

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

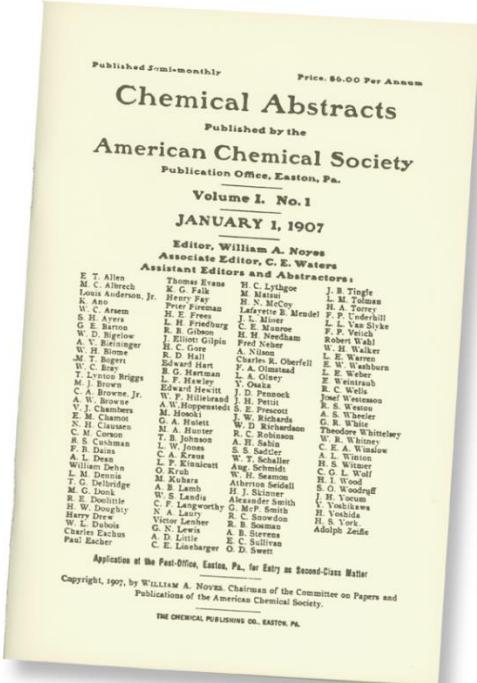


1907年，信息的汇集、管理发生了重大的变化

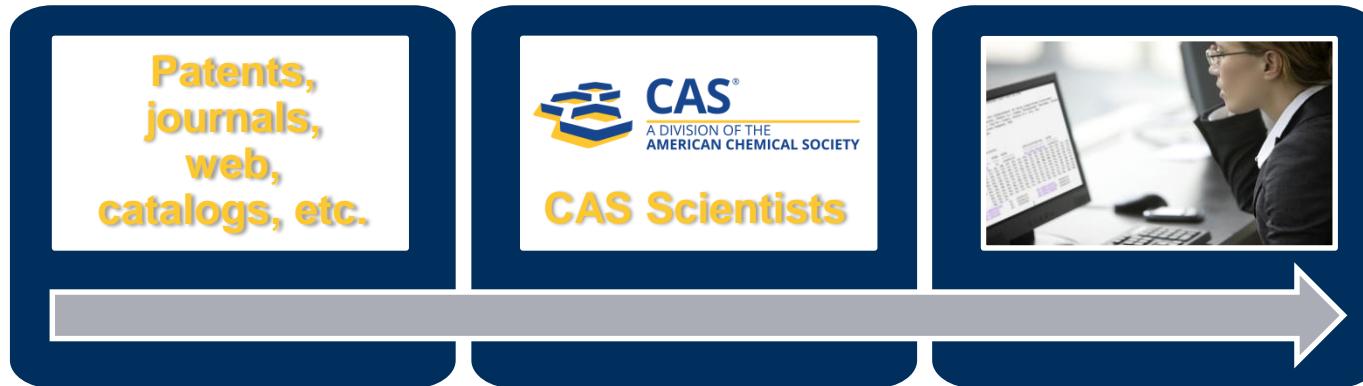


威廉·诺伊斯
(William A. Noyes)

- “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

ACS chemical
biology

BEILSTEIN JOURNAL
OF ORGANIC CHEMISTRY

division of polymer chemistry, inc
American Chemical Society

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



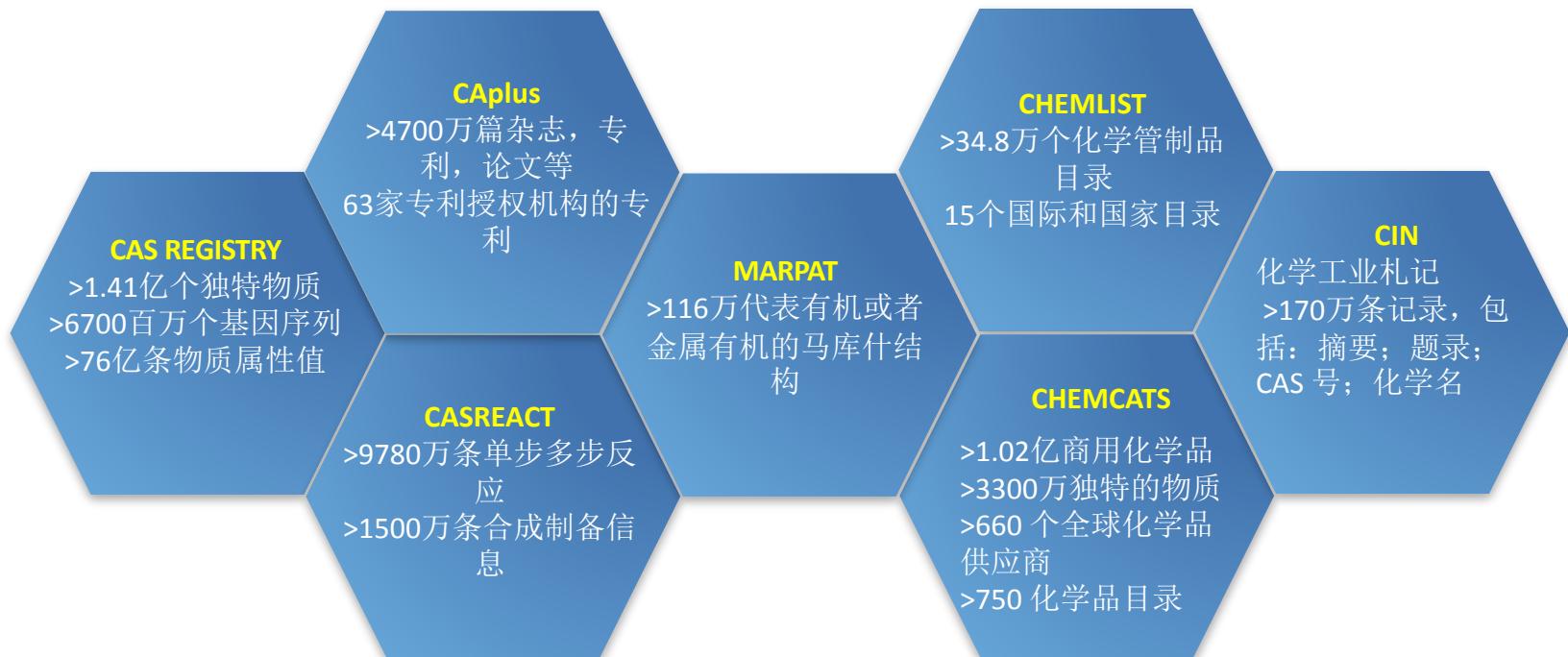
ACS Chemical
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THE JOURNAL OF
PHYSICAL CHEMISTRY
Letters

