

朱传娴

客户顾问

hzhu@acs-i.org

# 如何使用SciFinder获取医药信息

湖北医药学院

2019.6.4



# 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

# 美国化学文摘社—Chemical Abstracts Service

- ACS的分支机构
- 创建于1907年，简称“CAS”
- 最早创立了《化学文摘》
- 密切关注，索引和提炼着全球化学相关的文献和专利
- 总部座落于俄亥俄州的哥伦布市



# CAS数据库——源于化学，超越化学

## 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

# SciFinder覆盖的数据库



# CAS数据库最具价值的内容——人工索引


## 4. Process for preparation of novel sofosbuvir crystal

By: Zhou, Haohui; Lin, Guoliang; Wu, Yao; Zou, Wenjuan; Chan, Yunxia

Assignee: Beijing Winsunny Pharmaceutical Co., Ltd., Peop. Rep. China

The invention relates to a novel sofosbuvir crystal having high stability and soly. The novel sofosbuvir crystal is prepd. through crystg. sofosbuvir in pos. solvent and neg. solvent. The method has high repeatability, easy control, high yield, and high product purity.

### Patent Information

Patent No.	Kind	Language	Date	Application No.	Date
CN 105732751  PATENTPAK	A		Jul 6, 2016	CN 2014-10742897	Dec 9, 2014

### Priority Application

CN 2014-10742897	Dec 9, 2014
------------------	-------------

### Indexing


Carbohydrates (Section33-9)

Section cross-reference(s): 34, 63

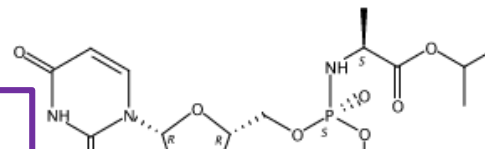
### Concepts

Crystallization	Drug bioavailability
Hepatitis C	Hepatitis C virus
Homo sapiens	Human
Pharmaceutical coated tablets	

### Substances

**1190307-88-0P Sofosbuvir**   
Absolute stereochemistry.

Page 2 in **PATENTPAK**



### Tips:

1. 98%以上的文献，都经过人工索引
2. 用Index Term标引文献中的重要技术术语
3. 用CAS RN标引出文献中的重要物质
4. 用CAS Role标引文献中重要物质的研究领域

# CAS人工标引解决的问题

- 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很好的解决了该问题，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。

# 提纲

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- 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登录网址: <https://scifinder.cas.org/>

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SciFinder® is a research discovery application that provides integrated access to the world's most comprehensive and authoritative source of references, substances and reactions in chemistry and related sciences.

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### News & Updates

**Welcome to SciFinder**

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Our new branding will also be phased into training and other support materials in the coming months. If you are a Key Contact and have questions, or need assistance updating logos on any of your organization's websites, please contact the [CAS Customer Center](#).

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**Introducing the PatentPak Interactive Patent Chemistry Viewer**  
The new [PatentPak interactive patent chemistry viewer](#) significantly reduces the time spent locating the important chemistry in a patent by using CAS scientists' direct links to key substances in the source patent.

**New Commercial Source Logos**

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9

# SciFinder主界面

检索完，请点击退出

工具栏

The screenshot shows the SciFinder web interface. At the top, there is a header bar with the SciFinder logo and navigation links like 'Explore', 'Saved Searches', and 'SciPlanner'. A search bar is prominently displayed in the center. To the left, a sidebar lists various search categories: REFERENCES, SUBSTANCES, and REACTIONS. On the right, there is a section for 'SAVED ANSWER SETS' showing a list of previously saved searches. The interface is annotated with several callouts in Chinese:

- 检索完，请点击退出**: A callout pointing to the 'Sign Out' button in the top right corner.
- 工具栏**: A callout pointing to the top navigation bar containing 'Explore', 'Saved Searches', and 'SciPlanner'.
- 检索入口**: A callout pointing to the main search input field.
- 已保存的结果集**: A callout pointing to the 'SAVED ANSWER SETS' list on the right.
- 定题追踪**: A callout pointing to the 'KEEP ME POSTED' section on the right.

**REFERENCES: RESEARCH TOPIC**

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

**Search**

[Advanced Search](#)

**REFERENCES**

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

**SUBSTANCES**

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

**REACTIONS**

- Reaction Structure

**SAVED ANSWER SETS**

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

[View All](#) | [Import](#)

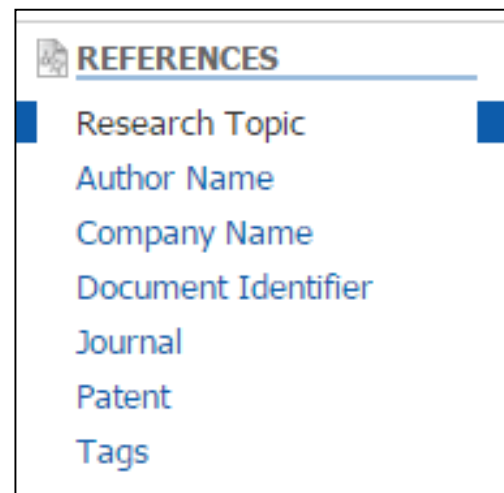
**KEEP ME POSTED**

You have no promises.  
Learn how to:  
[Create Keep Me Posted](#)

# 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：中药在白内障治疗中的应用

检索式：Chinese Medicine in Cataract

The screenshot displays the SciFinder web interface. At the top, there is a navigation bar with 'CAS Solutions' and the SciFinder logo. Below this is a menu with 'Explore', 'Saved Searches', and 'SciPlanner'. The left sidebar contains two main sections: 'REFERENCES' and 'SUBSTANCES'. Under 'REFERENCES', there are links for 'Research Topic', 'Author Name', 'Company Name', 'Document Identifier', 'Journal', 'Patent', and 'Tags'. Under 'SUBSTANCES', there are links for 'Chemical Structure' and 'Markush'. The main content area is titled 'REFERENCES: RESEARCH TOPIC' and features a search input field containing the text 'Chinese Medicine in Cataract'. Below the input field, there are 'Examples:' such as 'The effect of antibiotic residues on dairy products' and 'Photocyanation of aromatic compounds'. A prominent blue 'Search' button is located below the examples. At the bottom of the main 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 Cataract"

## REFERENCES ?

Select All Deselect All

1 of 5 Research Topic Candidates Selected

	References
<input type="checkbox"/> 37 references were found containing "Chinese Medicine in Cataract" as entered	37
<input checked="" type="checkbox"/> 323 references were found containing the two concepts "Chinese Medicine" and "Cataract" closely associated with one another.	323
<input type="checkbox"/> 464 references were found where the two concepts "Chinese Medicine" and "Cataract" were present anywhere in the reference	464
<input type="checkbox"/> 308536 references were found containing the concept "Chinese Medicine".	308536
<input type="checkbox"/> 86644 references were found containing the concept "Cataract".	86644

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

CAS Solutions

**SCIFINDER**  
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Preferences | SciFinder Help | Sign Out

Welcome Helen Zhu

Explore | Saved Searches | SciPlanner | Save | Print | Export

Research Topic "Chinese Medicine in Cataract" > references (322)

**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

Analyze by: Author Name

Li Jun 6

Name Not Translated 4

Ye Mingwei 4

Zhang Xiuhua 4

Li Shunguang 3

Li Xianqiang 3

Qin Zhengqiang 3

Wang Weilin 3

1. **Characterization effects and mechanism of Radix Angelicae dahuricae extracts on baicalin in Radix Scutellariae using in vivo and in vitro**

Quick View | Other Sources

By Liang Xin-Li; Liao Zheng-Gen; Zhu Jing-Yun; Zhao Guo-Wei; Yang Ming; Yin Rong-Li; Cao Yun-Chao; Zhang Jing; Zhao Li-Jun  
From Journal of ethnopharmacology (2012), 139(1), 52-7. | Language: English, Database: MEDLINE

ETHNOPHARMACOLOGICAL RELEVANCE: Angelicae Dahurica(Hoffm.)Benth.&Hook.f.ex Franch.&Sav combined with Scutellaria baicalensis Georgi. has been widely used as herb-pairs in traditional **Chinese medicine** (TCM) to treat migraine headache and **cataract**, but the underlying compatibility mechanism of the two herbs remains unknown. AIM OF STUDY: In the present work, we investigated the additive or synergistic effects of absorption behavior of Radix Angelicae dahuricae extracts on baicalin, and the absorption-enhancing mechanism of Radix Angelicae dahuricae extracts on baicalin. MATERIALS AND METHODS...

2. **Identification of a PRX variant in a Chinese family with congenital cataract by exome sequencing**

Quick View | Other Sources

By Yuan, L.; Yi, J.; Lin, Q.; Xu, H.; Deng, X.; Xiong, W.; Xiao, J.; Jiang, C.; Yuan, X.; Chen, Y.; et al  
From QJM (2016), 109(11), 731-735. | Language: English, Database: CAPLUS

Background: Congenital **cataract** is a common cause of childhood **vision** impairment or blindness with genetic and clin. heterogeneity. The aim of this study was to identify the disease-assocd. gene in a **Chinese** family with congenital **cataract**. Methods: A four-generation **Chinese** family with three enrolled patients suffering from congenital **cataract** was studied. Detailed family history and clin. data of all the members were collected and recorded. Exome sequencing was applied in the proband to screen potential genetic variants, and then Sanger sequencing was used to verify the variant within th...

Citing Reference: 帮助找到最重要的文献

# 文献检索结果

CAS Solutions

**SCIFINDER**  
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Preferences | SciFinder Help | Sign Out

Welcome Helen Zhu

Explore | Saved Searches | SciPlanner

Save | Print | Export

Research Topic "Chinese Medicine in Cataract" > **文献分析工具**

**REFERENCES** ?

Get Substances | Get Reactions | Get Related Citations | Tools

Create Keep Me Posted Alert | Send to SciPlanner

Display Options

Sort by: Citing References

0 of 322 References Selected

**Analyze** | Refine | Categorize

Analyze by: Author Name

Author	Count
Li Jun	6
Name Not Translated	4
Ye Mingwei	4
Zhang Xiuhua	4
Li Shunguang	3
Li Xianqiang	3
Qin Zhengqiang	3
Wang Weilin	3
Yan Huiwei	2

**获取原文**

1. **The absorption characterization effects and mechanism of Radix Angelicae dahuricae extracts on baicalin in Radix Scutellariae using in vivo and in vitro absorption models**

Quick View | **Other Sources**

By Liang Xin-Li; Liao Zheng-Gen; Zhu Jing-Yun; Zhao Guo-Wei; Yang Ming; Yin Rong-Li; Cao Yun-Chao; Zhang Jing; Zhao Li-Jun  
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Quick View | **Other Sources**

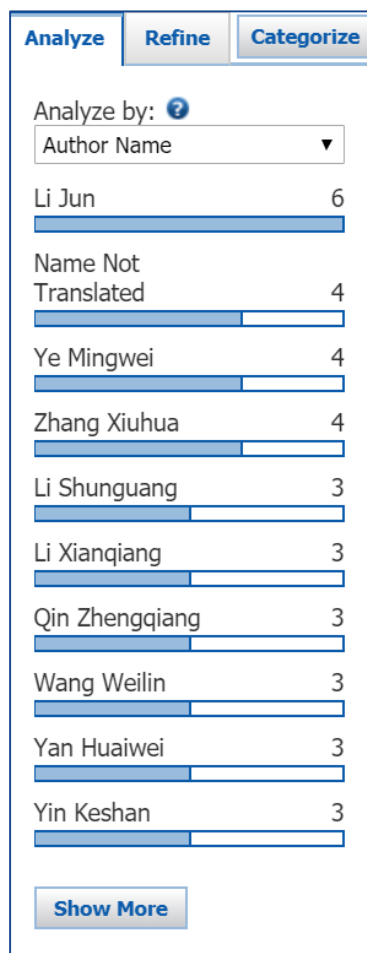
By Yuan, L.; Yi, J.; Lin, Q.; Xu, H.; Deng, X.; Xiong, W.; Xiao, J.; Jiang, C.; Yuan, X.; Chen, Y.; et al  
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SciFinder提供强大的文献处理工具，帮助处理文献

