

朱传娴

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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 solv. 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

Hepatitis C

Homo sapiens

Pharmaceutical coated tablets

Drug bioavailability

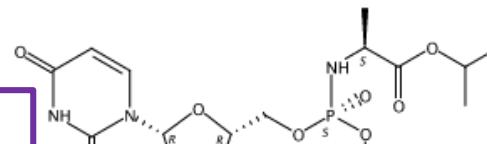
Hepatitis C virus

Human

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

- 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
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- SciFinder常见问题及解决

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[New Commercial Source Logos](#)

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检索入口

定题追踪

检索完, 请点击退出

Explore Saved Searches SciPlanner

REFERENCES: RESEARCH TOPIC

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

Search Advanced Search

REFRENCES

- 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

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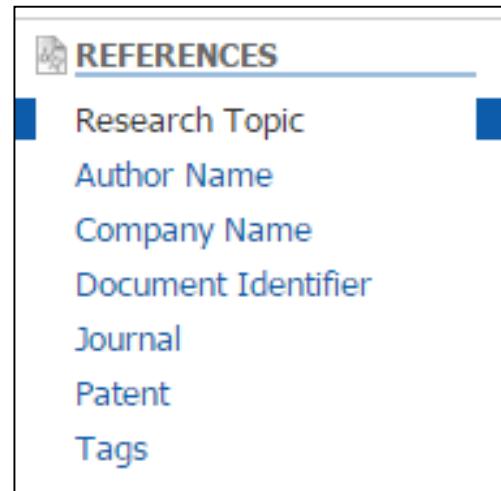
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■ 文献检索方法

- 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 shows the SciFinder interface. At the top, there is a navigation bar with 'CAS Solutions ▾', the SciFinder logo, and buttons for 'Explore ▾', 'Saved Searches ▾', and 'SciPlanner'. On the left, a sidebar under 'REFERENCES' lists 'Research Topic' (which is selected, indicated by a blue bar), 'Author Name', 'Company Name', 'Document Identifier', 'Journal', 'Patent', and 'Tags'. Below this is a section for 'SUBSTANCES' with 'Chemical Structure' and 'Markush' options. The main search area is titled 'REFERENCES: RESEARCH TOPIC ?' and contains the search term 'Chinese Medicine in Cataract' in a blue box. Below the search term, 'Examples:' are listed: 'The effect of antibiotic residues on dairy products' and 'Photocyanation of aromatic compounds'. A large blue 'Search' button is at the bottom of this section. Below the search button is a link to 'Advanced Search'. A purple box at the bottom right contains the text '关键词之间用介词连接： in, with, of...'. The SciFinder logo is at the bottom right of the page.

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

- | | | |
|-------------------------------------|--|--------|
| <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

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

REFERENCES ?

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Analyze Refine Categorize

Display Options

Sort by: Citing References ▾

Accession Number
Author Name
Citing References
Publication Year
Title

Page: 1 of 17

Li Jun 6
Name Not
Translated 4
Ye Mingwei 4
Zhang Xiuhua 4
Li Shuguang 3
Li Xianqiang 3
Qin Zhengqiang 3
Wang Weilin 3

Characterization effects and mechanism of Radix Angelicae dahuricae extracts on baicalin in Radix Scutellariae using in vivo and in vitro
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...
~5

2. Identification of a PRX variant in a Chinese family with congenital cataract by exome sequencing
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...
~3

Citing Reference: 帮助找到最重要的文献



文献检索结果

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

REFERENCES ②

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Sort by: Citing References ▾

0 of 322 References Selected

获取原文

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

Yan Huiwei 2

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
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...

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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

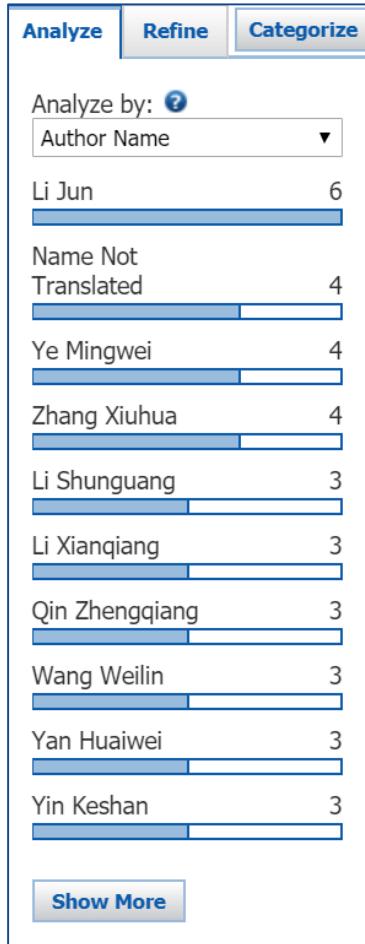
Background: Congenital **cataract** is a common cause of childhood **vision** impairment or blindness with genetic and clin. heterogeneity. The aim of this study was to identify the disease-assocd. gene in a **Chinese** family with congenital **cataract**. Methods: A four-generation **Chinese** family 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...

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文献检索结果的Analyze

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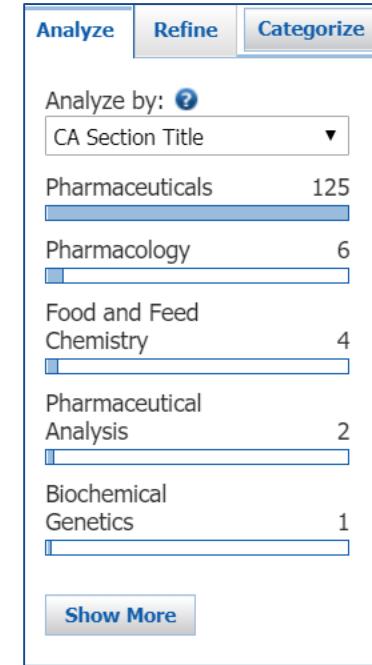
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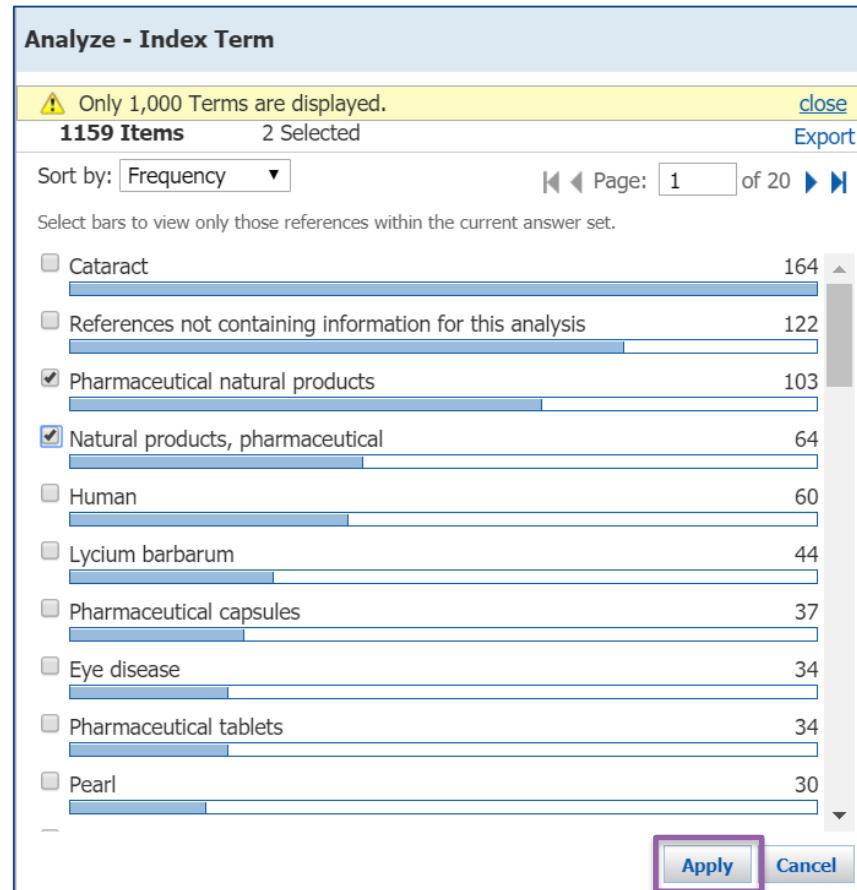
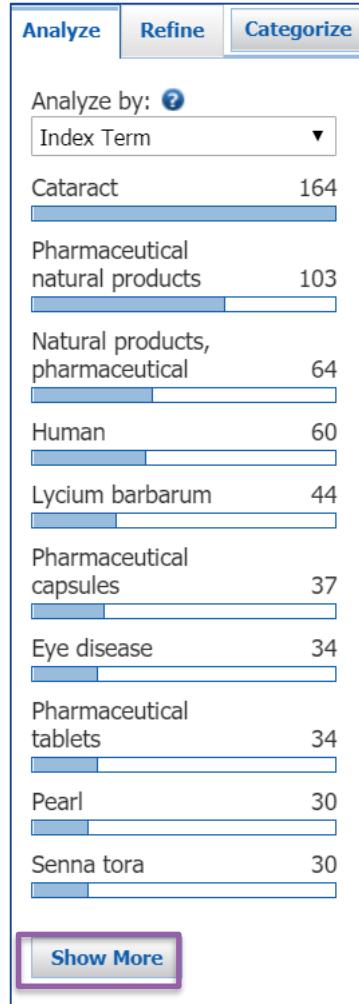
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- Author
- Company Name
- Document Type
- Publication Year
- Language
- Database

Document Type(s)

- Biography
- Book
- Clinical Trial
- Commentary
- Conference
- Dissertation
- Editorial
- Historical
- Journal
- Letter
- Patent
- Preprint
- Report
- Review

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Display Options

Sort by: Citing References

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 Zhongxiyi 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, preprns. contg. sulfur, anti-quinone preprns., inhibitors of aldose reductase (AR), vitamins and energy mixts., non-steroidal antiinflammatory drugs, **Chinese** herbal **medicine**, other drugs, and prospect in the future.

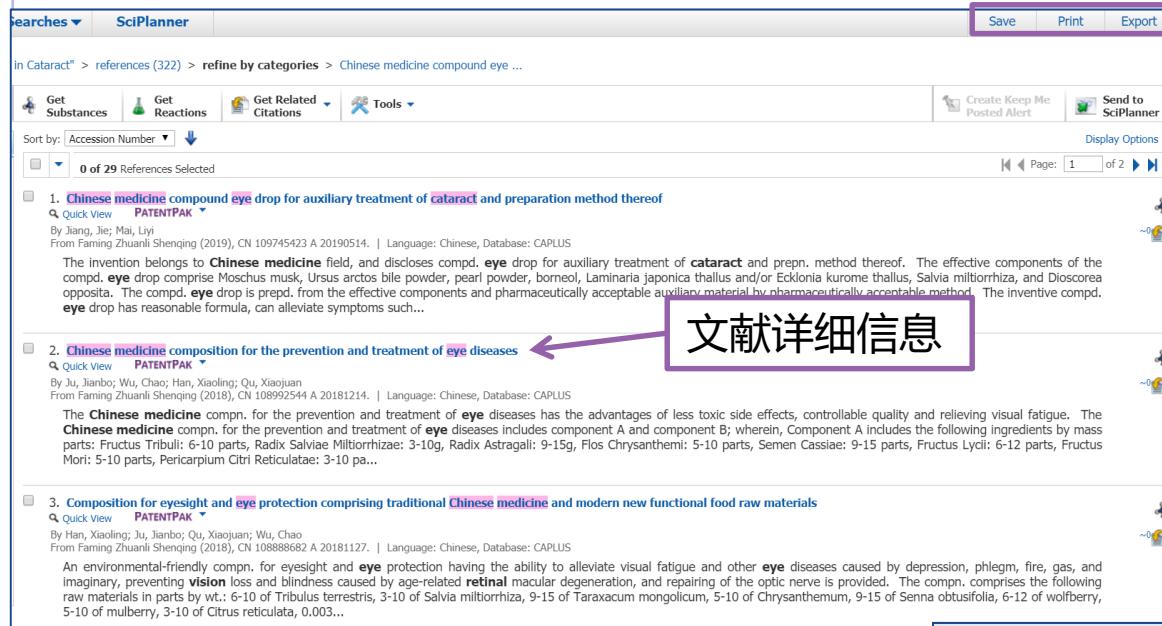
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文献检索结果的Categorize

