

匡金海

客户顾问

jkuang@acs-i.org

如何使用SciFinder获取科技信息

东北大学

2018.05.22



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 Analysis
- SciFinder常见问题及解决

美国化学文摘社—Chemical Abstracts Service

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

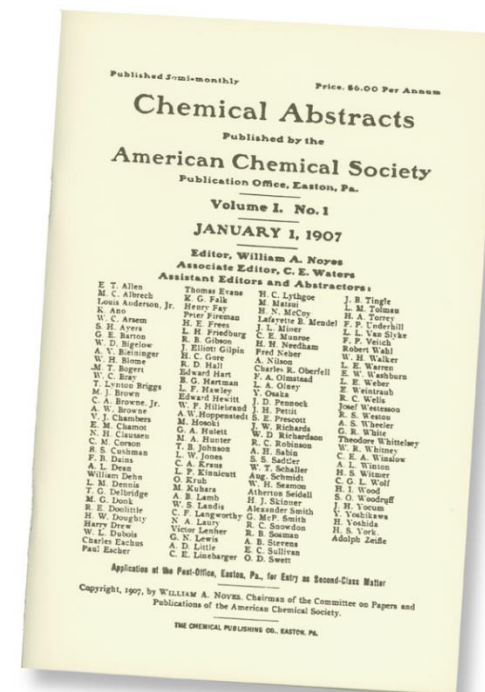


1907年，信息的汇集、管理发生了重大的变化



威廉·诺伊斯
(William A. Noyes)

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



CAS——构建最高质量的化学数据库



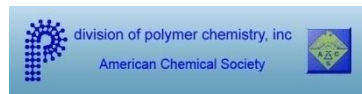
arXiv.org

Aldrichimica ACTA

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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：

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染料、有机颜料;合成橡胶;纺织品、纤维

应用化学各领域：

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物理、无机、分析化学各领域：

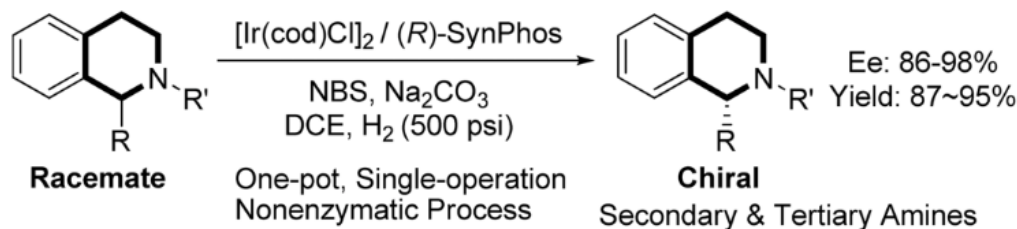
表面化学,催化剂,相平衡,核现象,电化学

CAS数据库最具价值的内容——人工标引

1. Concise Redox Deracemization of Secondary and Tertiary Amines with a Tetrahydroisoquinoline Core via a **Nonenzymatic Process**

By: Ji, Yue; Shi, Lei; Chen, Mu-Wang; Feng, Guang-Shou; Zhou, Yong-Gui

A concise deracemization of racemic secondary and tertiary amines with a tetrahydroisoquinoline core has been successfully realized by orchestrating a redox **process** consisted of N-bromosuccinimide oxidn. and iridium-catalyzed asym. hydrogenation. This compatible redox combination enables one-pot, single-operation deracemization to generate chiral 1-substituted 1,2,3,4-tetrahydroisoquinolines with up to 98% ee in 93% yield, offering a simple and scalable synthetic technique for chiral amines directly from racemic starting materials.



Indexing

Heterocyclic Compounds (One Hetero Atom) (Section27-17)

Concepts

Enantioselective synthesis
Oxidation

Hydrogenation catalysts

stereoselective prepn. of tetrahydroisoquinoline derivs. via iridium-catalyzed deracemization in presence of chiral phosphine ligands

Substances

12112-67-3 Dichlorobis(cyclooctadiene)diiridium
76189-55-4
133545-16-1
445467-61-8
503538-68-9 (S)-SynPhos

Chiral ligands

stereoselective prepn. of tetrahydroisoquinoline derivs. via iridium-catalyzed deracemization in presence of chiral phosphine ligands

stereoselective prepn. of tetrahydroisoquinoline derivs. via iridium-catalyzed deracemization in presence of chiral phosphine ligands

Catalyst use; Uses

QUICK LINKS

0 Tags, 0 Comments

SOURCE

Journal of the American Chemical Society
Volume137
Issue33
Pages10496-10499
Journal; Online Computer File
2015
CODEN:JACSAT
ISSN:0002-7863
DOI:10.1021/jacs.5b06659

COMPANY/ORGANIZATION

State Key Laboratory of Catalysis, Dalian Institute of Chemical Physics
Chinese Academy of Sciences
Dalian, Peop. Rep. China
116023

ACCESSION NUMBER

2015:1340032
CAN163:331216
CAPLUS

PUBLISHER

American Chemical Society

LANGUAGE

English

Tips:

98%以上的文献，都经过人工标引

用Index Term标引文献中的重要技术术语

用CAS RN标引出文献中的重要物质

用CAS Role标引文献中重要物质的研究领域

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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。

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PatentPak™

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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			atkina, Natalia Language: English; Database: CAPLUS												
By Beigelman, Le From PCT Int. App. Disclosed he phosphate, R methods of t medicament	<table border="1"> <thead> <tr> <th>Patent No.</th><th>Kind</th><th>Language</th></tr> </thead> <tbody> <tr> <td>WO 2016100441</td><td>A1</td><td>English</td></tr> </tbody> </table> <table border="1"> <thead> <tr> <th>Patent Family</th></tr> </thead> <tbody> <tr> <td>US 20160176911</td></tr> </tbody> </table>	Patent No.	Kind	Language	WO 2016100441	A1	English	Patent Family	US 20160176911	<table border="1"> <thead> <tr> <th>Kind</th><th>Language</th></tr> </thead> <tbody> <tr> <td>A1</td><td>English</td></tr> </tbody> </table>	Kind	Language	A1	English	B is substituted purine and pyrimidine nucleobase; dashed bond between R and R ⁴ is absent, then R is H, substituted each R ⁶ and R ⁷ are independently hydrogen or deuterium; R ⁵ 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.
Patent No.	Kind	Language													
WO 2016100441	A1	English													
Patent Family															
US 20160176911															
Kind	Language														
A1	English														

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: CAP



Search in SciFinder | View Detail
Analyst Markup Locations (1)
 page 130

CAS RN 1206126-39-7






[Search in SciFinder](#) | [View Detail](#)

Analyst Markup Locations (1)

 page 130

CAS RN 1206126-41-1	
SM, ST, SV, SY, TH, TJ, TM, TN, US, UZ, VC, VN, ZA, ZM, ZW.	

8. [By](#)
[From](#)

(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)				(10) International Publication Number WO 2016/11773 A1	
(51) International Patent Classification: <i>C07H 19/10</i> (2006.01) <i>C07H 19/73</i> (2006.01) <i>C07H 20/20</i> (2006.01) <i>A61K 31/7072</i> (2006.01) <i>C07H 19/11</i> (2006.01) <i>A61K 31/7076</i> (2006.01) <i>C07H 19/213</i> (2006.01) <i>A61K 31/708</i> (2006.01) <i>C07H 19/067</i> (2006.01) <i>A61P 31/14</i> (2006.01) <i>C07H 19/073</i> (2006.01)			(81) Designated States (unless indicated otherwise) AO, AT, AU, AZ, BA, CA, CH, CL, CN, CO, DZ, EC, EE, EG, ES, FR, GB, GR, HK, HU, IL, IN, JP, KE, KR, KZ, LA, LC, LK, LU, MG, MK, MN, MW, MX, MY, NG, NI, NO, NZ, OM, PA, PE, PG, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, SR, TH, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW		
(21) International Application Number: PCT/US2015/065981					
(22) International Filing Date: 16 December 2015 (16.12.2015)			(84) Designated States (unless indicated otherwise) kind of regional protection available: ALL designated states		
(25) Filing Language: English			(26) Publication Language: English		

WO 2016/106441

PCT/US2015/065981

**EXAMPLE 1
COMPOUND 1**

Chemical reaction scheme showing the synthesis of Compound 1 (1-1) and its subsequent transformations into compounds 1-2, 1-3, 1-4, 1-5, and 1-6.

The starting material is a nucleoside derivative, which is converted to Compound 1 (1-1) via a series of steps. Compound 1 (1-1) is then converted to 1-2, 1-3, 1-4, 1-5, and 1-6.

Reagents and conditions for the transformations:

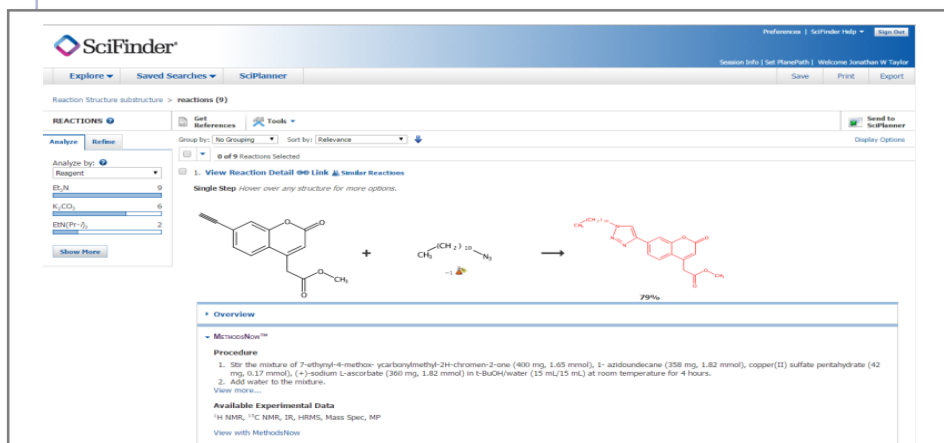
- 1-1 to 1-2: dichloromethane, pyridinium dichromate, acetic anhydride, tert-butanol
- 1-2 to 1-3: (CH₃)₃C-C(=O)-O-
- 1-3 to 1-4: Et₃SiO-C(=O)-
- 1-4 to 1-5: Et₃SiO-C(=O)-
- 1-5 to 1-6: (CH₃)₃C-C(=O)-O-

Route 2 shows the conversion of 1-4 to 1-5 via intermediate 1-4a.



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atorvastatin

Results (528)

Sort Relevance

Compare (0/3)

Analysis of Atorvastatin in Blood plasma by High-performance thin layer chromatography

CAS MN: 1-101-CAS-1389

View Details & Instructions

Add to Compare

Analyte	Atorvastatin
Matrix	Blood plasma
Other Materials	Material: 60 F ₂₅₄ silica gel HP TLC plates
Method Category	Active Pharmaceutical Ingredient and Metabolite Analysis
Technique	High-performance thin layer chromatography
Equipment Used	Automatic TLC Sampler 3
Source	HPTLC determination of atorvastatin in plasma Jamshidi, A.; Nateghi, A. R. Chromatographia (2007), 65 (11/12), 763-766. Vieweg Verlag/GWV Fachverlage GmbH

Document Sources

Abstract

单独的分析界面

提纲

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

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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, navigation links (Explore, Saved Searches, SciPlanner), and user information (Welcome Helen Zhu, Sign Out). Below the header is a search area with a text input field and a 'Search' button. To the left of the search area is a sidebar with categories: REFERENCES, SUBSTANCES, and REACTIONS. To the right is a sidebar with 'SAVED ANSWER SETS' and 'KEEP ME POSTED'. Annotations in Chinese point to various parts of the interface: '检索完，请点击退出' points to the Sign Out button; '工具栏' points to the top navigation bar; '检索入口' points to the search input field; '已保存的结果集' points to the SAVED ANSWER SETS sidebar; and '定题追踪' points to the KEEP ME POSTED sidebar.

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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

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SAVED ANSWER SETS

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

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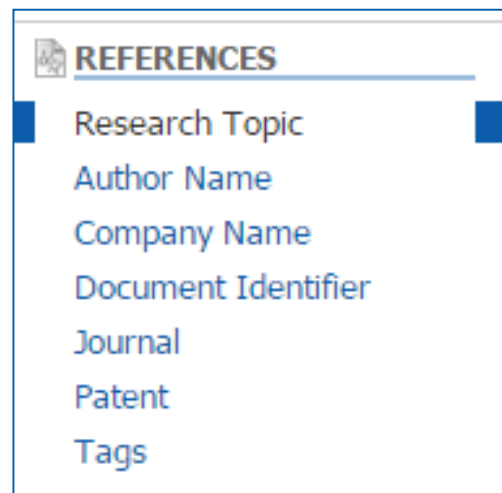
SciFinder检索——文献检索

■ 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
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文献检索——主题: 铝合金铸造

- 检索词：铝合金 铸造
- 检索式：casting of aluminum alloy

The screenshot displays the SciFinder web interface. At the top, there's a 'CAS Solutions' dropdown and the SciFinder logo. Below this is a navigation bar with 'Explore', 'Saved Searches', and 'SciPlanner'. The main content area shows the search results for the topic 'casting of aluminum alloy', indicating 23167 references. On the left, a sidebar lists various search filters under 'REFERENCES' and 'SUBSTANCES'. The main search area includes a text input field with the search term, a 'Search' button, and options for 'Advanced Search' and 'Always Show'.

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Research Topic "casting of aluminum alloy" > references (23167)

REFERENCES

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

SUBSTANCES

- Chemical Structure
- Markush

REFERENCES: RESEARCH TOPIC ?

casting of aluminum alloy

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

Search

Advanced Search ☒ Always Show

关键词之间可用介词连接：in, with, of...



主题检索的候选项

Select All Deselect All

0 of 5 Research Topic Candidates Selected

	References
<input type="checkbox"/> 3045 references were found containing "casting of aluminum alloy" as entered.	3045
<input type="checkbox"/> 23167 references were found containing the two concepts "casting" and "aluminum alloy" closely associated with one another.	23167
<input type="checkbox"/> 37003 references were found where the two concepts "casting" and "aluminum alloy" were present anywhere in the reference.	37003
<input type="checkbox"/> 729595 references were found containing the concept "casting".	729595
<input type="checkbox"/> 187686 references were found containing the concept "aluminum alloy".	187686

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“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；

文献检索结果

文献分析工具

REFERENCES ?

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Analyze Refine Categorize

Sort by: Accession Number

0 of 23167 References Selected

Page: 1 of 1159

Sample Analysis: ?

Author Name

Cui Jianzhong ≥ 130

Che Yun ≥ 104

Zhang Zhongke ≥ 98

Men Sanquan ≥ 95

Campbell John ≥ 81

Li Xiang ≥ 72

Tiryakioglu Murat ≥ 72

Cui Jian Zhong ≥ 64

Katgerman L ≥ 63

Rohatgi P K ≥ 63

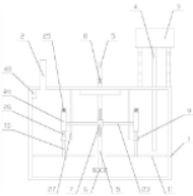
Show More

1. A kind of low-pressure casting equipment of high yield rate for producing aluminium alloy wheel hub [Machine Translation].

Quick View Other Sources

By Huang, Longhui

From Faming Zhuanli Shenqing (2018), CN 107962166 A 20180427. | Language: Chinese, Database: CAPLUS



[Machine Translation of Descriptors]. The invention relates to a kind of low-pressure casting equipment of high yield rate for producing aluminum alloy wheel hub, including crucible, inlet pipe, mold, riser pipe, purifn. mechanism and two elevating mechanisms, Purifn. mechanism includes purifn. pipe, nozzle, sliding block, rotating mechanism and two stirring mechanisms, Rotating mechanism includes translation component, movable plate, first gear and two transmission components, Transmission component includes the first rack, the second rack, second gear and the 3rd gear, inert gas is accessed to t...

2. A kind of aluminium alloys for automobile body sheets containing rare earth and preparation method thereof [Machine Translation].

Quick View Other Sources

By Jiang, Jiming; Jiang, Fengchan; Jiang, Huiyang; Chen, Zhibin; Lin, Jianhua

From Faming Zhuanli Shenqing (2018), CN 107974577 A 20180501. | Language: Chinese, Database: CAPLUS

[Machine Translation of Descriptors]. The present invention discloses a kind of aluminum alloys for automobile body sheets contg. rare earth and prepn. method thereof, which belongs to tech. field of aluminum alloy prepn. The described aluminum alloys for automobile body sheets contg. rare earth includes the following raw materials: titanium, zinc, iron, silicon, manganese, copper, carbon, chromium, boron, magnesium, molybdenum, tungsten, vanadium, rare earth elements, refining agents, sodium alc. ether sulfate, grain refiner and aluminum. The described aluminum alloys for automobile body shee...

3. A kind of machining process method of aluminium alloy machinery casting [Machine Translation].

Quick View Other Sources

By Zhu, Xu

文献检索结果：Refine

REFERENCES ?

Analyze Refine

Refine by: ?

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

Research Topic

corrosion resistant

Examples:

The effect of antibiotic resistance on dairy products

Photocyanation of aromatic compounds

Refine

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1. A kind of aluminum alloys for automobile body sheets containing rare earth and preparation method thereof [Machine Translation].
Quick View Other Sources
By Jiang, Jiming; Jiang, Fengchan; Jiang, Huiyang; Chen, Zhibin; Lin, Jianhua
From Faming Zhuanli Shenqing (2018), CN 107974577 A 20180501. | Language: Chinese, Database: CAPLUS
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2. A kind of high strength corrosion resistant pressure-casted aluminum alloy and its pressure casting method [Machine Translation].
Quick View PATENTPAK
By Fu, Yacheng; Wang, Shuncheng
From Faming Zhuanli Shenqing (2018), CN 107937765 A 20180420. | Language: Chinese, Database: CAPLUS
[Machine Translation of Descriptors]. A kind of high-strength **corrosion-resistant cast aluminum** and die **casting** method, its component and mass percent are: Si9.6-10.4%, Mg0.4~ 0.6%, Fe 0.3-0.5%, Ti0.1-0.3%, Tc0.01~ 0.03%, b 0.002-0.006%, Ba0.01~ 0.03%, Ge0.005-0.015%, the rest is Al and emerging impurity. The **casting** method includes the following steps: batching, melting **aluminum alloy** liq., refining degasification slagging-off, grain-refining agent added, modifier and silicon phase richer, alter and stir mold. The present invention optimizes Si, Mg main alloying elements on the basis of...

3. For haul train traction rod for ultra-high strength of 7 series aluminum alloy material for homogenizing heat treatment process [Machine Translation].
Quick View PATENTPAK
By Lin, Shunyan; Zhou, Zhijun; Wen, Qinghong; Yao, Yong; Lin, Lin
From Faming Zhuanli Shenqing (2018), CN 107937784 A 20180420. | Language: Chinese, Database: CAPLUS
[Machine Translation of Descriptors]. The present invention provides a 7xxx series **aluminum alloy** material homogenization heat treatment process, comprising the steps of, first, the **aluminum alloy** material through batching, melting and **casting** to obtain **aluminum alloy** ingot; then the above steps to obtain **aluminum alloy** ingot after homogenizing treatment at low temp. and high temp. homogenization heat treatment after homogenizing treatment to obtain **aluminum alloy** ingot. The present invention uses the "cold+ high-temp." homogenization heat treatment process, combined with alloying constituent...

