

匡金海

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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

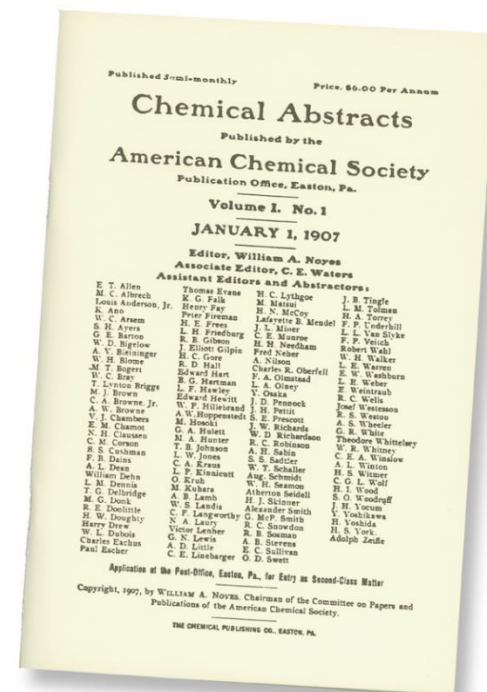


1907年，信息的汇集、管理发生了重大的变化



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



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A CAS SOLUTION

CAS——构建最高质量的化学数据库



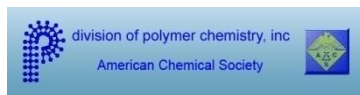
arXiv.org

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

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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  PATENTPAK	A		Jul 6, 2016	CN 2014-10742897	Dec 9, 2014

Priority Application

CN 2014-10742897	Dec 9, 2014
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Indexing

Carbohydrates (Section33-9)

Section cross-reference(s): 34, 63

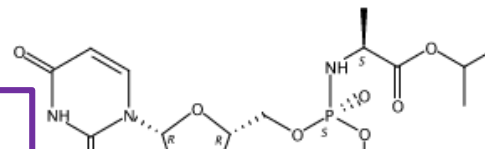
Concepts

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

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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

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

atkina, Natalia
guage: English, Database: CAPLUS

B is substituted purine and pyrimidine nucleobase; dashed bond between R and R⁴ is absent, then R is H, substituted each R⁶ and R⁷ are independently hydrogen or deuterium; R⁵ 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 prepn. method comprises reaction of (2'R)-2'-deoxy-2'-fluoro-2'-methyluridine with

ZOOM DOWNLOAD PDF

(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 31/702* (2006.01)
C07H 19/11 (2006.01) *A61K 31/706* (2006.01)
C07H 19/13 (2006.01) *A61K 31/708* (2006.01)
C07H 19/067 (2006.01) *A61P 31/14* (2006.01)
C07H 19/073 (2006.01)

(21) International Application Number:
PCT/US2015/065981

(22) International Filing Date:
16 December 2015 (16.12.2015)

(25) Filing Language:
English

(81) Designated States (for kind of national protection sought): AO, AT, AU, AZ, BA, BB, BG, BR, CA, CH, CL, CN, CO, CZ, DE, DK, EC, EE, EG, ES, FI, FR, GB, GR, HK, HU, IL, IN, JP, KZ, LA, LC, LK, LR, LS, LU, LY, MA, MD, ME, MK, MN, MW, MX, MY, NG, NI, NO, NZ, 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, GU, KE, MG, MW, MZ, NA, NG, SD, SI, SZ, TZ, UG, ZM, ZW); EAPC (AM, BY, KG, MD, ME, MK, MT, RU, TD, TM, UA, YU, ZJ); Eurasian (AZ, BY, GE, KZ, KG, MD, ME, MK, MT, RU, SJ, TJ, TM, UA, YU, ZJ); European (AL, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LT, LU, LV, MA, MC, NL, NO, PL, PT, RO, RS, SE, SI, SK, SM, SP, TR, UK, XK); African and Asian (AO, AU, BZ, CA, CH, CL, CN, CO, CZ, DE, DK, EC, EE, EG, ES, FI, FR, GB, GR, HK, HU, IL, IN, JP, KZ, LA, LC, LK, LR, LS, LU, LY, MA, MD, ME, MK, MN, MW, MX, MY, NG, NI, NO, NZ, 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).

Search in SciFinder | View Detail

Analyst Markup Locations (1)
page 130

CAS RN 1206126-39-7

Chemical structure of compound 1-1:

Search in SciFinder | View Detail

Analyst Markup Locations (1)
page 130

CAS RN 1206126-41-1

Chemical structure of compound 1-4a:

WO 2016/100441

PCT/US2015/065981

EXAMPLE 1 COMPOUND 1

Synthesis scheme for Compound 1:

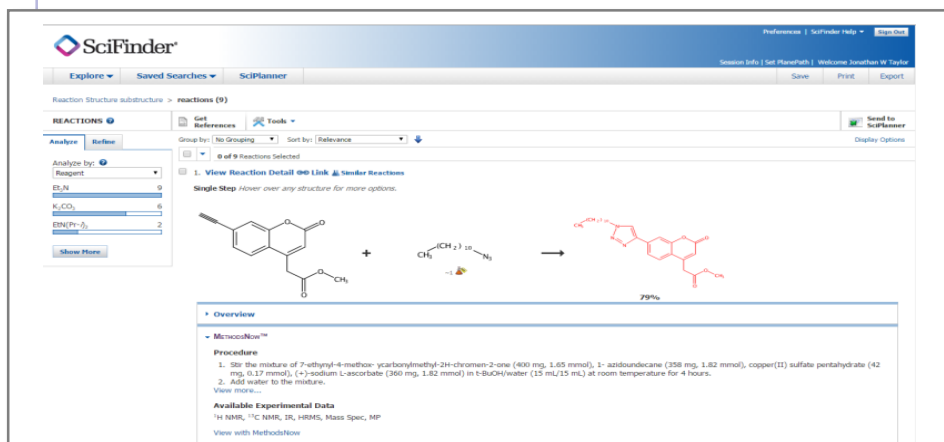
Route 2

dichloromethane
pyridinium dichromate
acetic anhydride
tert-butanol

SciFINDER®

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



嵌在SciFinder中的合成模块

METHODS

atovastatin

Results (528)

Sort Relevance

☐ ☐ ☐

☐ **Analysis of Atorvastatin in Blood plasma by High-performance thin layer chromatography**
CAS MN: 1-101-CAS-1389

Analyte	Atorvastatin
Matrix	Blood plasma
Other Materials	Material: 60 F ₂₅₄ silica gel HPTLC 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. View at Verlag/GWV Fachverlage GmbH

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



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

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

New Commercial Source Logos

SciFinder主界面

检索完，请点击退出

工具栏

The screenshot shows the SciFinder web interface. At the top, there is a header bar with the SciFinder logo and navigation links like 'Explore', 'Saved Searches', and 'SciPlanner'. A search bar is prominently displayed in the center. To the left, a sidebar lists various search categories: REFERENCES, SUBSTANCES, and REACTIONS. On the right, there is a section for 'SAVED ANSWER SETS' and a 'KEEP ME POSTED' notification. Several callout boxes with Chinese text point to specific features: '检索完，请点击退出' (After searching, click exit) points to the 'Sign Out' button; '工具栏' (Toolbar) points to the top navigation bar; '检索入口' (Search Entry) points to the main search bar; '已保存的结果集' (Saved Results Set) points to the 'SAVED ANSWER SETS' list; and '定题追踪' (Topic Tracking) points to the 'KEEP ME POSTED' section.

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Preferences | SciFinder Help | **Sign Out**

Welcome Helen Zhu

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

REFERENCES: RESEARCH TOPIC

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

Search

Advanced Search

SAVED ANSWER SETS

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

View All | Import

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检索入口

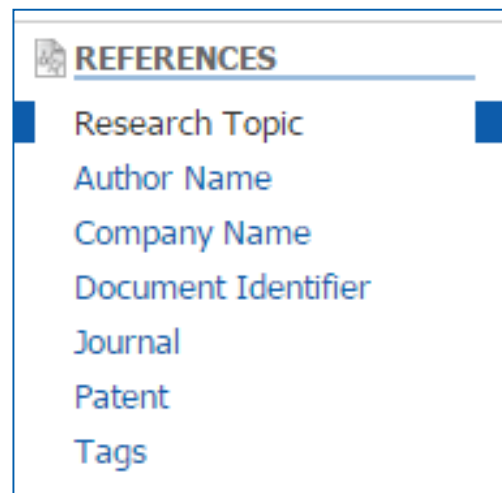
已保存的结果集

定题追踪

SciFinder检索——文献检索

■ 文献检索方法

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



■ 检索策略推荐

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

文献检索——主题

主题检索：木质复合材料的制备

检索式：prepare of wood composite



The screenshot displays the SciFinder web interface. At the top, the SciFinder logo is visible. Below it, there are navigation tabs: 'Explore', 'Saved Searches', and 'SciPlanner'. The 'Explore' tab is selected. The main search area is titled 'Research Topic "prepare of wood composite"'. On the left, there is a sidebar with two main sections: 'REFERENCES' and 'SUBSTANCES'. Under 'REFERENCES', there are options: 'Research Topic', 'Author Name', 'Company Name', 'Document Identifier', 'Journal', 'Patent', and 'Tags'. Under 'SUBSTANCES', there are options: 'Chemical Structure', 'Markush', and 'Molecular Formula'. The 'Research Topic' option is selected. The main search area contains a text input field with the text 'prepare of wood composite'. Below the input field, there are examples of search results: 'The effect of antibiotic residues on dairy products' and 'Photocyanation of aromatic compounds'. A blue 'Search' button is located below the examples. At the bottom of the search area, there are two checkboxes: '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
☐ 5648 references were found containing the two concepts "prepare" and "wood composite" closely associated with one another.	5648
☐ 10379 references were found where the two concepts "prepare" and "wood composite" were present anywhere in the reference.	10379
☐ 12228635 references were found containing the concept "prepare".	12228635
☐ 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** (Accession Number, Author Name, Citing References, Publication Year, Title) | Display Options

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

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Analyze Refine Categorize

Sort by: Accession Number ↓

0 of 5648 References Selected

Display Options

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 (BPP) 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...

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

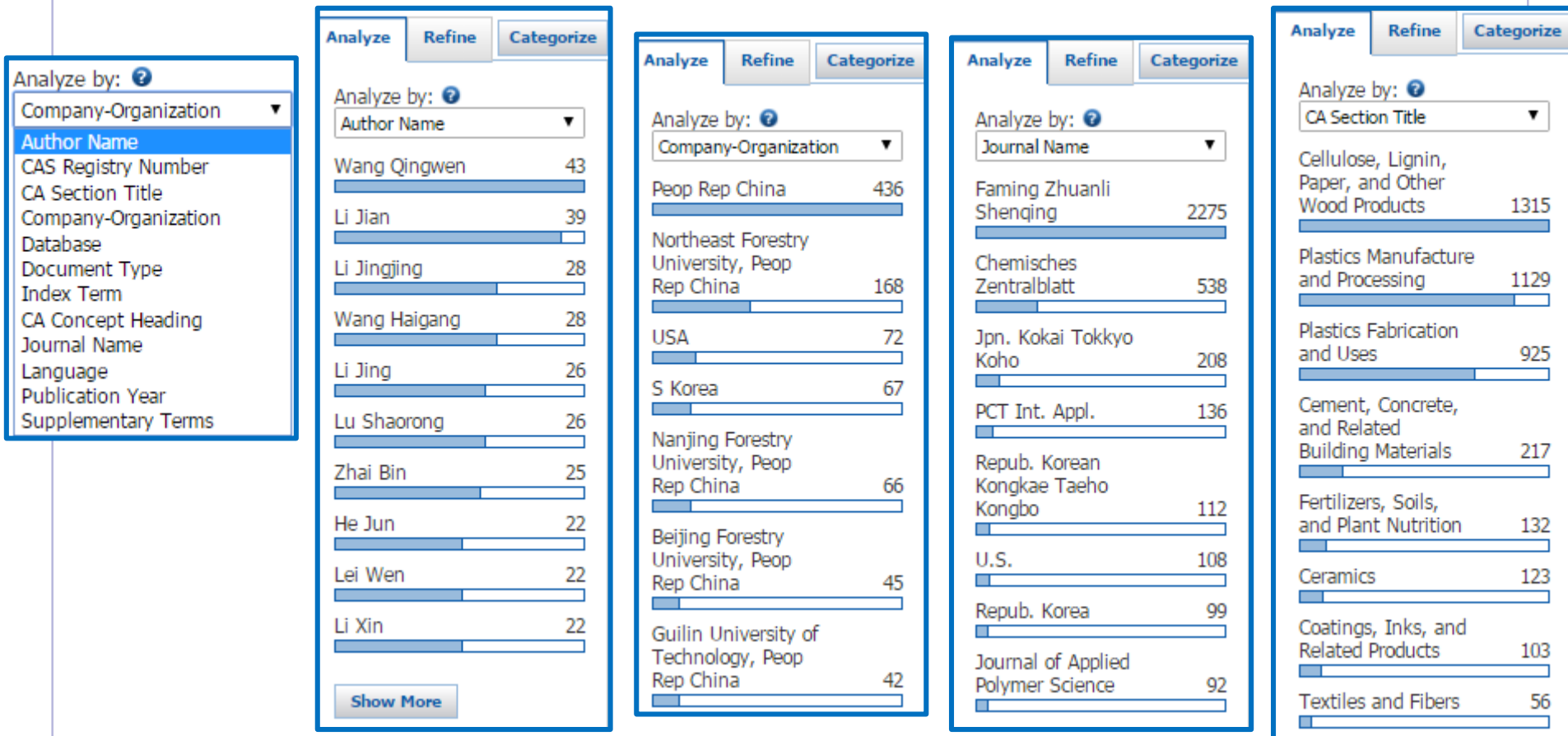
文献检索结果的Analyze

本领域研究人员

本领域研究机构、
合作伙伴、竞争对手

期刊

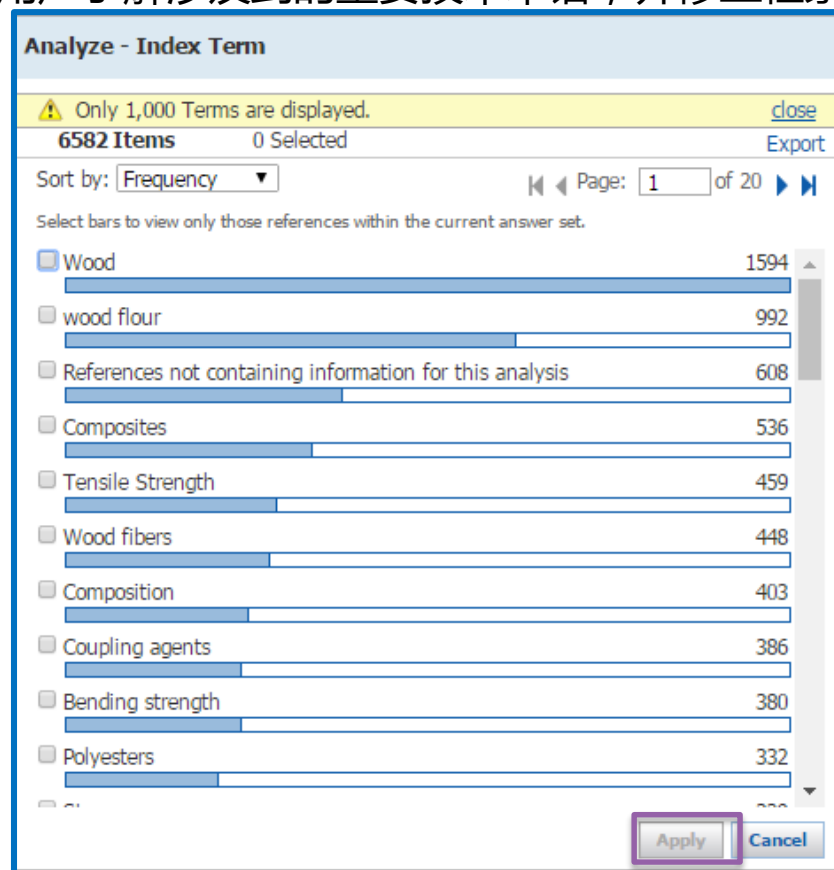
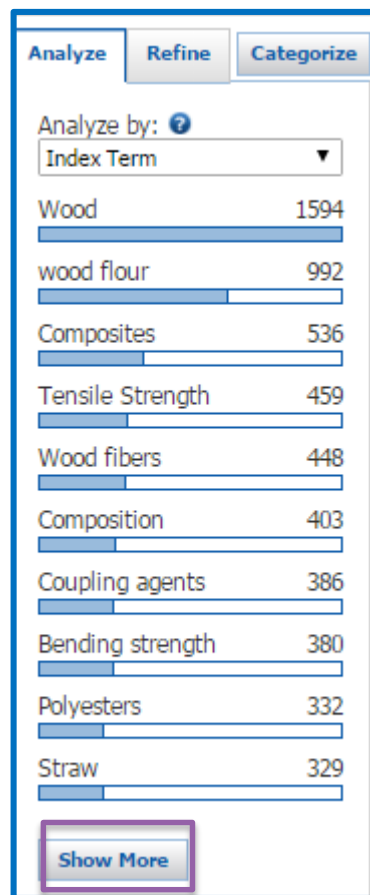
涉及学科领域



