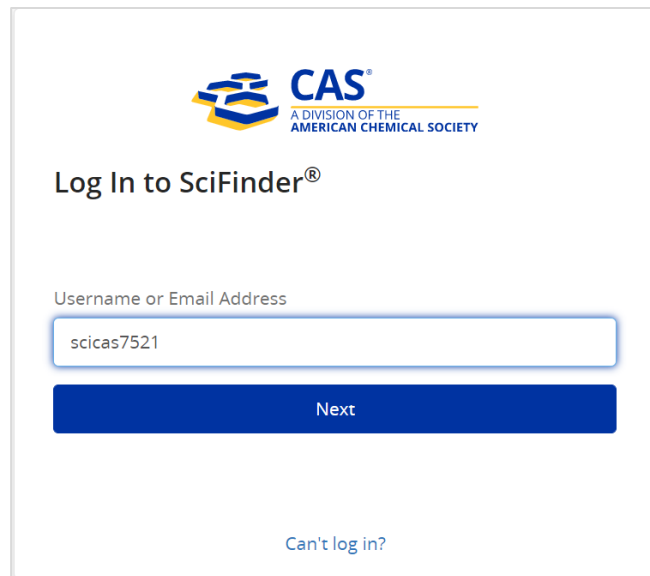
# SciFinder覆盖的数据库



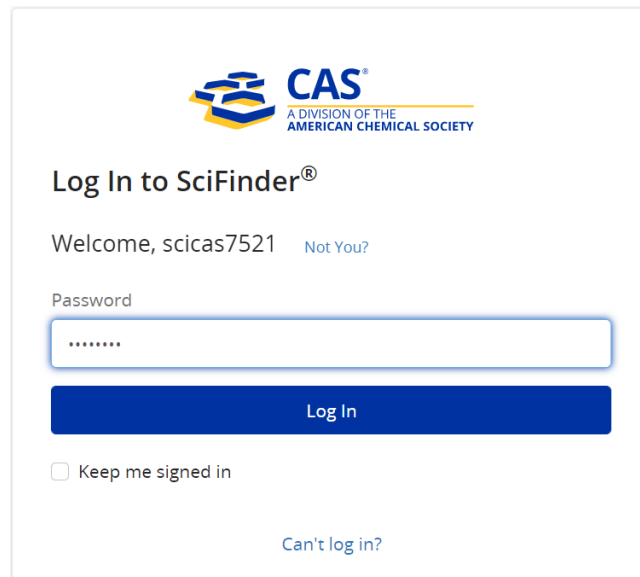
SciFinder是提供经CAS科学家人工标引内容的工具型数据库。

Sources: <https://www.cas.org/about/cas-content>

# SciFinder登录网址: <https://SciFinder.cas.org>



The screenshot shows the SciFinder login page. At the top is the CAS logo with the text "CAS A DIVISION OF THE AMERICAN CHEMICAL SOCIETY". Below the logo is the heading "Log In to SciFinder®". There is a text input field labeled "Username or Email Address" containing the text "scicas7521". Below the input field is a blue button labeled "Next". At the bottom of the page is a link that says "Can't log in?".



The screenshot shows the SciFinder login page after a successful login. At the top is the CAS logo with the text "CAS A DIVISION OF THE AMERICAN CHEMICAL SOCIETY". Below the logo is the heading "Log In to SciFinder®". The text "Welcome, scicas7521" is displayed, followed by a link "Not You?". There is a text input field labeled "Password" containing several dots. Below the input field is a blue button labeled "Log In". Below the button is a checkbox labeled "Keep me signed in". At the bottom of the page is a link that says "Can't log in?".

每个用户必须注册后才能使用

# SciFinder主界面

The screenshot shows the SciFinder web interface. At the top left is the SciFinder logo and 'CAS SOLUTIONS'. The top right has 'Preferences | SciFinder Help' and a 'Sign Out' button. Below the logo is a navigation bar with 'Explore', 'Saved Searches', and 'SciPlanner'. The main content area is titled 'REFERENCES: RESEARCH TOPIC' and features a search input field with examples: 'The effect of antibiotic residues on dairy products' and 'Photocyanation of aromatic compounds'. A 'Search' button is below the input field, and an 'Advanced Search' link is at the bottom. On the left, a sidebar lists search criteria under 'REFERENCES', 'SUBSTANCES', and 'REACTIONS'. On the right, a 'SAVED ANSWER SETS' panel lists various saved sets like 'CSF1R', 'jmc', 'EP 19870107847', etc. At the bottom right, there is a 'KEEP ME POSTED' section.

检索完, 请点击退出

工具栏

检索入口

已保存的结果集

定题追踪

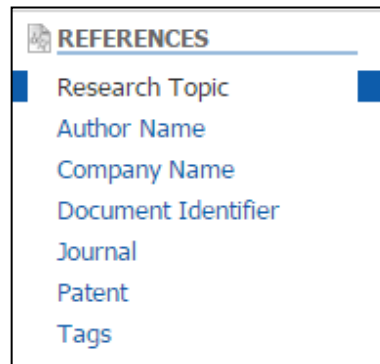
# SciFinder检索——文献检索

## 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



# 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 shows the SciFinder search interface. At the top, there are tabs for 'Explore', 'Saved Searches', and 'SciPlanner'. On the left, there is a sidebar with 'REFERENCES' and 'SUBSTANCES' sections. Under 'REFERENCES', options include 'Research Topic', 'Author Name', 'Company Name', 'Document Identifier', 'Journal', 'Patent', and 'Tags'. Under 'SUBSTANCES', options include 'Chemical Structure' and 'Markush'. The main search area is titled 'REFERENCES: RESEARCH TOPIC'. It features a search input field containing 'chinese medicine in COVID-19'. Below the input field, there are 'Examples:' such as 'The effect of antibiotic residues on dairy products' and 'Photocyanation of aromatic compounds'. A blue 'Search' button is positioned below the examples. At the bottom of the search area, 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 Save Print Export

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

REFERENCES ⓘ

Get Substances Get Reactions Get Related Citations Tools ▾

Create Keep Me Posted Alert Send to SciPlanner

Analyze Refine Categorize

Sort by: Citing References

Accession Number  
Author Name  
Citing References  
Publication Year  
Title  
Quick View Other Sources

Page: 1 of 52

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. **Diagnosis 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 significan...

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 signific...

3. **COVID-19 infection and rheumatoid arthritis: Faraway, so close!**  
By Favalli, Ennio Giulio; Ingegneri, 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 coronaviruses (SARS-CoV-2) is mainly supportive, even though several compds. 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 ...

Citing Reference: 帮助找到最重要的文献

# 文献结果集

Explore ▾ Saved Searches ▾ SciPlanner Save Print Export

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

REFERENCES

Get Substances Reactions Citations Tools

Create Keep Me Posted Alert Send to SciPlanner

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

文献分析工具

获取原文

- 1. Traditional Chinese exercise for COVID-19: A protocol for systematic review and meta-analysis**  
Quick View Other Sources  
By Duan, Yuanyuan; Xiong, Mengran; Wang, Heping; Yao, Xiaoyan; Liu, Henyuan; 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 work to convalescence therapy is very important, thus **Chinese** experts draw up Expert Consensus on Reh...
- 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...

SciFinder提供强大的文献处理工具，帮助处理文献



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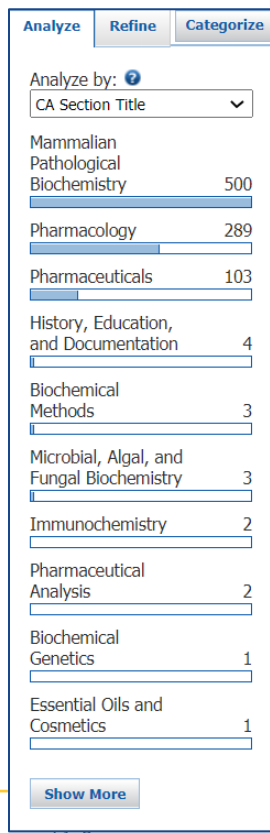


# 分析文献结果集——Analyze

期刊



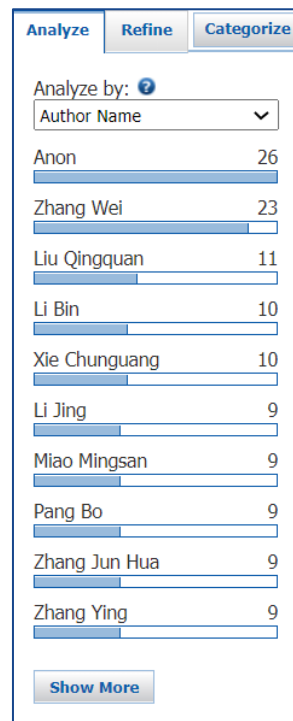
涉及学科领域



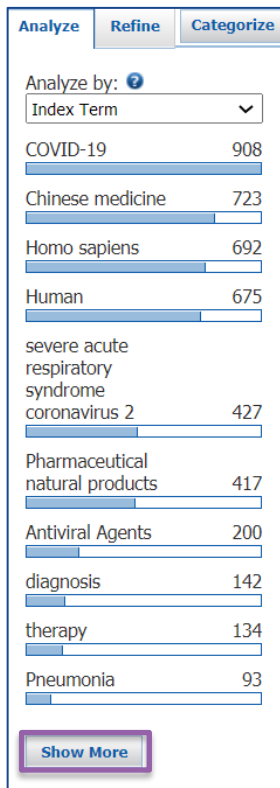
本领域研究机构、合作伙伴、竞争对手



本领域研究人员

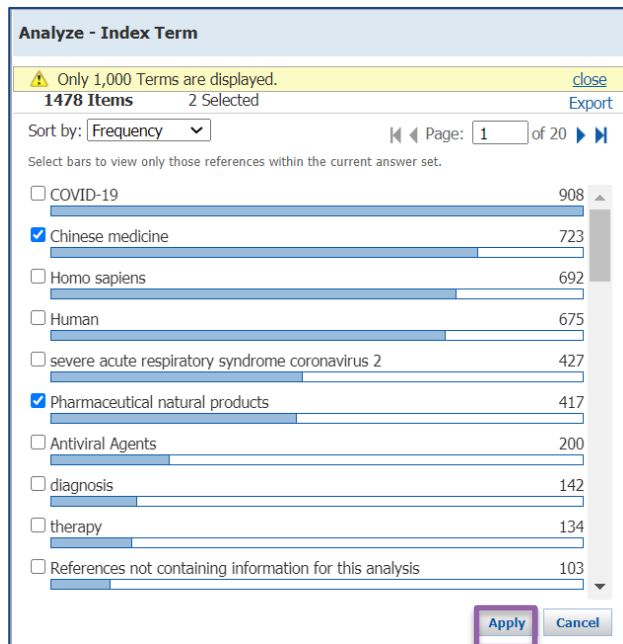


# 分析文献结果集——Analyze



Index Term:

帮助用户了解涉及到的重要技术术语，并修正检索词



选择感兴趣的内容，点击Apply



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# 筛选文献结果集——Refine

Analyze Refine Categorize

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

Get Substances Get Reactions Get Related Citations Tools

Send selected records to SciPlanner. Send to SciPlanner

Sort by: Accession Number

0 of 212 References Selected

Page: 1 of 11

- 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 come 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 ...
- 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, Yi; Sun, Yang; Guan, Manke; Shang, Hongcai  
From TMR Modern Herbal Medicine (2020), 3(3), 149-146. | 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...
- 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...
- 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 ...