# 文献检索结果的Analyze

## 本领域研究人员



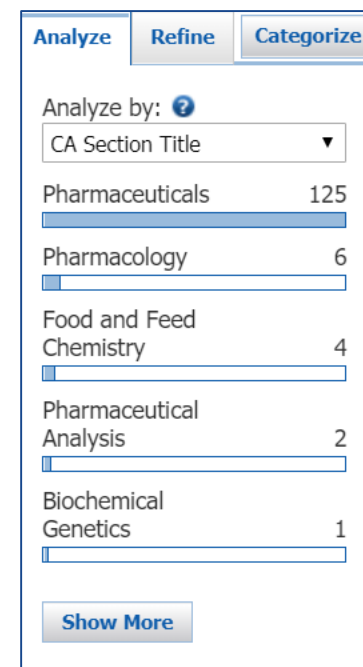
## 本领域研究机构、合作伙伴、竞争对手



## 期刊



## 涉及学科领域

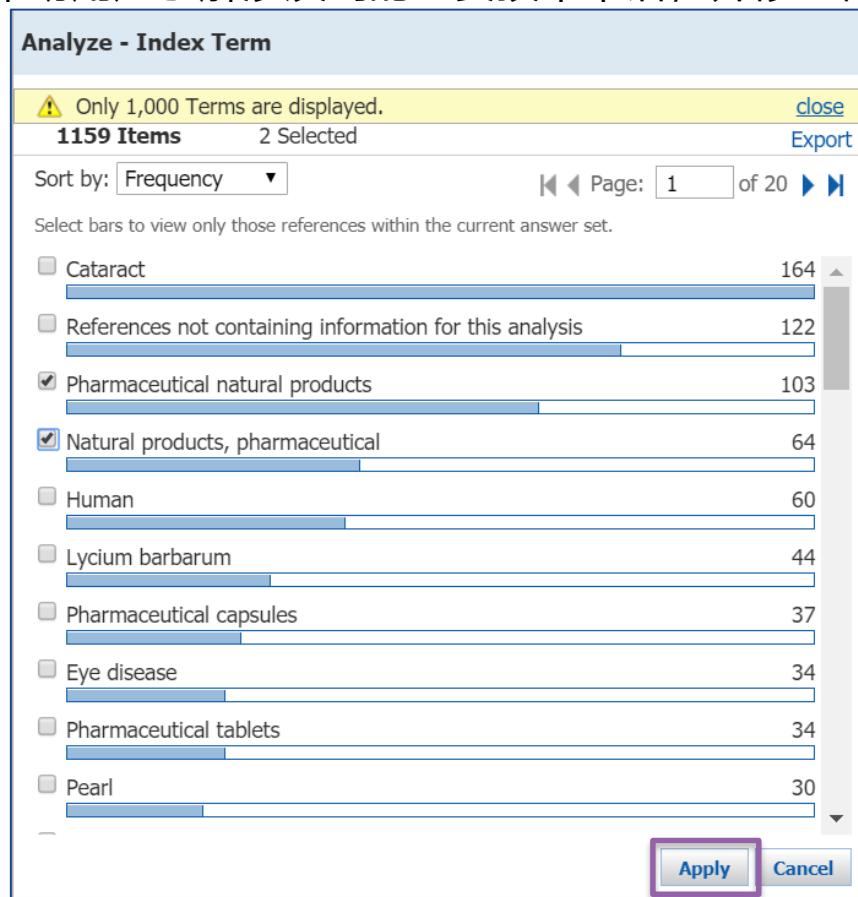
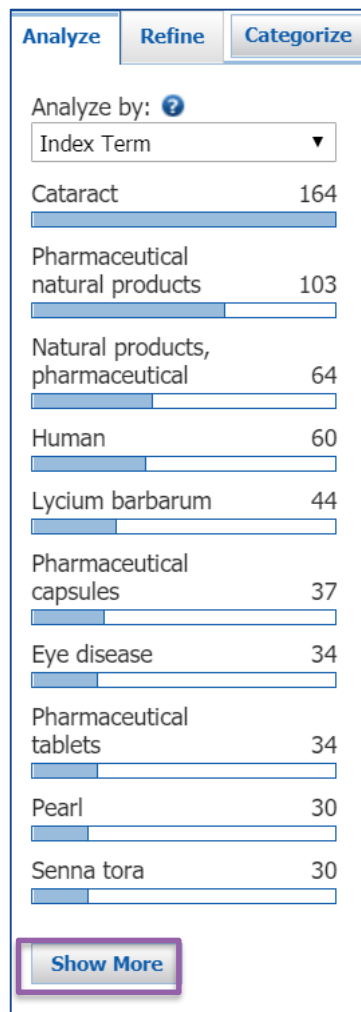




# 文献检索结果的Analyze

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



# 文献检索结果的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

Create Keep Me Posted Alert

Send to SciPlanner

Sort by: Citing References

Display Options

☐ 0 of 2 References Selected

☐ 1. Research progress in improving effect of Fructus Lycii on eyesight

Quick View

Other Sources

By Wang, Zhong-zhong; Lu, Xiao-li; Zhang, Zi-ping  
From Zhongguo Xinyao Zazhi (2013), 22(14), 1648-1651. | Language: Chinese, Database: CAPLUS

A review. As a precious traditional **Chinese medicine**, Fructus Lycii (Medlar) not only has several pharmacol. actions such as antioxidant, anti-aging, antitumor, lowering blood pressure, immunomodulative effects, but also has properties preventing age-related macular, diabetic retinopathy, senile **cataract**, glaucoma and other ophthalmic diseases. To provide consult and ref. for further research on this topic, we summarized the latest research progress in the improving effect of Fructus Lycii on eyesight in this review.

☐ 2. Research advances in drug treatment for cataract

Quick View

Other Sources

By Wang, Yan  
From Zhonghua Zhongxueyi Zazhi (2006), 7(6), 505-507. | Language: Chinese, Database: CAPLUS

A review. The research advances in drug treatment for **cataract** were introduced with several subsections as follow, inorg. ion, preps. contg. sulfur, anti-quinone preps., inhibitors of aldose reductase (AR), vitamins and energy mixts., non-steroidal antiinflammatory drugs, **Chinese** herbal **medicine**, other drugs, and prospect in the future.

Refine: 帮助用户迅速获得需要的文献

# 文献检索结果的Categorize

学科领域  
主分类

学科领域  
副分类

Index Term

选中的Index Term

**Categorize** ?

1. Select a heading and category.

Category Heading	Category
All	<b>Medicine (120)</b>
General chemistry	Substances in medicine (215)
Genetics & protein chemistry	Food (92)
Physical chemistry	Substances in food chemistry (25)
Polymer chemistry	Agriculture (7)
<b>Biotechnology</b>	Substances in biological uses (25)
Biology	Substances in adverse effects (14)
Technology	Toxicology & forensics (4)
Environmental chemistry	
Analytical chemistry	
Catalysis	

2. Select index terms of interest.

Index Terms	
Page: 1 of 2	
<a href="#">Select All</a> <a href="#">Deselect All</a>	
capsules	
<input type="checkbox"/> Pharmaceutical tablets	34
<input type="checkbox"/> Ethanol	22
<input type="checkbox"/> Ophthalmic solutions	21
<input checked="" type="checkbox"/> Salvia miltiorrhiza	20
<input type="checkbox"/> Pharmaceutical decoctions	18
<input type="checkbox"/> Pharmaceutical granules	18
<input type="checkbox"/> Ophthalmic drug delivery systems	16
<input type="checkbox"/> Pharmaceutical powders	15
<input checked="" type="checkbox"/> Alisma orientale	12
<input type="checkbox"/> Chinese medicine	12
<input type="checkbox"/> Pharmaceutical solutions	11

**Selected Terms**

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

**Biotechnology > Medicine (2 Terms)**

Biotechnology > Medicine > 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。

# 结果集的保存— Save, Print, Export

Searches ▾ SciPlanner Save Print Export

In Cataract\* > references (322) > refine by categories > Chinese medicine compound eye ...

Get Substances Get Reactions Get Related Citations Tools

Sort by: Accession Number

0 of 29 References Selected

1. Chinese medicine compound eye drop for auxiliary treatment of cataract and preparation method thereof  
PATENTPAK  
By Jiang, Jie; Mai, Liyi  
From Faming Zhuanli Shenqing (2019), CN 109745423 A 20190514. | Language: Chinese, Database: CAPLUS  
The invention belongs to Chinese medicine field, and discloses compd. eye drop for auxiliary treatment of cataract and prepn. method thereof. The effective components of the compd. eye drop comprise Moschus moschiferus, Ursus arctos bile powder, pearl powder, borneol, Laminaria japonica thallus and/or Ecklonia kurome thallus, Salvia miltiorrhiza, and Dioscorea opposita. The compd. eye drop is prepd. from the effective components and pharmaceutically acceptable auxiliary material by pharmaceutically acceptable method. The inventive compd. eye drop has reasonable formula, can alleviate symptoms such...

2. Chinese medicine composition for the prevention and treatment of eye diseases  
PATENTPAK  
By Ju, Jianbo; Wu, Chao; Han, Xiaoling; Qu, Xiaojuan  
From Faming Zhuanli Shenqing (2018), CN 108992544 A 20181214. | Language: Chinese, Database: CAPLUS  
The Chinese medicine compn. for the prevention and treatment of eye diseases has the advantages of less toxic side effects, controllable quality and relieving visual fatigue. The Chinese medicine compn. for the prevention and treatment of eye diseases includes component A and component B; wherein, Component A includes the following ingredients by mass parts: Fructus Tribuli: 6-10 parts, Radix Salviae Miltiorrhizae: 3-10g, Radix Astragali: 9-15g, Flos Chrysanthemi: 5-10 parts, Semen Cassiae: 9-15 parts, Fructus Lycii: 6-12 parts, Fructus Mori: 5-10 parts, Pericarpium Citri Reticulatae: 3-10 pa...

3. Composition for eyesight and eye protection comprising traditional Chinese medicine and modern new functional food raw materials  
PATENTPAK  
By Han, Xiaoling; Ju, Jianbo; Qu, Xiaojuan; Wu, Chao  
From Faming Zhuanli Shenqing (2018), CN 108886682 A 20181127. | Language: Chinese, Database: CAPLUS  
An environmental-friendly compn. for eyesight and eye protection having the ability to alleviate visual fatigue and other eye diseases caused by depression, phlegm, fire, gas, and imaginary, preventing vision loss and blindness caused by age-related retinal macular degeneration, and repairing of the optic nerve is provided. The compn. comprises the following raw materials in parts by wt.: 6-10 of Tribulus terrestris, 3-10 of Salvia miltiorrhiza, 9-15 of Taraxacum mongolicum, 5-10 of Chrysanthemum, 9-15 of Senna obtusifolia, 6-12 of wolfberry, 5-10 of mulberry, 3-10 of Citrus reticulata, 0.003...

Save: 保存在服务器上, 方便以后登陆查看, 每次可存1万条记录。

Export: 导出至本地电脑。

Print: 打印成PDF格式

文献详细信息

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

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

Export

\* Required

Export:

☒ All  
☐ Selected  
☐ Range

Example: 2-20

For:

Citation Manager

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

Offline review

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

Saving locally

☐ Answer Key eXchange (\*.alox)

Details:

File Name: \*

Reference\_06\_19\_2012\_100848

Format:

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

Include:

☐ Task History  
☐ Tags  
☐ Comments

Export Cancel

# 文献信息—题录、摘要、索引

## 2. Chinese medicine composition for the prevention and treatment of eye diseases

By: Ju, Jianbo; Wu, Chao; Han, Xiaoling; Qu, Xiaojuan  
Assignee: Xi'an Libang Pharmaceutical Co., Ltd., Peop. Rep. China

The Chinese medicine compn. for the prevention and treatment of eye diseases has the advantages of less toxic side effects, controllable quality and relieving visual fatigue. The Chinese medicine compn. for the prevention and treatment of eye diseases includes component A and component B; wherein, Component A includes the following ingredients by mass parts: Fructus Tribuli: 6-10 parts, Radix Salviae Miltiorrhizae: 3-10g, Radix Astragali: 9-15g, Flos Chrysanthemi: 5-10 parts, Semen Cassiae: 9-15 parts, Fructus Lycii: 6-12 parts, Fructus Mori: 5-10 parts, Pericarpium Citri Reticulatae: 3-10 parts, Xanthophyll: 0.003-0.012 part, Acer truncatum Bunge seed oil: 1-3 parts, zeaxanthin: 0.001-0.0044 part, milk: 20-50 parts, egg liq.: 5-20 parts, and plant juice: 2-5 parts.

### Patent Information

Patent No.	PatentPak Options	Kind	Language	Date	Application No.	Date
CN 108992544	<a href="#">PDF</a>   <a href="#">PDF+</a>   <a href="#">Viewer</a>	A		Dec 14, 2018	CN 2018-11062718	Sep 12, 2018

### Priority Application

CN 2018-11062718	Sep 12, 2018
------------------	--------------

### Indexing

Pharmaceutical (Chemical)

#### Concepts

重要概念

Pharmaceutical natural products

Chaihu; Chinese medicine compn. for the prevention and treatment of eye diseases

Acer truncatum  
Asthenopia

Adenophora  
Buddleja

文献详情界面包括:

1. 标题
2. 摘要
3. 文献中重要的技术术语
4. 文献中重要的物质
5. 书目信息
6. 获得文献中的物质, 反应
7. 参考文献
8. 链接原文

#### Substances

重要物质

557-04-0 Magnesium stearate	Page 7 in <a href="#">PATENTPAK</a>
9004-32-4 Sodium carboxymethylcellulose	Page 7 in <a href="#">PATENTPAK</a>
9004-53-9 Dextrin	Page 8 in <a href="#">PATENTPAK</a>
9004-61-9 Hyaluronic acid	Page 7 in <a href="#">PATENTPAK</a>
9063-38-1 Sodium Carboxymethyl starch	Page 7 in <a href="#">PATENTPAK</a>

Chinese medicine compn. for the prevention and treatment of eye diseases

Modifier or additive use; Therapeutic use; Biological study; Uses

472-70-8 Cryptoxanthin	Page 2 in <a href="#">PATENTPAK</a>
507-70-0	Page 2 in <a href="#">PATENTPAK</a>
1309-38-2 Magnetitum, biological studies	Page 2 in <a href="#">PATENTPAK</a>
7235-40-7 $\beta$ -Carotene	Page 2 in <a href="#">PATENTPAK</a>
11103-57-4 Vitamin A	Page 2 in <a href="#">PATENTPAK</a>

### QUICK LINKS

0 Tags, 0 Comments

### PATENT INFORMATION

Dec 14, 2018  
CN 108992544  
A

### APPLICATION

Sep 12, 2018  
CN 2018-11062718

### PRIORITY

Sep 12, 2018  
CN 2018-11062718

### SOURCE

Faming Zhuanli Shenqing  
16pp.  
Patent  
2018  
CODEN:CNXXEV

### ACCESSION NUMBER

2018:2488106  
CAN170:140195  
CAPLUS

### LANGUAGE

Chinese

# 文献检索——中草药

主题检索：五味子

检索式： Wuweizi, Schisandra chinensis

第一步：中文名检索

The screenshot shows the SciFinder web interface. At the top, there are tabs for 'Explore', 'Saved Searches', and 'SciPlanner'. Below the tabs, a breadcrumb trail reads: 'Research Topic "wuweizi" > references (153) > The influence of Schisandrin B...'. On the left side, there is a sidebar with two main sections: 'REFERENCES' and 'SUBSTANCES'. Under 'REFERENCES', there are options: 'Research Topic', 'Author Name', 'Company Name', 'Document Identifier', 'Journal', 'Patent', and 'Tags'. Under 'SUBSTANCES', there are options: 'Chemical Structure' and 'Markush'. The main content area is titled 'REFERENCES: RESEARCH TOPIC'. It contains a search input field with the text 'wuweizi'. Below the input field, there are examples: 'The effect of antibiotic residues on dairy products' and 'Photocyanation of aromatic compounds'. A blue 'Search' button is located below the examples. At the bottom of the main content area, there is a link for 'Advanced Search'.

This screenshot shows a selection interface for search results. At the top, there are two buttons: 'Select All' and 'Deselect All'. Below these buttons, it says '1 of 2 Research Topic Candidates Selected'. There are two rows of results, each with a checkbox and a description. The first row has a checked checkbox and the text '173 references were found containing "wuweizi" as entered.'. The second row has an unchecked checkbox and the text '328 references were found containing the concept "wuweizi".'. At the bottom of the interface, there is a button labeled 'Get References'.