文献检索结果的Analyze

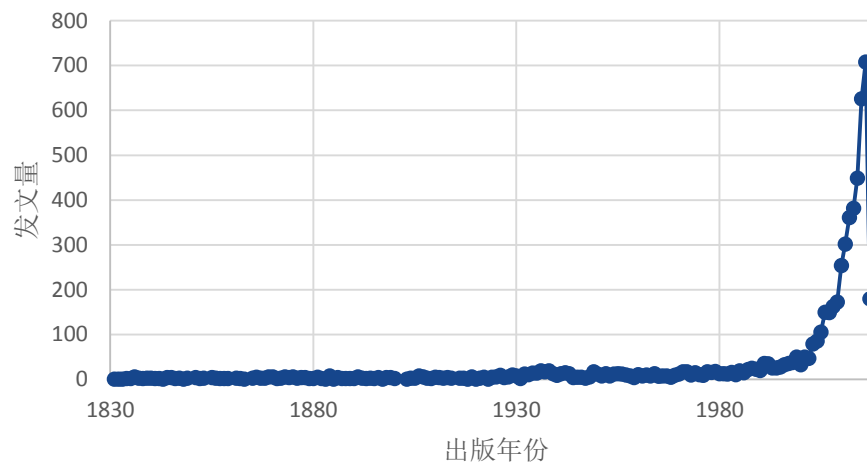
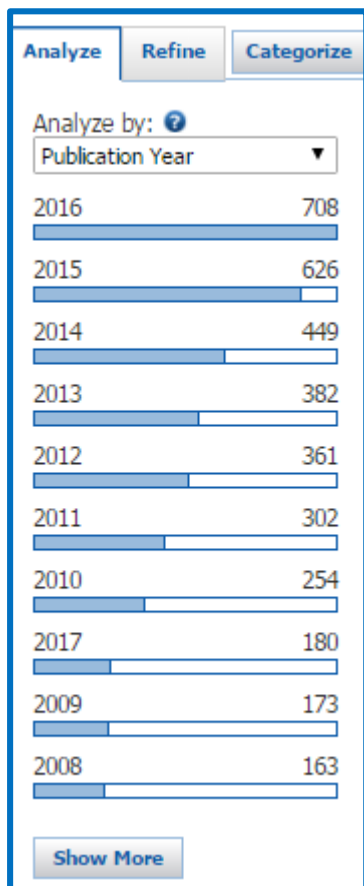
Index Term :

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

AnalyzeRefineCategorize

Refine by: ?

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

Company Name

china

Examples:
3M
DuPont

Refine

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Sort by: Accession Number

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0 of 2953 References Selected

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

Quick ViewOther Sources

By Hao, Jianxiu; Wang, Haigang; Wang, Weihong; Wang, Qingwen
From Fuhe Callao 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...

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

Quick ViewOther 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 ViewOther 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.

Category Heading	Category
All	Substances in technology (3338)
Technology	Materials & products (769)
Polymer chemistry	Construction (113)
General chemistry	Processes & apparatus (383)
Physical chemistry	Metallurgy (83)
Genetics & protein chemistry	Ceramics (36)
Biotechnology	Formed, removed, & other substances (241)
Environmental chemistry	Power & fuel topics (61)
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Biology	
Analytical chemistry	

2. Select index terms of interest.

Index Terms	
Page: 1 of 2	
Select All Deselect All	
☐ Wood flour	701
☐ Wood	662
☐ Wood fibers	324
☐ Boards	162
☐ Construction materials	76
☐ Wood chips	68
☒ Floors	60
☐ Poplar wood	59
☐ Wood boards	57
☐ Fiberboard	49
☐ Cement	45
☐ Granulation	39
☐ Pine wood	35
☐ Thermal insulators	35
☐ Impregnation	33
☐ Floor coverings	31

Selected Terms

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

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Technology > Construction > 1 Index Term(s) Selected

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

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

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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

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File Name: *

Reference_06_19_2012_100848

Format:

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

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☐ Tags
☐ Comments

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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 extruder, rotating 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 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	重要概念	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

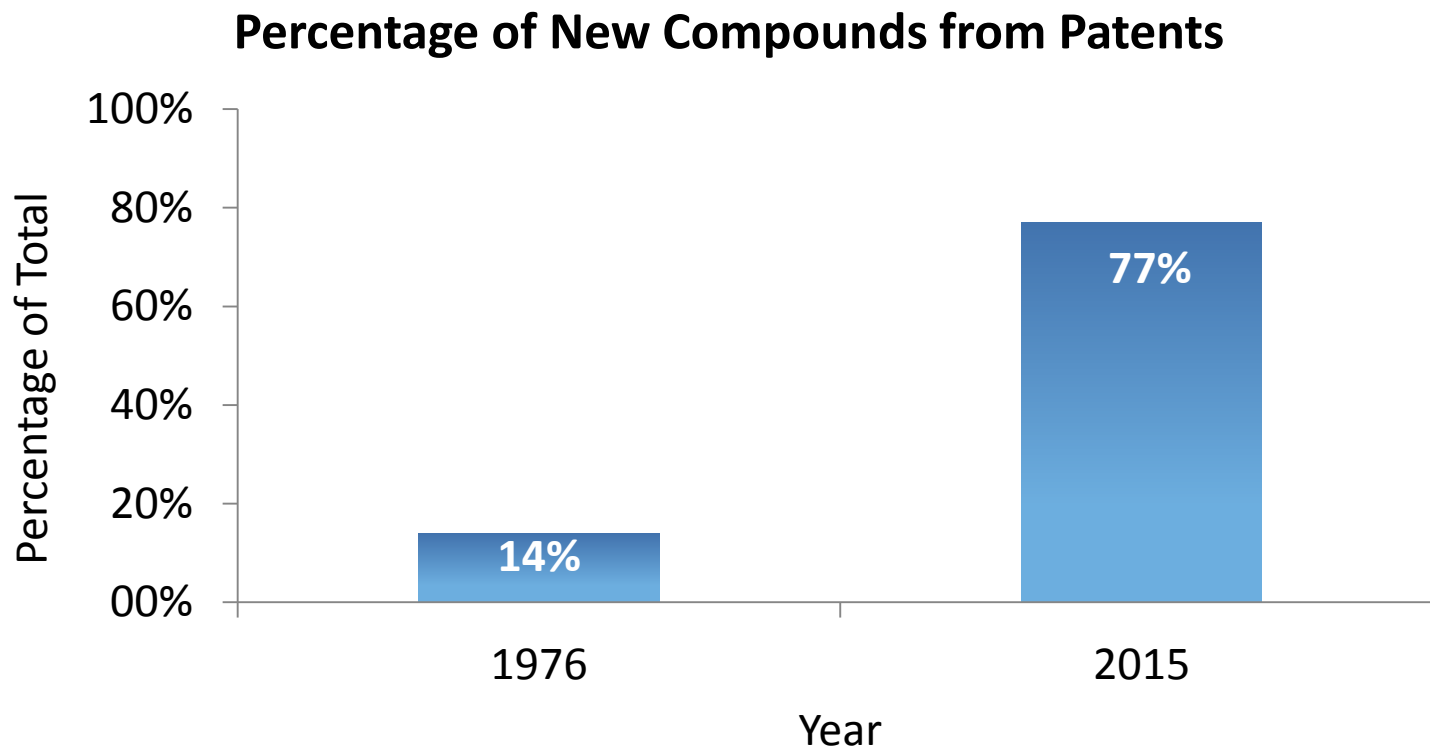
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- 主题检索时，使用介词 in, with, of 等作为连接词
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PatentPakTM

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

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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- β -carboline for the treatment of ear disease

Quick View PatentPak

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

The invention relates to a compound of the formula (I) and pharmaceutical compositions thereof useful in the treatment of acute and chronic inner ear diseases.

6-fluoro-9-methyl-1H-Indole-3-ethanamine hydrochloride with 2,2-dihydroxyacetic acid followed by decarboxylation and redn. and

Patent No.	Kind	Language
EP 2853533	Interactive	German

Patent Family

Patent No.	Kind	Language
WO 2015044434	A2	German
WO 2015044434	A3	German

9. Preparation of indolo-substituted 9-methyl- β -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

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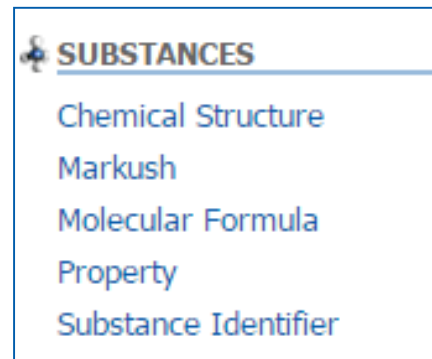
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- 美国化学文摘社简介
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 - 文献检索 (PatentPak)
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- 理化性质检索
- 物质标识符检索：化学名称，CAS RN



■ 物质检索策略推荐

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Reaction Structure structure variable only at spe... > reactions (29) > refine "structure variable only at spe..." (29)

 **REFERENCES**

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

 **SUBSTANCES**

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

SUBSTANCES: SUBSTANCE IDENTIFIER ?

sunset yellow

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

Search

提示：

1. 一次最多可输入25个物质。
2. 每行一个物质标识符。

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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

»
🔍

C₁₆ H₁₂ N₂ O₇ S₂ · 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

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[Explore by Structure](#)

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SUBSTANCE DETAIL ?
Return

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Get Reactions

Get Commercial Sources

由物质获得文献，反应，供应商等信息

CAS Registry Number 2783-94-0
(Component: 5859-11-0)
~2,889 ~65

C₁₆ H₁₂ N₂ O₇ S₂ · 2 Na
2-Naphthalenesulfonic acid, 6-hydroxy-5-[2-(4-sulfohenyl)diazenyl]-, sodium salt (1:2)
Other Names
2-Naphthalenesulfonic acid, 6-hydroxy-5-[(4-sulfohenyl)azo]-, disodium salt (9CI)
C.I. Food Yellow 3 (7CI)
C.I. Food Yellow 3, disodium salt (8CI)
Sunset Yellow FCF (6CI)
1-*p*-Sulfohenylazo-2-hydroxynaphthalene-6-sulfonate disodium salt
[View more...](#)

• 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

Value

Condition

Note

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

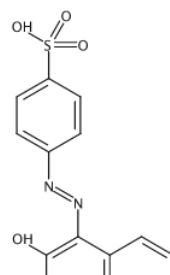
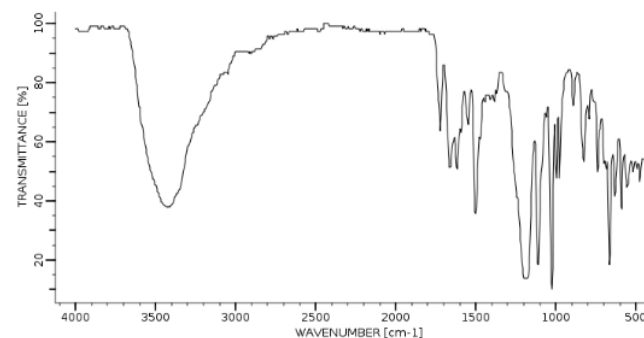
IR Absorption Spectrum

See spectrum

IR Absorption Spectrum

See full text

IR Absorption Spectrum



SPECTRUM ID
BR036790

CAS REGISTRY NUMBER
2783-94-0

FORMULA
 $C_{16}H_{12}N_2O_7S_2 \cdot 2Na$

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

SPECTROMETER
BIO-RAD DIGILAB FT-IR OR EQUIVALENT

SOURCE
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SUBSTANCES

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

Property dropdown menu:

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

Search

Search Results (Molecular Weight):

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寻找分子量在250-400之间的物质

物质结果集的筛选——Refine

SUBSTANCES

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0 of 49251077 Substances Selected

Page: 1 of 3283406

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

Structure Editor:

Click to Edit

Search type: **Exact Structure**

Only retrieve substances

1. **2088740-67-2**

Absolute stereochemistry., Double bond geometry as shown.

C₂₁ H₂₈ O₇
INDEX NAME NOT YET ASSIGNED
[Key Physical Properties](#)

2. **2088740-65-0**

Absolute stereochemistry., Rotation (+), Double bond geometry as shown.

C₂₀ H₂₆ O₇
INDEX NAME NOT YET ASSIGNED
[Key Physical Properties](#)

3. **2088740-64-9**

Absolute stereochemistry., Rotation (+), Double bond geometry as shown.

C₁₉ H₂₄ O₇
INDEX NAME NOT YET ASSIGNED
[Key Physical Properties](#)

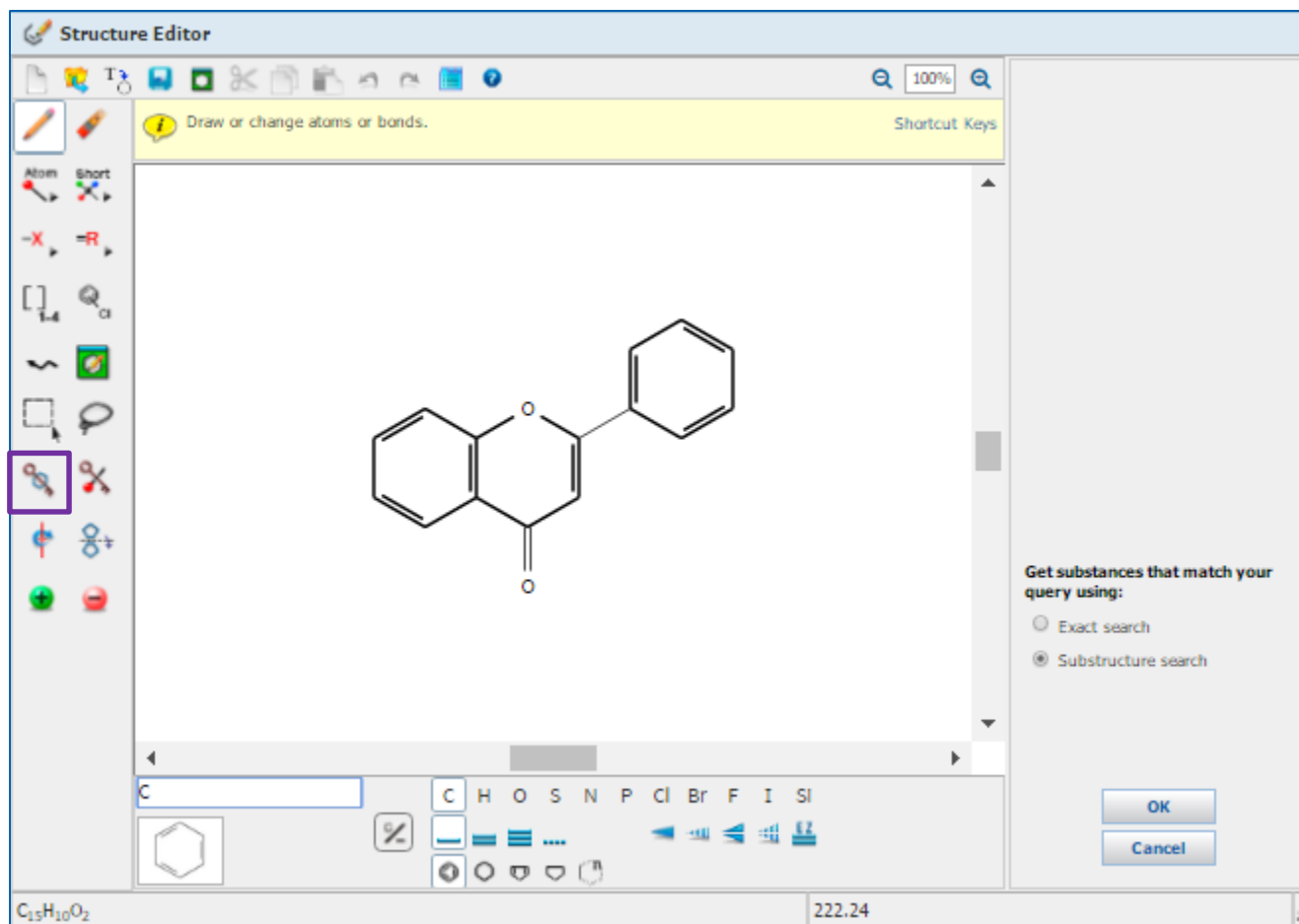
4. **2088740-61-6**

5. **2088740-58-1**

6. **2088740-43-4**

4500多万个结构，
如何筛选黄酮类物质？

物质结果集的筛选——Refine



锁环工具：避免在被锁定的环结构上出现新的环结构

SUBSTANCES ?