Refine: 帮助用户迅速获得需要的文献

# 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.      2. Select index terms of interest.

Category Heading	Category	Index Terms	Selected Terms
All	Miscellaneous substances (321)	<b>Select All</b> <b>Deselect All</b>	Click 'x' to remove the category from 'Selected Terms'
General chemistry	Substances in property studies (208)	<input checked="" type="checkbox"/> Pharmaceutical decoctions 60 ▲	+ Physical chemistry > Gas, liquid, & solid phenomena (2 Terms)
<b>Physical chemistry</b>	<b>Gas, liquid, &amp; solid phenomena (22)</b>	<input checked="" type="checkbox"/> Pharmaceutical injections 20	
Polymer chemistry	Substances in processes (28)	<input type="checkbox"/> Sputum 9	
Biotechnology	Mechanics (4)	<input type="checkbox"/> Blood plasma 5	
Biology	Particle phenomena (3)	<input type="checkbox"/> Convalescent plasma 5	
Technology	Thermodynamics (3)	<input type="checkbox"/> Binding energy 2	
Analytical chemistry	Spectra & spectroscopy (3)	<input type="checkbox"/> Blood serum 2	
Environmental chemistry	Electric & magnetic phenomena (2)	<input type="checkbox"/> Body fluid 2	
Synthetic chemistry	Subatomics (1)	<input type="checkbox"/> Disorder 2	
Catalysis		<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 ▼	

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

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

Get Substances Get Reactions Get Related Citations Tools

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, Qu; Cui, Liao; Luo, Hui; Luo, Lianxiang  
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**  
By Zeng, Mengjie; Li, Lijun; Wu, Zhiqian  
From PLoS One (2020), 15(9), e0238028. | 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)**  
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-Wen; 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-ba...

**4. A case of treatment of a new coronavirus pneumonia patient with consistent fever using Fenghuolun theory by professor Du Shaohui**  
By Yang, Hai; Du, Shao-hui; 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.

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## 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, Jiao; 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) ≥ 30% and drug-like (DL) ≥ 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 TGFB1. According to the std. of p < .05, GO function was enriched in 108 biol. processes, 16 cell processes and 2 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 comparison of pos. and neg. 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.

**重要概念**

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)

Intercellular adhesion molecule 1  
Peroxisome proliferator-activated receptor γ  
Transcription factor STAT1  
Type II interferons

Interleukin 1β  
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

### Substances

**重要物质**

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  
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520-18-3 Kaempferol

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Animal Experiment Center  
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# PatentPak——专利工作流程解决方案

By Orhan, Ilkay Erdogan; Kartal, Murat  
From Turkish Journal of Pharmaceutical Sciences (2015), 12(3), 279-286. | Language: English, Database: CAPLUS

Hypericum perforation L. (St. John's Wort) is a reputed plant with a long service to humankind. In the current study, antioxidant activity of the methanol ext. of the aerial parts of if H. perforatum growing in Turkey along with hyperoside and hyperforin was evaluated by 2,2-diphenyl-1-picrylhydrazyl (DPPH) radical scavenging, metal-chelation, and ferric-reducing antioxidant power (FRAP) assays. The major components including chlorogenic acid, the flavonoid derivs.; rutin, hyperoside, quercitrin, quercetin, and biapigenin, the naphthodianthrone; pseudohypericin and hypericin, and the phlor...

28. **Flavaspidic acid BB of phloroglucinol derivatives of Drosera fragrans and antibacterial application**  
PATENTPAK  
Quick View

Patent No.	PatentPak Options	Kind	Language
CN 107837247	PDF   PDF+   Viewer	A	Chinese

By Shen, Zhibin  
From Faming Zhuanli (2017), 13(1), 1-4. | Language: Chinese, Database: CAPLUS

The invention provides a flavaspidic acid BB derivative, which is shown as structure I. Flavaspidic acid BB has good antibacterial applications, can effectively inhibit the growth of drug-resistant bacteria, provides the antibacterial solution to drug-resistant bacteria. Exptl. result shows that the compd. has relatively strong antibacterial effect, esp. has good curative effect against the drug-resistant bacteria.

29. **Electrochemical properties of carbon aerogels with freeze-drying**  
Quick View | Other Sources

By Xu, Yuelong; Yan, Meifang; Liu, Zhenfa  
From IOP Conference Series: Materials Science and Engineering (2017), 231(2017 2nd International Seminar on Advances in Materials Science and Engineering), 012093/1-012093/5. | Language: English, Database: CAPLUS

Carbon aerogels (CAs) were prepd. via a sol-gel process by polymn. of phloroglucinol, resorcinol and formaldehyde using 2,4-dihydroxybenzoic acid as catalyst with freeze-drying. The electrochem. properties were characterized using cyclic voltammetry, galvanostatic charge-discharge measurements and electrochem. impedance spectroscopy (EIS). The specific capacitance of corresponding CAs was up to 131 F g<sup>-1</sup> and 105 F g<sup>-1</sup> at the d. of 0.5 A g<sup>-1</sup> and 1.0 A g<sup>-1</sup>, resp.

30. **Organic acid catalyzed carbon aerogels with freeze-drying**  
Quick View | Other Sources

By Xu, Yuelong; Yan, Meifang; Liu, Zhenfa  
From IOP Conference Series: Materials Science and Engineering (2017), 231(2017 2nd International Seminar on Advances in Materials Science and Engineering), 012113/1-012113/5. | Language: English, Database: CAPLUS

Carbon aerogels (CAs) were synthesized via a sol-gel process by condensation-polymn. of phloroglucinol, resorcinol and formaldehyde using 2,4-dihydroxybenzoic acid as catalyst with freeze-drying. The effects of the freeze-drying method on the texture and pore structure were studied. Meanwhile the structure of carbon aerogels was characterized by X-ray diffraction (XRD), SEM (SEM) and a surface-area analyzer. The results show that the freeze-drying method and acid catalyst were good for the sp. surface area of carbon aerogel, up to 765m<sup>2</sup> g<sup>-1</sup>, and pore size distribution.

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By Orman, İskay Erogan; Kartal, Murat  
From Turkish Journal of Pharmaceutical Sciences (2015), 12(2): 279-286. | Language: English, Database: CAPLUS

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CAS RN 1404-90-6  
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5. 根据权利要求4所述香鳞毛蕨间苯三酚类化合物黄绵马酸BB的应用,其特征在在于,所述耐药性的革兰氏阳性致病菌是对头孢唑啉、万古霉素和/或达托霉素产生耐药性的革兰氏阳性致病菌。

6. 根据权利要求4或5所述香鳞毛蕨间苯三酚类化合物黄绵马酸BB的应用,其特征在在于,所述耐药性革兰氏阳性致病菌为耐药的金黄色葡萄球菌和/或表皮葡萄球菌。

7. 权利要求1至6所述香鳞毛蕨间苯三酚类化合物黄绵马酸BB的化学合成方法,其特征在在于,包括以下步骤:

- S1. 合成2',4',6'-三羟基-3'-丁酰基苯丁酮;
- S2. 合成4,4-二甲基-3,5-二羟基-2,6-二丁酰基-2,5-环己二烯酮;
- S3. 合成4,4-二甲基-3,5-二羟基-2-丁酰基-2,5-环己二烯酮;
- S4. 合成2,4,6-三甲氧基苯甲醚;
- S5. 合成2-甲基,3,5-二甲氧基苯甲醚;
- S6. 合成3'-甲基-2',4',6'-三甲氧基苯丁酮;
- S7. 合成3'-甲基-2',4',6'-三羟基苯丁酮;
- S8. 合成4,4-二甲基-3,5-二羟基-2-丁酰基-6-(5-甲基-2,4,6-三羟基-3-丁酰基苯基)-2,5-环己二烯酮。

8. 权利要求7所述香鳞毛蕨间苯三酚类化合物黄绵马酸BB的化学合成方法,其特征在在于:

- S1. 合成2',4',6'-三羟基-3'-丁酰基苯丁酮;

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# PatentPak——专利工作流程解决方案

28. Flavaspidic acid BB of phloroglucinol derivatives of Dryopteris fragrans and antibacterial application

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CAS RN 2216756-37-3

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- S3. 合成4,4-二甲基-3,5-二羟基-2-丁酰基-2,5-环己二烯酮;
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- S6. 合成3'-甲基-2',4',6'-三甲氧基苯丁酮;
- S7. 合成3'-甲基-2',4',6'-三羟基苯丁酮;
- S8. 合成4,4-二甲基-3,5-二羟基-2-丁酰基-6-(5-甲基-2,4,6-三羟基-3-丁酰基苯基)-2,5-环己二烯酮。

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- S1. 合成2',4',6'-三羟基-3'-丁酰基苯丁酮;

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28. Flavaspidic acid BB of phloroglucinol derivatives of *Dryopteris fragrans* and antibacterial application

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5. 根据权利要求4所述香鳞毛蕨间苯三酚类化合物黄绵马酸BB的应用,其特征在于,所述耐药性的革兰氏阳性致病菌是对头孢唑啉、万古霉素和/或达托霉素产生耐药性的革兰氏阳性致病菌。

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S2. 合成4,4-二甲基-3,5-二羟基-2,6-二丁酰基-2,5-环己二烯酮;

S3. 合成4,4-二甲基-3,5-二羟基-2-丁酰基-2,5-环己二烯酮;

S4. 合成2,4,6-三甲氧基苯甲醛;

S5. 合成2-甲基,3,5-二甲氧基苯甲醛;

S6. 合成3'-甲基-2',4',6'-三甲氧基苯丁酮;

S7. 合成3'-甲基-2',4',6'-三羟基苯丁酮;