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CAS数据库——源于化学，超越化学

生物化学：

农化产品管控信息,生化遗传学,发酵,免疫化学,药理学

有机化学各领域：

氨基酸,生物分子,碳水化合物,有机金属化合物,类固醇

大分子化学各领域：

纤维素、木质素、造纸;涂料、墨水
染料、有机颜料;合成橡胶;纺织品、纤维

应用化学各领域：

大气污染,陶瓷,精油、化妆品,化石燃料,黑色金属、合金

物理、无机、分析化学各领域：

表面化学,催化剂,相平衡,核现象,电化学

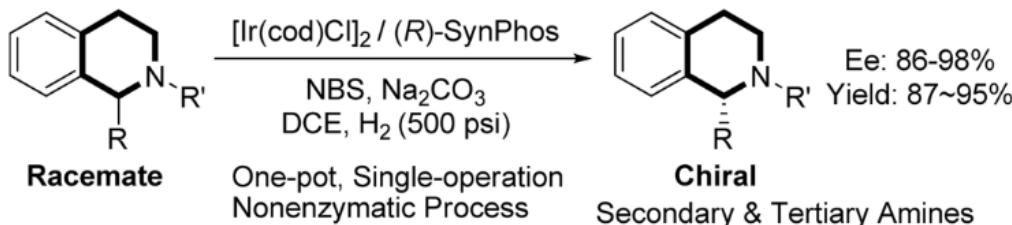


CAS数据库最具价值的内容——人工标引

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
503539-69-0

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

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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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
CPLUS

PUBLISHER

American Chemical Society

LANGUAGE

English



CAS人工标引解决的问题

- 检索词的同义词拓展：解决不同科研人员由于教育背景、语言、表达习惯不同导致的对同一个技术术语描述的差异。
- 用名称、分子式等检索化合物，会导致检索不全、不准的问题。CAS RN很好的解决了该问题，帮助检索人员实现精准定位化合物的目标。
- 利用SciFinder中的标引信息（Index Term，CAS RN，CAS Role），提高效率，启发思路。

CAS最新动向—解决方案

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 **CHEMZENT™**
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CAS最新动向—解决方案

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

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

Quick View PATENTPAK ▾

By Beigelman, Le From PCT Int. App. atkina, Natalia Language: English, Database: CAPLUS

Patent No. WO 201600441 Kind A1 Language English

Patent Family US 20160176911 A1 English

B is substituted purine and pyrimidine nucleobase; dashed bond between R and R⁴ is absent, then R is H, substituted each R⁶ and R⁷ are independently hydrogen or deuterium; R⁵ is -OH or F; methods of synthesizing nucleotide analogs and as a HCV infection with one or more nucleotide analogs. Thus, nucleotide II was prep'd. and tested as antiviral agent and of a hepatitis C virus.

7. Process for preparation of sofosbuvir

Quick View PATENTPAK ▾

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

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

ZOOM DOWNLOAD PDF

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

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Analyst Markup Locations (1) page 130

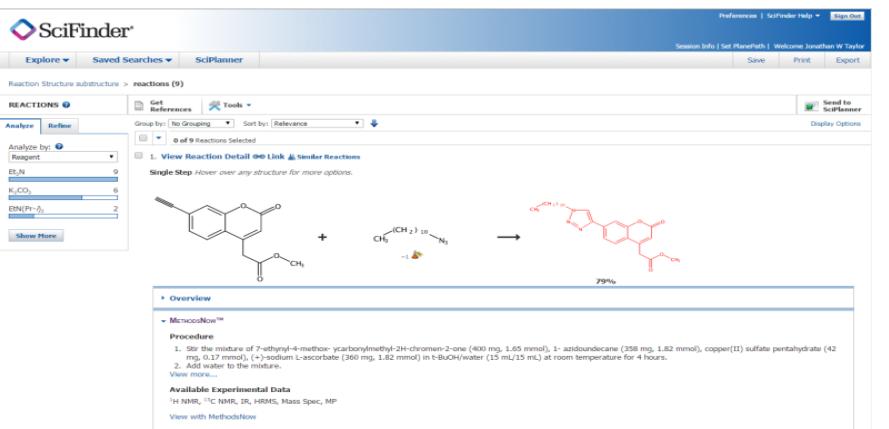
WO 2016/100441

PCT/US2015/065981

EXAMPLE 1
COMPOUND 1

CAS最新动向—解决方案

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



SciFinder

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Reactions (9)

Group by: No Grouping Sort by: Relevance

0 of 9 Reactions Selected

View Reaction Detail < Link Similar Reactions

Single Step Hover over any structure for more options.

Reaction Structure substructure > Reactions (9)

Analyzer by: Reactant

Et₃N 9

K₂CO₃ 6

EtN(Pt)₂ 2

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Overview

MethodsNow™

Procedure

1. Stir the mixture of 2-ethyl-4-methoxy-ycarbonylmethyl-2H-chromen-2-one (400 mg, 1.65 mmol), 1-azidoundecane (358 mg, 1.82 mmol), copper(II) sulfate pentahydrate (42 mg, 0.17 mmol), (+)-medium L-ascorbate (360 mg, 1.82 mmol) in t-BuOH/water (15 mL/15 mL) at room temperature for 4 hours.