4. A kind of high-performance aluminum alloy thick plate and preparation method thereof [Machine Translation].
Quick View PATENTPAK
By Han, Shuai; Xie, Yancui; Wang, Dawei; Yu, Lili; Geng, Guangchao; Chen, Shiyu; Zang, Jiaji; Xu, Hanji; Lu, Xiaohan; Zheng, Xinran
From Faming Zhuanli Shenqing (2018), CN 107937779 A 20180420. | Language: Chinese, Database: CAPLUS
[Machine Translation of Descriptors]. The invention discloses a kind of high-performance **aluminum alloy** thick plate and prepn. method thereof, and relates to a kind of high-performance **aluminum alloy** thick plate and prepn. method thereof. The purpose of the invention is to solve the problems of poor strength, toughness, **corrosion resistance** and fatigue property, and failure to meet the use std. requirements of the market of the plate manuf. with the existing high-performance **aluminum alloy** manufg. method and prepg. method. Elements in the **aluminum alloy** thick plate of the invention include Si,...

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 Accession Number Author Name Citing References Publication Year Title

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Page: 1 of 80

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1. **Arm spacing on mechanical properties and corrosion resistance of Al 9 Wt Pct Si and Zn 27 Wt Pct Al alloys**

By Osorio, Wislei R.; Goulart, Pedro R.; Santos, Givanildo A.; Moura Neto, Carlos; Garcia, Amauri
From Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science (2006), 37A(8), 2525-2538. | Language: English, Database: CAPLUS

Mech. properties and **corrosion resistance** (CR) of metallic alloys depend strongly on the solidification microstructural arrangement. The correlation of **corrosion** behavior and mech. properties with microstructure parameters can be useful for planning solidification conditions to achieve a desired level of final properties. The influence of heat-transfer solidification variables on the microstructural array of both Al - 9% Si and Zn - 27% Al **alloy castings** was studied and correlations between the as-cast dendritic microstructure, CR, and tensile mech. properties were developed. Exptl. results...

2. **Magnesium diecasting alloy AJ62x with superior creep resistance, ductility and diecastability**

Quick View Other Sources
By Pekguleryuz, M.; Labelle, P.; Argo, D.; Baril, E.
Edited by Kaplan, Howard I
From Magnesium Technology 2003, Proceedings of the Symposium held during the 2003 TMS Annual Meeting, San Diego, CA, United States, ar. 2-6, 2003 (2003), 201-206. | Language: English, Database: CAPLUS

Magnesium diecasting alloys for elevated temp. applications are coming of age. Several research centers and companies have been working on **alloy** systems based on alk. earth and rare earth alloying addns. to push the limits for the creep performance of Mg-based diecasting alloys. Noranda's Mg-Al-Sr based alloys have shown superior creep performance and high-temp. performance at temps. as high as 150-175° and stress levels of 50-70 MPa. The most recent **alloy** formulation AJ62x (Mg-6Al-2Sr) has in addn. shown excellent **castability**, and superior hot-tear **resistance**. Based on these attributes AJ...

3. **Pitting corrosion of rheocast A356 aluminium alloy in 3.5 wt.% NaCl solution**

Quick View Other Sources
By Arrabal, R.; Mingo, B.; Pardo, A.; Moledano, M.; Matykina, E.; Rodriguez, I.
From Corrosion Science (2013), 73, 342-355. | Language: English, Database: CAPLUS

In this study, the microstructure and **corrosion** behavior of rheocast and gravity-cast A356 **aluminum** alloys were examd. and compared. Scanning Kelvin probe force microscopy (SKPFM) results proved that large potential differences between iron-contg. intermetallics and the α -Al matrix were responsible for the initiation of the attack at the intermetallics/ α -Al interfaces. For longer immersion times, **corrosion** attack proceeded through the eutectic areas. Semisolid processing refined the eutectic silicon and iron-intermetallics and reduced the p.d. between secondary phases and the matrix. This ...

4. **Novel applications of CrN (PVD) coatings deposited at 200°**

Quick View Other Sources
By Navinsek, B.; Panjan, P.
From Surface and Coatings Technology (1995), 74-75(1-3, Pt. 2), 919-26. | Language: English, Database: CAPLUS

Citing Reference: 帮助找到最重要的文献

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Smelting	343
Tensile strength	310
Corrosion-resistant materials	306
Melting	276
annealing	258
Purification	215
heat treatment	197
Quenching (cooling)	193

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1. A kind of **aluminum alloy** for automobile body sheets containing rare earth and preparation method thereof [Machine Translation].
Quick View Other Sources
By Jiang, Jiming; Jiang, Fengchan; Jiang, Huiyang; Chen, Zhibin; Lin, Jianhua
From Faming Zhuanli Shenqing (2018), CN 107974577 A 20180501. | Language: Chinese, Database: CAPLUS
[Machine Translation of Descriptors]. The present invention discloses a kind of **aluminum alloy** for automobile body sheets contg. rare earth and prepn. method thereof, which belongs to tech. field of **aluminum alloy** prepn. The described **aluminum alloy** for automobile body sheets contg. rare earth includes the following raw materials: titanium, zinc, iron, silicon, manganese, copper, carbon, chromium, boron, magnesium, molybdenum, tungsten, vanadium, rare earth elements, refining agents, sodium alc. ether sulfate, grain refiner and **aluminum**. The described **aluminum alloy** for automobile body shee...

2. A kind of high strength corrosion resistant pressure-casted **aluminum alloy** and its pressure casting method [Machine Translation].
Quick View PATENTPAK
By Fu, Yacheng; Wang, Shuncheng
From Faming Zhuanli Shenqing (2018), CN 107937765 A 20180420. | Language: Chinese, Database: CAPLUS
[Machine Translation of Descriptors]. A kind of high-strength **corrosion-resistant cast aluminum** and die **casting** method, its component and mass percent are: Si9.6-10.4%, Mg0.4~ 0.6%, Fe 0.3-0.5 %, Ti0.1-0.3%, Tc0.01~ 0.03%, b 0.002-0.006%, Ba0.01~ 0.03%, Ge0.005-0.015%, the rest is Al and emerging impurity. The **casting** method includes the following steps: batching, melting **aluminum alloy** liq., refining degasification slagging-off, grain-refining agent added, modifier and silicon phase richer, alter and stir mold. The present invention optimizes Si, Mg main alloying elements on the basis of...

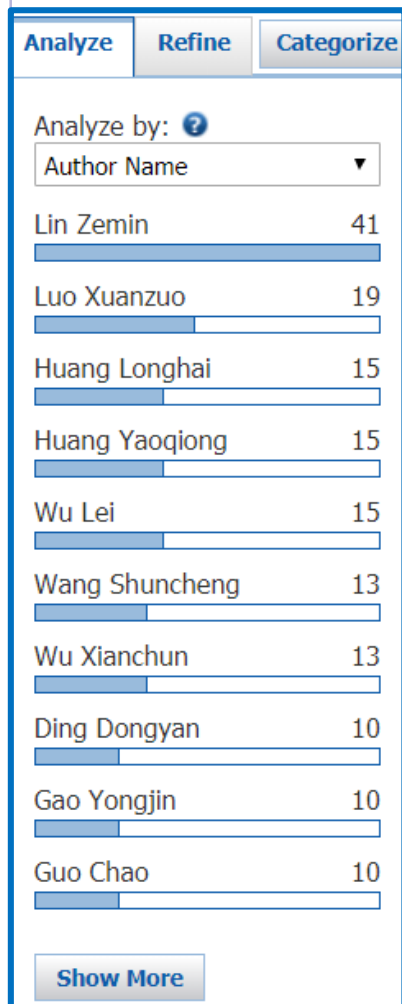
3. For haul train traction rod for ultra-high strength of 7 series **aluminum alloy** material for homogenizing heat treatment process [Machine Translation].
Quick View PATENTPAK
By Lin, Shunyan; Zhou, Zhijun; Wen, Qinghong; Yao, Yong; Lin, Lin
From Faming Zhuanli Shenqing (2018), CN 107937847 A 20180420. | Language: Chinese, Database: CAPLUS
[Machine Translation of Descriptors]. The present invention provides a 7xxx series **aluminum alloy** material homogenization heat treatment process, comprising the steps of, first, the **aluminum alloy** material through batching, melting and **casting** to obtain **aluminum alloy** ingot; then the above steps to obtain **aluminum alloy** ingot after homogenizing treatment at low temp. and high temp. homogenization heat treatment after homogenizing treatment to obtain **aluminum alloy** ingot. The present invention uses the "cold+ high-temp." homogenization heat treatment process, combined with alloying constituen...

4. A kind of high-performance **aluminum alloy** thick plate and preparation method thereof [Machine Translation].
Quick View PATENTPAK

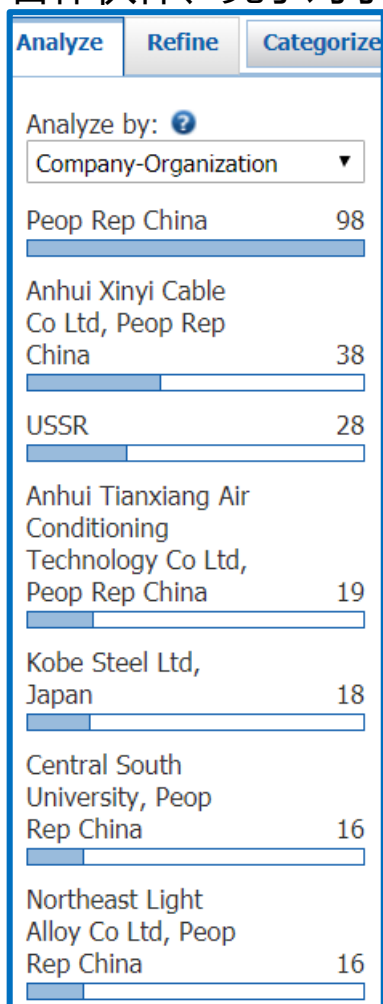
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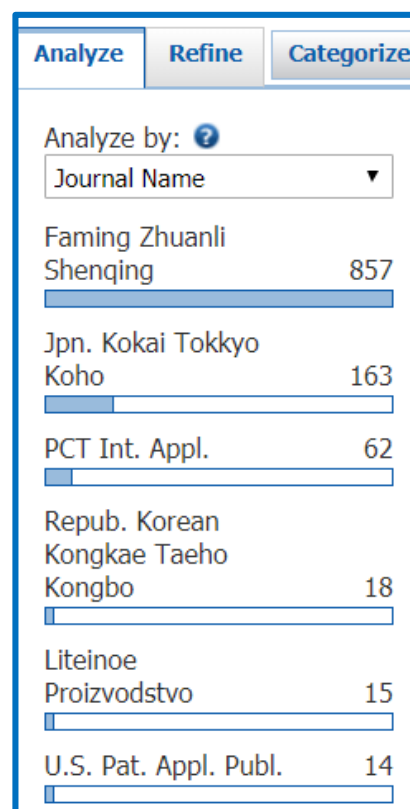
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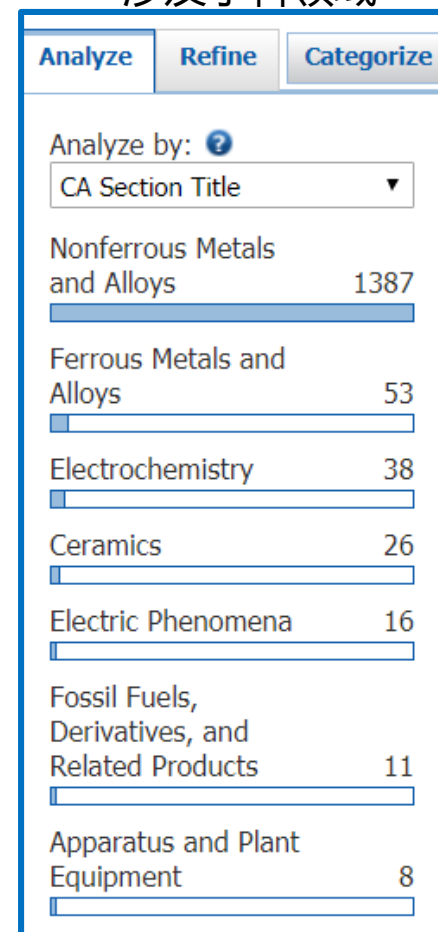
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Index Term ▼

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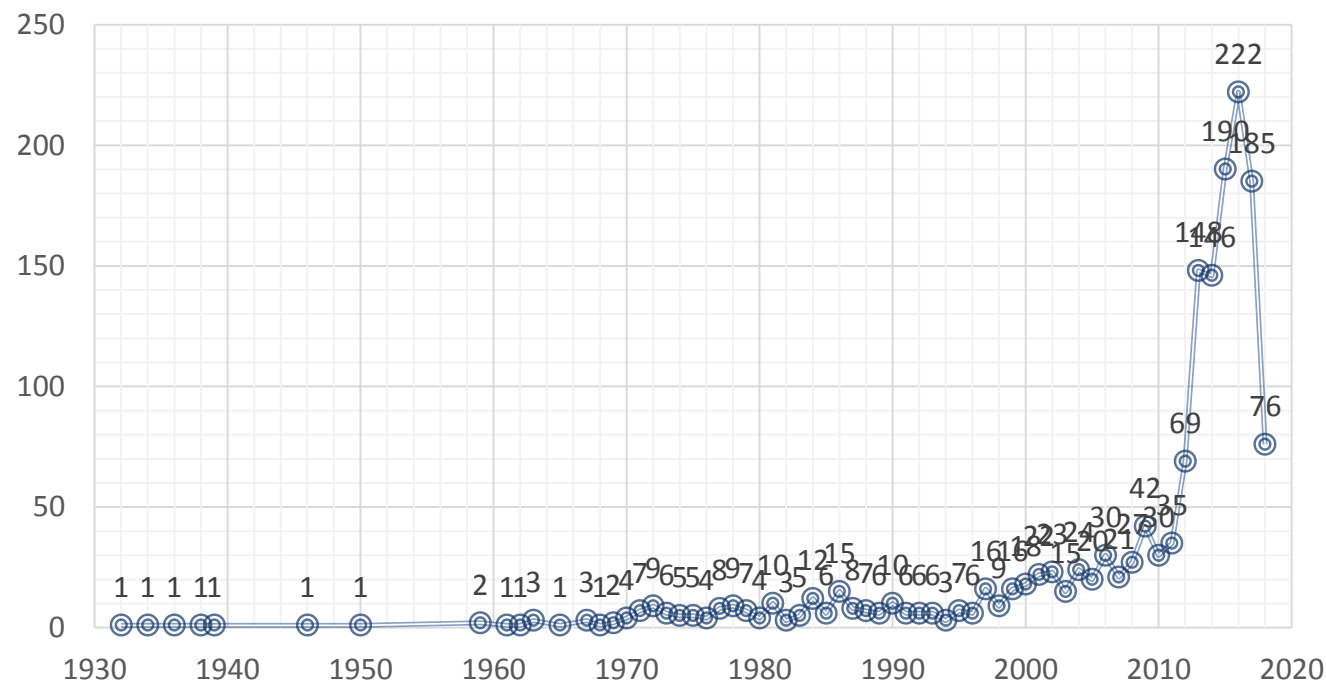
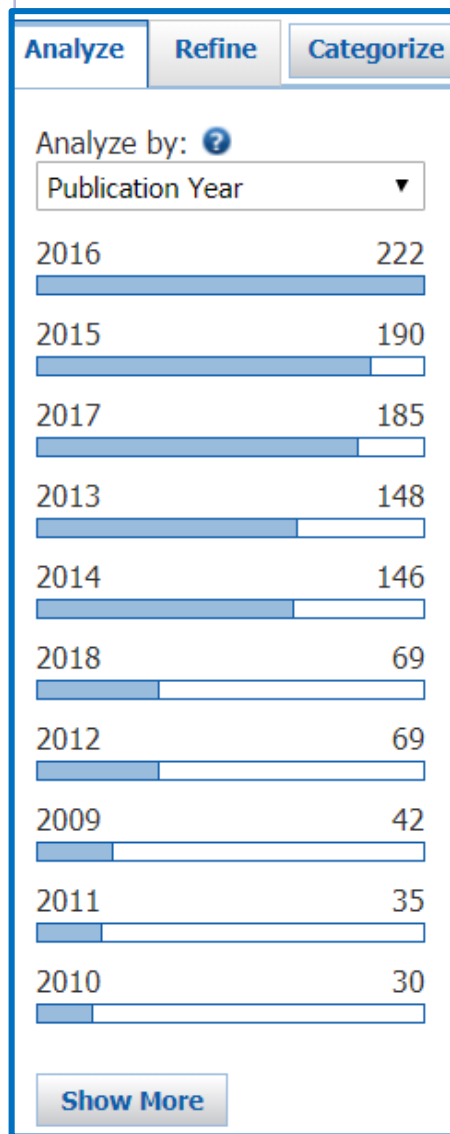
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<input type="checkbox"/> corrosion resistance	479
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学科领域
副分类

Index Term

选中的Index Term

Categorize ?

1. Select a heading and category.

Category Heading	Category
All	Substances in technology (3117)
Technology	Processes & apparatus (432)
General chemistry	Metallurgy (239)
Physical chemistry	Materials & products (410)
Synthetic chemistry	Formed, removed, & other substances (132)
Polymer chemistry	Construction (45)
Biotechnology	Ceramics (20)
Environmental chemistry	Power & fuel topics (14)
Genetics & protein chemistry	Imaging & recording (8)
Analytical chemistry	
Catalysis	
Biology	

2. Select index terms of interest.

Index Terms	
Page: 1 of 3	
Select All Deselect All	
<input type="checkbox"/> Magnesium	85
<input type="checkbox"/> Zinc	81
<input type="checkbox"/> Copper	78
<input type="checkbox"/> Titanium	68
<input type="checkbox"/> Nickel	63
<input type="checkbox"/> Iron	49
<input type="checkbox"/> Chromium	47
<input type="checkbox"/> Forging	47
<input type="checkbox"/> Manganese	42
<input checked="" type="checkbox"/> Cast alloys, aluminum	35
<input type="checkbox"/> Zirconium	34
<input type="checkbox"/> Cast iron	31
<input type="checkbox"/> AL9	29
<input type="checkbox"/> Rare earth metals	25
<input type="checkbox"/> Strontium	25
<input type="checkbox"/> Alloying	21
<input type="checkbox"/> Steel	21

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

- ✕ Technology > Metallurgy (1 Terms)

Technology > Metallurgy > 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。

结果集的保存— Save, Print, Export

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Save : 保存在服务器上, 方便以后登陆查看, 每次可存1万条记录。

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文献信息—题录、摘要、索引

2. Evaluation of corrosion resistance for the new surface treatment process for aluminum die cast products. Alugy process

By: Takada, Koji

ADC-12 aluminum alloy die castings after Alugy treatment or further coated with a resin were evaluated for corrosion resistance. Excellent corrosion resistance was obtained over the conventionally anodic oxidized castings. The Alugy process will enhance the scope in usage of aluminum die castings.