S8. 合成4,4-二甲基-3,5-二羟基-2-丁酰基-6-(5-甲基-2,4,6-三羟基-3-丁酰基苯基)-2,5-环己二烯酮。

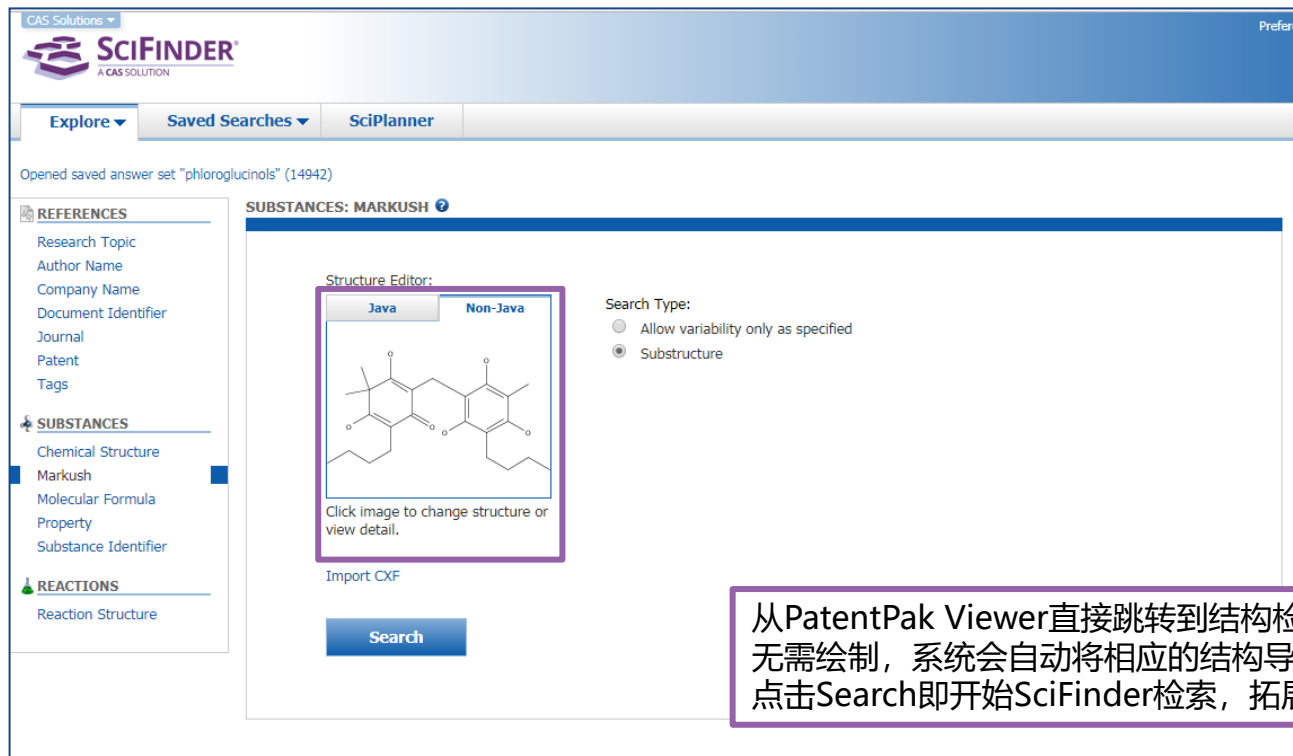
8. 权利要求7所述香鳞毛蕨间苯三酚类化合物黄绵马酸BB的化学合成方法,其特征在于,包括以下步骤:

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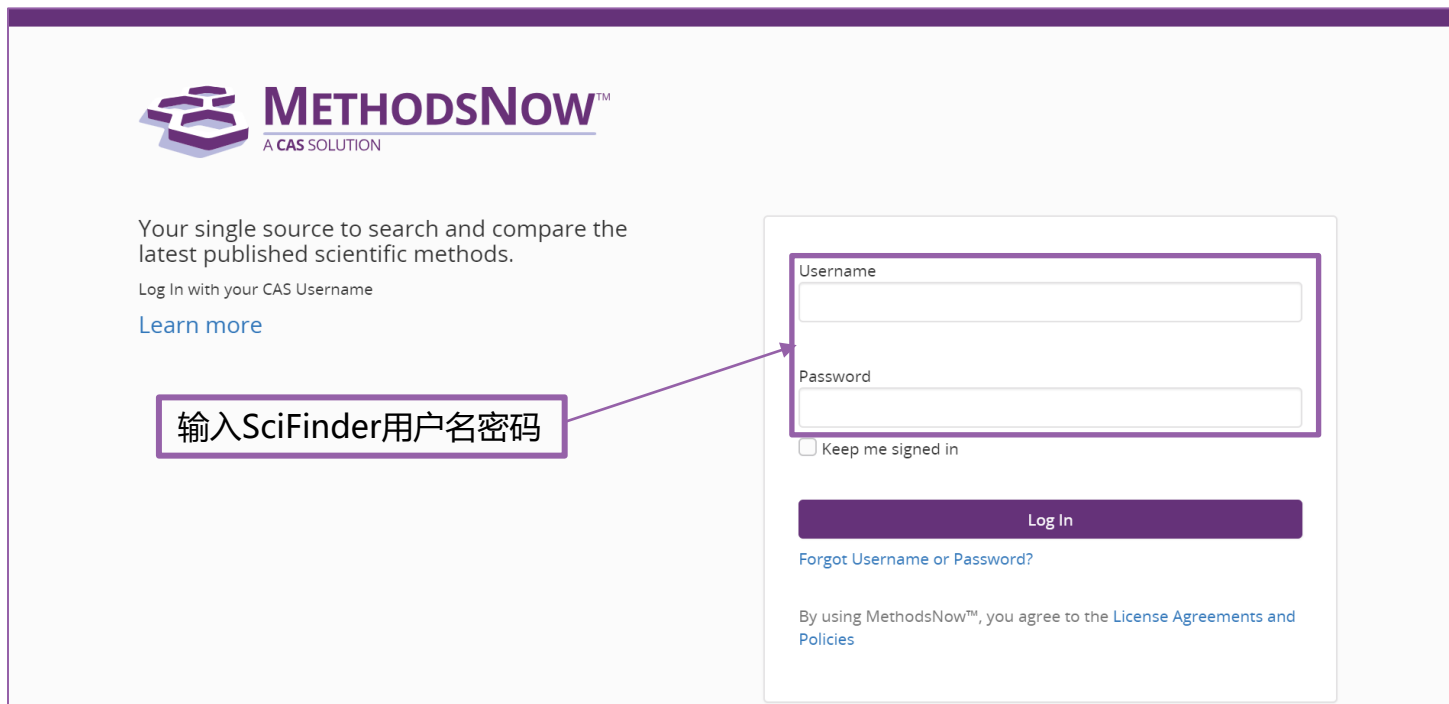
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▼ **Year**

**Results** (318)

**Analysis of Clopidogrel in Drugs by Spectrophotometry**  
CAS MN: 1-101-CAS-61399

[View Details & Instructions](#) [Add to Compare](#)

Analyte	Clopidogrel
Matrix	Drugs
Other Materials	Reagent: Hydrochloric acid; 1,10-Phenanthroline; Iron chloride (FeCl <sub>3</sub> ); Phosphoric acid Material: 10 mL volumetric flask
Method Category	Active Pharmaceutical Ingredient and Metabolite Analysis
Technique	Spectrophotometry
Equipment Used	Spectrophotometer
Source	<b>Assay of Clopidogrel by visible spectrophotometry</b> Anupama, B.; Jagathi, V.; Aparna, A.; Madhubabu, M.; Lakshmi Annapurna, V. International Journal of Pharma and Bio Sciences (2011), 2 (2), 105-108. Muthu Prasanna P.

限定目标分析物



# 利用MethodsNow检索文献——直接获得分析实验方法

The screenshot displays the MethodsNow search interface. On the left, a 'Matrix' filter window is open, showing a list of search criteria. The 'Pharmaceutical tablets' option is selected and highlighted with a purple box. A purple arrow points from this box to a purple box containing the text '进一步限定分析介质' (Further limit analysis medium). Below the filter window, there are 'Apply' and 'Cancel' buttons. On the right, the 'Results' section shows 102 results. The top result is 'Analysis of Clopidogrel in Pharmaceutical tablets by Spectrophotometry'. A purple box highlights the 'View Details & Instructions' button, with a purple arrow pointing to a purple box containing the text '查看详细实验方法' (View detailed experimental method). Below the result, there is a table with columns for 'Analyte' and 'Clopidogrel', and rows for 'Matrix', 'Other Materials', 'Method Category', 'Technique', 'Equipment Used', and 'Source'. The 'Source' row includes the text: 'Spectrophotometric methods for the determination of clopidogrel' by Aparna, A.; Anupama, B.; Vindya, G.; Rao, P. Bhaskara; Rao, G. Devala, International Journal of Chemical Sciences (2010), 8 (4), 2529-2532. Sadguru Publications. There is also a 'Full Text' button and an 'Abstract' dropdown menu.

# 利用MethodsNow检索文献——直接获得分析实验方法

Method Detail (1 of 102) ← Prev Next →

Analysis of Clopidogrel in Pharmaceutical tablets by Spectrophotometry  
CAS MN: 1-101-CAS-191095

Method Category: Active Pharmaceutical Ingredient and Metabolite Analysis  
Technique: Spectrophotometry

## 实验材料

Materials	Role	Image	CAS RN
Clopidogrel	analyte	<a href="#">View Structure</a>	113665-84-2
Pharmaceutical tablets	matrix		
Iron chloride (FeCl <sub>3</sub> )	reagent	<a href="#">View Structure</a>	7705-08-0
3-Methyl-2-benzothiazolinone hydrazone	reagent	<a href="#">View Structure</a>	1128-67-2
Methanol	reagent	<a href="#">View Structure</a>	67-56-1
Hydrochloric acid	reagent	<a href="#">View Structure</a>	7647-01-0

Source

Spectrophotometric methods for the determination of clopidogrel  
Aparna, A.; Anupama, B.; Vindya, G.; Rao, P. Bhaskara; Rao, G. Devala  
International Journal of Chemical Sciences (2010), 8 (4), 2529 - 2532. Sadguru Publications  
CODEN: IJCSIL | ISSN: 0972768X

[Full Text](#)

Abstract ^

Two simple and sensitive spectrophotometric methods have been developed for the estimation of clopidogrel in pure and pharmaceutical dosage forms. Method A is based on the formation of charge transfer complex of the drug with chloranilic acid ( $\lambda_{max}$  515 nm). Method B is based on oxidative coupling of the drug with 3-Me 2-benzothiazolinone hydrazone (MBTH;  $\lambda_{max}$  630 nm). The absorbance of the colored species was measured against the reagent blank. These methods have been statistically evaluated and found to be precise and accurate.

Equipment Used  
Spectrophotometer

## Conditions

Instrument  
Detection wavelength: 630 nm

## Instructions

### 详细步骤

**Preparation of 3-Methyl 2-benzothiazolinone hydrazone (MBTH)**

1. Prepare an aqueous solution of MBTH at 0.2% w/v.

**Preparation of ferric chloride solution**

1. Prepare a solution of ferric chloride (0.7% w/v) in 0.5 N hydrochloric acid.

**Preparation of standard solution of clopidogrel**

1. Accurately weigh 100 mg of clopidogrel and dissolve in 100 mL of methanol to obtain a stock solution of 1 mg/mL.
2. Dilute this solution further to get working standard solution of 100 µg/mL.

**Spectrophotometric analysis for determination of clopidogrel using MBTH reagent**

1. Transfer aliquots of working standard solution of clopidogrel ranging from 0.5 - 2.5 mL into a series of 10 mL volumetric flasks.
2. Add 2 mL of ferric chloride to these flasks.
3. Shake the contents and keep aside for 2 minutes.
4. Add 1.5 mL of MBTH reagent and keep for 10 min.
5. Dilute the volume upto 10 mL with distilled water.
6. Measure the absorbance of the green colored chromogen at 630 nm against reagent blank.
7. Calculate the amount of clopidogrel present in the sample solution from its calibration curve.