学科领域 主分类	学科领域 副分类	Index Term	选中的Index Term																																					
<p>Categorize </p> <p>1. Select a heading and category.</p> <table border="1"><thead><tr><th>Category Heading</th><th>Category</th></tr></thead><tbody><tr><td>All</td><td>Medicine (120)</td></tr><tr><td>General chemistry</td><td>Substances in medicine (215)</td></tr><tr><td>Genetics & protein chemistry</td><td>Food (92)</td></tr><tr><td>Physical chemistry</td><td>Substances in food chemistry (25)</td></tr><tr><td>Polymer chemistry</td><td>Agriculture (7)</td></tr><tr><td>Biotechnology</td><td>Substances in biological uses (25)</td></tr><tr><td>Biology</td><td>Substances in adverse effects (14)</td></tr><tr><td>Technology</td><td>Toxicology & forensics (4)</td></tr><tr><td>Environmental chemistry</td><td></td></tr><tr><td>Analytical chemistry</td><td></td></tr><tr><td>Catalysis</td><td></td></tr></tbody></table> <p>2. Select index terms of interest.</p> <table border="1"><thead><tr><th>Index Terms</th></tr></thead><tbody><tr><td>capsules</td></tr><tr><td><input type="checkbox"/> Pharmaceutical tablets 34</td></tr><tr><td><input type="checkbox"/> Ethanol 22</td></tr><tr><td><input type="checkbox"/> Ophthalmic solutions 21</td></tr><tr><td><input checked="" type="checkbox"/> Salvia miltiorrhiza 20</td></tr><tr><td><input type="checkbox"/> Pharmaceutical decoctions 18</td></tr><tr><td><input type="checkbox"/> Pharmaceutical granules 18</td></tr><tr><td><input type="checkbox"/> Ophthalmic drug delivery systems 16</td></tr><tr><td><input type="checkbox"/> Pharmaceutical powders 15</td></tr><tr><td><input checked="" type="checkbox"/> Alisma orientale 12</td></tr><tr><td><input type="checkbox"/> Chinese medicine 12</td></tr><tr><td><input type="checkbox"/> Pharmaceutical solutions 11</td></tr></tbody></table> <p>Selected Terms</p> <p>Click 'x' to remove the category from 'Selected Terms'</p> <p><input checked="" type="checkbox"/> Biotechnology > Medicine (2 Terms)</p> <p>Biotechnology > Medicine > 2 Index Term(s) Selected</p> <p>OK Cancel</p>				Category Heading	Category	All	Medicine (120)	General chemistry	Substances in medicine (215)	Genetics & protein chemistry	Food (92)	Physical chemistry	Substances in food chemistry (25)	Polymer chemistry	Agriculture (7)	Biotechnology	Substances in biological uses (25)	Biology	Substances in adverse effects (14)	Technology	Toxicology & forensics (4)	Environmental chemistry		Analytical chemistry		Catalysis		Index Terms	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
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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



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

Sort by: Accession Number ▾

0 of 29 References Selected

1. Chinese medicine compound eye drop for auxillary treatment of cataract and preparation method thereof

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

3. Composition for eyesight and eye protection comprising traditional Chinese medicine and modern new functional food raw materials

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文献详细信息

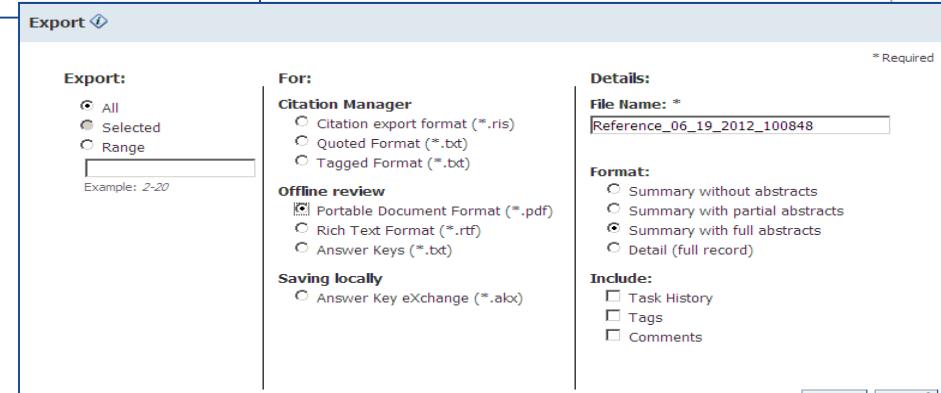
Save: 保存在服务器上，方便以后登陆查看，每次可存1万条记录。

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Export: All Selected Range Example: 2-20

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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

文献信息一题录、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	PDF PDF+ Viewer	A		Dec 14, 2018	CN 2018-11062718	Sep 12, 2018

Priority Application

CN 2018-11062718	Sep 12, 2018
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Indexing

Concepts	重要概念
	Pharmaceutical natural products
	Chaihu; Chinese medicine compn. for the prevention and treatment of eye diseases
Acer truncatum	Adenophora
Asthenopia	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 PATENTPAK
9004-32-4 Sodium carboxymethylcellulose	Page 7 in PATENTPAK
9004-53-9 Dextrin	Page 8 in PATENTPAK
9004-61-9 Hyaluronic acid	Page 7 in PATENTPAK
9063-38-1 Sodium Carboxymethyl starch	Page 7 in PATENTPAK
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 PATENTPAK
507-70-0	Page 2 in PATENTPAK
1309-38-2 Magnetitum, biological studies	Page 2 in PATENTPAK
7235-40-7 β-Carotene	Page 2 in PATENTPAK
11103-57-4 Vitamin A	Page 2 in PATENTPAK

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 Zhanli Shengqing
16pp.
Patent
2018
CODEN:CNXXEV

ACCESSION NUMBER
2018:2488106
CAN170:140195
CAPLUS

LANGUAGE
Chinese

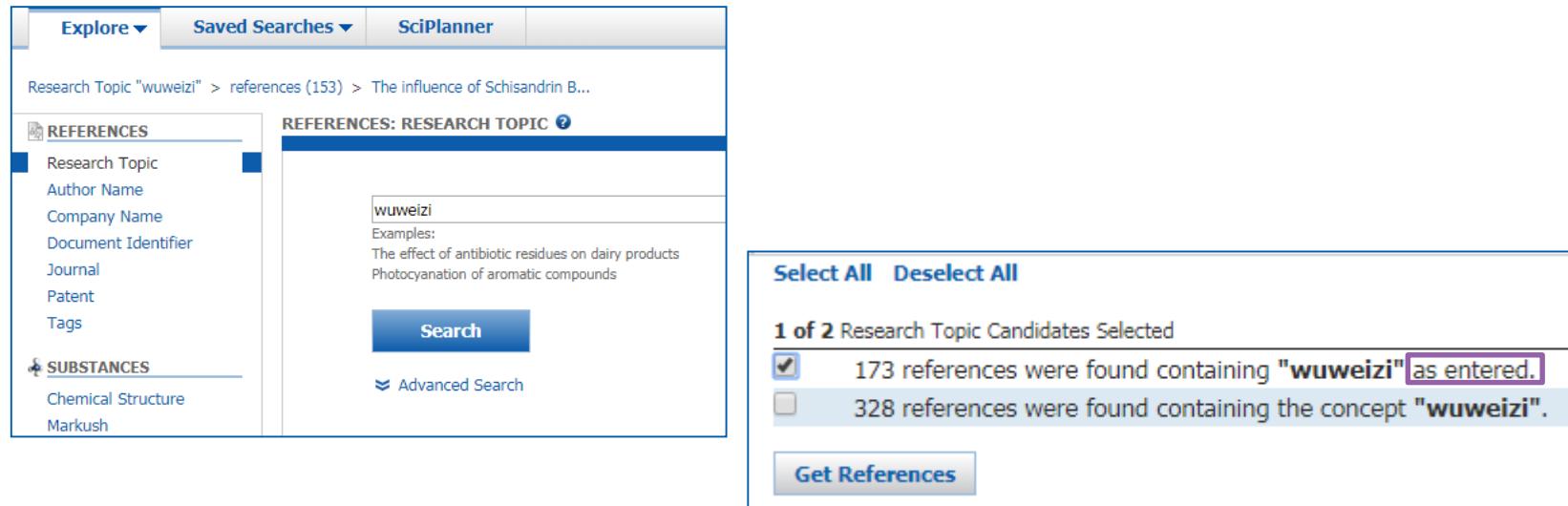


文献检索——中草药

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 interface with the following details:

- Header:** Explore ▾, Saved Searches ▾, SciPlanner
- Breadcrumbs:** Research Topic "wuweizi" > references (153) > The influence of Schisandr... (partially visible)
- Left Sidebar (REFERENCES):**
 - Research Topic
 - Author Name
 - Company Name
 - Document Identifier
 - Journal
 - Patent
 - Tags
- Left Sidebar (SUBSTANCES):**
 - Chemical Structure
 - Markush
- Search Panel:**
 - REFRENCES: RESEARCH TOPIC** (highlighted)
 - wuweizi** (search term)
 - Examples:
The effect of antibiotic residues on dairy products
Photocyanation of aromatic compounds
 - Search** button
 - Advanced Search** link
- Bottom Panel:**
 - Select All Deselect All**
 - 1 of 2 Research Topic Candidates Selected**
 - 173 references were found containing "**wuweizi**" as entered.
 - 328 references were found containing the concept "**wuweizi**".
 - Get References** button

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

Sort by: Accession Number ⓘ Display Options

0 of 153 References Selected

Page: 1 of 8

Analyze by: ⓘ

Author Name

Author Name	Count
Huang Min	3
Olaide 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

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 β -amyloid protein A β 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

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

Sort by: Accession Number ▾

0 of 17542 References Selected

Remove Duplicates Combine Answer Sets Add Tag

Display Options Page: 1 of 878

Analyze by: Author Name

Retrieving data...

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 Zuanli Shenqing [Machine Translation components: Gard, chinenesis 8-12 g, Medicata Fermentata]

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	Date Saved
wuweizi (153)	Nov 3, 2017
Research Topic "wuweizi" > references (153)	
poo (91)	Oct 20, 2017
Research Topic "suzuki reaction with catalyst" > references (91)	
r4r (139)	Oct 20, 2017
Research Topic "Modification of Azithromycin" > references (139)	
1996化工学报 (220)	Oct 9, 2017
Journal "Huanggong Xuebao" with limiters > references (497) > citing references (220)	
小剂量 (212)	Oct 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

wuder, characterized by the following weight of 5-25 g, Dolichos lablab 15-25 gram, **Schisandra chinensis** 8-12 g, Raphani Semen 8-12 grams, 8-12 g, Massa

SCI-FINDER® A CAS SOLUTION

文献检索——中草药

CAS Solutions ▾ Preferences | SciFinder Help ▾ Sign Out

SCI-FINDER®
A CAS SOLUTION

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 ▾

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

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].

By Jin, Yunlong
From Faming Zhanli 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].