2. Add water to the mixture.

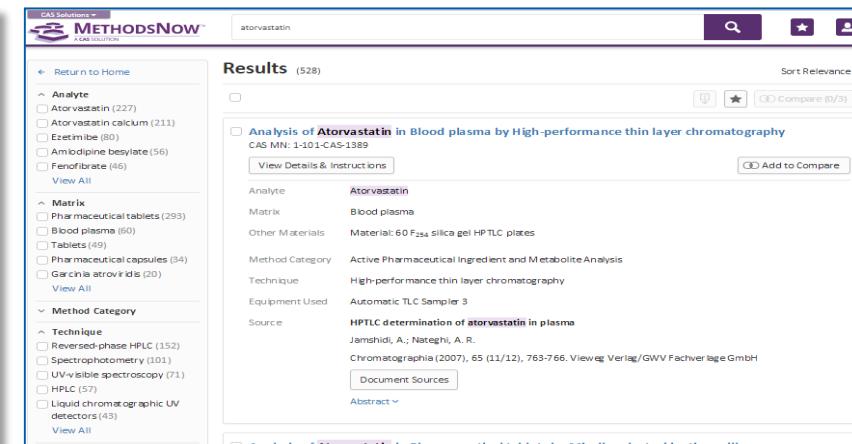
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Available Experimental Data

¹H NMR, ¹³C NMR, IR, HRMS, Mass Spec, MP

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嵌在SciFinder中的合成模块



CAS Solutions METHODSNow A CAS SOLUTION

Return to Home

Analyte

- Atorvastatin (227)
- Atorvastatin calcium (211)
- Ezetimibe (80)
- Amiodipine besylate (56)
- Fenofibrate (46)

View All

Matrix

- Pharmaceutical tablets (293)
- Blood plasma (60)
- Tablets (49)
- Pharmaceutical capsules (34)
- Garcinia atroviridis (20)

Method Category

Technique

- Reversed-phase HPLC (152)
- Spectrophotometry (101)
- UV-visible spectrosocopy (71)
- HPLC (57)
- Liquid chromatographic UV detectors (43)

View All

Results (528)

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

CAS MN: 1:101-CAS-1389

View Details & Instructions

Analyte: Atorvastatin

Matrix: Blood plasma

Other Materials: Material: 60 F₂₅₄ silica gel HPTLC plates

Method Category: Active Pharmaceutical Ingredient and Metabolite Analysis

Technique: High-performance thin layer chromatography

Equipment Used: Automatic TLC Sampler 3

Source: HPTLC determination of atorvastatin in plasma

Jamshidi, A.; Natajghi, A. R.

Chromatographia (2007), 65 (11/12), 763-766. Vieweg Verlag/GWV Fachverlage GmbH

Document Source

Abstract

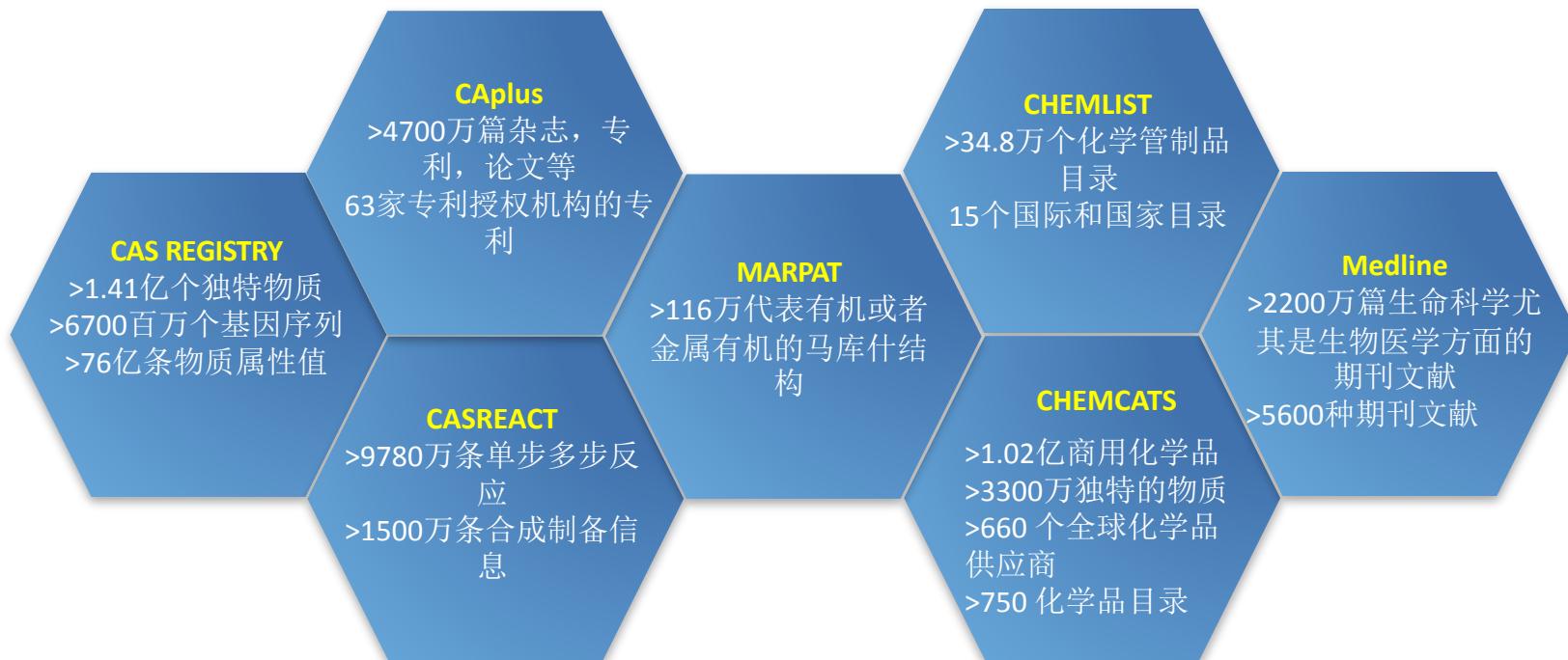
单独的分析界面



提纲

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

SciFinder覆盖的数据库



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REFERENCES: RESEARCH TOPIC

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

Search Advanced Search

REFRENCES

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

SUBSTANCES

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

REACTIONS

- Reaction Structure

SAVED ANSWER SETS

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

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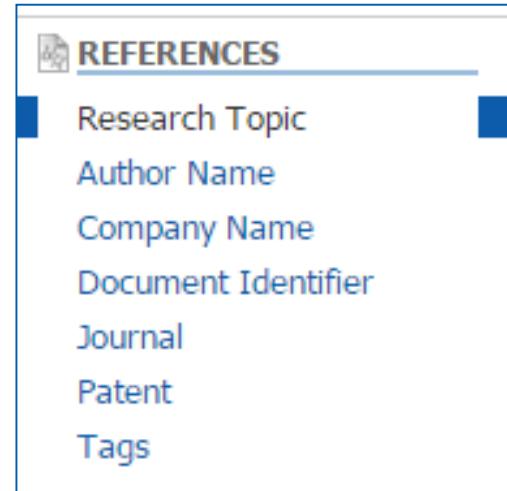
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SciFinder检索——文献检索