## Validation

### 数据有效性验证

Linearity Range	5 - 25 µg/mL
Recovery	99.36% from 75 mg label claim pharmaceutical tablets (sample data)
Accuracy	1.496 and 2.214% (range of error) at 0.05 and 0.01 significance level respectively
Precision	1.79% (RSD)

# 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

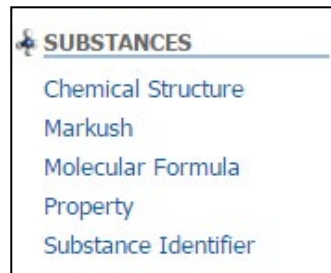
# 提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
  - 文献检索 (PatentPak及MethodsNow-ANA的应用)
  - 物质检索
  - Markush检索
  - 反应检索 (MethodsNow-SYN的应用)
  - SciPlanner
- SciFinder常见问题及解决

# 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

# 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。

# 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- $\alpha$ -glutamyl-L- $\alpha$ -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   ~62 

$C_{34}H_{60}N_{14}O_{12}S$

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

**Molecular Weight**

888.99

**Density (Predicted)**

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

**pKa (Predicted)**

Value:  $4.43 \pm 0.10$  | Condition: Most Acidic Temp: 25 °C

**Other Names**

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

Acetyl hexapeptide 8

Acetyl hexapeptide-3

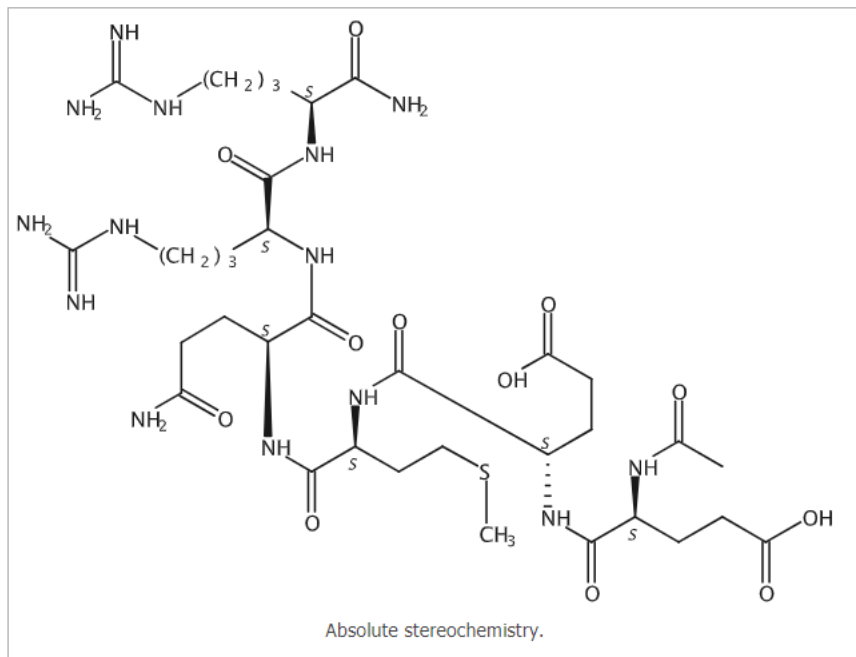
Argireline

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	<a href="#">See spectrum</a>		(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

# 物质检索——Property explore

Property Explore interface showing a dropdown menu for selecting a property. The selected property is **Molecular Weight**. The input field shows a range of **250-400** with examples: 44, 25-35, >125.

寻找分子量在250-400之间的物质

# 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

CC(C)Cc1ccc(cc1)NCCc2cc(Br)ncn2

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

Key Physical Properties

2. 1986293-21-3

CCOC1=CN=C(N(C)CC(F)F)N1CCCl

$C_{11}H_{16}ClF_2N_3O$   
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**

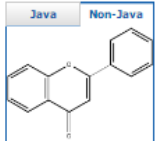
Analyze Refine

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**

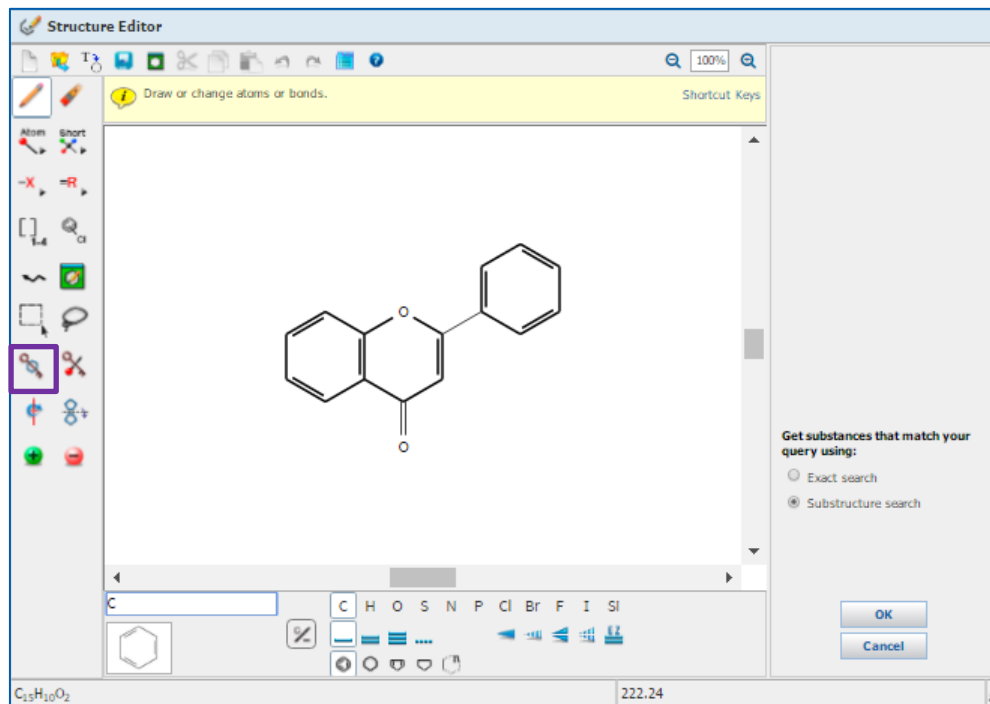
Only retrieve substances that:

- 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

$C_{15}H_{10}O_2$  222.24

锁环工具：避免在被锁定的环结构上出现新的环结构

# 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**   
  
**C<sub>17</sub>H<sub>14</sub>O<sub>2</sub>**  
4H-1-Benzopyran-4-one, 2-(3,5-dimethylphenyl)-  
▶ **Key Physical Properties**

2. **912915-64-1**   
  
**C<sub>15</sub>H<sub>10</sub>O<sub>4</sub>**  
4H-1-Benzopyran-4-one, 2-(3,5-dihydroxyphenyl)-  
▶ **Key Physical Properties**

4. **6665-68-5**

5. **22395-22-8**

从4500多万个结构中

筛选出16901个黄酮类物质



A DIVISION OF THE  
AMERICAN CHEMICAL SOCIETY

# 物质检索——分子式

检索(N H4) Sm (S O4)2 (H2 O)4, Ammonium Samarium Bis(sulfate(VI)) Tetrahydrate

Property "Experimental - Electric Conduc..." > substances (51)

REFERENCES

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

SUBSTANCES

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

SUBSTANCES: MOLECULAR FORMULA

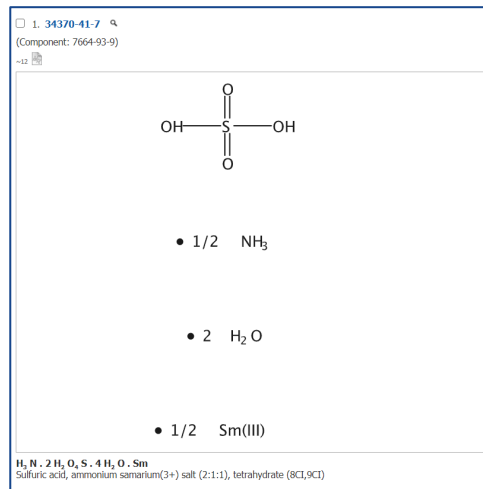
H3 N . 2 H2 O4 S . 4 H2 O . Sm

Examples:  
H4SiO4  
(C3H6O.C2H4O)x

Search

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. 金属盐：金属离子和阴离子间用点 (.) 分开
2. 不同组份之间用点 (.) 分开



# 物质检索——结构

The screenshot displays the CAS Substance Search interface. On the left, a navigation menu is organized into three sections: **REFERENCES** (Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, Tags), **SUBSTANCES** (Chemical Structure, Markush, Molecular Formula, Property, Substance Identifier), and **REACTIONS** (Reaction Structure). The **Chemical Structure** option is highlighted with a purple box. The main content area is titled **SUBSTANCES: CHEMICAL STRUCTURE** and features a **Structure Editor** window with **Java** and **Non-Java** tabs, a **Click to Edit** prompt, and an **Import CXF** button. To the right, the **Search Type** options are **Exact Structure**, **Substructure** (selected), and **Similarity**, along with a **Show precision analysis** checkbox. A **ChemDraw** logo is visible in the bottom right corner of the main area. At the bottom of the interface, there is a blue **Search** button and a link to **Advanced Search** with a checked **Always Show** option.

# 物质检索——结构

The image shows a screenshot of the 'Structure Editor' software interface. The interface is annotated with numerous Chinese labels pointing to specific tools and features. On the left side, a vertical toolbar contains icons for drawing and editing, with labels such as '橡皮' (Eraser), '铅笔' (Pencil), '元素周期表' (Periodic Table), '可变基团' (Variable Group), '重复基团工具' (Repeat Group Tool), '碳链工具' (Carbon Chain Tool), '选择工具' (Select Tool), '环锁定工具' (Ring Lock Tool), '旋转工具' (Rotate Tool), '正电子' (Positron), and '负电子' (Negatron). The top right corner features a 'Drawing Editor' panel with radio buttons for 'Structure', 'Reaction', and 'Markush', and a 'Structure and Reaction Switch Function' label. The bottom right corner has a search panel titled 'Get substances that match your query using:' with options for 'Exact search', 'Substructure search', and 'Similarity search', and a 'Structure Search Selection' label. The bottom center shows a 'Common Rings, Multi-ring Tools' label pointing to a ring selection tool. The bottom left has a 'Carbon atoms and single bond recovery tool' label. The bottom center also has a 'Single and double bonds, RS configuration, uncertain bond definition tool' label. The bottom right has a 'Mirror rotation tool' label. The bottom center has an 'Atom and bond definition tool' label. The bottom center has a 'Template tool' label. The bottom center has a 'Variable position connection tool' label. The bottom center has an 'R group definition tool' label. The bottom center has a 'Common groups' label. The bottom center has a 'Structure and reaction switch function' label. The bottom center has a 'Structure search selection' label. The bottom center has a 'Mirror rotation tool' label. The bottom center has a 'Single and double bonds, RS configuration, uncertain bond definition tool' label. The bottom center has a 'Common rings, multi-ring tools' label. The bottom center has a 'Carbon atoms and single bond recovery tool' label. The bottom center has a 'Positron' label. The bottom center has a 'Rotate tool' label. The bottom center has a 'Ring lock tool' label. The bottom center has a 'Select tool' label. The bottom center has a 'Carbon chain tool' label. The bottom center has a 'Repeat group tool' label. The bottom center has a 'Variable group' label. The bottom center has a 'Periodic table' label. The bottom center has a 'Pencil' label. The bottom center has an 'Eraser' label.