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

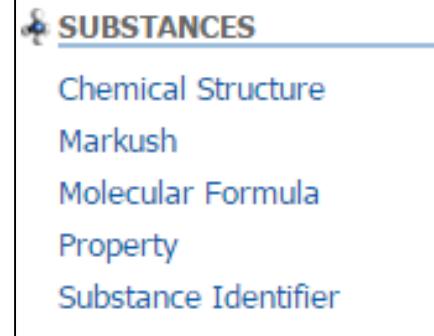
提纲

- 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 shows the SciFinder interface. At the top, there is a navigation bar with 'CAS Solutions ▾', the SciFinder logo, and menu items 'Explore ▾', 'Saved Searches ▾', and 'SciPlanner'. On the left, there are two main sections: 'REFERENCES' (with links to Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, and Tags) and 'SUBSTANCES' (with links to Chemical Structure, Markush, Molecular Formula, Property, and Substance Identifier). The main content area is titled 'SUBSTANCES: SUBSTANCE IDENTIFIER ?'. It contains a text input field with the placeholder 'qinghaosu', a note 'Enter one per line. Examples: 50-00-0 999815 Acetaminophen', and a 'Search' button.

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.

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

CAS Registry Number 63968-64

 ~4,864  ~131 

C₁₅ H₂₂ O₅
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**S*,6*R*,8*a**S*,9*R*,12*S*,12*a**R*)-

Molecular Weight
282.33

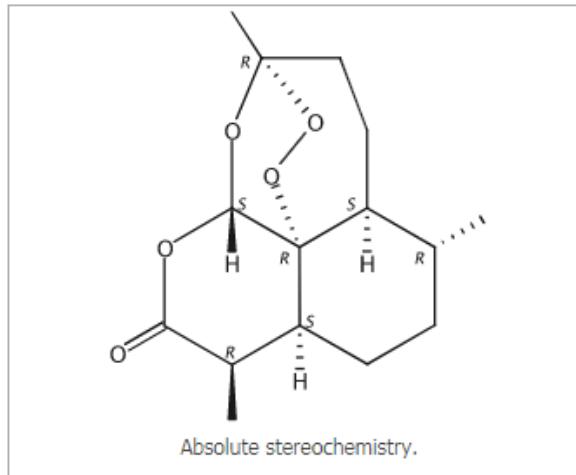
Melting Point (Experimental)
Value: 156-157 °C

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

Density (Experimental)
Value: 1.300 g/cm³

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**B*,6*B*,8*a**B*,9*a*,12*B*,12*a**R*^{*}]-
(3*R*,5*a**S*,6*R*,8*a**S*,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...](#)

由物质获得文献, 反应, 供应商等信息



物质详情

实验数据与实验谱图

EXPERIMENTAL PROPERTIES

EXPERIMENTAL SPECTRA

[1H NMR](#) [13C NMR](#) [Hetero NMR](#) [IR](#) [Mass](#) [Raman](#) [UV and Visible](#) [Additional Spectra](#)

13C NMR Properties

Value

Condition

Note

Carbon-13 NMR Spectrum

[See spectrum](#)

(3) ACD

Carbon-13 NMR Spectrum

[See spectrum](#)

(4) ACD

Carbon-13 NMR Spectrum

[See full text](#)

1 of 8

(5) CAS

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

[1H NMR](#) [13C NMR](#)

1H NMR Properties

Value

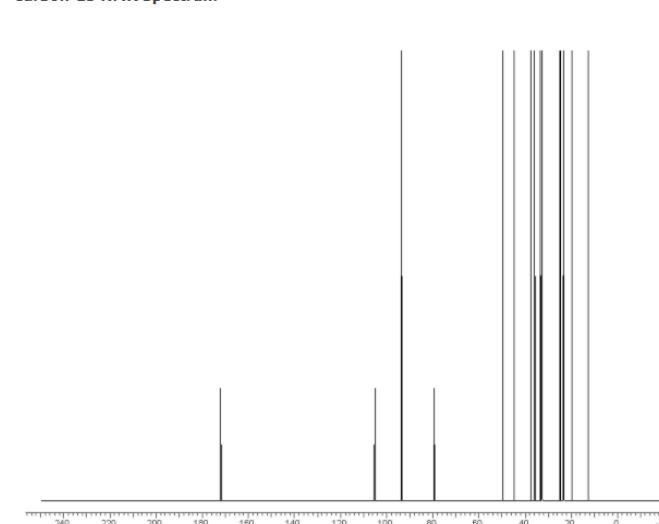
Proton NMR Spectrum

[See spectrum](#)

Notes

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

Carbon-13 NMR Spectrum



Print

SPECTRUM ID
7MED36_38.C

CAS REGISTRY NUMBER
63968-64-9

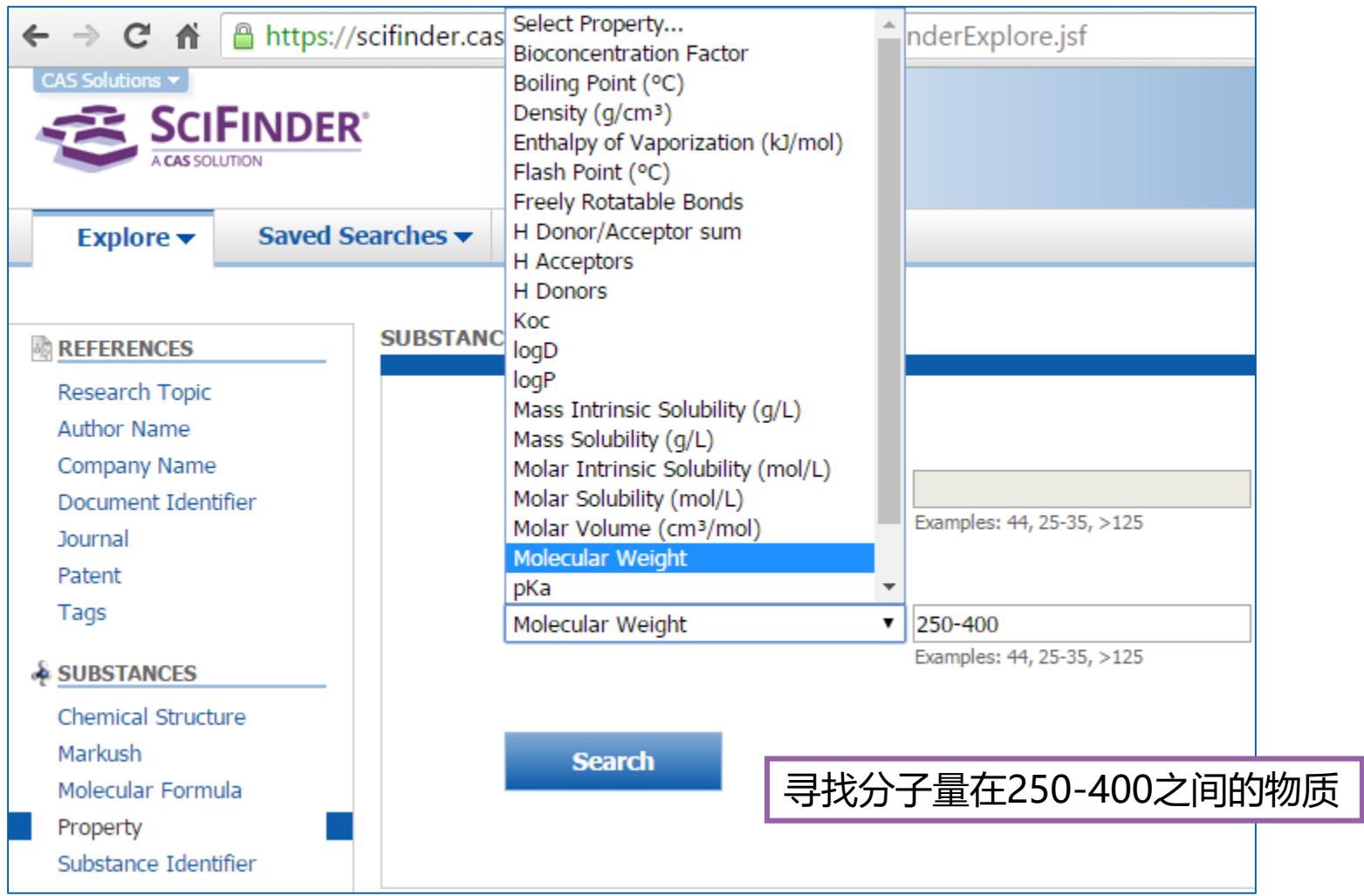
FORMULA
C₁₅ H₂₂ O₅

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

NUCLEUS
13C

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

物质检索——Property explore



https://scifinder.cas.org

CAS Solutions

SCI-FINDER®
A CAS SOLUTION

Explore ▾ Saved Searches ▾

REFERENCES

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

SUBSTANCES

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

Select Property...

- Bioconcentration Factor
- Boiling Point (°C)
- Density (g/cm³)
- Enthalpy of Vaporization (kJ/mol)
- Flash Point (°C)
- Freely Rotatable Bonds
- H Donor/Acceptor sum
- H Acceptors
- H Donors
- Koc
- logD
- logP
- Mass Intrinsic Solubility (g/L)
- Mass Solubility (g/L)
- Molar Intrinsic Solubility (mol/L)
- Molar Solubility (mol/L)
- Molar Volume (cm³/mol)
- Molecular Weight**
- pKa
- Molecular Weight

Search

Examples: 44, 25-35, >125

250-400

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

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

Sort by: CAS Registry Number

0 of 45142315 Substances Selected

1. 1986293-22-4

CN(CCCc1ccccc1)c2ccnc(Br)c2

C₁₅ H₁₇ Br N₂
3-Pyridinamine, 2-bromo-*N*-(3-phenylbutyl)-

Key Physical Properties

2. 1986293-21-3

CCN(CCC(F)F)c1ccnc2c1CCOC2

C₁₁ H₁₆ Cl F₂ N₃ O
4-Pyrimidinamine, *N*-(2-chloroethyl)-*N*-(2,2-difluoroethyl)-6-ethoxy-5-methyl-