Analyze Refine

Refine by: ?

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

Structure Editor:

Java Non-Java

Click image to change structure or view detail.

Search type: **Substructure**

Only retrieve substances that:

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

Refine

物质检索结果集

从4900多万个结构中
筛选出8415个黄酮类物质

0 of 8415 Substances Selected

Sort by: Relevance

Refine by: [?](#)

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

Structure Editor:

[Java](#) [Non-Java](#)

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

1. **1772897-96-7** [?](#)

~0 ~1

C₁₇ H₁₆ O₂
4#-1-Benzopyran-4-one, 2-(3,5-dimethylphenyl)-2,3-dihydro-
▶ **Key Physical Properties**

2. **1438763-28-0** [?](#)

~2

C₁₇ H₁₆ O₂
4#-1-Benzopyran-4-one, 2-(4-ethylphenyl)-2,3-dihydro-, (2R)-
▶ **Key Physical Properties**

3. **958734-07-1** [?](#)

~1

C₁₅ H₁₂ O₄
4#-1-Benzopyran-4-one, 2-(3,5-dihydroxyphenyl)-2,3-dihydro-
▶ **Key Physical Properties**

4. **1772047-03-6** [?](#)

~1 ~1

5. **21785-09-1** [?](#)

~169 ~19

6. **72984-48-6** [?](#)

~31

物质检索——分子式

REFERENCES

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

SUBSTANCES

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

REACTIONS

- Reaction Structure

SUBSTANCES: MOLECULAR FORMULA

Examples:
H4SiO4
(C3H6O.C2H4O)x

Search

金属盐：金属离子和阴离子间用点 (.) 分开

1. **151-21-3**

(Component: 151-41-7)

~84904 ~276

Chemical structure diagram showing the structure of Sulfuric acid monododecyl ester sodium salt (1:1). The structure consists of a central sulfur atom (S) double-bonded to two oxygen atoms (O) and single-bonded to a hydroxyl group (OH) and an ester group (O-CH2-CH2-...-CH2-CH3). The ester chain is represented as (CH2)11-CH3. Below the structure, the sodium ion (Na+) is indicated.

C₁₂H₂₆O₄S.Na
Sulfuric acid monododecyl ester sodium salt (1:1)

► **Key Physical Properties**

- Regulatory Information
- Spectra
- Experimental Properties

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

物质检索——结构

REFERENCES

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

SUBSTANCES

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

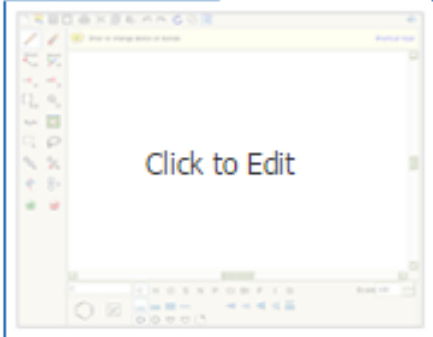
REACTIONS

- Reaction Structure

SUBSTANCES: CHEMICAL STRUCTURE ?

Structure Editor:

Java Non-Java



Search Type:

- ☐ Exact Structure
- ☒ Substructure
- ☐ Similarity

☐ Show precision analysis

 **ChemDraw**
Launch a SciFinder substance or reaction

Import CXF

Search

 Advanced Search ☒ Always Show

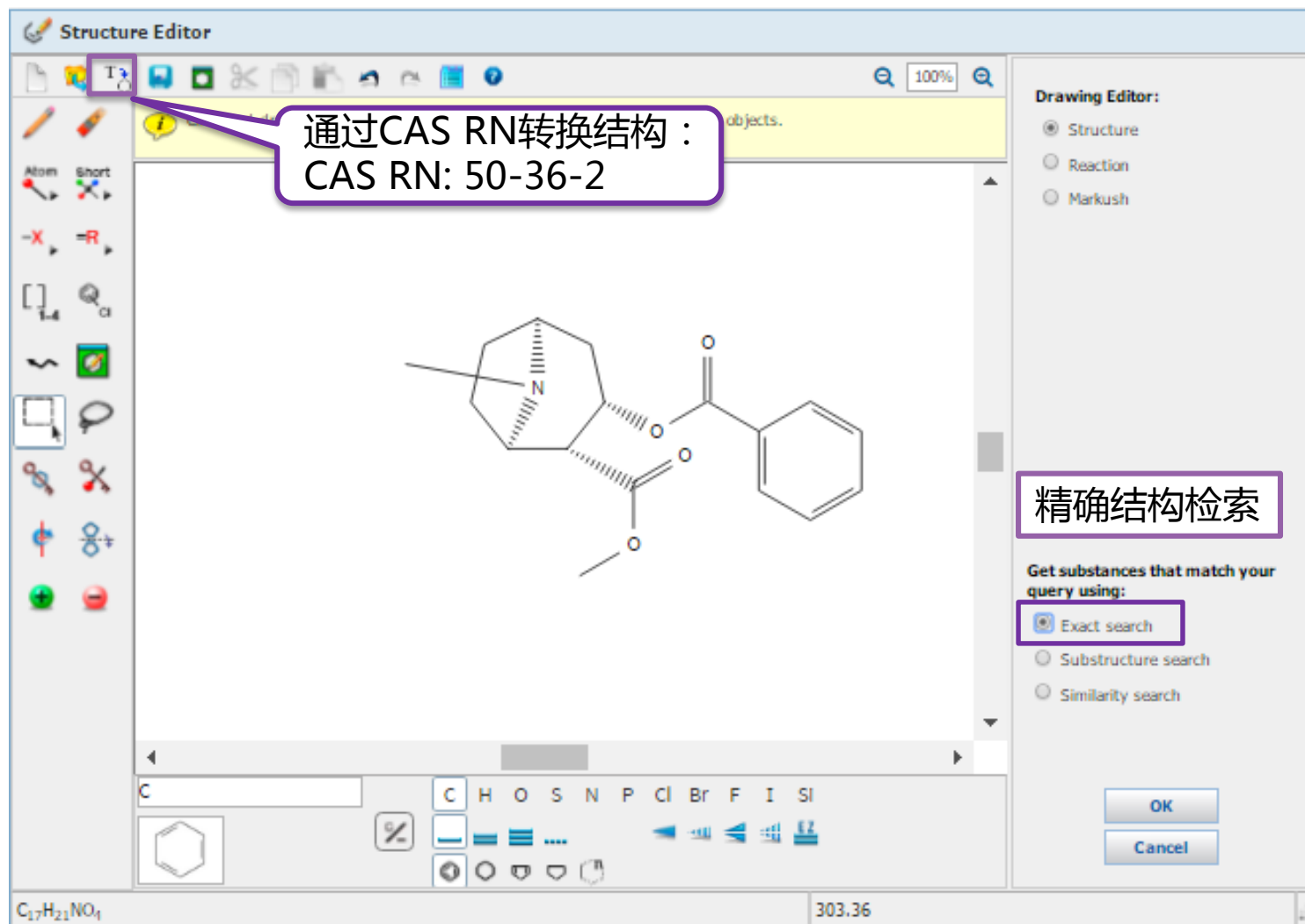
物质检索——结构

The image shows the SciFinder Structure Editor window with various tools and features labeled in Chinese:

- 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** (Select Tool)
- 环锁定工具** (Ring Locking Tool)
- 旋转工具** (Rotate Tool)
- 正电子** (Positron)
- 负电子** (Electron)
- C原子和单键恢复工具** (C Atom and Single Bond Recovery Tool)
- 常用基团** (Common Groups)
- 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** (Snare Selection Tool)
- 原子锁定工具** (Atom Locking Tool)
- 镜面旋转工具** (Mirror Rotation Tool)
- 单双键，RS构型，不确定键定义工具** (Single/Double Bond, RS Configuration, Uncertain Bond Definition Tool)
- 结构检索选择** (Structure Search Selection)
- 常见环，多元环工具** (Common Rings, Polycyclic Rings Tool)

The interface includes a toolbar with icons for drawing and editing, a central workspace for the chemical structure, and a right-hand panel for search options (Exact search, Substructure search, Similarity search) and buttons for '确定' (OK) and '取消' (Cancel).

物质检索——精确结构检索



精确结构检索结果

Get References Get Reactions Get Commercial Sources Tools Create Posted

Sort by: Relevance 0 of 6 Substances Selected

1. **668-19-9**
~18 ~1
Absolute stereochemistry.
C₁₇H₂₁N O₄
8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-[(benzoyloxy)-8-methyl-, methyl ester, (1*R*, 2*R*, 3*R*, 5*S*)-
▶ Key Physical Properties
Spectra

可卡因

2. **114599-38-1**
~5
Absolute stereochemistry.
668-19-9
C₁₇H₂₁N O₄
88-89-1
C₆H₃N₃O₇

C₁₇H₂₁N O₄ · C₆H₃N₃O₇
Alcococaine, picrate (6CI)

可卡因组合物

3. **109496-04-0**
~1
Absolute stereochemistry.
C₁₇H₂₁N O₄ · Cl H
Alcococaine, hydrochloride (6CI)

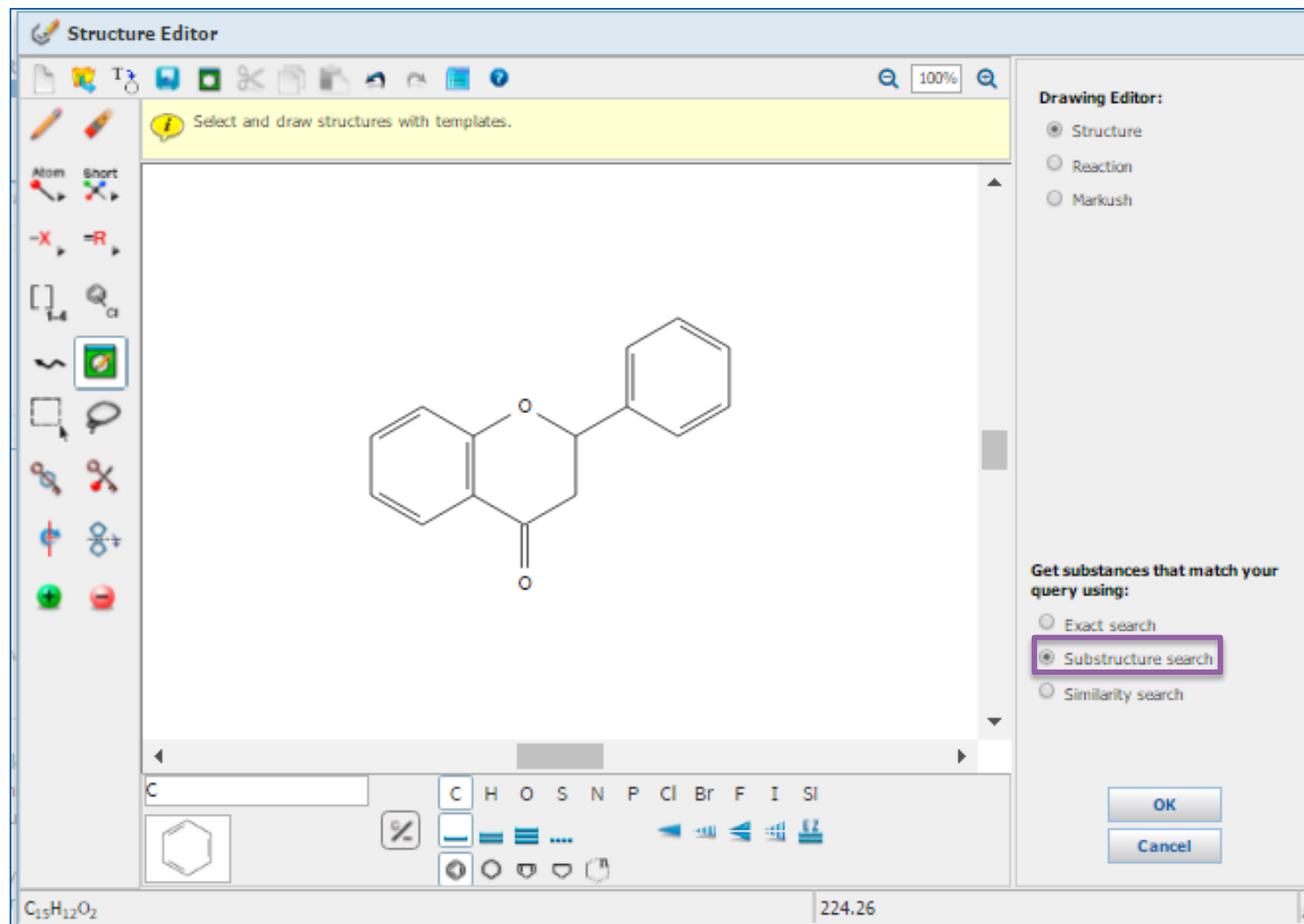
盐酸可卡因

物质检索——精确结构检索

- 精确结构检索：

获得被检索结构的盐，混合物，配合物，聚合物等，被检结构不能被取代

物质检索——亚结构检索

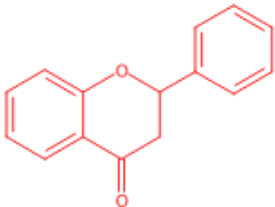


物质检索——亚结构检索

0 of 23824 Substances Selected

1. 487-26-3

~2093

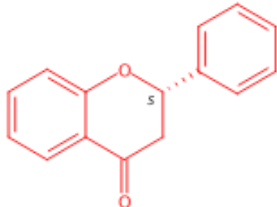


C₁₅H₁₂O₂
4-phenyl-4H-benzopyran-4-one, 2,3-dihydro-2-phenyl-

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

2. 17002-31-2

~244



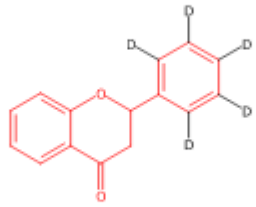
Absolute stereochemistry...Rotation (-).