橡皮

结构 and 反应切换功能

铅笔

元素周期表

可变基团

重复基团工具

碳链工具

选择工具

环锁定工具

旋转工具

正电子

C原子和单键恢复工具

常用基团

R基团定义工具

可变位置连接工具

模版工具

索套选择工具

原子锁定工具

镜面旋转工具

结构检索选择

负电子

单双键, RS构型, 不确定键定义工具

常见环, 多元环工具



# 物质检索——精确结构检索

## 检索青蒿素的组合物

Structure Editor

Click and drag to select objects. Ctrl-click to select or deselect objects.

Atom Short

Structure Editor

Enter CAS Registry Number, SMILES, or InChI:  
63968-64-9

Examples:  
50-00-0  
CCCO  
InChI=1S/C3H8O/c1-2-3-4/h4H,2-3H2,1H3

OK Cancel

Drawing Editor:

Structure  
 Reaction  
 Markush

Get substances that match your query using:

Exact search  
 Substructure search  
 Similarity search

OK Cancel

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

C<sub>15</sub>H<sub>22</sub>O<sub>5</sub> 282.34

精确结构检索

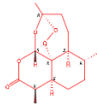
# 精确结构检索结果集

0 of 59 Substances Selected

Page: 1 of 2

1. **63968-64-9**

~6058 ~132



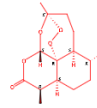
Absolute stereochemistry.

**C<sub>15</sub>H<sub>22</sub>O<sub>5</sub>**  
 3,12-Epoxy-12H-pyrano[4,3-j]-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




Absolute stereochemistry.

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

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



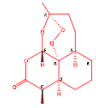
90-34-6  
 C<sub>15</sub>H<sub>21</sub>N<sub>3</sub>O



**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-j]-1,2-benzodioxepin-10(3H)-one, octahydro-3,6,9-trimethyl-, (3R,5aS,6R,8aS,9R,12S,12aR)-, mixt. with N-(6-methoxy-8-quinolinyl)-1,4-pentanediamine and 4,4'-(1,3-propanediyl)di-1-piperazine]bis[7-chloroquinoline]

3. **1201556-23-1**

~10




Absolute stereochemistry.


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

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

173531-57-2  
 C<sub>24</sub>H<sub>26</sub>ClN<sub>2</sub>O



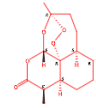
7664-38-2  
 H<sub>3</sub>O<sub>4</sub>P



**C<sub>24</sub>H<sub>26</sub>ClN<sub>2</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-j]-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



Absolute stereochemistry.

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

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-j]-1,2-benzodioxepin-10(3H)-one (1:1)

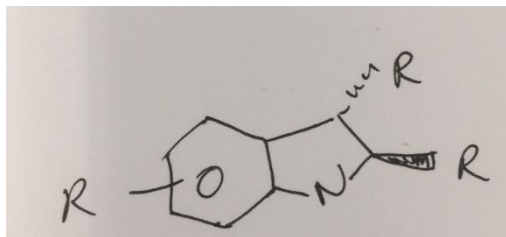
# 物质检索——精确结构检索

- 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

具有下图母核结构的药物分子



The screenshot shows the CAS Structure Editor software interface. The main window displays a chemical structure of a bicyclic core with two 'A' substituents. The interface includes a toolbar on the left with various drawing tools, a top menu bar, and a right sidebar with search options. The search options include 'Structure', 'Reaction', and 'Markush'. The 'Variables' panel on the right lists various search criteria such as 'Any halogen', 'Any metal', 'Any atom except H', etc. The bottom of the interface shows a search bar and a list of search results.

# 物质检索——亚结构检索

Select All Deselect All

1 of 5 Stereo Candidates Selected

	Substances
<input checked="" type="checkbox"/> Absolute stereo match	304
<input type="checkbox"/> Absolute stereo mirror image	60
<input type="checkbox"/> Relative stereo match	656
<input type="checkbox"/> Stereo that doesn't match query	3388
<input type="checkbox"/> No stereo in answer structure	17327

Get Substances

选择绝对立体构型完全匹配的候选项

# 物质检索——亚结构检索

查看结果集，根据适应症或靶点信息选取分子

Chemical Structure substructure > substances (304)

STANCES 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 304 Substances Selected Page: 1 of 7

Analyze by: Bioactivity Indicators

- Antibiotic agents 9
- Antidiabetic agents 9
- Antiobesity agents (all) 9
- Cardiovascular agents (all) 9

Show More

1. 2096301-64-1

Absolute stereochemistry, Rotation (+).

Chemical Structure substructure > substances (304)

STANCES 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 304 Substances Selected Page: 1 of 7

Analyze by: Target Indicators

- Enzymes (all) 167
- Receptors (all) 15
- Lipoproteins (all) 9

Show More

1. 2096301-64-1

Absolute stereochemistry, Rotation (+).

C<sub>26</sub>H<sub>28</sub>N<sub>2</sub>O<sub>5</sub>

2. 2096301-63-0

Absolute stereochemistry, Rotation (+).

3. 2030136-54-8

Absolute stereochemistry, Rotation (+).

C<sub>19</sub>H<sub>26</sub>BrN  
1-#Indole, 5-bromo-2-[(1*R*)-1-ethenyl-1,5-dimethyl-4-hexen-1-yl]-2,3-dihydro-3-methyl-, (2*S*,3*S*)-

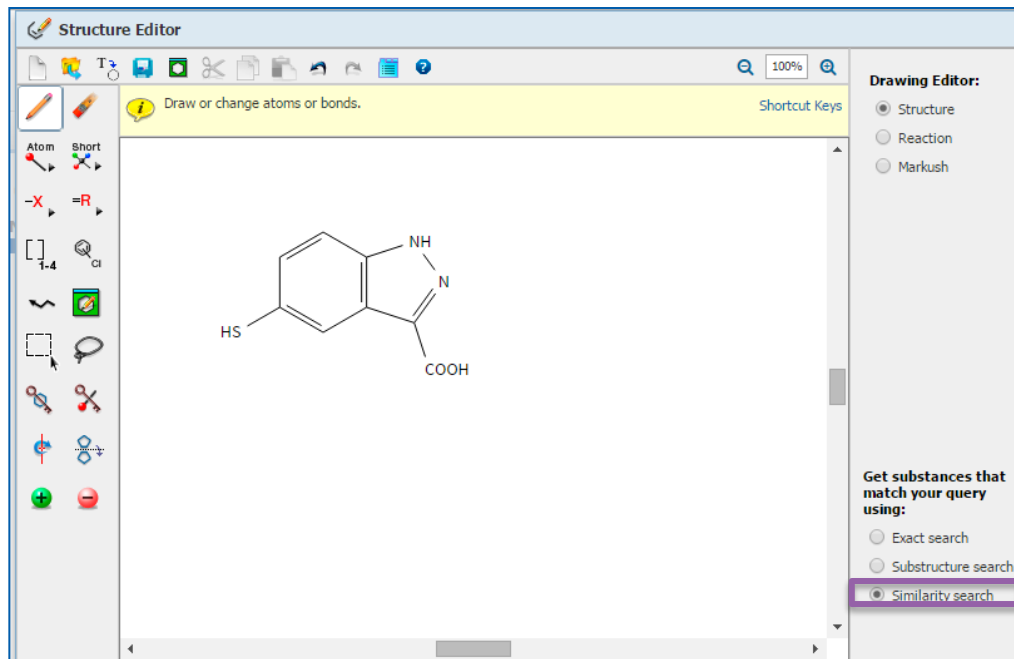
Key Physical Properties

# 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>9</sub> F N<sub>2</sub> O<sub>2</sub>**  
1H-Benz[*g*]indazole-3-carboxylic acid, 8-fluoro-1-methyl-

▶ Key Physical Properties

母体结构变化



CAS<sup>®</sup>

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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 (PatentPak及MethodsNow-ANA的应用)
  - 物质检索
  - Markush检索
  - 反应检索 (MethodsNow-SYN的应用)
  - SciPlanner
- SciFinder常见问题及解决

# 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



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(43) 申请公布日 2015.09.30

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(22) 申请日 2014.03.30 *C07K 1/06*(2006.01)  
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38号 *A61P 25/28*(2006.01)  
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(51) Int. Cl.

*C07K 5/087*(2006.01)  
*C07K 5/083*(2006.01)

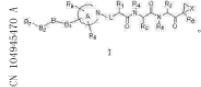
权利要求书3页 说明书24页 附图4张

(54) 发明名称

杂环构建的三肽环酰胺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酰胺类化合物,以Carfilzomib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, 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

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

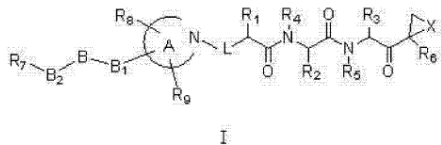
# Markush检索

CN 104945470 A

权利要求书

1/3 页

1. 一种杂环构建的三肽环氧化物类化合物,具有下述结构通式 I:



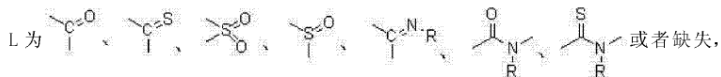
其中:

$R_1, R_2, R_3$  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,  $R_0, R_0$  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、杂环芳基、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

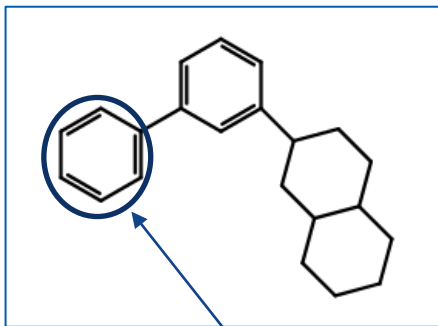


CAS<sup>®</sup>

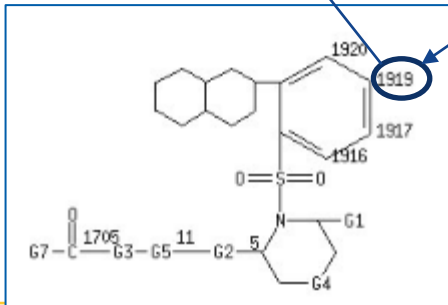
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# Markush检索

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



# Markush检索

Structure Editor

Click a ring system to block it from further ring fusion. Click a chain to block it from ring formation.