■ 文献检索方法

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



■ 检索策略推荐

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

文献检索——主题: 铝合金铸造

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

The screenshot shows the SciFinder interface with the following details:

- Header:** CAS Solutions, SCIFINDER, A CAS SOLUTION
- Navigation:** Explore, Saved Searches, SciPlanner
- Search Results:** Research Topic "casting of aluminum alloy" > references (23167)
- Left Sidebar (REFERENCES):**
 - Research Topic (selected)
 - Author Name
 - Company Name
 - Document Identifier
 - Journal
 - Patent
 - Tags
- Right Panel (REFERENCES: RESEARCH TOPIC):**
 - Search bar: casting of aluminum alloy
 - Examples:
 - The effect of antibiotic residues on dairy products
 - Photocyanation of aromatic compounds
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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 |

Get References

“Concepts”表示对主题词做了同义词的扩展；

“Closely associated with one another”表示同时出现在一个句子中；

“were present anywhere in the reference”表示同时出现在一篇文献中；



文献检索结果

文献分析工具

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Sort by: Accession Number 

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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

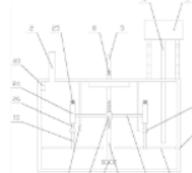
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0 of 23167 References Selected

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

By Huang, Longhui
From Faming Zhanli Shengqing (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 ...



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

By Jiang, Jiming; Jiang, Fengchan; Jiang, Huiyang; Chen, Zhibin; Lin, Jianhua
From Faming Zhanli Shengqing (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 sheet...

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

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 re on dairy products

Photocyanation of aroma compounds

Refine

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Sort by: Accession Number ▾ 0 of 1582 References Selected Page: 1 of 80

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 Zhanli Shengqing (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 prepnr. method thereof, which belongs to tech. field of **aluminum alloy** prepnr. 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...

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 Zhanli Shengqing (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** lgq., 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 Zhanli Shengqing (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 constitut...

4. **A kind of high-performance aluminum alloy thick plate and preparation method thereof [Machine Translation].**
Quick View PATENTPAK
By Han, Shuai; Xie, Yan cui; Wang, Dawei; Yu, Lili; Geng, Guangchao; Chen, Shiyu; Zang, Jiaji; Xu, Hanji; Lu, Xiaohan; Zheng, Xinran
From Faming Zhanli Shengqing (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 prepnr. method thereof, and relates to a kind of high-performance **aluminum alloy** thick plate and prepnr. 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 manufd. with the existing high-performance **aluminum alloy** manufg. method and prepgr. method. Elements in the **aluminum alloy** thick plate of the invention include Si,...

按被引次数排序— Citing References

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Page: 1 of 80

1. Publication Year | Citing References | Sources

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.; Mohedano, 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

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~370

~330

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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 Zhanli Shengqing (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...

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 Zhanli Shengqing (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 Zhanli Shengqing (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

Index Term

Casting of metals 951

corrosion resistance 479

Smelting 343

Tensile strength 310

Corrosion-resistant materials 306

Melting 276

annealing 258

Purification 215

heat treatment 197

Quenching (cooling) 193

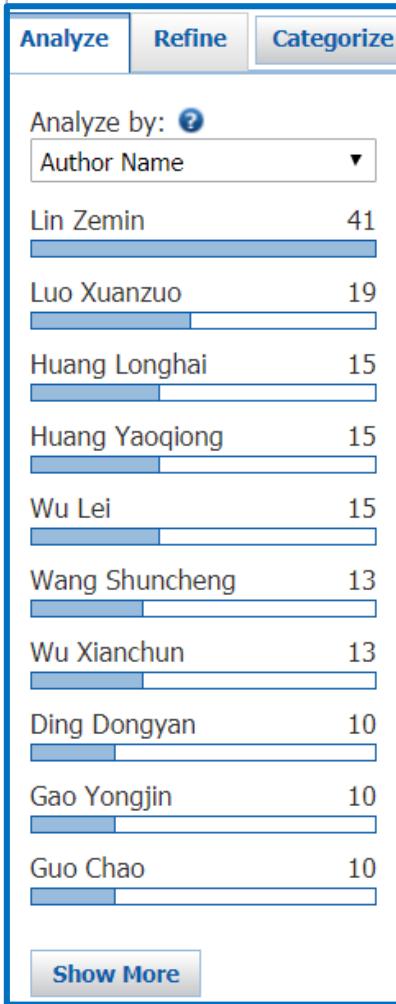
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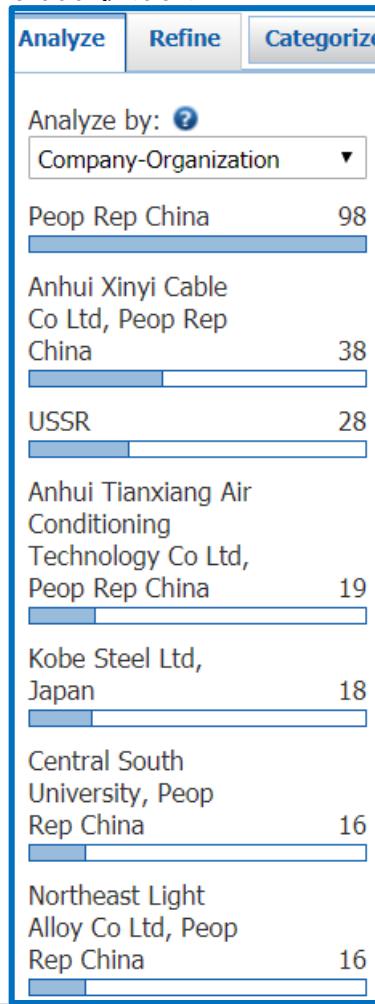