# 文献检索——中草药

Explore ▼ Saved Searches ▼ SciPlanner Save Print Export

⚠ 20 duplicates were automatically removed.

Research Topic "wuweizi" > references (153)

REFERENCES ⓘ

Get Substances Get Reactions Get Related Citations Tools ▼

Create Keep Me Posted Alert Send to SciPlanner

Analyze Refine Categorize

Analyze by: ⓘ

Author Name

Huang Min 3

Olalde Rangel Jose Angel 3

Wang Ying 3

Zhang Hanqi 3

Bi Hui Chang 2

Chang Cui 2

Chen Da Shuai 2

Chen Daofeng 2

Chen Ye Gao 2

Sort by: Accession Number ▼

0 of 153 References Selected

1. Method of producing soap for acne improvement

Quick View PATENTPAK

By Kim, Seong Jae

From Repub. Korean Kongkae Taeho Kongbo (2017), KR 2017110911 A 20171012. | Language: Korean, Database: CAPLUS

Title method comprises the steps of (A) mixing an anti-inflammatory nanocapsule and a molten soap base, (B) mixing the first mixt. and an essential oil, and (C) aging the second mixt. placed in a soap mold.

2. The influence of Schisandrin B on a model of Alzheimer's disease using  $\beta$ -amyloid protein A $\beta$ 1-42-mediated damage in SH-SY5Y neuronal cell line and underlying mechanisms

Quick View Other Sources

By Zhang, Ming; Zheng, Hong-xia; Gao, Yang-yang; Zheng, Bo; Liu, Jing-ping; Wang, He; Yang, Zhan-jun; Zhao, Zhi-ying

From Journal of Toxicology and Environmental Health, Part A: Current Issues (2017), Ahead of Print. | Language: English, Database: CAPLUS

Schisandrin B, an active substance, is derived from Chinese herb fruit **Wuweizi**, which exerts various pharmacol. activities ameliorating Alzheimer's disease (AD). The aim of this study was to further extend our examn. for the use of schisandrin

**Save This Answer Set**

\* Required

**Save:**

☒ All answers

☐ Only selected answers

**Title: \***

wuweizi

**Description:**

OK Cancel

# 文献检索——中草药

## 第二步：拉丁名检索

Explore ▾ Saved Searches ▾ SciPlanner

Research Topic "wuweizi" > references (153)

**REFERENCES**

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

**SUBSTANCES**

- Chemical Structure
- Markush

**REFERENCES: RESEARCH TOPIC ?**

Schisandra chinensis

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

**Search**

≡ Advanced Search

Select All Deselect All

1 of 2 Research Topic Candidates Selected

		References
<input type="checkbox"/>	16475 references were found containing "Schisandra chinensis" as entered.	16475
<input checked="" type="checkbox"/>	17542 references were found containing the concept "Schisandra chinensis".	17542

**Get References**



# 文献检索——中草药

Explore ▾ Saved Searches ▾ SciPlanner

Save Print Export

Duplicates not removed. Answer set exceeds 10,000 reference limit.

Research Topic "Schisandra chinensis" > references (17542)

REFERENCES ⓘ

Get Substances Get Reactions Get Related Citations View Only CHEMZENT Tools ▾

Create Keep Me Posted Alert Send to SciPlanner

Analyze Refine Categorize

Analyze by: ⓘ  
Author Name ▾  
Retrieving data...

Sort by: Accession Number ▾  
0 of 17542 References Selected

Remove Duplicates  
Combine Answer Sets  
Add Tag

Display Options  
Page: 1 of 878

☐ 1. Ameliorating effect of *Alpinia oxyphylla*-*Schisandra chinensis* herb pair on cognitive impairment in a mouse model of Alzheimer's disease  
Quick View Other Sources  
By Wang, Mengshi; Bi, Wenchuan; Fan, Kaiyue; Li, Tongde; Yan, Tingxu; Xiao, Feng; He, Bosai; Bi, Kaishun; Jia, Ying  
From Biomedicine & Pharmacotherapy (2017), Ahead of Print. | Language: English, Database: CAPLUS  
Alzheimer's disease (AD) is the most common cause of dementia. In our previous study, we found both *Alpinia oxyphylla* and *Schisandra chinensis* can improve the cognitive function of AD. To investigate whether the *Alpinia oxyphylla* - *Schisandra chinensis* herb pair (ASHP) has ameliorating effect on cognitive impairment, we used scopolamine to induce learning and memory impairments, as a mouse model of AD. Subsequently, we carried out Y-maze test and Morris water maze test to observe the behavior of mice. Finally, the level of Acetylcholine (ACh) and muscarinic receptor (M1) receptors, the act...

☐ 2. One kind of pig for promoting digestion and calming the nerves and powder [Machine Translation].  
Quick View Other Sources  
By Jin, Yunlong  
From Faming Zhuanli Shen  
[Machine Translation]  
components: Gardenia  
*Schisandra chinensis* 8-12 g,  
Medicata Fermenta

☐ 3. One kind of se-ric  
Quick View Other Sources  
By Dong, Jun

Combine Answer Sets

Select saved answer set(s) to combine with your current answer set (17542):

63 Answer Sets 1 Selected

Reference Answer Set Details	Date Saved
<input checked="" type="checkbox"/> wuweizi (153) Research Topic "wuweizi" > references (153)	Nov 3, 2017
<input type="checkbox"/> poo (91) Research Topic "suzuki reaction with catalyst" > references (91)	Oct 20, 2017
<input type="checkbox"/> r4r (139) Research Topic "Modification of Azithromycin" > references (139)	Oct 20, 2017
<input type="checkbox"/> 1996化工学报 (220) Journal "Huangong Xuebao" with limiters > references (497) > citing references (220)	Oct 9, 2017
<input type="checkbox"/> 本草纲目 (2123)	Sep 11, 2017

Select an option for combining the answer sets:

☒ Combine Include all answers from both sets

☐ Intersect Include only answers that appear in both sets

☐ Exclude Include only answers from current answer set (17542) that are not in wuweizi (153)

☐ Exclude Include only answers from wuweizi (153) that are not in current answer set (17542)

Combine Answer Sets Cancel

powder, characterized by the following weight of  
-25 g, Dolichos lablab 15-25 gram, *Schisandra*  
ram, Raphani Semen 8-12 grams, 8-12 g, Massa


ACS / Proprietary and Confidential / Do Not Distribute

SCI FINDER®  
A CAS SOLUTION

25

# 文献检索——中草药

CAS Solutions

 **SCIFINDER**  
A CAS SOLUTION

Preferences | SciFinder Help | Sign Out

Welcome Helen Zhu

Explore | Saved Searches | SciPlanner

Save | Print | Export

⚠ Duplicates not removed. Answer set exceeds 10,000 reference limit.

Research Topic "Schisandra chinensis" > references (17542) > Combine Reference Answer Sets "wuweizi (153)" (17590)

REFERENCES ?

Get Substances | Get Reactions | Get Related Citations | View Only CHEMZENT | Tools

Create Keep Me Posted Alert | Send to SciPlanner

Analyze | Refine | Categorize

Sort by: Accession Number

Display Options

0 of 17590 References Selected

Page: 1 of 880

Analyze by: Author Name

Kvasenkov O I	544
Zhuravskaya Skalova D V	204
Name Not Translated	183
Yan Chao	125
Choi Young Whan	75
Wang Lei	62
Wang Wei	53
Liu Yonghong	50
Ye Zhengliang	50

☐ 1. **Ameliorating effect of *Alpinia oxyphylla*-*Schisandra chinensis* herb pair on cognitive impairment in a mouse model of Alzheimer's disease**  
Quick View | Other Sources  
By Wang, Mengshi; Bi, Wenchuan; Fan, Kaiyue; Li, Tongde; Yan, Tingxu; Xiao, Feng; He, Bosai; Bi, Kaishun; Jia, Ying  
From Biomedicine & Pharmacotherapy (2017), Ahead of Print. | Language: English, Database: CAPLUS  
Alzheimer's disease (AD) is the most common cause of dementia. In our previous study, we found both *Alpinia oxyphylla* and *Schisandra chinensis* can improve the cognitive function of AD. To investigate whether the *Alpinia oxyphylla* - *Schisandra chinensis* herb pair (ASHP) has ameliorating effect on cognitive impairment, we used scopolamine to induce learning and memory impairments, as a mouse model of AD. Subsequently, we carried out Y-maze test and Morris water maze test to observe the behavior of mice. Finally, the level of Acetylcholine (ACh) and muscarinic receptor (M1) receptors, the act...

☐ 2. **One kind of pig for promoting digestion and calming the nerves and powder [Machine Translation].**  
Quick View | Other Sources  
By Jin, Yunlong  
From Faming Zhuanli Shenqing (2017), CN 107308398 A 20171103. | Language: Chinese, Database: CAPLUS  
[Machine Translation of Descriptors]. The present invention discloses a feed for promoting digestion and tranquilizing powder, characterized by the following weight of components: Gardenia Fructus 8-12 g, Paeoniae Radix Alba 8-12 gram, fritillaria 8-12 g, Pueraria 8-12 grams, jujube kernel 15-25 g, Dolichos lablab 15-25 gram, Schisandra chinensis 8-12 g, Pericarpium Citri Reticulatae Viride 8-12 grams, Crataegus pinnatifida Bge. Hordei Fructus Germinatus 5-7 gram, Raphani Semen 8-12 grams, 8-12 g, Massa Medicata Fermentata 10-14 gram, Magnoliae Officinalis Cortex 10-14 gram, Aurantii Fructus...

☐ 3. **One kind of se-rich hepatoprotective health rice wine [Machine Translation].**  
Quick View | Other Sources  
By Dong, Jun

全面的结果集

# 文献检索小结

- 主题检索时，使用介词 in, with, of 等作为连接词
- 跟据检索要求选择合适的候选项
- 通过SciFinder 的Analyze/Refine功能来缩小检索的范围
- 尝试将不同的Analyze/Refine功能组合起来用，会有更多的收益
- 使用Categorize可以让系统来实现自动分类
- 中草药的检索需要分别检中文名和拉丁名

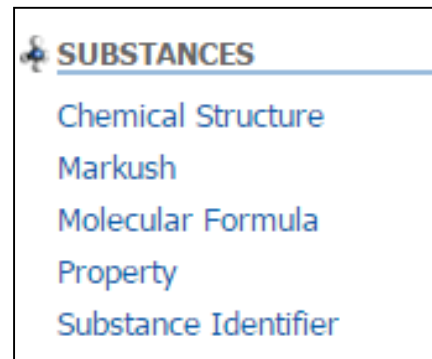
# 提纲

- 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检索选项——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

The screenshot displays the SciFinder web interface. At the top, there is a 'CAS Solutions' dropdown menu and the SciFinder logo with the tagline 'A CAS SOLUTION'. Below this is a navigation bar with 'Explore', 'Saved Searches', and 'SciPlanner' tabs. On the left side, there is a sidebar menu with two main sections: 'REFERENCES' and 'SUBSTANCES'. Under 'REFERENCES', there are links for Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, and Tags. Under 'SUBSTANCES', there are links for Chemical Structure, Markush, Molecular Formula, Property, and Substance Identifier. The 'SUBSTANCE IDENTIFIER' link is highlighted with a blue bar. The main content area is titled 'SUBSTANCES: SUBSTANCE IDENTIFIER' and contains a search input field with the text 'qinghaosu'. Below the input field, there is a note 'Enter one per line.' and 'Examples:' followed by '50-00-0', '999815', and 'Acetaminophen'. A blue 'Search' button is located at the bottom of the search area.

提示:

1. 一次最多可输入25个物质。
2. 每行一个物质标识符。

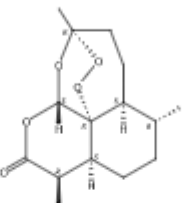
物质标识符包括CAS RN和化学名称，化学名称可以是通用名称、商品名、俗名。

# SciFinder中的物质记录

点击CAS RN 获得物质详细信息

1. **63968-64-9** 🔍

~4864 📄 ~131 🧪



Absolute stereochemistry.

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

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

**CAS Registry Number:** 63968-64-9

- 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** ?  
Return

Get ReferencesGet ReactionsGet Commercial Sources

由物质获得文献，反应，供应商等信息

CAS Registry Number 63968-64

~4,864 ~131

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

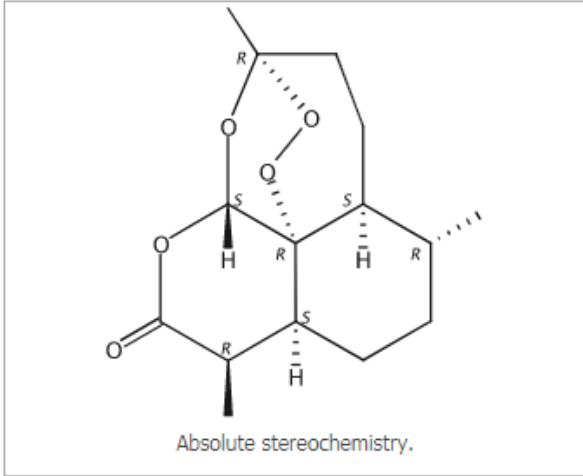
**Molecular Weight**  
282.33

**Melting Point (Experimental)**  
Value: 156-157 °C

**Boiling Point (Predicted)**  
Value: 389.9±42.0 °C | Condition: Press: 760 Torr

**Density (Experimental)**  
Value: 1.300 g/cm<sup>3</sup>

**Other Names**  
3,12-Epoxy-12*H*-pyrano[4,3-*j*]-1,2-benzodioxepin-10(3*H*)-one,  
octahydro-3,6,9-trimethyl-, [3*R*-(3*a*,5*a*β,6β,8*a*β,9*a*,12β,12*a**R*<sup>\*</sup>)]-  
(3*R*,5*a*,6*R*,8*a*,9*R*,12*S*,12*a*,*R*)-Octahydro-3,6,9-trimethyl-3,12-epoxy-  
12*H*-pyrano[4,3-*j*]-1,2-benzodioxepin-10(3*H*)-one  
(+)-Arteannuin  
(+)-Artemisinin  
(+)-Qinghaosu  
View more...



