

匡金海

客户顾问

jkuang@acsi.info

# 如何使用SciFinder获取科技信息

北京林业大学

2017.04.07



# 提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
  - 文献检索 ( PatentPak )
  - 物质检索 ( 聚合物检索 )
  - Markush检索
  - 反应检索 ( MethodsNow Synthesis )
  - SciPlanner
  - MethodsNow
- 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

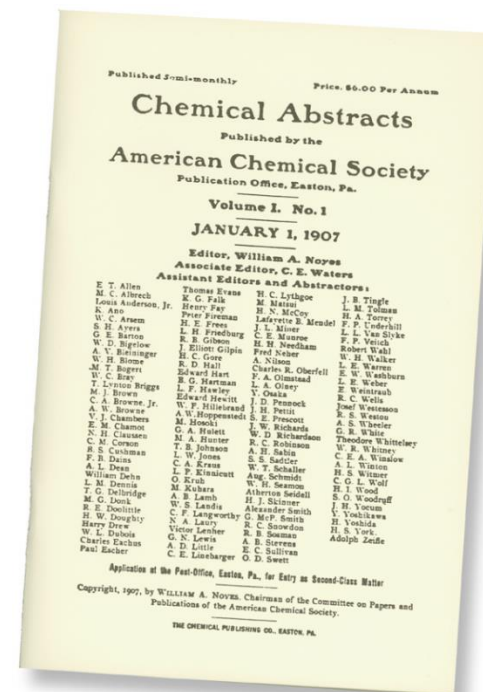


# 1907年，信息的汇集、管理发生了重大的变化



威廉·诺伊斯  
(William A. Noyes)

- “化学文摘”创刊
- 当年编制近12,000条文摘
- 今天，CAS每年收录、创建来自期刊、专利和其他已公开信息的文摘达到了100余万条



# CAS——构建最高质量的化学数据库



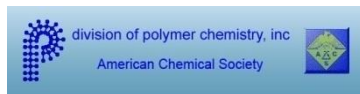
arXiv.org

Aldrichimica ACTA

ACS  
chemical  
biology



BEILSTEIN JOURNAL  
OF ORGANIC CHEMISTRY



J | A | C | S  
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

ACS Chemical  
Neuroscience



THE JOURNAL OF  
PHYSICAL CHEMISTRY  
Letters

SCIFINDER<sup>®</sup>  
A CAS SOLUTION

# CAS——构建最高质量的化学数据库



# 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



# 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 <a href="#">PATENTPAK</a>	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

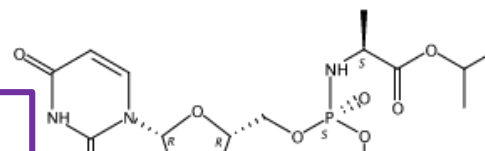
### Concepts

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。

# CAS最新动向—解决方案

## PatentPak™

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*A Solution Powered by CAS*

 **METHODSNOW™**  
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 **CHEMZENT™**  
A CAS SOLUTION

 **SCIFINDER®**  
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# CAS最新动向—解决方案

- CAS于2015年2月正式发布PatentPak™
- 专利工作流程解决方案
- 极大节约用户在研究专利时的时间
- 快速查找定位专利中的关键化学信息

6. Preparation of substituted nucleosides, nucleotides and analogs thereof as antiviral agents

Quick View PATENTPAK

By Beigelman, Le...  
From PCT Int. App...

Patent No.	Kind	Language
WO 2016100441	A1	English

Patent Family

US 20160176911	A1	English
----------------	----	---------

Disclosed he...  
phosphate, R...  
methods of t...  
medicament

atkina, Natalia  
Language: English, Database: CAPLUS

B is substituted purine and pyrimidine nucleobase; dashed bond between R and R<sup>4</sup> is absent, then R is H, substituted each R<sup>6</sup> and R<sup>7</sup> are independently hydrogen or deuterium; R<sup>5</sup> is -OH or F; methods of synthesizing nucleotide analogs and as a HCV infection with one or more nucleotide analogs. Thus, nucleotide II was prepd. and tested as antiviral agent and of a hepatitis C virus.

7. Process for preparation of sofosbuvir

Quick View PATENTPAK

By Li, Zebiao; Zhu, Mingmin; Zhang, Qinghai; Zhu, Gongfeng; Zhang, Zhaoguo; Lin, Yanfeng  
From Faming Zhuanli Shenqing (2016), CN 105669804 A 20160615. | Language: Chinese, Database: CAPLUS

The prep. method comprises reaction of (2'R)-2'-deoxy-2'-fluoro-2'-methylyridine with

ZOOM: - +

DOWNLOAD PDF: [Icon]

(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(19) World Intellectual Property Organization  
International Bureau

(43) International Publication Date  
23 June 2016 (23.06.2016)

WIPO PCT

(51) International Patent Classification:  
C07H 19/10 (2006.01) C07H 19/13 (2006.01)  
C07H 19/20 (2006.01) A61K 31/7072 (2006.01)  
C07H 19/11 (2006.01) A61K 31/7076 (2006.01)  
C07H 19/213 (2006.01) A61K 31/708 (2006.01)  
C07H 19/067 (2006.01) A61P 31/14 (2006.01)  
C07H 19/073 (2006.01)

(81) Designated States (kind of national protection):  
AO, AT, AU, AZ, BA, BB, BG, BR, BZ, CA, CH, CL, CN, CO, CZ, DE, DK, EC, EE, EG, ES, FI, FR, GB, GR, HK, HU, ID, IL, IN, JP, KE, KG, KH, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, NZ, OC, OM, PA, PE, PG, PH, PL, PT, RU, SE, SG, SK, SL, SM, ST, SV, SY, TH, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW.

(84) Designated States (unless otherwise indicated, for every kind of regional protection available): ARIPO (BW, GH, GM, KE, LU, MG, MW, MZ, NA, NG, SD, SI, SS, SZ, TZ, UG, ZM, ZW), EPO (AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, JP, KR, LK, LT, LU, LV, MA, MD, ME, MK, MN, MW, MX, MY, NZ, OC, OM, PA, PE, PG, PH, PL, PT, RU, SE, SG, SK, SL, SM, ST, SV, SY, TH, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW).

Chemical structure of a nucleoside derivative with R groups.

Search in SciFinder | View Detail

Analyst Markup Locations (1)  
page 130

CAS RN 1206126-39-7

Search in SciFinder | View Detail

Analyst Markup Locations (1)  
page 130

CAS RN 1206126-41-1

WO 2016/100441

PCT/US2015/065981

EXAMPLE 1 COMPOUND 1

Chemical reaction scheme showing the synthesis of Compound 1 from various precursors (1-1, 1-2, 1-3, 1-4, 1-5, 1-6) and Route 2.

Reagents: dichloromethane, pyridinium dichromate, acetic anhydride, tert-butanol.



# CAS最新动向—解决方案

- CAS于2016年2月正式发布MethodsNow™
- 最大方法信息合集
- 来自重要的全文信息资源：CAS高质量标引、全新的、增值的方法
- 满足合成和分析研究工作者的需求

SciFinder  
SciPlanner  
Reaction Structure substructure > reactions (9)  
Analyze by: Reagent, E/N, K<sub>2</sub>CO<sub>3</sub>, EN(Ph-<sub>2</sub>)  
1. View Reaction Detail [Link] [Send to SciPlanner]  
Single Step viewer over any structure for more options.  
Overview  
Microcosm™  
Procedure  
1. Stir the mixture of 7-methyl-4-methoxy-2-methyl-5-(4-methylphenyl)-2H-chromen-2-one (480 mg, 1.05 mmol), 1-iodooctane (388 mg, 1.82 mmol), copper(II) sulfate pentahydrate (42 mg, 0.17 mmol), (+)-sodium L-ascorbate (360 mg, 1.82 mmol) in t-BuOH/water (15 mL/15 mL) at room temperature for 4 hours.  
2. Add water to the mixture.  
View more...  
Available Experimental Data  
1H NMR, 13C NMR, IR, HRMS, Mass Spec, MP  
View with MethodsNow

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CAS Solutions  
METHODS NOW  
atorvastatin  
Results (528)  
Sort Relevance  
Analyte  
 Atorvastatin (227)  
 Atorvastatin calcium (211)  
 Ezetimibe (80)  
 Amlodipine besylate (56)  
 Fenofibrate (46)  
View All  
Matrix  
 Pharmaceutical tablets (293)  
 Blood plasma (60)  
 Tablets (49)  
 Pharmaceutical capsules (34)  
 Garcinia atrovitidis (20)  
View All  
Method Category  
Technique  
 Reversed-phase HPLC (152)  
 Spectrophotometry (101)  
 UV-visible spectroscopy (71)  
 HPLC (57)  
 Liquid chromatographic UV detectors (43)  
View All  
Analysis of Atorvastatin in Blood plasma by High-performance thin layer chromatography  
CAS MN: 1-101-CAS-1389  
View Details & Instructions  
Add to Compare  
Analyte: Atorvastatin  
Matrix: Blood plasma  
Other Materials: Material: 60 F254 silica gel HP TLC plates  
Method Category: Active Pharmaceutical Ingredient and Metabolite Analysis  
Technique: High-performance thin layer chromatography  
Equipment Used: Automatic TLC Sampler 3  
Source: HPTLC determination of atorvastatin in plasma  
Jamshidi, A.; Nateghi, A. R.  
Chromatographia (2007), 65 (11/12), 763-766. Vieweg Verlag/GWV Fachverlage GmbH  
Document Sources  
Abstract

单独的分析界面

# 提纲

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

# SciFinder覆盖的数据库



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# 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 left is the SciFinder logo with the text 'CAS Solutions' and 'A CAS SOLUTION'. To the right of the logo is a navigation bar with 'Explore', 'Saved Searches', and 'SciPlanner'. Further right are links for 'Preferences', 'SciFinder Help', and a 'Sign Out' button. Below the navigation bar is a search area with a text input field, a 'Search' button, and an 'Advanced Search' link. On the left side, there is a sidebar menu with categories: 'REFERENCES' (Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, Tags), 'SUBSTANCES' (Chemical Structure, Markush, Molecular Formula, Property, Substance Identifier), and 'REACTIONS' (Reaction Structure). On the right side, there is a 'SAVED ANSWER SETS' section listing various search results like 'CSF1R', 'jmc', 'EP 19870107847', etc. Below that is a 'KEEP ME POSTED' section with a message 'You have no proxies.' and a link to 'Learn how to: Create Keep Me Posted'. Chinese callouts are placed over the interface: '工具栏' points to the top navigation bar; '检索入口' points to the search input field; '已保存的结果集' points to the 'SAVED ANSWER SETS' list; and '定题追踪' points to the 'KEEP ME POSTED' section. The user's name 'Welcome Helen Zhu' is visible in the top right corner.

已保存的结果集

检索入口

定题追踪



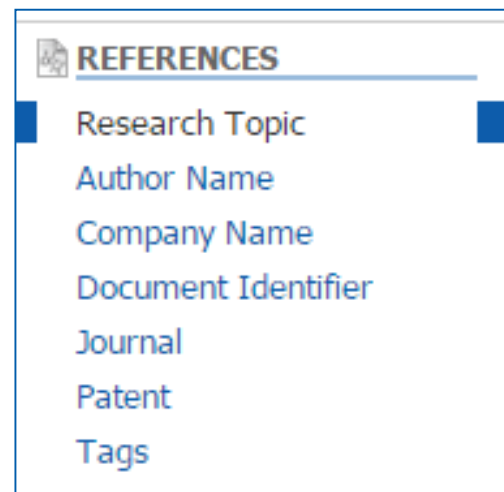
# SciFinder检索——文献检索

## ■ 文献检索方法

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

## ■ 检索策略推荐

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



# 文献检索——主题

主题检索：木质复合材料的制备

检索式：prepare of wood composite

The screenshot displays the SciFinder search interface. At the top, the SciFinder logo is visible, along with navigation tabs for 'Explore', 'Saved Searches', and 'SciPlanner'. Below the navigation, the search topic 'prepare of wood composite' is entered. The interface is divided into two main sections: 'REFERENCES' and 'SUBSTANCES'. The 'REFERENCES' section is active, showing a list of search criteria: Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, and Tags. The 'SUBSTANCES' section is also visible, with options for Chemical Structure, Markush, and Molecular Formula. The search results area shows the entered query 'prepare of wood composite' and provides examples of search results: 'The effect of antibiotic residues on dairy products' and 'Photocyanation of aromatic compounds'. A 'Search' button is present, along with options for 'Advanced Search' and 'Always Show'.

Research Topic "prepare of wood composite"

**REFERENCES**

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

**SUBSTANCES**

- Chemical Structure
- Markush
- Molecular Formula

**REFERENCES: RESEARCH TOPIC**

prepare of wood composite

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

**Search**

Advanced Search  Always Show

关键词之间用介词连接：in, with, of...

# 主题检索的候选项

Select All Deselect All

0 of 4 Research Topic Candidates Selected

	References
<input type="checkbox"/> 5648 references were found containing the two concepts "prepare" and "wood composite" closely associated with one another.	5648
<input type="checkbox"/> 10379 references were found where the two concepts "prepare" and "wood composite" were present anywhere in the reference.	10379
<input type="checkbox"/> 12228635 references were found containing the concept "prepare".	12228635
<input type="checkbox"/> 31524 references were found containing the concept "wood composite".	31524

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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Sort by: **Citing References** (selected)  
Accession Number  
Author Name  
Citing References  
Publication Year  
Title

Page: 1 of 283

1. **Properties and morphology of impact modified polypropylene-wood flour composites**  
By Oksman, Kristiina; Clemons, Craig  
From Journal of Applied Polymer Science (1998), 67(9), 1503-1513. | Language: English, Database: CAPLUS  
The mech. properties and morphol. of polypropylene (I)/**wood flour**, I/WF, **composites** with different impact modifiers and maleated I (MAPP) as a compatibilizer were studied. Two different ethylene/propylene/diene terpolymers (EPDM) and 1 maleated styrene-ethylene/butylene-styrene triblock copolymer (SEBS-MA) were used as impact modifiers in the I/WF systems. All 3 elastomers increased the impact strength of the I/WF **composites**, but the addn. of maleated EPDM and SEBS gave the greatest improvements in impact strength. Addn. of MAPP did not affect the impact properties of the **composites**, but it...

2. **Mechanical properties of biodegradable composites from poly lactic acid (PLA) and microcrystalline cellulose (MCC)**  
By Mathew, Aji P.; Oksman, Kristina; Sain, Mohini  
From Journal of Applied Polymer Science (2005), 97(5), 2014-2025. | Language: English, Database: CAPLUS  
Biodegradable **composites** were **prepd.** using microcryst. cellulose (MCC) as the reinforcement and poly(lactic acid) (PLA) as a matrix. PLA is polyester of lactic acid and MCC is cellulose derived from high quality **wood** pulp by acid hydrolysis to remove the amorphous regions. The **composites** were **prepd.** with different MCC contents, up to 25 wt %, and **wood flour** (WF) and **wood pulp** (WP) were used as ref. materials. Generally, the MCC/PLA **composites** showed lower mech. properties compared to the ref. materials. The dynamic mech. thermal anal. (DMTA) showed that the storage modulus was increased wit...

3. **Polypropylene-wood fiber composites: effect of treatment and mixing conditions on mechanical properties**

Citing Reference: 帮助找到最重要的文献

# 按被引次数排序— Citing References

文献分析工具

REFERENCES ?

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Analyze Refine Categorize

Sort by: Accession Number ↓

0 of 5648 References Selected

Display Options Page: 1 of 283

Analyze by: Author Name

Wang Qingwen	43
Li Jian	39
Li Jingjing	28
Wang Haigang	28
Li Jing	26
Lu Shaorong	26
Zhai Bin	25
He Jun	22
Lei Wen	22
Li Xin	22

1. Improved toughness of wood flour/HDPE composites with elastomers

Quick View Other Sources

By Hao, Jianxiu; Wang, Haigang; Wang, Weihong; Wang, Qingwen  
From Fuhe Cailiao Xuebao (2016), 33(5), 976-983. | Language: Chinese, Database: CAPLUS

Three kinds of elastomers, polyolefin elastomer (POE), elastomer modified polyethylene (BPB) and graft modified polyolefin elastomer (A669), were introduced to **prepn.** process of **wood** flour/high d. polyethylene (WF/HDPE) **composite** to improve the toughness of **wood-plastic composites**. The kinds and contents of toughening agents which could simultaneously improve the toughness and maintain the rigidity of WF/HDPE **composites** were detd. by the impact strength and flexural elastic modulus test of WF/HDPE **composites**. The toughening principles were analyzed by the aid of the crystrn. behavior, thermal...

2. Compound wood nizi its pharmaceutical composition in the preparation of analgesic application of [Machine Translation].

Quick View Other Sources

By Yin, Qiang; Wang, Changhong; Mu, Dandan; Ma, Xuan; Yin, Hailong; Liu, Lacai; Cheng, Xuemei; Cheng, Juanjuan; Huang, Lu; Liu, Zijia; et al  
From Faming Zhuanli Shenqing (2017), CN 106540119 A 20170329. | Language: Chinese, Database: CAPLUS

[Machine Translation of Descriptors]. The invention discloses a kind of compound **wooden** Nizi its analgesic pharmaceutical **composition** in the **preparation** of a medicament for, the said timber Nizi compound and its pharmaceutical **composition** is comprised of fennel root bark, Peganum harmala, Pimpinella anisum fruit, Flos Chrysanthemi, celery root, Cichorium glandulosum and/or Cichorium intybus, Nigella glandulifera seed, chicory root, dracocephalum, grass seeds, Glycyrrhiza uralensis Fisch, Ocimum basilicum fruits and abelmoschus seed. The drug can be effectively applied to the treatment of neu...