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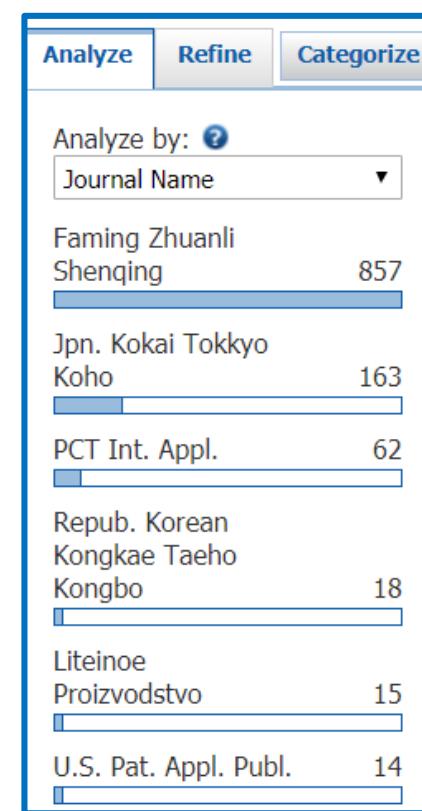
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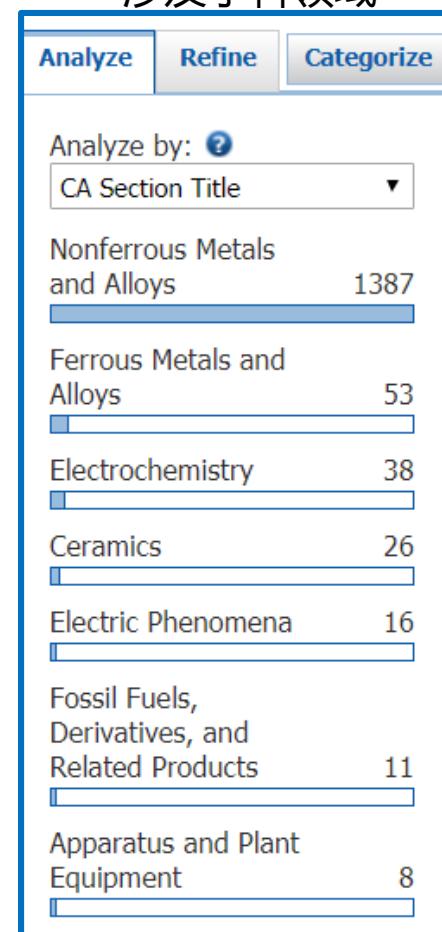
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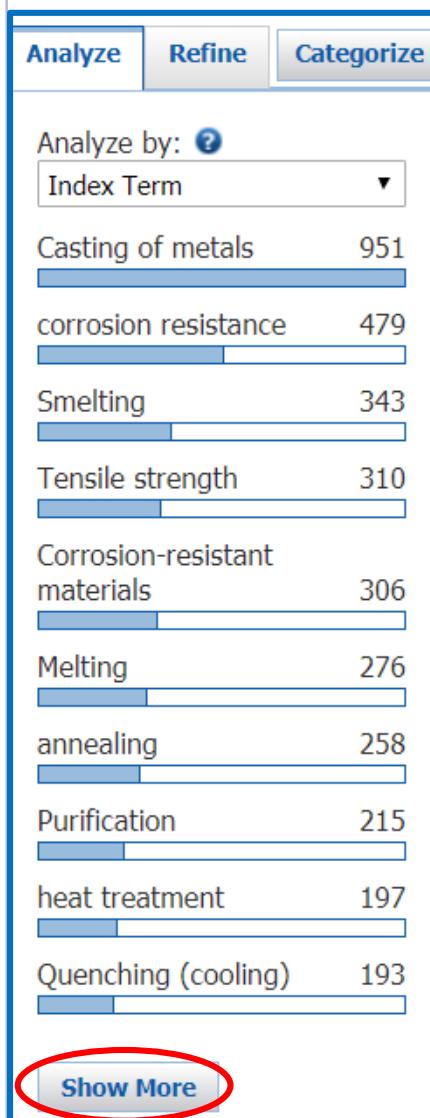


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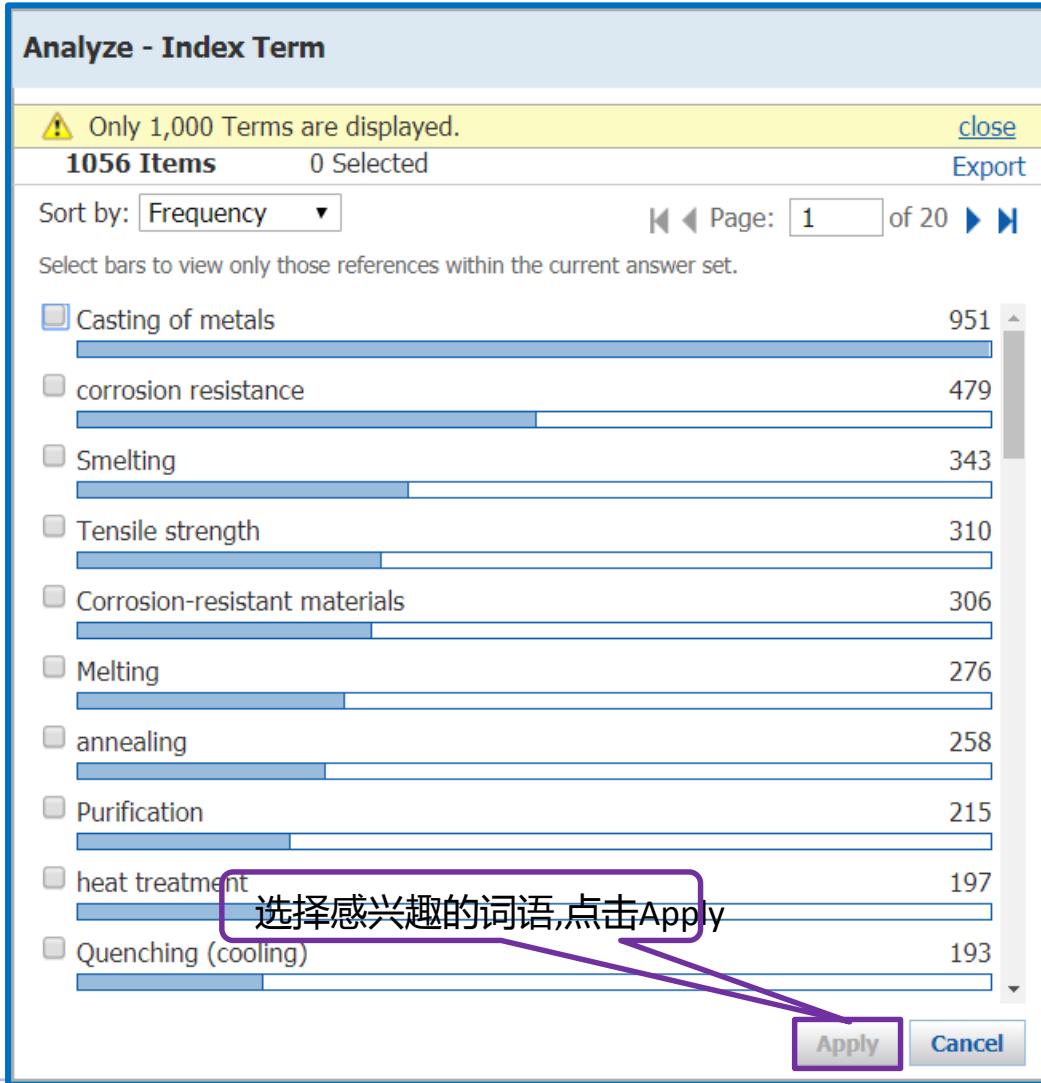