Absolute stereochemistry.

物质详情



## EXPERIMENTAL PROPERTIES

## EXPERIMENTAL SPECTRA

## 实验数据与实验谱图

**<sup>1</sup>H NMR** **<sup>13</sup>C NMR** Hetero NMR IR Mass Raman UV and Visible Additional Spectra

### <sup>13</sup>C NMR Properties

	Value	Condition	Note
Carbon-13 NMR Spectrum	<a href="#">See spectrum</a>		(3)ACD
Carbon-13 NMR Spectrum	<a href="#">See spectrum</a>		(4)ACD
Carbon-13 NMR Spectrum	<a href="#">See full text</a>	1 of 8	(5)CAS

### Notes

(3) ACD: Spectral data were obtained from Advanced Chemistry Development, Inc.

(4) Han, Jaehong; Journal of Natural Products 2001, V64(9), P1201-1205 CAPLUS 🔍

(5) Yadav, J. S.; Tetrahedron 2010, V66(11), P2005-2009 CAPLUS 🔍

## 预测数据与预测谱图

## PREDICTED PROPERTIES

## PREDICTED SPECTRA

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

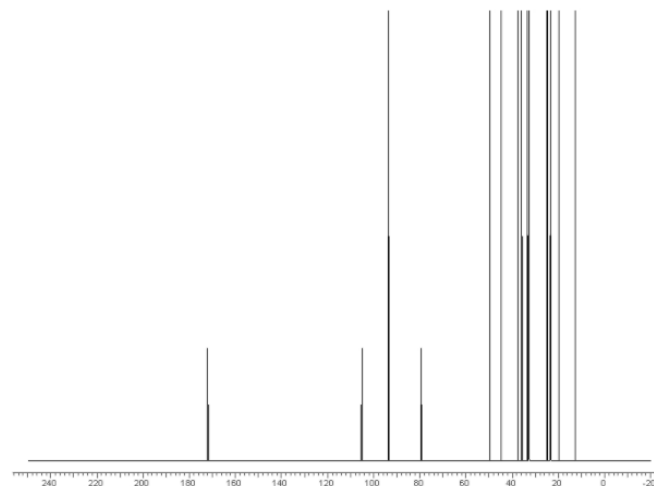
### <sup>1</sup>H NMR Properties

	Value
Proton NMR Spectrum	<a href="#">See spectrum</a>

### Notes

(28) Predicted NMR data calculated using Advanced Chemistry Development, Inc. (ACD/

Carbon-13 NMR Spectrum



SPECTRUM ID  
7MED36\_38.C

CAS REGISTRY NUMBER  
63968-64-9

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

CAS INDEX NAME  
3,12-Epoxy-12H-pyrano[4,3-β]-1,2-benzodioxepin-10(3H)-one, octahydro-3,6,9-trimethyl-, (3R,5aS,6R,8aS,9R,12S,12aR)-

NUCLEUS  
13C

SOURCE  
Spectral data were obtained from Advanced Chemistry Development, Inc.

# 物质检索——Property explore

The screenshot shows the SciFinder web interface for property exploration. The browser address bar displays <https://scifinder.cas>. The SciFinder logo is visible at the top left. The 'Explore' tab is selected, and the 'SUBSTANCES' section is active in the left sidebar. A dropdown menu for 'Select Property...' is open, listing various properties, with 'Molecular Weight' highlighted. Below the dropdown, a search range of '250-400' is entered, with examples '44, 25-35, >125' shown. A 'Search' button is located at the bottom center. On the right side, a text box contains the Chinese text: 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** 🔍

~0

**C<sub>15</sub> H<sub>17</sub> Br N<sub>2</sub>**  
3-Pyridinamine, 2-bromo-*N*-(3-phenylbutyl)-

▶ **Key Physical Properties**

2. **1986293-21-3** 🔍

~0

**C<sub>11</sub> H<sub>16</sub> Cl F<sub>2</sub> N<sub>3</sub> O**  
4-Pyrimidinamine, *N*-(2-chloroethyl)-*N*-(2,2-difluoroethyl)-6-ethoxy-5-methyl-

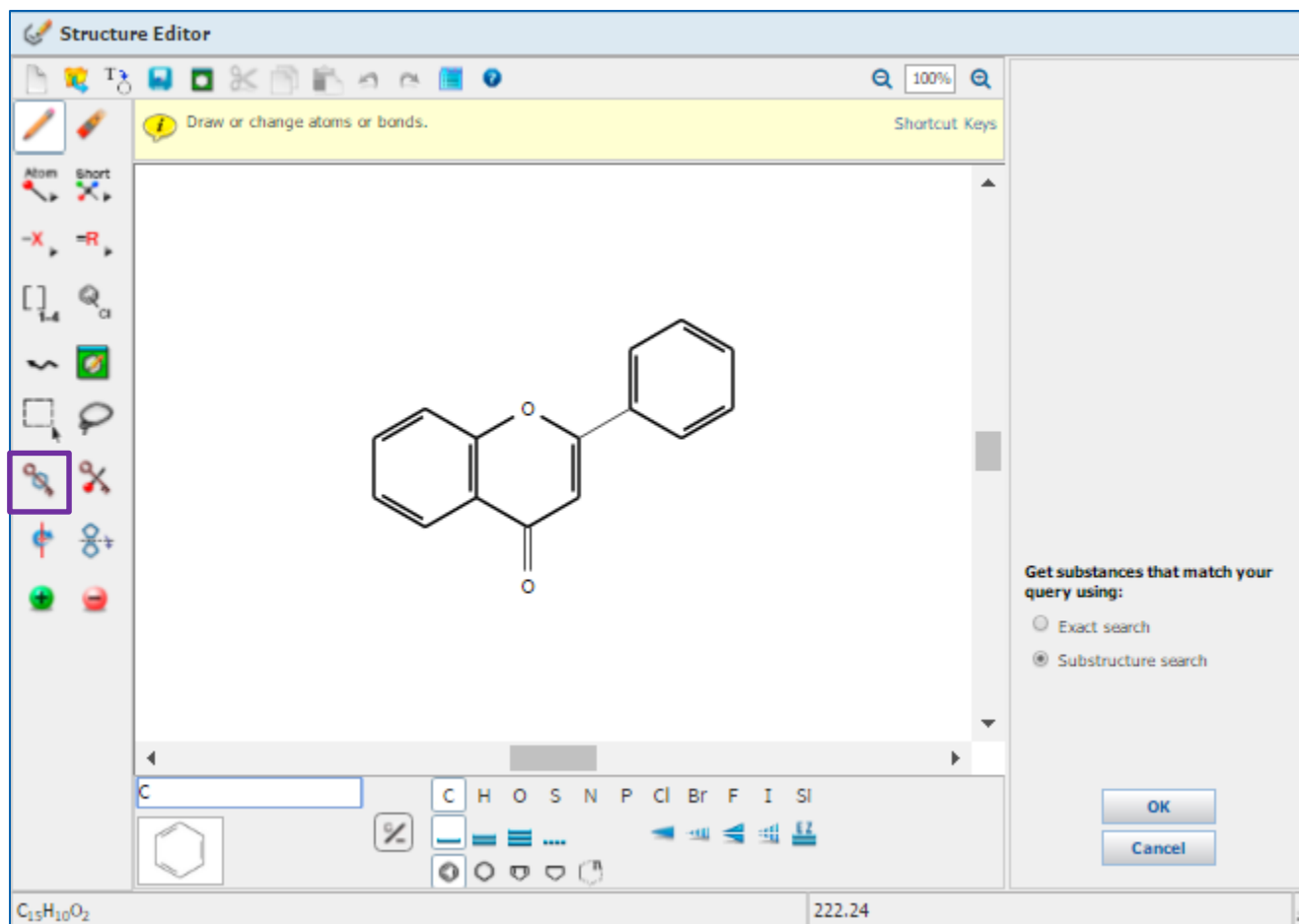
▶ **Key Physical Properties**

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



锁环工具：避免在被锁定的环结构上出现新的环结构

**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

# 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>**  
4/4'-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>**  
4/4'-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

# 物质检索——分子式

**REFERENCES**

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

**SUBSTANCES**

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

**REACTIONS**

- Reaction Structure

**SUBSTANCES: MOLECULAR FORMULA**

Examples:  
H4SiO4  
(C3H6O,C2H4O)x

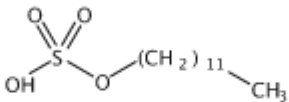
**Search**

无机金属盐：金属离子和阴离子间用点 (.) 分开

1. **151-21-3**

(Component: 151-41-7)

~84904 ~276



• Na

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

**Key Physical Properties**

- Regulatory Information
- Spectra
- Experimental Properties

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

# 物质检索——结构

**REFERENCES**

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

**SUBSTANCES**

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

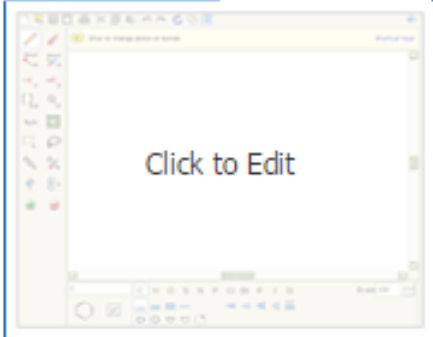
**REACTIONS**

- Reaction Structure

## SUBSTANCES: CHEMICAL STRUCTURE ?

Structure Editor:


Java Non-Java



Search Type:


- ☐ Exact Structure
- ☒ Substructure
- ☐ Similarity

☐ Show precision analysis

 **ChemDraw**  
Launch a SciFinder substance or reaction

Import CXF

**Search**

 Advanced Search ☒ Always Show

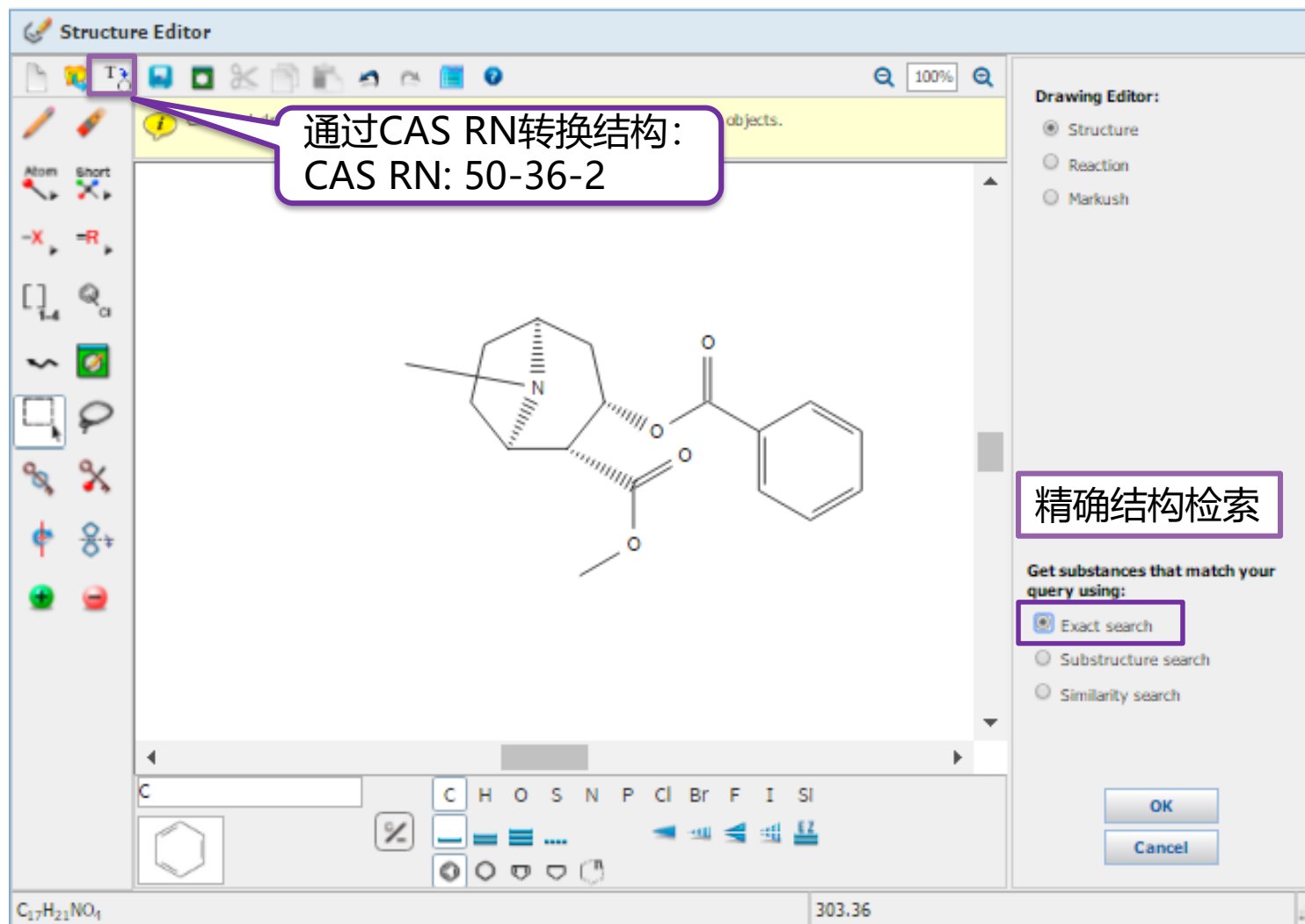
# 物质检索——结构

The image shows the SciFinder Structure Editor interface with various tools labeled in Chinese. The labels are as follows:

- 橡皮 (Eraser)
- 结构和反应切换功能 (Structure and Reaction Switching Function)
- 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 (Selection Tool)
- 环锁定工具 (Ring Locking Tool)
- 旋转工具 (Rotation Tool)
- 正电子 (Positron)
- C原子和单键恢复工具 (C Atom and Single Bond Restoration Tool)
- 常用基团 (Common Group)
- R基团定义工具 (R Group Definition Tool)
- 可变位置连接工具 (Variable Position Connection Tool)
- 模版工具 (Template Tool)
- 索套选择工具 (Loop Selection Tool)
- 原子锁定工具 (Atom Locking Tool)
- 镜面旋转工具 (Mirror Rotation Tool)
- 单双键, RS构型, 不确定键定义工具 (Single/Double Bond, RS Configuration, Uncertain Bond Definition Tool)
- 结构检索选择 (Structure Search Selection)
- 负电子 (Negatron)
- 常见环, 多元环工具 (Common Ring, Polycyclic Tool)



# 物质检索——精确结构检索



# 精确结构检索结果

Get References

Get Reactions

Get Commercial Sources

Tools

Create Posted

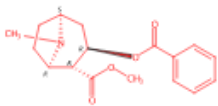
Sort by: Relevance

0 of 6 Substances Selected

1. 668-19-9

~18

~1



Absolute stereochemistry.