环锁定

Structure Editor

Structure

Reaction

Markush

Get substances that match your query using:

Exact search

Substructure search

Similarity search

OK

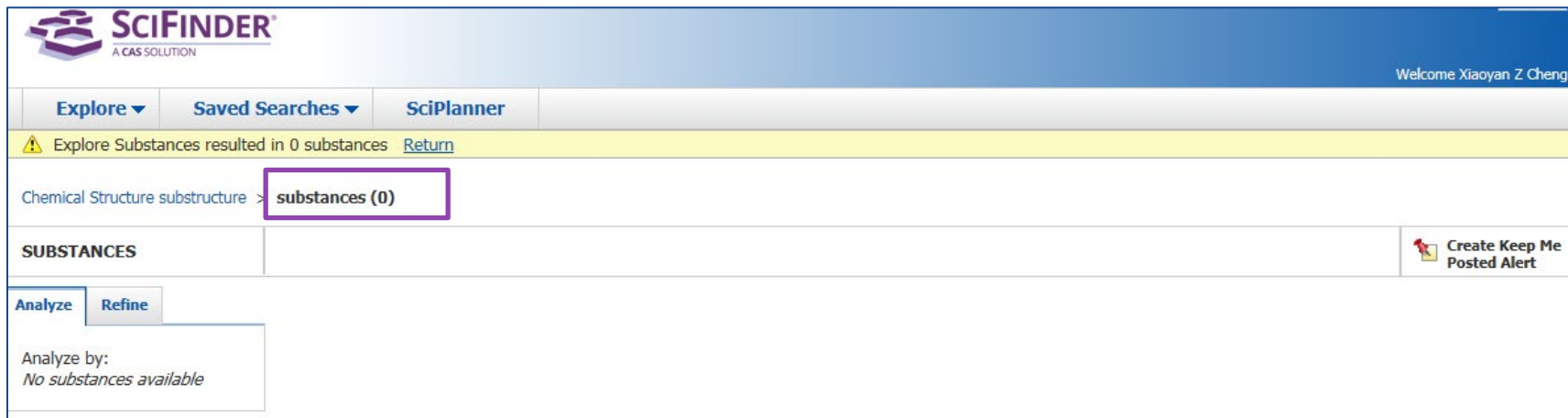
Cancel

C<sub>22</sub>H<sub>26</sub> 290.45

结构检索

亚结构检索

# Markush检索

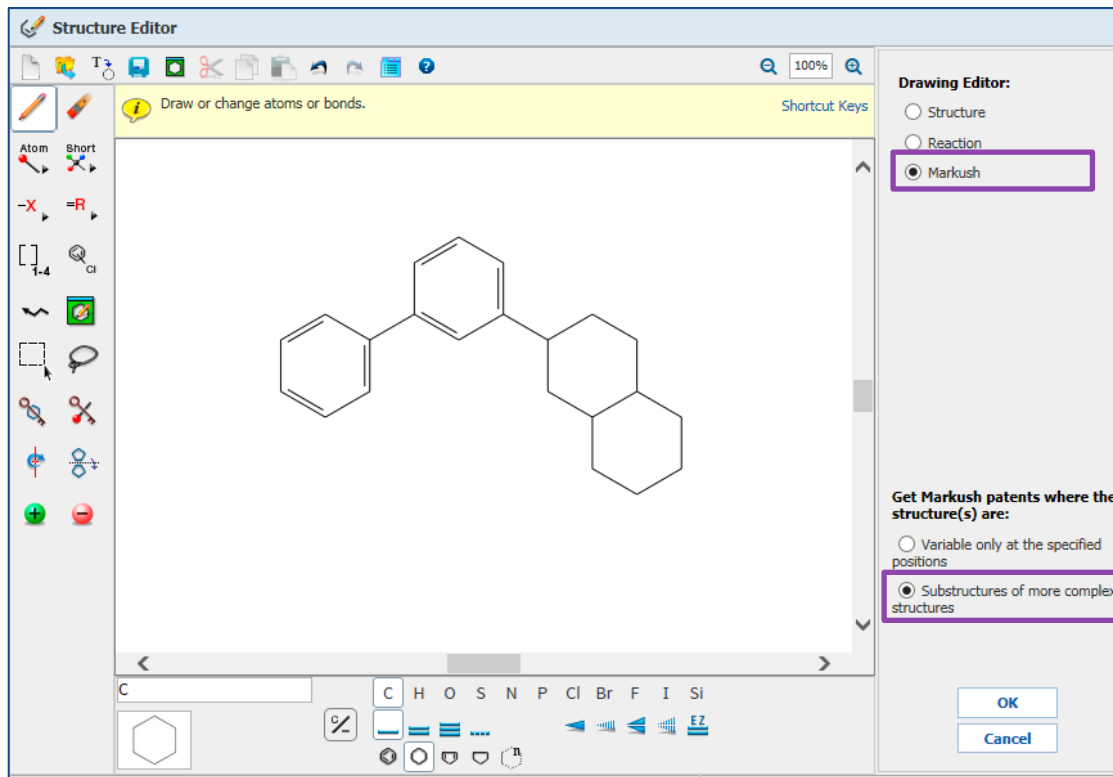


The screenshot displays the SciFinder web interface. At the top left is the SciFinder logo with the tagline 'A CAS SOLUTION'. On the top right, it says 'Welcome Xiaoyan Z. Cheng'. Below the header are navigation tabs: 'Explore', 'Saved Searches', and 'SciPlanner'. A yellow warning banner states: 'Explore Substances resulted in 0 substances [Return](#)'. The search input field contains 'Chemical Structure substructure' and shows 'substances (0)'. Below the search bar, there are buttons for 'Analyze' and 'Refine'. A dropdown menu under 'Analyze' shows 'Analyze by: No substances available'. On the right side of the interface, there is a 'Create Keep Me Posted Alert' button.

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

0 of 24 References Selected

**1. Compounds for the modulation of proprotein convertase subtilisin/kexin type 9 (PCSK9)**  
Quick View PATENTPAK  
By Bowers, Simeon; Karbarz, Mark; Zhu, Jiang; Barta, Thomas E.; Bourne, Jonathan William; Pandey, Anjali  
From PCT Int. Appl. (2020), WO 2020252383 A2 20201217. | Language: English, Database: CAPLUS

The present disclosure relates to novel compds. capable of binding to PCSK9, thereby modulating PCSK9 biol. activity. Also provided are compns. comprising these compds., methods of prep. the compds., and methods for use of the compds. in the treatment of PCSK9-related conditions and diseases.

**2. 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  $R^1-Ar^1-N(Ar^2-R^3)-Ar^3-R^2$ , 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.

**3. 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.

**4. 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

$$P-\left\{S_0-X^1\right\}_{k1}-A^1-Z^1-B^1-Z^2-A^2-R^2 \quad (I)$$

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, F, I, etc.

Markush检索结果集: 24项专利!



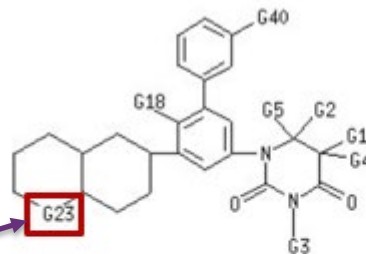
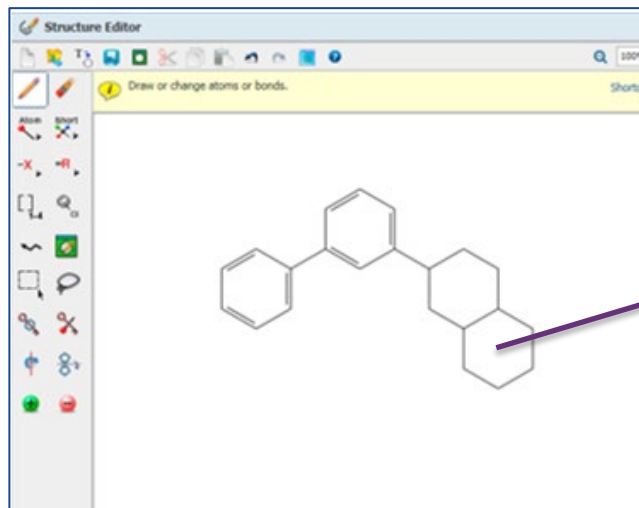
# Markush检索

## 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:

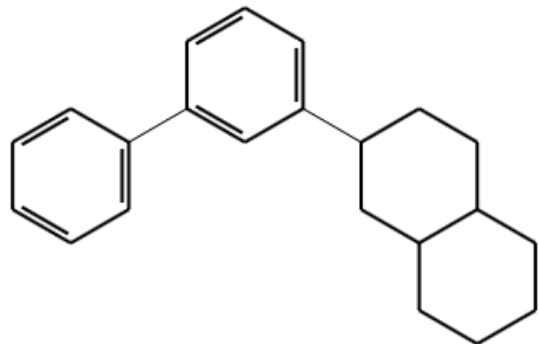
Note:

claim 1

or salts

also incorporates claim 15

## Markush检索



亚结构检索结果集：0

Markush检索结果集：24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 (PatentPak及MethodsNow-ANA的应用)
  - 物质检索
  - Markush检索
  - 反应检索 (MethodsNow-SYN的应用)
  - SciPlanner
- SciFinder常见问题及解决

# SciFinder检索——反应检索

- 反应检索方法

结构式

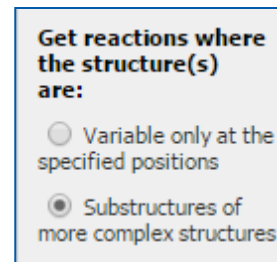
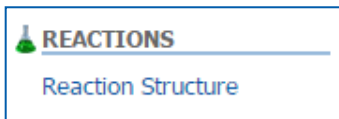
- 常用获取方法

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

The screenshot shows the Structure Editor software interface. The main window is titled "Structure Editor" and contains a toolbar with various drawing tools. Four specific tools are highlighted with purple boxes and Chinese labels:

- 反应箭头** (Reaction Arrow): Points to the reaction arrow tool in the toolbar.
- 反应原子标记工具** (Reaction Atom Marking Tool): Points to the tool that allows marking atoms in a reaction.
- 官能团列表** (Functional Group List): Points to the list of functional groups at the bottom left of the interface.
- 反应位置标记工具** (Reaction Position Marking Tool): Points to the tool that allows marking reaction positions on a structure.

Other visible elements include the "Drawing Editor" panel on the right with radio buttons for "Structure", "Reaction", and "Markush", and a status bar at the bottom showing "16.04".

# SciFinder反应检索——原子和环被锁定

The screenshot shows the SciFinder Structure Editor interface. The main window displays a chemical reaction: nitrobenzene (reactant) is converted to aniline (product). The interface includes a toolbar on the left with various drawing tools, a central workspace for the reaction, and a 'Drawing Editor' panel on the right. In the 'Drawing Editor' panel, the 'Reaction' radio button is selected. Below it, the 'Get reactions where the structure(s) are:' section has two options: 'Variable only at the specified positions' (which is highlighted by a callout box) and 'Substructures of more complex structures'. The callout box contains the Chinese text '原子和环被锁定' (Atoms and rings are locked).