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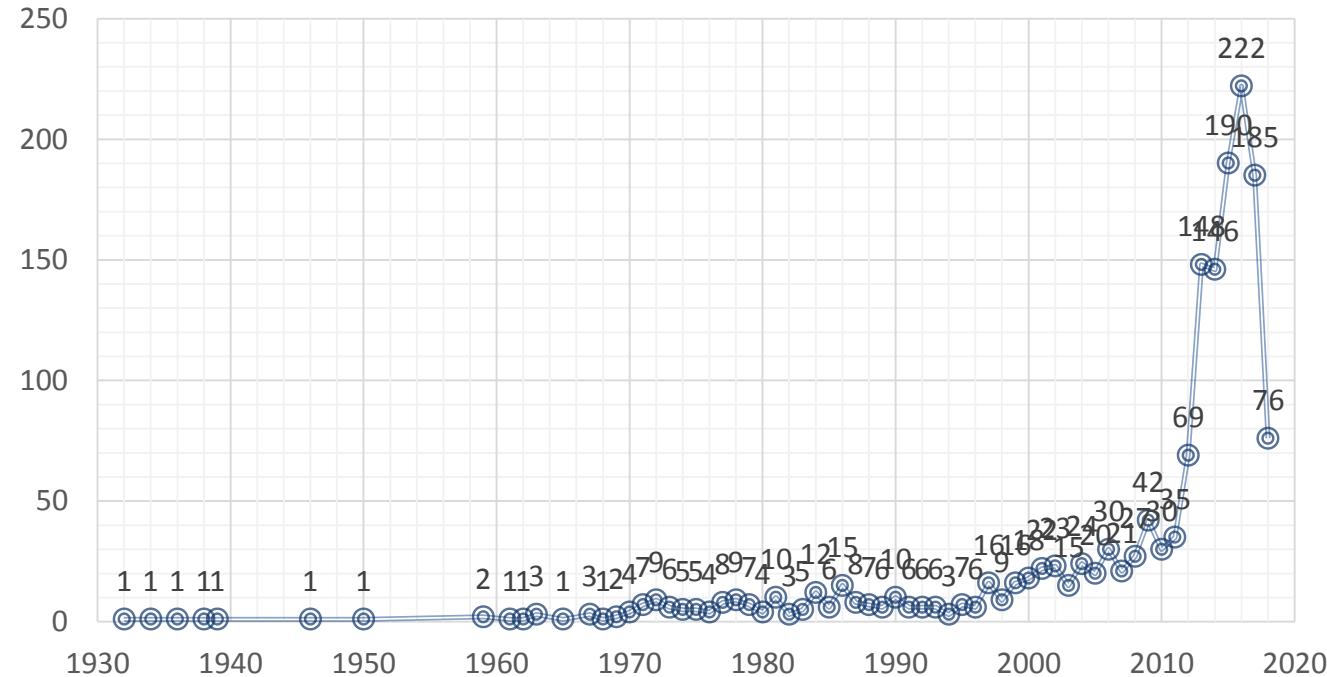
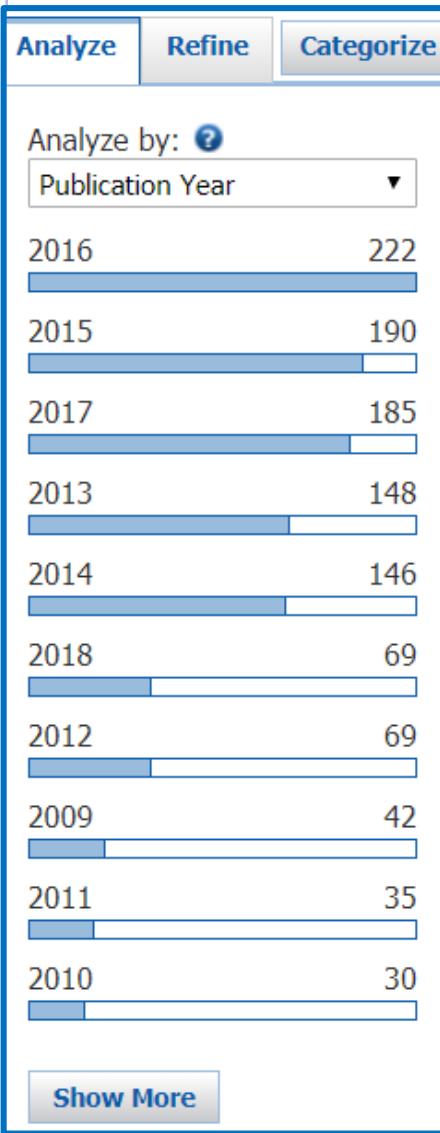
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Index Term

选中的Index Term

Categorize 

1. Select a heading and category.

Category Heading	Category
All	Substances in technology (3117)
Technology	Processes & apparatus (432)
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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	