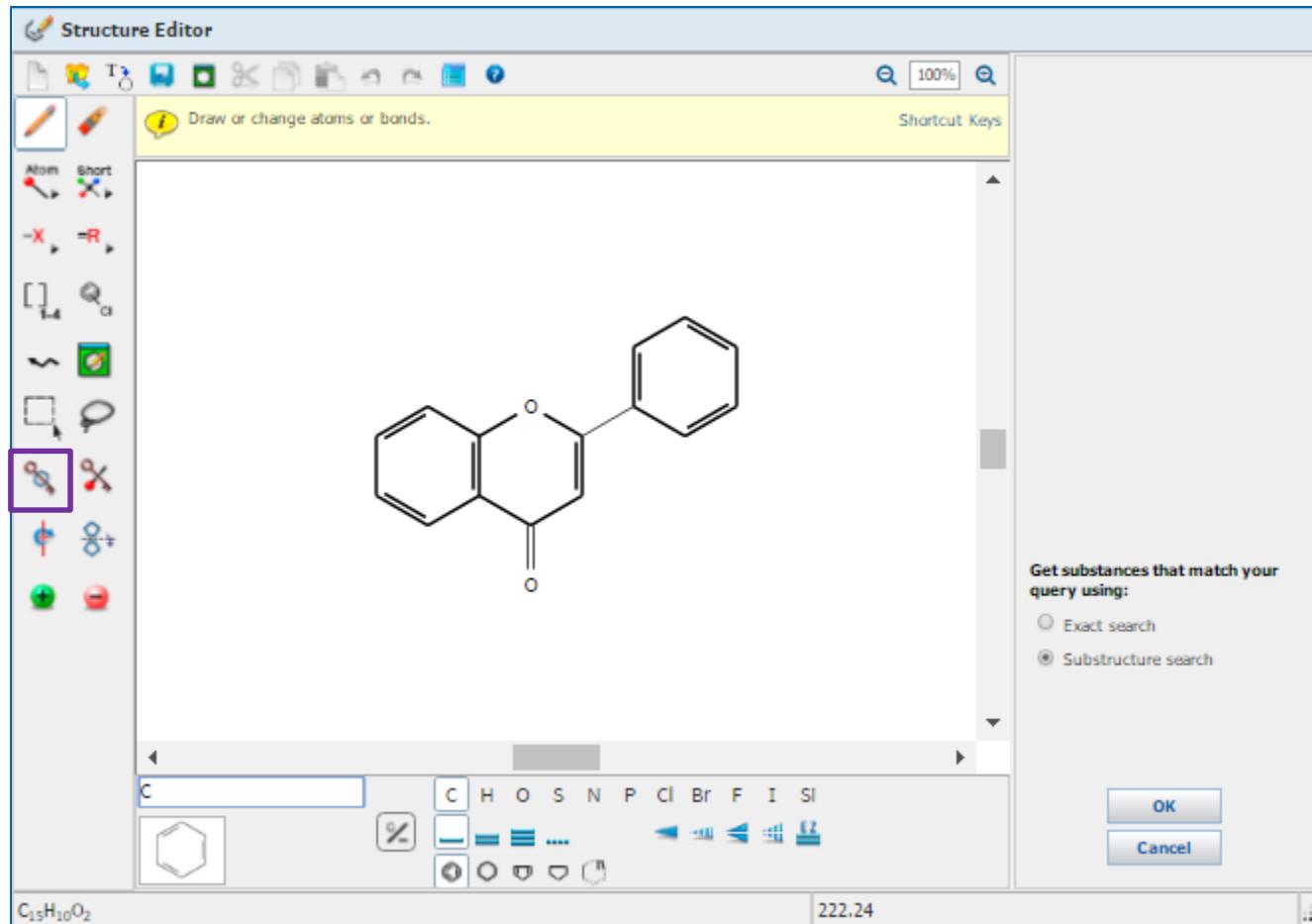
Key Physical Properties

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

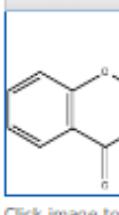
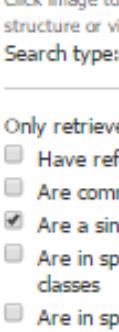
SUBSTANCES 

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

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

SUBSTANCES ? Get References Get Reactions Get Commercial Sources Tools

Analyze Refine Sort by: Relevance ▼ ▼

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

0 of 16901 Substances Selected

1. 1373355-19-1 ?

~3 Get References Get Reactions Get Commercial Sources

C1=C2C=C(C=C2C(=O)c3ccccc3)C=C1c4ccccc4

C17H14O2
4H-1-Benzopyran-4-one, 2-(3,5-dimethylphenyl)-

► Key Physical Properties

2. 912915-64-1 ?

~6 Get References Get Reactions Get Commercial Sources

C15H10O4
4H-1-Benzopyran-4-one, 2-(3,5-dihydroxyphenyl)-

► Key Physical Properties

4. 6665-68-5 ?

~38 Get References Get Reactions Get Commercial Sources

C1=C2C=C(C=C2C(=O)c3ccccc3)C=C1Cc4ccccc4

5. 22395-22-8 ?

~269 Get References Get Reactions Get Commercial Sources

CC1=C2C=C(C=C2C(=O)c3ccccc3)C=C1Oc4ccccc4

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

无机金属盐：金属离子和阴离子间用点（.）分开

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

C₁₂H₂₆O₄S.Na

Examples:
H₄SiO₄
(C₃H₆O.C₂H₄O)_x

Search

1. 151-21-3 (Component: 151-41-7)

~84904 ~276

CC(C)CCCCCCCCCCCC(=O)O[Na+].Na

C₁₂H₂₆O₄S.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

 **SciFinder**[®]
A CAS SOLUTION

物质检索——结构

REFERENCES

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

SUBSTANCES

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

REACTIONS

- Reaction Structure

SUBSTANCES: CHEMICAL STRUCTURE [?](#)

Structure Editor:

Java Non-Java

Click to Edit

Import CXF

Search

Advanced Search Always Show

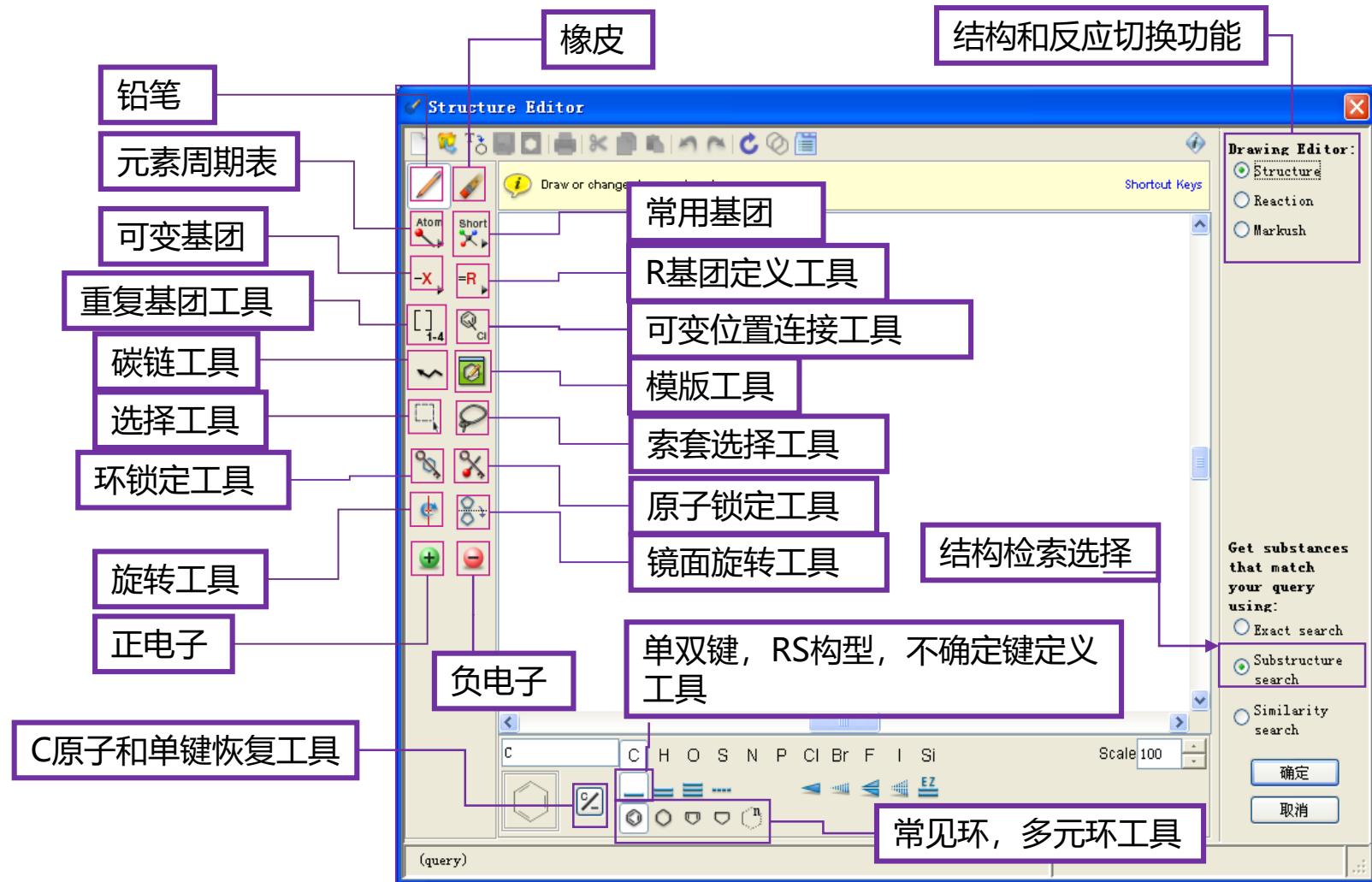
Search Type:

- Exact Structure
- Substructure
- Similarity

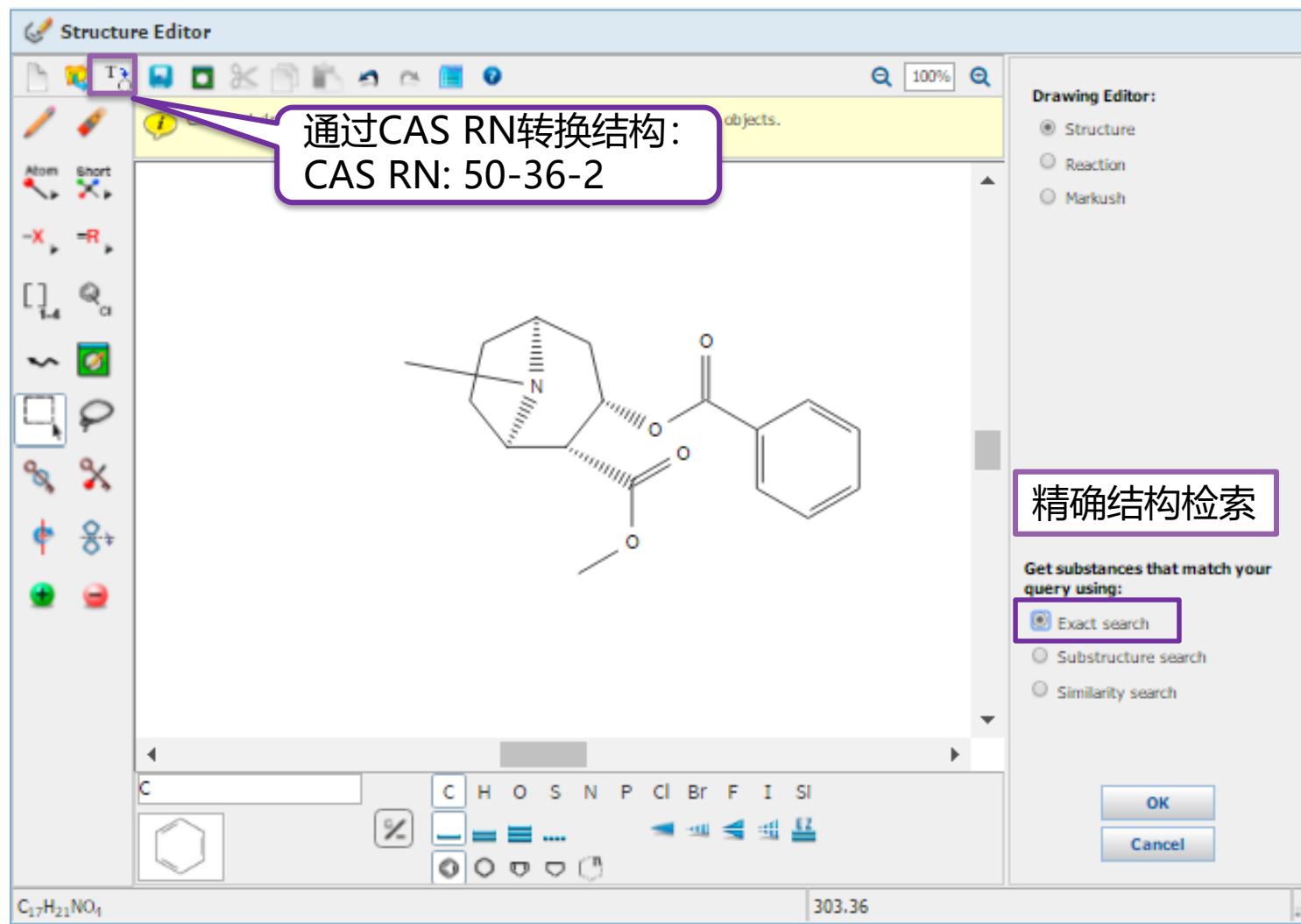
Show precision analysis

 **ChemDraw®**
Launch a SciFinder substance or reaction search

物质检索——结构



物质检索——精确结构检索

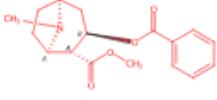


精确结构检索结果

Get References | Get Reactions | Get Commercial Sources | Tools ▾ | Create Posted

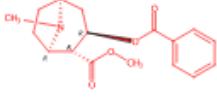
Sort by: Relevance ▾

0 of 6 Substances Selected

1. 668-19-9  Absolute stereochemistry.