**$C_{17}H_{21}NO_4$**   
8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(benzoyloxy)-8-methyl-, methyl ester, (1*R*,2*R*,3*R*,5*S*)-

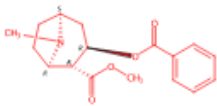
Key Physical Properties

Spectra

可卡因

2. 114599-38-1

~5

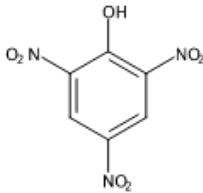


Absolute stereochemistry.

**668-19-9**  
 **$C_{17}H_{21}NO_4$**

88-89-1

**$C_6H_3N_3O_7$**

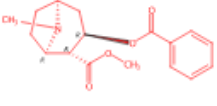


**$C_{17}H_{21}NO_4 \cdot C_6H_3N_3O_7$**   
Alcococaine, picrate (6CI)

可卡因组合物

3. 109496-04-0

~1



Absolute stereochemistry.

**$C_{17}H_{21}NO_4 \cdot ClH$**   
Alcococaine, hydrochloride (6CI)

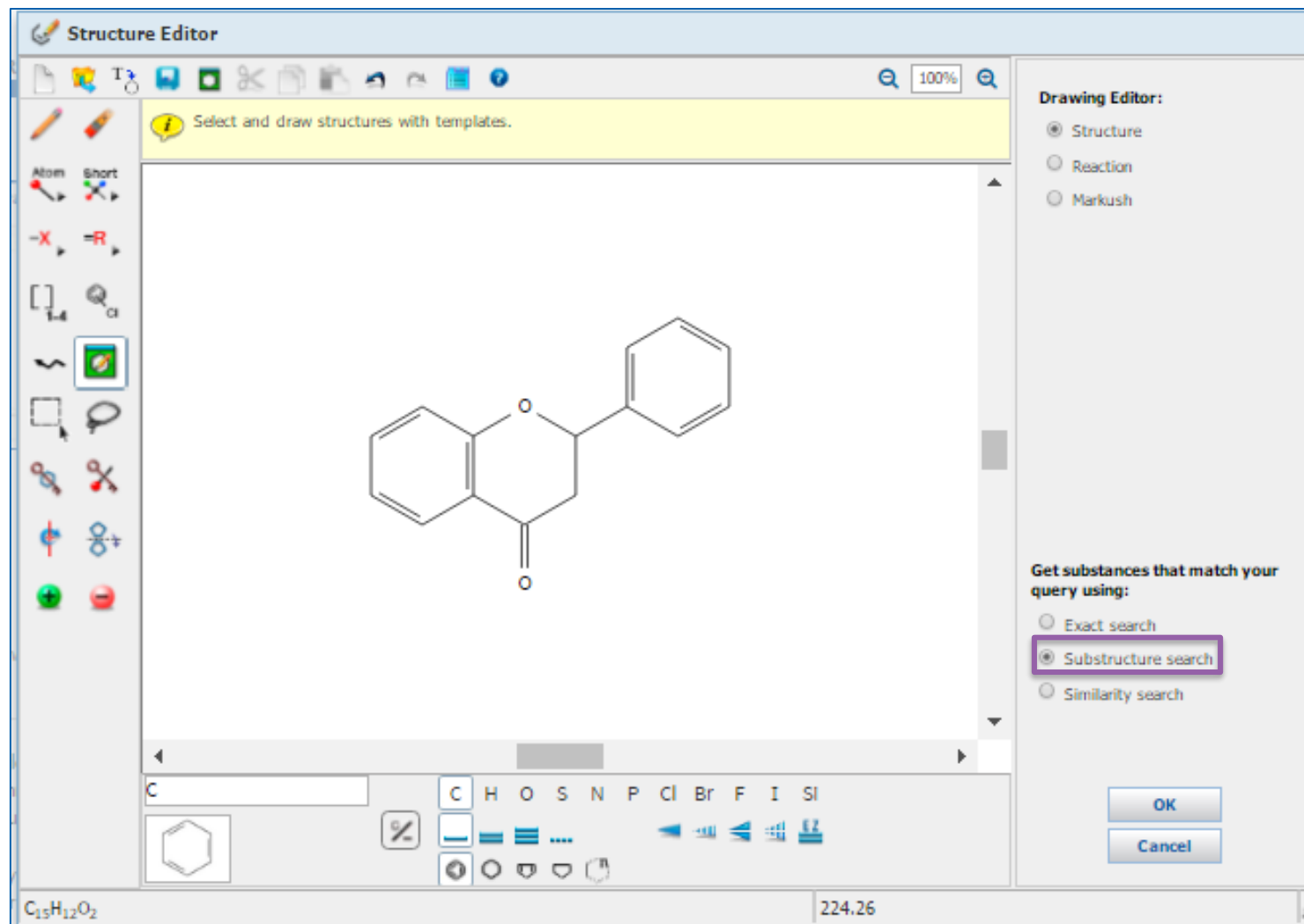
盐酸可卡因

# 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

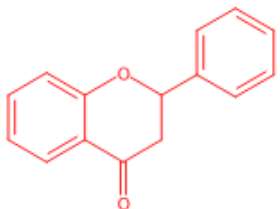
# 物质检索——亚结构检索



# 物质检索——亚结构检索

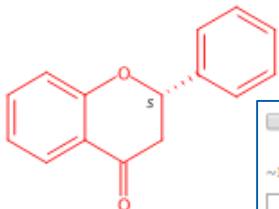
0 of 23824 Substances Selected

1. 487-26-3



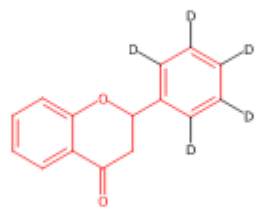
C15H11O2  
4H-1-Benzopyran-4-one, 2-phenyl-

2. 17002-31-2



Absolute stereochemistry, Rotat

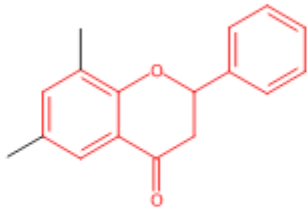
10. 146196-91-0



C15H4D4O2  
e, 2,3-dihydro-2-(phenyl- $\alpha$ )-(9CI)

同位素

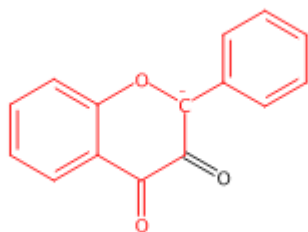
281. 123251-10-5



C17H16O2  
4H-1-Benzopyran-4-one, 2,3-dihydro-6,8-dimethyl-

取代物

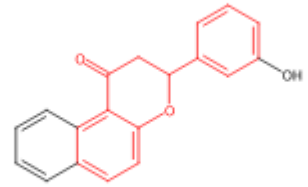
295. 780723-19-5



C15H9O3  
2H-1-Benzopyran-3,4-dione, 2-phenyl-, ion(1-)

离子

284. 136116-23-9



C19H14O3  
1H-Naphtho[2,1-b]pyran-1-one, 2,3-dihydro-3-(3-hydroxyphenyl)-

稠环物质

Key Physical Properties

Experimental Properties

ACS / Proprietary and Confidential / Do Not Distribute

# 亚结构检索结果的限定

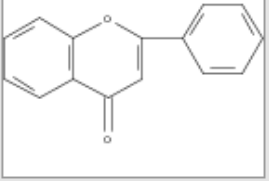
## 化学结构的再次限定

Analysis Refine

Refine by: ⓘ

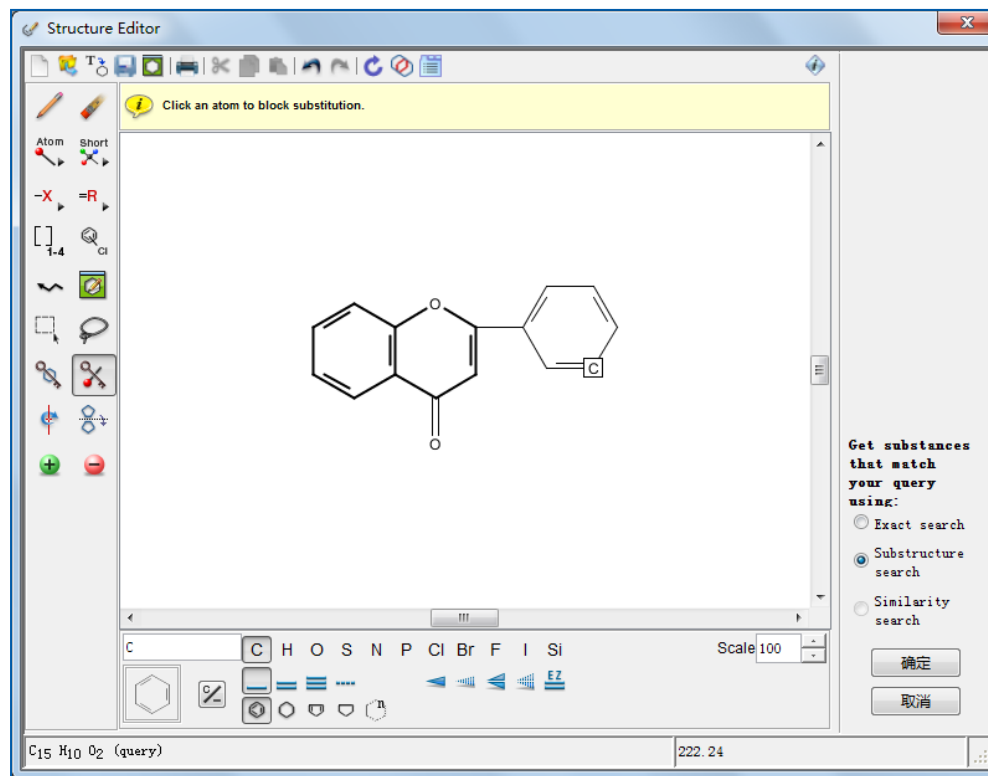
- ☒ Chemical Structure
- ☐ Isotope-Containing
- ☐ Metal-Containing
- ☐ Commercial Availability
- ☐ Property Availability
- ☐ Property Value
- ☐ Reference Availability
- ☐ Atom Attachment

Chemical Structure:



Click image to change structure or view detail

Search type: **Substructure**



环锁定

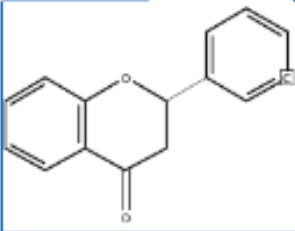


原子锁定

# 亚结构检索结果的限定

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

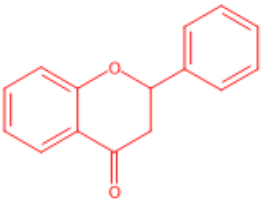
Get References Get Reactions Get Commercial Sources Tools

Sort by: Relevance

0 of 13826 Substances Selected

1. 487-26-3

~2093

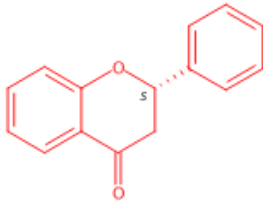


$C_{15}H_{12}O_2$   
4H-1-Benzopyran-4-one, 2,3-dihydro-2-phenyl-

Key Physical Properties  
Regulatory Information  
Spectra  
Experimental Properties

2. 17002-31-2

~244



Absolute stereochemistry., Rotation (-).

$C_{15}H_{12}O_2$   
4H-1-Benzopyran-4-one, 2,3-dihydro-2-phenyl-, (2S)-

Key Physical Properties  
Experimental Properties

4. 104550-32-5

~3

5. 75524-43-5

~2

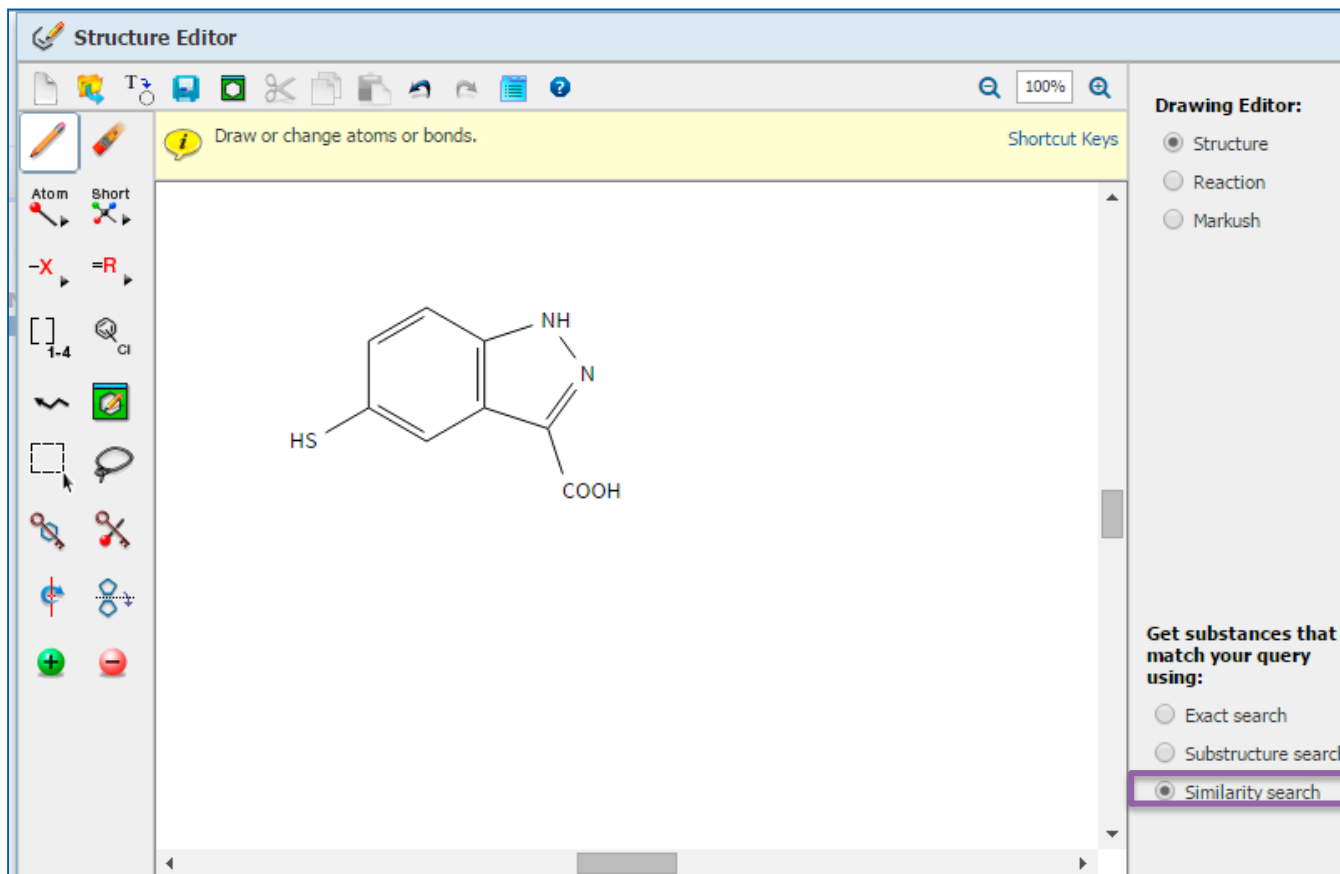
# 物质检索——亚结构检索

- 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"/> $\geq 99$ (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