3. Preparation method of wood-plastic environment-friendly composite exhibition board [Machine Translation].

Quick View Other Sources

Citing Reference: 帮助找到最重要的文献

# 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

Analyze by: ?

- Company-Organization
- Author Name**
- CAS Registry Number
- CA Section Title
- Company-Organization
- Database
- Document Type
- Index Term
- CA Concept Heading
- Journal Name
- Language
- Publication Year
- Supplementary Terms

Analyze Refine Categorize

Analyze by: ?

Author Name

Wang Qingwen	43
Li Jian	39
Li Jingjing	28
Wang Haigang	28
Li Jing	26
Lu Shaorong	26
Zhai Bin	25
He Jun	22
Lei Wen	22
Li Xin	22

Show More

Analyze Refine Categorize

Analyze by: ?

Company-Organization

Peop Rep China	436
Northeast Forestry University, Peop Rep China	168
USA	72
S Korea	67
Nanjing Forestry University, Peop Rep China	66
Beijing Forestry University, Peop Rep China	45
Guilin University of Technology, Peop Rep China	42

Analyze Refine Categorize

Analyze by: ?

Journal Name

Faming Zhuanli Shenqing	2275
Chemisches Zentralblatt	538
Jpn. Kokai Tokkyo Koho	208
PCT Int. Appl.	136
Repub. Korean Kongkae TaeHo Kongbo	112
U.S.	108
Repub. Korea	99
Journal of Applied Polymer Science	92

Analyze Refine Categorize

Analyze by: ?

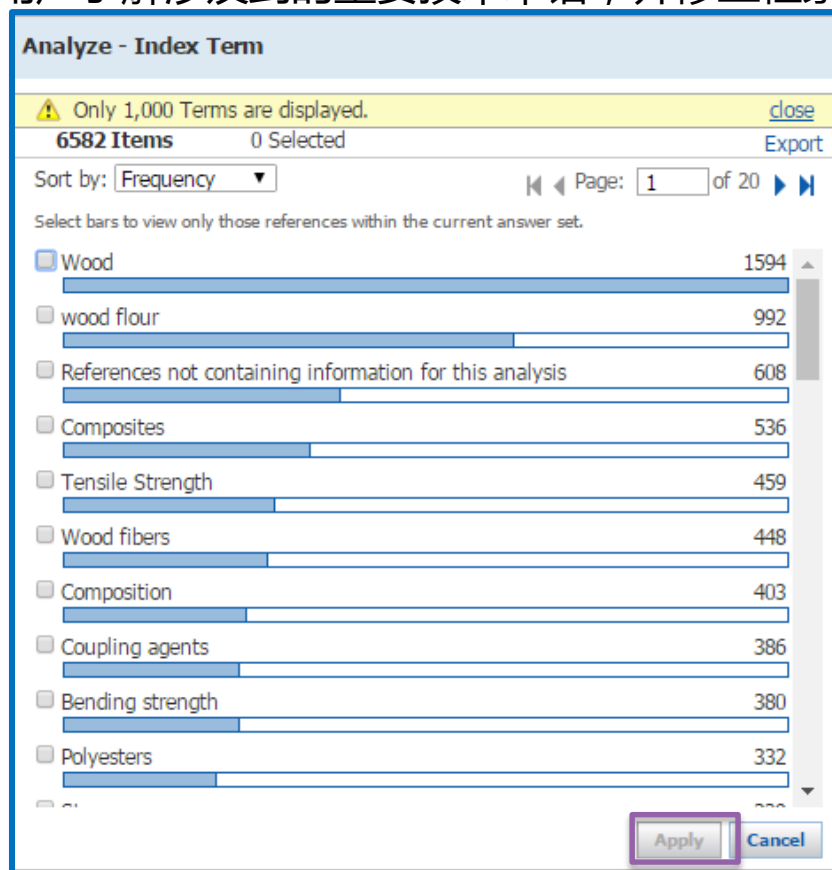
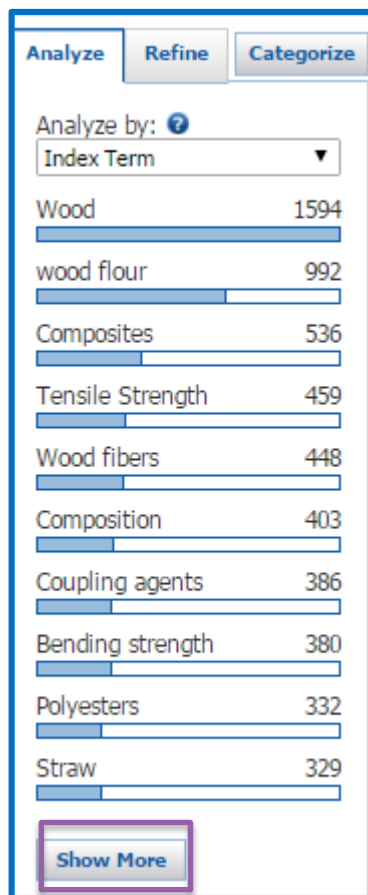
CA Section Title

Cellulose, Lignin, Paper, and Other Wood Products	1315
Plastics Manufacture and Processing	1129
Plastics Fabrication and Uses	925
Cement, Concrete, and Related Building Materials	217
Fertilizers, Soils, and Plant Nutrition	132
Ceramics	123
Coatings, Inks, and Related Products	103
Textiles and Fibers	56

# 文献检索结果的Analyze

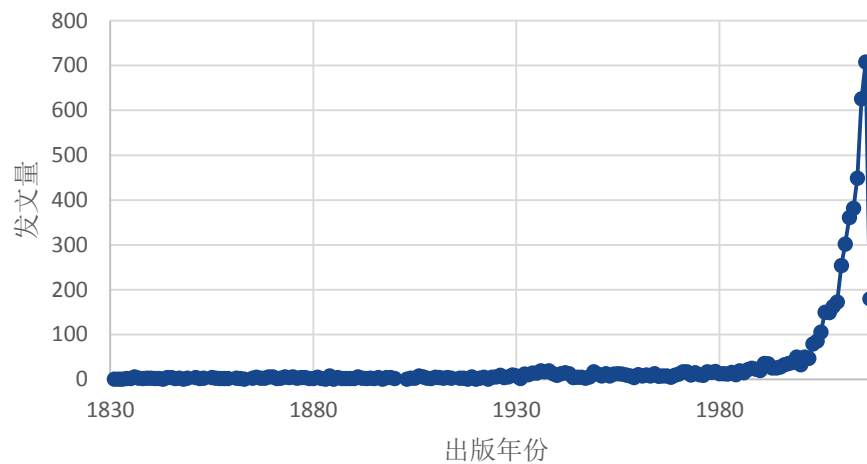
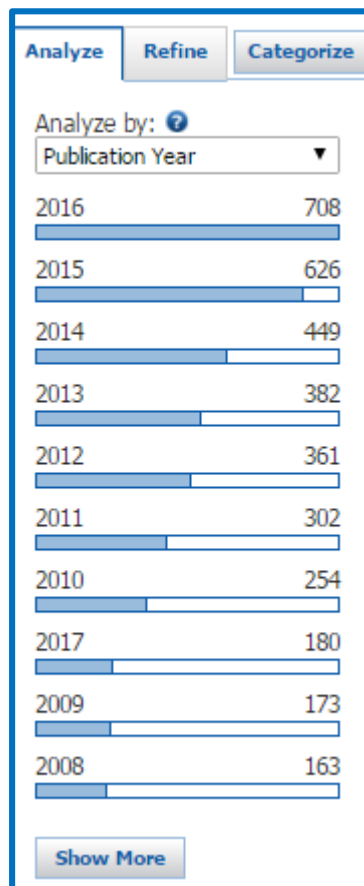
Index Term :

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Analyze



Publication Year: 分析领域发展趋势



# 文献检索结果的Refine

Analyze Refine Categorize

Refine by: ?

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

Company Name

Examples:

3M

DuPont

Refine

Get Substances Get Reactions Get Related Citations Tools

Sort by: Accession Number

0 of 2953 References Selected

Page: 1 of 148

- Improved toughness of wood flour/HDPE composites with elastomers**  
Quick View Other Sources  
By Hao, Jianxiu; Wang, Haigang; Wang, Weihong; Wang, Qingwen  
From Fuhe Calliao Xuebao (2016), 33(5), 976-983. | Language: Chinese, Database: CAPLUS  
Three kinds of elastomers, polyolefin elastomer (POE), elastomer modified polyethylene (BPB) and graft modified polyolefin elastomer (A669), were introduced to **prepn.** process of **wood flour**/high d. polyethylene (WF/HDPE) **composite** to improve the toughness of **wood-plastic composites**. The kinds and contents of toughening agents which could simultaneously improve the toughness and maintain the rigidity of WF/HDPE **composites** were detd. by the impact strength and flexural elastic modulus test of WF/HDPE **composites**. The toughening principles were analyzed by the aid of the crystn. behavior, thermal...
- Compound wood nizi its pharmaceutical composition in the preparation of analgesic application of [Machine Translation].**  
Quick View Other Sources  
By Yin, Qiang; Wang, Changhong; Mu, Dandan; Ma, Xuan; Yin, Hailong; Liu, Lacai; Cheng, Xuemei; Cheng, Juanjuan; Huang, Lu; Liu, Zijia; et al  
From Faming Zhuanli Shenqing (2017), CN 106540119 A 20170329. | Language: Chinese, Database: CAPLUS  
[Machine Translation of Descriptors]. The invention discloses a kind of compound **wooden Nizi** its analgesic pharmaceutical **composition** in the **preparation** of a medicament for, the said timber Nizi compound and its pharmaceutical **composition** is comprised of fennel root bark, Peganum harmala, Pimpinella anisum fruit, Flos Chrysanthemi, celery root, Cichorium glandulosum and/or Cichorium intybus, Nigella glandulifera seed, chicory root, dracocephalum, grass seeds, Glycyrrhiza uralensis Fisch, Ocimum basilicum fruits and abelmoschus seed. The drug can be effectively applied to the treatment of neu...
- Preparation method of wood-plastic environment-friendly composite exhibition board [Machine Translation].**  
Quick View Other Sources  
By Qian, Zhigang  
From Faming Zhuanli Shenqing (2017), CN 106543756 A 20170329. | Language: Chinese, Database: CAPLUS  
[Machine Translation of Descriptors]. The present invention relates to a kind of **prepn.** method of **wood-plastic environment-friendly composite** exhibition board, and the following steps are specifically included:(1) **prepg.** raw materials;(2) making **wood-plastic environment-friendly composite** material;(3) molding **wood-plastic environment-friendly composite** exhibition board, obtaining the **wood-plastic environment-friendly composite** exhibition board by hot-pressing mode.By using above-mentioned tech. scheme, **wood-plastic environment-friendly composite** exhibition board widely suitable for exhibition...

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.      2. Select index terms of interest.

Category Heading	Category	Index Terms	Selected Terms
All	Substances in technology (3338)	Page: 1 of 2 Select All   Deselect All	Click 'X' to remove the category from 'Selected Terms'
<b>Technology</b>	Materials & products (769)	<input type="checkbox"/> Wood flour 701	<input checked="" type="checkbox"/> Technology > Construction (1 Terms)
Polymer chemistry	<b>Construction (113)</b>	<input type="checkbox"/> Wood 662	
General chemistry	Processes & apparatus (383)	<input type="checkbox"/> Wood fibers 324	
Physical chemistry	Metallurgy (83)	<input type="checkbox"/> Boards 162	
Genetics & protein chemistry	Ceramics (36)	<input type="checkbox"/> Construction materials 76	
Biotechnology	Formed, removed, & other substances (241)	<input type="checkbox"/> Wood chips 68	
Environmental chemistry	Power & fuel topics (61)	<input checked="" type="checkbox"/> Floors 60	
Synthetic chemistry	Imaging & recording (13)	<input type="checkbox"/> Poplar wood 59	
Catalysis		<input type="checkbox"/> Wood boards 57	
Biology		<input type="checkbox"/> Fiberboard 49	
Analytical chemistry		<input type="checkbox"/> Cement 45	
		<input type="checkbox"/> Granulation 39	
		<input type="checkbox"/> Pine wood 35	
		<input type="checkbox"/> Thermal insulators 35	
		<input type="checkbox"/> Impregnation 33	
		<input type="checkbox"/> Floor coverings 31	

Technology > Construction > 1 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

composite > references (5648) > refine "china" (2953) > refine by categories > Preparation of wear-resistant ...

Get Substances Get Reactions Get Related Citations Tools

Sort by: Accession Number

0 of 60 References Selected

1. Water-resistant wear-resistant floor and preparation method thereof

Quick View PATENTPAK

By Yang, Xiaorong

From Faming Zhuanli Shenqing (2017), CN 106351417 A 20170125. | Language: Chinese, Database: CAPLUS

The title water-resistant wear-resistant floor comprises substrate, coating layer, and surface layer (plant epidermis), wherein the substrate is **prepd.** by bonding two layers of double-layer **composite** plate; and the surface layer is wrapped with coating layer. The above **composite** plate comprises two solid **wood** plates and polyurethane sandwiched therebetween; and the above coating layer is **prepd.** from polyvinyl chloride resin 40-80, epoxy resin 20-40, chloroprene rubber 10-20, ethylene-propylene-diene monomer rubber 5-10, talc powder 20-40, sericite powder 15-30, glass fiber 10-20, titanium dio...

2. Preparation of wear-resistant composite fiberboard capable of being used as environment-friendly floor

Quick View PATENTPAK

By Fei, Genhua

From Faming Zhuanli Shenqing (2017), CN 106349728 A 20170125. | Language: Chinese, Database: CAPLUS

The raw material of the **composite** fiberboard comprises scrap **wood** 7-15, crop straw 8-12, flax fiber 3-6, silicon dioxide 4-9, polyurethane 5-15, polyacrylate 5-8, ethylene-vinyl acetate copolymer 3-6, carbonic acid fiber 4-9, nickel dibutylthiocarbamate 1-2, zinc borate 1-3, m-phenylenediamine 2-5, phthalide 3-5, sodium tartrate 1-4, 2,4-diaminobenzenesulfonic acid 1-3, silane coupling agent 1-4, antioxidant 2-3 and adhesive 2-5 parts. The **prepn.** method comprises the steps of: (1) weighing material; (2) soaking scrap **wood**, crop straw and flax fiber in 0.5 % sodium hypochlorite for 3-6 h to ob...

3. Process for production of eucalyptus solid wood composite floor from composite urea formaldehyde resin

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。

Export : 导出至本地电脑。

Print : 打印成PDF格式

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

Export:

All

Selected

Range

Example: 2-20

For:

Citation Manager

Citation export format (\*.ris)

Quoted Format (\*.txt)

Tagged Format (\*.bt)

Offline review

Portable Document Format (\*.pdf)

Rich Text Format (\*.rtf)

Answer Keys (\*.bt)

Saving locally

Answer Key eXchange (\*.akx)

Details:

\* Required

File Name: \*

Reference\_06\_19\_2012\_100848

Format:

Summary without abstracts

Summary with partial abstracts

Summary with full abstracts

Detail (full record)

Saving locally:

Task History

Tags

Comments

Export Cancel

# 文献信息—题录、摘要、索引

## 2. Preparation of wear-resistant composite fiberboard capable of being used as environment-friendly floor

By: Fei, Genhua

Assignee: Suzhou Baisike Energy-saving Environmental Protection Technology Co., Ltd., Peop. Rep. China

The raw material of the composite fiberboard comprises scrap wood 7-15, crop straw 8-12, flax fiber 3-6, silicon dioxide 4-9, polyurethane 5-15, polyacrylate 5-8, ethylene-vinyl acetate copolymer 3-6, carbonic acid fiber 4-9, nickel dibutylthiocarbamate 1-2, zinc borate 1-3, m-phenylenediamine 2-5, phthalide 3-5, sodium tartrate 1-4, 2,4-diaminobenzenesulfonic acid 1-3, silane coupling agent 1-4, antioxidant 2-3 and adhesive 2-5 parts. The prepn. method comprises the steps of: (1) weighing material; (2) soaking scrap wood, crop straw and flax fiber in 0.5 % sodium hypochlorite for 3-6 h to obtain softened mixt.; (3) drying and cutting the softened mixt., adding the dried and cut softened mixt., silicon dioxide and antioxidant to a hot melt of polyurethane at a speed of 100-1300 rpm at 250-400 °C for 55 min; (4) screening the mixt. obtained in step (3) to remove large-particle matter; (5) adding the mixt. obtained in step (4) to a twin-screw mixer, carrying out mixing reaction at 550-650 °C for 45-75 min while adding polyurethane, polyacrylate, ethylene-vinyl acetate copolymer, carbonic acid fiber, nickel dibutylthiocarbamate, zinc borate, m-phenylenediamine, phthalide, sodium tartrate, 2,4-diaminobenzenesulfonic acid and silane coupling agent in sequence; (6) adding the mixt. obtained in step (5) to a twin-screw extruder, cooling while adding adhesive under stirring with stirring speed of 150-300 rpm for 45 min, and (7) adding the mixt. obtained in step (6) in a twin-screw extruder, extruding, compression molding and cooling to obtain composite fiberboard finished product. The composite fiberboard has good wear resistance, is environment friendly, and can be used as environment friendly floor.