Indexing

Nonferrous Metals and Alloys (Section56-10)

重要概念

Concepts

Cast metals and alloys

aluminum alloys, evaluation of corrosion resistance of Alugy treated

Physical, engineering or chemical process; Properties; Process

重要物质

Substances

37321-78-1 ADC-12

die-castings; evaluation of corrosion resistance of Alugy treated

Physical, engineering or chemical process; Properties; Process

书目信息

QUICK LINKS

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SOURCE

Kinki Aruminyumu Hyomen
Shori Kenkyukai Kaishi
Volume169
Pages1-4
Journal
1994
CODEN:KAHKA7
ISSN:0285-6689

COMPANY/ORGANIZATION

Takada Laboratories, Inc.
Nagoya, Japan 464

ACCESSION NUMBER

1995:223124
CAN122:36526
CAPLUS

PUBLISHER

Kinki Aruminyumu Hyomen
Shori Kenkyukai

LANGUAGE

Japanese

Supplementary Terms

corrosion resistance aluminum die casting; Alugy process aluminum die casting

Tags

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Comments

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No comments

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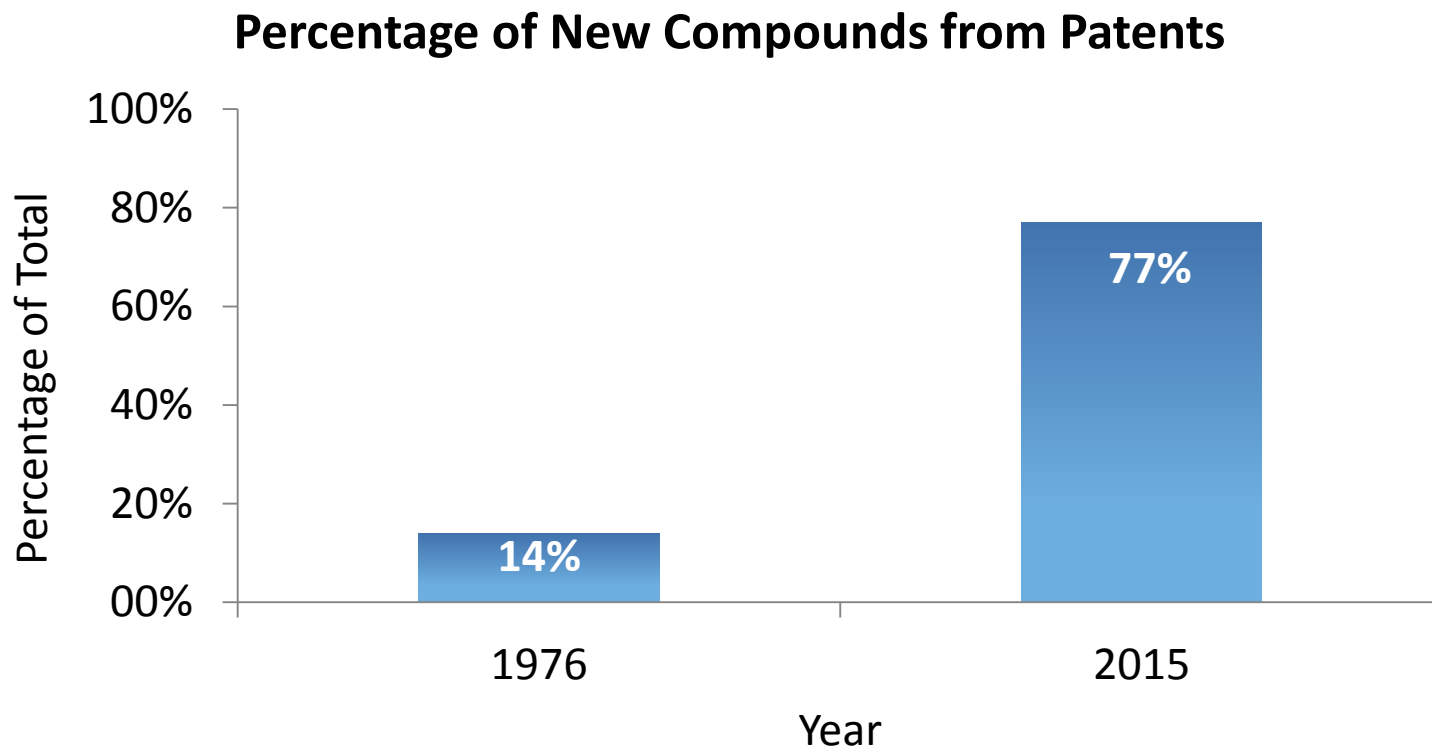
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- 使用Categorize可以让系统来实现自动分类

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：

330. Organic light emitting device comprising polar matrix

Quick View

PATENTPAK

By Denker, U
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Patent No.	PatentPak Options	Kind	Language
WO 2016207229	PDF PDF+ Viewer	A1	English
Patent Family			
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Fig.1

PatentPak——专利工作流程解决方案

专利PDF文件

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The screenshot displays the PatentPak interface, which is a web-based tool for viewing and downloading patent documents. The interface includes a sidebar on the left with a search bar and a list of key substances. The main area shows a patent document with text and chemical structures. Annotations highlight specific features:

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- Download Patent PDF File:** A button labeled "LOAD PDF" with a location pin icon, located next to the "DOWNLOAD PDF" button.
- PatentPak Viewer:** A text box pointing to a red location pin icon on the chemical structure of the starting material, indicating that clicking the pin will quickly locate the substance information in the PDF file.

The patent document content includes the following text:

followed by... acetate (50 mL) ... desired compound was obtained in 70 % yield (5.71 g). Finally, the

The pure sublimed compound was amorphous, with no detectable melting peak on the DSC curve, glass transition onset at 86 °C, and started to decompose at 490 °C.

Synthesis example 2
(9,9-dihexyl-9H-fluorene-2,7-diyl)bis-diphenylphosphine oxide (E8)

The chemical reaction scheme shows the synthesis of (9,9-dihexyl-9H-fluorene-2,7-diyl)bis-diphenylphosphine oxide (E8) from a dibromide precursor. The reaction conditions are:

- 1) n-BuLi, THF, -78 °C
- 2) ClP(Ph)₂, THF, -50 °C to RT
- 3) H₂O₂, DCM, RT

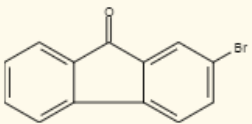
PatentPak——专利工作流程解决方案

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PAGE 52 / 69 ZOOM DOWNLOAD PDF

Key Substances in Patent

CAS RN 3096-56-8

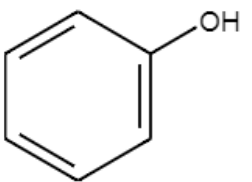


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Analyst Markup Locations (2)

- page 51
- page 51

CAS RN 108-95-2




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Analyst Markup Locations (2)

- page 51

Synthesis of 2-bromospiro[fluorene-9,9'-xanthene]



Chemical Formula: $C_{13}H_7BrO$
Molecular Weight: 259.10

Chemical Formula: $C_{13}H_7BrO$
Molecular Weight: 259.10

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2-Bromo-9-fluorenone (10.00 g, 1.0 eq, 38.6 mmol) and phenol (34.9 g, 9.6 eq., 0.37 mol) were placed in a two-necked flask and degassed with argon. Methanesulfonic acid (10.0 mL, 4.0 eq, 0.15 mol) was added, and the resulting mixture was refluxed for 4 days at 135°C. After cooling to room temperature, DCM (80 mL) and water (130 mL) were added. Upon stirring, the material precipitates. After filtration

PatentPak——专利工作流程解决方案

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Key Substances in Patent

CAS RN 3096-56-8

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Structure Markush Reactions

CAS RN 108-95-2

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Analyst Markup Locations (2)

page 51

Synthesis of 2-bromospiro[fluorene-9,9'-fluorene]

CAS Registry Number 3096-56-8

$C_{13}H_7BrO$
9H-Fluoren-9-one, 2-bromo-
Molecular Weight 259.10
Melting Point (Experimental)
Value: 141-142 °C

Chemical Formula: $C_{13}H_7BrO$

Chemical Formula: $C_{26}H_{15}BrO$
Molecular Weight: 411.30

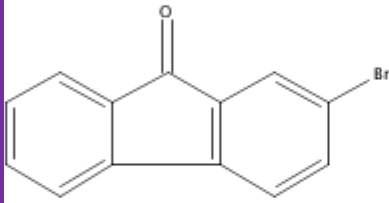
2-Bromo-9-fluorenone (10.00 g, 1.0 eq, 38.6 mmol) and phenol (34.9 g, 9.6 eq., 0.37 mol) were placed in a two-necked flask and degassed with argon. Methanesulfonic acid (10.0 mL, 4.0 eq, 0.15 mol) was added, and the resulting mixture was refluxed for 4 days at 135°C. After cooling to room temperature, DCM (80 mL) and water (130 mL) were added. Upon stirring, the material precipitates. After filtration

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SUBSTANCES: CHEMICAL STRUCTURE ?

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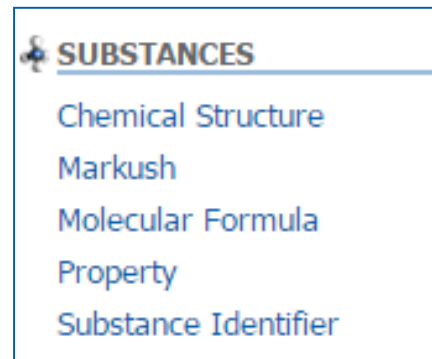
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 - MethodsNow Analysis
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■ 物质检索方法

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- 物质标识符检索：化学名称，CAS RN



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- 无机物，合金：分子式检索
- 高分子化合物：分子式检索和结构检索

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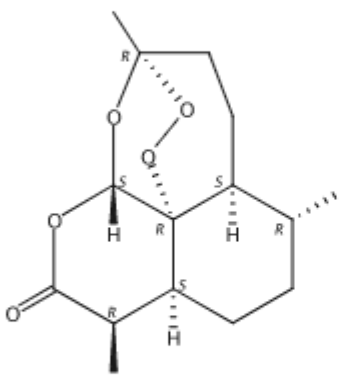
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0 of 1 Substance Selected

1. 63968-64-9

~5009 ~123



Absolute stereochemistry.

C₁₅ H₂₂ O₅
3,12-Epoxy-12H-pyrano[4,3-f]-1,2-benzodioxepin-10(3H)-one, octahydro-3,6,9-trimethyl-, (3R,5aS,6R,8aS,9R,12S,12aR)-

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

CAS Registry Number: 63968-64-9

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C₁₅ H₂₂ O₅
3,12-Epoxy-12*H*-pyrano[4,3-*j*]-1,2-benzodioxepin-10(3*H*)-one,
octahydro-3,6,9-trimethyl-, (3*R*,5*aS*,6*R*,8*aS*,9*R*,12*S*,12*aR*)-

Molecular Weight
282.33

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

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

Density (Experimental)
Value: 1.300 g/cm³

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

由物质获得文献，反应，供应商等信息

Absolute stereochemistry.

物质详情

通过物质获得文献

Get References

Limit results to:

<input type="checkbox"/> Adverse Effect, including toxicity	<input type="checkbox"/> Preparation
<input type="checkbox"/> Analytical Study	<input type="checkbox"/> Process
<input type="checkbox"/> Biological Study	<input type="checkbox"/> Properties
<input type="checkbox"/> Combinatorial Study	<input type="checkbox"/> Prophetic in Patents
<input type="checkbox"/> Crystal Structure	<input type="checkbox"/> Reactant or Reagent
<input type="checkbox"/> Formation, nonpreparative	<input type="checkbox"/> Spectral Properties
<input type="checkbox"/> Miscellaneous	<input type="checkbox"/> Uses
<input type="checkbox"/> Occurrence	

For each sequence, retrieve:

☐ Additional related references, e.g., activity studies, disease studies.

Get **Cancel**

Chinese Labels:

- 分析化学 (Analytical Study)
- 晶体结构 (Crystal Structure)
- 制备 (Preparation)
- 工艺 (Process)
- 谱图性质性质 (Spectral Properties)

EXPERIMENTAL PROPERTIES

Biological Chemical Density Flow and Diffusion Lipinski Optical and Scattering Structure Related Thermal

Structure Related Properties

Property	Value
Bond Angle	See full text
Bond Length	See full text
Permeability	See full text
X-Ray Diffraction Pattern	See full text

Notes

- (2) Galasso, V.; Chemical Physics 2007, V335(2-3), P141-154 CAPLUS
 (23) Du-Cuny, Lei; Bioorganic & Medicinal Chemistry 2009, V17(19), P
 (25) Sahoo, Nanda Gopal; Journal of Pharmaceutical Sciences 2009, V

实验数据与实验谱图

Note

(2)CAS

(2)CAS

1 of 4

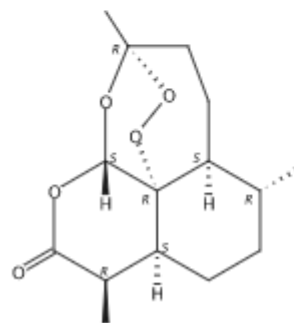
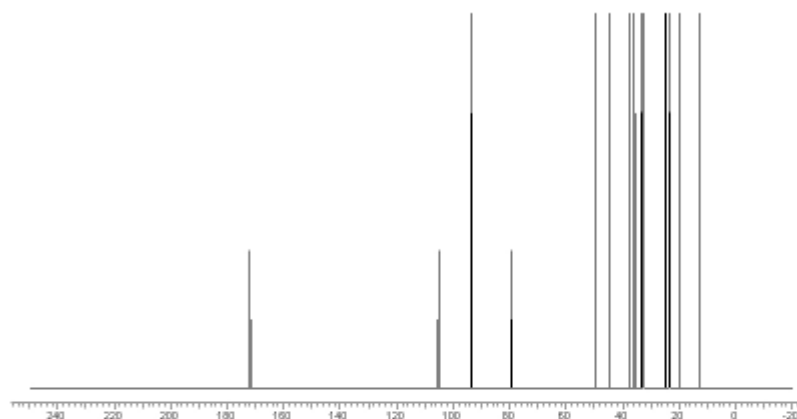
EXPERIMENTAL SPECTRA

¹H NMR ¹³C NMR Hetero NMR IR Mass Raman

¹³C NMR Properties

Property	Value
Carbon-13 NMR Spectrum	See spectrum
Carbon-13 NMR Spectrum	See spectrum
Carbon-13 NMR Spectrum	See full text

Carbon-13 NMR Spectrum



Abraham, et al.

FORMULA

C₁₅H₂₂O₅

CAS INDEX NAME

3,12-Epoxy-12H-pyrano[4,3-*f*]-1,2-benzodioxepin-10(3*H*)-one, octahydro-3,6,9-trimethyl-, (3*R*,5*a*,5*b*,8*a*,5*g*,12*S*,12*a*,*R*)-

NUCLEUS

¹³C

SOURCE

Spectral data were obtained from Advanced Chemistry Development, Inc.

物质检索——理化性质性质检索

SUBSTANCES: PROPERTY ?

☒ Experimental

Select Property...
Select Property...
Boiling Point (°C)
Density (g/cm³)
Electric Conductance (S)
Electric Conductivity (S/cm)
Electric Resistance (ohm)
Electric Resistivity (ohm*cm)
Glass Transition Temp. (°C)
Magnetic Moment (μB)
Median Lethal Dose (LD50) (mg/kg)
Melting Point (°C)
Optical Rotatory Power (degrees)
Refractive Index
Tensile Strength (MPa)

Examples: 44, 25-35, >125

Examples: 44, 25-35, >125

Explore

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

Examples: 44, 25-35, >125

Examples: 44, 25-35, >125

Examples: 44, 25-35, >125

Search

物质检索——理化性质检索：寻找电阻率大于125ohm的含铁物质

SUBSTANCES: PROPERTY ?

☒ Experimental

Electric Resistivity (ohm*cm) ▼

Select Property...

Boiling Point (°C)

Density (g/cm³)

Electric Conductance (S)

Electric Conductivity (S/cm)

Electric Resistance (ohm)

Electric Resistivity (ohm*cm)

Glass Transition Temp. (°C)

Magnetic Moment (μB)

Median Lethal Dose (LD50) (mg/kg)

Melting Point (°C)

Optical Rotatory Power (degrees)

Refractive Index

Tensile Strength (MPa)

>125

Examples: 44, 25-35, >125

Examples: 44, 25-35, >125

SciFinder物质检索结果

SUBSTANCES

Get References Get Reactions Get Commercial Sources Tools Create Keep Me Posted Alert Send to SciPlanner

Analyze Refine

Sort by: CAS Registry Number

0 of 241 Substances Selected

Page: 1 of 17

Analyze by:
Substance Role

Properties 228
Preparation 199
Uses 187
Process 169
Reactant or Reagent 126
Analytical Study 118
Formation, Nonpreparative 111
Biological Study 110
Occurrence 99
Miscellaneous 91

1. **1260101-12-9**
~1
1260101-11-8
 $C_{48}H_{40}N_8O_6U$

14797-73-0
 ClO_4

2. **1260101-08-3**
~1
1260101-07-2
 $C_{72}H_{60}N_{12}O_6Th$

3. **1260101-01-6**
~1
1260101-00-5
 $C_{60}H_{64}N_8O_{14}U$

14797-73-0
 ClO_4

通过分析/限定工具筛选结果

SUBSTANCES ?

Analyze Refine

Analyze by: ?

Elements

O

C

H

N

Fe

S

Mn

Zn

Cu

Se

Show More

Get References Get Reactions Get Commercial Sources Tools

Sort by: CAS Registry Number

0 of 34 Substances Selected

1. 1228647-06-0

Component	Component Ratio
O	22
Zn	0.8
Cu	0.4
Co	0.8
Ba	2
Mn	0.8
Fe	11.2

Ba . Co . Cu . Fe . Mn . O . Zn

Barium cobalt copper iron manganese zinc oxide

(Ba₂Co_{0.8}Cu_{0.4}Fe_{11.2}Mn_{0.8}Zn_{0.8}O₂₂)

Experimental Properties

2. 1228647-05-9

Component	Component Ratio
O	22
Zn	0.8
Cu	0.4
Co	0.8
Ba	2
Mn	0.6
Fe	11.4

Ba . Co . Cu . Fe . Mn . O . Zn

Barium cobalt copper iron manganese zinc oxide

(Ba₂Co_{0.8}Cu_{0.4}Fe_{11.4}Mn_{0.6}Zn_{0.8}O₂₂)

Experimental Properties

3. 1228647-04-8

Component	Component Ratio
O	22
Zn	0.8
Cu	0.4
Co	0.8
Ba	2
Mn	0.4
Fe	11.6

Ba . Co . Cu . Fe . Mn . O . Zn

Barium cobalt copper iron manganese zinc oxide

(Ba₂Co_{0.8}Cu_{0.4}Fe_{11.6}Mn_{0.4}Zn_{0.8}O₂₂)

Experimental Properties

4. 1228647-02-6

5. 1072928-27-8

6. 1072928-25-6

Create Keep Me Posted Alert


Send to SciPlanner

Display Options

Page: 1 of 3

分子式检索


CAS Solutions ▾

 **SciFINDER**
A CAS SOLUTION

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: MOLECULAR FORMULA ?

Examples:
H4SiO4
(C3H6O.C2H4O)x

Search

分子式书写规则—Hill 规则

- 单一组分物质：
 - 对于不含C的物质，按照字母顺序排序
 - 对于含C的物质，C、H写在前面，其他的按照字母顺序排列
 - 相邻的两个元素之间必须有区分号，即数字或者空格，倘若数字为1，那么可以用空格来区分
 - 区分大小写
- 多组分物质：
 - 每一组分必须遵照单一组分物质的分子式来书写。
 - 不同组分之间的排序按照各组分的首元素的字母顺序排序，但是含C组分的一定排在不含C的组分前面。**用点将不同的组分分开**
 - 倘若不同组分的首元素相同，则看元素数量多少，数量多的排在前面，若元素数量一样，则按次元素的顺序排列。

合金的检索

检索铁、锰、镍合金

The screenshot displays the SciFinder web interface. The top navigation bar includes 'Explore', 'Saved Searches', and 'SciPlanner'. The main search area shows the molecular formula 'Fe . Mn . Ni' with 1095 substances found. A left sidebar lists various search criteria like 'Research Topic', 'Author Name', and 'Substances'. The main results area is divided into a list of substances and a detailed view of the selected results. The detailed view shows a table of components and their percentages for each substance.