C₁₅H₁₂O₂
4-phenyl-4H-benzopyran-4-one, 2,3-dihydro-

▶ **Key Physical Properties**
Experimental Properties

10. 146196-91-0

~1



C₁₅H₇D₅O₂
4-(2,3,4,5-tetradeuteriophenyl)-4H-benzopyran-4-one, 2,3-dihydro-2-(phenyl-d₄)- (9CI)

Spectra

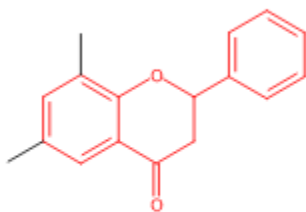
同位素

亚结构检索结果

281. 123251-10-5

~3   ~1 

取代物



$C_{17}H_{16}O_2$

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

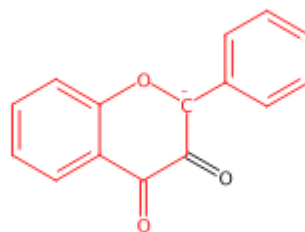
► Key Physical Properties

Experimental Properties

295. 780723-19-5

~0 

离子



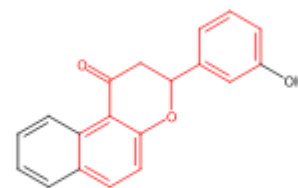
$C_{15}H_9O_3$

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

284. 136116-23-9

~2 

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



SCIFINDER®
A CAS SOLUTION

亚结构检索结果的限定

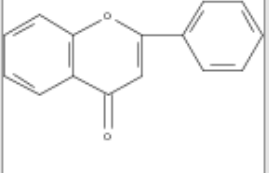
化学结构的再次限定

Analysis Refine

Refine by: ⓘ

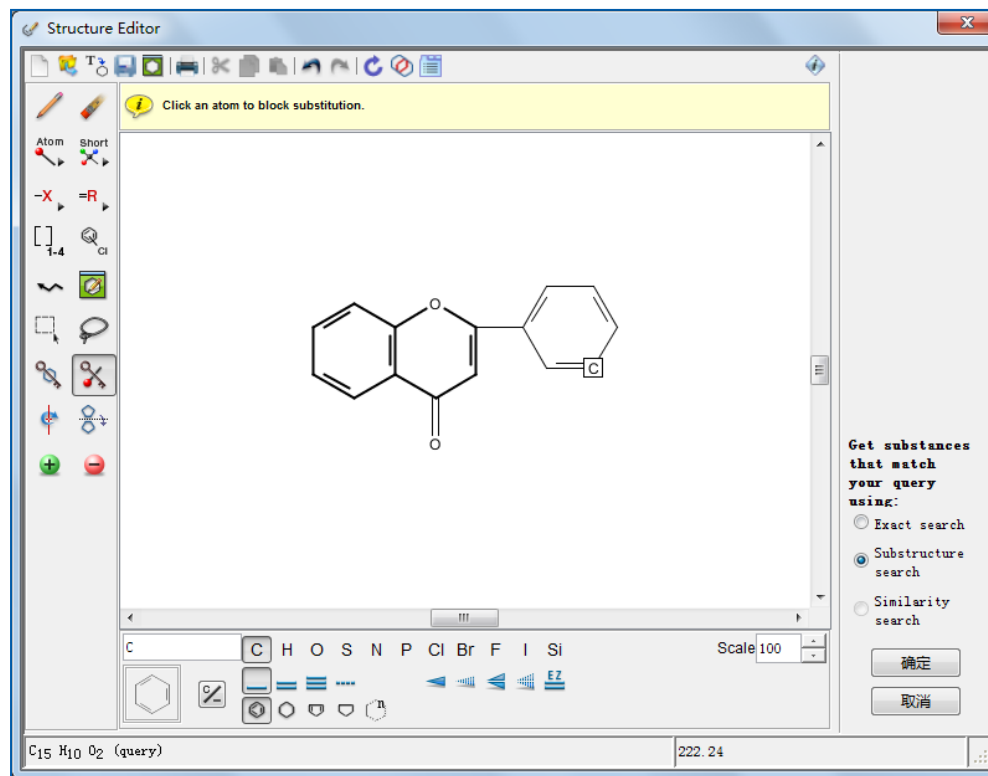
- ☒ Chemical Structure
- ☐ Isotope-Containing
- ☐ Metal-Containing
- ☐ Commercial Availability
- ☐ Property Availability
- ☐ Property Value
- ☐ Reference Availability
- ☐ Atom Attachment

Chemical Structure:



Click image to change structure or view detail

Search type: **Substructure**



环锁定

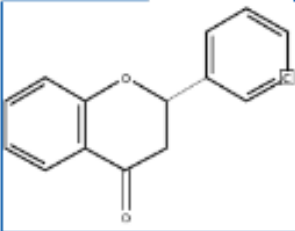


原子锁定

亚结构检索结果的限定

Structure Editor:

Java Non-Java



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

Only retrieve substances that:

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

Refine

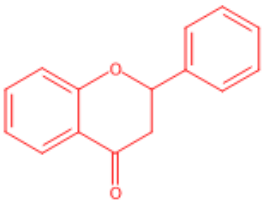
Get References Get Reactions Get Commercial Sources Tools

Sort by: Relevance

0 of 13826 Substances Selected

1. **487-26-3**

~2093

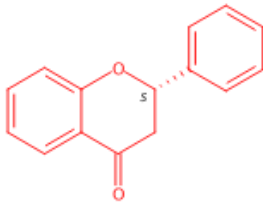


C₁₅H₁₂O₂
4*H*-1-Benzopyran-4-one, 2,3-dihydro-2-phenyl-

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

2. **17002-31-2**

~244



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

▶ **Key Physical Properties**
Experimental Properties

Absolute stereochemistry, Rotation (-).

4. **104550-32-5**

~3

5. **75524-43-5**

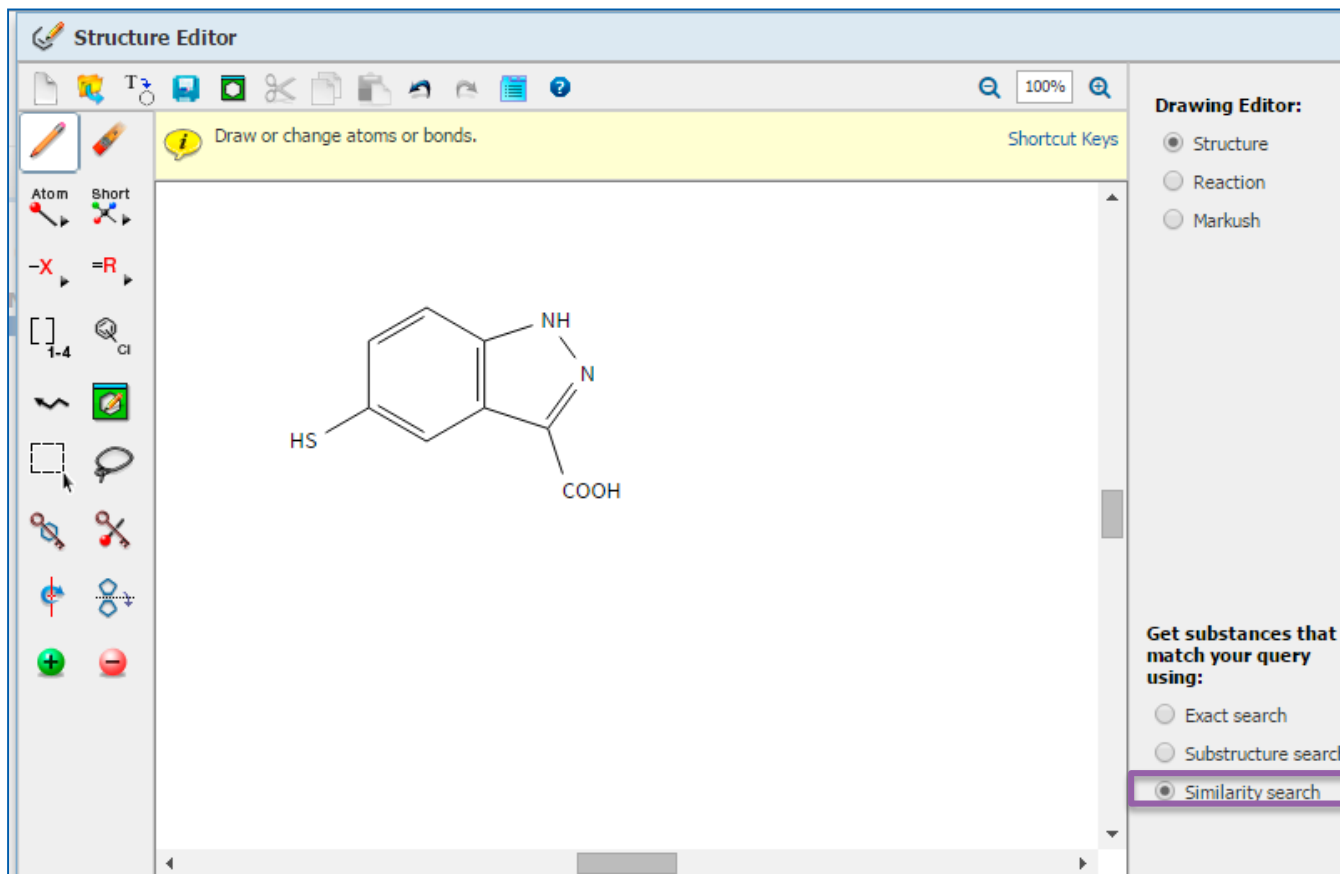
~2

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
☐ ≥ 99 (most similar)	0
☐ 95-98	0
☐ 90-94	0
☐ 85-89	11
☐ 80-84	34
☐ 75-79	84
☐ 70-74	267
☐ 65-69	696
☐ 0-64 (least similar)	1818

Get Substances

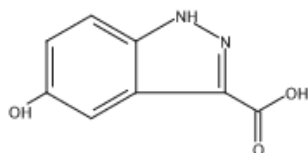
评分越高，相似度越高，结构越相似

Score: 88

☐ 1. 885518-94-5

取代基变化

~1 ~35



$C_8H_6N_2O_3$

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

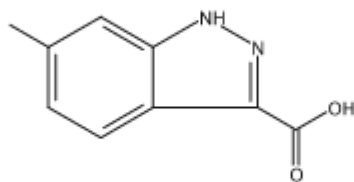
► Key Physical Properties

Score: 86

☐ 5. 858227-12-0

取代基位置变化

~7 ~41



$C_9H_8N_2O_2$

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

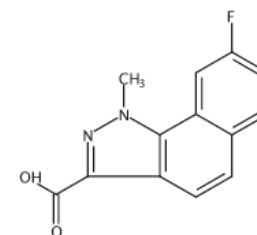
► Key Physical Properties

Score: 65

☐ 541. 1100422-

母体结构变化

~1



$C_{13}H_9FN_2O_2$

1H-Benz[7]indazole-3-carboxylic acid, 8-fluoro-1-methyl-

► Key Physical Properties



SCIFINDER®
A CAS SOLUTION

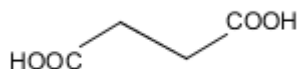
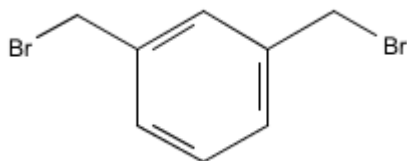
物质检索——相似结构检索

- 相似结构检索：

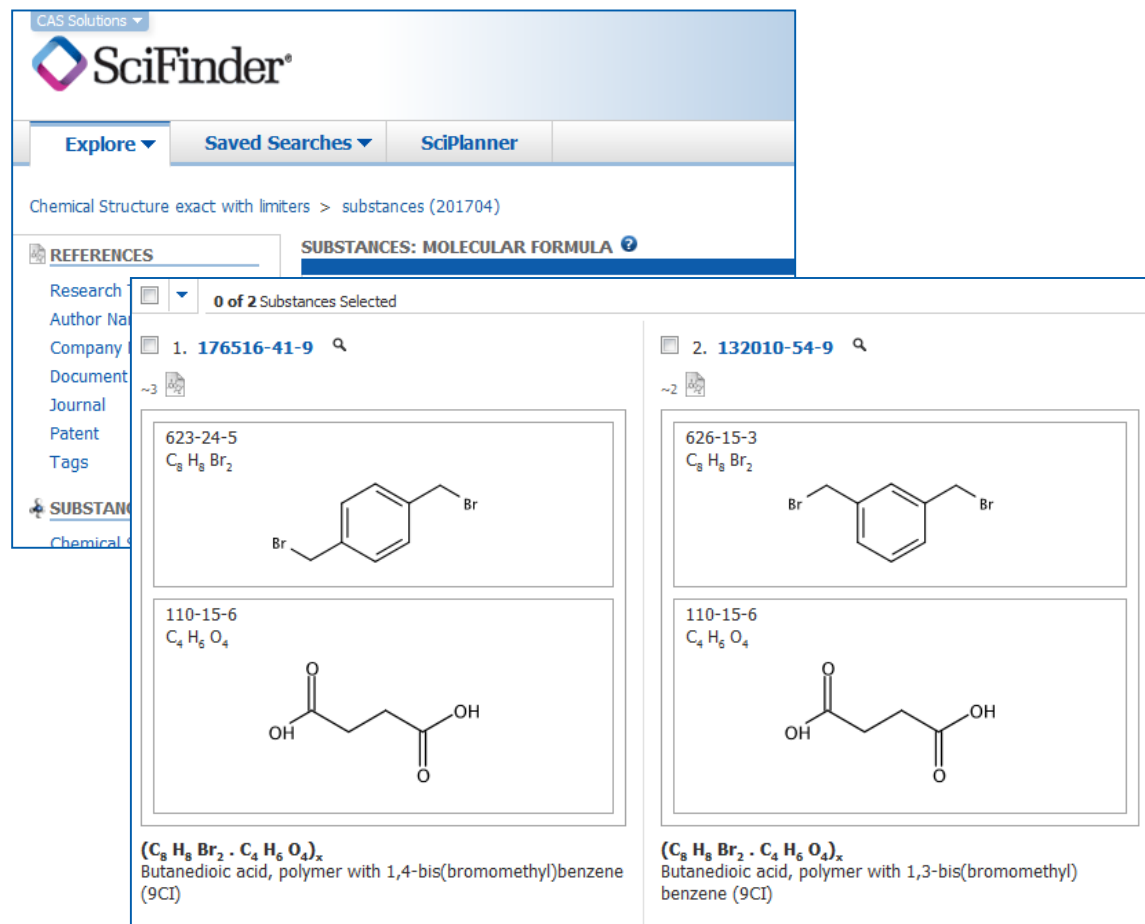
获得片段或整体结构与被检索结构相似的结果，母体结构可以被取代，也可以被改变

聚合物的检索

已知起始原料的聚合物



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



0 of 2 Substances Selected

1. 176516-41-9

623-24-5
 $C_8 H_8 Br_2$

110-15-6
 $C_4 H_6 O_4$

$(C_8 H_8 Br_2 \cdot C_4 H_6 O_4)_x$
Butanedioic acid, polymer with 1,4-bis(bromomethyl)benzene (9CI)

2. 132010-54-9

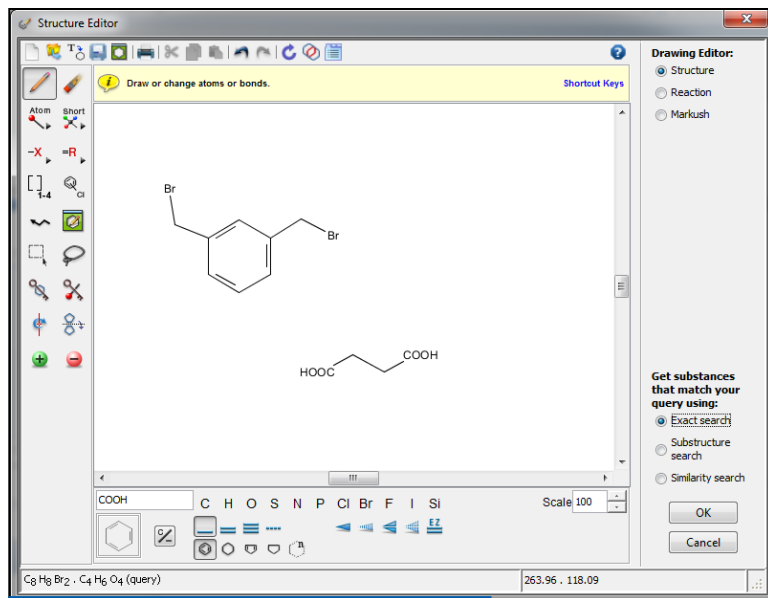
626-15-3
 $C_8 H_8 Br_2$

110-15-6
 $C_4 H_6 O_4$

$(C_8 H_8 Br_2 \cdot C_4 H_6 O_4)_x$
Butanedioic acid, polymer with 1,3-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 | ☒ Single component
☐ Commercially available
☐ Included in references |
| Classes | ☐ Alloys
☐ Coordination compounds
☐ Incompletely defined
☐ Mixtures
☒ Polymers
☐ Organics, and others not listed |
| Studies | ☐ Analytical
☐ Biological
☐ Preparation
☐ Reactant or reagent |