### Patent Information

Patent No.	Kind	Language	Date	Application No.	Date
CN 106349728	PATENTPAK A		Jan 25, 2017	CN 2016-10839302	Sep 22, 2016

### Priority Application

CN 2016-10839302			Sep 22, 2016
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### Indexing

Cellulose, Lignin, Paper, and Other Wood Products (Section43-2)

### Concepts

Polycarbonates

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

重要概念

重要物质

### Substances

83-86-3

84-74-2 Dibutyl phthalate

Page 2 in PATENTPAK

Page 2 in PATENTPAK

书目信息

### QUICK LINKS

0 Tags, 0 Comments

### PATENT INFORMATION

Jan 25, 2017  
CN 106349728  
A

### APPLICATION

Sep 22, 2016  
CN 2016-10839302

### PRIORITY

Sep 22, 2016  
CN 2016-10839302

### SOURCE

Faming Zhuanli Shenqing  
8pp.  
Patent  
2017  
CODEN:CNXXEV

### ACCESSION NUMBER

2017:139362  
CAN166:295950  
CAPLUS



# 文献检索小结

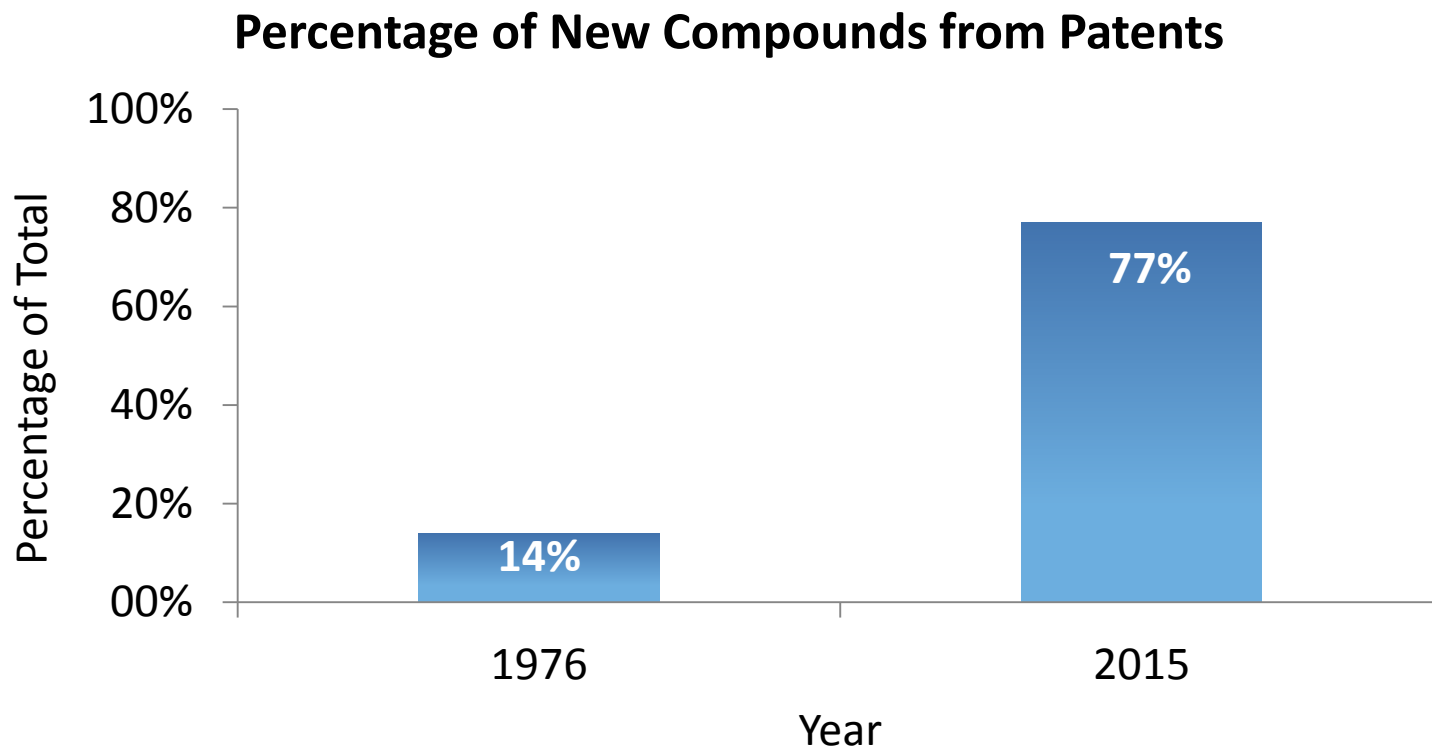
- 主题检索时，使用介词 **in, with, of** 等作为连接词
- 跟据检索要求选择合适的候选项
- 通过SciFinder 的**Analyze/Refine**功能来缩小检索的范围
- 尝试将不同的**Analyze/Refine**功能组合起来用，会有更多的收益
- 使用**Categorize**可以让系统来实现自动分类

# PatentPak<sup>TM</sup>

## 专利工作流程解决方案



# 越来越多的新化合物倾向于首先通过专利公布



# PatentPak——专利工作流程解决方案

在SciFinder检索结果中，看到PatentPak图标即可点击

点击专利号，获取PatentPak Viewer

The claimed herbicidal formulations contain active ingredients from the group of N-(1,3,4-oxadiazol-2-yl)-arylcarboxylic acid amides (I; where A = N or C-alkyl, C-halogenalkyl, etc., R = alkyls, halogenalkyls, etc., X = alkyls and substituted alkyls, and Z = H, halogens, and substituted alkyls). The claimed amides can be formulated in mixts. with other herbicides and optional herbicide safeners. The herbicide combinations were evaluated against 15 test weeds. The herbicidal formulations are suitable for weed control in agricultural crops (esp. genetically modified crops) and other useful pl...

## 8. Preparation of 6-fluoro-9-methyl- $\beta$ -carboline for the treatment of ear disease

Quick View

PatentPak

By Rommelspacher  
From Eur. Pat. Appl.

Patent No.	Kind	Language
<a href="#">EP 2853533</a>	Interactive	German

### Patent Family

<a href="#">WO 2015044434</a>	A2	German
<a href="#">WO 2015044434</a>	A3	German

... methyl- $\beta$ -carboline (I) and pharmaceutical compns. thereof useful in the treatment of acute and chronic inner ear diseases. ... 6-1-methyl-1H-Indole-3-ethanamine hydrochloride with 2,2-dihydroxyacetic acid followed by decarboxylation and redn. and

## 9. Preparation of fluoro-substituted 9-methyl- $\beta$ -carbolines for the treatment of ear diseases

Quick View

PatentPak

By Rommelspacher, Hans; Enzensperger, Christoph  
From PCT Int. Appl. (2015), WO 2015044434 A2 20150402. | Language: German, Database: CAPLUS



# PatentPak——专利工作流程解决方案

PatentPak浏览器

下载带有物质信息汇总表格的专利PDF文件

The screenshot displays the PatentPak viewer interface. At the top, there are navigation controls including 'PAGE 38 / 75', 'ZOOM', and buttons for 'DOWNLOAD PDF' and 'LOAD PDF'. On the left side, there is a sidebar with 'Key Substances in Patent' and two chemical structures with their respective CAS RNs: 1689575-79-8 and 24335-20-4. The main content area shows a patent document with a section titled 'Beispiele' and a specific example 'Beispiel 1a: Synthese von 6-Fluor-9-methyl-β-carbolin'. The text describes the synthesis process, mentioning reagents like 5-Fluor-1-methyltryptamin and Glyoxalsäurehydrat. A callout points to a lightbulb icon in the text, indicating that clicking it allows for quick navigation to the corresponding material information in the PDF file.

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专利PDF文件

在PatentPak Viewer中点击物质下面的灯泡，快速定位到PDF文件中的物质信息

# 节省您最宝贵的资源——时间



- 即时获得来自世界上31家专利授权机构的逾900万份专利PDF文件，且数量持续增加
- 专利族涵盖了多种语言
- 通过CAS登记号获得物质在专利文献中的相关信息
- 专利研究安全保密
- 每日更新
- SciFinder检索功能中内置交互式浏览器

# 提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
  - 文献检索 ( PatentPak )
  - 物质检索 ( 聚合物检索 )
  - Markush检索
  - 反应检索 ( MethodsNow Synthesis )
  - SciPlanner
  - MethodsNow
- 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



## SUBSTANCES

Chemical Structure

Markush

Molecular Formula

Property

Substance Identifier

## ■ 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 navigation bar with 'CAS Solutions' and the SciFinder logo. Below this, there are tabs for 'Explore', 'Saved Searches', and 'SciPlanner'. The main content area shows a breadcrumb trail: 'Reaction Structure structure variable only at spe... > reactions (29) > refine "structure variable only at spe..." (29)'. On the left, there is a sidebar 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' option is highlighted. The main search area is titled 'SUBSTANCES: SUBSTANCE IDENTIFIER' and contains a text input field with the text 'sunset yellow'. Below the input field, there is a note: 'Enter one per line. Examples: 50-00-0, 999815, 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。

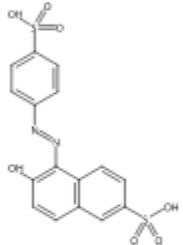
# SciFinder中的物质记录


点击CAS RN 获得物质详细信息

1. **2783-94-0** 

(Component: 5859-11-0)

~2889   ~65 



» 

**C<sub>16</sub> H<sub>12</sub> N<sub>2</sub> O<sub>7</sub> S<sub>2</sub> · 2 Na**  
2-Naphthalenesulfonic acid, 6-hydroxy-5-[2-(4-sulfophenyl)diazenyl]-, sodium salt (1:2)

Regulatory Information  
Spectra

**CAS Registry Number: 2783-94-0**

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

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

# SciFinder中的物质记录

**SUBSTANCE DETAIL** ?

[Get References](#) [Get Reactions](#) [Get Commercial Sources](#)

[Return](#)

**CAS Registry Number** 2783-94-0

(Component: 5859-11-0)

~2,889 ~65

**C<sub>16</sub> H<sub>12</sub> N<sub>2</sub> O<sub>7</sub> S<sub>2</sub> · 2 Na**  
2-Naphthalenesulfonic acid, 6-hydroxy-5-[2-(4-sulfophenyl)diazenyl]-, sodium salt (1:2)

**Other Names**  
2-Naphthalenesulfonic acid, 6-hydroxy-5-[(4-sulfophenyl)azo]-, disodium salt (9CI)  
C.I. Food Yellow 3 (7CI)  
C.I. Food Yellow 3, disodium salt (8CI)  
Sunset Yellow FCF (6CI)  
1-*p*-Sulfophenylazo-2-hydroxynaphthalene-6-sulfonate disodium salt  
[View more...](#)

由物质获得文献，反应，供应商等信息

• 2 Na

物质详情

## EXPERIMENTAL PROPERTIES

Biological Chemical Structure Related

### Structure Related Properties

X-Ray Diffraction Pattern

### Value

See full text

### Note

(4)CAS

实验数据与实验谱图

### Notes

(4) Park, Seul-Ki; Advanced Functional Materials 2011, V21(11), P2129-2139 CAPLUS

## EXPERIMENTAL SPECTRA

IR Mass UV and Visible

### IR Properties

IR Absorption Spectrum

See spectrum

(1)BIORAD

IR Absorption Spectrum

See spectrum

(1)BIORAD

IR Absorption Spectrum

See spectrum

(1)BIORAD

IR Absorption Spectrum

See spectrum

IR Absorption Spectrum

See spectrum

IR Absorption Spectrum

See spectrum

IR Absorption Spectrum

See spectrum

IR Absorption Spectrum

See spectrum

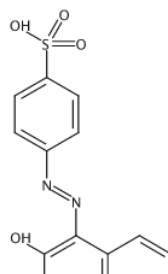
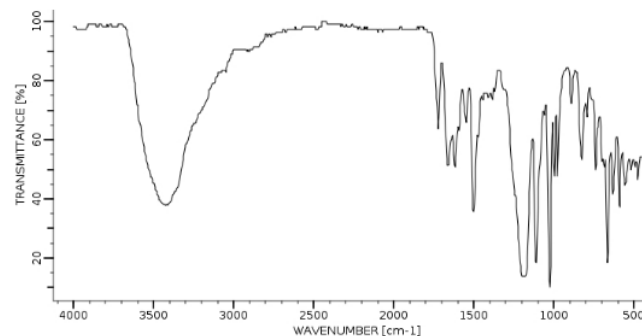
IR Absorption Spectrum

See spectrum

IR Absorption Spectrum

See full text

### IR Absorption Spectrum



SPECTRUM ID  
BR036790

CAS REGISTRY NUMBER  
2783-94-0

FORMULA  
C<sub>16</sub> H<sub>12</sub> N<sub>2</sub> O<sub>7</sub> S<sub>2</sub> · 2 Na

CAS INDEX NAME  
2-Naphthalenesulfonic acid, 6-hydroxy-5-[2-(4-sulfophenyl)diazenyl]-, sodium salt (1:2)

SPECTROMETER  
BIO-RAD DIGILAB FT-IR OR EQUIVALENT

SOURCE  
Infrared spectral data from the Bio-Rad/Sadtler IR Data Collection was obtained from Bio-Rad Laboratories, Philadelphia, PA (US). Copyright © Bio-Rad Laboratories. All Rights Reserved.



# 物质检索——Property explore

The screenshot shows the SciFinder web interface. The browser address bar displays <https://scifinder.cas>. The SciFinder logo is visible at the top left. The main navigation area includes 'Explore' and 'Saved Searches' tabs. On the left, there are two panels: 'REFERENCES' and 'SUBSTANCES'. The 'SUBSTANCES' panel is active, showing a list of properties: Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, Tags, Chemical Structure, Markush, Molecular Formula, Property, and Substance Identifier. A dropdown menu is open over the 'Property' field, listing various properties. 'Molecular Weight' is selected and highlighted in blue. Below the dropdown, a search input field contains the value '250-400'. Below the input field, there are two examples: 'Examples: 44, 25-35, >125' and 'Examples: 44, 25-35, >125'. A blue 'Search' button is located below the input field. A purple-bordered callout box on the right contains the text: 寻找分子量在250-400之间的物质.

# 物质结果集的筛选——Refine

0 of 49251077 Substances Selected

1. 2088740-67-2

2. 2088740-65-0

3. 2088740-64-9

4. 2088740-61-6

5. 2088740-58-1

6. 2088740-43-4

Structure Editor:  
Java Non-Java  
Click to Edit

Search type: Exact Structure  
Only retrieve substances

4500多万个结构，  
如何筛选黄酮类物质？

# 物质结果集的筛选——Refine

Structure Editor

Draw or change atoms or bonds.