Substances: MOLECULE

Fe . Mn . Ni
Examples:
H4SiO4
(C3H6O.C2H4O)

Search

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

SUBSTANCES
Chemical Structure

Substances (1095)

Sort by: CAS Registry Number

0 of 1095 Substances Selected

1. 1850365-63-7
~1

Component	Component Percent
Fe	80
Mn	16
Ni	5

Fe . Mn . Ni
Iron alloy, base, Fe 80,Mn 16,Ni 5

2. 1835656-90-0
~1

Component	Component Percent
Fe	92
Ni	8.3
Mn	0.1

Fe . Mn . Ni
Iron alloy, base, Fe 92,Ni 8.3,Mn 0.1

3. 1835656-89-7
~1

Component	Component Percent
Fe	91
Ni	8.4
Mn	0.1

Fe . Mn . Ni
Iron alloy, base, Fe 91,Ni 8.4,Mn 0.1

4. 1821204-48-1
~1

Component	Component Percent
Mn	60
Ni	25
Fe	15

5. 1818872-06-8
~1

Component	Component Percent
Fe	65
Ni	35
Mn	0.5

6. 1816304-50-3
~1

Component	Component Percent
Fe	72
Ni	25
Mn	2.9

合金物质以列表形式呈现

合金的检索

检索参杂铁、锰、镍原子的合金

The screenshot displays the SciFinder software interface. On the left, the 'Structure Editor' window shows a chemical structure with atoms Fe, Mn, and Ni. The main window, titled 'SUBSTANCES', shows search results for the query 'Fe, Mn, Ni (query)'. The results are sorted by 'CAS Registry Number' and display 8 results. Each result includes a table of components and their percentages, and a note about the index name not yet being assigned.

Structure Editor:

Draw or change atoms or bonds. Shortcuts: Structure, Reaction, Markush.

Fe, Mn, Ni (query)

SUBSTANCES

Get References, Get Reactions, Get Commercial Sources, Tools

Sort by: CAS Registry Number

0 of 205650 Substances Selected

Display Options

Page: 1 of 4113

1. 2078047-46-6

Component	Component Percent
Fe	67
Cr	20
Ni	5.4
Mo	5.3
Mn	1.6
Ta	0.3

C, Cr, Fe, Mn, Mo, Ni, Ta
INDEX NAME NOT YET ASSIGNED

2. 2077985-45-4

Component	Component Percent
Fe	98
Mn	0.7
Ni	0.6
C	0.1
Si	0.1

C, Fe, Mn, Ni, Si
INDEX NAME NOT YET ASSIGNED

3. 2077985-44-3

Component	Component Percent
Fe	96
Ni	2.2
Mn	1.3
Si	0.3

Fe, Mn, Ni, Si
INDEX NAME NOT YET ASSIGNED

4. 2077962-09-3

Component	Component Percent
Fe	75
Cr	19
Ni	3.9
Mn	1.2
Si	0.9
C	0.4

C, Cr, Fe, Mn, Ni, Si
INDEX NAME NOT YET ASSIGNED

5. 2077962-06-0

Component	Component Percent
Fe	74
Cr	18
Mn	5.4
Ni	1
Si	0.7
C	0.4

C, Cr, Fe, Mn, Ni, Si
INDEX NAME NOT YET ASSIGNED

6. 2077946-90-6

Component	Component Percent
Fe	93 - 96
Ni	2.8 - 3.5
Cr	1 - 1.5
Mn	0.3 - 0.5
Mo	0 - 0.5
C	0.3 - 0.4
Si	0.2 - 0.4
Cu	0 - 0.3

7. 2077930-92-6

Component	Component Percent
Fe	97
Cr	1.2
Mn	0.8
C	0.2
Cu	0.2
Mo	0.2
Si	0.2
Ni	0.1

8. 2077913-93-8

Component	Component Percent
Fe	60 - 82
Cr	16 - 18
Ni	2.5 - 6
Cu	0 - 3.5
Mo	0 - 3.5
W	0 - 3.5
Mn	0 - 2
Co	0 - 1.5
Si	0 - 0.5

物质检索——结构

REFERENCES

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

SUBSTANCES

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

REACTIONS

- Reaction Structure

SUBSTANCES: CHEMICAL STRUCTURE ?

Structure Editor:

Java Non-Java

Click to Edit

Search Type:

- ☐ Exact Structure
- ☒ Substructure
- ☐ Similarity

☐ Show precision analysis

ChemDraw
Launch a SciFinder substance or reaction

Import CXF

Search

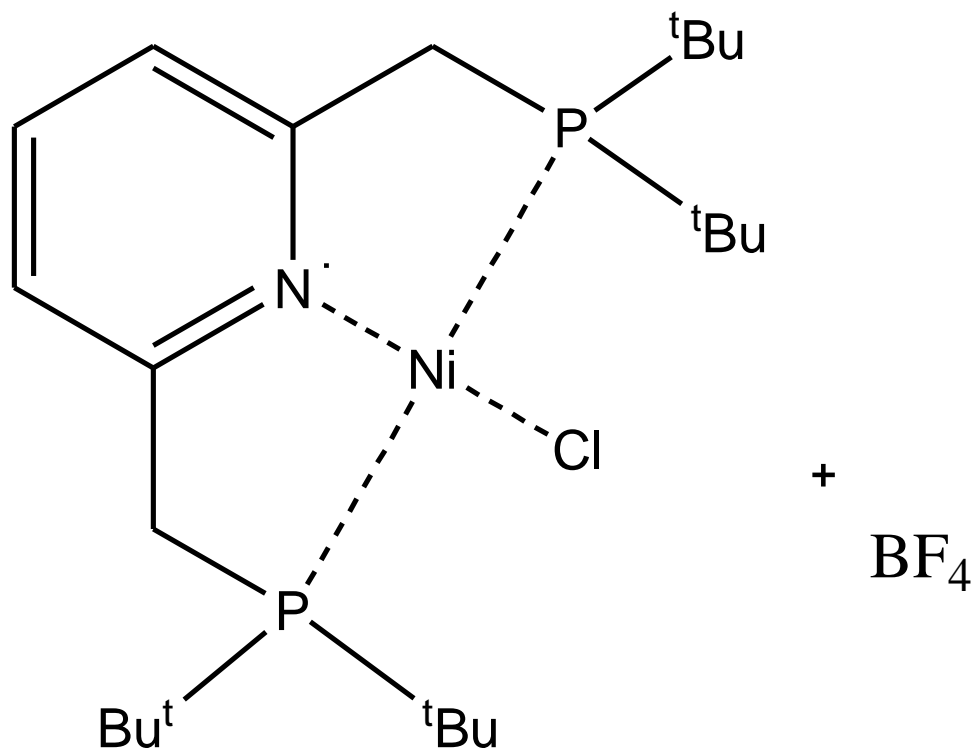
[Advanced Search](#) ☒ Always Show

物质检索——结构

The image shows the SciFinder Structure Editor window with various toolbars and panels. Labels in Chinese boxes point to specific features:

- 橡皮** (Eraser): Points to the eraser icon in the top toolbar.
- 结构和反应切换功能** (Structure and reaction switching function): Points to the 'Structure' and 'Reaction' radio buttons in the 'Drawing Editor' panel.
- 铅笔** (Pencil): Points to the pencil icon in the top toolbar.
- 元素周期表** (Periodic table): Points to the 'Atom' button in the left toolbar.
- 可变基团** (Variable group): Points to the 'Short' button in the left toolbar.
- 重复基团工具** (Repeat group tool): Points to the 'R' button in the left toolbar.
- 碳链工具** (Carbon chain tool): Points to the '1-4' button in the left toolbar.
- 选择工具** (Select tool): Points to the selection icon in the left toolbar.
- 环锁定工具** (Ring lock tool): Points to the lock icon in the left toolbar.
- 旋转工具** (Rotate tool): Points to the rotation icon in the left toolbar.
- 正电子** (Positron): Points to the '+' button in the left toolbar.
- 负电子** (Electron): Points to the '-' button in the left toolbar.
- C原子和单键恢复工具** (C atom and single bond recovery tool): Points to the 'C' button in the bottom toolbar.
- 常用基团** (Common groups): Points to the 'Draw or change' button in the top toolbar.
- R基团定义工具** (R group definition tool): Points to the 'R' button in the left toolbar.
- 可变位置连接工具** (Variable position connection tool): Points to the '1-4' button in the left toolbar.
- 模版工具** (Template tool): Points to the template icon in the left toolbar.
- 索套选择工具** (Lasso select tool): Points to the lasso icon in the left toolbar.
- 原子锁定工具** (Atom lock tool): Points to the lock icon in the left toolbar.
- 镜面旋转工具** (Mirror rotate tool): Points to the rotation icon in the left toolbar.
- 结构检索选择** (Structure search selection): Points to the 'Exact search', 'Substructure search', and 'Similarity search' radio buttons in the 'Drawing Editor' panel.
- 单双键, RS构型, 不确定键定义工具** (Single/double bond, RS configuration, uncertain bond definition tool): Points to the bond type buttons in the bottom toolbar.
- 常见环, 多元环工具** (Common rings, polycyclic tool): Points to the ring icons in the bottom toolbar.

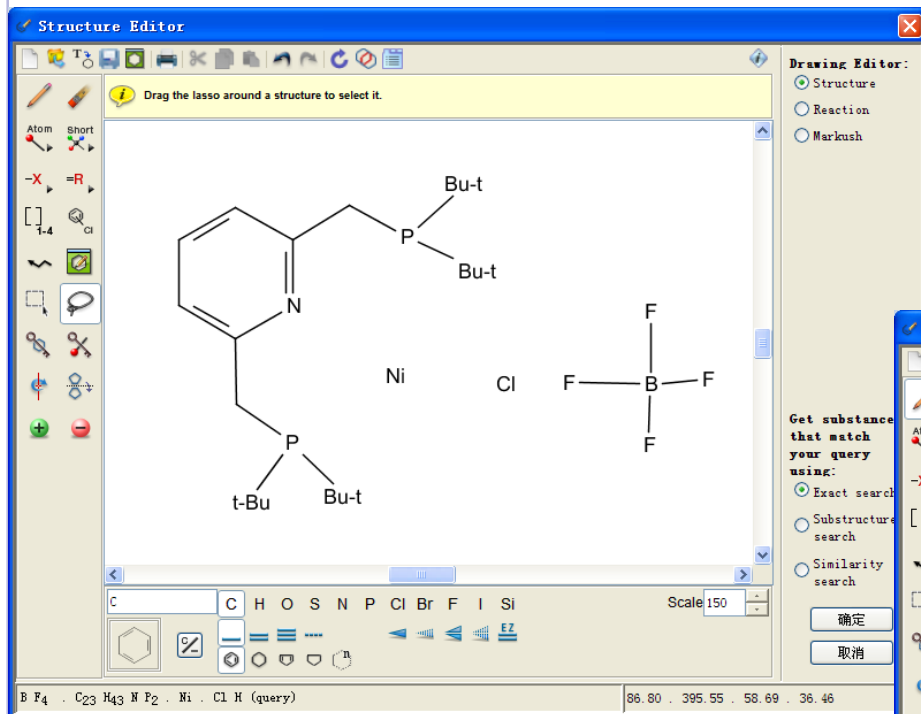
物质检索——精确结构检索



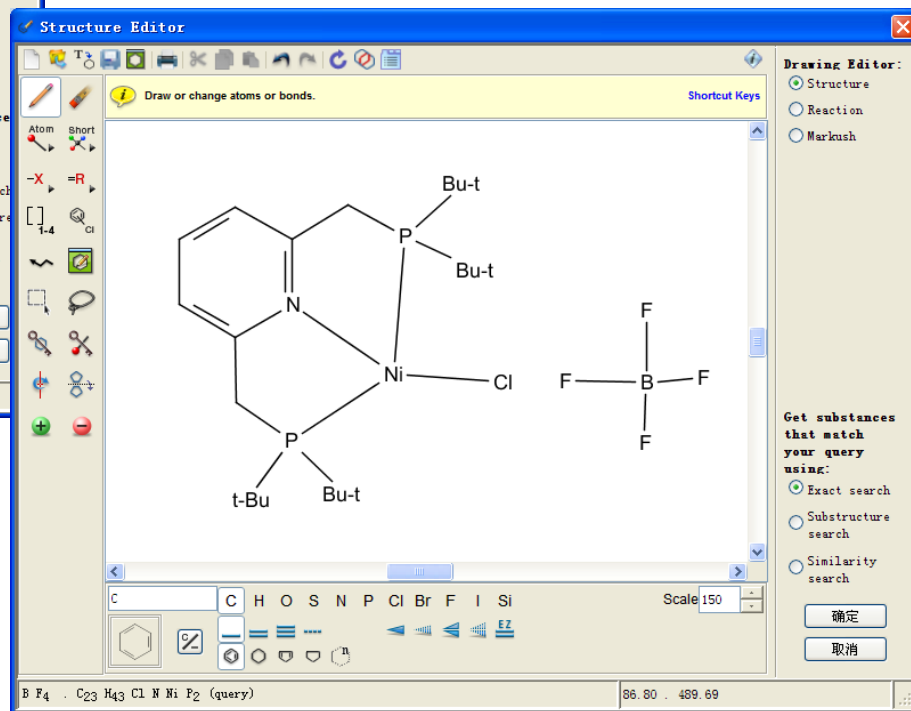
该结构中包含：

配体
金属
阳离子
阴离子

物质检索——精确结构检索



任何一种结构,使用精确结构都可以检索到



精确结构检索结果

SUBSTANCES

Get References Get Reactions Get Commercial Sources Tools

Analyze **Refine**

Analyze by:

Substance Role

Preparation 1

Properties 1

Reactant or Reagent 1

Show More

Sort by: CAS Registry Number

0 of 1 Substance Selected

1. **1136166-99-8**

~1

1136166-98-7
C₂₃ H₄₃ Cl N Ni P₂

14874-70-5
B F₄

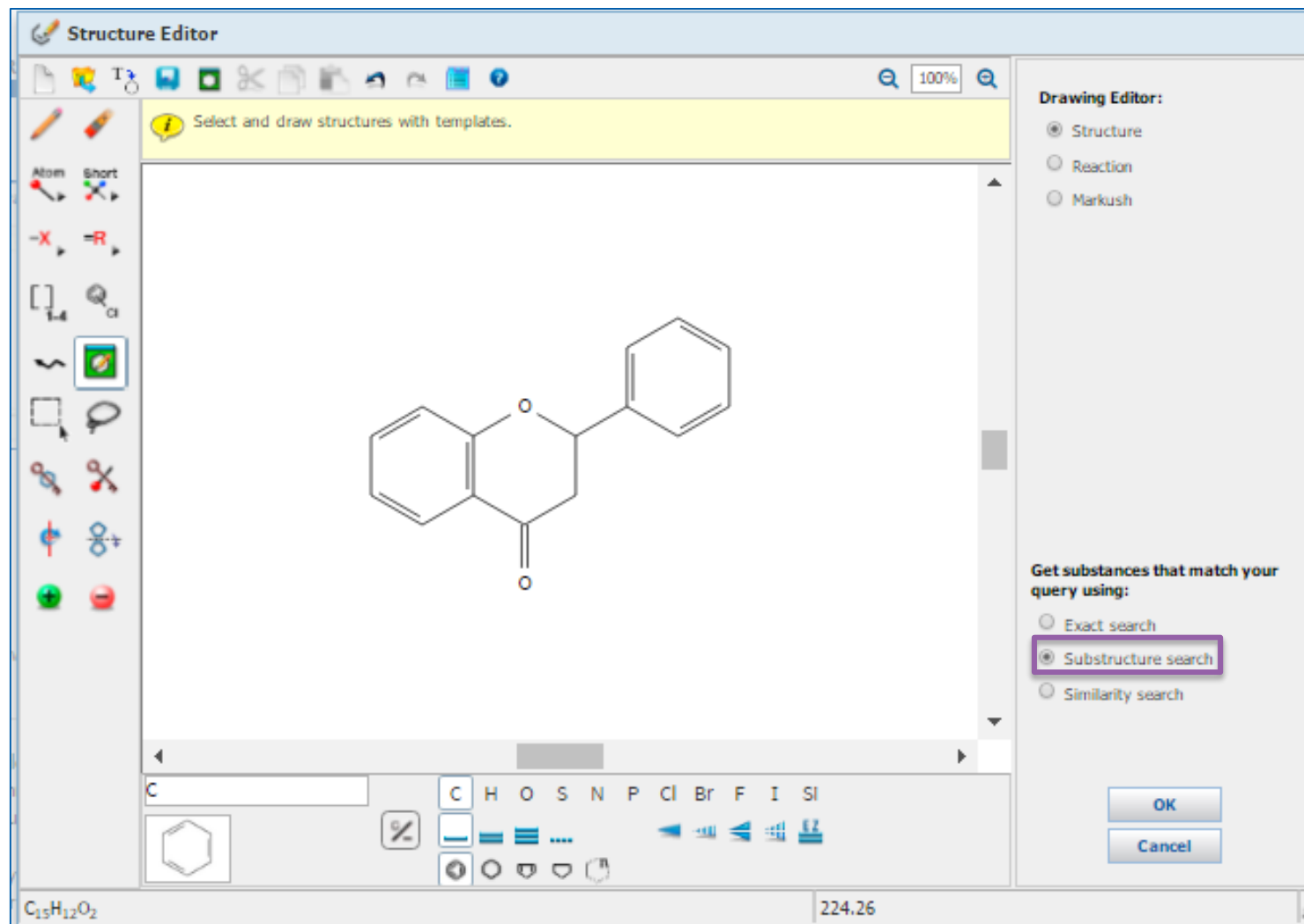
C₂₃ H₄₃ Cl N Ni P₂ · B F₄
 Nickel(1+), [2,6-bis[[bis(1,1-dimethylethyl)phosphino-κP]methyl]pyridine-κN]chloro-, (5P-4-3)-, tetrafluoroborate(1-) (1:1)

物质检索——精确结构检索

- 精确结构检索：

获得被检索结构的盐，混合物，配合物，聚合物等，被检结构不能被取代

物质检索——亚结构检索



物质检索——亚结构检索

0 of 23824 Substances Selected

1. **487-26-3**

~2093 ~69

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 ~4

Absolute stereochemistry...Rotation (-).