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Index Terms																																
  Page: 1 of 3  																																
Select All Deselect All																																
<table border="1"><tbody><tr><td><input type="checkbox"/> Zinc</td><td>81</td></tr><tr><td><input type="checkbox"/> Copper</td><td>78</td></tr><tr><td><input type="checkbox"/> Titanium</td><td>68</td></tr><tr><td><input type="checkbox"/> Nickel</td><td>63</td></tr><tr><td><input type="checkbox"/> Iron</td><td>49</td></tr><tr><td><input type="checkbox"/> Chromium</td><td>47</td></tr><tr><td><input type="checkbox"/> Forging</td><td>47</td></tr><tr><td><input type="checkbox"/> Manganese</td><td>42</td></tr><tr><td><input checked="" type="checkbox"/> Cast alloys, aluminum</td><td>35</td></tr><tr><td><input type="checkbox"/> Zirconium</td><td>34</td></tr><tr><td><input type="checkbox"/> Cast iron</td><td>31</td></tr><tr><td><input type="checkbox"/> AL9</td><td>29</td></tr><tr><td><input type="checkbox"/> Rare earth metals</td><td>25</td></tr><tr><td><input type="checkbox"/> Strontium</td><td>25</td></tr><tr><td><input type="checkbox"/> Alloying</td><td>21</td></tr><tr><td><input type="checkbox"/> Steel</td><td>21</td></tr></tbody></table>	<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
<input type="checkbox"/> Zinc	81																															
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<input type="checkbox"/> Manganese	42																															
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1. Conversion bath with nitrate for corrosion-resistant coating on aluminum alloys

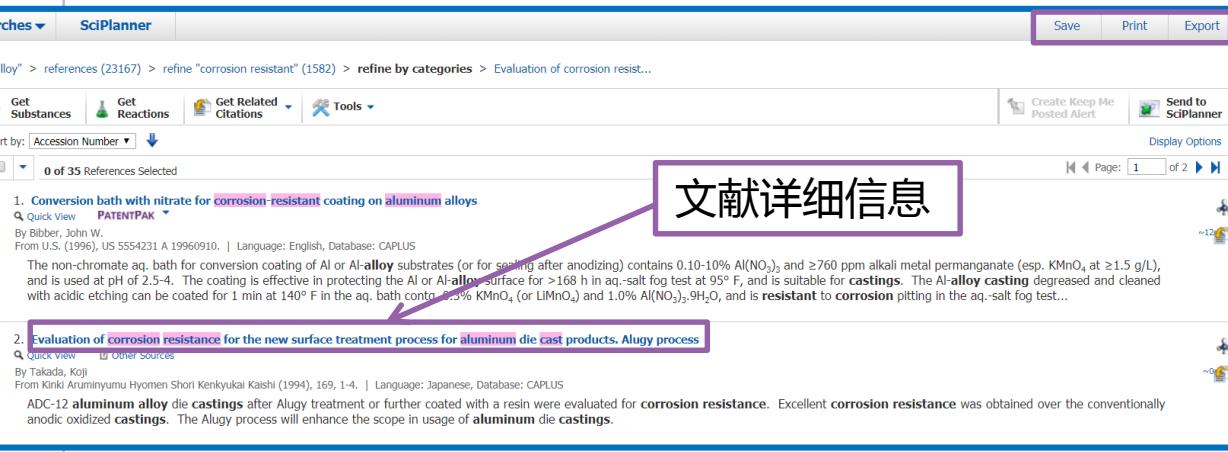
2. Evaluation of corrosion resistance for the new surface treatment process for aluminum die cast products. Alugy process

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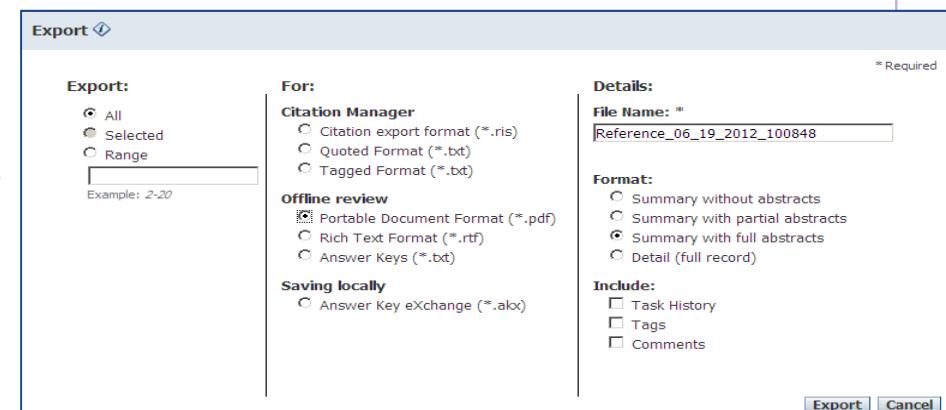
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文献信息一题录、摘要、索引

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

Supplementary Terms

corrosion resistance aluminum die casting; Alugy process aluminum die casting

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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
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LANGUAGE
Japanese



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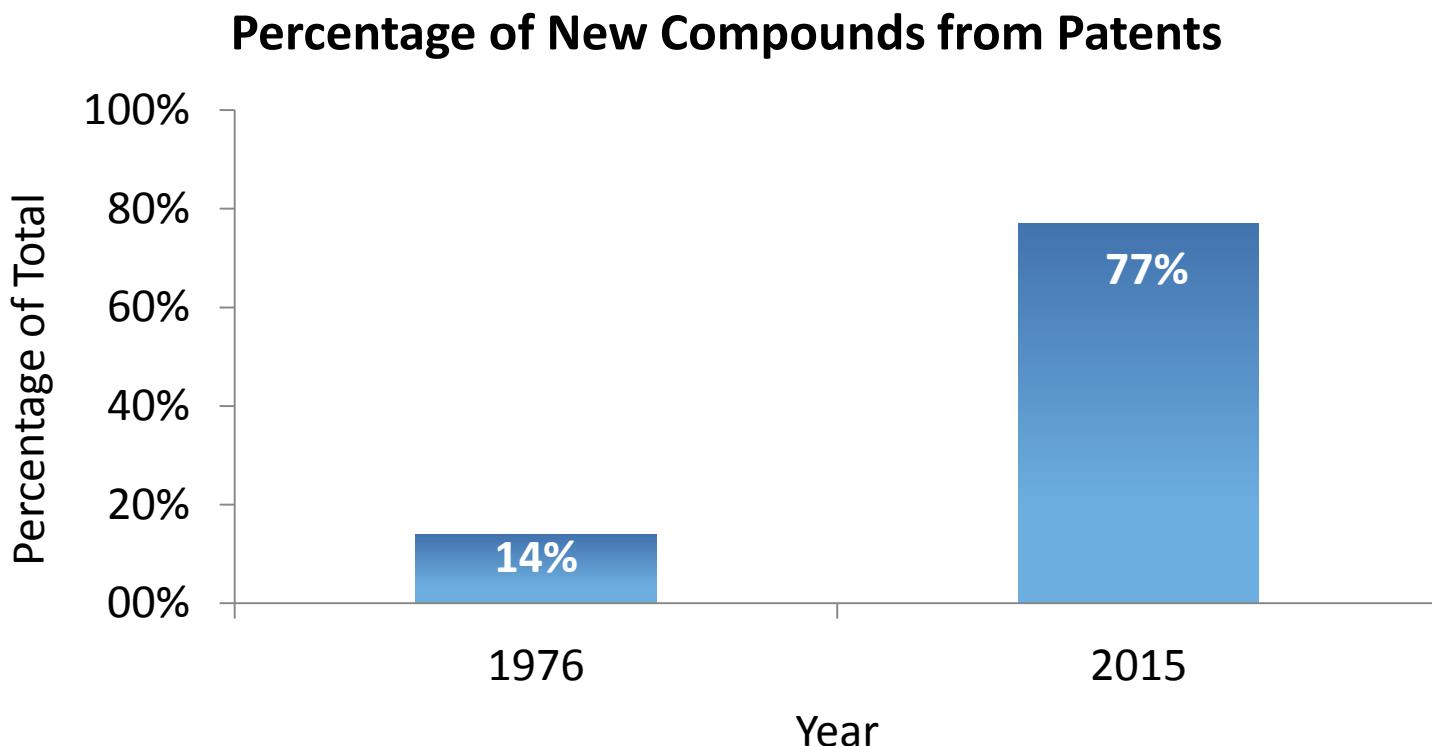
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By Denker, U
From PCT Int