Shortcut Keys

100%

Atom Short

Get substances that match your query using:

- Exact search
- Substructure search

OK

Cancel

$C_{15}H_{10}O_2$

222.24

锁环工具：避免在被锁定的环结构上出现新的环结构

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

从4900多万个结构中

筛选出8415个黄酮类物质

Create Keep Me  
Posted Alert

Send to  
SciPlanner

Display Options

Page: 1 of 561

SUBSTANCES

Get  
References

Get  
Reactions

Get Commercial  
Sources

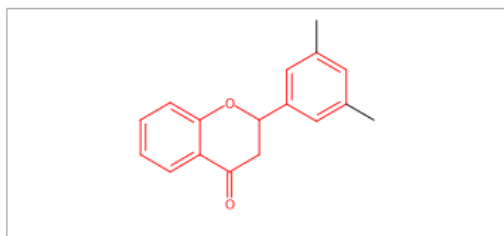
Tools

Sort by: Relevance

0 of 8415 Substances Selected

1. 1772897-96-7

~0 ~1

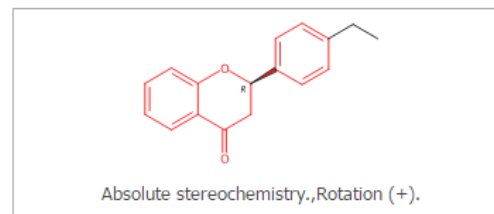


**C<sub>17</sub> H<sub>16</sub> O<sub>2</sub>**  
4#-1-Benzopyran-4-one, 2-(3,5-dimethylphenyl)-2,3-dihydro-

▶ Key Physical Properties

2. 1438763-28-0

~2

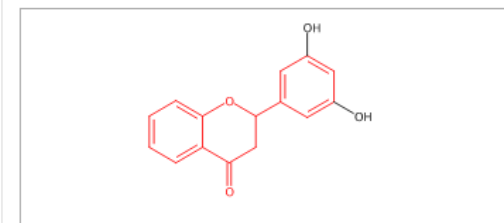


**C<sub>17</sub> H<sub>16</sub> O<sub>2</sub>**  
4#-1-Benzopyran-4-one, 2-(4-ethylphenyl)-2,3-dihydro-, (2*R*)-

▶ Key Physical Properties

3. 958734-07-1

~1

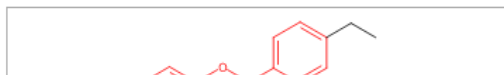


**C<sub>15</sub> H<sub>12</sub> O<sub>4</sub>**  
4#-1-Benzopyran-4-one, 2-(3,5-dihydroxyphenyl)-2,3-dihydro-

▶ Key Physical Properties

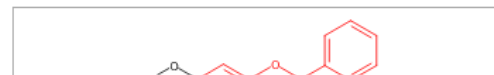
4. 1772047-03-6

~1



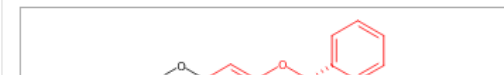
5. 21785-09-1

~169 ~19



6. 72984-48-6

~31

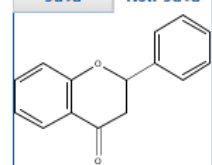


Refine by:

- 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**

# 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**

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

金属盐：金属离子和阴离子间用点 (.) 分开

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

# 物质检索——结构

**REFERENCES**

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

**SUBSTANCES**

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

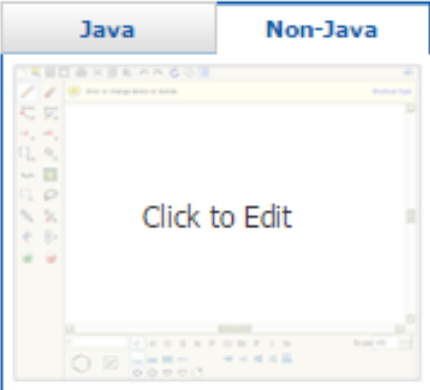
**REACTIONS**

- Reaction Structure

## SUBSTANCES: CHEMICAL STRUCTURE

Structure Editor:

Java Non-Java



Click to Edit

Search Type:

- Exact Structure
- Substructure
- Similarity

Show precision analysis

**ChemDraw**  
Launch a SciFinder substance or reaction

Import CXF

**Search**

[Advanced Search](#)  Always Show

# 物质检索——结构

The image shows a screenshot of the Structure Editor software interface, which is used for drawing and editing chemical structures. The interface includes a toolbar on the left with various drawing tools, a central workspace for drawing, and a right-hand panel for drawing settings and search options. The following labels point to specific features in the software:

- 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 Recovery 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 (Lasso Selection Tool)
- 原子锁定工具 (Atom Locking Tool)
- 镜面旋转工具 (Mirror Rotation Tool)
- 结构检索选择 (Structure Search Selection)
- 单双键, RS构型, 不确定键定义工具 (Single/Double Bond, RS Configuration, Uncertain Bond Definition Tool)
- 常见环, 多元环工具 (Common Ring, Poly-ring Tool)
- 负电子 (Negatively Charged Electron)

# 物质检索——精确结构检索

The screenshot displays the Structure Editor software interface. The main window shows a chemical structure of a complex molecule. A callout box points to the 'I' icon in the top toolbar, with the text: 通过CAS RN转换结构：CAS RN: 50-36-2. On the right side, the Drawing Editor panel is visible, with the 'Exact search' option selected under the heading 'Get substances that match your query using:'. The bottom status bar shows the molecular formula C<sub>17</sub>H<sub>21</sub>NO<sub>4</sub> and the molecular weight 303.36.

通过CAS RN转换结构：  
CAS RN: 50-36-2

精确结构检索

Get substances that match your query using:

- Exact search
- Substructure search
- Similarity search

OK  
Cancel

C<sub>17</sub>H<sub>21</sub>NO<sub>4</sub> 303.36



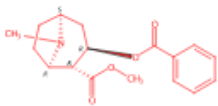
# 精确结构检索结果

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

Sort by: Relevance

0 of 6 Substances Selected

1. **668-19-9**



Absolute stereochemistry.

**C<sub>17</sub>H<sub>21</sub>N O<sub>4</sub>**  
8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(benzoyloxy)-8-methyl-, methyl ester, (1*R*, 2*R*, 3*R*, 5*S*)-

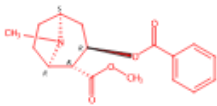
Key Physical Properties  
Spectra

**可卡因**

2. **114599-38-1**

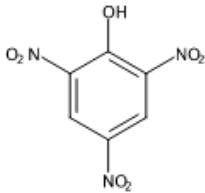
**可卡因组合物**

668-19-9  
C<sub>17</sub>H<sub>21</sub>N O<sub>4</sub>



Absolute stereochemistry.

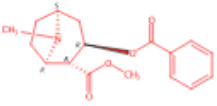
88-89-1  
C<sub>6</sub>H<sub>3</sub>N<sub>3</sub>O<sub>7</sub>



**C<sub>17</sub>H<sub>21</sub>N O<sub>4</sub> · C<sub>6</sub>H<sub>3</sub>N<sub>3</sub>O<sub>7</sub>**  
Alcocaine, picrate (6CI)

3. **109496-04-0**

(Component: 668-19-9)



\* HCl

Absolute stereochemistry.

**C<sub>17</sub>H<sub>21</sub>N O<sub>4</sub> · Cl H**  
Alcocaine, 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

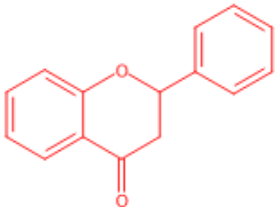
The screenshot displays the 'Structure Editor' window. The central workspace shows a chemical structure of a benzodioxane derivative with a phenyl group. The interface includes a toolbar on the left with various drawing tools, a top toolbar with file operations, and a right-hand panel with search settings. The search settings panel is titled 'Get substances that match your query using:' and has three radio button options: 'Exact search', 'Substructure search' (which is selected and highlighted with a purple box), and 'Similarity search'. Below these options are 'OK' and 'Cancel' buttons. At the bottom of the window, the molecular formula  $C_{15}H_{12}O_2$  and the molecular weight 224.26 are displayed.

# 物质检索——亚结构检索

0 of 23824 Substances Selected

1. 487-26-3

~2093

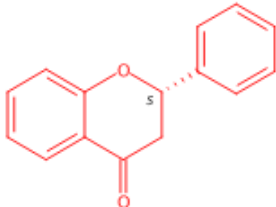


$C_{15}H_{12}O_2$   
4-phenyl-4H-1-benzopyran-4-one, 2,3-dihydro-2-phenyl-

Key Physical Properties  
Regulatory Information  
Spectra  
Experimental Properties

2. 17002-31-2

~244



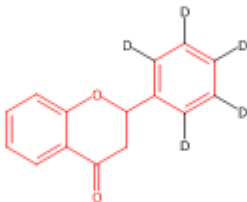
Absolute stereochemistry...Rotation (-).

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

Key Physical Properties  
Experimental Properties

10. 146196-91-0

~1 ~5



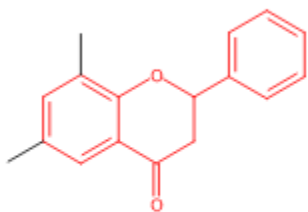
$C_{15}H_7D_5O_2$   
4-(2,3,4,5-tetradeuteriophenyl)-4H-1-benzopyran-4-one, 2,3-dihydro-2-(phenyl-d<sub>4</sub>)- (9CI)

Spectra

同位素

# 亚结构检索结果

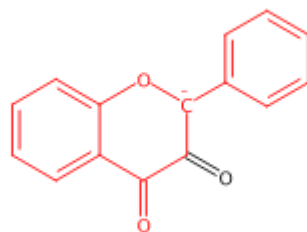
取代物



$C_{17}H_{16}O_2$   
4H-1-Benzopyran-4-one, 2,3-dihydro-6,8-dimethyl-

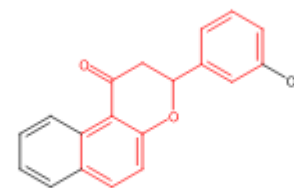
▶ Key Physical Properties  
Experimental Properties

离子



$C_{15}H_9O_3$   
2H-1-Benzopyran-3,4-dione, 2-phenyl-, ion(1-)

稠环物质



$C_{19}H_{14}O_3$   
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

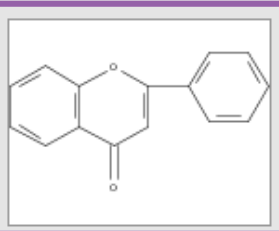
## 化学结构的再次限定

Analysis Refine

Refine by: ⓘ

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

Chemical Structure:

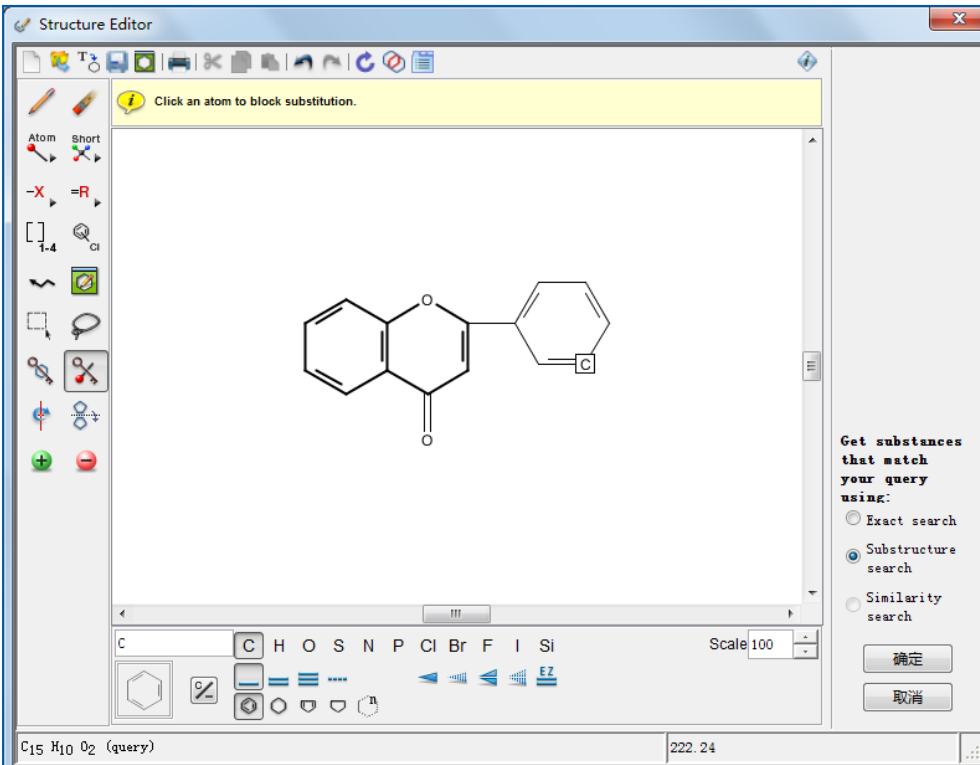


Click image to change structure or view detail

Search type: **Substructure**

Structure Editor

Click an atom to block substitution.



Get substances that match your query using:

- Exact search
- Substructure search
- Similarity search

确定 取消

C<sub>15</sub> H<sub>10</sub> O<sub>2</sub> (query) 222.24



环锁定

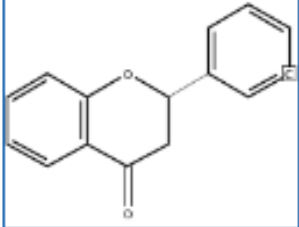


原子锁定

# 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

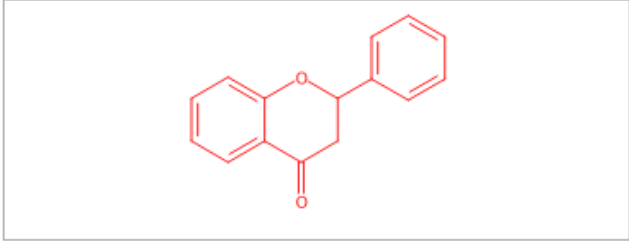
**Refine**

Get References Get Reactions Get Commercial Sources Tools

Sort by: Relevance

0 of 13826 Substances Selected

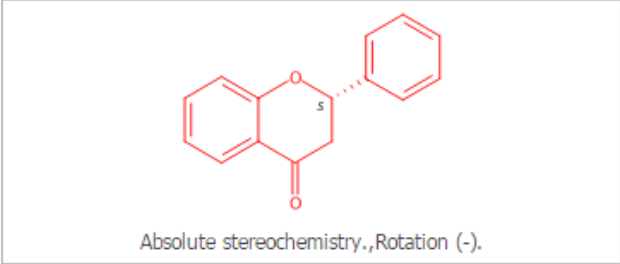
1. 487-26-3  
~2093



$C_{15}H_{12}O_2$   
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

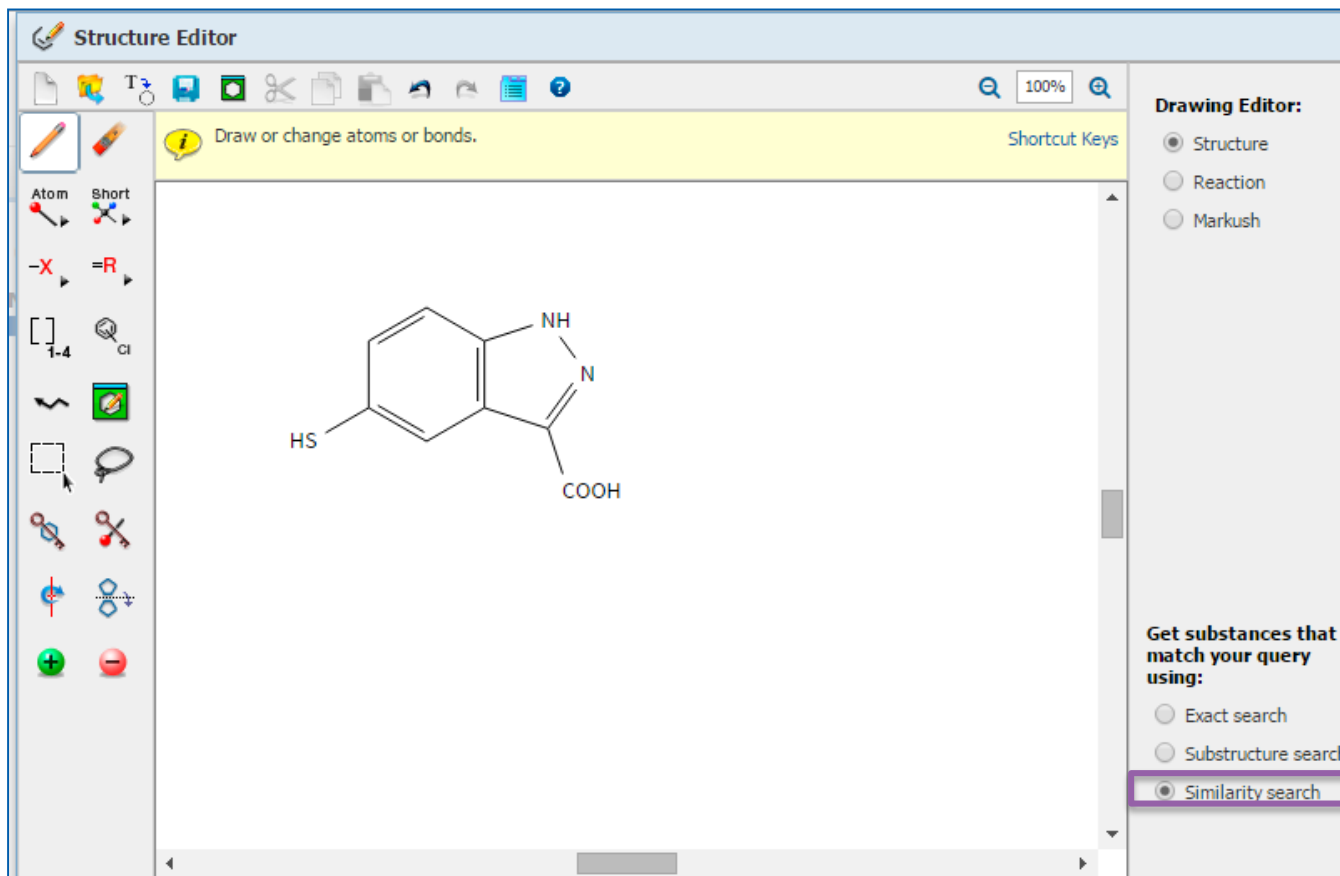
# 物质检索——亚结构检索

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

Get Substances

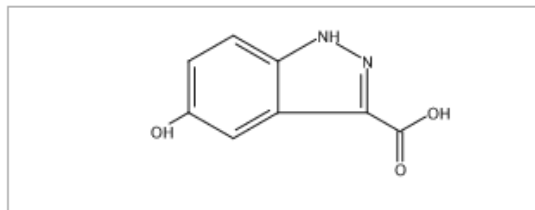
评分越高，相似度越高，结构越相似

Score: 88

1. 885518-94-5

取代基变化

~1 ~35



$C_8 H_6 N_2 O_3$

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

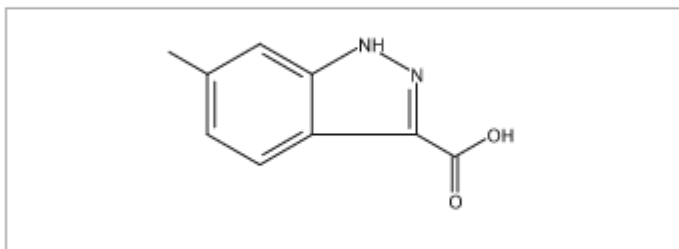
▶ Key Physical Properties

Score: 86

5. 858227-12-0

取代基位置变化

~7 ~41



$C_9 H_8 N_2 O_2$

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

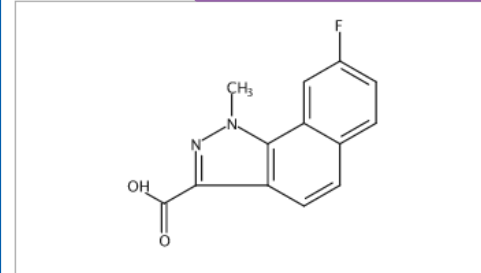
▶ Key Physical Properties

Score: 65

541. 1100422-

母体结构变化

~1



$C_{13} H_9 F N_2 O_2$

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

▶ Key Physical Properties



**SCIFINDER**<sup>®</sup>  
A CAS SOLUTION

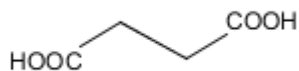
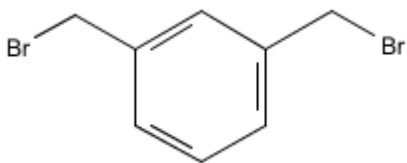
# 物质检索——相似结构检索