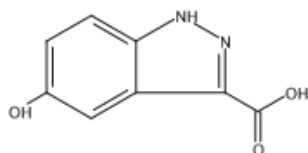
相似度越高，结构越相似

Score: 88

☐ 1. 885518-94-5

取代基变化

~1 ~35



$C_8H_6N_2O_3$

1H-Indazole-3-carboxylic acid, 5-hydroxy-

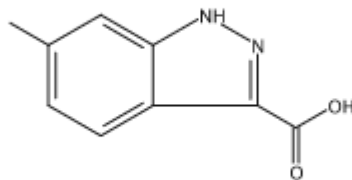
► Key Physical Properties

Score: 86

☐ 5. 858227-12-0

取代基位置变化

~7 ~41



$C_9H_8N_2O_2$

1H-Indazole-3-carboxylic acid, 6-methyl-

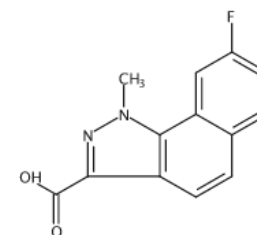
► Key Physical Properties

Score: 65

☐ 541. 1100422-

母体结构变化

~1



$C_{13}H_9FN_2O_2$

1H-Benz[g]indazole-3-carboxylic acid, 8-fluoro-1-methyl-

► Key Physical Properties



**SCIFINDER®**  
A CAS SOLUTION

# 物质检索——相似结构检索

- 相似结构检索：

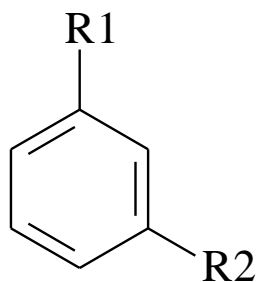
获得片段或整体结构与被检索结构相似的结果，母体结构可以被取代，也可以被改变

# 提纲

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

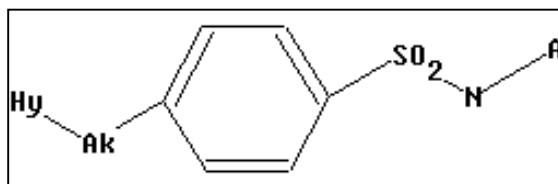
# Markush检索

- 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
- 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
  - 专利中所陈述的预测物质，不会被分配CAS RN
  - Markush检索，能检索到通过结构检索检不到的专利




R1 = H, Br, Cl, I

R2 = Br, Cl, I, —CH<sub>2</sub>—halogen, —CH(CH<sub>3</sub>)—halogen,



可用SciFinder中的Markush检索  
查看专利中化合物结构保护范围。

# Markush检索

 **SCIFINDER**  
A CAS SOLUTION

Welcome Helen Zhu

Explore ▼ Saved Searches ▼ SciPlanner Save Print Export

Markush substructure > references (1969) > Compounds and methods for anti...

REFERENCES ⓘ

Get Substances Get Reactions Get Related Citations Tools ▼ Create Keep Me Posted Alert Send to SciPlanner

Analyze Refine Categorize

Sort by: Accession Number ▼

0 of 1969 References Selected

Page: 1 of 99

Analyze by: Document Type ▼

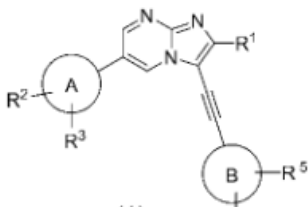
Patent 1969

Journal 1

Show More

全部是专利

☐ 1. Compounds and methods for anticoagulation therapy  
PATENTPAK  
Quick View  
By Allende Rodriguez, Mikel; Hermida Santos, Jose; Montes Diaz, Ramon; Oyarzabal Santamarina, Julen  
From PCT Int. Appl. (2016), WO 2016120432 A1 20160804. | Language: English, Database: CAPLUS  
The invention relates to certain compds. that are inducers of Heat shock 70 kDa protein 1A/1B (HSPA1A/B) and their use for anticoagulation therapy; and to a method for anticoagulation therapy that comprises the administration of one of these inducer compds. It has been here proved that induction of Heat shock 70 kDa protein 1A/1B by administration of one of these inducer compds. has antithrombotic effects without accelerating or altering bleeding time.

☐ 2. Preparation of new imidazopyrimidine derivatives as negative allosteric modulators of metabotropic glutamate receptor subtype 2 (mGlu2 receptor)  
PATENTPAK  
Quick View  
By Urashima, Kuniko; Tojo, Kengo; Koike, Shoko; Masumoto, Shuji  
From Jpn. Kokai Tokkyo Koho (2016), JP 2016132660 A 20160725. | Language: Japanese, Database: CAPLUS  


The title imidazo[1,2-a]pyrimidine derivs. I [R<sup>1</sup> = H or halogen; ring A Ph or pyridyl; R<sup>2</sup>, R<sup>3</sup> (same or different) = hydrogen, halogen, C<sub>1-4</sub> alkyl or C<sub>1-4</sub> alkoxy each optionally substituted with 1-5 halogen atoms; or in case where R<sup>2</sup> and R<sup>3</sup> are at the adjacent substitution position, R<sup>2</sup> and R<sup>3</sup> together with ring A form C<sub>5-8</sub> carbocyclic ring (optionally substituted with 1-5 halogen or 1-2 hydroxy group) or 5- or 6-membered satd. heterocyclic ring; ring B = Ph or pyridyl; R<sup>4</sup>, R<sup>5</sup> (same or different) = H, halogen, hydroxy, amino, -C(O)OR<sup>a</sup>, -C(O)NR<sup>a</sup>R<sup>b</sup>, SO<sub>3</sub>H, SO<sub>2</sub>NR<sup>a</sup>R<sup>b</sup>, SO<sub>2</sub>R<sup>b</sup>, or NR<sup>a</sup>SO<sub>2</sub>R<sup>b</sup>; R<sup>a</sup>, R<sup>b</sup> (same...

# 提纲

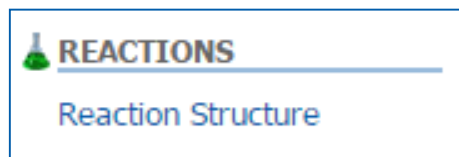
- 美国化学文摘社简介
- SciFinder简介及检索方式
  - 文献检索
  - 物质检索
  - Markush检索
  - 反应检索
  - SciPlanner
- SciFinder常见问题及解决