CN1[C@H]2[C@H](C[C@H]1C(=O)OC(=O)c3ccccc3)C(=O)OC2

可卡因

2. 114599-38-1  Absolute stereochemistry.

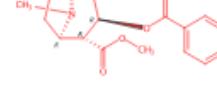
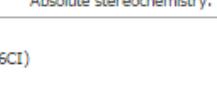
CN1[C@H]2[C@H](C[C@H]1C(=O)OC(=O)c3ccccc3)C(=O)OC2

可卡因组合物

668-19-9
C12H21NO4

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

3. 109496-04-0  (Component: 668-19-9)  Absolute stereochemistry.

CN1[C@H]2[C@H](C[C@H]1C(=O)OC(=O)c3ccccc3)C(=O)OC2

盐酸可卡因

88-89-1
C6H3N3O7

3,4-dinitrophenol, 2-hydroxy-

O=[N+]([O-])c1cc(O)c([N+]([O-])=[N+]([O-])=O)cc1[N+]([O-])=[N+]([O-])=O

C17H21NO4.C6H3N3O7

Allococaine, picrate (6CI)

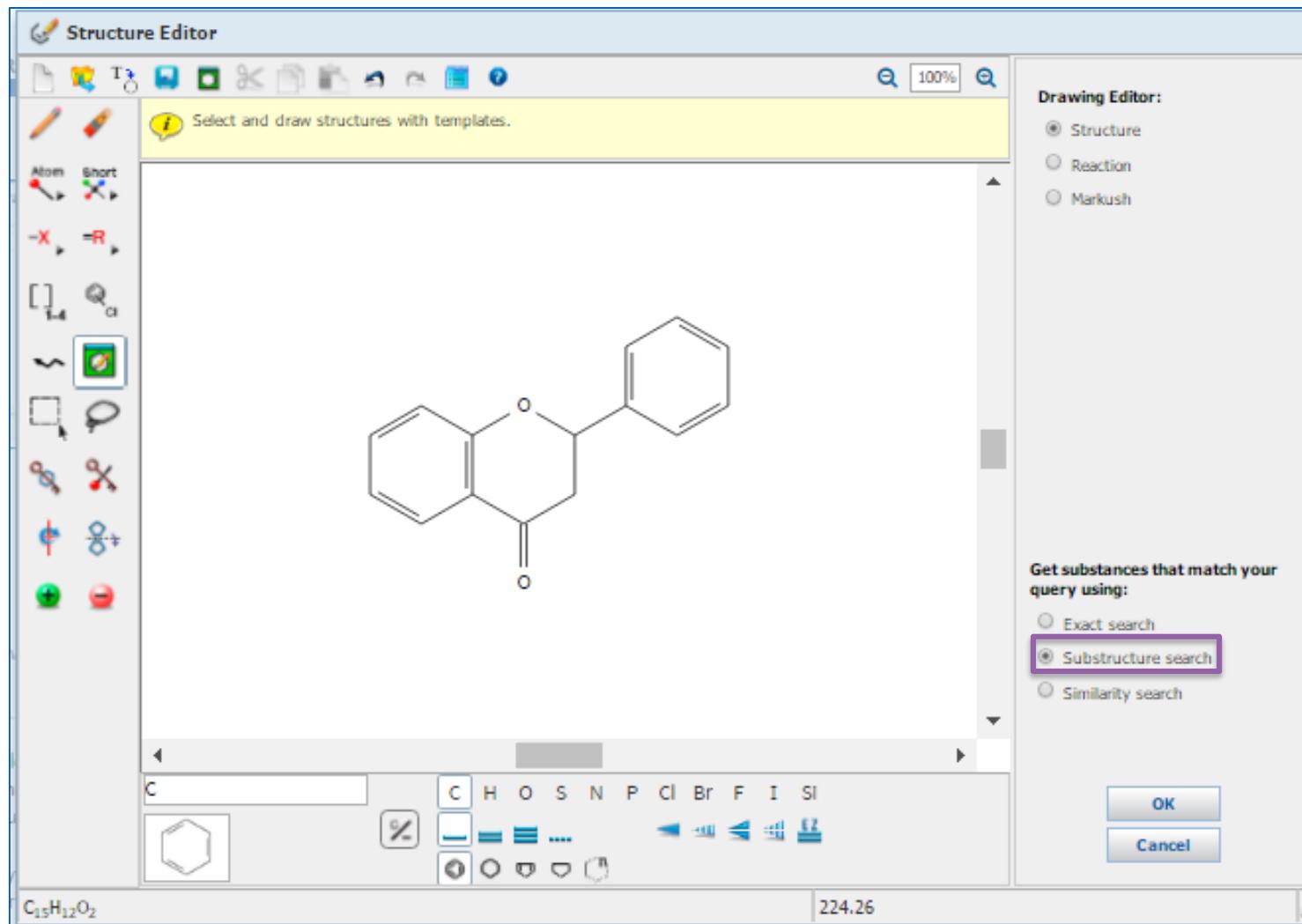
物质检索——精确结构检索

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

~2093 ~69

C1=C2C=C(C=C2C(=O)C3=C(C=C(C=C3)C=C4C=CC=C4)C=C1)C=C3C=C4C=C(C=C4)C=C3

C15H14O2
4H-1-Benzopyran-4-one, 2-phenyl-,
Key Physical Properties

2. 17002-31-2

~244 ~4

C1=C2C=C(C=C2C(=O)C3=C(C=C(C=C3)C=C4C=CC=C4)C=C1)C=C3C=C4C=C(C=C4)C=C3

Absolute stereochemistry., Rotat

10. 146196-91-0

~1 ~5

C15H14D2O2
2,3-dihydro-2-(phenyl-d3)- (9CI)

同位素

281. 123251-10-5

~3 ~1

取代物

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

295. 780723-19-5

~0

离子

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

284. 136116-23-9

~2

稠环物质

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

Key Physical Properties

亚结构检索结果的限定

Analysis Refine

Refine by: Chemical Structure

Isotope-Containing

Metal-Containing

Commercial Availability

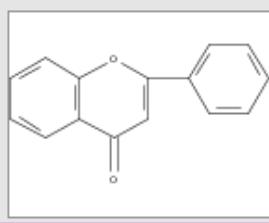
Property Availability

Property Value

Reference Availability

Atom Attachment

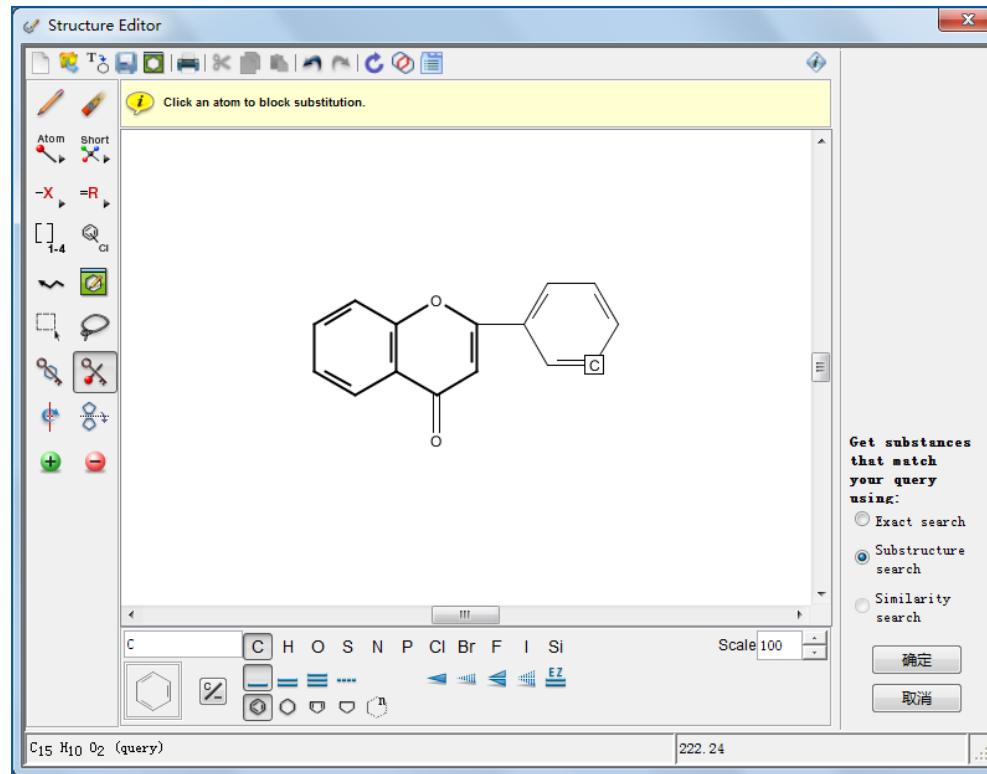
Chemical Structure:



Click image to change structure or view detail

Search type: **Substructure**

化学结构的再次限定



环锁定

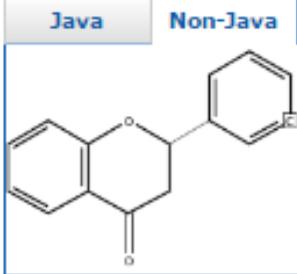


原子锁定

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

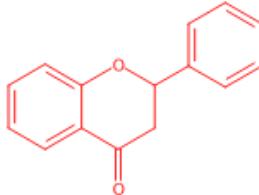
Get References Get Reactions Get Commercial Sources Tools

Sort by: Relevance

0 of 13826 Substances Selected

1. 487-26-3

~2093



C₁₅H₁₂O₂
4H-1-Benzopyran-4-one, 2,3-dihydro-2-phenyl-

Key Physical Properties

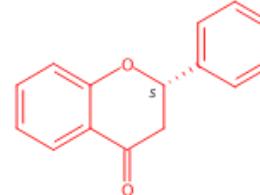
Regulatory Information
Spectra
Experimental Properties

4. 104550-32-5

~3

2. 17002-31-2

~244



Absolute stereochemistry, Rotation (-).