- 相似结构检索：

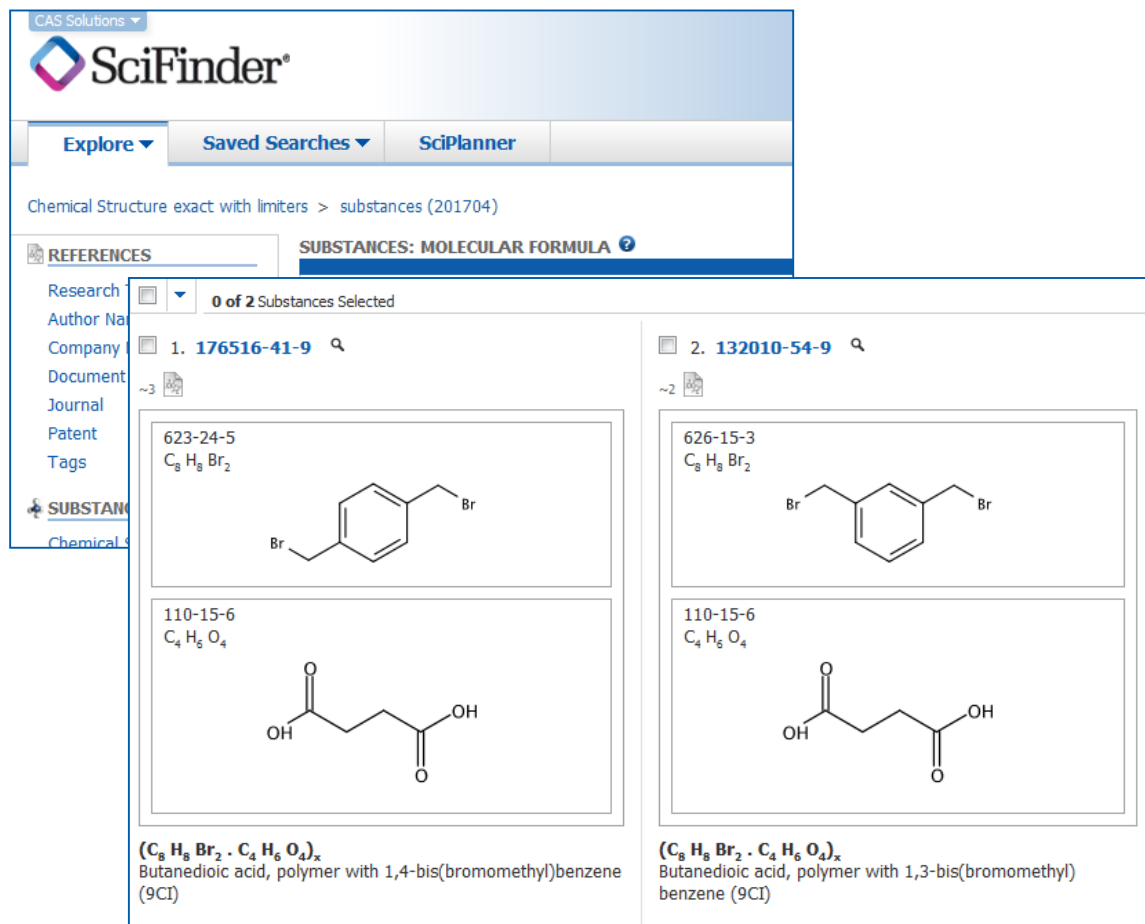
获得片段或整体结构与被检索结构相似的结果，母体结构可以被取代，也可以被改变

# 聚合物的检索

已知起始原料的聚合物



$(C_8 H_8 Br_2 \cdot C_4 H_6 O_4)_x$



The screenshot shows the SciFinder interface with search results for the molecular formula  $(C_8 H_8 Br_2 \cdot C_4 H_6 O_4)_x$ . The results are displayed in a grid format, showing two entries:

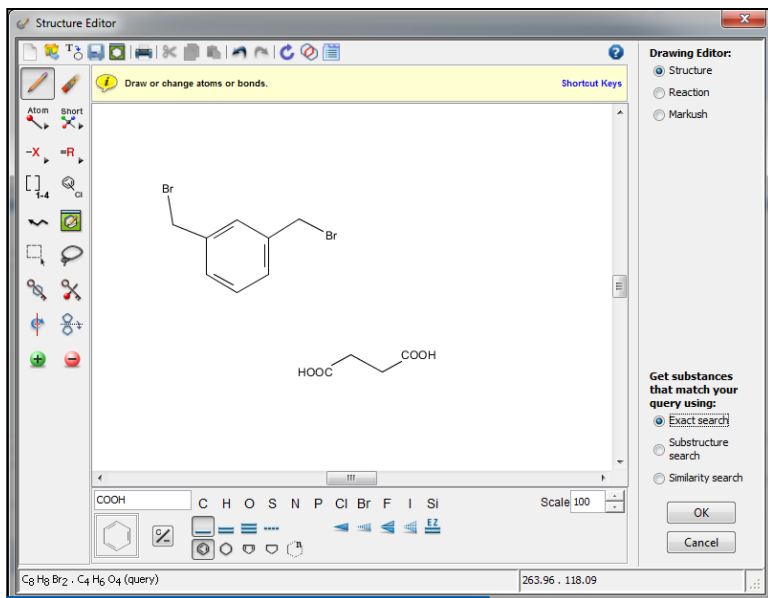
- Entry 1: 176516-41-9. Chemical structure: 1,4-bis(bromomethyl)benzene. Molecular formula:  $C_8 H_8 Br_2$ .
- Entry 2: 132010-54-9. Chemical structure: Butanedioic acid. Molecular formula:  $C_4 H_6 O_4$ .

The search results also show the molecular formula  $(C_8 H_8 Br_2 \cdot C_4 H_6 O_4)_x$  and the name of the polymer: Butanedioic acid, polymer with 1,4-bis(bromomethyl)benzene (9CI).

分子式检索后会得到同分异构体



# 聚合物的检索



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

单一组分

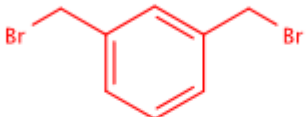
聚合物

0 of 1 Substance Selected

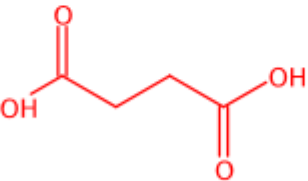
1. **132010-54-9** 🔍

~2

626-15-3  
C<sub>8</sub> H<sub>8</sub> Br<sub>2</sub>



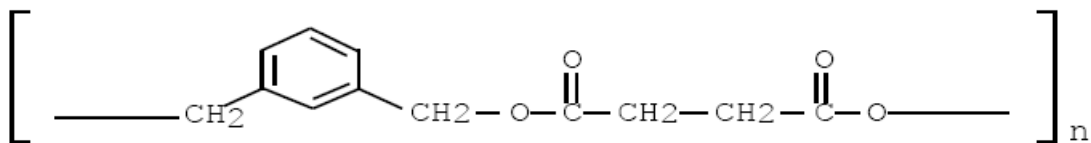
110-15-6  
C<sub>4</sub> H<sub>6</sub> O<sub>4</sub>



**(C<sub>8</sub> H<sub>8</sub> Br<sub>2</sub> . C<sub>4</sub> H<sub>6</sub> O<sub>4</sub>)<sub>x</sub>**  
 Butanedioic acid, polymer with 1,3-bis(bromomethyl)benzene (9CI)

# 聚合物的检索

已知重复单元的聚合物



(C<sub>12</sub> H<sub>12</sub> O<sub>4</sub>)<sub>n</sub>

SciFinder®  
Welcome Helen Zhu

Explore Saved Searches SciPlanner Save Print Export

Molecular Formula "(C<sub>12</sub> H<sub>12</sub> O<sub>4</sub>)<sub>n</sub>" > substances (45)

STANCES Get References Get Reactions Get Commercial Sources Tools

Sort by: CAS Registry Number

0 of 45 Substances Selected

1. 1801551-81-4 [Chemical Structure] (C <sub>12</sub> H <sub>12</sub> O <sub>4</sub> ) <sub>n</sub> INDEX NAME NOT YET ASSIGNED	2. 1637772-98-5 [Chemical Structure] (C <sub>12</sub> H <sub>8</sub> O <sub>4</sub> ) <sub>n</sub> Poly[oxy-1,4-butanedioxyoxycarbonyl(1,4-phenylene-2,3,5,6-d)carbonyl]	3. 1421756-46-8 [Chemical Structure] (C <sub>12</sub> H <sub>12</sub> O <sub>4</sub> ) <sub>n</sub> Poly[oxy((1,4-phenyl-1,2-ethanedioxy)oxy(1,4-dioxo-1,4-butanedioxy)]
4. 1392419-56-5 [Chemical Structure]	5. 1353713-96-8 [Chemical Structure] Substance Image	6. 1341223-97-9 [Chemical Structure] Substance Image

Click to view detail  
Substance Image Cannot Be Displayed 1421756-46-8

# 聚合物的检索

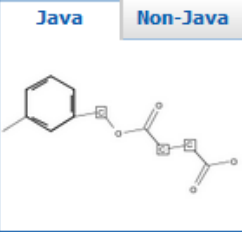
Analyze Refine

Refine by: ?

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

Structure Editor:

Java Non-Java

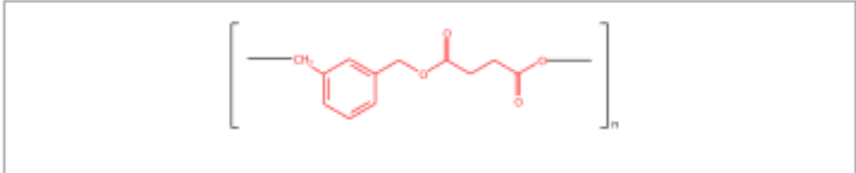


Click image to change structure or view detail.  
Search type: **Substructure**

0 of 1 Substance Selected

1. 132010-11-8

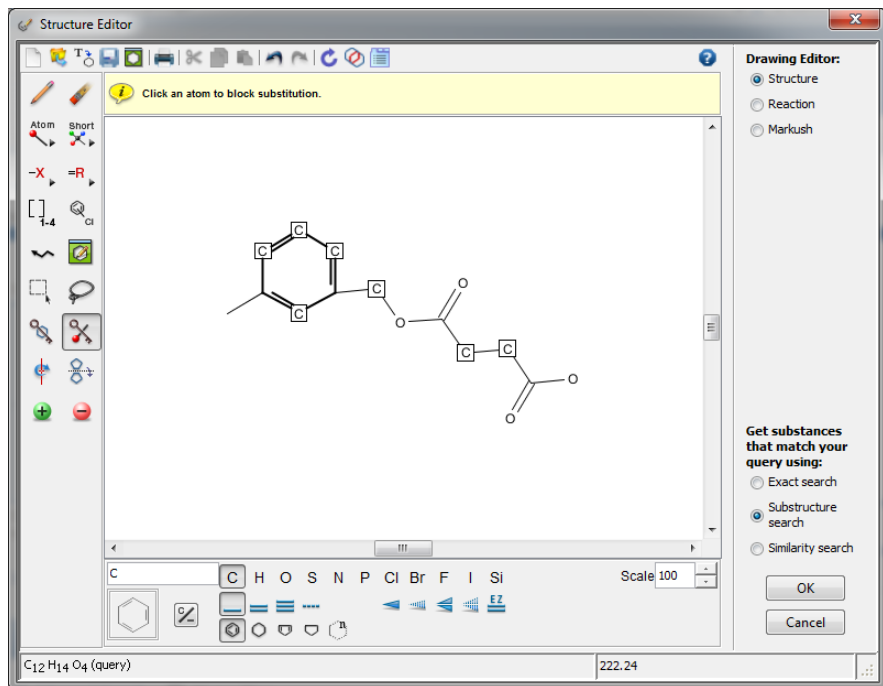
~2



$(C_{12} H_{12} O_4)_n$   
Poly[oxy(1,4-dioxo-1,4-butanediyl)oxymethylene-1,3-phenylenemethylene] (9CI)

利用结构特征进行Refine，迅速查找需要的物质

# 聚合物检索



绘制好SRU后用亚结构检索  
因为两段为开放状态

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

单一组分

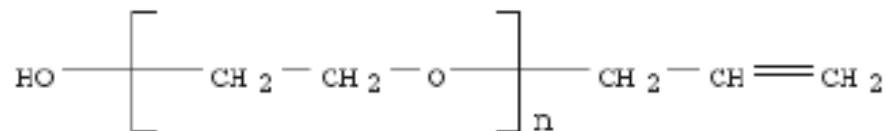
聚合物

The screenshot shows the SciFinder search results interface. At the top, it says "0 of 1 Substance Selected". Below that, the first result is listed as "1. 132010-11-8" with a magnifying glass icon. Underneath the result number is a chemical structure of a polymer repeat unit, shown in red, enclosed in brackets with a subscript 'n'. The structure is a poly[oxy(1,4-dioxo-1,4-butanediyl)oxymethylene-1,3-phenylenemethylene]. Below the structure, the chemical formula  $(C_{12}H_{12}O_4)_n$  is displayed, followed by the full name of the polymer: Poly[oxy(1,4-dioxo-1,4-butanediyl)oxymethylene-1,3-phenylenemethylene] (9CI).



# 聚合物的检索

含端基和SRUs的聚合物



Explore ▾ Saved Searches ▾ SciPlanner

REFERENCES

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

SUBSTANCES: MOLECULAR FORMULA ?

(C<sub>2</sub> H<sub>4</sub> O)<sub>n</sub> C<sub>3</sub> H<sub>6</sub> O

Examples:  
H<sub>4</sub>SiO<sub>4</sub>  
(C<sub>3</sub>H<sub>6</sub>O.C<sub>2</sub>H<sub>4</sub>O)<sub>x</sub>

Search

SUBSTANCES

(C<sub>2</sub> H<sub>4</sub> O)<sub>n</sub> C<sub>3</sub> H<sub>6</sub> O

↑  
SRU部分

↑  
两端部分

0 of 4 Substances Selected

1. 1500029-22-0

~3

(C<sub>2</sub> H<sub>4</sub> O)<sub>n</sub> C<sub>3</sub> H<sub>6</sub> O  
Poly(oxy-1,2-ethanediyl), α-(1-methylethenyl)-ω-hydroxy-

2. 191403-44-8

~5

(C<sub>2</sub> H<sub>4</sub> O)<sub>n</sub> C<sub>3</sub> H<sub>6</sub> O  
Poly(oxy-1,2-ethanediyl), α-1-propen-1-yl-ω-hydroxy-

3. 50856-25-2

~57

(C<sub>2</sub> H<sub>4</sub> O)<sub>n</sub> C<sub>3</sub> H<sub>6</sub> O  
Poly(oxy-1,2-ethanediyl), α-ethenyl-ω-methoxy-

4. 27274-31-3

~1115

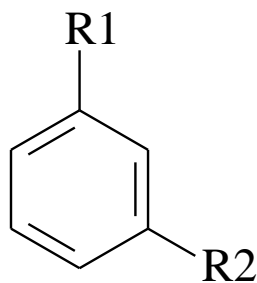
(C<sub>2</sub> H<sub>4</sub> O)<sub>n</sub> C<sub>3</sub> H<sub>6</sub> O  
Poly(oxy-1,2-ethanediyl), α-2-propen-1-yl-ω-hydroxy-  
Regulatory Information

# 提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
  - 文献检索 (PatentPak)
  - 物质检索 ( 聚合物检索 )
  - Markush检索
  - 反应检索 ( MethodsNow Synthesis )
  - SciPlanner
  - MethodsNow
- SciFinder常见问题及解决

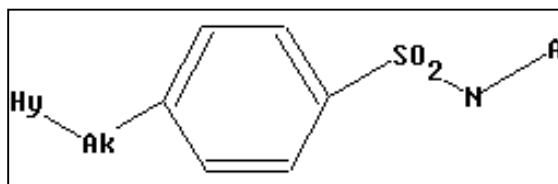
# Markush检索

- 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—halogen,  
|  
CH<sub>3</sub>



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

100%

Atom Short

-X =R

Hy-Ak SO<sub>2</sub>-N-A

**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

A C H O S N P Cl Br F I Si

# Markush检索

SCIFINDER<sup>®</sup>  
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

Display Options

Analyze by: Document Type

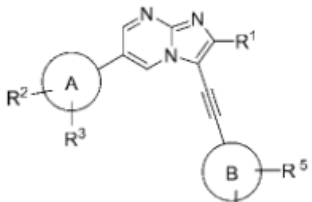
Patent	1969
Journal	1

Show More

1. **Compounds and methods for anticoagulation therapy**  
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)**  
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 [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>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...