# SciFinder检索选项——反应检索

- 反应检索方法

结构式



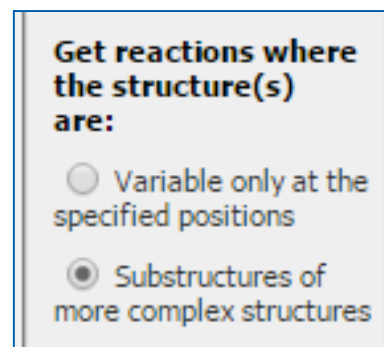
- 常用获取方法

已知物质：由物质获取反应

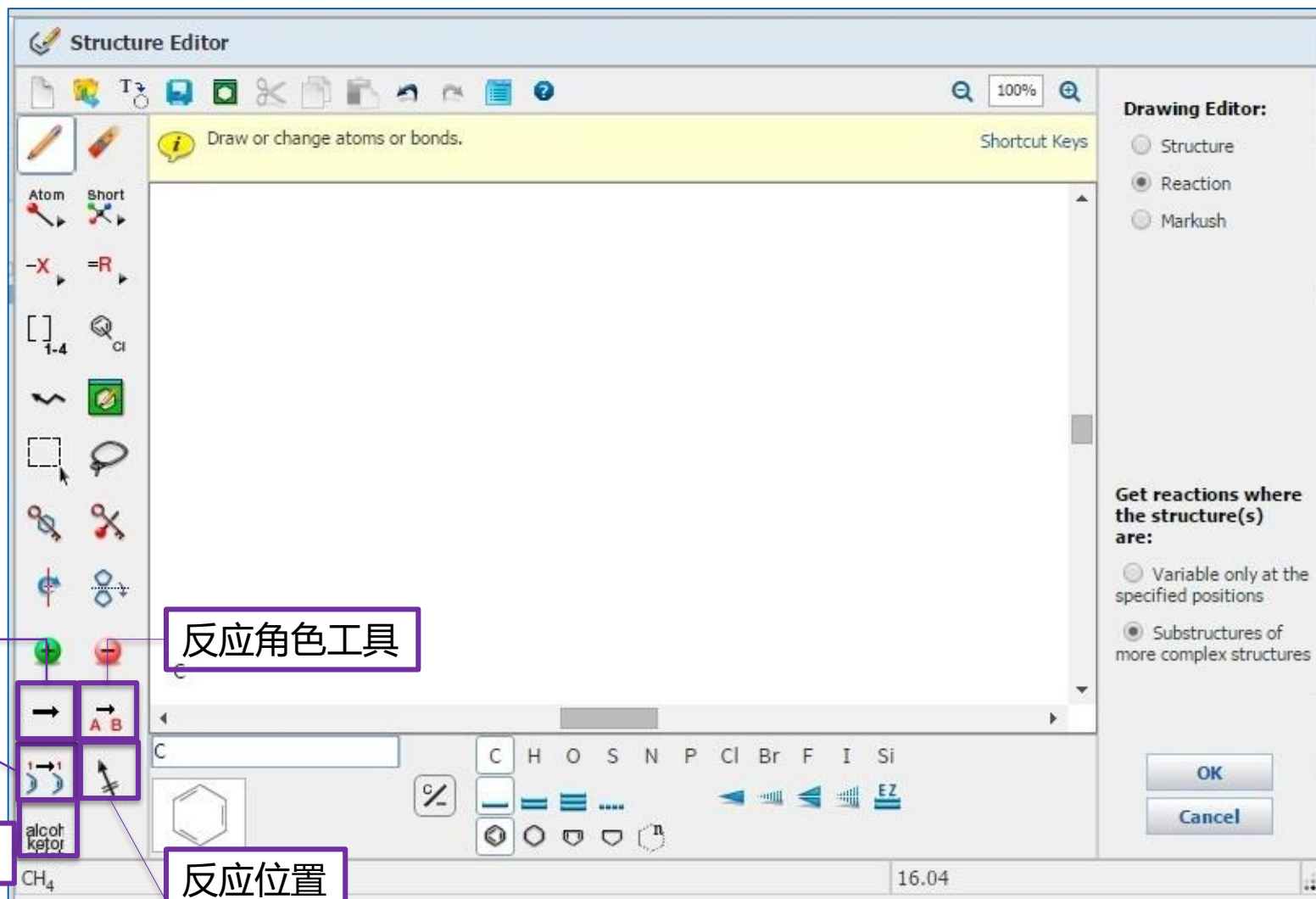
已知文献：从文献中获取反应

精确结构反应检索

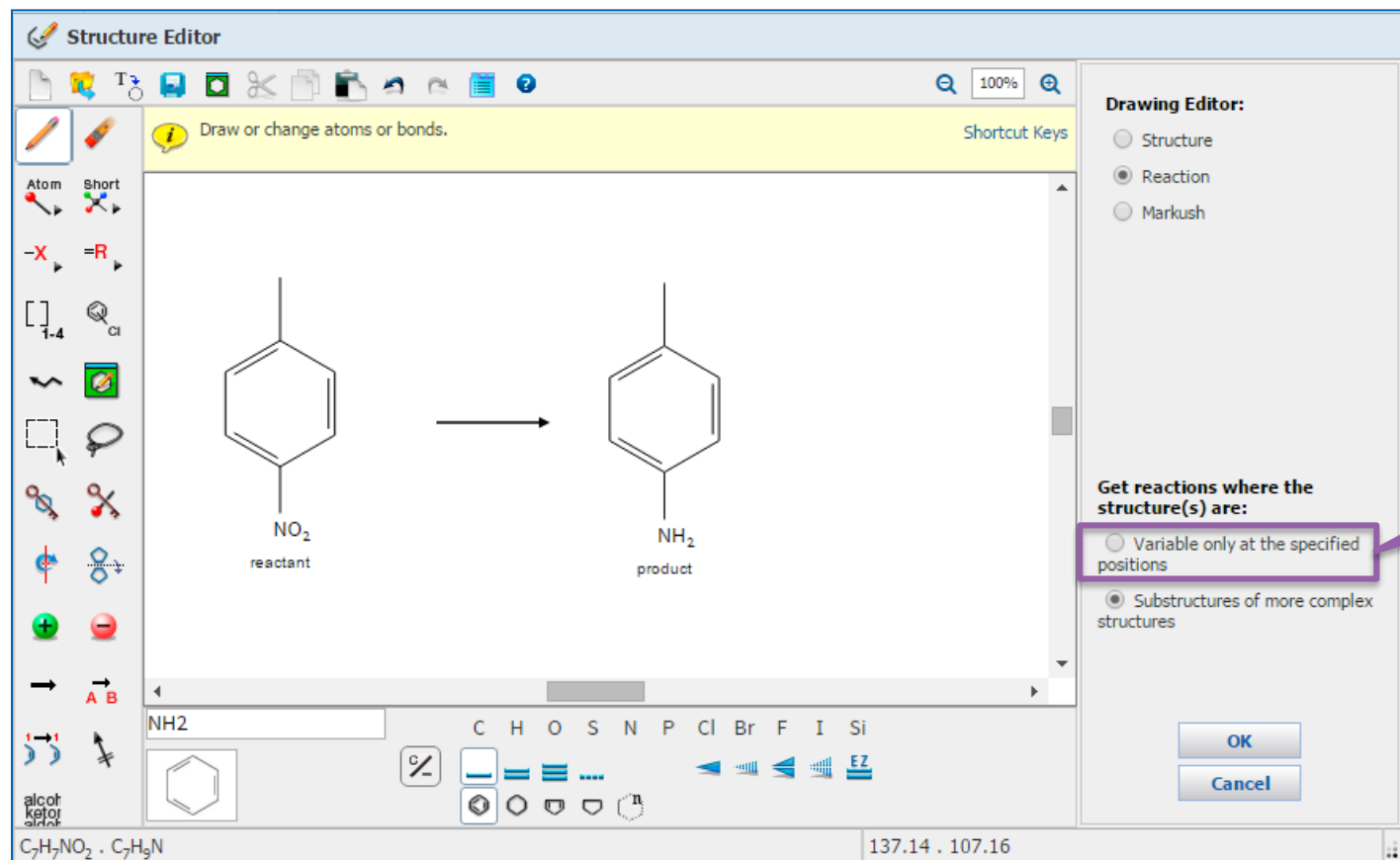
亚结构反应检索



# 反应绘制工具



# SciFinder反应检索——精确反应检索



精确反应检索

# 反应检索结果

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

获取相似反应

Get References Tools

Group by: **Document** Sort by: Relevance

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

Single Step Hover over any structure for more options.

Cc1ccc(cc1)[N+](=O)[O-]  $\rightarrow$  Cc1ccc(cc1)N

~102 ~122

**100%**

**Overview**

**Steps/Stages**

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

**Notes**

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

**References**

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

# 获取相似反应

选择相似反应的相似限制:

Broad: 仅反应中心相似

Medium: 反应中心及附属原子和键

Narrow: 反应中心及扩展的原子和键

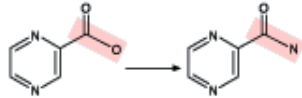
**Get Similar Reactions ?**

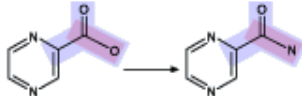
**Retrieve similar reactions from:**

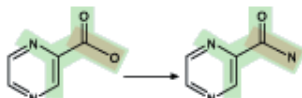
- ☒ All reactions
- ☐ Current answer set

**Include this level of similarity:**

- ☒ Broad - Reaction centers only (2934)


- ☐ Medium - Reaction centers plus adjacent atoms and bonds (109)


- ☐ Narrow - Reaction centers plus extended atoms and bonds (95)



Get Reactions

Cancel

# 按照反应类型排序

Group by: Transformation ▼ Sort by: Frequency ▼ ↓

☐ 0 of 560 Reactions Selected

☐ 1. Reduction of Nitro Compounds to Amines  
538 Reactions

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

☐ 2. Reduction of Nitro to Azo Compounds  
11 Reactions

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

☐ 3. Reduction of Nitro to Azoxy Compounds  
11 Reactions

$$\text{Ar-NO}_2 \longrightarrow \text{Ar-N}^+=\text{N-Ar} \begin{matrix} \text{O}^- \\ | \end{matrix}$$

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

**REACTIONS** ?

Get References Tools

Analyze Refine

Analyze by: Reagent

H<sub>2</sub> 148

**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


Show More

Group by: No Grouping Sort by: Relevance

0 of 512 Reactions Selected

1. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.



**Overview**

Steps/Stages

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

**Notes**

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

**References**

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

# SciFinder囊括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



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



# 官能团反应检索

## 寻找羟基转化为氨基的反应

Structure Editor

Drag the reaction arrow to specify reaction direction.

ALCOHOLS  
reactant

AMINES  
product

Functional Groups

Enter 3 or more characters...

Alcohols (13)

ALCOHOLS is a class that includes: Allyl Alcohol, Cyanohydrin, Cyclic Alcohol, Enol, Glycol, Halohydrin, Hemiacetal, Hyd...

ALCOHOLS

Allyl Alcohol

Cyanohydrin

C-OH

C=O-H

HO-C-C-OH

Cyclic Alcohol

Enol

Glycol

X-C-C-OH

HO-C-O-C

N-OH

X-C-OH

C

H

Halohydrin

Hemiacetal

Hydroxylamine

Phenol

Primary Alcohol

Secondary Alcohol

Get reaction structure(s)

Variable positions

Substructure complex structure

Formula is not available

# 通过后处理工具筛选反应—Refine

[Explore ▾](#)[Saved Searches ▾](#)[SciPlanner](#)[Save](#)[Print](#)[Export](#)[Reaction Structure substructure](#) > [reactions \(1851074\)](#)**REACTIONS** ⓘ

Get References

Tools ▾

Send to SciPlanner

[Analyze](#)[Refine](#)

Refine by: ⓘ

- ☐ Reaction Structure
- ☒ Product Yield
- ☐ Number of Steps
- ☐ Reaction Classification
- ☐ Excluding Reaction Classification
- ☐ Non-participating functional groups

Product Yield:

 %

Upper Limit

Example: 80

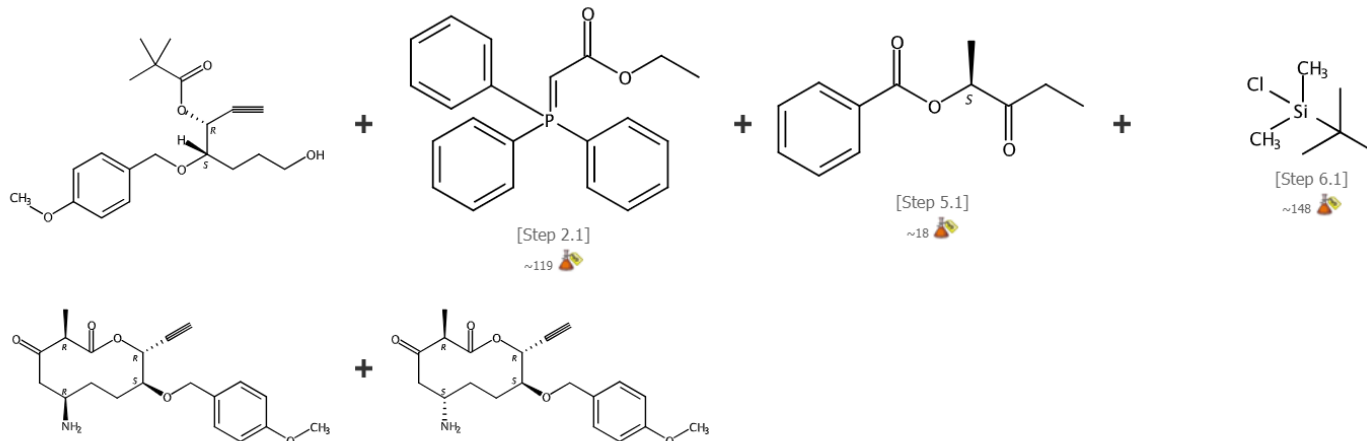
 %

Lower Limit

Example: 20

☐ Include answers that have no product yield[Refine](#)Group by: [No Grouping](#) ▾Sort by: [Accession Number](#) ▾☐ ▾ 0 of 1851074 Reactions Selected

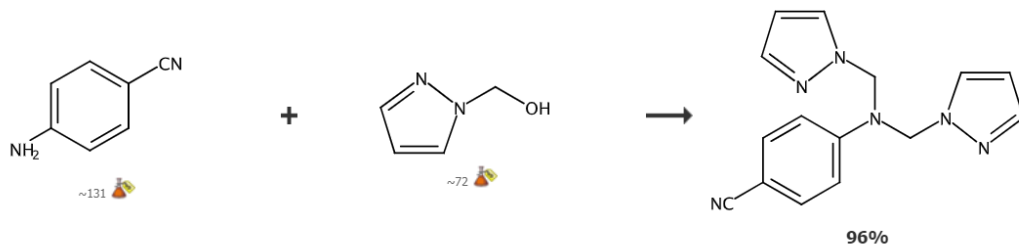
Page: 1 of 37022

[Display Options](#)☐ 1. [View Reaction Detail](#) ⓘ [Link](#)13 Steps *Hover over any structure for more options.*[Overview](#)

# 通过后处理工具筛选反应—Refine

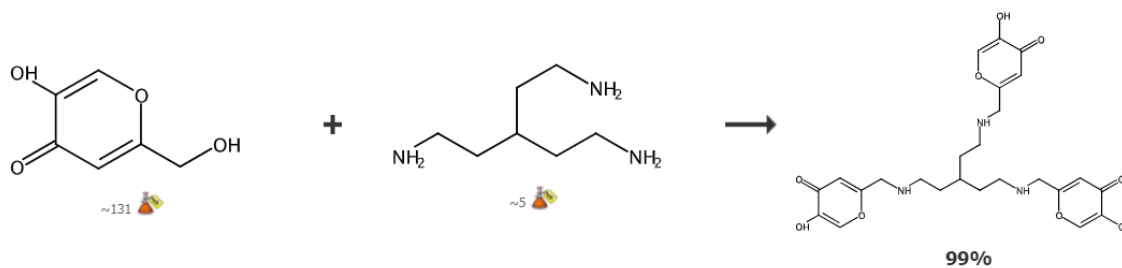
## 1. [View Reaction Detail](#) [Link](#) [Similar Reactions](#)

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



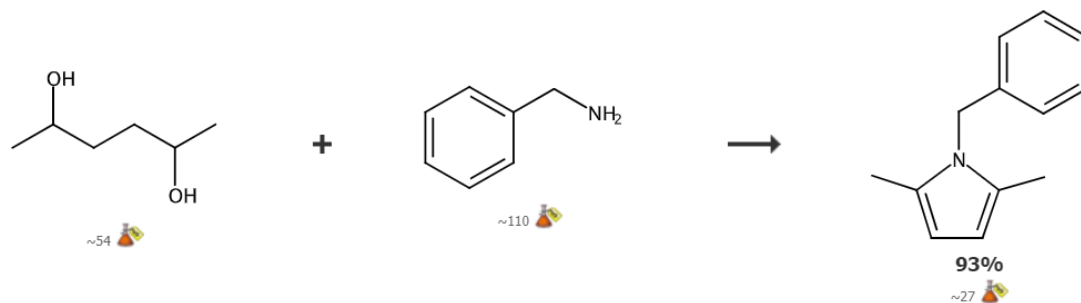
## 3. [View Reaction Detail](#) [Link](#) [Similar Reactions](#)

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



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

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



# 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

# SciPlanner使用简介

3. View Reaction Detail [Link](#) **勾选想要的反应**

3 Steps Hover over any structure for more options.

**点击Send to SciPlanner**

**进入SciPlanner 新建文件**

**将刚推送过来的反应拖至编辑面板**

**Send to SciPlanner**

**Display Options**

**Overview**

**Steps/Stages**

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

**Notes**

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

**References**

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

SciPlanner [SciPlanner\\_11\\_19\\_2015\\_112612](#)

**Workspace** **Edit** **View** **GoTo**

New  
Open  
Save  
Duplicate  
Import  
Export  
Print  
Close

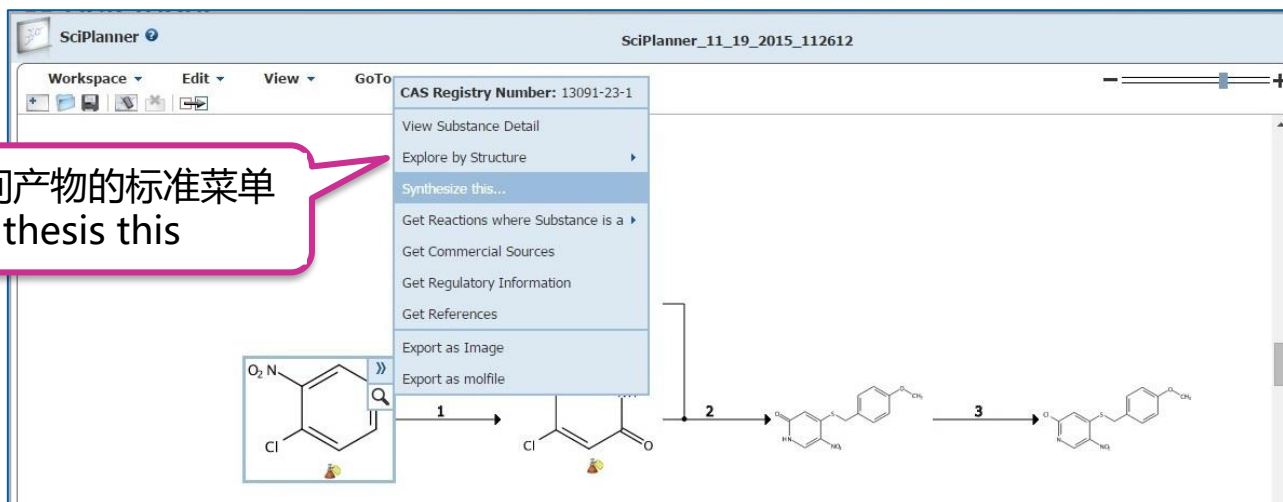
Your Workspace is empty.