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

▶ **Key Physical Properties**
Experimental Properties

10. **146196-91-0**

~1 ~5

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

Spectra

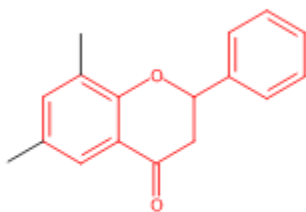
同位素

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-

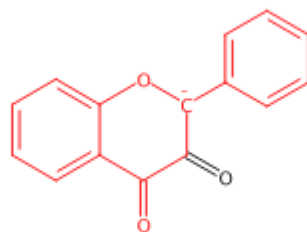
► Key Physical Properties

Experimental Properties

295. 780723-19-5

~0

离子



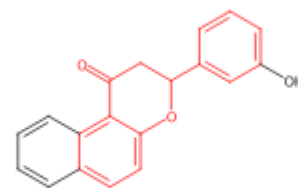
$C_{15}H_9O_3$

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

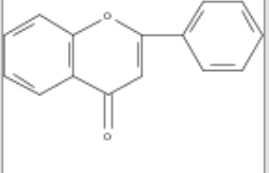
化学结构的再次限定

Analysis Refine

Refine by: ⓘ

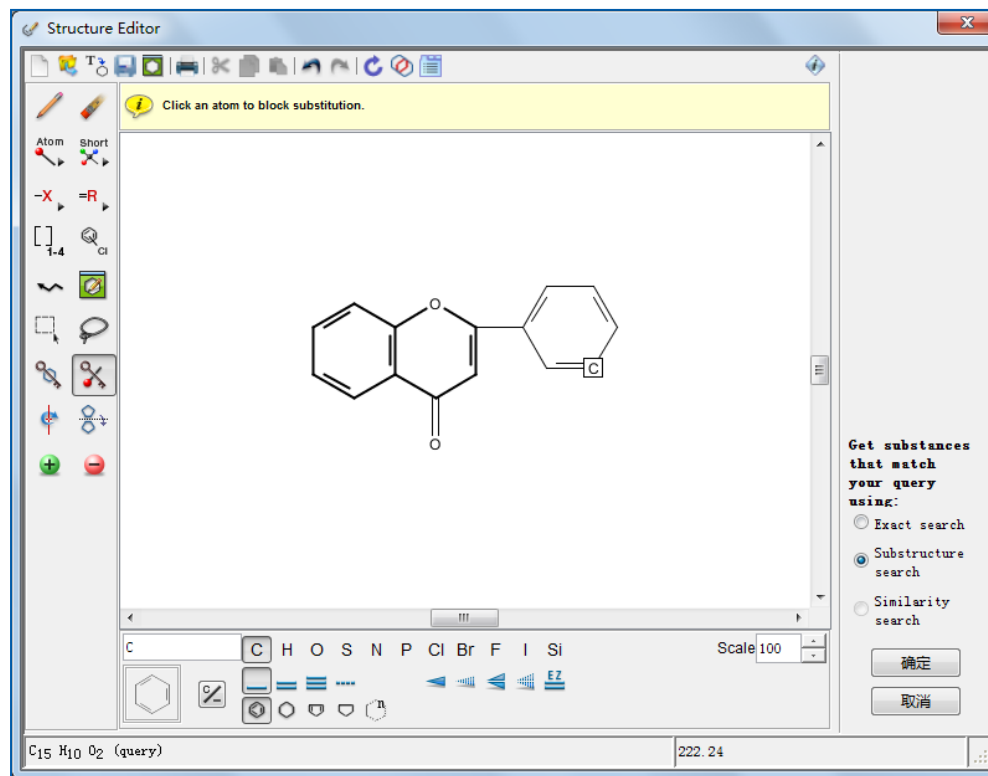
- ☒ Chemical Structure
- ☐ Isotope-Containing
- ☐ Metal-Containing
- ☐ Commercial Availability
- ☐ Property Availability
- ☐ Property Value
- ☐ Reference Availability
- ☐ Atom Attachment

Chemical Structure:



Click image to change structure or view detail

Search type: **Substructure**



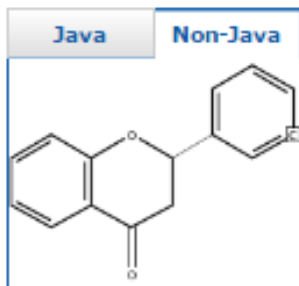
环锁定



原子锁定

亚结构检索结果的限定

Structure Editor:



Click image to change structure or view detail.

Search type: **Substructure**

Only retrieve substances that:

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

Refine

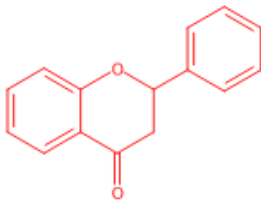
Get References Get Reactions Get Commercial Sources Tools

Sort by: Relevance

0 of 13826 Substances Selected

1. 487-26-3

~2093

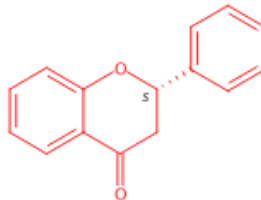


C₁₅H₁₂O₂
4H-1-Benzopyran-4-one, 2,3-dihydro-2-phenyl-

Key Physical Properties
Regulatory Information
Spectra
Experimental Properties

2. 17002-31-2

~244



Absolute stereochemistry., Rotation (-).

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

Key Physical Properties
Experimental Properties

4. 104550-32-5

~3

5. 75524-43-5

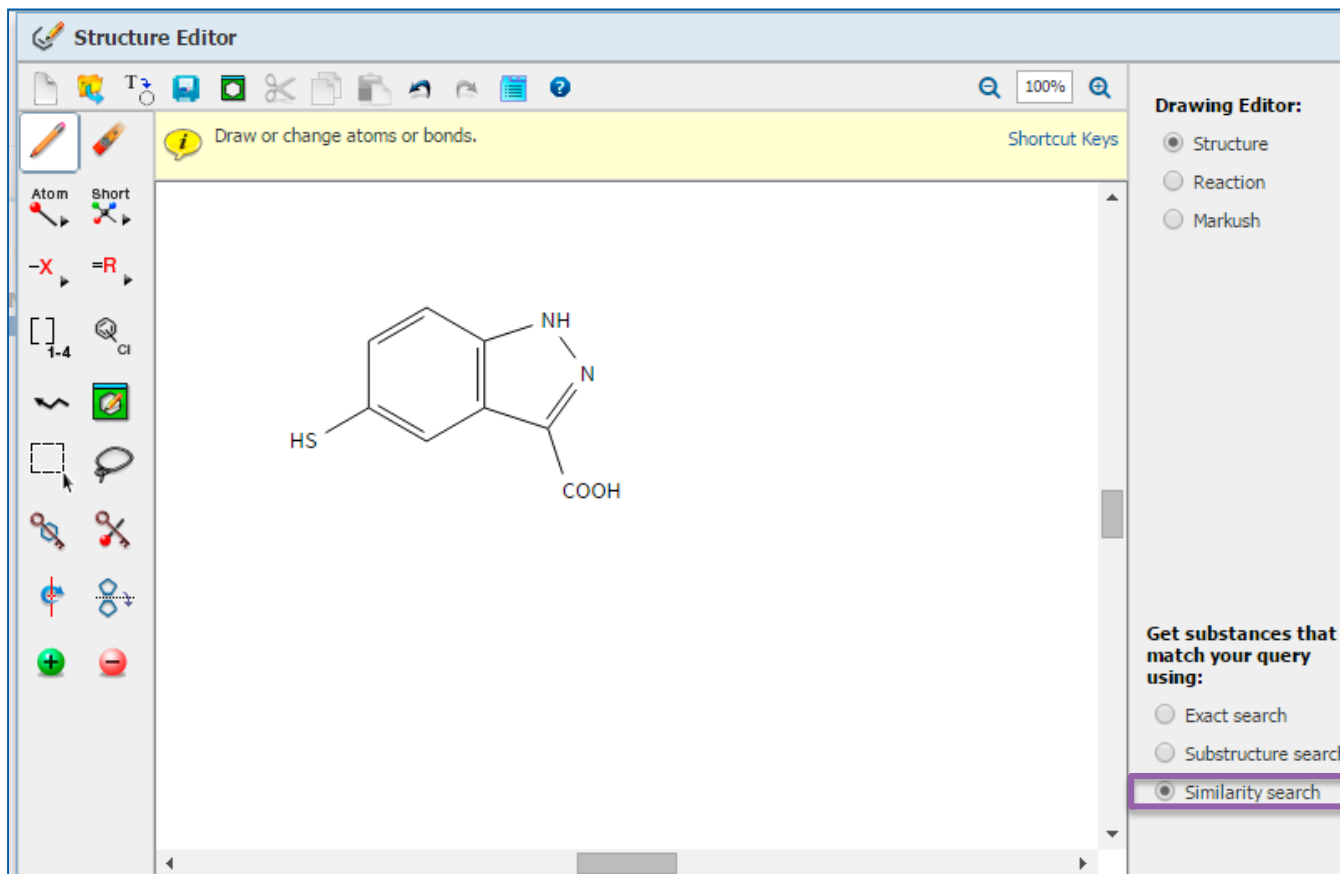
~2

物质检索——亚结构检索

- 亚结构检索：

包括精确结构检索结果，及被检索结构的修饰结构

物质检索——相似结构检索



相似结构检索结果

Select All Deselect All

0 of 6 Similarity Candidates Selected

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

Get Substances

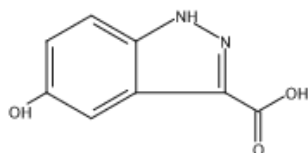
评分越高，相似度越高，结构越相似

Score: 88

☐ 1. 885518-94-5

取代基变化

~1 ~35



$C_8H_6N_2O_3$

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

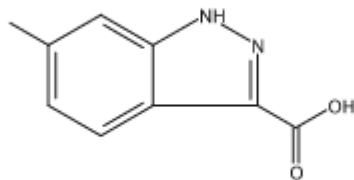
► Key Physical Properties

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-

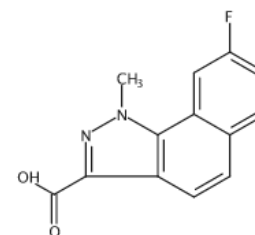
► Key Physical Properties

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

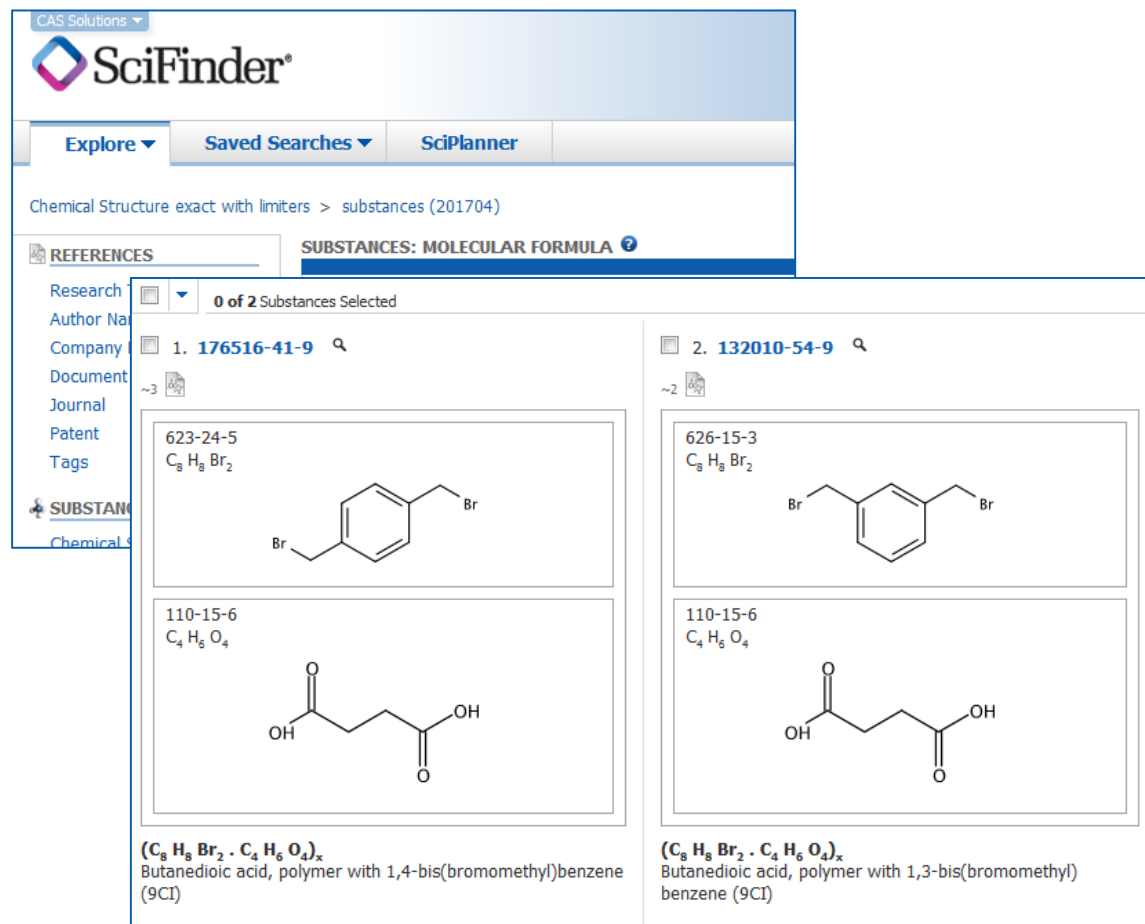
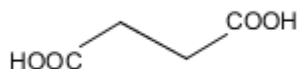
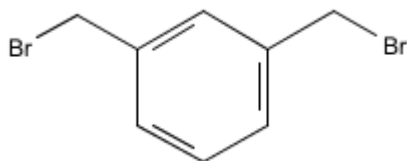
物质检索——相似结构检索

- 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



CAS Solutions
SciFinder®

Explore ▾ Saved Searches ▾ SciPlanner

Chemical Structure exact with limiters > substances (201704)

REFERENCES SUBSTANCES: MOLECULAR FORMULA ?

0 of 2 Substances Selected

1. 176516-41-9

2. 132010-54-9

623-24-5
 $C_8 H_8 Br_2$

626-15-3
 $C_8 H_8 Br_2$

110-15-6
 $C_4 H_6 O_4$

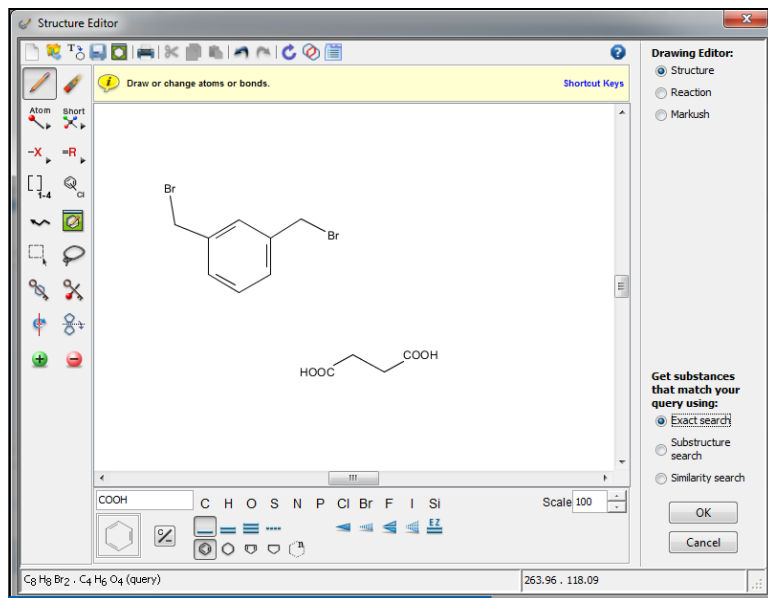
110-15-6
 $C_4 H_6 O_4$

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

$(C_8 H_8 Br_2 \cdot C_4 H_6 O_4)_x$
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 | <input checked="" type="checkbox"/> Single component
<input type="checkbox"/> Commercially available
<input type="checkbox"/> Included in references |
| Classes | <input type="checkbox"/> Alloys
<input type="checkbox"/> Coordination compounds
<input type="checkbox"/> Incompletely defined
<input type="checkbox"/> Mixtures
<input checked="" type="checkbox"/> Polymers
<input type="checkbox"/> Organics, and others not listed |
| Studies | <input type="checkbox"/> Analytical
<input type="checkbox"/> Biological
<input type="checkbox"/> Preparation
<input type="checkbox"/> Reactant or reagent |

单一组分

聚合物

0 of 1 Substance Selected

1. **132010-54-9** 🔍

~2

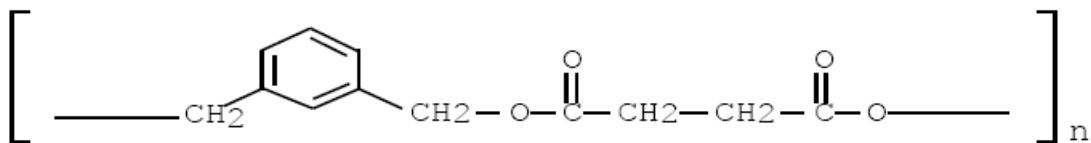
626-15-3
C₈ H₈ Br₂

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[®] interface showing search results for the molecular formula (C₁₂ H₁₂ O₄)_n. The results list includes:

- 1. 1801551-81-4
- 2. 1637772-98-5
- 3. 1421756-46-8
- 4. 1392419-56-5
- 5. 1353713-96-8
- 6. 1341223-97-9

Substance 3 (1421756-46-8) detail view shows the chemical structure and the text: "Substance Image Cannot Be Displayed 1421756-46-8".

聚合物的检索

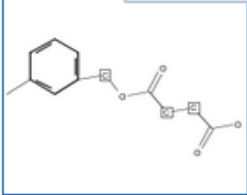
Analyze Refine

Refine by: ?