全部是专利

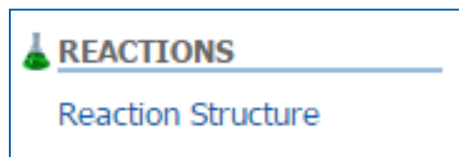
# 提纲

- 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 ( 聚合物检索 )
  - Markush检索
  - 反应检索 ( MethodsNow Synthesis )
  - SciPlanner
  - MethodsNow
- 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



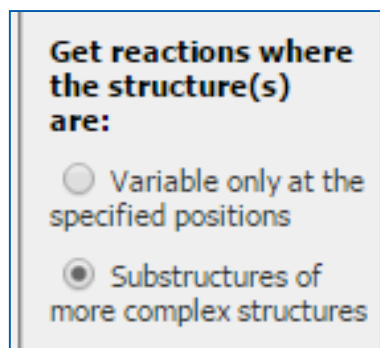
- 常用获取方法

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

The screenshot shows the Structure Editor window with various toolbars and a central canvas. The interface includes a top toolbar with icons for file operations, a left toolbar with drawing tools, a central canvas with a yellow status bar, and a right sidebar with drawing editor options. The bottom of the window features a chemical element palette and a status bar.

**Structure Editor**  
Draw or change atoms or bonds. Shortcut Keys

**Drawing Editor:**

- Structure
- Reaction
- Markush

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

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

**Annotations:**

- 反应箭头 (Reaction Arrow)
- 反应原子标记工具 (Reaction Atom Marking Tool)
- 官能团列表 (Functional Group List)
- 反应角色工具 (Reaction Role Tool)
- 反应位置标记工具 (Reaction Position Marking Tool)



# SciFinder反应检索——精确反应检索

The screenshot displays the SciFinder Structure Editor interface. The central workspace shows a chemical reaction: nitrobenzene (reactant) is converted to aniline (product). The reactant is a benzene ring with a nitro group ( $\text{NO}_2$ ) at the bottom position, and the product is a benzene ring with an amino group ( $\text{NH}_2$ ) at the bottom position. An arrow points from the reactant to the product. Below the structures, the text "reactant" and "product" are visible. The interface includes a drawing toolbar on the left with various icons for atoms, bonds, and rings. At the bottom, there is a search bar containing "NH2" and a list of elements: C, H, O, S, N, P, Cl, Br, F, I, Si. The status bar at the bottom shows the molecular formula  $\text{C}_7\text{H}_7\text{NO}_2 \cdot \text{C}_7\text{H}_7\text{N}$  and the coordinates 137.14 . 107.16. On the right side, the "Drawing Editor" panel is open, showing three radio buttons: "Structure", "Reaction" (which is selected), and "Markush". Below this, the text "Get reactions where the structure(s) are:" is followed by two radio buttons: "Variable only at the specified positions" and "Substructures of more complex structures". A purple callout box with the text "精确反应检索" (Precise Reaction Search) points to the "Variable only at the specified positions" option. The "OK" and "Cancel" buttons are at the bottom of the panel.

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章，通过Group by Document合并。

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

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

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

~102 100% ~122

**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

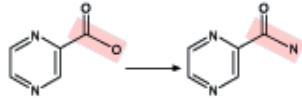
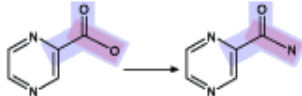
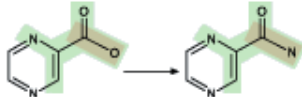
Narrow：反应中心及扩展的原子和键

### 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)  


# 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

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

更精确的查找需要的反应

# 反应检索结果的筛选

获得特定物质做还原剂的反应

**REACTIIONS** Get References Tools Send to SciPlann

Analyze **Refine**

Analyze by: Reagent

H <sub>2</sub>	148
<b>NaBH<sub>4</sub></b>	<b>51</b>
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.*

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

~102 100% ~122

**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

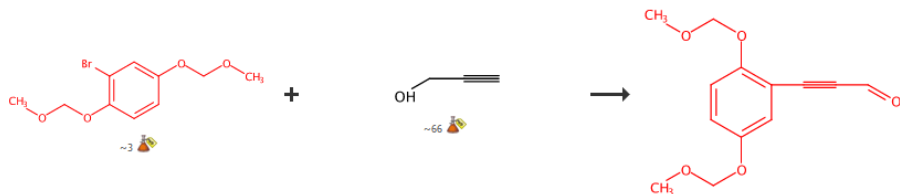


General/Typical Procedure: **General Procedure for Nitroarene Reductions.** Molecular hydrogen was added with a balloon filled with 1 atm of H<sub>2</sub> to a mixture of nitroarene (0.3 mmol), Cs<sub>2</sub>CO<sub>3</sub> (0.3 mmol), anisole as internal standard (0.3 mmol), and NHC-Pd-rGO (6 × 10<sup>-3</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

# SciFinder囊括最大的反应实验过程合集

2 Steps Hover over any structure for more options.



## Overview Steps/Stages

- 1.1 C: Pd(PPh<sub>3</sub>)<sub>4</sub>, S: BuNH<sub>2</sub>, 21 h, 100°C
- 2.1 R: DMSO, R: Cl(O=)CC(=O)Cl, S: CH<sub>2</sub>Cl<sub>2</sub>, 15 min, -78°C
- 2.2 S: CH<sub>2</sub>Cl<sub>2</sub>, -78°C; 2 h, -78°C
- 2.3 R: Et<sub>3</sub>N, 30 min, -78°C; -78°C → rt
- 2.4 R: H<sub>2</sub>O, R: NH<sub>4</sub>Cl, 30 min, rt

## Notes

1) key step, alternate catalyst concentration, catalyst (CuI) and temperature, Sonogashira coupling, 2) key intermediate, Swern oxidation, Swern method shown, Reactants: 2, Reagents: 5, Catalysts: 1, Solvents: 2, 5 Most stages in any one step: 4

## References

Synthesis of Bioactive Speciosins G and P from *Hexagonia speciosa*  
[Quick View](#) [Other Sources](#)  
 By Guerrero-Vasquez, Guillermo A. et al  
 From Journal of Natural Products, 77(9), 2029-2036; 2014

## Experimental Procedure:

我们可以做得更好

- 更好的阅读体验?
- 这些数字代表什么?
- 查免费的Supporting Information? 可能只有图谱。

## Experimental Procedure

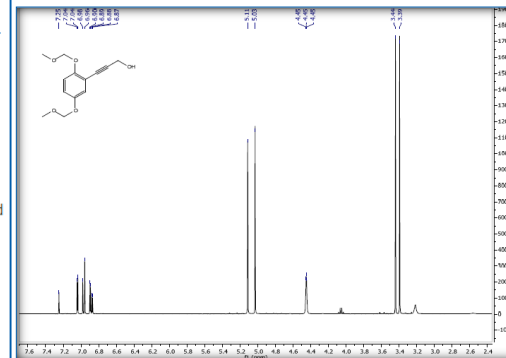


### Step 1

**General Procedure for the Sonogashira Coupling.**<sup>8,10,11</sup> Compounds **6a**<sup>31</sup> and **16**<sup>8</sup> were synthesized according to literature procedures. Aryl halide **6a** or **16** (9.21 mmol) in *n*-butylamine (6.4 mL) was placed in a flame-dried round-bottomed flask under an argon atmosphere. A mixture of terminal alkynes **7**, **25**, **26**, or **27** (9.21 mmol) in *n*-butylamine (10 mL) and Pd(Ph<sub>3</sub>)<sub>4</sub> (5% or 3%) was added, with the optional addition of CuI (3%) where appropriate. The mixture was heated for 21 h at 98 °C and poured into H<sub>2</sub>O (80 mL). The product was extracted with EtOAc (3 × 80 mL). The combined organic layers were washed with brine, dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>, and evaporated under reduced pressure. The crude product was purified by silica gel column chromatography (EtOAc/hexanes, 10–50%). *3*-(2,5-bis(methoxymethoxy)phenyl)prop-2-yn-1-ol<sup>2</sup> (**8**). Yield 96%; colorless oil. IR (KBr)  $\nu_{\max}$  3310, 2230 cm<sup>-1</sup>; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz)  $\delta$  3.46 (3H, s, H-4b), 3.51 (3H, s, H-1b), 4.51 (2H, s, H-1a), 5.09 (2H, s, H-4a), 5.17 (2H, s, H-1a), 6.95 (1H, dd, *J* = 9 and 3.0 Hz, H-5), 7.03 (1H, d, *J* = 9.0 Hz, H-6), 7.10 (1H, d, *J* = 3.0 Hz, H-3); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz)  $\delta$  51.81 (C-9), 56.05 (C-4b), 56.38 (C-1b), 81.74 (C-7), 91.56 (C-8), 95.14 (C-4a), 95.88 (C-4b), 114.19 (C-2), 117.13 (C-5), 118.50 (C-3), 121.20 (C-6), 151.95 (C-4), 153.06 (C-1); HRESIMS *m/z* 275.0900 [M + Na]<sup>+</sup> (calcd for C<sub>13</sub>H<sub>16</sub>O<sub>5</sub> 275.0896).

### Step 2

**Generation of the Key Aldehyde.**<sup>17</sup> Oxalyl chloride (272.3  $\mu$ L, 3.12 mmol) in dry CH<sub>2</sub>Cl<sub>2</sub> (9 mL) was added to a stirred solution of DMSO (332  $\mu$ L, 4.68 mmol) in dry CH<sub>2</sub>Cl<sub>2</sub> (1.5 mL) under an argon atmosphere at -78 °C. The mixture was stirred for 15 min, and the alcohol **8** (393.5 mg, 1.56 mmol) or alcohol **17** (300 mg, 1.56 mmol) in dry CH<sub>2</sub>Cl<sub>2</sub> (12 mL) was added dropwise (Note: Swern oxidation could be scaled-up to 1.56 mmol of starting material). After the starting material had been consumed (nearly 2 h), Et<sub>3</sub>N (1.88 mL, 7.8 mmol) was added. The reaction mixture was stirred at -78 °C for a further 30 min and was allowed to warm to rt and quenched with saturated NH<sub>4</sub>Cl and H<sub>2</sub>O, and the mixture was stirred for 30 min. The organic phase was decanted off, and the aqueous layer was extracted with CH<sub>2</sub>Cl<sub>2</sub> (3 × 30 mL). The combined organic layers were washed with brine, dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>, and evaporated under reduced pressure. *3*-(2,5-bis(methoxymethoxy)phenyl)prop-2-ynal (**9**). Yield 91%; colorless oil. IR (KBr)  $\nu_{\max}$  1660, 2194 cm<sup>-1</sup>; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz)  $\delta$  3.46 (3H, s, H-4b), 3.51 (3H, s, H-1b), 5.10 (2H, s, H-4a), 5.21 (2H, s, H-1a), 7.09 (1H, dd, *J* = 9.2 and 1.2 Hz, H-6), 7.12 (1H, dd, *J* = 9.1 and 2.2 Hz, H-5), 7.22 (1H, dd, *J* = 2.2 and 1.3 Hz, H-3), 9.44 (1H, s, H-9); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz)  $\delta$  56.18 (C-4b), 56.54 (C-1b), 92.05 (C-8), 92.27 (C-7), 95.22 (C-4a), 95.58 (C-1a), 110.70 (C-2), 116.72 (C-6), 122.0 (C-5), 122.09 (C-3), 151.85 (C-4), 154.88 (C-1), 176.92 (C-9); HRESIMS *m/z* 273.0741 [M + Na]<sup>+</sup> (calcd for C<sub>13</sub>H<sub>14</sub>O<sub>5</sub> 273.0739).



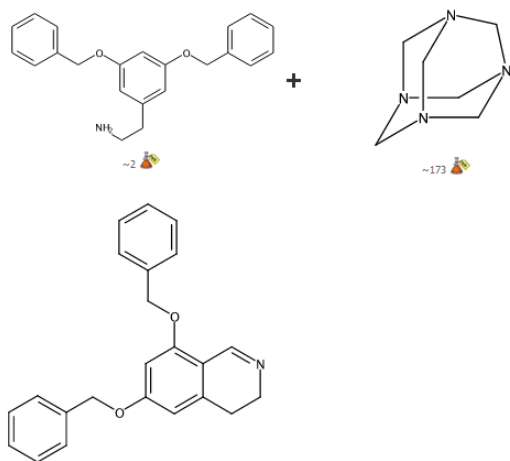
# MethodsNow Synthesis

## MethodsNow

### Asymmetric formal synthesis of schulzeines A and C

By Jang, Jaebong; Jung, Jong-Wha; Ahn, Jaeseung; Sim, Jaehoon; Chang, Dong-Jo; Kim, Dae-Duk; Suh, Young-Ger  
From Organic & Biomolecular Chemistry, 10(27), 5202-5204; 2012  
Published by Royal Society of Chemistry

Reaction Steps 1 2 3 4 5 6 7 8 9 10 11



多步反应中，原文没有描述  
的实验过程以灰色标示

<b>Products</b>	Isoquinoline, 3,4-dihydro-6,8-bis(phenylmethoxy)-, 95%, CAS RN: 1384461-35-1
<b>Reactants</b>	Benzeneethanamine, 3,5-bis(phenylmethoxy)-, CAS RN: 188662-05-7 Hexamethylenetetramine, CAS RN: 100-97-0
<b>Solvents</b>	Trifluoroacetic acid, CAS RN: 76-05-1 Acetic acid, CAS RN: 64-19-7
<b>Procedure</b>	<ol style="list-style-type: none"> <li>1. Add hexamethylenetetramine (3.1 g, 22.1 mmol) to the mixture of 2-(3,5-bis(benzyloxy)phenyl)ethanamine (2.0 g, 11.0 mmol), AcOH (12 mL) and TFA (3 mL) under argon</li> <li>2. Stir the mixture for 3 hours at 90°C.</li> <li>3. Dilute the reaction mixture with H<sub>2</sub>O.</li> <li>4. Basify with potassium carbonate and extract with CH<sub>2</sub>Cl<sub>2</sub>.</li> <li>5. Wash the combined organic layers with brine.</li> <li>6. Dry over MgSO<sub>4</sub> and concentrate in vacuo.</li> <li>7. Purify the residue by column chromatography on silica gel (5 to 10% EtOAc in hexane) to obtain 6,8-bis(benzyloxy)-3,4-dihydroisoquinoline.</li> </ol>
<b>Scale</b>	gram
<b><sup>1</sup>H NMR</b>	(CDCl <sub>3</sub> , 400 MHz) δ 8.69 (s, 1H), 7.43 - 7.29 (m, 10H), 6.45 (d, <i>J</i> = 1.88 Hz, 2H), 6.36 (s, 1H), 5.05 (s, 2H), 5.04 (s, 2H), 3.67 (t, 2H), 2.65 (t, 2H)
<b><sup>13</sup>C NMR</b>	(CDCl <sub>3</sub> , 100 MHz) δ 161.9, 157.7, 155.2, 140.0, 136.3, 128.6, 128.5, 128.1, 128.0, 127.4, 127.1, 111.9, 105.3, 98.5, 70.1, 46.5, 26.0
<b>IR</b>	(thin film, neat) ν <sub>max</sub> 3062, 3032, 2935, 1736, 1620, 1603, 1575, 1497, 1442, 1377, 1351, 1309 cm <sup>-1</sup>
<b>HRMS</b>	(FAB+) calcd for C <sub>23</sub> H <sub>22</sub> N <sub>2</sub> (M+H <sup>+</sup> ) 344.1651; found 344.1658
<b>Mass Spec</b>	(FAB+) <i>m/z</i> 344 (M+H <sup>+</sup> )
<b>State</b>	yellow solid
<b>CAS Method Number</b>	3-614-CAS-200055

物质信息

实验过程

图谱信息

保存/导出方法

Print/Export Close



# 亚结构反应检索

通过C-H活化对苯并噁唑或者恶唑进行烷基化

The screenshot shows the ChemDraw Structure Editor interface. On the left, the Structure Editor toolbar includes a button labeled "=R" which is highlighted with a purple box and an arrow pointing to the R-group Definitions dialog. The main window displays a chemical structure of a benzimidazole derivative with an R1 group attached to the C2 position. The R-group Definitions dialog box is open on the right, showing the definition R1 = O, S. Below the definition, there is a periodic table with the elements O and S highlighted in purple. The dialog also includes sections for Variables and Shortcuts, and buttons for Close and Cancel.

# 亚结构反应检索

The screenshot displays the Structure Editor interface. The main workspace shows a chemical reaction: a reactant (a benzimidazole-like structure with an R1 group and a hydrogen atom) reacting to form a product (the same structure with an Ak group instead of the hydrogen). A purple arrow points from the Ak variable in the product to the Variables dialog box.

**Structure Editor**

Drag the reaction arrow to specify reaction direction.