C₁₅H₁₂O₂
4H-1-Benzopyran-4-one, 2,3-dihydro-2-phenyl-, (2S)-

Key Physical Properties

Experimental Properties

5. 75524-43-5

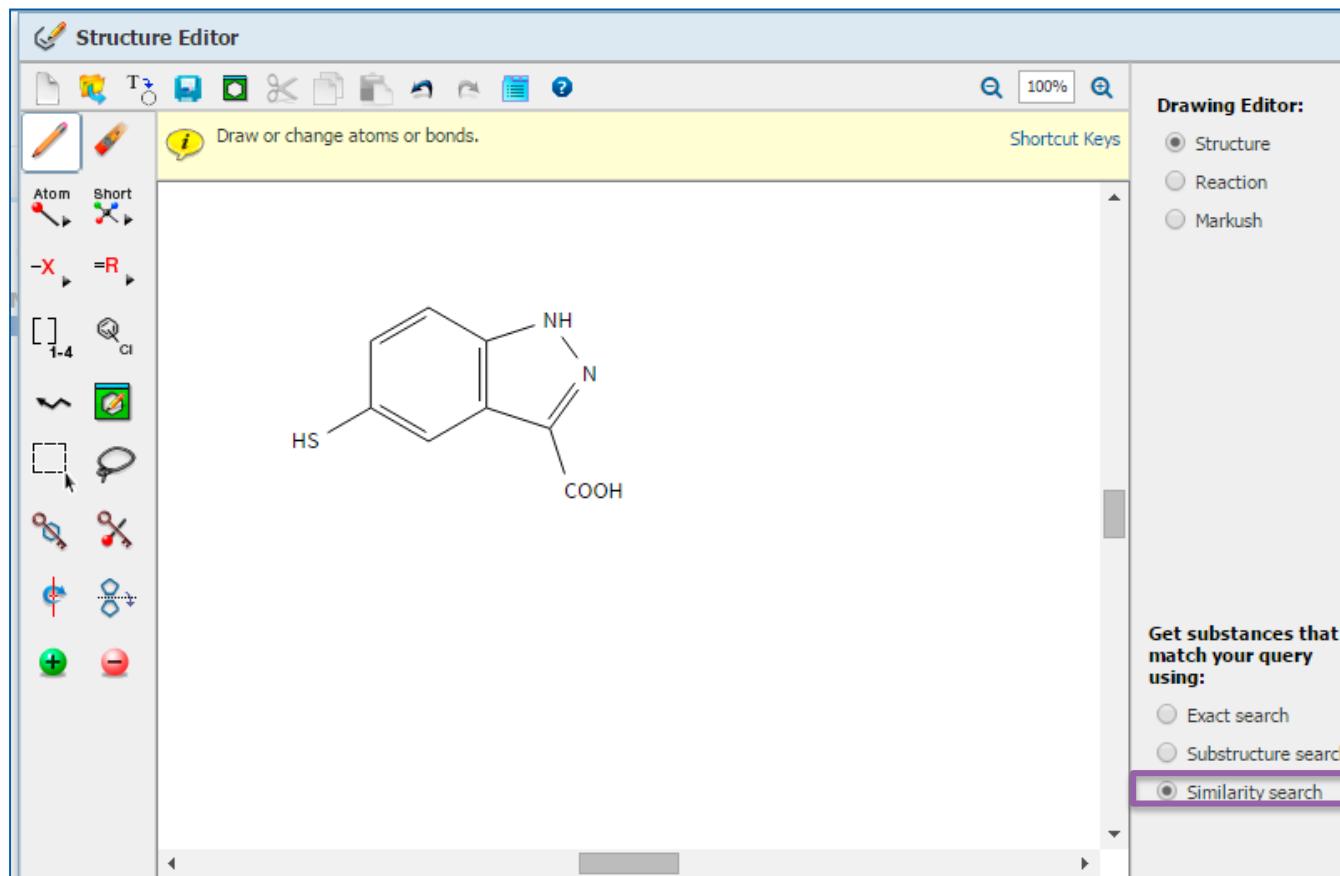
~2

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"/> ≥ 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

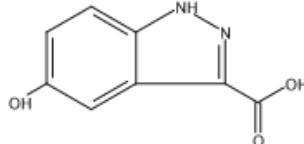
Get Substances

相似度越高，结构越相似

Score: 88

1. 885518-94-5

取代基变化



C₈ H₆ N₂ O₃

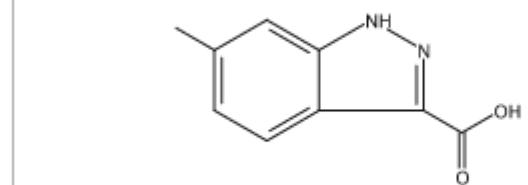
1H-Indazole-3-carboxylic acid, 5-hydroxy-

► Key Physical Properties

Score: 86

5. 858227-12-0

取代基位置变化



C₉ H₈ N₂ O₂

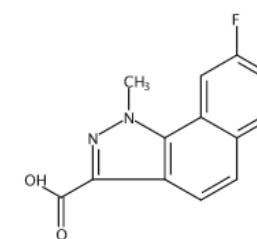
1H-Indazole-3-carboxylic acid, 6-methyl-

► Key Physical Properties

Score: 65

541. 1100422-

母体结构变化



C₁₃ H₉ FN₂O₂

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

► Key Physical Properties



SCI-FINDER®
A CAS SOLUTION

物质检索——相似结构检索

- 相似结构检索：

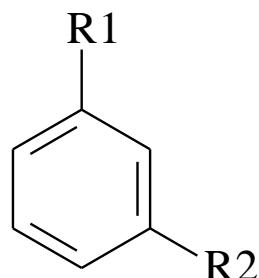
获得片段或整体结构与被检索结构相似的结果，母体结构可以被取代，也可以被改变

提纲

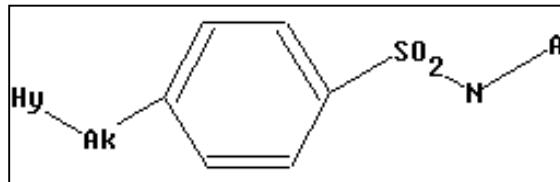
- 美国化学文摘社简介
- SciFinder简介及检索方式
 - 文献检索
 - 物质检索
 - Markush检索
 - 反应检索
 - SciPlanner
- SciFinder常见问题及解决

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



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

Structure Editor

Draw or change atoms or bonds.

Shortcut Keys

Drawing Editor:

- Structure
- Reaction
- Markush

Get Markush patents where the structure(s) are:

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

OK Cancel

Hy Ak

SCI-FINDER®
A CAS SOLUTION

Markush检索



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

Display Options

Page: 1 of 99

Analyze by:	
Document Type	1969
Patent	1969
Journal	1
Show More	

全部是专利

1. Compounds and methods for anticoagulation therapy

[Quick View](#) PATENTPAK

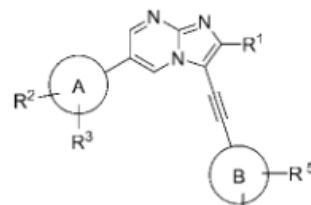
By Allende Rodriguez, Mikel; Hermida Santos, Jose; Montes Diaz, Ramon; Oyarzabal Santamarina, Julen
From PCT Int. Appl. (2016), WO 2016120432 A1 20160804. | Language: English, Database: CAPLUS

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)

[Quick View](#) PATENTPAK

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 [R¹ = H or halogen; ring A Ph or pyridyl; R², R³ (same or different) = hydrogen, halogen, C₁₋₄ alkyl or C₁₋₄ alkoxy each optionally substituted with 1-5 halogen atoms; or in case where R² and R³ are at the adjacent substitution position, R² and R³ together with ring A form C₅₋₈ 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; R⁴, R⁵ (same or different) = H, halogen, hydroxy, amino, -C(O)OR^a, -C(O)NR^aR^b, SO₃H, SO₂NR^aR^b, SO₂R^b, or NR^aSO₂R^b; R^a, R^b (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