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

Structure Editor:

Java Non-Java

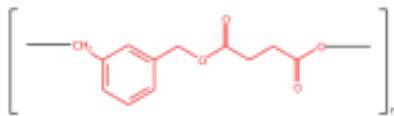


Click image to change structure or view detail.
Search type: **Substructure**

0 of 1 Substance Selected

1. 132010-11-8

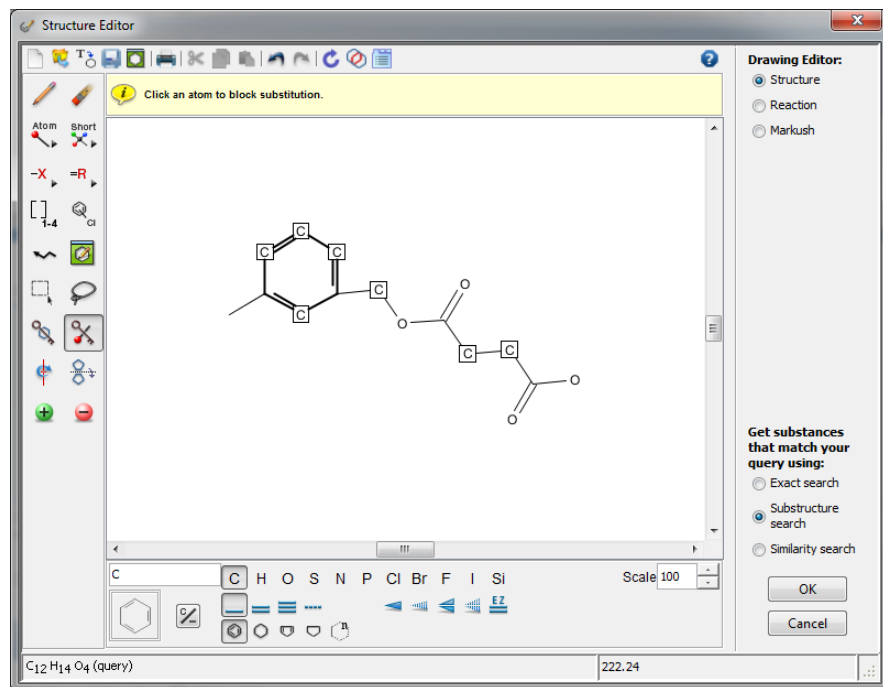
~2



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

利用结构特征进行Refine，迅速查找需要的物质

聚合物检索



绘制好SRU后用亚结构检索
因为两段为开放状态

- Characteristics
- ☒ 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

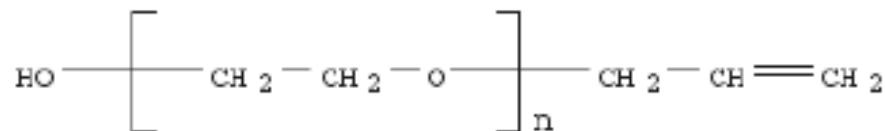
1. 132010-11-8

~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

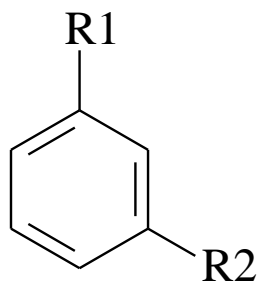
$(\text{C}_2 \text{ H}_4 \text{ O})_n \text{ C}_3 \text{ H}_6 \text{ O}$
Poly(oxy-1,2-ethanediyl), α-2-propen-1-yl-ω-hydroxy-
Regulatory Information

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
 - Markush检索
 - 反应检索 (MethodsNow Synthesis)
 - SciPlanner
 - MethodsNow Analysis
- SciFinder常见问题及解决

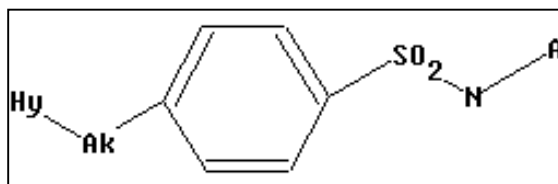
Markush检索

- 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

 **SCIFINDER**
A CAS SOLUTION

Welcome Helen Zhu

Explore ▾ Saved Searches ▾ SciPlanner Save Print Export

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

REFERENCES ⓘ

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

Analyze Refine Categorize

Sort by: Accession Number ▾

0 of 1969 References Selected

Page: 1 of 99

Analyze by: Document Type ▾

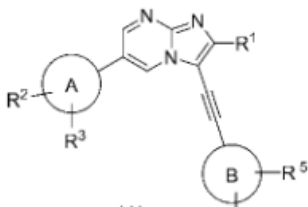
Patent 1969

Journal 1

Show More

全部是专利

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

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


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

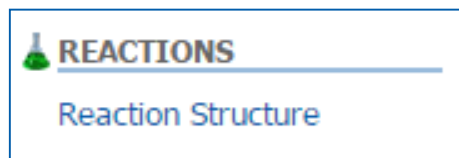
提纲

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



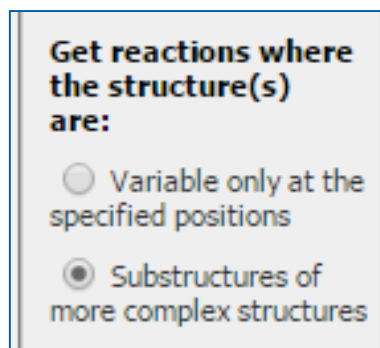
- 常用获取方法

已知物质：由物质获取反应

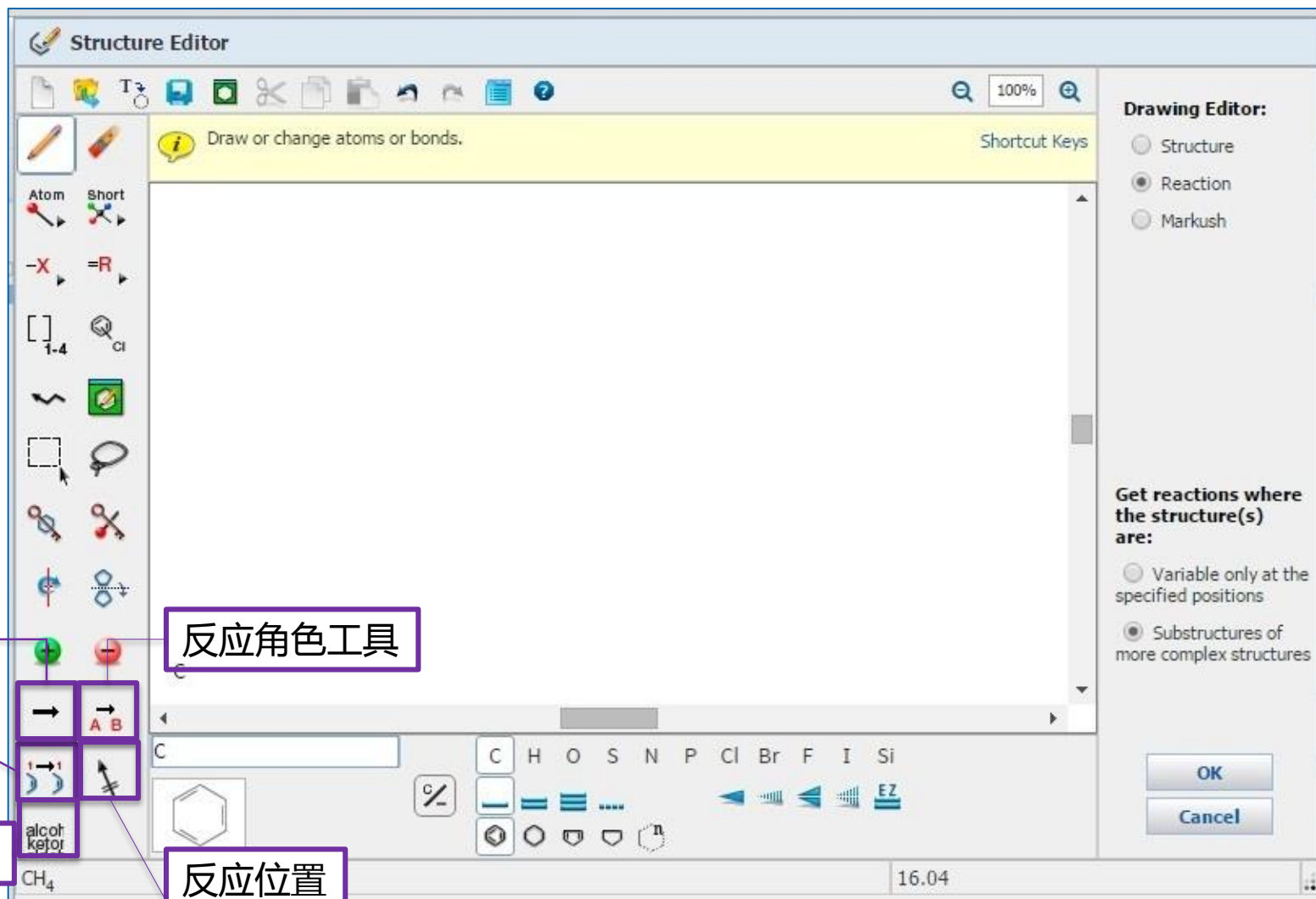
已知文献：从文献中获取反应

精确结构反应检索

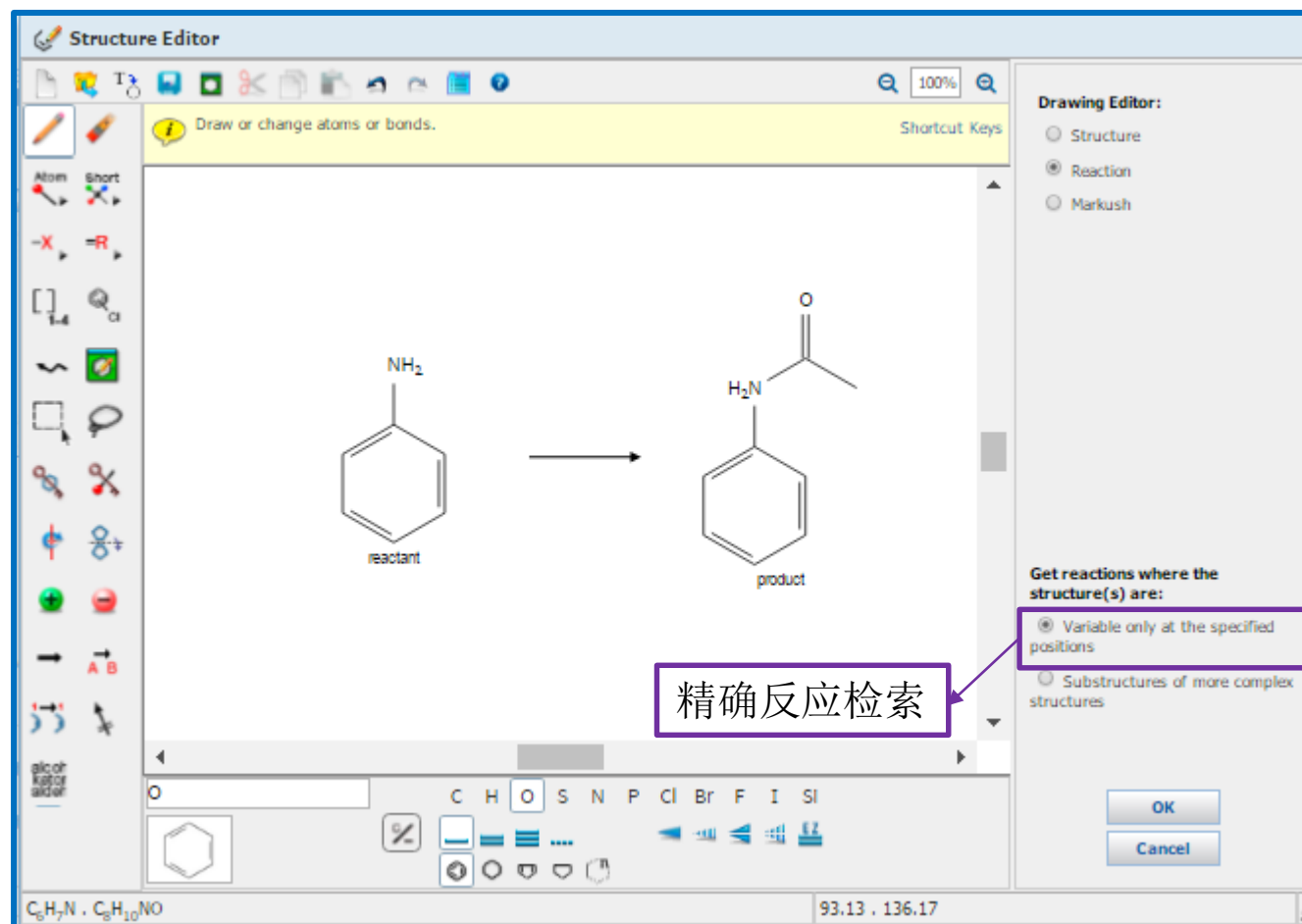
亚结构反应检索



反应绘制工具



SciFinder反应检索——精确反应检索



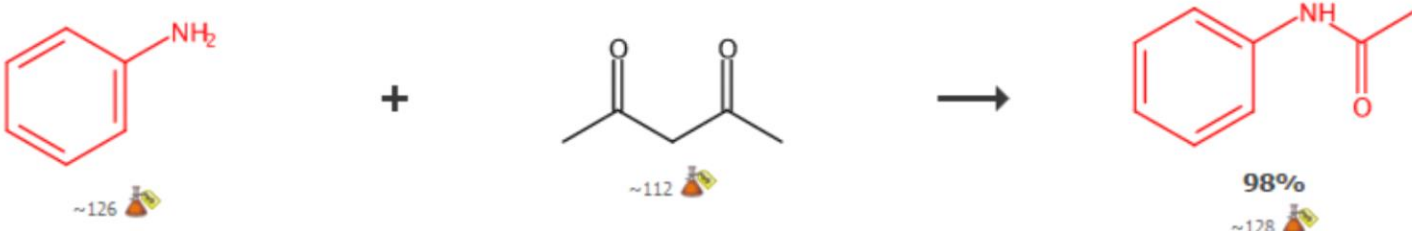
反应检索结果

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

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

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

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


~126 + ~112 → 98% ~128

Overview

Steps/Stages

1.1 R:H₂O, R:O₂, C:SiO₂ (sulfuric acid), C:H₂SO₄ (silica), 2 h, 120°C, 1 atm

Notes

green chemistry-reagent, silica supported and used, no solvent, aerobic, optimization optimized on temperature, Reactants: 2, Most stages in any one step: 1

References

获取相似反应

获取相似反应

选择相似反应的相似限制：

- Broad：仅反应中心相似
- Medium：反应中心及附属原子和键
- Narrow：反应中心及扩展的原子和键

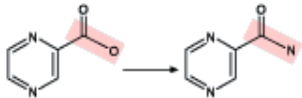
Get Similar Reactions ?

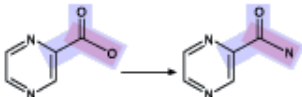
Retrieve similar reactions from:

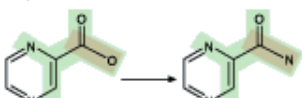
- ☒ All reactions
- ☐ Current answer set

Include this level of similarity:

- ☒ Broad - Reaction centers only (2934)


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


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



Get Reactions

Cancel

按照反应类型排序

Group by: Transformation Sort by: Frequency

0 of 605 Reactions Selected

1. Acylation of Nitrogen Nucleophiles by Anhydrides or Dicarboxates
188 Reactions

$$\text{R}-\text{C}(=\text{O})-\text{O}-\text{C}(=\text{O})-\text{R}^2 + \text{R}^1-\text{NH}-\text{R}^1 \longrightarrow \text{R}-\text{C}(=\text{O})-\text{N}(\text{R}^1)_2 + \text{R}^2-\text{C}(=\text{O})-\text{OH}$$

2. Acylation of Nitrogen Nucleophiles by Carboxylic Acids
81 Reactions

$$\text{R}-\text{C}(=\text{O})-\text{OH} + \text{R}^1-\text{NH}-\text{R}^1 \longrightarrow \text{R}-\text{C}(=\text{O})-\text{N}(\text{R}^1)_2$$

更精确的查找需要的反应

3. Acylation of Nitrogen Nucleophiles by Acyl/ Thioacyl/ Carbamoyl Halides and Analogs
55 Reactions

$$\text{R}-\text{C}(=\text{Y})-\text{X} + \text{R}^1-\text{NH}-\text{R}^1 \longrightarrow \text{R}-\text{C}(=\text{Y})-\text{N}(\text{R}^1)_2$$

Y = O, S, NR'

反应检索结果的筛选

Analyze

Refine

Analyze by: ?
Solvent ▼

H ₂ O	99
CH ₂ Cl ₂	65
MeCN	55
THF	27
PhMe	26
AcOH	25
CHCl ₃	22
DMF	15
DMSO	15
Me ₂ CO	15

Show More

Group by: No Grouping ▼ Sort by: Relevance ▼

0 of 606 Reactions Selected

1. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.

Nc1ccccc1
~126

+

CC(=O)CC(=O)C
~112

→

CC(=O)Nc1ccccc1
98%
~128

▼ Overview

Steps/Stages

1.1 R:H₂O, R:O₂, C:SiO₂ (sulfuric acid), C:H₂SO₄ (silica), 2 h, 120°C, 1 atm

Notes

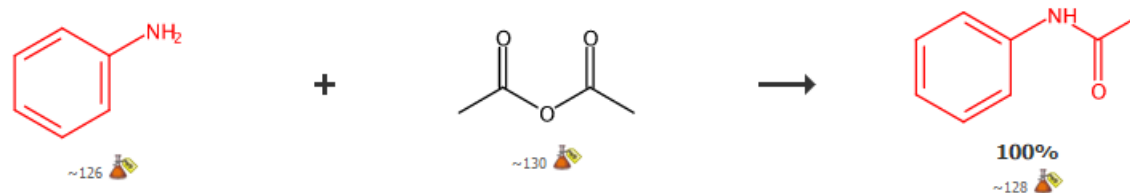
green chemistry-reagent, silica supported and used, no solvent, aerobic, optimization optimized on temperature, Reactants: 2, Most stages in any one step: 1

References

Silica sulfuric acid mediated acylation of a

筛选用水作溶剂的反应

SciFinder囊括最大的反应实验过程合集



▼ Overview

Steps/Stages

1.1 S:CH₂Cl₂, 20-120 min, rt

Notes

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

References

Indole Synthesis via Rhodium Catalyzed Oxidative Coupling of Acetanilides and Internal Alkynes

Quick View Other Sources

By Stuart, David R. et al

From Journal of the American Chemical Society, 130(49), 16474-16475; 2008

不用阅读全文，直接获得包含
实验过程的反应记录

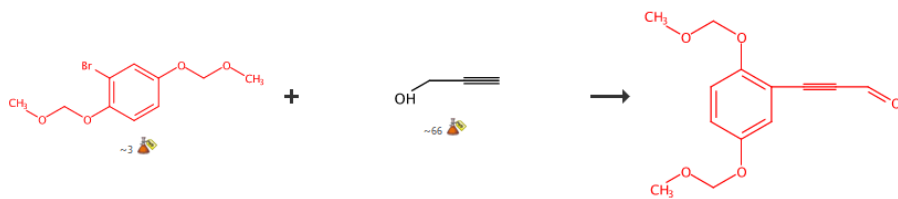
▼ Experimental Procedure



Representative procedure for the preparation of acetanilides: Aniline (10.1 mL, 109.7 mmol, 1 eq) was added to a round-bottom flask via syringe and fitted with a rubber septum. The flask was purged with argon and dry DCM (300 mL, 0.4 M) was added. Acetic anhydride (12.5 mL, 132.2 mmol, 1.2 eq) was added and the reaction was stirred at room temperature and monitored by TLC. Upon completion (generally a couple of hours, but as short as 20 minutes) the reaction mixture was washed with a saturated solution of sodium carbonate, the organic layers dried with MgSO₄ and the solvent removed under reduced pressure. The product was obtained in quantitative yield (14.8 g). In most cases analytically pure acetanilides can be obtained after extraction however if necessary purification by flash chromatography with ethyl acetate/pet. ether was used (see below for specific conditions). **Acetanilide (1a):** The above procedure was followed to afford the product in quantitative yield. This compound can also be purchased from commercial sources (CAS: 103-84-4). ¹H NMR (400 MHz, CDCl₃, 293 K): δ 7.50 (d, J = 7.8 Hz, 2H), 7.32 (t, J = 7.9 Hz, 2H), 7.10 (t, J = 7.4 Hz, 1H), 2.17 (s, 3H). The signal for the exchangeable NH does not appear in the spectrum.

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, R: 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

Notes

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

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?
- 去免费的Supporting Information查? 可能只有图谱。

Experimental Procedure

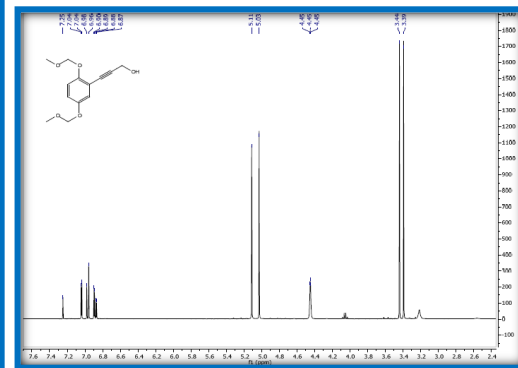
NATURAL
PRODUCTS

Step 1

General Procedure for the Sonogashira Coupling.^{8,10,11} Compounds **6a**³¹ 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 (**8**). 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, s, H-1a), 5.09 (2H, s, H-4a), 5.17 (2H, s, H-1a), 6.95 (1H, dd, *J* = 9 and 3.0 Hz, H-5), 7.03 (1H, d, *J* = 9.0 Hz, H-6), 7.10 (1H, d, *J* = 3.0 Hz, H-3); 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 C₁₃H₁₆O₅ 275.0896).