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

**SCI FINDER®**  
A CAS SOLUTION

# SciPlanner使用简介

打开中间产物的标准菜单  
选择Synthesize this

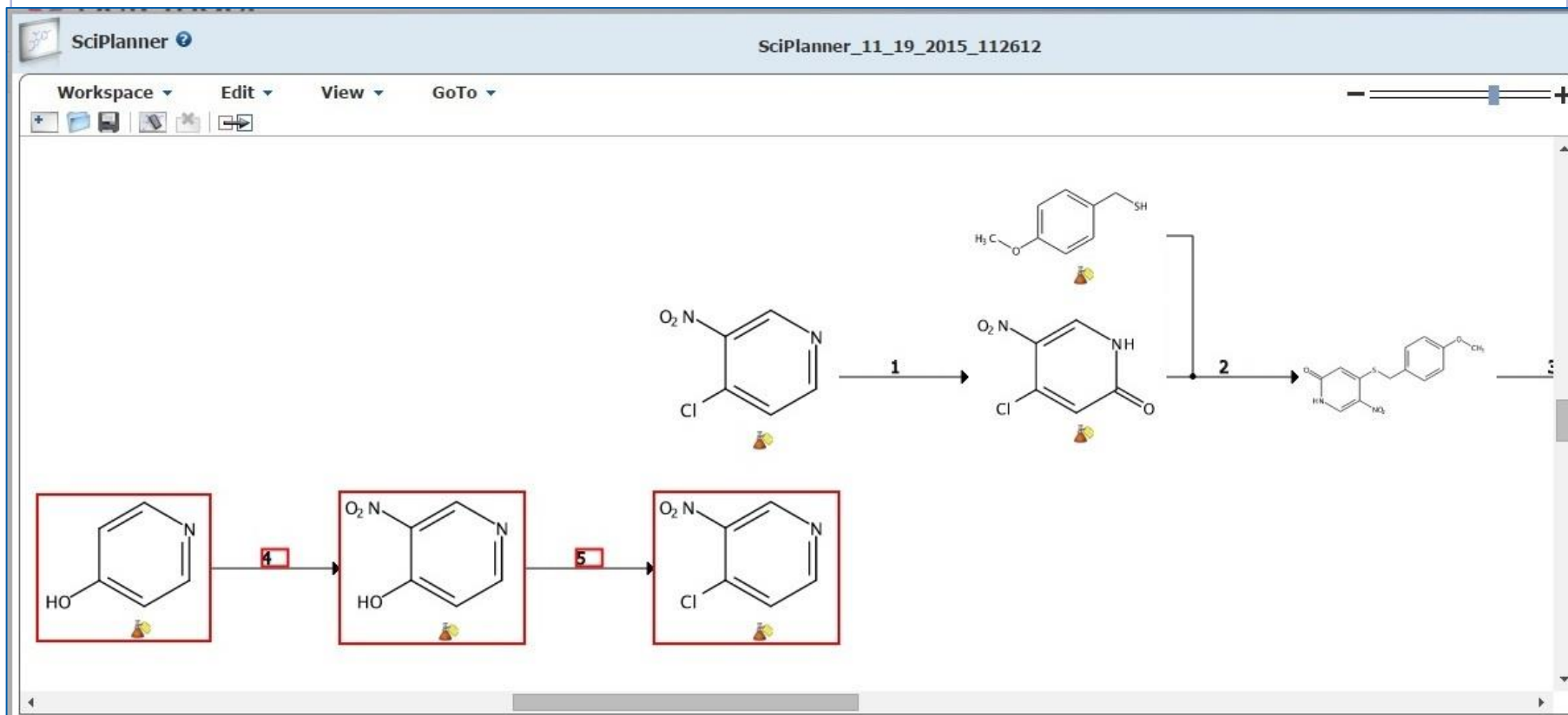


在检索到的反应中选择感兴趣的反应

继续推送到SciPlanner



# SciPlanner使用简介



步骤同前，将推送过来的反应拖到编辑面板中，可以看到两条反应中存在同样的结构

# SciPlanner使用简介

SciPlanner 11\_19\_2015\_112612

Workspace Edit View GoTo

New  
Open  
Save  
Duplicate  
Import  
**Export**  
Print  
Close

点击 Workspace, 选择 Export 导出结果

用鼠标将两个同样的结构拖至重叠, 两条反应合并

选择适当的输出格式, 输出结果

**Export**

**For:**

**Offline Review**

- ☒ Portable Document Format (\*.pdf)
- ☐ Citations (\*.ris)
- ☐ Image (\*.png)

**Saving Locally**

- ☐ SciPlanner eXchange (\*.pkx)

**Details:**

**File Name:** \*

SciPlanner\_11\_19\_2015\_112612

**Title**

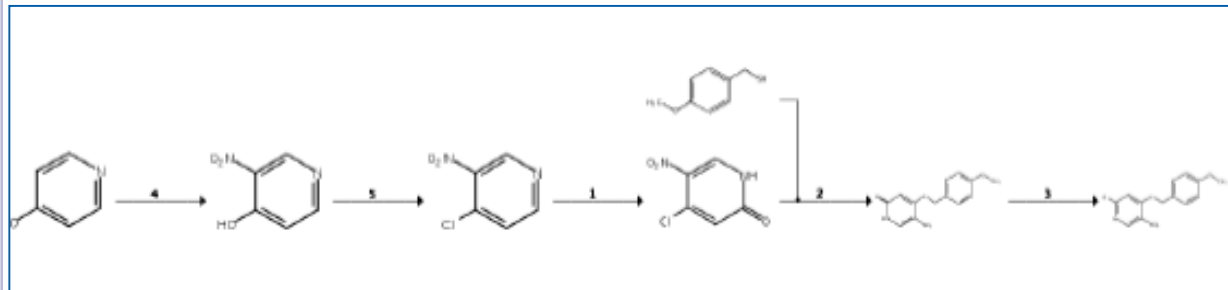
**Include:**

- ☒ SciPlanner Image
- ☒ Reaction Details
- ☒ Substance Details
- ☒ Reference Details

**Export** **Cancel**



# 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	Reactants: 1, Reagents: 2, Solvents: 2, Steps: 1, Stages: 2	90%
	1.2 R:K <sub>2</sub> CO <sub>3</sub> , S:H <sub>2</sub> O, cooled, pH 10	Transformation: 1. Formation of Alkyl Halides from Alcohols	

## References

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		
<p>1228150-22-8</p> <p>C<sub>13</sub>H<sub>12</sub>N<sub>2</sub>O<sub>4</sub>S 2(1H)-Pyridine, 4-[[4-methoxyphenyl]methyl]thio-5-nitro- Related Info: ~ 2 References Reactions</p>	<p>1228150-23-9</p> <p>C<sub>13</sub>H<sub>11</sub>ClN<sub>2</sub>O<sub>4</sub>S Pyridine, 2-chloro-4-[[4-methoxyphenyl]methyl]thio-5-nitro- Related Info: ~ 2 References Reactions</p>	<p>13091-23-1</p> <p>C<sub>5</sub>H<sub>3</sub>ClN<sub>2</sub>O<sub>2</sub> Pyridine, 4-chloro-3-nitro- Related Info: ~ 301 References Reactions ~ 100 Commercial Sources Regulatory Information</p>
<p>5435-54-1</p> <p>C<sub>6</sub>H<sub>4</sub>N<sub>2</sub>O<sub>3</sub> 4-Pyridinol, 3-nitro- Related Info: ~ 113 References Reactions ~ 197 Commercial Sources Regulatory Information</p>	<p>6258-60-2</p> <p>C<sub>8</sub>H<sub>10</sub>O S Benzenemethanethiol, 4-methoxy- Related Info: ~ 749 References Reactions ~ 71 Commercial Sources Regulatory Information</p>	<p>626-64-2</p> <p>C<sub>5</sub>H<sub>5</sub>N O 4-Pyridinol Related Info: ~ 1351 References Reactions ~ 160 Commercial Sources Regulatory Information</p>
<p>850663-54-6</p> <p>C<sub>6</sub>H<sub>3</sub>ClN<sub>2</sub>O<sub>3</sub> 2(1H)-Pyridine, 4-chloro-5-nitro- Related Info: ~ 22 References Reactions ~ 138 Commercial Sources</p>		

# 提纲

- 美国化学文摘社简介
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# 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

[首页](#)[本馆概况](#)[资源](#)[服务](#)[读者意见](#)[党建工作](#)[校外访问](#)

当前日期: 2019年6月4

当前位置: 首页 / 资源 / 正文

日 星期二

## SciFinder

发布日期: 2019年05月07日 来源: 点击: [140]

数据库名称	SciFinder
数据库链接	<p>读者注册地址: <a href="https://scifinder.cas.org/registration/index.html?corpKey=6BE07969X86F35040X3C9C945423CF0CF467">https://scifinder.cas.org/registration/index.html? corpKey=6BE07969X86F35040X3C9C945423CF0CF467</a></p> <p>SciFinder检索网址: <a href="https://scifinder.cas.org/">https://scifinder.cas.org/</a> (试用至2019年5月31日)</p>



# 如何获取SciFinder账号

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

- CONTACT INFORMATION--**: Includes input fields for First Name, Last Name, Email, Confirm Email, Phone Number, and Fax Number. It also features dropdown menus for Area of Research and Job Title.
- USERNAME AND PASSWORD--**: Includes input fields for Username, Password, and Re-enter Password. A small "Tips" link is visible next to the Password field.
- SECURITY INFORMATION--**: Includes a dropdown menu for Security Question and an input field for the Answer. A small "Why?" link is visible next to the Answer field.

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

请注意：

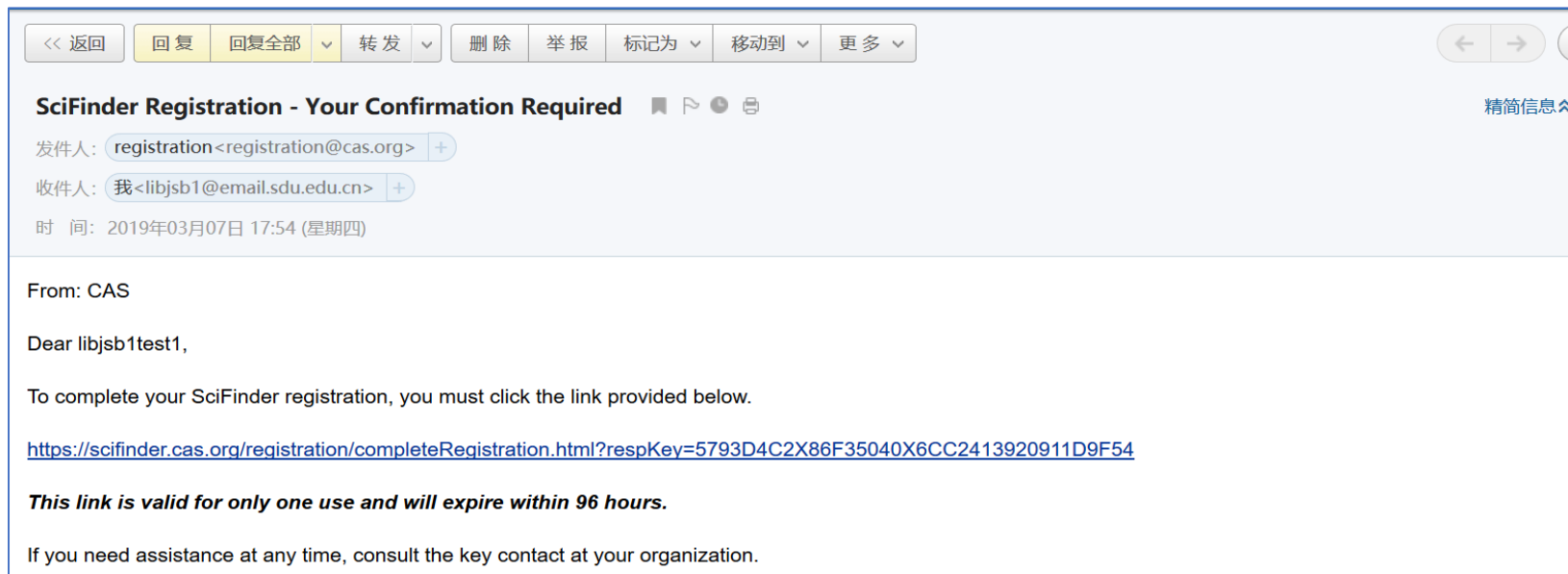
1. 必须输入**真实姓名**和邮箱。  
2. 用户名必须是唯一的，且包含 5-15 个字符。它可以只包含字母或字母组合、数字和/或以下特殊字符：

- - (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. 从下拉列表中选择一个密码提示问题并给出答案。  
单击 Register (注册) 。

# 如何获取SciFinder账号



打开并阅读 CAS 的电子邮件（必须在48小时内点击，否则需要重新注册）

注意垃圾邮件、未知邮件、订阅邮件等来自@cas.org的邮件

# 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.

注册成功后直接点击<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
- 请提供真实姓名信息
- 严禁过量下载
- 严禁账号分享
- 严禁将账号用于非学术研究

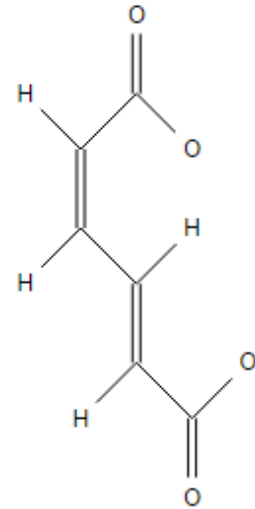


更多培训资料请访问

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

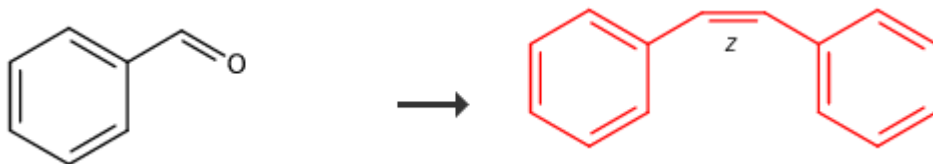
# 上机练习

- 检索“中药在帕金森病（**Parkinson's disease**）治疗中的应用”的文献。被引次数最高的文献来自哪份期刊？发文最多的研究机构是哪家？该研究领域专利多还是期刊多？
- 找出分析五味子素（**Schisandrin**）的相关文献？用TLC方法做分析的文献？
- 检索环系上含有以下结构片段的天然产物



# 上机练习

1. 检索以下反应:



2. 检索保护吡啶环上N原子而环上的羟基不受影响的反应?

美国化学文摘社北京代表处

010-62508026

china@acs-i.org