**Drawing Editor:**

- Structure
- Reaction
- Markush

**Variables**

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

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

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

Buttons: Close, OK, Cancel

Bottom status bar: Formula is not available

# 通过后处理工具筛选反应--Analyze

通过催化剂筛选反应

Analyze Refine

Analyze by: ?  
Catalyst

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

Group by: No Grouping Sort by: Accession Number

No Grouping  
Document  
Transformation

1. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.

~57  
~52  
83%

Overview

Steps/Stages

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

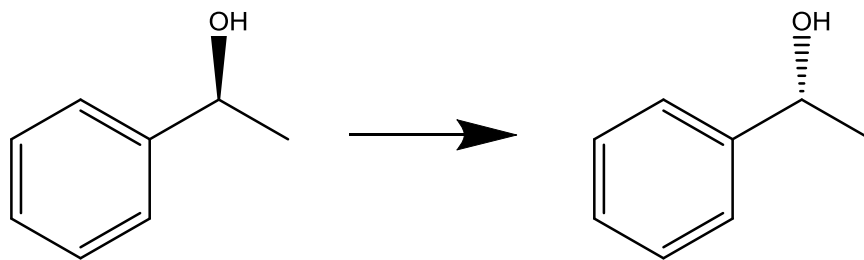
Notes

catalyst prepared and used, screw cap tube used, Reactants: 2, Reagents: 2, Catalysts: 1, Solvents: one step: 3

References

ACS / Proprietary and Confidential / Do Not Distribute

## 案例：如何获取手性翻转反应



# 案例：如何获取手性翻转反应

检索思路：

- 1). 先获取反应物物质，然后再获取其作为反应物的反应，得到检索结果集1。
- 2). 先获取产物物质，然后再获取其作为产物的反应，得到检索结果集2。
- 3). 两个结果集取交集。

Substances: CHEMICAL STRUCTURE

Structure Editor:

Java Non-Java

Search Type:

- Exact Structure
- Substructure
- Similarity

Show precision analysis

ChemDraw

Launch a SciFinder substa  
More

Import CXF

Search

1 of 52 Substances Selected

1. 1445-91-6

~3499

Absolute stereochemistry, Rotation (-).

$C_8H_{10}O$   
Benzenemethanol,  $\alpha$ -methyl-, (aS)-

Key Physical Properties  
Regulatory Information  
Spectra  
Experimental Properties

Get Reactions

Retrieve reactions for:

- All substances
- Selected substances

Limit results by reaction role:

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

Get Cancel

# 案例：如何获取手性翻转反应

ances (52) > get reactions (7938)


Get References | Tools

Group by: No Grouping | Sort by: Accession Number

0 of 7938 Reactions Selected

1. View Reaction Detail [Link](#)

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



### Combine Answer Sets

Select an option for combining the two selected saved answer sets:

- Combine** Include all reactions from both sets
- Intersect** Include only reactions that appear in both sets
- Exclude** Include only answers from 2 that are not in 1
- Exclude** Include only answers from 1 that are not in 2

2 of 50 Reaction A

- 2 (4185)  
产物  
Chemical Structure e
- 1 (7938)  
反应物  
Chemical Structure e
- 2 (3888)  
Chemical Structure e
- 1 (9519)  
Chemical Structure e
- 手性2 (172)

Combine Answer Sets | Cancel

# 聚合物改性案例：甲基丙烯酸甲酯对聚乙二醇的改性反应

思路：

1. 从物质检索出发，先检索到聚乙二醇的物质信息
2. 从物质获取反应，获得聚乙二醇参与的反应信息
3. 限定反应，通过接枝物质的结构（甲基丙烯酸甲酯）来限定反应
4. 获得聚合物的改性反应

# 检索聚乙二醇物质信息：物质识别号检索

Explore ▾ Saved Searches ▾ SciPlanner

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: SUBSTANCE IDENTIFIER ⓘ

PEG

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

Search

substances (1)

Get References Get Reactions Get Commercial Sources Tools ▾

Sort by: CAS Registry Number ▾ ↓

0 of 1 Substance Selected

1. 25322-68-3 🔍

~233271 ~437

$$\text{OH} \left[ \text{---} \text{CH}_2 \text{---} \text{CH}_2 \text{---} \text{O} \right]_n \text{H}$$

**(C<sub>2</sub> H<sub>4</sub> O)<sub>n</sub> H<sub>2</sub> O**  
Poly(oxy-1,2-ethanediyl), α-hydro-ω-hydroxy-

▶ **Key Physical Properties**

- Regulatory Information
- Spectra
- Experimental Properties



# 从物质获取反应信息：获取聚乙二醇作为反应物的反应

Sample Analysis: [?](#)  
Reagent ▼

HOCH <sub>2</sub> CH <sub>2</sub> OH polymer	≥ 7928
HCl	≥ 6993
Et <sub>3</sub> N	≥ 5713
DCC	≥ 5143
NaOH	≥ 4539
K <sub>2</sub> CO <sub>3</sub>	≥ 3583
NaN <sub>3</sub>	≥ 3358
NaHCO <sub>3</sub>	≥ 3314
H <sub>2</sub>	≥ 3069
NaBH <sub>4</sub>	≥ 2996

[Show More](#)

0 of 39274 Reactions Selected Page: 1 of 2619

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

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

22336. [View Reaction Detail](#) [Link](#)

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

Overview  
Steps/Stage

1.1 S:EtC(=O)  
1.2 80°C

[Step 3.1]  
~128

# 限定反应：根据参与反应的甲基丙烯酸甲酯，限定反应结构

The screenshot displays the SciFinder Structure Editor interface. On the left, the 'REACTIIONS' panel is active, with the 'Refine' tab selected. Under 'Refine by:', the 'Reaction Structure' option is highlighted with a red box. Below it, several other refinement criteria are listed: Product Yield, Number of Steps, Reaction Classification, Excluding Reaction Classification, and Non-participating functional groups. The main workspace shows the chemical structure of methyl methacrylate (MMA) labeled as 'reactant'. The structure is a 2D skeletal structure with a methyl group, a methacrylate group, and a methyl ester group. The status bar at the bottom indicates the molecular formula  $C_5H_8O_2$  and the molecular weight 100.12. On the right side, there are options to 'Get reactions where the structure(s) are:' with radio buttons for 'Variable only at the specified positions' (selected) and 'Substructures of more complex structures'. 'OK' and 'Cancel' buttons are at the bottom right.

# 获得改性后的聚合物：获得甲基丙烯酸甲酯 (MMA) 接枝的PEG

Analyze Refine

Group by: No Grouping Sort by: Relevance

0 of 156 Reactions Selected

1. View Reaction Detail Link

Single Step Hover over any structure for more options.

### MMA封端的PEG

OH-[CH2-CH2-O]n-H + CH2=C(CH3)COOCH3 → CH2=C(CH3)COO-[CH2-CH2-O]n-O-CO-C(CH3)=CH2

2. Overview Steps/Stages

1.1 R:NaOH, 1.2 R:Phenol

3. View Reaction Detail Link

Single Step Hover over any structure for more options.

### PMMA和PEG共聚物

OH-[CH2-CH2-O]n-H + CH2=C(CH3)COOCH3 → [CH2-CH2-O]n-[CH2-C(CH3)(COOCH3)]m

1.1 C:(PhCO<sub>2</sub>)<sub>2</sub>, S:CH<sub>2</sub>Cl<sub>2</sub>, 6 h, 80°C

Notes  
thermal, Reactants: 2, Catalysts: 1, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References  
Chemistry modification of PMMA-g-PEG copolymer  
Quick View Other Sources  
By Rosa, Juliana dos Santos et al  
From Macromolecular Symposia, 343(1), 78-87; 2014

# 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 ( 聚合物检索 )
  - Markush检索
  - 反应检索 ( MethodsNow Synthesis )
  - SciPlanner
  - MethodsNow
- 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** [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

**进入SciPlanner 新建文件**

SciPlanner SciPlanner\_11\_19\_2015\_112612 **将刚推送过来的反应拖至编辑面板**

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.

# SciPlanner使用简介

SciPlanner 11\_19\_2015\_112612

Workspace Edit View GoTo

CAS Registry Number: 13091-23-1

- 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

打开中间产物的标准菜单  
选择Synthesis this

1 2 3

Get References Tools

Send selected records to SciPlanner. Send to SciPlanner

Group by: No Grouping Sort by: Accession Number

1 of 34 Reactions Selected

1. View Reaction Detail

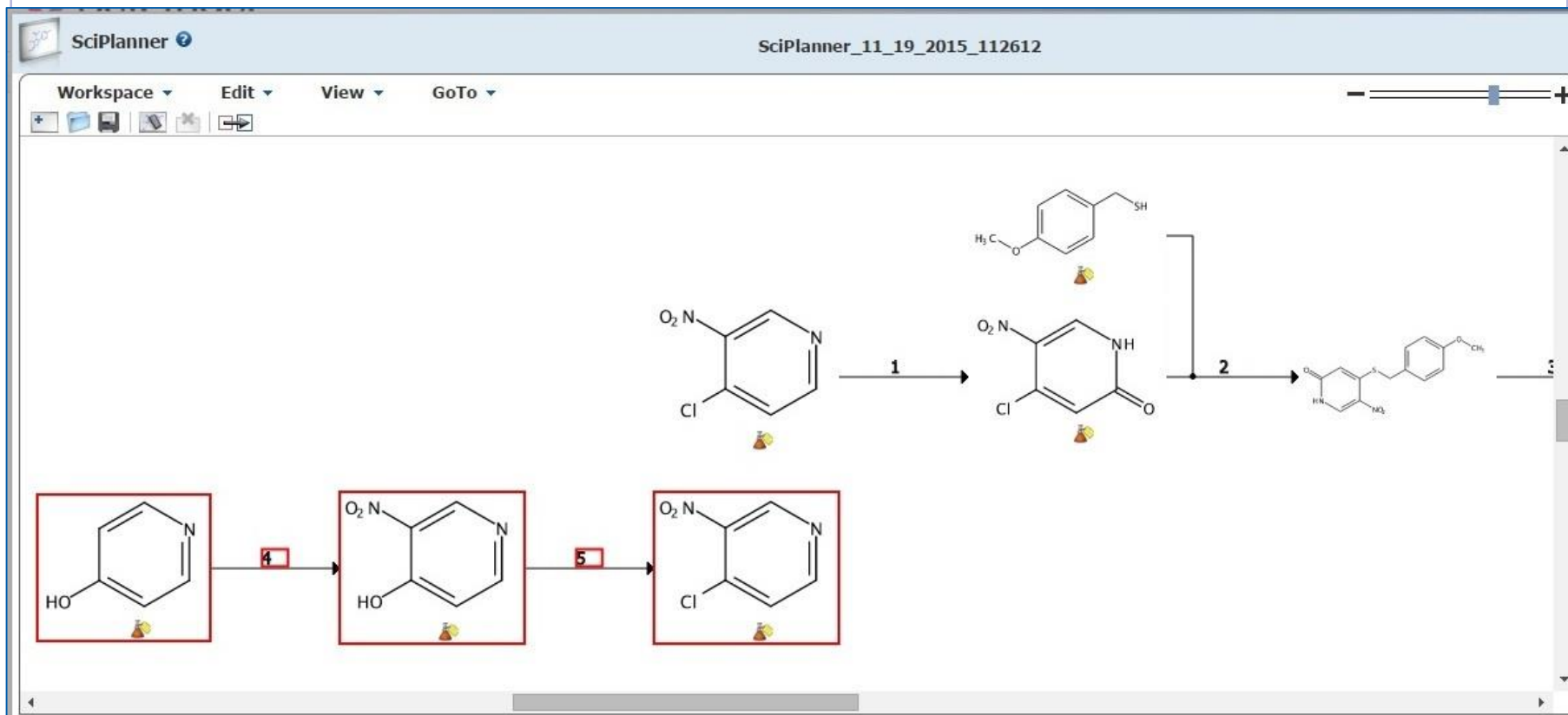
2 Steps Hover over any structure for more options.

在检索到的反应中选择感兴趣的反应

继续推送到SciPlanner

~161 ~192

# SciPlanner使用简介



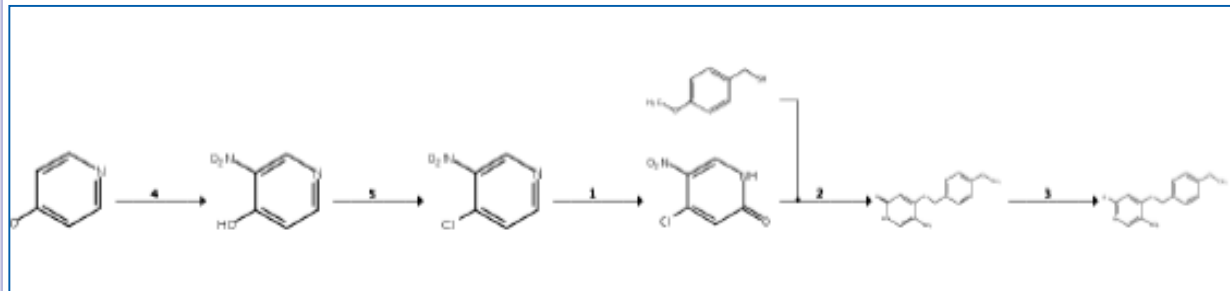
步骤同前，将推送过来的反应拖到编辑面板中，可以看到两条反应中存在同样的结构

# SciPlanner使用简介

The screenshot displays the SciPlanner software interface. The top menu bar includes 'Workspace', 'Edit', 'View', and 'GoTo'. A 'Workspace' dropdown menu is open on the left, listing options: New, Open, Save, Duplicate, Import, **Export**, Print, and Close. The main workspace shows a chemical reaction sequence: a starting material (a pyridine ring with a nitro group and a hydroxyl group) reacts (step 4) to form a pyridine ring with a nitro group and a chlorine atom. This intermediate then reacts (step 5) to form another pyridine ring with a nitro group and a chlorine atom. Finally, this intermediate reacts (step 1) to form a pyridine ring with a nitro group and a chlorine atom, which is then converted to a pyridine ring with a nitro group and a chlorine atom, and finally to a pyridine ring with a nitro group and a chlorine atom. A pink callout box points to the 'Export' option in the menu with the text: '点击 Workspace, 选择 Export 导出结果'. Another pink callout box points to the reaction steps with the text: '用鼠标将两个同样的结构拖至重叠, 两条反应合并'. A third pink callout box points to the 'Export' dialog box with the text: '选择适当的输出格式, 输出结果'. The 'Export' dialog box is open on the right, showing options for 'Offline Review' (Portable Document Format (\*.pdf), Citations (\*.ris), Image (\*.png)) and 'Saving Locally' (SciPlanner eXchange (\*.pkx)). The 'Details' section includes 'File Name: \*' (SciPlanner\_11\_19\_2015\_112612) and 'Title'. The 'Include' section has checkboxes for 'SciPlanner Image', 'Reaction Details', 'Substance Details', and 'Reference Details'. 'Export' and 'Cancel' buttons are at the bottom right.



# SciPlanner导出结果



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

Substance Information		
<p>1228150-22-8</p> <p>C<sub>13</sub>H<sub>12</sub>N<sub>2</sub>O<sub>4</sub>S 2-(1H)-Pyridinone, 4-[[4-methoxyphenyl)methyl]thio]-5-nitro-</p> <p>Related Info: ~ 2 References Reactions</p>	<p>1228150-23-9</p> <p>C<sub>13</sub>H<sub>11</sub>ClN<sub>2</sub>O<sub>3</sub>S Pyridine, 2-chloro-4-[[4-methoxyphenyl)methyl]thio]-5-nitro-</p> <p>Related Info: ~ 2 References Reactions</p>	<p>13091-23-1</p> <p>C<sub>6</sub>H<sub>3</sub>ClN<sub>2</sub>O<sub>2</sub> Pyridine, 4-chloro-3-nitro-</p> <p>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-</p> <p>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-</p> <p>Related Info: ~ 749 References Reactions ~ 71 Commercial Sources Regulatory Information</p>	<p>626-64-2</p> <p>C<sub>6</sub>H<sub>7</sub>N O 4-Pyridinol</p> <p>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)-Pyridinone, 4-chloro-5-nitro-</p> <p>Related Info: ~ 22 References Reactions ~ 136 Commercial Sources</p>		

# 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 ( 聚合物检索 )
  - Markush检索
  - 反应检索 ( MethodsNow Synthesis )
  - SciPlanner
  - **MethodsNow**
- SciFinder常见问题及解决

# MethodsNow™ 是一个完整的 CAS 解决方案



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- Historical Analysis / Dating: 考古分析，同位素分析
- Environmental Analysis: 土壤/空气/水分析，农药残留分析...
- Agricultural Applications / Analysis: 除草剂分析...
- Food Analysis: 脂肪酸分析，脂肪酸酯分析，蛋白质分析...
- Fuels / Geology / Biofuels: 生物燃料分析，油气分析，石油产品分析，煤炭加工...
- Miscellaneous: 化妆品分析，爆炸物分析，纳米材料分析...