 **REACTIONS**
Reaction Structure

- 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

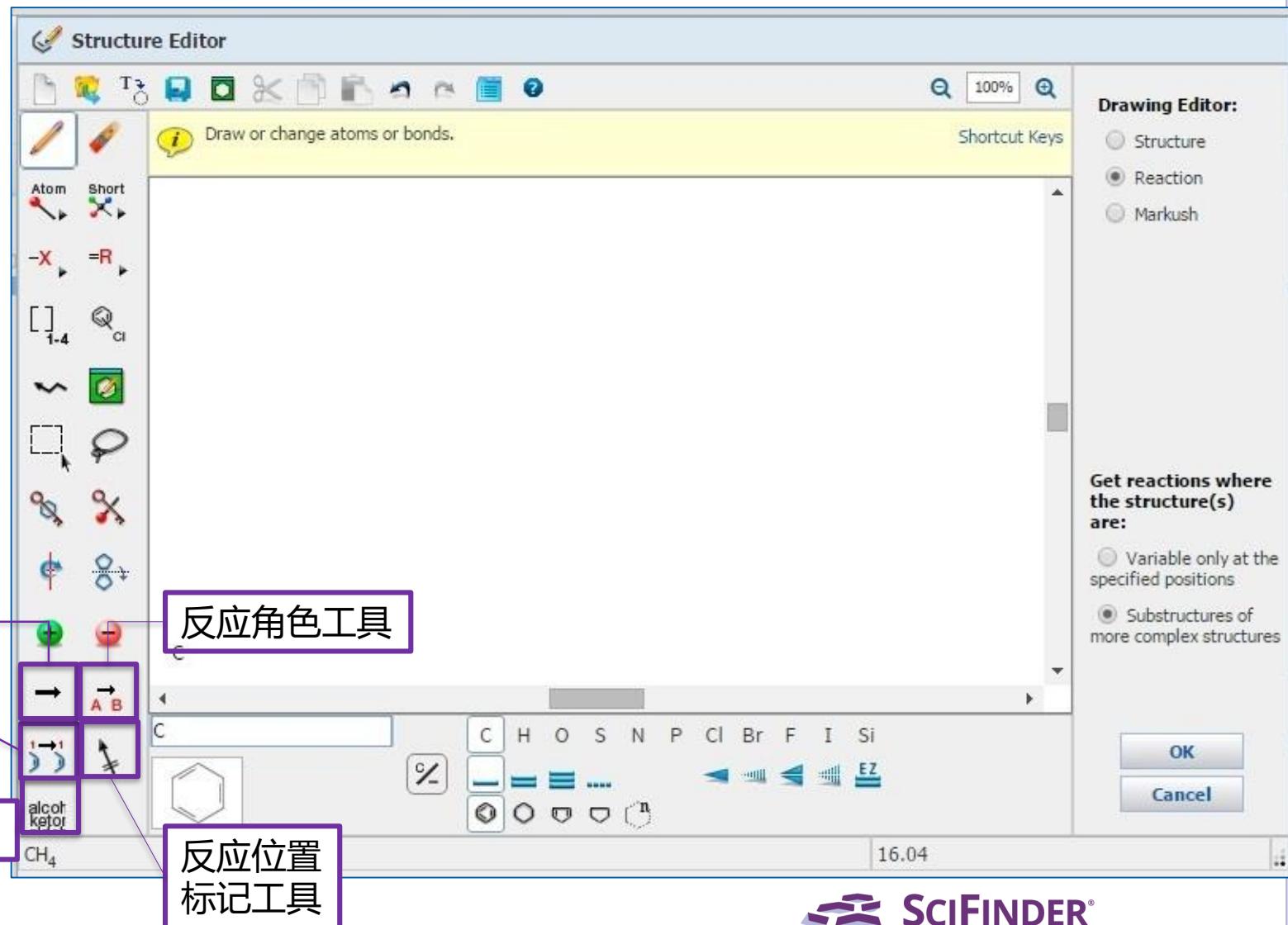
- 精确结构反应检索

- 亚结构反应检索

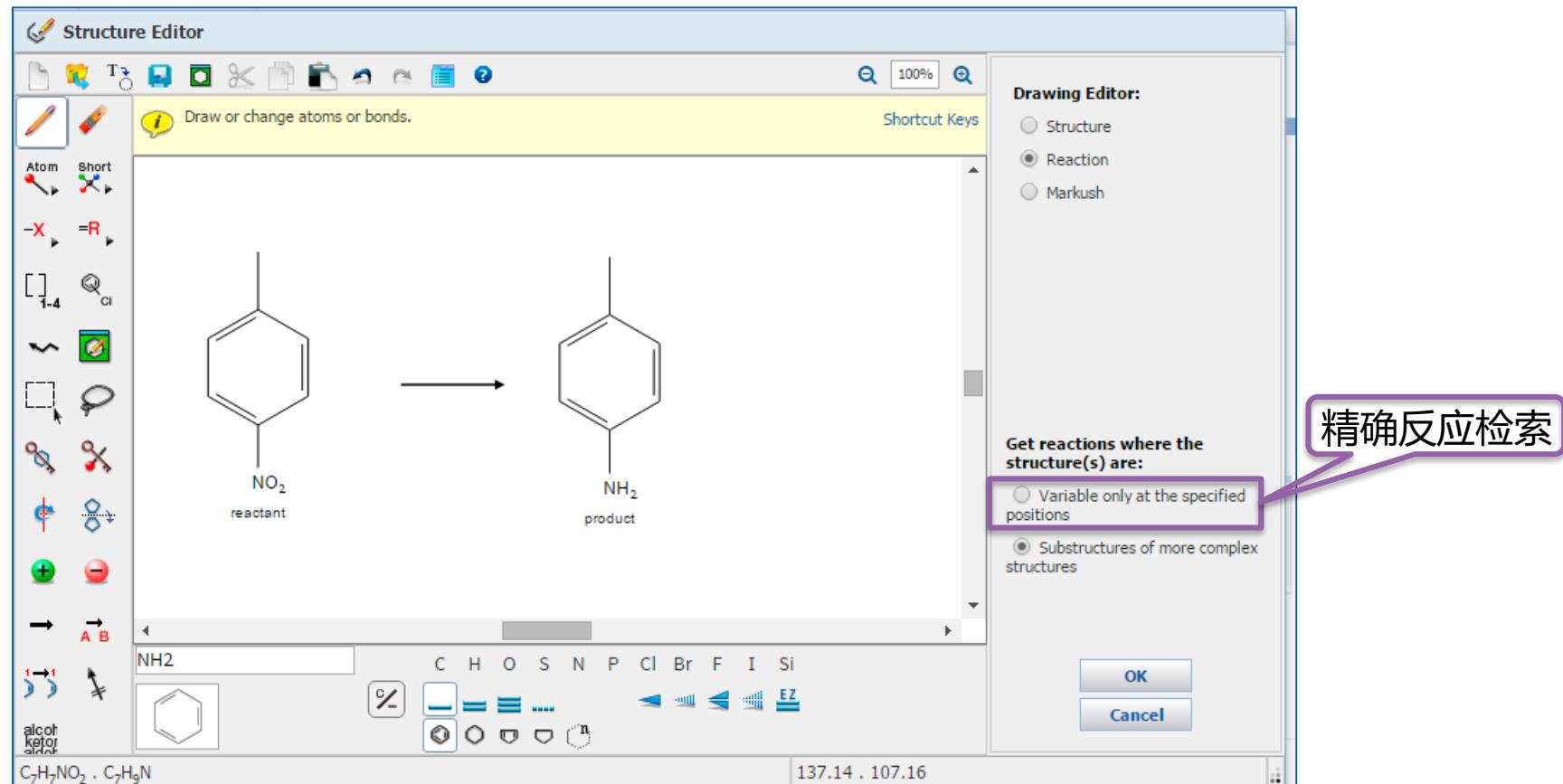
**Get reactions where
the structure(s)
are:**

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

反应绘制工具



SciFinder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。

Get References Tools ▾ Send to SciPlanner

Group by: **No Grouping** Sort by: **Relevance** Display Option

No Grouping Document Selected Transformation

1. View Reaction Detail Similar Reactions

Single Step Hover over any structure for more options.

Chemical reaction: 4-nitroanisole (O₂N-C₆H₄-CH₃) is converted to 4-aminanisole (NH₂-C₆H₄-CH₃). The yield is 100%. The reaction conditions are ~102 °C and ~122 °C.

Overview

Steps/Stages

1.1 R:NaBH₄, C:1832616-28-0, C:Ru, S:H₂O, 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

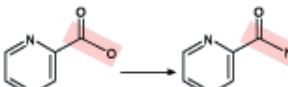
Narrow: 反应中心及扩展的原子和键

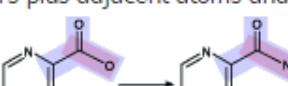
Get Similar Reactions [?](#)

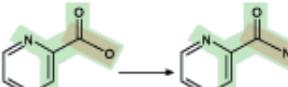
Retrieve similar reactions from:

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

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

2. Reduction of Nitro to Azo Compounds
11 Reactions

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

3. Reduction of Nitro to Azoxy Compounds
11 Reactions

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

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 ②

Get References Tools ▾ Send to SciPlann

Analyze Refine

Group by: No Grouping Sort by: Relevance

0 of 512 Reactions Selected

Page: 1 of 11

Analyze by: Reagent

Reagent	Count
H ₂	148
NaBH ₄	51
N ₂ H ₄ ·H ₂ O	43
KOH	17
CO	16
HCO ₂ H	16
NH ₄ ⁺ · HCO ₂ ⁻	16
H ₂ O	14
N ₂ H ₄	14
NaOH	14

Single Step Hover over any structure for more options.

1. View Reaction Detail



Overview

Steps/Stages

1.1 R:NaBH₄, C:1832616-28-0, C:Ru, S:H₂O, 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:H₂, R:Cs₂CO₃, C:1610424-70-8, C:1034343-98-0 (oxide), S:PhMe, 2 h, 100°C, 1 atm 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

Notes

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 H₂ to a mixture of nitroarene (0.3 mmol), Cs₂CO₃ (0.3 mmol), anisole as internal standard (0.3 mmol), and NHC-Pd-rGO (6×10^{-3} mmol, based on metal) in toluene (5 mL). The system was then evacuated and backfilled with H₂ 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

Get reaction structure(s)

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

Enol

Glycol

Cyclic Alcohol

Hydroxylamine

Halohydrin

Hemiacetal

N—OH

Phenol

Primary Alcohol

Secondary Alcohol

Cancel

AMINES

alcohols

ketones

aldehydes

C H O S N P Cl Br F I Si

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 ▾

Analyze Refine

Group by: No Grouping Sort by: Accession Number

0 of 1851074 Reactions Selected

Display Options

Send to SciPlanner

Refine by: ?

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

Product Yield: 100 %

Upper Limit: Example: 80

90 %

Lower Limit: Example: 20

Include answers that have no product yield

Refine

1. View Reaction Detail [Link](#)

13 Steps Hover over any structure for more options.

[Step 2.1] ~119

[Step 5.1] ~18

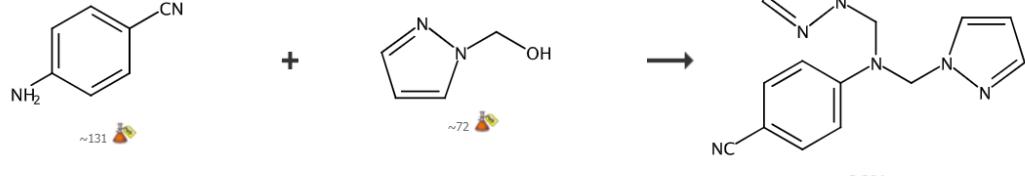
[Step 6.1] ~148

Overview

通过后处理工具筛选反应—Refine

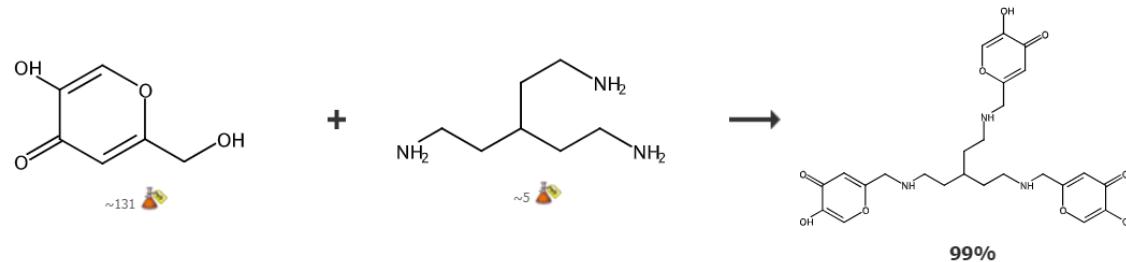
1. [View Reaction Detail](#) [Link](#) [Similar Reactions](#)

Single Step Hover over any structure for more options.



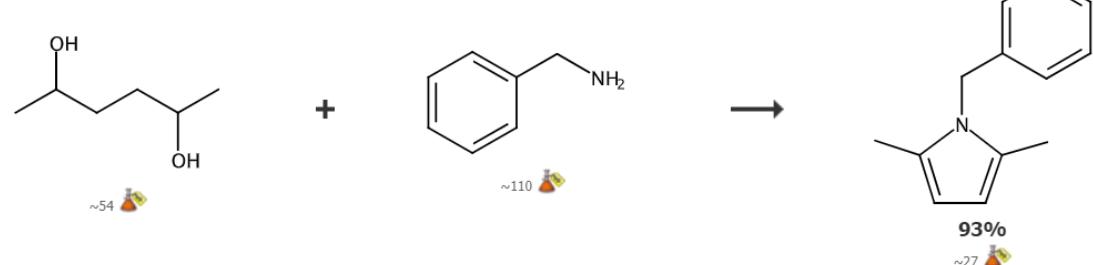
3. [View Reaction Detail](#) [Link](#) [Similar Reactions](#)