原子和环被锁定



# 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。

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

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

O=[N+]([O-])c1ccc(C)cc1 → Nc1ccc(C)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

# 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

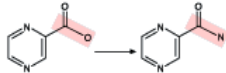
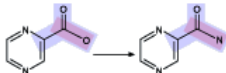
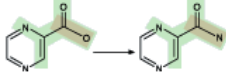
Narrow: 反应中心及扩展的原子和键

### 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)  


# 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

$$\text{Ar-NO}_2 \longrightarrow \begin{array}{c} \text{Ar} \quad \text{Ar} \\ \diagdown \quad / \\ \text{N}=\text{N} \end{array}$$

3. Reduction of Nitro to Azoxy Compounds  
11 Reactions

$$\text{Ar-NO}_2 \longrightarrow \begin{array}{c} \text{O}^- \\ | \\ \text{Ar} \quad \text{Ar} \\ \diagdown \quad / \\ \text{N}^+=\text{N} \end{array}$$

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 search interface for chemical reactions. On the left, a 'Reagents' list is shown with a bar chart indicating the number of reactions for each reagent. A purple box highlights 'NaBH<sub>4</sub>' with a count of 51. An arrow points from this box to the main reaction view. The main view shows a reaction scheme where 4-nitrotoluene is reduced to 4-aminotoluene using NaBH<sub>4</sub> as the reagent. The yield is 100%. Below the reaction, the 'Overview' section lists the reaction conditions: 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. The 'References' section contains a link to a paper: 'Fabrication of Ruthenium Nanoparticles in Porous Organic Polymers: Towards Advanced Heterogeneous Catalytic Nanoreactors'. A purple box highlights this reference, with an arrow pointing to the text '获得文献详情' (Obtain literature details).

Reagent	Count
H <sub>2</sub>	198
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>2</sub> <sup>-</sup>	16
H <sub>2</sub> O	14
N <sub>2</sub> H <sub>4</sub>	14
NaOH	14

**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, 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

# 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  
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

通过C-H活化对苯并噁唑或者恶唑进行烷基化

The screenshot displays the ChemDraw Structure Editor interface. The main window shows a benzimidazole derivative with an R1 group at the 2-position. A purple arrow points from the R1 group in the structure to the R-group definition panel on the right. The R-group definition panel is titled "R-group Definitions" and shows a list of R1 through R10. The R1 definition is set to "O, S". Below this, the "Atoms" section shows a periodic table with the element "S" (Sulfur) highlighted in a purple box. The "Variables" and "Shortcuts" sections are also visible.

Structure Editor

Draw or change atoms or bonds.

R-group Definitions

R1 R2 R3 R4 R5 R6 R7 R8 R9 R10

R1 = O, S

Atoms

H																			He
Li	Be									B	C	N	O	F					Ne
Na	Mg									Al	Si	P	S	Cl	Ar				
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr		
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe		
Cs	Ba		Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn		
Fr	Ra																		
Lanthanides		La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu			
Actinides		Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr			

Variables

Shortcuts

Close

Cancel

Formula is not available

# 亚结构反应检索

The screenshot displays the Structure Editor interface. The main workspace shows a chemical reaction: a benzimidazole derivative with an R1 group and a hydrogen atom at the 2-position (reactant) reacts to form the same derivative with an R1 group and a variable group 'Ak' at the 2-position (product). A purple arrow points from the 'Ak' variable in the product to the 'Variables' dialog box.

**Structure Editor**

Draw or change atoms or bonds. Shortcut Keys

**Drawing Editor:**

- Structure
- Reaction
- Markush

**Variables**

X	Any halogen
M	Any metal
A	Any atom except H
Q	Any atom except C or H
<b>Ak</b>	Any carbon chain
Cy	Any cycle
Cb	Any carbocycle
Hy	Any heterocycle

**Get reactions where the structure(s) are:**

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

Formula is not available

# 亚结构反应检索

The screenshot displays the 'Structure Editor' window. The main workspace shows a chemical reaction: a benzimidazole derivative with an R1 group and a hydrogen atom at the 2-position (labeled 'reactant') reacts to form a benzimidazole derivative with an R1 group and an 'Ak' group at the 2-position (labeled 'product').

On the right side, the 'Drawing Editor' panel has three radio buttons: 'Structure', 'Reaction' (which is selected), and 'Markush'. Below this, the section 'Get reactions where the structure(s) are:' contains two radio buttons: 'Variable only at the specified positions' and 'Substructures of more complex structures' (which is selected and highlighted with a purple box).

At the bottom of the window, there is a search bar containing 'Ak', a list of elements (C, H, O, S, N, P, Cl, Br, F, I, Si), and a 'Formula is not available' message.



# 通过后处理工具筛选反应——Analyze

通过催化剂筛选反应

The screenshot displays the 'Analyze' interface in Reaxys. On the left, a list of catalysts is shown with their respective counts:

Catalyst	Count
CuI	28
312696-09-6	17
AgNO <sub>3</sub>	17
(MeOCH <sub>2</sub> CH <sub>2</sub> ) <sub>2</sub> O	16
NaI	15
1905414-33-6	14
CoBr <sub>2</sub>	11
Me <sub>2</sub> SiCH <sub>2</sub> MgCl	10
Ph <sub>2</sub> P(CH <sub>2</sub> ) <sub>3</sub> PPh <sub>2</sub>	10
658062-48-7	9

The 'Analyze by:' dropdown menu is set to 'Catalyst'. A purple box highlights this dropdown, with an arrow pointing to the text '通过催化剂筛选反应'. The 'Group by:' dropdown is set to 'Document', and 'Sort by:' is set to 'Accession Number'. The main view shows a reaction scheme for the synthesis of a fluorinated benzothiazole derivative. The reaction involves a long-chain alkyl iodide and a fluorinated benzothiazole derivative, yielding the product in 83% yield. Below the reaction scheme, the 'Overview' section lists the steps/stages:

- 1.1 R:LiO-Bu-*t*, C:1905414-33-6, S:Dioxane, 16 h, 100°C
- 1.2 S:H<sub>2</sub>O, rt
- 1.3 R:HCl, S:H<sub>2</sub>O, neutralized

The 'Notes' section contains the following text: 'catalyst prepared and used, screw cap tube used, Reactants: 2, Reagents: 2, Catalysts: 1, Solvents: one step: 3'. The 'References' section is currently empty.

# 通过后处理工具筛选反应--Analyze

CAS Solutions  
SCIFINDER  
A CAS SOLUTION

Preferences | SciFinder Help | Sign Out

Welcome Helen Zhu

Explore | Saved Search | **筛选出有实验步骤的反应** | Save | Print | Export

Reaction Structure substructure with limiters > reactions (282)

REACTIONS

Send to SciPlanner

Analyze Refine

Analyze by:

Group by: No Grouping Sort by: Accession Number

0 of 282 Reactions Selected

1. View Reaction Detail

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

C[CH-](F)(F)F.[K+].BrC1=CC=C2N=CN=C21>>CC(C)C1=CC=C2N=CN=C2S1

~76  ~108  78%

Overview

2. View Reaction Detail

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

# 通过后处理工具筛选反应--Analyze

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

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

**Overview**

**METHODS NOW™**

**Procedure**

1. Add one equivalent of indole, 3 equivalents of benzothiazole to a Chemglass vial.
2. Purge the vial for 5 minutes under vacuum.

[View more...](#)

**Available Experimental Data**

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

[View with MethodsNow](#)

**MethodsNow**

**C-H Functionalization of Heteroarenes Using Unactivated Alkyl Halides through Visible-Light Photoredox Catalysis under Basic Conditions**

By Bissonnette, Noah B.; Boyd, Michael J.; May, Gregory D.; Giroux, Simon; Nuhant, Philippe  
 From Journal of Organic Chemistry, 83(18), 10933-10940, 2018  
 Published by American Chemical Society

<b>Products</b>	2-(1-Methylethyl)benzothiazole, 72%, CAS RN: 17626-86-7
<b>Reactants</b>	Isopropyl iodide, CAS RN: 75-30-9 Benzothiazole, CAS RN: 95-16-9
<b>Reagents</b>	2,2,6,6-Tetramethylpiperidine, CAS RN: 768-66-1
<b>Catalysts</b>	Iridium(III), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine-κ <sup>N,N'</sup> ][bis(2-(2-pyridinyl)-κ <sup>N</sup> phenyl)-hexafluorophosphate(1-)](1:1), CAS RN: 676525-77-2

<b>Solvents</b>	Methanol, CAS RN: 67-56-1
<b>Procedure</b>	<ol style="list-style-type: none"> <li>1. Add one equivalent of indole, 3 equivalents of benzothiazole and 2.5 mol % of [Ir(ppy)<sub>3</sub>]/(dtbbpy)]PF<sub>6</sub> to a vial (1 dram, ~3.7 mL), 15 × 45 mm, 13-425 thread with red pressure relief cap Chemglass vial.</li> <li>2. Purge the vial for 5 minutes under vacuum.</li> <li>3. Fill the vial with nitrogen gas.</li> <li>4. Add MeOH (0.5 mL), 3.1 equivalents of Et<sub>3</sub>N and 1 equivalent of indole to the reaction mixture under N<sub>2</sub> atmosphere.</li> <li>5. Remove the nitrogen line.</li> <li>6. Add 3 equivalents of benzothiazole to the reaction mixture.</li> <li>7. Irradiate the vial under blue LED light.</li> <li>8. Stir the reaction mixture overnight at room temperature at 1000 rpm with a small cooling fan (approximately 16 hours).</li> <li>9. After the completion of the reaction, add 0.25 equivalent of 1,4-dinitrobenzene to the vial.</li> <li>10. Evaporate the volatiles using a V10 Biotage system.</li> <li>11. Load the crude mixture onto a 40 g ISCO column using hexane/ethyl acetate (100:0 to 0:100) as eluents.</li> </ol>
<b>Transformation</b>	Friedel-Crafts Alkylation
<b><sup>1</sup>H NMR</b>	(400 MHz, chloroform-d) δ 7.98 (dd, <i>J</i> = 8.2, 1.2 Hz, 1H), 7.85 (dd, <i>J</i> = 8.0, 1.3 Hz, 1H), 7.45 (ddd, <i>J</i> = 8.3, 7.2, 1.3 Hz, 1H), 7.34 (ddd, <i>J</i> = 8.3, 7.3, 1.2 Hz, 1H), 3.43 (hept, <i>J</i> = 6.9 Hz, 1H), 1.48 (d, <i>J</i> = 6.9 Hz, 6H).
<b><sup>13</sup>C NMR</b>	(101 MHz, chloroform-d) δ 178.7, 153.3, 134.8, 126.0, 124.7, 122.7, 121.7, 34.2, 23.1 (2C).
<b>HRMS</b>	(ESI), m/z: calcd for C <sub>10</sub> H <sub>12</sub> NS[M + H] <sup>+</sup> : 178.0690, found: 178.0687.
<b>CAS Method Number</b>	3-085-CAS-19169886

# 提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
  - 文献检索 (PatentPak及MethodsNow-ANA的应用)
  - 物质检索
  - Markush检索
  - 反应检索 (MethodsNow-SYN的应用)
  - **SciPlanner**
- SciFinder常见问题及解决