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输入SciFinder的账号密码



# MethodsNow – Analysis(www.methodsnow.com)

检索/高级检索



方法分类



历史检索



The screenshot shows the MethodsNow website interface. At the top, there is a navigation bar with the logo 'METHODSNOW A CAS SOLUTION' and links for 'Saved' and 'Account'. Below the navigation bar is a search section with the heading 'Search' and a search input field. A callout bubble points to the search input field with the text '保存结果集'. Below the search input field is a link for 'Advanced Search'. The main content area is titled 'Browse Method Categories' and lists various categories such as 'Agricultural Applications / Analysis', 'Bioassays', 'Biomolecule Isolation', 'Environmental Analysis', 'Food Analysis', 'Organic Compound Analysis', 'Pharmacology / Toxicology', 'Polymer Analysis', and 'Water Analysis'. A callout bubble points to the 'Organic Compound Analysis' category with the text '点击一个类别 浏览相关方法'. Below the categories is a 'Recent Searches' section with a list of search results, including 'hplc lycopene analysis'. A callout bubble points to the 'hplc lycopene analysis' entry with the text '点击历史检索 重新运行检索'. Another callout bubble points to the 'X' icon next to the search entry with the text '点击“X” 删除检索历史'.

# 高级检索

The image shows two overlapping screenshots of the CAS MethodsNow Advanced Search interface. The top screenshot shows the main search area with a 'Keyword' field and a dropdown menu for logical operators. A callout box points to the dropdown menu with the text '逻辑运算符 : and, or, not'. Another callout box points to a close button on the right with the text '删除检索条件'. The bottom screenshot shows the 'Add Search Criteria' dropdown menu open, listing search options: Keyword, Analyte, Matrix, Method Category, Technique, CAS Method Number, and Publication Name. A callout box points to this list with the text '检索选项 : 关键词、分析物、基质、方法分类、技术、CAS Method Number、期刊名'. The interface includes the MethodsNow logo, 'CAS Solutions' dropdown, 'Saved' and 'Account' icons, and a 'Return to Home' link.

逻辑运算符 : and, or, not

删除检索条件

增加检索条件

检索选项 : 关键词、分析物、  
基质、方法分类、技术、CAS  
Method Number、期刊名

# 案例：利用超临界萃取法分析叶片中的酚类物质

CAS Solutions



Search

此处只需输入一个关键词即可，MethodsNow会自动进行同义词查找

Enter keyword, matrix, analyte, etc.

supercritical



supercritical extraction

supercritical fluid chromatographic chiral stationary phases

supercritical fluid chromatography

Browse Method Categories

Agricultural Applications / Analysis

Fuels / Geology / Biofuels

Pharmacology / Toxicology

Bioassays

Historical Analysis / Dating

Polymer Analysis

Biomolecule Isolation

Miscellaneous

Water Analysis

Environmental Analysis

Organic Compound Analysis

Food Analysis

Organometallics / Inorganics

Recent Searches

supercritical extraction



member





# 结果显示

典型分析方法标题格式：通过某技术手段在某基质中分析某物质

限定分析物、基质、方法等条件

The screenshot displays the METHODS NOW search results page. The search query is "supercritical extraction". The results are sorted by relevance. A list of filters is on the left, including Analyte (Phenols, Palmitic acid, Limonene, Myrcene,  $(\pm)$ - $\alpha$ -Pinene), Matrix (Leaf, Root, Zingiber officinale, Seed, Coffee products), Method Category, and Technique (Supercritical extraction). The main results area shows a single result: "Analysis of Lutein A in Pharmaceutical natural products by HPLC" with CAS MN: 1-131-CAS-120642. The result details include Analyte (Rubixanthin; Lutein A; Zeaxanthin; *cis*- $\beta$ -Carotene;  $\beta$ -Carotene; Carotenes), Matrix (Rosa canina; Pharmaceutical natural products), Other Materials (Reagent: Ethanol; Hexane; Material: Spherisorb column (5  $\mu$ m, 4.6 x 250 mm, ODS1); Stainless steel column; Glass beads (1 mm diameter)), Method Category (Natural Product Isolation Analysis), Technique (Liquid chromatography spectrometric detectors; HPLC; Supercritical extraction), and Equipment Used (HPLC system; Diode array detector (DAD); Supercritical extraction apparatus; Thermostatic chamber). Callouts highlight the search bar, filter sidebar, result title, "View Details & Instructions" button, "Add to Compare" button, and action buttons (Export, Save).

导出方法

保存方法

查看方法详情

方法对比

# 结果显示

## Analysis of Phenols in *Calophyllum brasiliense* by Supercritical extraction

CAS MN: 2-105-CAS-52171

Method Category: Antioxidant Assay

Technique: Spectrophotometry; Soxhlet extractor; **Supercritical extraction**

Materials	Role	Image	CAS RN
Mammea A/BB	analyte	<a href="#">View Structure</a>	6916-62-7
Xanthone	analyte	<a href="#">View Structure</a>	90-47-1
Coumarin	analyte	<a href="#">View Structure</a>	91-64-5
Phenols	analyte		
Biflavonoids	analyte		
<i>Calophyllum brasiliense</i>	matrix		
Leaf	matrix		
Sieves (30 and 50 mesh)	material		
Dichloromethane	reagent	<a href="#">View Structure</a>	75-09-2
Methanol	reagent	<a href="#">View Structure</a>	67-56-1
DPPH radical	reagent	<a href="#">View Structure</a>	1898-66-4

## 实验材料

### Source

Comparing conventional and **supercritical extraction** of (-)-mammea A/BB and the antioxidant activity of *Calophyllum brasiliense* extracts

Goncalves, Renata Menoci; Lemos, Caroline Ortega Terra; Leal, Ivana Correa Ramos; Nakamura, Celso Vataru; Cortez, Diogenes Aparicio Garcia; da Silva, Edson Antonio; Cabral, Vladimir Ferreira; Cardozo-Filho, Lucio

Molecules (2013), 18, 6215 - 6229. MDPI AG

CODEN: MOLEFW | ISSN: 14203049 | DOI: 10.3390/molecules18066215

[Document Sources](#)

### Abstract ^

*Calophyllum brasiliense* is a rich source of bioactive coumarins, xanthones and biflavonoids. The aim of the study was to compare the phenol contents and the antioxidant activity of *C. brasiliense* extracts obtained by conventional and supercritical fluid extraction (SFE) methods, as well as the quantification of crude extracts and (-)-mammea A/BB yields. Dichloromethane and hexane were used as solvents for the conventional extractions and SFE was developed using supercritical CO<sub>2</sub>; the kinetic curves were modeled using a second-order empirical model. The dichloromethane extract presented the best total yield, although it showed the lowest content of (-)-mammea A/BB. The concentration of the coumarin was considerably higher in concerning the ed to be more

### Instructions

#### Organic solvent extraction using Soxhlet apparatus

1. Collect the leaves of *Calophyllum brasiliense* Cambess.
2. Dry the plant material in a circulating air oven (QUIMIS Q-31) at 313 K temperature.
3. Mill the leaves in a home processor (WALITA RI7625) after 72 h.
4. Use Tyler sieves (W. S. Tyler, Mentor, OH, USA) to classify the samples according to particle size.
5. Select the leaves trapped in the 30 and 50 mesh sieves for the extraction.
6. Perform the organic solvent extraction for 300 min using a Soxhlet apparatus.
7. Use dichloromethane as a solvent due to the differences in terms of polarity and dielectric constant.
8. Set the boiling point at 313 K and the dielectric constant at 8.93.
9. Express the yields obtained for each solvent extraction and calculate in relation to the initial dry weight sample.

#### Determination of antioxidant activity by DPPH (2,2-diphenyl-1-picrylhydrazyl) method

1. Dilute the extracts in methanol up to concentrations from 25 to 350 µg/mL.
2. Add 2,850 µl of the DPPH solution (0.6 mM) to 150 µL of sample.
3. Substitute the volume of the samples by distilled water for the blank control.
4. Keep the reaction for 1 h at room temperature, in the dark.
5. Measure the absorbance at 515 nm.
6. Express the antioxidant activity (AA%) as a percentage of DPPH radical elimination, calculate according to the following equation:  $AA\% = [(1 - A_{sample})/A_{blank}] \times 100$ , where A.blank represents the absorbance of the blank and A.sample represents the absorbance of the extract solution.
7. Calculate the concentration of the extracts resulting in 50% of inhibition (IC<sub>50</sub>) from the inhibition percentage plotting graph.

### Validation

Inhibitory Activity 206.58 µg/mL (IC<sub>50</sub>)

## 文献信息

## Equipment Used

Oven, Q-31, QUIMIS

Processor, RI7625, WALITA

Spectrophotometer, UV-1203, Shimadzu

## Conditions

Instrument

Detection wavelength - 515 nm

## 设备条件

## 实验步骤及数据有效性

# 对比不同分析方法

导出对比  
PDF文件

	1	2	3
Title	Analysis of Phenols in <i>Calophyllum brasiliense</i> by Supercritical extraction	Analysis of Phenols in <i>Calophyllum brasiliense</i> by Supercritical extraction	Analysis of Phenols in <i>Calophyllum brasiliense</i> by Supercritical extraction
CAS Method Number	2-105-CAS-52171	1-131-CAS-62310	1-131-CAS-52140
Method Category	Antioxidant Assay	Natural Product Isolation	
Technique	Spectrophotometry; Soxhlet extractor; Supercritical extraction	Spectrophotometry; Soxhlet extractor	
Analyte	Mammea A/BB; Xanthone; Coumarin; Phenols; Biflavonoids	Phenols	
Matrix	<i>Calophyllum brasiliense</i> ; Leaf	<i>Calophyllum brasiliense</i> ; Leaf	
Other Materials	Dichloromethane; Methanol; DPPH radical; Sieves (30 and 50 mesh)	Methanol; Sodium carbonate; Folin-Ciocalteu reagent; Sieves (30 and 50 mesh)	
Equipment Used	Oven, Q-31, QUIMIS; Processor, RI7625, WALITA; Spectrophotometer, UV-1203, Shimadzu	Oven, Q-31, QUIMIS; Processor, RI7625, WALITA; Spectrophotometer, UV-1203, Shimadzu; Syringe pumps.	Oven, Q-31, QUIMIS; Processor, RI7625, WALITA; Spectrophotometer, UV-1203, Shimadzu; Syringe pumps.
Conditions	Instrument: Detection wavelength - 515 nm	Instrument: Detection wavelength - 760 nm	Instrument: Detection wavelength - 760 nm
Source	Comparing conventional and supercritical extraction of (-)-mammea A/BB and the antioxidant	Comparing conventional and supercritical extraction of (-)-mammea A/BB and the antioxidant	Comparing conventional and supercritical extraction of (-)-mammea A/BB and the antioxidant
Method	Organic solvent extraction using Soxhlet apparatus 1. Collect the leaves of <i>Calophyllum brasiliense</i> Cambout	Supercritical Fluid Extraction (SFE) 1. Collect the leaves of <i>Calophyllum brasiliense</i> Cambout	Supercritical Fluid Extraction (SFE) 1. Collect the leaves of <i>Calophyllum brasiliense</i> Cambout
Inhibitory Activity	206.58 µg/mL (IC <sub>50</sub> )		
Concentration		26.98 ± 2.90 mg of GAE/g of extract	15.06 ± 1.75 mg of GAE/g of extract

# 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 ( 聚合物检索 )
  - Markush检索
  - 反应检索 ( MethodsNow Synthesis )
  - SciPlanner
  - MethodsNow
- 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
- 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



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Beijing Forestry University Library

图书馆首页

资源

服务

本馆概况

首页 >> 资源 >> 电子资源 >> 试用资源

试用资源 / TRIAL RESOURCES

## SciFinder--全球权威科学研究工具

资源网址	语种/类型	揭示深度	起止年限	涉及学科	访问次数
访问入口	外文 / 综合	全文	试用截止日期至2017年4月26日	化学	

SciFinder 检索网址:

[URL-1: https://scifinder.cas.org/](https://scifinder.cas.org/)

[URL-2: https://origin-scifinder.cas.org/](https://origin-scifinder.cas.org/)

同时开通: **MethodsNow** 实验方法信息数据库 <http://www.methodsnow.com/>

**PatentPakTM——专利工作流程解决方案** 读者在SciFinder中找到需要的专利文献后, 在相应的文献标题下可看到PatentPak按钮, 点击该按钮即可使用。

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读者在使用SciFinder之前必须进行注册, 需提供学校名、所在院系、姓名及邮箱信息发送邮件至 [China@acsi.info](mailto:China@acsi.info), 请在24小时查收邮件, 点击邮件中的注册链接完成注册。注册后系统将自动发送一个链接到您所填写的email邮箱中, 激活此链接即可完成注册。参考“[SciFinder注册说明](#)”。



# 如何获取SciFinder账号

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

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

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

请注意：

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

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

3. 密码必须包含 7-15 个字符，并且至少**包含三种以下字符**：

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

例：abc@123

4. 从下拉列表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

From: CAS

Dear user,

To complete your SciFinder registration, you must click the link provided below. By clicking the link, you agree to all of the following terms and conditions:

- I will not share my username and password with any other person.
- I will search only for myself and not for others or other organizations.
- I will not use any automated program or script for extracting or downloading CAS data, or any other systematic retrieval of data.
- I may retain a maximum of 5,000 Records at any given time for personal use or to share within a Project team for the duration of the Project.
- My organization's SciFinder License and the CAS Information Use Policies (<http://www.cas.org/legal/infopolicy.html>) apply to my use of SciFinder.
- I will contact my SciFinder Key Contact if I have questions.

If you do not accept these terms and conditions, do not click the link and delete this e-mail message.

<https://scifinder.cas.org/registration/completeRegistration.html?respKey=B8CB6727-86F3-F014-11E6-D312D80AC094>

*This link is valid for only one use and will expire within 48 hours.*

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

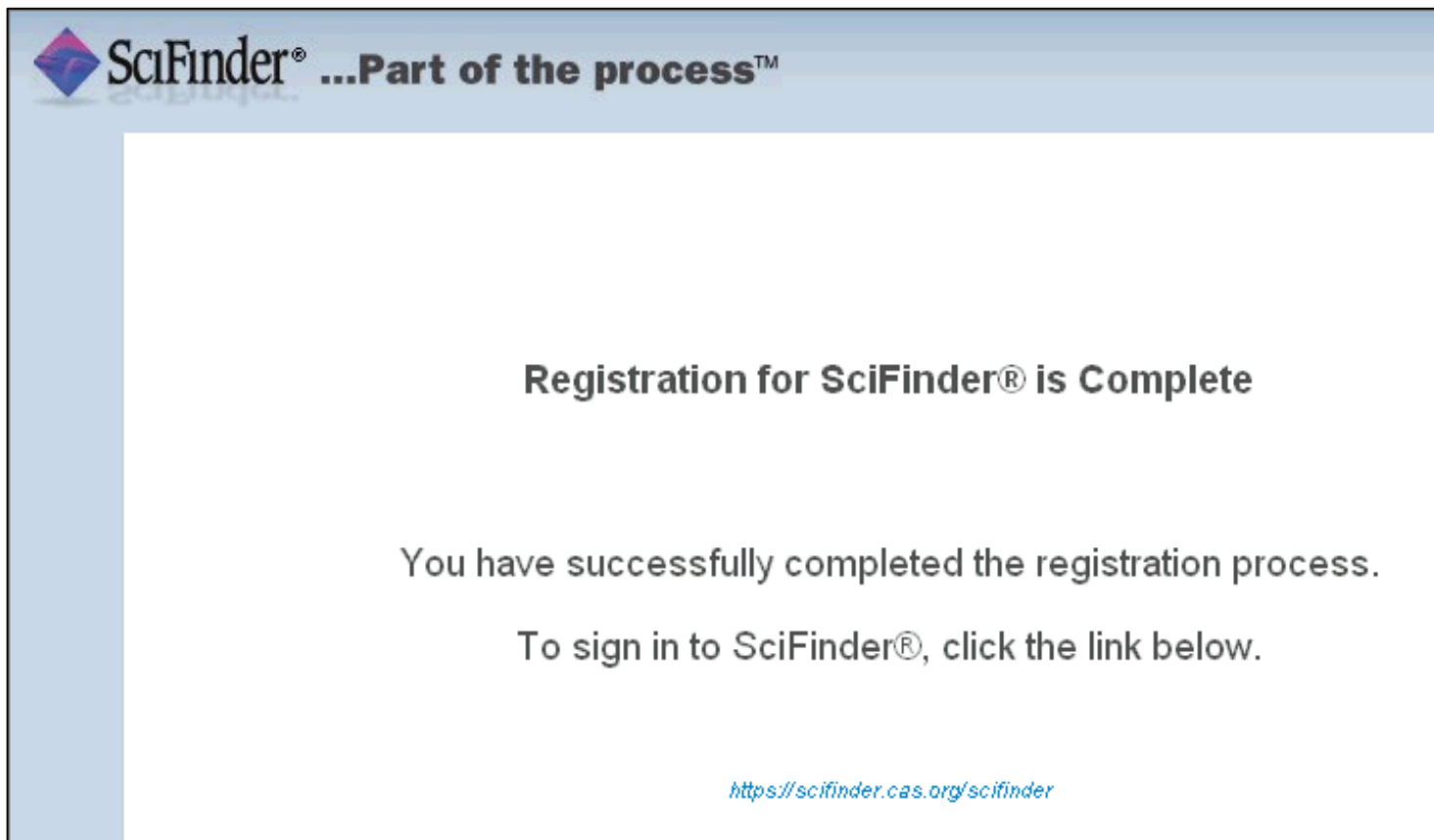
打开并阅读 CAS 的电子邮件（必须在48小时内点击，否则需要重新注册）

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



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- 严禁账号分享
- 严禁将账号用于非学术研究

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