单一组分

聚合物

0 of 1 Substance Selected

1. **132010-54-9** 🔍

~2

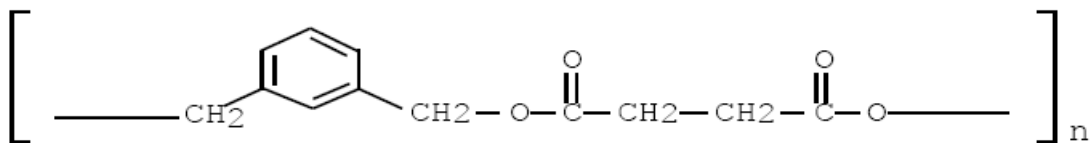
626-15-3
C₈ H₈ Br₂

110-15-6
C₄ H₆ O₄

(C₈ H₈ Br₂ . C₄ H₆ O₄)_x
 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



(C₁₂ H₁₂ O₄)_n

SciFinder®

Molecular Formula "(C₁₂ H₁₂ O₄)_n" > substances (45)

Sort by: CAS Registry Number

0 of 45 Substances Selected

1. 1801551-81-4	2. 1637772-98-5	3. 1421756-46-8
(C ₁₂ H ₁₂ O ₄) _n INDEX NAME NOT YET ASSIGNED	(C ₁₂ H ₁₂ O ₄) _n Poly[oxy-1,4-butanediylloxycarbonyl(1,4-phenylene-2,3,5,6-dioxo)carbonyl]	(C ₁₂ H ₁₂ O ₄) _n Poly[oxy((1,4-phenyl-1,2-ethanediyl)oxy(1,4-dioxo-1,4-butanediyl))]
4. 1392419-56-5	5. 1353713-96-8	6. 1341223-97-9
	Substance Image	Substance Image

聚合物的检索

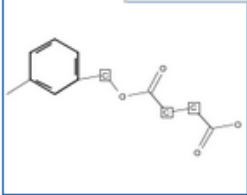
Analyze Refine

Refine by: ?

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

Structure Editor:

Java Non-Java

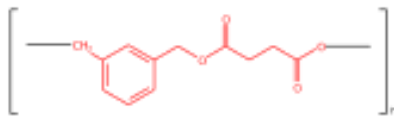


Click image to change structure or view detail.
Search type: **Substructure**

0 of 1 Substance Selected

1. 132010-11-8

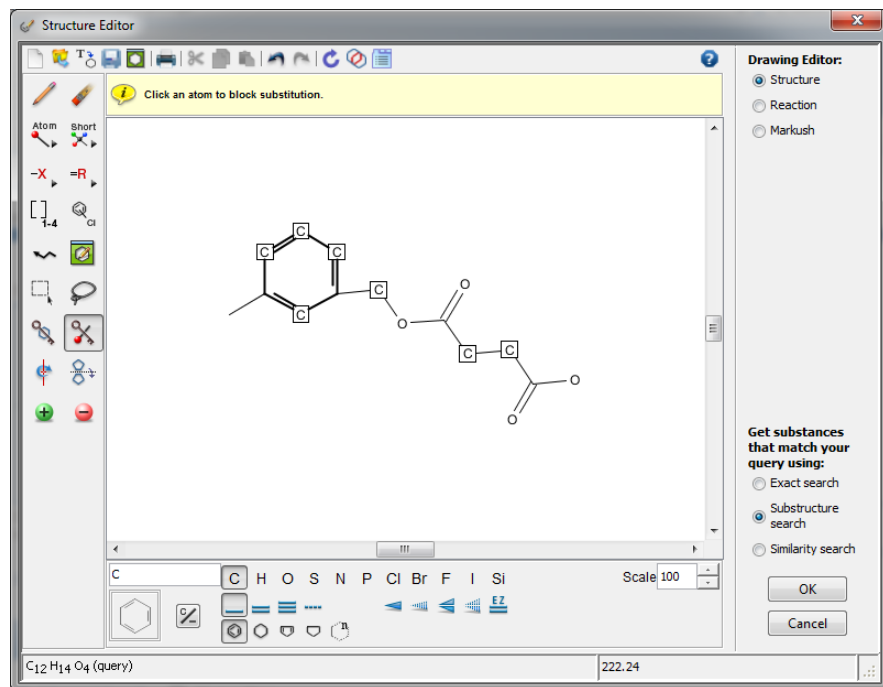
~2



$(C_{12}H_{12}O_4)_n$
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
- ☒ Single component
 - ☐ Commercially available
 - ☐ Included in references
- Classes
- ☐ Alloys
 - ☐ Coordination compounds
 - ☐ Incompletely defined
 - ☐ Mixtures
 - ☒ Polymers
 - ☐ Organics, and others not listed
- Studies
- ☐ Analytical
 - ☐ Biological
 - ☐ Preparation
 - ☐ Reactant or reagent

单一组分

聚合物

0 of 1 Substance Selected

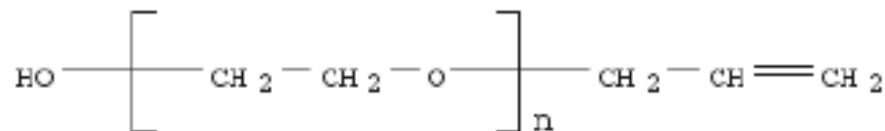
1. 132010-11-8

~2

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

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 ?

$(\text{C}_2 \text{ H}_4 \text{ O})_n \text{ C}_3 \text{ H}_6 \text{ O}$

Examples:
H₄SiO₄
(C₃H₆O.C₂H₄O)_x

Search

SUBSTANCES



↑
SRU部分

↑
两端部分

0 of 4 Substances Selected

1. 1500029-22-0

~3

$(\text{C}_2 \text{ H}_4 \text{ O})_n \text{ C}_3 \text{ H}_6 \text{ O}$
Poly(oxy-1,2-ethanediyl), α-(1-methylethenyl)-ω-hydroxy-

2. 191403-44-8

~5

$(\text{C}_2 \text{ H}_4 \text{ O})_n \text{ C}_3 \text{ H}_6 \text{ O}$
Poly(oxy-1,2-ethanediyl), α-1-propen-1-yl-ω-hydroxy-

3. 50856-25-2

~57

$(\text{C}_2 \text{ H}_4 \text{ O})_n \text{ C}_3 \text{ H}_6 \text{ O}$
Poly(oxy-1,2-ethanediyl), α-ethenyl-ω-methoxy-

4. 27274-31-3

~1115

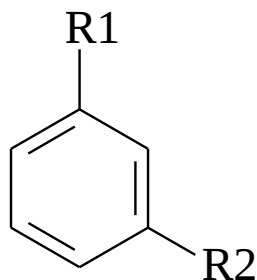
$(\text{C}_2 \text{ H}_4 \text{ O})_n \text{ C}_3 \text{ H}_6 \text{ O}$
Poly(oxy-1,2-ethanediyl), α-2-propen-1-yl-ω-hydroxy-
Regulatory Information

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

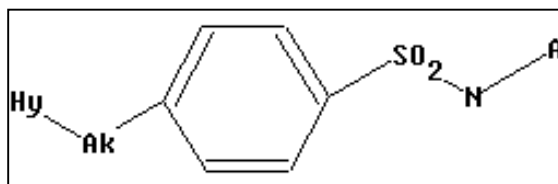
Markush检索

- 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, —CH₂—halogen, —CH(CH₃)—halogen,



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

1-4 Cl

Hy-Ak

SO₂-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



[Explore](#)
[Saved Searches](#)
[SciPlanner](#)
[Save](#)
[Print](#)
[Export](#)

Welcome Helen Zhu

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

REFERENCES

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[Send to SciPlanner](#)

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[Refine](#)
[Categorize](#)

Sort by: [Accession Number](#)

0 of 1969 References Selected

Page: 1 of 99

Analyze by:

Document Type

Patent 1969

Journal 1

Show More

全部是专利

1. **Compounds and methods for anticoagulation therapy**

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

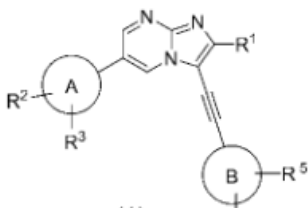
By Allende Rodriguez, Mikel; Hermida Santos, Jose; Montes Diaz, Ramon; Oyarzabal Santamarina, Julen
From PCT Int. Appl. (2016), WO 2016120432 A1 20160804. | Language: English, Database: CAPLUS

The invention relates to certain compds. that are inducers of Heat shock 70 kDa protein 1A/1B (HSPA1A/B) and their use for anticoagulation therapy; and to a method for anticoagulation therapy that comprises the administration of one of these inducer compds. It has been here proved that induction of Heat shock 70 kDa protein 1A/1B by administration of one of these inducer compds. has antithrombotic effects without accelerating or altering bleeding time.

2. **Preparation of new imidazopyrimidine derivatives as negative allosteric modulators of metabotropic glutamate receptor subtype 2 (mGlu2 receptor)**

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

By Urashima, Kuniko; Tojo, Kengo; Koike, Shoko; Masumoto, Shuji
From Jpn. Kokai Tokkyo Koho (2016), JP 2016132660 A 20160725. | Language: Japanese, Database: CAPLUS



The title imidazo[1,2-a]pyrimidine derivs. I [R¹ = H or halogen; ring A Ph or pyridyl; R², R³ (same or different) = hydrogen, halogen, C₁₋₄ alkyl or C₁₋₄ alkoxy each optionally substituted with 1-5 halogen atoms; or in case where R² and R³ are at the adjacent substitution position, R² and R³ together with ring A form C₅₋₈ carbocyclic ring (optionally substituted with 1-5 halogen or 1-2 hydroxy group) or 5- or 6-membered satd. heterocyclic ring; ring B = Ph or pyridyl; R⁴, R⁵ (same or different) = H, halogen, hydroxy, amino, -C(O)OR^a, -C(O)NR^aR^b, SO₃H, SO₂NR^aR^b, SO₂R^b, or NR^aSO₂R^b; R^a, R^b (same...