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

勾选想要的反应

3 Steps Hover over any structure for more options.

Send to SciPlanner

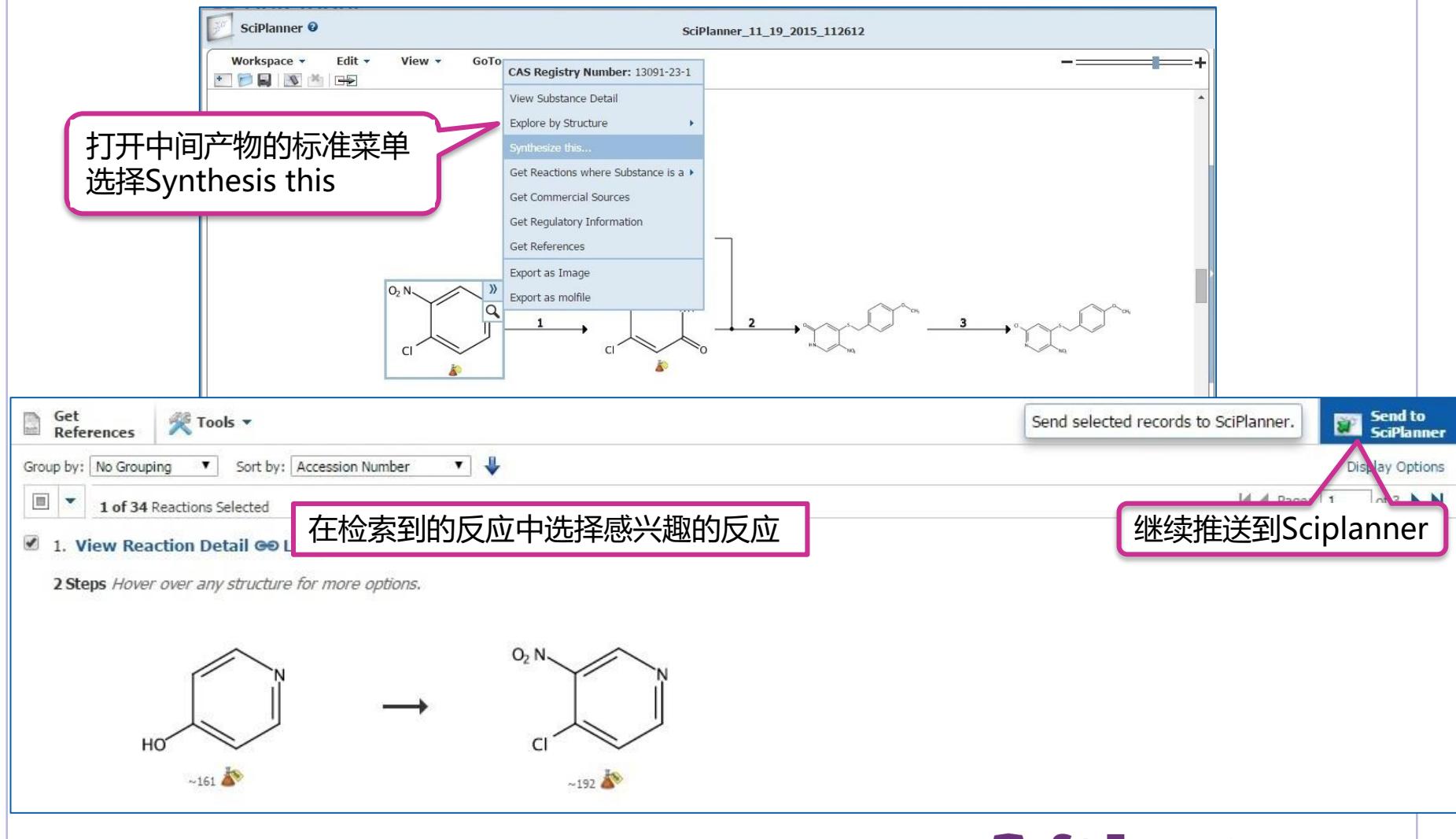
Display Options

进入SciPlanner 新建文件

将刚推送过来的反应拖至编辑面板

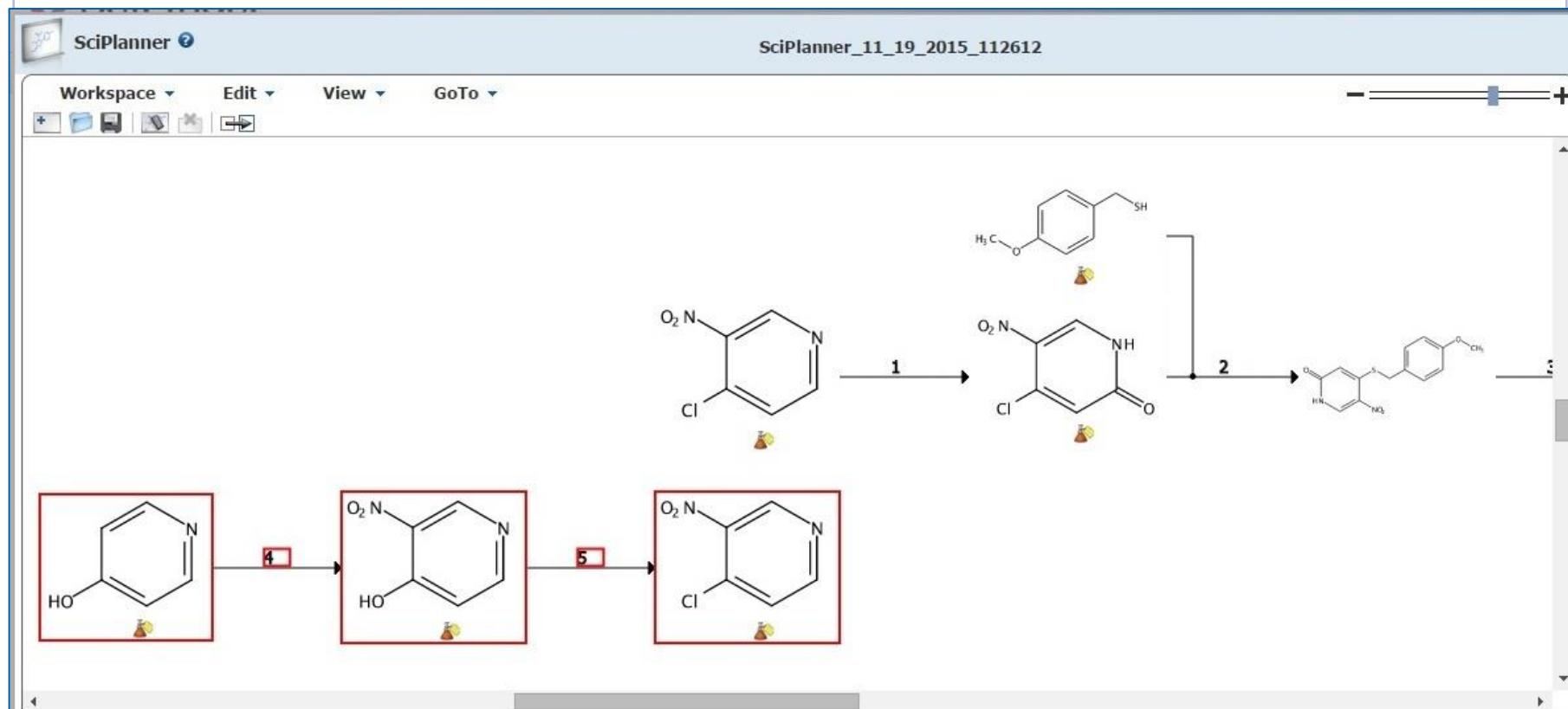
The screenshot shows the SciPlanner interface. At the top, a reaction scheme is displayed with two reactants and a product. The first reactant is 4-nitro-2-chloropyridine, the second is 4-methoxybenzenethiol, and the product is 2-(4-methoxybenzenethio)pyridine-4-nitro. The reaction is labeled [Step 2.1]. Below the reaction, the 'Overview' section is expanded, showing 'Steps/Stages' with three entries: 1.1, 2.1, and 3.1. The 'Notes' section indicates 2 reactants, 5 reagents, 1 solvent, 3 steps, and 1 stage. The 'References' section lists 'Syntheses of 4- and 6-substituted thiazolo[4,5-c]pyridines'. The bottom part of the screenshot shows the SciPlanner workspace, which is currently empty. A reaction preview is visible on the right side of the workspace.

SciPlanner使用简介



 **SciFinder**
A CAS SOLUTION

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 2015

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

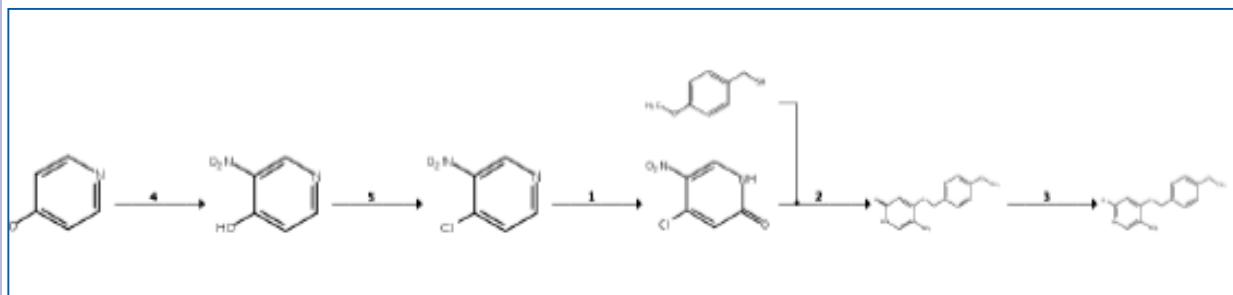
Include:

SciPlanner Image
 Reaction Details
 Substance Details
 Reference Details

Export Cancel



SciPlanner导出结果



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

Substance Information		
1228150-22-8 C ₁₃ H ₁₂ N ₂ O ₅ S 2(1H)-Pyridone, 4-[(4-methoxyphenyl)methyl]thio]-5-nitro- Related Info: ~ 2 References Reactions	1228150-23-9 C ₁₃ H ₁₁ ClN ₂ O ₅ S Pyridine, 2-chloro-4-[(4-methoxyphenyl)methyl]thio]-5-nitro- Related Info: ~ 2 References Reactions	13091-23-1 C ₆ H ₃ ClN ₂ O ₂ Pyridine, 4-chloro-3-nitro- Related Info: ~ 301 References Reactions ~ 100 Commercial Sources Regulatory Information
5435-54-1 C ₆ H ₄ N ₂ O ₃ 4-Pyridinol, 3-nitro- Related Info: ~ 113 References Reactions ~ 197 Commercial Sources Regulatory Information	6258-60-2 C ₈ H ₁₀ OS Benzenemethanethiol, 4-methoxy- Related Info: ~ 749 References Reactions ~ 71 Commercial Sources Regulatory Information	626-64-2 C ₆ H ₅ N ₂ O 4-Pyridinol Related Info: ~ 1351 References Reactions ~ 160 Commercial Sources Regulatory Information
850663-54-6 C ₆ H ₃ ClN ₂ O ₃ 2(1H)-Pyridone, 4-chloro-5-nitro- Related Info: ~ 22 References Reactions ~ 136 Commercial Sources		

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

首页

本馆概况

资源

服务

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校外访问

当前日期: 2019年6月4日

当前位置: 首页 / 资源 / 正文

日 一 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: https://scifinder.cas.org/registration/index.html? corpKey=6BE07969X86F35040X3C9C945423CF0CF467</p> <p>SciFinder检索网址: https://scifinder.cas.org/ (试用至2019年5月31日)</p>



如何获取SciFinder账号

The registration form is divided into three main sections:

- CONTACT INFORMATION:** Fields for First Name, Last Name, Email, Confirm Email, Phone Number, Fax Number, Area of Research (dropdown), and Job Title (dropdown).
- USERNAME AND PASSWORD:** Fields for Username, Password, and Re-enter Password. There are "Tips" links next to the Password and Re-enter Password fields.
- SECURITY INFORMATION:** Fields for Security Question (dropdown) and Answer. There is a "Why?" link next to the Answer field.

At the bottom are "Register>>" and "Clear All" buttons.

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 @、#、%、&、*)
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

SciFinder Registration - Your Confirmation Required

发件人: registration<registration@cas.org> +

收件人: 我<libjsb1@email.sdu.edu.cn> +

时间: 2019年03月07日 17:54 (星期四)

From: CAS

Dear libjsb1test1,

To complete your SciFinder registration, you must click the link provided below.

<https://scifinder.cas.org/registration/completeRegistration.html?respKey=5793D4C2X86F35040X6CC2413920911D9F54>

This link is valid for only one use and will expire within 96 hours.

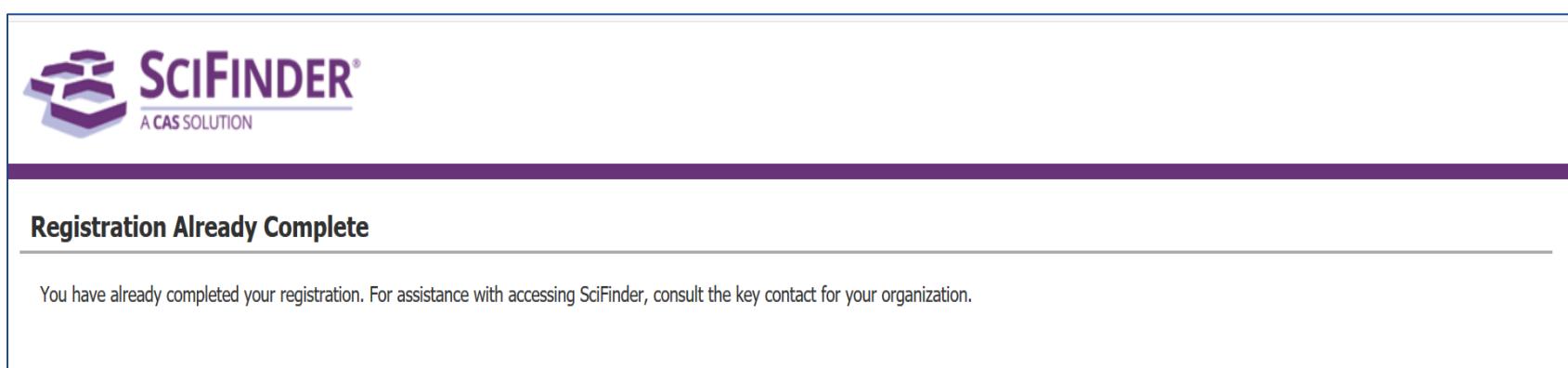
If you need assistance at any time, consult the key contact at your organization.

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



The image shows a screenshot of a SciFinder registration confirmation page. At the top left is the SciFinder logo with the text "A CAS SOLUTION". Below the logo, a purple horizontal bar contains the text "Registration Already Complete". Underneath this bar, a message reads: "You have already completed your registration. For assistance with accessing SciFinder, consult the key contact for your organization." The entire page is enclosed in a light blue border.

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

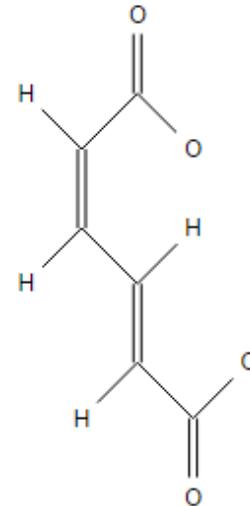
更多培训资料请访问

www.cas-china.org



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. 检索保护吲哚环上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