# 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

~192 [Step 2.1] ~72

▼ 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**

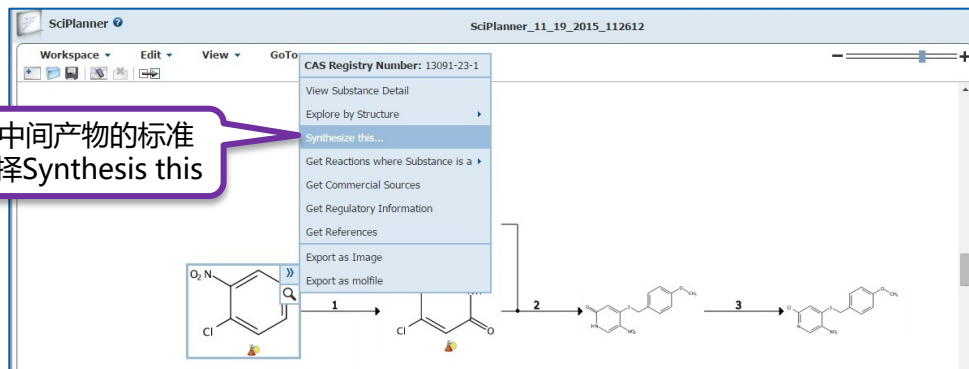
Syntheses of 4- and 6-substituted thiazolo[4,5-c]pyridines

3. 进入SciPlanner 新建文件

4. 将刚推送过来的反应拖至编辑面板

# SciPlanner使用简介

5. 打开中间产物的标准菜单选择Synthesize this



6. 在检索到的反应中选择感兴趣的反应

Get References Tools

Send selected records to SciPlanner. Send to SciPlanner

Group by: No Grouping Sort by: Accession Number

1 of 34 Reactions Selected

1. View Reaction Detail

2 Steps Hover over any structure for more options.

HO

~161

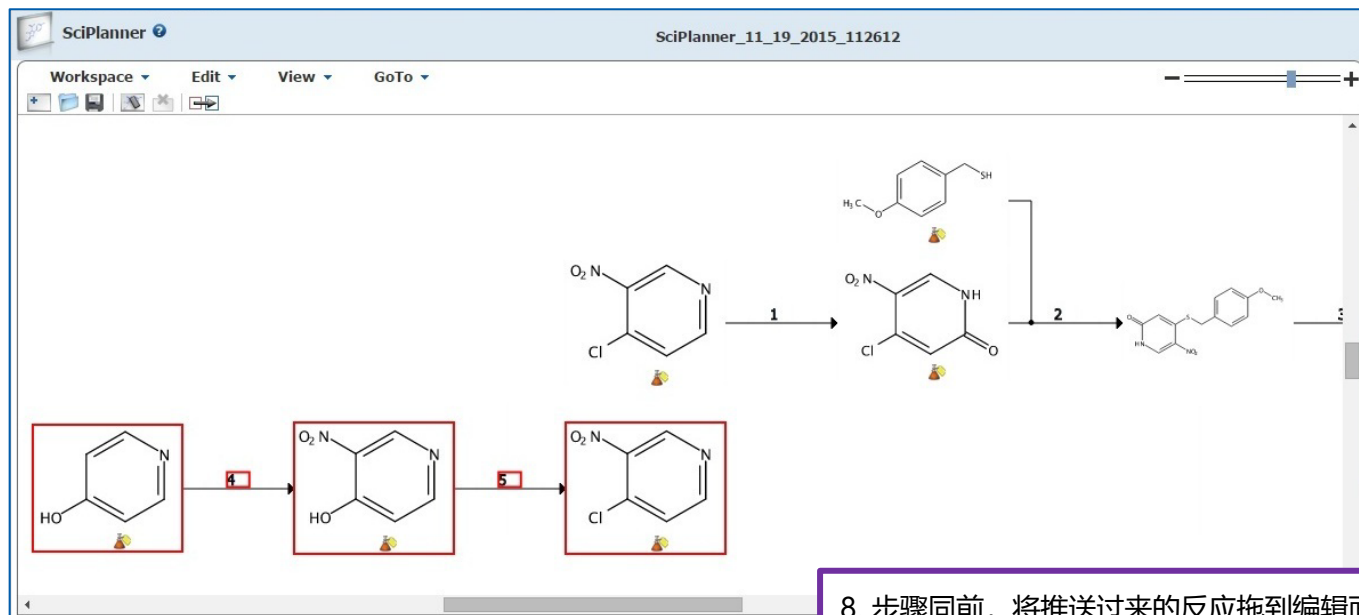
O<sub>2</sub>N

Cl

~192

7. 继续推送到SciPlanner

# SciPlanner使用简介



# SciPlanner使用简介

The screenshot displays the SciPlanner software interface with a chemical reaction workflow and an export dialog box. The workflow consists of four chemical structures connected by arrows labeled 4, 5, 1, and 2. Structure 1 is a pyridine ring with a nitro group and a hydroxyl group. Structure 2 is a pyridine ring with a nitro group and a chlorine atom. Structure 3 is a pyridine ring with a nitro group and a chlorine atom, and a hydroxyl group. Structure 4 is a pyridine ring with a nitro group and a chlorine atom, and an amide group. The export dialog box is open, showing options for offline review and saving locally. The 'Export' button is highlighted.

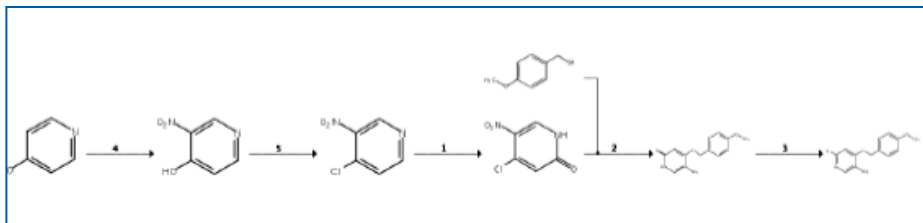
10. 点击 Workspace, 选择Export 导出结果

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



# SciPlanner导出结果



Reaction	Stages	Notes	Yield
5	1.1 R:POCl <sub>3</sub> , S:PhMe, 0°C → rt, 16 h, rt → 110°C 1.2 R:K <sub>2</sub> CO <sub>3</sub> , S:H <sub>2</sub> O, cooled, pH 10	<b>Reactants:</b> 1, <b>Reagents:</b> 2, <b>Solvents:</b> 2, <b>Steps:</b> 1, <b>Stages:</b> 2  <b>Transformation:</b> 1. Formation of Alkyl Halides from Alcohols	<b>90%</b>
<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 Poloek, Anurach et al From Journal of Materials Chemistry C: Materials for Optical and Electronic Devices, 2(48), 10343-10356; 2014			

Substance Information		
<b>1228150-22-8</b>  C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> O <sub>5</sub> S 2-(1-(4-methoxyphenyl)methylthio)-5-nitro-2(1H)-pyridone <b>Related Info:</b> ~ 2 References Reactions	<b>1228150-23-9</b>  C <sub>12</sub> H <sub>11</sub> ClN <sub>3</sub> O <sub>5</sub> S Pyridine, 2-(chloro-4-nitro-methoxyphenyl)methylthio-5-nitro- <b>Related Info:</b> ~ 2 References Reactions	<b>13091-23-1</b>  C <sub>5</sub> H <sub>3</sub> ClN <sub>2</sub> O <sub>2</sub> Pyridine, 4-nitro-3-nitro- <b>Related Info:</b> ~ 361 References Reactions ~ 100 Commercial Sources Regulatory Information
<b>5435-54-1</b>  C <sub>5</sub> H <sub>4</sub> N <sub>2</sub> O 4-Pyridinol, 3-nitro- <b>Related Info:</b> ~ 115 References Reactions ~ 167 Commercial Sources Regulatory Information	<b>6258-66-2</b>  C <sub>7</sub> H <sub>10</sub> O <sub>2</sub> S Benzenemethanethiol, 4-methoxy- <b>Related Info:</b> ~ 749 References Reactions ~ 71 Commercial Sources Regulatory Information	<b>626-44-2</b>  C <sub>5</sub> H <sub>4</sub> N <sub>2</sub> O 4-Pyridinol <b>Related Info:</b> ~ 1551 References Reactions ~ 100 Commercial Sources Regulatory Information
<b>850663-54-6</b>  C <sub>12</sub> H <sub>7</sub> ClN <sub>3</sub> O <sub>5</sub> 2-(1-(4-chloro-5-nitro- <b>Related Info:</b> ~ 22 References Reactions ~ 136 Commercial Sources		



**CAS**  
 A DIVISION OF THE  
 AMERICAN CHEMICAL SOCIETY

# 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

## 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 form, divided 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--**: Includes input fields for Username (with a '7ps' character count indicator), Password, and Re-enter Password.
- SECURITY INFORMATION--**: Includes a dropdown menu for 'Security Question' (set to 'Select one') and an 'Answer' input field (with a 'Why?' character count indicator).

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

请注意:

1. 必须输入真实姓名和**学校**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) 。

- 登录学校图书馆网站找到SciFinder数据库说明页，按照提示进行注册

# 如何获取SciFinder账号



## Registration Already Complete

You have already completed your registration. For assistance with accessing SciFinder, consult the key contact for your organization.

点击激活链接后注册成功。

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

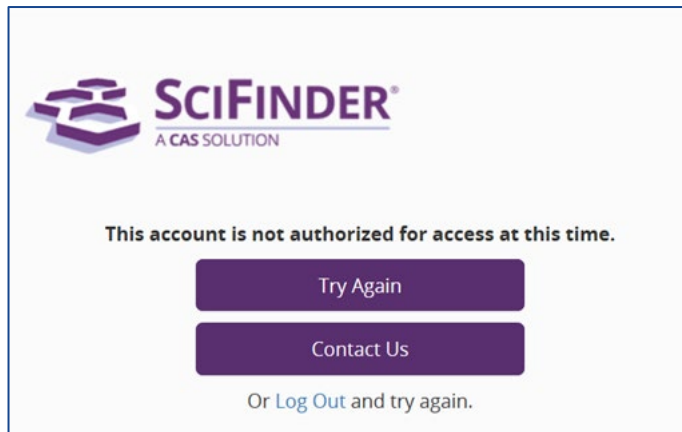
# SciFinder常见问题

## Unauthorized IP Address

User registration is available only from IP addresses specified by the key contact at your organization. Please try to register again from an authorized location.

- 检查注册链接是否正确
- 确认连入校园网，且不是通过VPN连接
- 如果链接正确，且在校园网内，请联系图书馆或[china@acs-i.org](mailto:china@acs-i.org)

# 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](mailto:china@acs-i.org)



更多培训资料请访问

<https://www.cas.org/support/training/scifinder>

# 谢谢!



欢迎联系:

美国艾赛思国际有限公司北京代表处  
ACS International Ltd Beijing Rep Office

[china@acs-i.org](mailto:china@acs-i.org)

[www.cas.org](http://www.cas.org)