SCIFINDER
A CAS SOLUTION

ACS / Proprietary and Confidential / Do Not Distribute

69

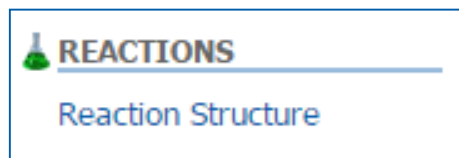
提纲

- 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



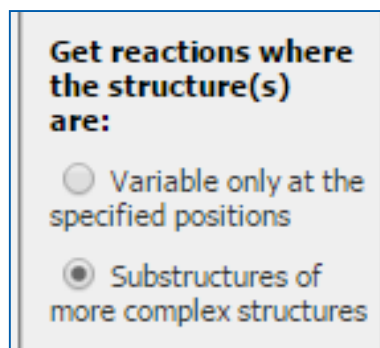
- 常用获取方法

已知物质：由物质获取反应

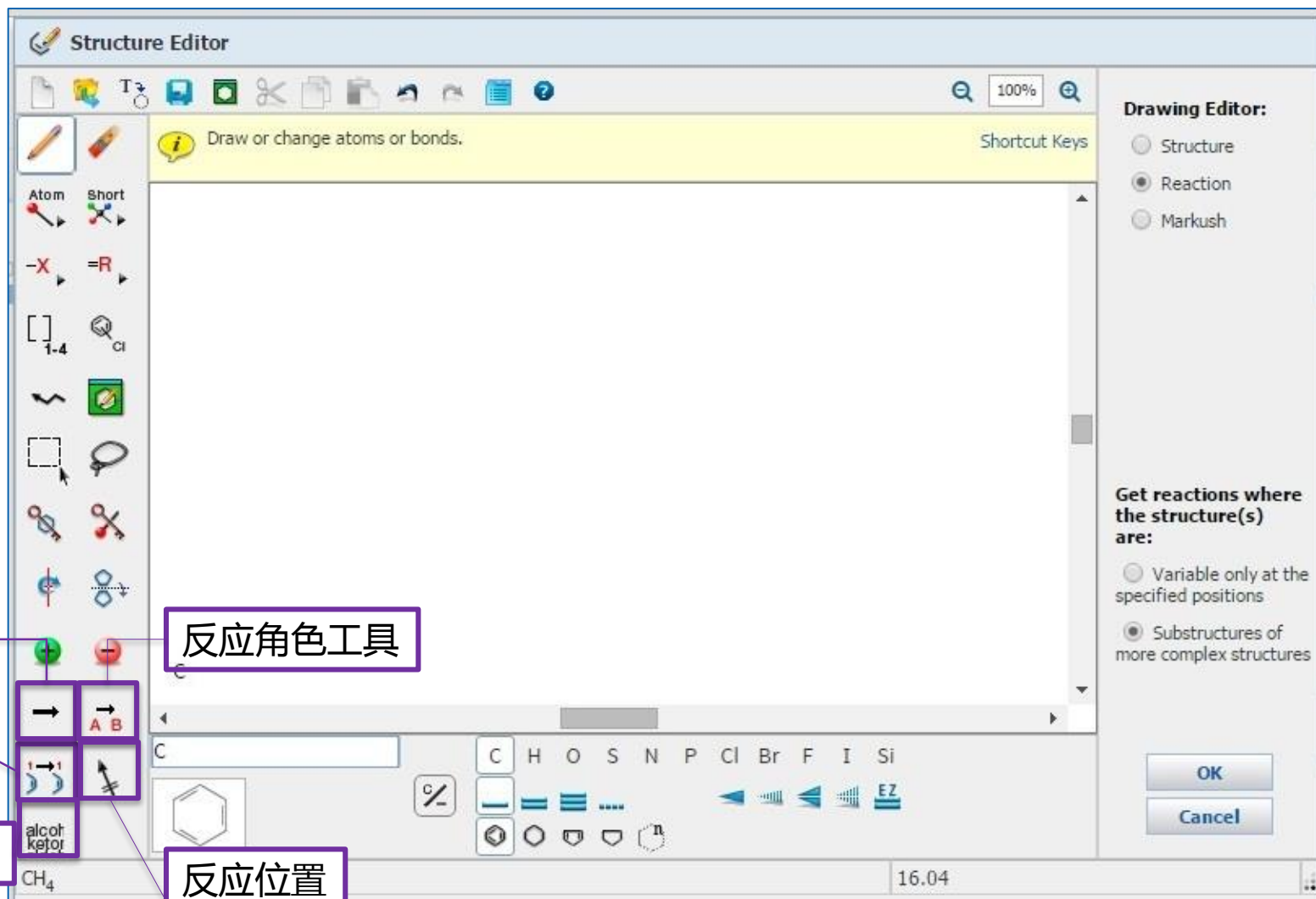
已知文献：从文献中获取反应

精确结构反应检索

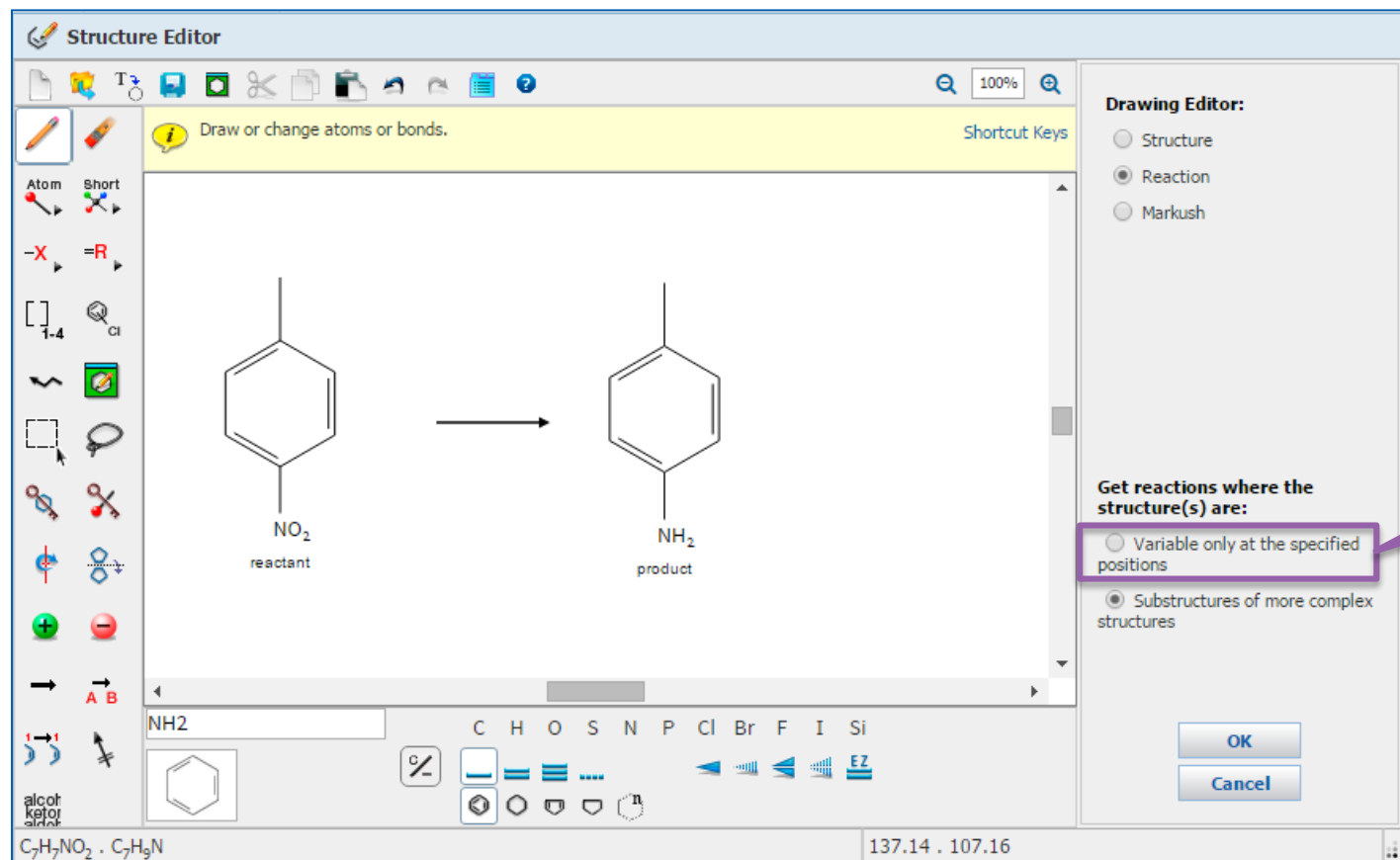
亚结构反应检索



反应绘制工具



SciFinder反应检索——精确反应检索



精确反应检索

反应检索结果

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

Get References Tools

Group by: No Grouping No Grouping Document Transformation Sort by: Relevance Selected

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

Single Step Hover over any structure for more options.



Overview

Steps/Stages

1.1 R:NaBH₄, C:1832616-28-0, C:Ru, S:H₂O, S:THF, 45 min, 25°C

Notes

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

References

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

获取相似反应

选择相似反应的相似限制：

Broad：仅反应中心相似

Medium：反应中心及附属原子和键

Narrow：反应中心及扩展的原子和键

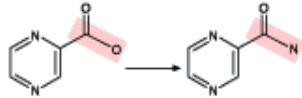
Get Similar Reactions ?

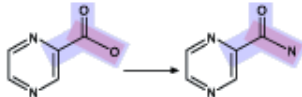
Retrieve similar reactions from:

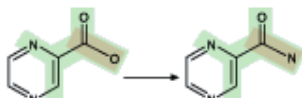
- ☒ All reactions
- ☐ Current answer set

Include this level of similarity:

- ☒ Broad - Reaction centers only (2934)


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


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



Get Reactions

Cancel

按照反应类型排序

Group by: Transformation ▼ Sort by: Frequency ▼

☐ 0 of 560 Reactions Selected

☐ 1. Reduction of Nitro Compounds to Amines
538 Reactions

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

☐ 2. Reduction of Nitro to Azo Compounds
11 Reactions

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

☐ 3. Reduction of Nitro to Azoxy Compounds
11 Reactions

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

更精确的查找需要的反应

反应检索结果的筛选

获得特定物质做还原剂的反应

REACTIONS ?

Get References Tools

Analyze Refine

Analyze by: Reagent

H₂ 148

NaBH₄ 51

N₂H₄·H₂O 43

KOH 17

CO 16

HCO₂H 16

NH₄⁺·HCO₂⁻ 16

H₂O 14

N₂H₄ 14

NaOH 14

Show More

Group by: No Grouping Sort by: Relevance

0 of 512 Reactions Selected

1. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.



Overview

Steps/Stages

1.1 R:NaBH₄, C:1832616-28-0, C:Ru, S:H₂O, S:THF, 45 min, 25°C

Notes

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

References

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

SciFinder囊括最大的反应实验过程合集

Single Step Hover over any structure for more options.



▼ Overview

Steps/Stages

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

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

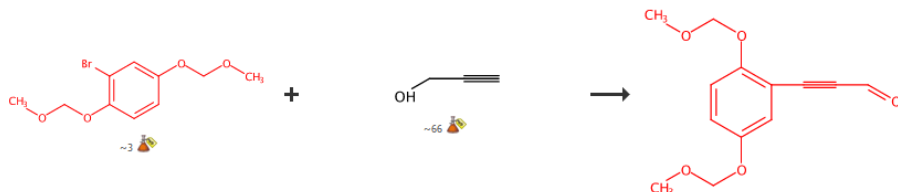


General/Typical Procedure: **General Procedure for Nitroarene Reductions.** Molecular hydrogen was added with a balloon filled with 1 atm of H₂ to a mixture of nitroarene (0.3 mmol), Cs₂CO₃ (0.3 mmol), anisole as internal standard (0.3 mmol), and NHC-Pd-rGO (6 × 10⁻³ mmol, based on metal) in toluene (5 mL). The system was then evacuated and backfilled with H₂ in cycles for three times before putting the reaction vessel in an oil bath at 100°C for 2h. Yields were determined by GC analyses using anisole (0.3 mmol) as internal standard. Products were identified according to spectroscopic data of the commercially available compounds. Entry: 4; Yield 100%.

不用阅读全文，直接获得包含实验过程的反应记录

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(PPh₃)₄, S: BuNH₂, 21 h, 100°C
2.1 R: DMSO, R: Cl(O=)CC(=O)Cl, S: CH₂Cl₂, 15 min, -78°C
2.2 S: CH₂Cl₂, -78°C; 2 h, -78°C
2.3 R: Et₃N, 30 min, -78°C; -78°C → rt
2.4 R: H₂O, R: NH₄Cl, 30 min, rt

Notes

1) key step, alternate catalyst concentration, catalyst (CuI) and temperature, Sonogashira coupling, 2) key intermediate, Swern oxidation, 3) method shown, Reactants: 2, Reagents: 5, Catalysts: 1, Solvents: 2, Steps: 4. 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

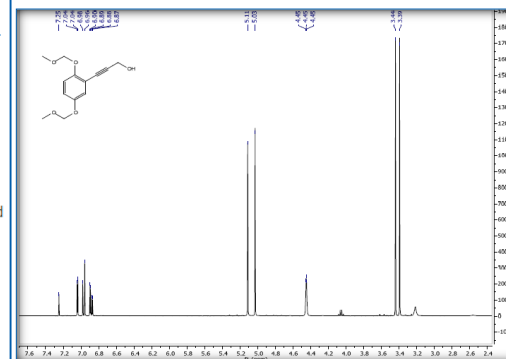


Step 1

General Procedure for the Sonogashira Coupling.^{5,10,11} Compounds **6a**²¹ and **16**⁸ 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(PPh₃)₄ (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 H₂O (80 mL). The product was extracted with EtOAc (3 × 80 mL). The combined organic layers were washed with brine, dried over anhydrous Na₂SO₄, 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**²² (**6**): Yield 96%; colorless oil. IR (KBr) ν_{max} 3310, 2230 cm⁻¹; ¹H NMR (CDCl₃, 400 MHz) δ 3.46 (3H, s, H-4b), 3.51 (3H, s, H-1b), 4.51 (2H, t, H-3, H-4a), 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); ¹³C NMR (CDCl₃, 100 MHz) δ 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]⁺ (calcd for C₁₁H₁₀O₄, 275.0896).

Step 2

Generation of the Key Aldehyde.¹⁷ Oxalyl chloride (272.3 μ L, 3.12 mmol) in dry CH_2Cl_2 (9 mL) was added to a stirred solution of DMSO (332 μ L, 4.68 mmol) in dry CH_2Cl_2 (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_2Cl_2 (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_3N (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 NaHCO_3 and H_2O , and the mixture was stirred for 30 min. The organic phase was decanted off, and the aqueous layer was extracted with CH_2Cl_2 (3 $\times$ 30 mL). The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4 , and evaporated under reduced pressure. **3-[2,5-Bis(methoxymethoxy)phenyl]prop-2-ynal** (**9**): Yield 91%; colorless oil. IR (KBr) ν_{max} 1660, 2194 cm^{-1} ; ^1H NMR (CDCl_3 , 400 MHz) δ 3.46 (3s, H-4b), 3.51 (3s, 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); ^{13}C NMR (CDCl_3 , 100 MHz) δ 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]⁺ (calcd for $\text{C}_{13}\text{H}_{14}\text{O}_5$, 273.0739).



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。



SciFinder®
A CAS SOLUTION

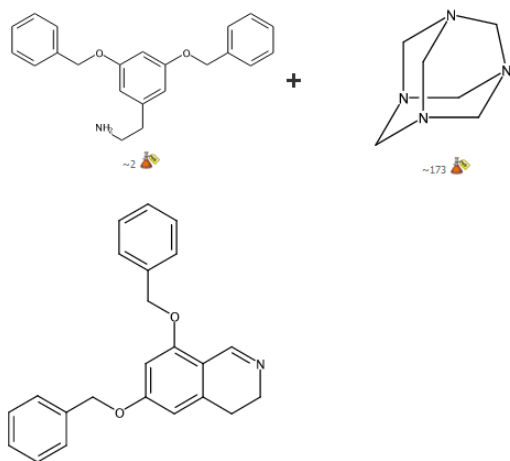
MethodsNow Synthesis

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

Products	Isoquinoline, 3,4-dihydro-6,8-bis(phenylmethoxy)-, 95%, CAS RN: 1384461-35-1
Reactants	Benzeneethanamine, 3,5-bis(phenylmethoxy)-, CAS RN: 188662-05-7 Hexamethylenetetramine, CAS RN: 100-97-0
Solvents	Trifluoroacetic acid, CAS RN: 76-05-1 Acetic acid, CAS RN: 64-19-7
Procedure	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. 2. Stir the mixture for 3 hours at 90°C. 3. Dilute the reaction mixture with H ₂ O. 4. Basify with potassium carbonate and extract with CH ₂ Cl ₂ . 5. Wash the combined organic layers with brine. 6. Dry over MgSO ₄ and concentrate in vacuo. 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.
Scale	gram
¹ H NMR	(CDCl ₃ , 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)
¹³ C NMR	(CDCl ₃ , 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
IR	(thin film, neat) ν _{max} 3062, 3032, 2935, 1736, 1620, 1603, 1575, 1497, 1442, 1377, 1351, 1309 cm ⁻¹
HRMS	(FAB+) calcd for C ₂₃ H ₂₂ NO ₂ (M+H ⁺) 344.1651; found 344.1658
Mass Spec	(FAB+) <i>m/z</i> 344 (M+H ⁺)
State	yellow solid
CAS Method Number	3-614-CAS-200055

物质信息

实验过程

图谱信息

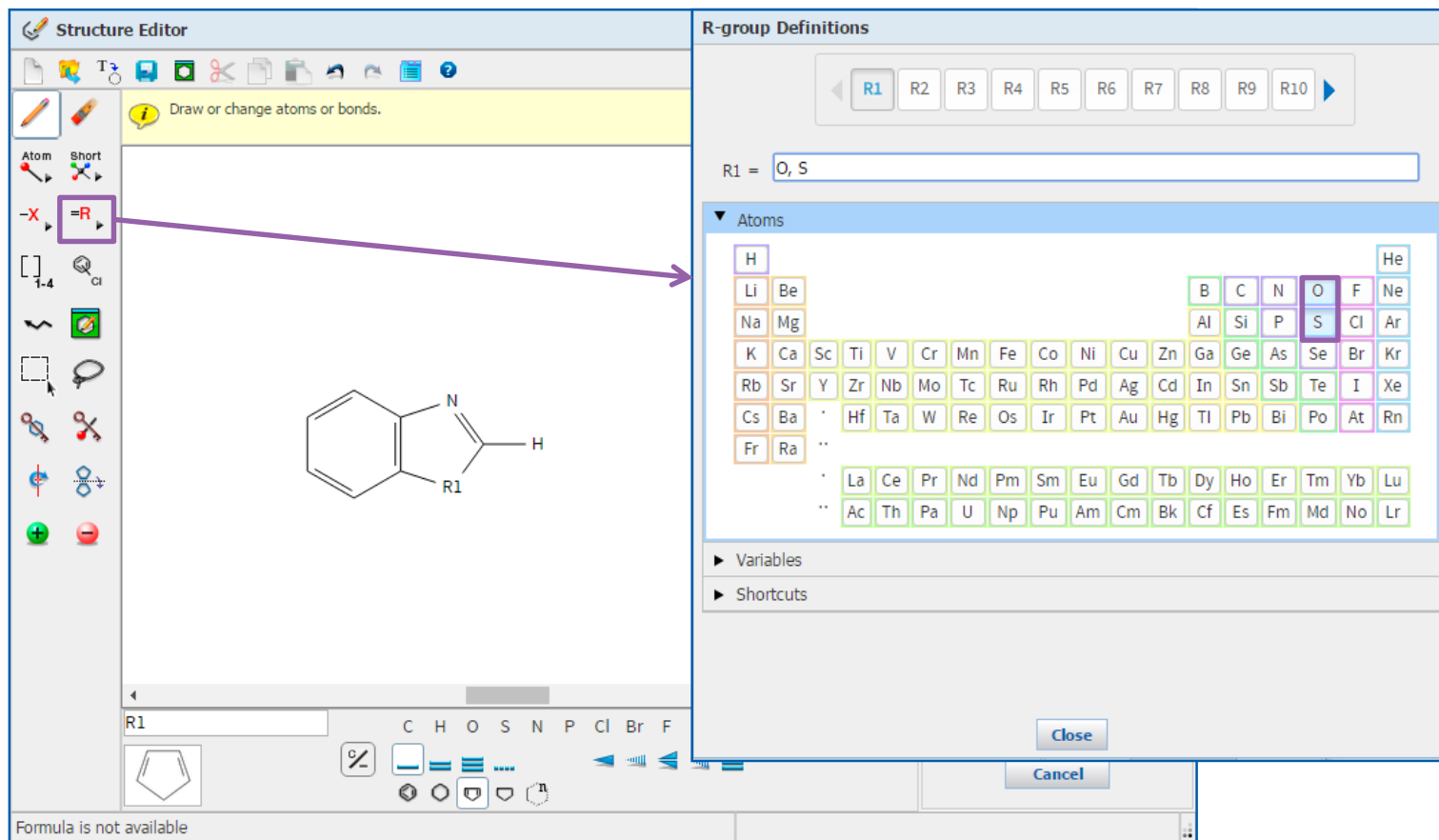
保存/导出方法

Print/Export

Close

亚结构反应检索

通过C-H活化对苯并噻唑或者恶唑进行烷基化



亚结构反应检索

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

Reactant: A benzimidazole derivative with a substituent R1 and a hydrogen atom at the 2-position.