Step 2

Generation of the Key Aldehyde.¹⁷ Oxalyl chloride (272.3 μ L, 3.12 mmol) in dry CH₂Cl₂ (9 mL) was added to a stirred solution of DMSO (332 μ L, 4.68 mmol) in dry CH₂Cl₂ (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 CH₂Cl₂ (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), Et₃N (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 NH₄Cl and H₂O, and the mixture was stirred for 30 min. The organic phase was decanted off, and the aqueous layer was extracted with CH₂Cl₂ (3 × 30 mL). The combined organic layers were washed with brine, dried over anhydrous Na₂SO₄, 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 (CDCl₃, 400 MHz) δ 3.46 (3H, s, H-4b), 3.51 (3H, s, H-1b), 5.10 (2H, s, H-4a), 5.21 (2H, s, H-1a), 7.09 (1H, dd, *J* = 9.2 and 1.2 Hz, H-6), 7.12 (1H, dd, *J* = 9.1 and 2.2 Hz, H-5), 7.22 (1H, dd, *J* = 2.2 and 1.3 Hz, H-3), 9.44 (1H, s, H-9); ¹³C NMR (CDCl₃, 100 MHz) δ 56.18 (C-4b), 56.54 (C-1b), 92.05 (C-8), 92.27 (C-7), 95.22 (C-4a), 95.88 (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 C₁₃H₁₄O₅ 273.0739).



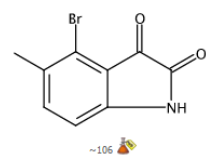
MethodsNow Synthesis

MethodsNow

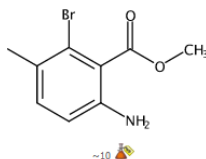
A New Method for Synthesis of Nolatrexed Dihydrochloride

By Zhao, Xueqing; Li, Fei; Zhuang, Weiping; Xue, Xiaowen; Lian, Yuanyang; Fan, Jianhui; Fang, Dongsheng
From Organic Process Research & Development, 14(2), 346-350; 2010
Published by American Chemical Society

Reaction Steps **1** **2** **3**



+



Products	Benzoic acid, 6-amino-2-bromo-3-methyl-, methyl ester, 84%, CAS RN: 147149-88-0
Reactants	1H-Indole-2,3-dione, 4-bromo-5-methyl-, CAS RN: 147149-84-6 Methanol, CAS RN: 67-56-1
Reagents	Potassium persulfate, CAS RN: 7727-21-1 Sodium methoxide, CAS RN: 124-41-4 Hydrochloric acid, CAS RN: 7647-01-0 Sodium dithionite, CAS RN: 7775-14-6
Solvents	Methanol, CAS RN: 67-56-1 Water, CAS RN: 7732-18-5
Procedure	<ol style="list-style-type: none"> 1. Add sodium methoxide (22.6%, 4.80 kg, 20.1 mol) to a mixture of 4-bromo-5-methylisatin (6.67 mol) and anhydrous methanol (6.70 L). 2. Add K₂S₂O₈ (1.90 kg, 7.03 mol) to the mixture in parts 10°C with an ice-water bath. 3. After addition the reactant mixture turns yellow, continue the stirring for 1 hour at room temperature. 4. Adjust the reaction mixture to pH 8-9 with aqueous 36% HCl (1.24 L) 15 °C. 5. Destroy the excessive K₂S₂O₈ by aqueous 5% Na₂S₂O₄ solution (450 mL). 6. After rotary evaporation under a reduced pressure at 55 °C, Leave a brown liquid. 7. Mix the mixture with CH₂Cl₂ (6 L) and H₂O (4 L). 8. Separate the organic phase. 9. Extract the aqueous phase with CH₂Cl₂ (4 L). 10. Dry the combined organic phases over Na₂SO₄. 11. Concentrate the combined organic phases with a rotavapor. 12. Distill the resulted brown liquid under high vacuum.
Scale	milligram
¹H NMR	CDCl ₃ : δ 2.28 (s, 3 H, Ar-CH ₃), 3.91 (s, 3 H, -OCH ₃), 4.26 (br s, 2 H, NH ₂), 6.54 (d, J = 8.2 Hz, 1 H, Ar-H), 7.00 (d, J = 8.2 Hz, 1 H, Ar-H).
IR	KBr cm ⁻¹ : 3472, 3382, 2953, 2924, 1716, 1622, 1480, 1277, 816.

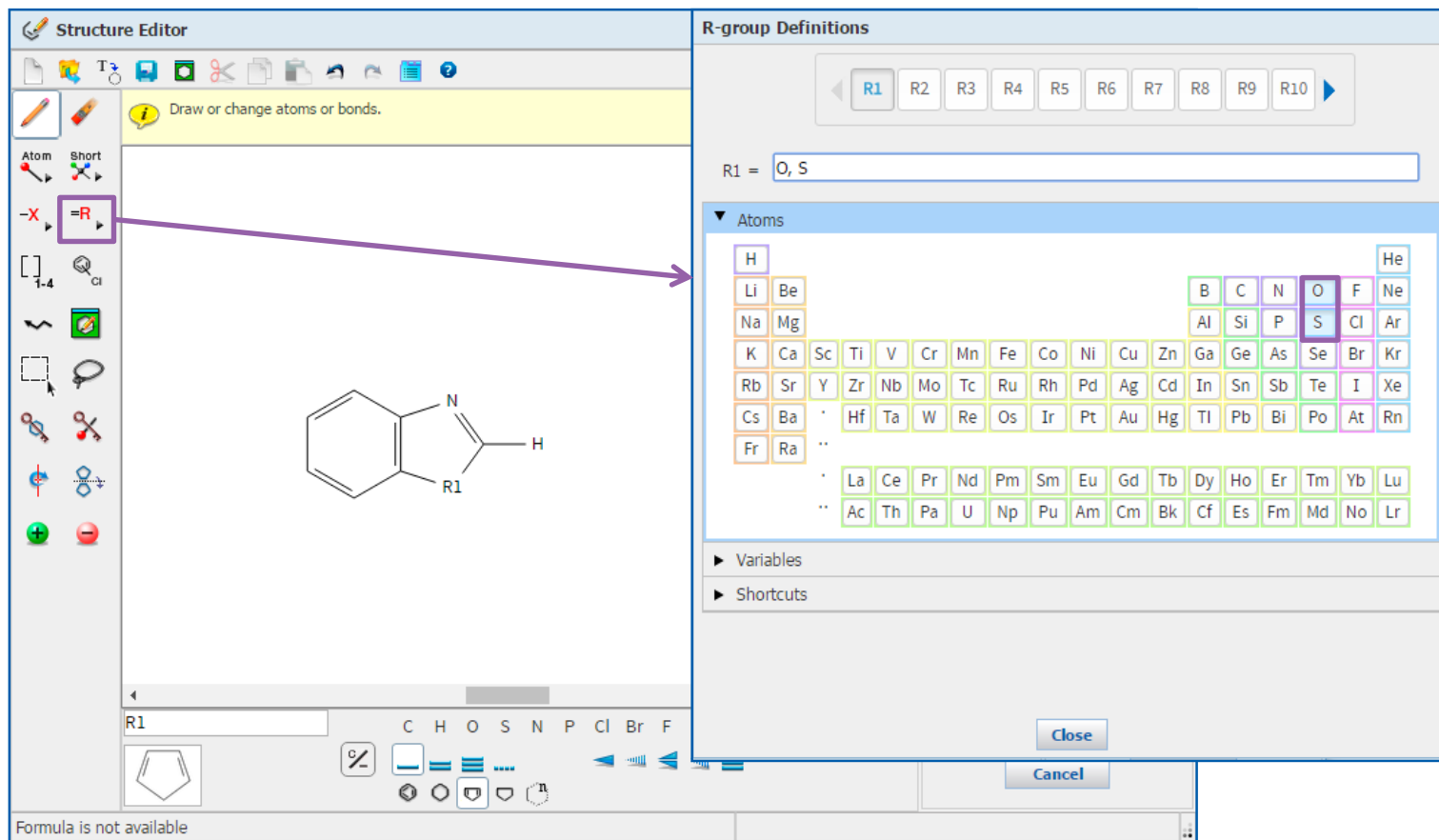
物质信息

实验过程

图谱信息

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

Chemical Reaction:

Reactant: A benzimidazole ring with a substituent R1 and a hydrogen atom (H) attached to the nitrogen atom.

Product: A benzimidazole ring with a substituent R1 and a carbon chain (Ak) attached to the nitrogen atom.

Formulas:

Reactant: C1=NC2=CC=CC=C2N1C(R1)=C

Product: C1=NC2=CC=CC=C2N1C(R1)=CAk

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 Sort by: Accession Number

☐ No Grouping
☒ Document
☐ Transformation

1. **View Reaction Detail** **Similar Reactions**

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

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

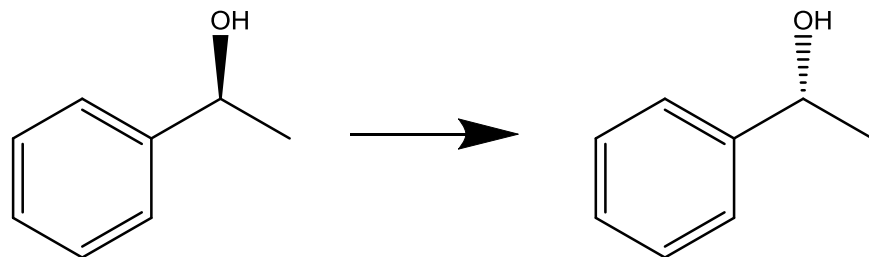
Notes

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



1. View Reaction Detail [Link](#)

Single Step Hover over any structure for more options.



6. View Reaction Detail [Link](#)

Single Step Hover over any structure for more options.



4. View Reaction Detail [Link](#)

Single Step Hover over any structure for more options.



94. View Reaction Detail [Link](#)

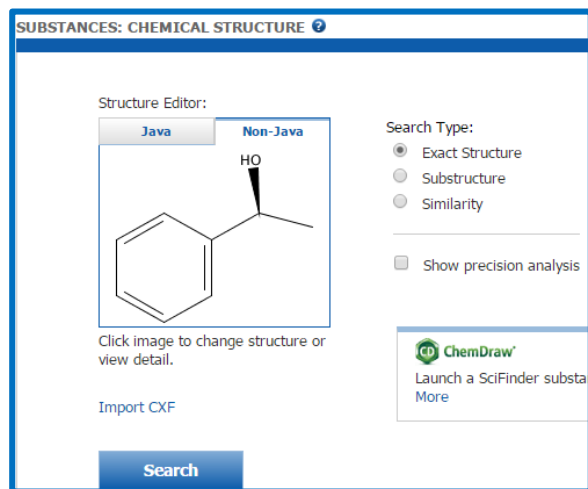
Single Step Hover over any structure for more options.



案例：如何获取手性翻转反应

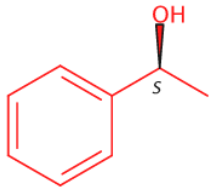
检索思路：

- 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



Absolute stereochemistry, Rotation (-).

C₉H₁₀O
Benzenemethanol, α-methyl-, (αS)-

► 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

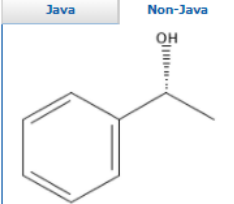
检索思路：

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

SUBSTANCES: CHEMICAL STRUCTURE

Structure Editor:

Java Non-Java



Click image to change structure or view detail.

Import CXF

Search

Search Type:

- ☒ Exact Structure
- ☐ Substructure
- ☐ Similarity

☐ Show precision analysis

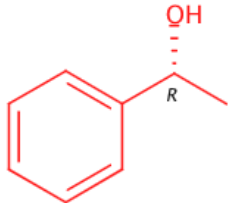
ChemDraw

Launch a SciFinder substance

1 of 54 Substances Selected

1. 1517-69-7

~3531 ~94



Absolute stereochemistry, Rotation (+).

C₈H₁₀O
Benzenemethanol, α-methyl-, (αR)-

Key Physical 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** Send to SciPlanner

Group by: No Group

0 of 79

1. View Reaction Set

4 Steps Hover over any structure for more options.

Chemical structures: NC(=O)C, CC(=O)C, CC1(C)CC1, NC1(C)CC1, C/C=C/C(O)C

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

反应检索结果集

Get References

Tools ▾

Send to SciPlanner

Group by: No Grouping ▾ Sort by: Accession Number ▾

Display Options

0 of 27 Reactions Selected

Page: 1 of 2

1. View Reaction Detail Link

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



Overview

Steps/Stages

1.1 S:H₂O, S:M , 360 h, 30°C



Notes

biotransformation, ee=92%, resting cells of the yeast *C. albicans* used, stereoselective, Reactants: 1, Solvents: 2, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Deracemization of 1-phenylethanol via tandem biocatalytic oxidation and reduction

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)

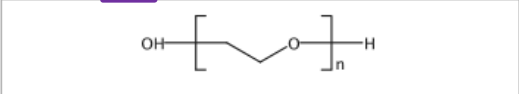
Get References Get Reactions Get Commercial Sources Tools ▾

Sort by: CAS Registry Number ▾

☐ 0 of 1 Substance Selected

☐ 1. **25322-68-3** 🔍

~233271   ~437 



(C₂ H₄ O)_n H₂ O
Poly(oxy-1,2-ethanediyl), α-hydro-ω-hydroxy-

▶ **Key Physical Properties**

- Regulatory Information
- Spectra
- Experimental Properties

从物质获取反应信息：获取聚乙二醇作为反应物的反应

Sample Analysis: [?](#)

Reagent ▼

HOCH 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](#)

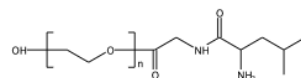
0 of 39274 Reactions Selected
Page: 1 of 2619

☐ 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.*



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 interface for refining reaction structures. The main window is the "Structure Editor", which shows the chemical structure of methyl methacrylate (MMA) as the reactant. The left sidebar contains a "REFINEMENT" panel with a "Refine by:" dropdown menu. The "Reaction Structure" option is selected and highlighted with a red box. Below this, other refinement options like "Product Yield", "Number of Steps", "Reaction Classification", "Excluding Reaction Classification", and "Non-participating functional groups" are listed. The "Structure Editor" panel at the bottom left shows the MMA structure. The right sidebar contains a "Get reactions where the structure(s) are:" section with two radio buttons: "Variable only at the specified positions" (selected) and "Substructures of more complex structures". The "OK" and "Cancel" buttons are at the bottom right. 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 *Hover over any structure for more options.*

MMA封端的PEG

3. View Reaction Detail

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

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 (PatentPak)
 - 物质检索
 - Markush检索
 - 反应检索 (MethodsNow Synthesis)
 - SciPlanner
 - MethodsNow Analysis
- 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

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.

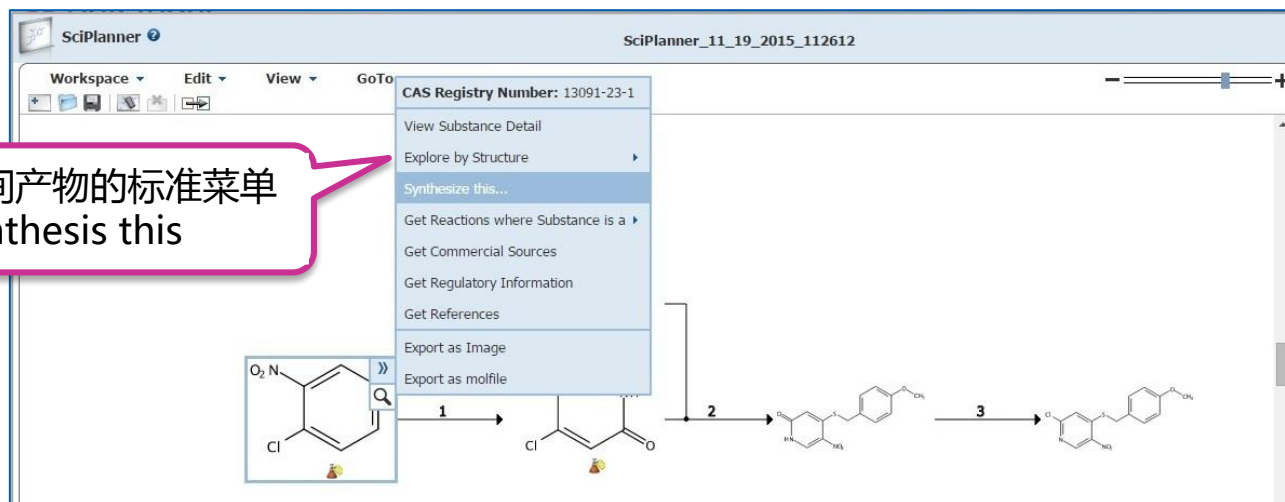
Notes
Reactants: 2, Reagents: 5, Solvents: 1, Steps: 3, Stages: 3, Most stages in any one step: 1

References
Syntheses of 4- and 6-substituted thiazolo[4,5-c]pyridines
Quick View [Other](#)
By Huang, Yuhua et al

Clear Reactions

SciPlanner使用简介

打开中间产物的标准菜单
选择Synthesize this

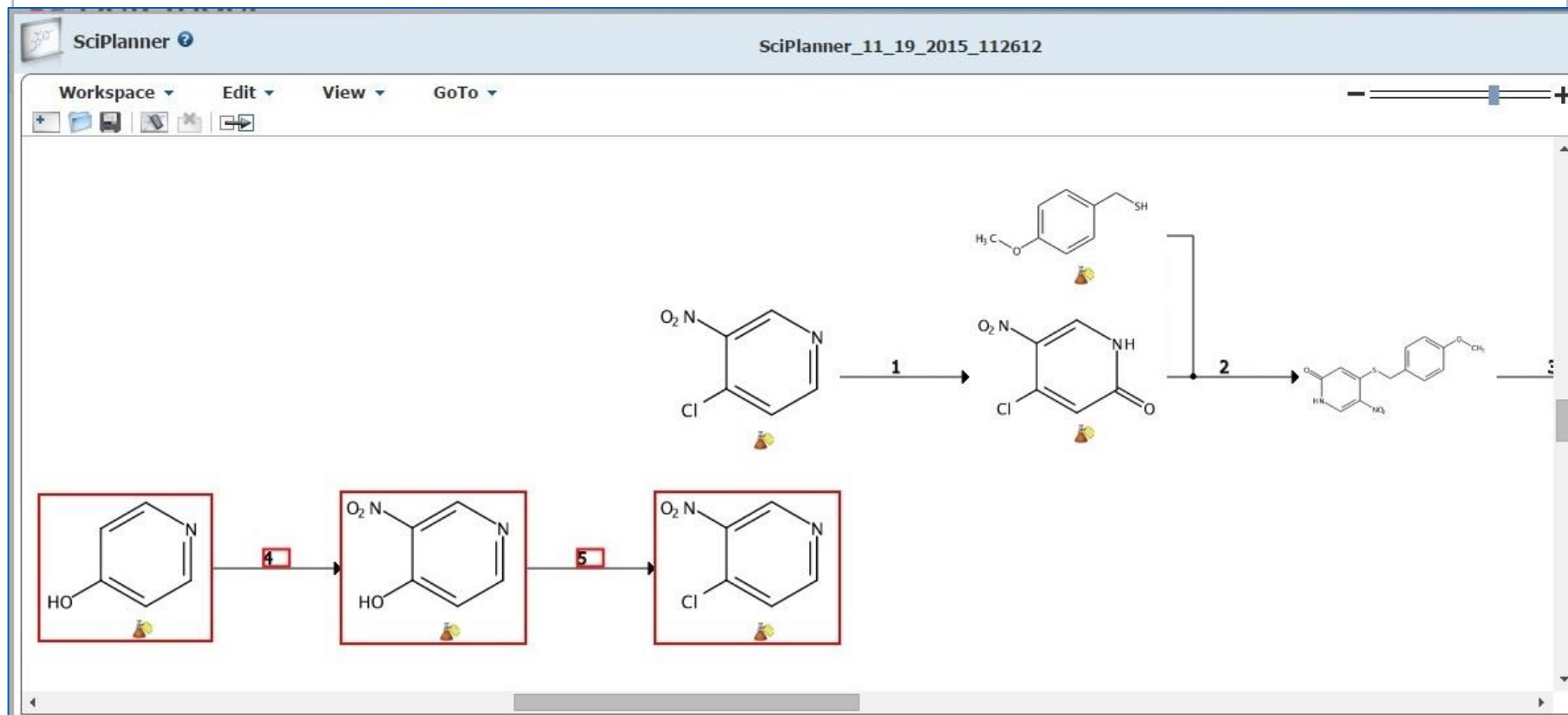


在检索到的反应中选择感兴趣的反应

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

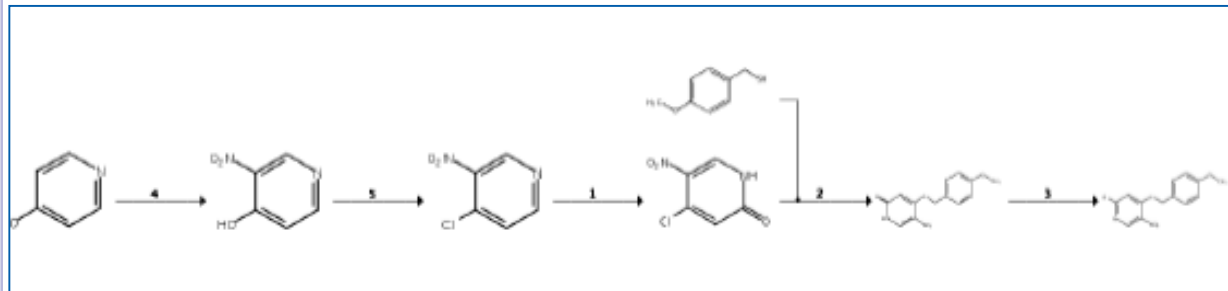
Title

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		
<p>1228150-22-8</p> <p>C₁₃H₁₂N₂O₄S 2(1H)-Pyridone, 4-[[4-methoxyphenyl]methyl]thio-5-nitro- Related Info: ~ 2 References Reactions</p>	<p>1228150-23-9</p> <p>C₁₃H₁₁ClN₂O₄S Pyridine, 2-chloro-4-[[4-methoxyphenyl]methyl]thio-5-nitro- Related Info: ~ 2 References Reactions</p>	<p>13091-23-1</p> <p>C₅H₃ClN₂O₂ Pyridine, 4-chloro-3-nitro- Related Info: ~ 301 References Reactions ~ 100 Commercial Sources Regulatory Information</p>
<p>5435-54-1</p> <p>C₅H₄N₂O₃ 4-Pyridinol, 3-nitro- Related Info: ~ 113 References Reactions ~ 197 Commercial Sources Regulatory Information</p>	<p>6258-60-2</p> <p>C₈H₁₀O S Benzenemethanethiol, 4-methoxy- Related Info: ~ 749 References Reactions ~ 71 Commercial Sources Regulatory Information</p>	<p>626-64-2</p> <p>C₅H₅N O 4-Pyridinol Related Info: ~ 1351 References Reactions ~ 160 Commercial Sources Regulatory Information</p>
<p>850663-54-6</p> <p>C₁₃H₉ClN₂O₄ 2(1H)-Pyridone, 4-chloro-5-nitro- Related Info: ~ 22 References Reactions ~ 136 Commercial Sources</p>		

提纲

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

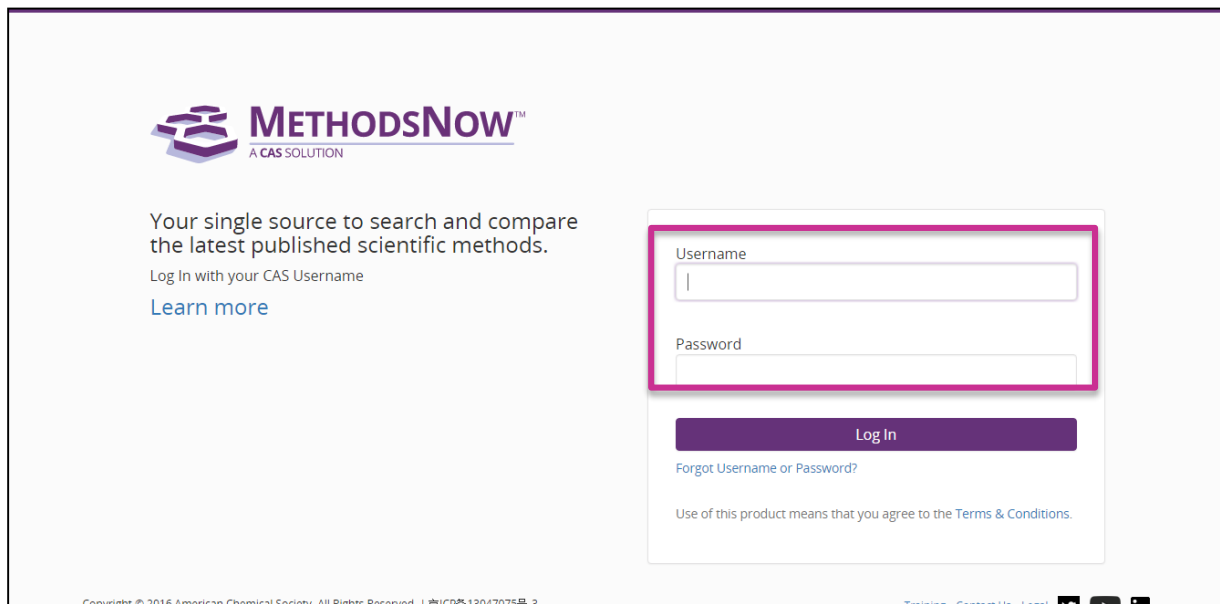


MethodsNow – Analysis(www.methodsnow.com)

- 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

MethodsNow – Analysis(www.methodsnow.com)



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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 bubble points to the 'Saved' link with the text '保存结果集'. Below the search section is a 'Browse Method Categories' section with a grid of category links. A callout bubble points to the 'Organic Compound Analysis' link with the text '点击一个类别 浏览相关方法'. Below the categories is a 'Recent Searches' section with a list of search terms. A callout bubble points to the 'hplc lycopene analysis' entry with the text '点击历史检索 重新运行检索'. Another callout bubble points to the 'X' icon next to the search entry with the text '点击“X” 删除检索历史'.

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 shows 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 explain the functionality of various elements.

Annotations:


- 逻辑运算符：and, or, not (Logical operators: and, or, not)
- 删除检索条件 (Delete search criteria)
- 增加检索条件 (Add search criteria)
- 检索选项：关键词、分析物、基质、方法分类、技术、CAS Method Number、期刊名 (Search options: Keyword, Analyte, Matrix, Method Category, Technique, CAS Method Number, Journal Name)



Interface Elements:

- CAS Solutions
- METHODSNow™ A CAS SOLUTION
- Return to Home
- Advanced Search
- Keyword
- AND
- Matrix
- AND
- Analyte
- Add Search Criteria
- Search Button
- Publication Name
- Keyword
- Analyte
- Matrix
- Method Category
- Technique
- CAS Method Number
- Publication Name
- Saved
- Account

案例：高效液相色谱法测定血液中罗红霉素的含量

CAS Solutions

 **METHODSNow™**
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 Saved  Account

Search

Enter keyword, matrix, analyte, etc.

roxithromycin

Q

[Advanced Search](#)

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	

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

导出方法

保存方法

限定分析物、基质、方法等条件

查看方法详情

方法对比

Analysis of Roxithromycin in Blood plasma by HPLC-tandem mass spectrometry
CAS MN: 1-101-CAS-1241367

View Details & Instructions

Add to Compare

Analyte	Roxithromycin; Ambroxol hydrochloride
Matrix	Blood plasma
Other Materials	Reagent: Methanol; Acetonitrile; Ammonium acetate; Heparin Material: C ₁₈ analytical column (150 mm x 4.6 mm, 5 μm)
Method Category	Active Pharmaceutical Ingredient and Metabolite Analysis
Technique	HPLC-tandem mass spectrometry
Equipment Used	LC-MS/MS system; LC pump; Autosampler; Triple-quadrupole tandem mass spectrometer
Source	Simultaneous determination and pharmacokinetic study of roxithromycin and ambroxol hydrochloride in human plasma by LC-MS/MS Hang, Tai-jun; Zhang, Meng; Song, Min; Shen, Jian-ping; Zhang, Yin-di Clinica Chimica Acta (2007), 382 (1-2), 20-24. Elsevier Ltd.

Document Sources

结果显示

Method Detail (2 of 5)

Analysis of Roxithromycin in Blood plasma by HPLC

CAS MN: 1-101-CAS-67878

Method Category: Active Pharmaceutical Ingredient and Metabolite Analysis

Technique: Fluorescence; HPLC

Materials	Role
Roxithromycin	analyte
Blood plasma	matrix
Column, 125 x 4.6 mm i.d. LiChrospher RP-18e	material
SPE Bakerbond cartridges, C18	material

设备条件

Equipment Used

HPLC system, HP 1100, Hewlett-Packard, Waldbronn, Germany

Autosampler, G1313A

Conditions

Chromatographic

HPLC : mobile phase : 700 ml of acetonitrile + 300 ml of a 0.05 mol/L column oven : at 40 °C, fluorescence detector excitation wavelength

实验材料

Source

Determination of roxithromycin in human plasma by HPLC with fluorescence and UV absorbance detection: Application to a pharmacokinetic study

Glowka, Franciszek K.; Karazniewicz-Lada, Marta

Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences (2007), 852 (1-2), 669 - 673. Elsevier B.V.

CODEN: JCBAAL | ISSN: 15700232 | DOI: 10.1016/j.jchromb.2007.02.022

Document Sources

Abstract

A selective HPLC method with fluorescence detection for the determination of roxithromycin (ROX) in human plasma was described. After solid-phase extraction (SPE), ROX and erythromycin (internal standard, I.S.) were derivatized by treatment with 9-fluorenylmethyl chloroformate (FMOC-Cl). Optimal resolution of fluorescence derivatives of ROX and I.S. was obtained during one anal. run using reversed phase, C₁₈ column. The mobile phase was composed of potassium dihydrogenphosphate solution, pH 7.5 and acetonitrile. Fluorescence of the compounds was measured at the maximum excitation, 255 nm and emission, 313 nm, of ROX derivatives. Validation parameters of the method were also established. After SPE, differences in recoveries of ROX and erythromycin from human plasma were observed. The linear range of the standard curve of ROX in plasma was 0.5-10.0 mg/l. The validated method was successfully applied for pharmacokinetic studies of ROX after administration of a single tablet of ROX.

Instructions

Standards Preparation

1. Prepare stock solutions of roxithromycin (ROX) and erythromycin (I.S.) with 1 g/L, each in methanol.
2. Prepare standard solutions: 5.0, 7.5, 15.0, 20.0, 50.0, 75.0 and 100.0 mg/L of ROX and 200.0 mg/L of I.S. in methanol.
3. Transfer the volume of 50 µL aliquots of the sample to a glass vial containing 0.5 mL blank human plasma.

Solid phase extraction procedure

1. Process the resulting plasma samples containing: 0.5, 0.75, 1.5, 2.0, 5.0, 7.5 and 10.0 mg/l of ROX and 20.0 mg/l of I.S. according to the SPE.
2. Add the volume of 0.5 ml of a phosphate buffer, pH 7.5 (prepared as a mixture of 85.2 ml of 1/15 M Na₂HPO₄ and 14.8 ml 1/15 M KH₂PO₄).
3. Transfer the samples into C18 SPE Bakerbond cartridges (J.T. Baker Mallinckrodt Deventer, Holland).
4. Wash the absorbed analytes with water and elute with methanol.
5. Evaporate the organic liquid to dryness at 40 °C.

Derivatization

1. Dissolve the residue in 200 µL aliquots of acetonitrile and transfer the sample to a glass reaction vial.
2. Add a 100 µL aliquots of a 2.5 mg/L 9-fluorenylmethyl chloroformate (FMOC-Cl) in acetonitrile and 100 µL aliquots of a phosphate buffer, pH 7.5.
3. Incubate the sample at 40 °C for 40 min.
4. Inject an aliquot 100 µL after derivatization, onto the chromatographic system.

HPLC

1. Prepare the mobile phase by mixing 700 mL of acetonitrile with 300 mL of a 0.05 mol/L solution of potassium dihydrogenphosphate in water, adjust to pH 7.5 with a 10% sodium hydroxide solution.
2. Determine ROX and I.S. in human plasma in a chromatograph model HP 1100 (Hewlett-Packard, Waldbronn, Germany).
3. Set at a flow rate of quaternary pump at 2 mL/min, a column oven at 40 °C and a fluorescence detector model HP 1046A and G13 21 A-1100, at an excitation wavelength (Ex) of 255 nm and emission wavelength (Em) of 315 nm.
4. Inject the samples (100 µL) using autosampler model G1313A.
5. Perform the separation on a 125 x 4.6 mm i.d. LiChrospher RP-18e column packed with 5 µm particles, with a guard column (LiChrospher RP-18e), both from Merck.

文献信息

实验步骤

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 Roxithromycin in Blood plasma by HPLC-tandem mass spectrometry	Analysis of Roxithromycin in Blood plasma by HPLC	Analysis of Roxithromycin in Blood plasma by High-performance liquid chromatography-mass spectrometry	
CAS Method Number	1-101-CAS-1241367	1-101-CAS-67878	1-101-CAS-10378	
Method Category	Active Pharmaceutical Ingredient and Metabolite Analysis	Active Pharmaceutical Ingredient and Metabolite Analysis	Active Pharmaceutical Ingredient and Metabolite Analysis	
Technique	HPLC-tandem mass spectrometry			
Analyte	Roxithromycin; Ambroxol hydrochloride			
Matrix	Blood plasma			
Other Materials	Methanol; Acetonitrile; Ammonium acetate; Heparin; C ₁₈ analytical column (150 mm x 4.6 mm, 5 µm)	Column, 125 x 4.6 mm i.d. LiChrospher RP-18e; SPE Bakerbond cartridges, C18	Acetonitrile; Column (250 mm x 4.6 mm i.d., 5 µm)	
Equipment Used	LC-MS/MS system, Thermo Finnigan, San Jose, CA; LC pump, Surveyor, Thermo Finnigan, San Jose, CA; View All	HPLC system, HP 1100, Hewlett-Packard, Waldbronn, Germany; Autosampler, G1313A	HPLC, 1100, Agilent; Mass detector	
Conditions	Instrument: Column: C ₁₈ analytical column; column temperature: 30 °C; mobile phase: mixture of methanol View All	Chromatographic: HPLC : mobile phase : 700 ml of acetonitrile + 300 ml of a 0.05 mol/L solution of potassium View All	Instrument: Detection- SIM mode. Chromatographic: Injection volume- 20 µL; mobile phase- (75:25, v/v) of View All	
Source	Simultaneous determination and pharmacokinetic study of roxithromycin and ambroxol View All	Determination of roxithromycin in human plasma by HPLC with fluorescence and UV absorbance View All	Stochastic resonance is applied to quantitative analysis for weak chromatographic signal of View All	
Preparation	Collection of plasma samples	Standards Preparation	Plasma samples	



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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 Analysis
- 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

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

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

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

请注意：

1.必须输入真实姓名和学校域名邮箱。
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>

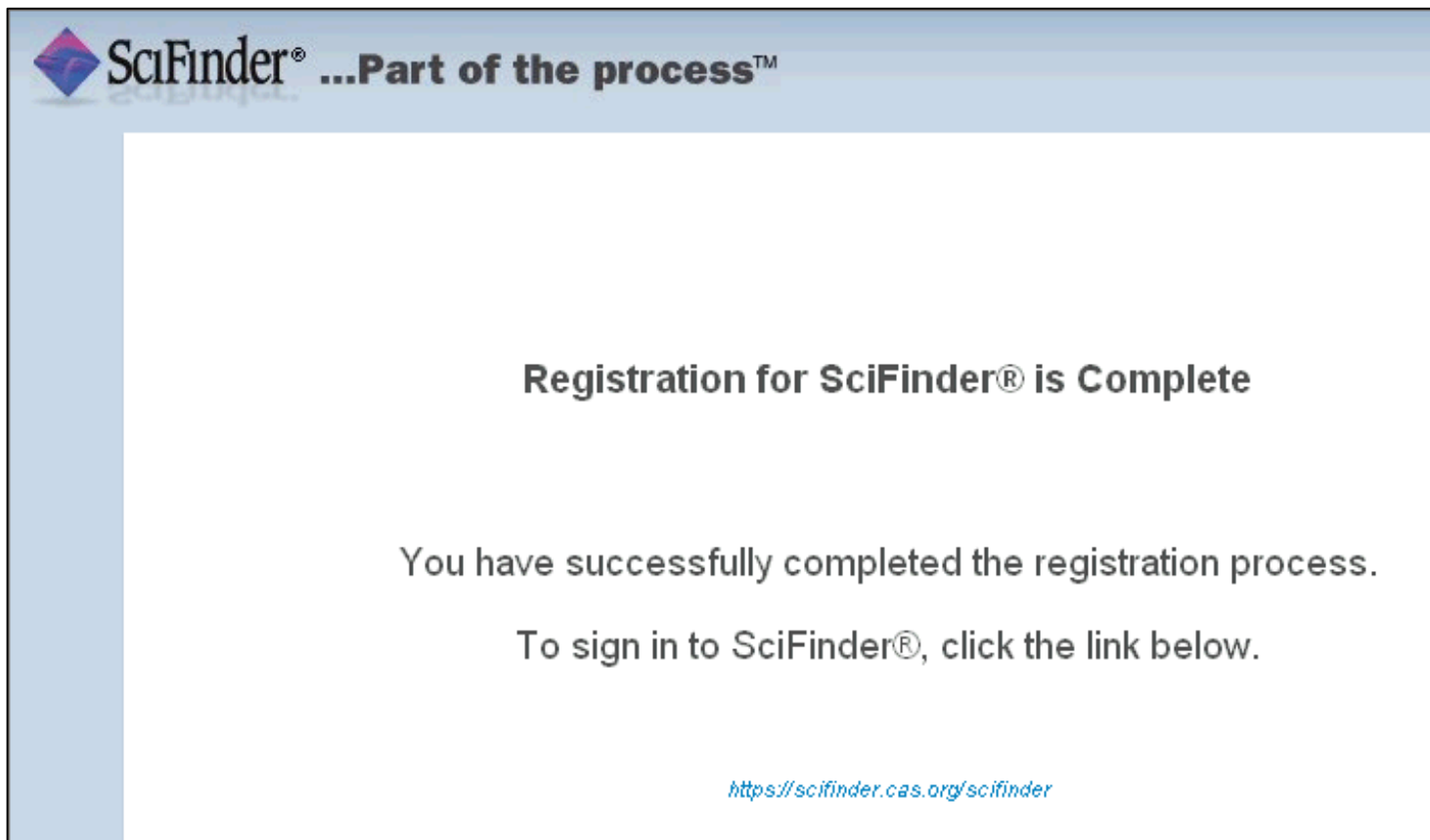
This link is valid for only one use and will expire within 48 hours.

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

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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
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- 严禁账号分享
- 严禁将账号用于非学术研究

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