Product: A benzimidazole derivative with a substituent R1 and a substituent Ak at the 2-position.

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 ₃	17
(MeOCH ₂ CH ₂) ₂ O	16
NaI	15
1905414-33-6	14
CoBr ₂	11
Me ₃ SiCH ₂ MgCl	10
Ph ₂ P(CH ₂) ₃ PPh ₂	10
658062-48-7	9

Group by: No Grouping
No Grouping
Document
Transformation

Sort by: Access Number

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:H₂O, rt
- 1.3 R:HCl, S:H₂O, neutralized

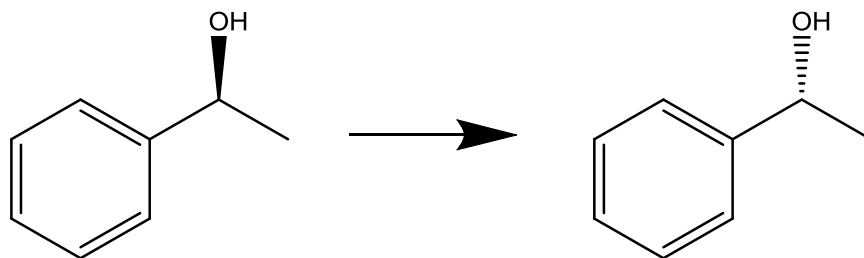
Notes

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

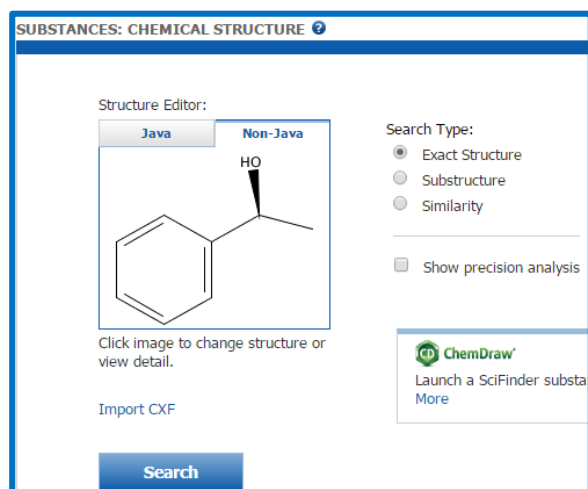
案例：如何获取手性翻转反应



案例：如何获取手性翻转反应

检索思路：

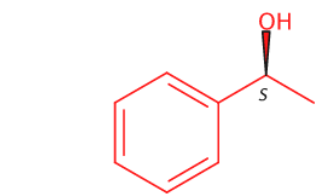
- 1). 先获取反应物物质，然后再获取其作为反应物的反应，得到检索结果集1。
- 2). 先获取产物物质，然后再获取其作为产物的反应，得到检索结果集2。
- 3). 两个结果集取交集。



1 of 52 Substances Selected

1. 1445-91-6

~3499   ~90 



Absolute stereochemistry, Rotation (-).

C₈H₁₀O
Benzenemethanol, α -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.

NH₂ O

Combine Answer Sets

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)

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

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

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

(C₂H₄O)_n H₂O
 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 ₂ CH ₂ OH polymer	≥ 7928
HCl	≥ 6993
Et ₃ N	≥ 5713
DCC	≥ 5143
NaOH	≥ 4539
K ₂ CO ₃	≥ 3583
NaN ₃	≥ 3358
NaHCO ₃	≥ 3314
H ₂	≥ 3069
NaBH ₄	≥ 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

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 'REACTANTS' section is active, showing a list of refinement criteria. The 'Reaction Structure' option is selected and highlighted with a red box. Below this, the 'Structure Editor' section shows a preview of the reactant structure, methyl methacrylate, with the label 'reactant' underneath it. The main workspace shows the chemical structure of methyl methacrylate, labeled 'reactant'. The right sidebar contains 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'. The bottom status bar shows the molecular formula $C_5H_8O_2$ and the molecular weight 100.12.

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

Analyze by: ?

Reagent

NaN ₃	23
DCC	17
NaOH	17
Et ₃ N	16
(NH ₄) ₂ S ₂ O ₈	12
NH ₃	11
NH ₄ Cl	11
MeOH	10
25190-89-0	8
9004-82-4	8

Show More

Group by: No Grouping

Sort by: Relevance

0 of 156 Reactions Selected

Page: 1 of 11

1. View Reaction Detail

Single Step

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

+

$\text{CH}_2=\text{C}(\text{CH}_3)\text{COOCH}_3$

→

$\text{CH}_2=\text{C}(\text{CH}_3)\text{COO}-[\text{CH}_2\text{CH}_2\text{O}]_n\text{O}-\text{COC}(\text{CH}_3)=\text{CH}_2$

MMA封端的PEG

3. View Reaction Detail

Single Step

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

+

$\text{CH}_2=\text{C}(\text{CH}_3)\text{COOCH}_3$

→

$\text{CH}_2=\text{C}(\text{CH}_3)\text{COO}-[\text{CH}_2\text{CH}_2\text{O}]_n\text{O}-\text{COC}(\text{CH}_3)=\text{CH}_2$

PMMA和PEG共聚物

Overview

Steps/Stages

1.1 R:NaOH,

1.2 R:Phenol

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

进入SciPlanner 新建文件

将刚推送过来的反应拖至编辑面板

Send to SciPlanner

Display Options

Overview

Steps/Stages

1.1 R: NH₃, R: t-BuOK, R: t-BuOOH, S: THF
2.1 R: NaH, S: THF
3.1 R: POCl₃, reflux

Notes

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

References

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

SciPlanner [SciPlanner_11_19_2015_112612](#)

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

New
Open
Save
Duplicate
Import
Export
Print
Close

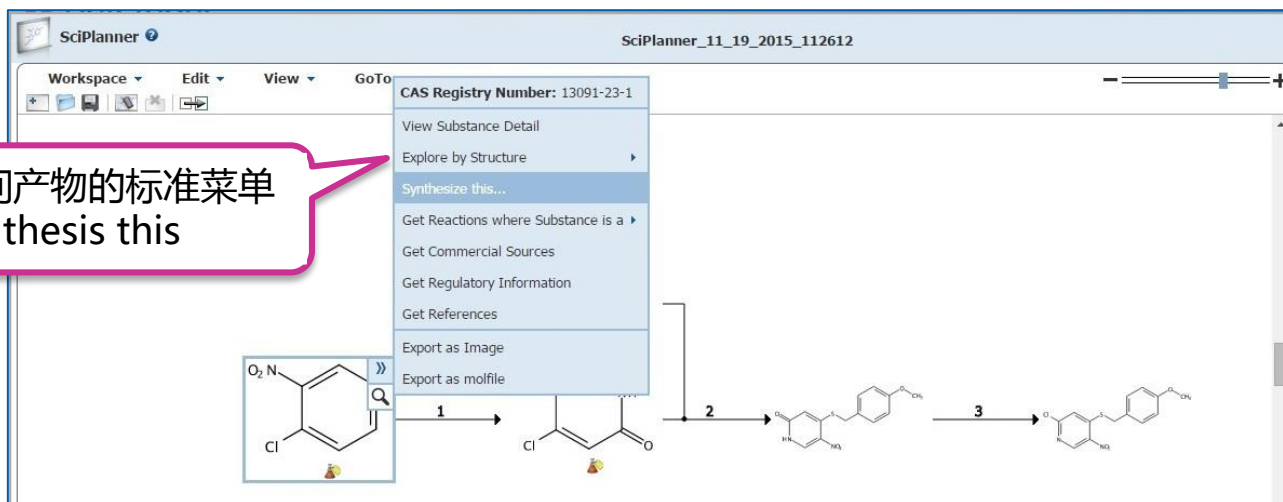
Your Workspace is empty.

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

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SciPlanner使用简介

打开中间产物的标准菜单
选择Synthesize this

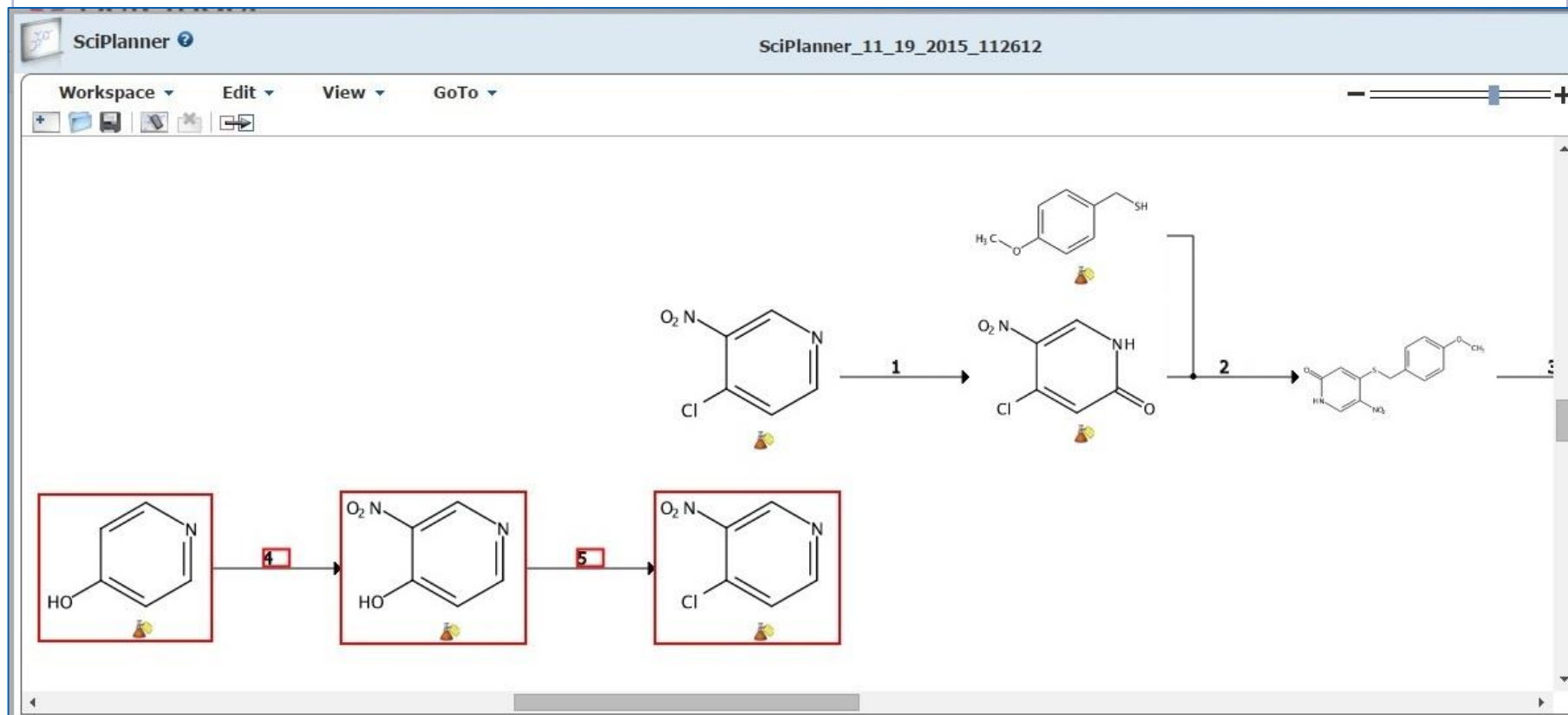


在检索到的反应中选择感兴趣的反应

继续推送到SciPlanner



SciPlanner使用简介



步骤同前，将推送过来的反应拖到编辑面板中，可以看到两条反应中存在同样的结构

SciPlanner使用简介

SciPlanner 11_19_2015_112612

Workspace Edit View GoTo

New
Open
Save
Duplicate
Import
Export
Print
Close

点击 Workspace, 选择 Export 导出结果

用鼠标将两个同样的结构拖至重叠, 两条反应合并

选择适当的输出格式, 输出结果

Export

For:

Offline Review

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

Saving Locally

- ☐ SciPlanner eXchange (*.pkx)

Details:

File Name: *

SciPlanner_11_19_2015_112612

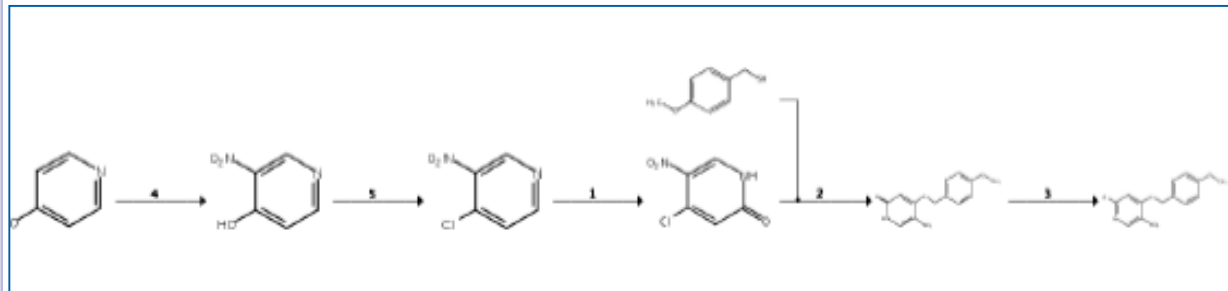
Title

Include:

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

Export **Cancel**

SciPlanner导出结果



Reaction	Stages	Notes	Yield
5	1.1 R:POCl ₃ , S:PhMe, 0°C → rt; 16 h, rt → 110°C	Reactants: 1, Reagents: 2, Solvents: 2, Steps: 1, Stages: 2	90%
	1.2 R:K ₂ CO ₃ , S:H ₂ O, cooled, pH 10	Transformation: 1. Formation of Alkyl Halides from Alcohols	

References

High color rendering index and color stable hybrid white efficient OLEDs with a double emitting layer structure using a single phosphorescence dopant of heteroleptic platinum complexes

By Poloek, Anurach et al

From Journal of Materials Chemistry C: Materials for Optical and Electronic Devices, 2(48), 10343-10356; 2014

Substance Information		
1228150-22-8 C₁₃H₁₂N₂O₄S 2(1H)-Pyridine, 4-[[4-methoxyphenyl]methyl]thio-5-nitro- Related Info: ~ 2 References Reactions	1228150-23-9 C₁₃H₁₁ClN₂O₄S Pyridine, 2-chloro-4-[[4-methoxyphenyl]methyl]thio-5-nitro- Related Info: ~ 2 References Reactions	13091-23-1 C₅H₃ClN₂O₂ Pyridine, 4-chloro-3-nitro- Related Info: ~ 301 References Reactions ~ 100 Commercial Sources Regulatory Information
5435-54-1 C₅H₄N₂O₃ 4-Pyridinol, 3-nitro- Related Info: ~ 113 References Reactions ~ 197 Commercial Sources Regulatory Information	6258-60-2 C₈H₁₀O S Benzenemethanethiol, 4-methoxy- Related Info: ~ 749 References Reactions ~ 71 Commercial Sources Regulatory Information	626-64-2 C₅H₅N O 4-Pyridinol Related Info: ~ 1351 References Reactions ~ 160 Commercial Sources Regulatory Information
850663-54-6 C₁₃H₉ClN₂O₄ 2(1H)-Pyridine, 4-chloro-5-nitro- Related Info: ~ 22 References Reactions ~ 138 Commercial Sources		

提纲

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 - 文献检索
 - 物质检索 (聚合物检索)
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 - 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



- 最大的方法信息合集，聚焦核心化学市场
- 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
- 分析与合成两个模块
- 逾百万的合成和分析方法合集——数量持续增加!

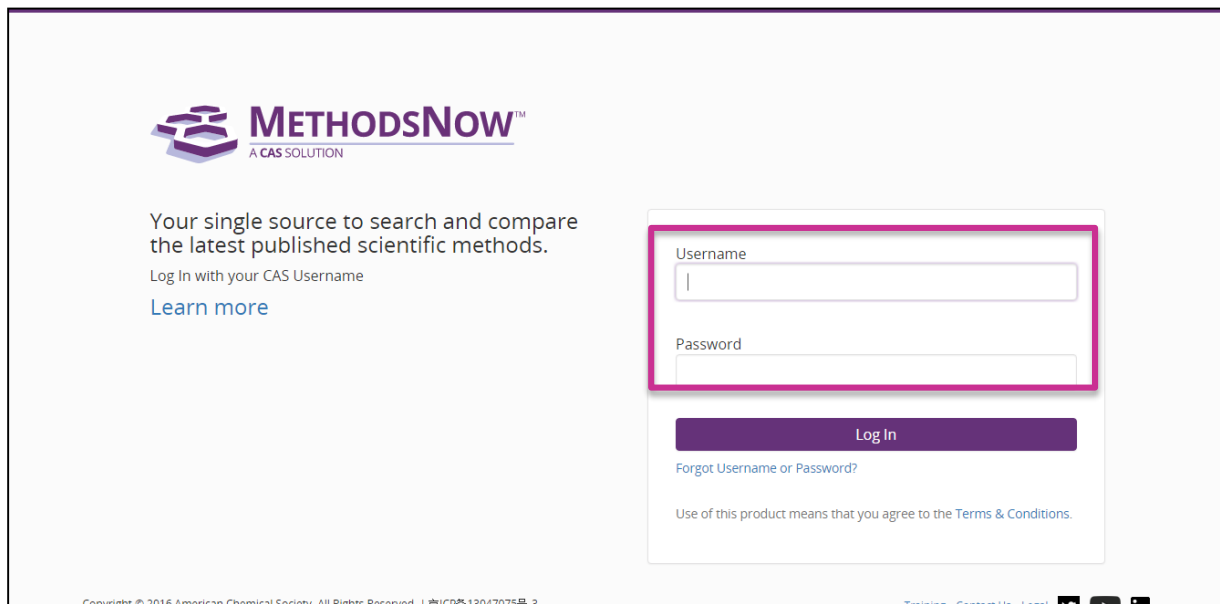


MethodsNow – Analysis(www.methodsnow.com)

- Organic Compound Analysis: 天然产物分离分析，手性分离，活性药物成分及代谢产物分析...
- Organometallics / Inorganics: 地质分析，无机物分析，金属有机化合物分析
- Pharmacology / Toxicology: 成瘾药物检测，有毒物检测...
- Bioassays: 生物探针，生物标定细胞实验，生物标定药物实验，生物医学材料分析，生物分子/生物组织分离测定...
- Water Analysis: 阴阳离子分析，元素测定，痕量元素分析，废水分析，生物标记公共卫生分析...
- 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...

目前有13个大类，45个小类。某些子项目属于多种方法分类

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MethodsNow – Analysis(www.methodsnow.com)

检索/高级检索



方法分类



历史检索



The screenshot shows the MethodsNow Analysis web interface. At the top, there is a header with 'CAS Solutions' and 'METHODSNow™ A CAS SOLUTION'. On the right, there are links for 'Saved' (with a star icon) and 'Account' (with a user icon). Below the header is a 'Search' section with a text input field labeled 'Enter keyword, matrix, analyte, etc.' and a search button. A callout '保存结果集' (Save Results Set) points to the 'Saved' link. Below the search section is a 'Browse Method Categories' section with a grid of category links. A callout '点击一个类别 浏览相关方法' (Click a category to browse related methods) points to the 'Organic Compound Analysis' link. Below the categories is a 'Recent Searches' section with a list of search terms. A callout '点击历史检索 重新运行检索' (Click history search to re-run search) points to the 'hplc lycopene analysis' link. On the right side of the 'Recent Searches' section, there is a callout '点击“X” 删除检索历史' (Click 'X' to delete search history) pointing to a close button.

CAS Solutions

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★ Saved Account

Search

Enter keyword, matrix, analyte, etc.

Advanced Search

Browse Method Categories

Agricultural Applications / Analysis
Bioassays
Biomolecule Isolation
Environmental Analysis
Food Analysis

Organic Compound Analysis
Inorganic / Organometallics / Inorganics

Pharmacology / Toxicology
Polymer Analysis
Water Analysis

Recent Searches

hplc lycopene analysis

保存结果集

点击一个类别
浏览相关方法

点击历史检索
重新运行检索

点击“X”
删除检索历史

高级检索

The image displays two overlapping screenshots of the CAS MethodsNow Advanced Search interface. The top screenshot shows the main search form with fields for Keyword, Matrix, and Analyte, along with logical operators (AND, OR, NOT) and a search button. The bottom screenshot shows a dropdown menu for selecting search criteria, including Publication Name, Keyword, Analyte, Matrix, Method Category, Technique, CAS Method Number, and Publication Name. Annotations in Chinese provide instructions on how to use these features.

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

The screenshot shows the MethodsNow search interface. At the top, there is a navigation bar with 'CAS Solutions' and 'METHODSNow™ A CAS SOLUTION' on the left, and 'Saved' and 'Account' on the right. The main section is titled 'Search' with the prompt 'Enter keyword, matrix, analyte, etc.'. A search bar contains the text 'supercritical', and a dropdown menu shows suggestions: 'supercritical extraction', 'supercritical fluid chromatographic chiral stationary phases', and 'supercritical fluid chromatography'. A callout box with a purple border and an arrow pointing to the search bar contains the text: '此处只需输入一个关键词即可，MethodsNow会自动进行同义词查找'. Below the search bar, there is a 'Browse Method Categories' section with a grid of categories: Agricultural Applications / Analysis, Bioassays, Biomolecule Isolation, Environmental Analysis, Food Analysis, Fuels / Geology / Biofuels, Historical Analysis / Dating, Miscellaneous, Organic Compound Analysis, Organometallics / Inorganics, Pharmacology / Toxicology, Polymer Analysis, and Water Analysis. At the bottom, there is a 'Recent Searches' section with two entries: 'supercritical extraction' and 'member', each with a close button (X).

CAS Solutions

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Saved Account

Search

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

CAS Solutions

METHODSNow
A CAS SOLUTION

"supercritical extraction"

Results (581)

Sort Relevance

导出方法

保存方法

View Details & Instructions

查看方法详情

Add to Compare

方法对比

Limiting Analysis Conditions: Analyte, Matrix, Method Category, Technique

Analyte	Rubixanthin; Lutein A; Zeaxanthin; <i>cis</i> - β -Carotene; β -Carotene; Carotenes
Matrix	Rosa canina; Pharmaceutical natural products
Other Materials	Reagent: Ethanol; Hexane Material: Spherisorb column (5 μ m, 4.6 x 250 mm, ODS1); Stainless steel column; Glass beads (1 mm diameter) View All
Method Category	Natural Product Isolation Analysis
Technique	Liquid chromatography spectrometric detectors; HPLC; Supercritical extraction
Equipment Used	HPLC system; Diode array detector (DAD); Supercritical extraction apparatus; Thermostatic chamber

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	View Structure	6916-62-7
Xanthone	analyte	View Structure	90-47-1
Coumarin	analyte	View Structure	91-64-5
Phenols	analyte		
Biflavonoids	analyte		
<i>Calophyllum brasiliense</i>	matrix		
Leaf	matrix		
Sieves (30 and 50 mesh)	material		
Dichloromethane	reagent	View Structure	75-09-2
Methanol	reagent	View Structure	67-56-1
DPPH radical	reagent	View Structure	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 CO₂; 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 (IC₅₀) from the inhibition percentage plotting graph.

Validation

Inhibitory Activity 206.58 µg/mL (IC₅₀)

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

			Expand All Collapse All		
	1	2	3		
Title	Analysis of Phenols in Calophyllum brasiliense by Supercritical extraction	Analysis of Phenols in Calophyllum brasiliense by Supercritical extraction	Analysis of Phenols in Calophyllum brasiliense 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		Equipment Used	Oven, Q-31, QUIMIS; Processor, RI7625, WALITA; Spectrophotometer, UV-1203, Shimadzu; Syringe pumps. View All
Technique	Spectrophotometry; Soxhlet extractor; Supercritical extraction	Spectrophotometry; Soxhlet extractor		Conditions	Instrument: Detection wavelength - 515 nm Instrument: Detection wavelength - 760 nm Instrument: Detection wavelength - 760 nm
Analyte	Mammea A/BB; Xanthone; Coumarin; Phenols; Biflavonoids	Phenols		Source	Comparing conventional and supercritical extraction of (-)-mammea A/BB and the antioxidant View All
Matrix	Calophyllum brasiliense; Leaf	Calophyllum brasiliense		Method	Organic solvent extraction using Soxhlet apparatus 1. Collect the leaves of Calophyllum brasiliense Combretaceae View All
Other Materials	Dichloromethane; Methanol; DPPH radical; Sieves (30 and 50 mesh)	Methanol; Sodium carbonate; Folin-Ciocalteu (30 and 50 mesh)		Inhibitory Activity	206.58 µg/mL (IC ₅₀)
				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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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/>

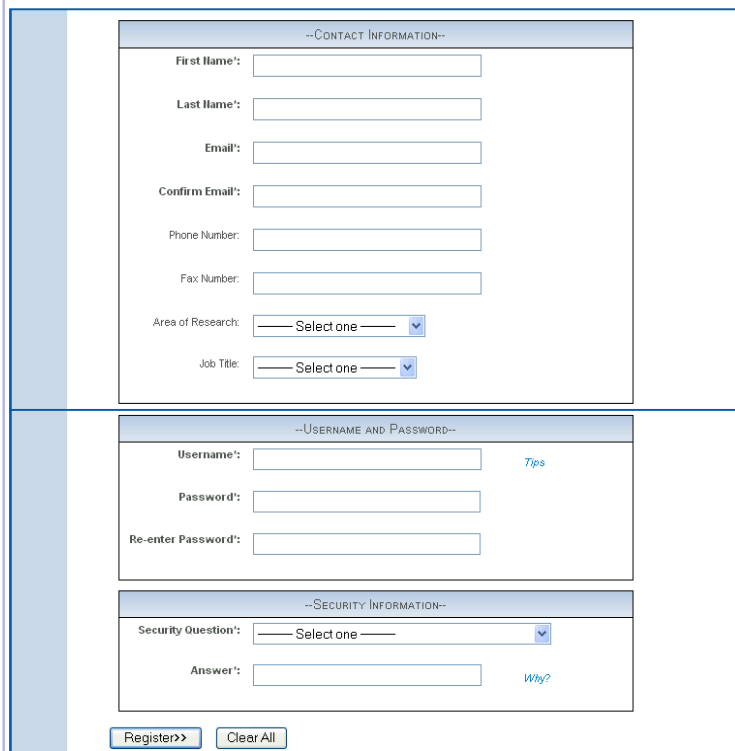
PatentPakTM——专利工作流程解决方案 读者在SciFinder中找到需要的专利文献后, 在相应的文献标题下可见到PatentPak按钮, 点击该按钮即可使用。

SciFinder 注册须知:

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, 并在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 registration form is divided into three main sections: Contact Information, Username and Password, and Security Information. The Contact Information section includes fields for First Name, Last Name, Email, Confirm Email, Phone Number, Fax Number, Area of Research (a dropdown menu), and Job Title (a dropdown menu). The Username and Password section includes fields for Username, Password, and Re-enter Password, with a 'Tips' link next to the Password field. The Security Information section includes a Security Question (a dropdown menu) and an Answer field, with a 'Why?' link next to the Answer field. At the bottom of the form are two buttons: 'Register>>' and 'Clear All'.

--CONTACT INFORMATION--

First Name:

Last Name:

Email:

Confirm Email:

Phone Number:

Fax Number:

Area of Research:

Job Title:

--USERNAME AND PASSWORD--

Username:

Password: [Tips](#)

Re-enter Password:

--SECURITY INFORMATION--

Security Question:

Answer: [Why?](#)

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.

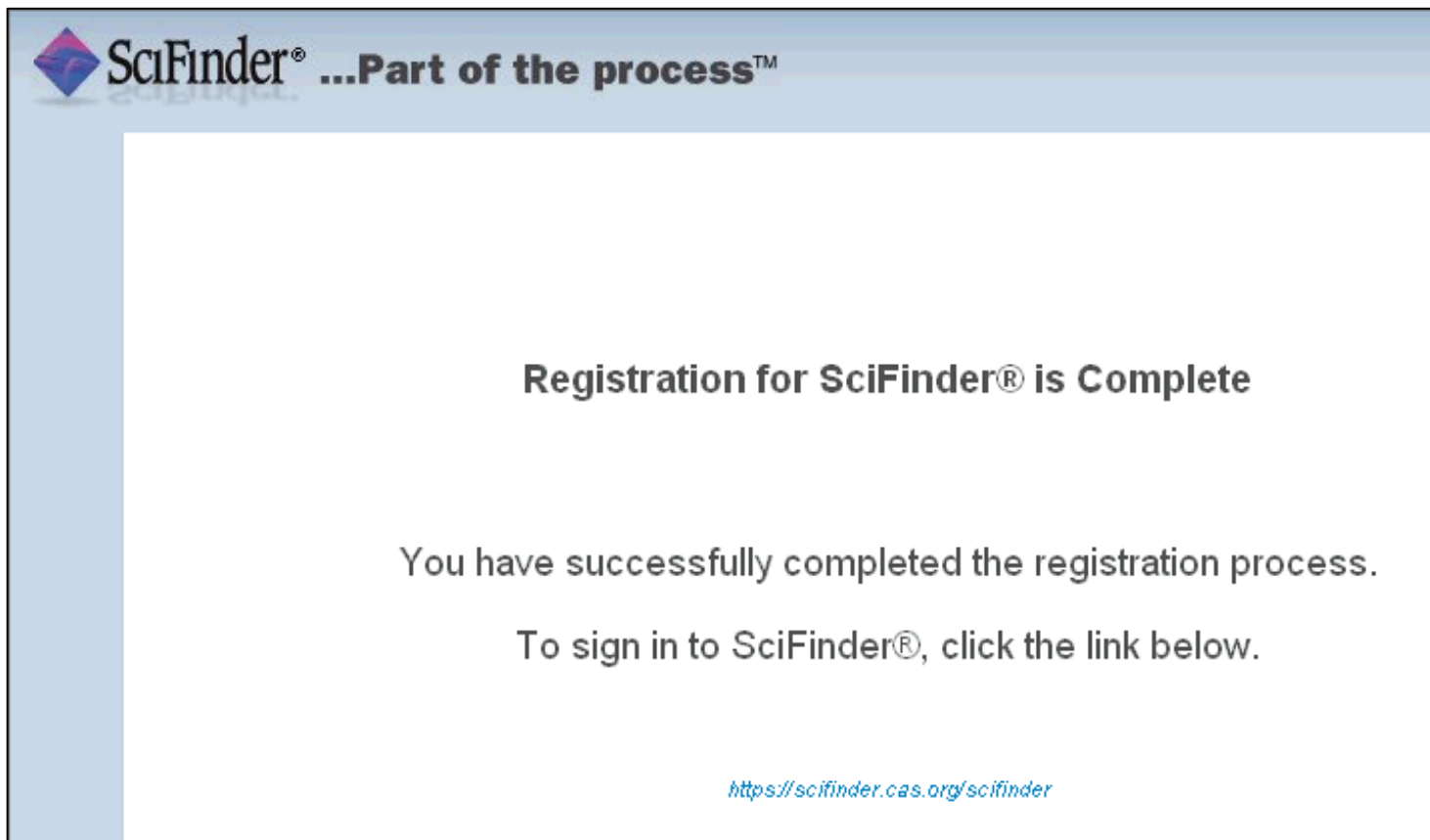
If you need assistance at any time, consult the key contact at your organization.

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



账号注册成功，登录scifinder.cas.org开始使用SciFinder

SciFinder使用注意事项

- 一人注册一个帐号
- 请提供真实姓名信息
- 严禁过量下载
- 严禁账号分享
- 严禁将账号用于非学术研究

更多培训资料请访问

www.cas-china.org

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