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an electronic device comprising ≥ 1 light emitting layer between an anode and
prising between the cathode and the anode ≥ 1 mixed layer comprising (i) in
ectropos. element selected from Li, Na, K, Be, Sc, Y, La, Lu, Ti and V, and (ii)
n transport matrix compd. comprising ≥ 1 polar group selected from a
wherein the redn. potential of the substantially covalent electron transport
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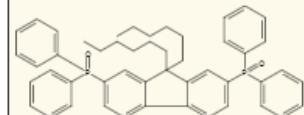


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CAS RN 1798388-23-4

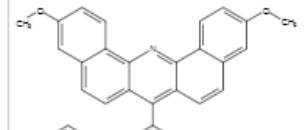


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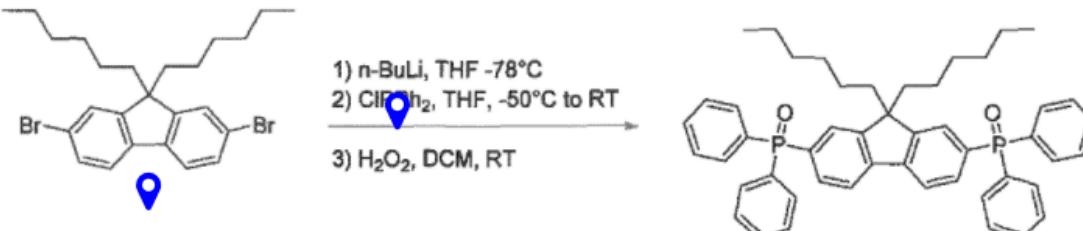
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followed by: acetate (50 mL) was added to the desired compound twice. obtained in 70 % yield (5.71 g). Finally, the

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



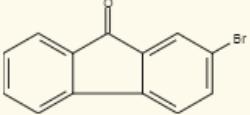
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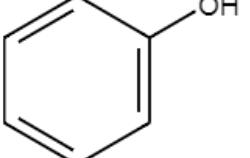
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page 51
page 51

CAS RN 108-95-2



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Analyst Markup Locations (2)
page 51

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



Chemical Formula: C₁₃H₇BrO
Molecular Weight: 259,10

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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Key Substances in Patent

CAS RN 3096-56-8

CAS Registry Number 3096-56-8
~368 ~114
C₁₃H₇BrO
9H-Fluoren-9-one, 2-bromo-
Molecular Weight
259.10
Melting Point (Experimental)
Value: 141-142 °C

Chemical Formula: C₁₃H₇BrO

Chemical Formula: C₂₅H₁₅BrO
Molecular Weight: 411.30

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

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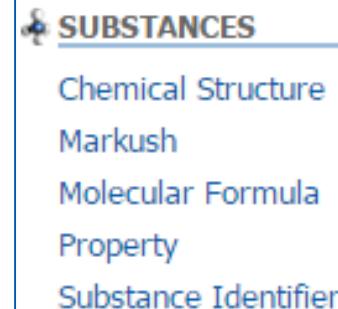
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- 分子式检索
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1. 63968-64-9

~5009 ~123

Absolute stereochemistry.

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

Key Physical Properties
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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*,5a*S*,6*R*,8a*S*,9*R*,12*S*,12a*R*)-

Molecular Weight
282.33

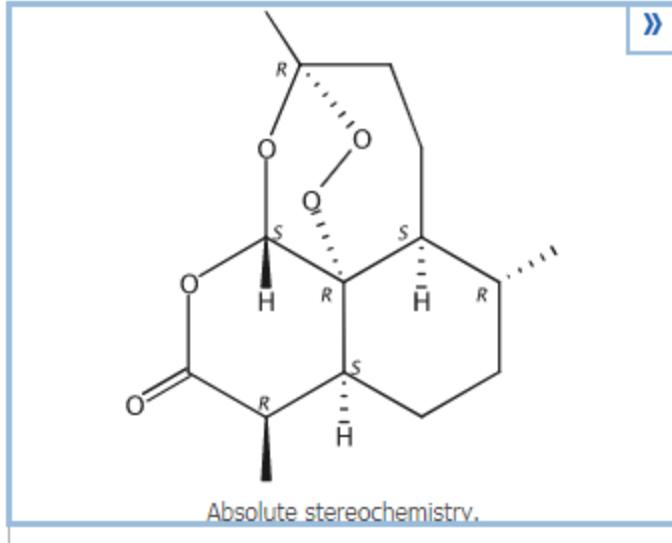
Melting Point (Experimental)
Value: 156-157 °C

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

Density (Experimental)
Value: 1.300 g/cm³

Other Names
3,12-Epoxy-12*H*-pyrano[4,3-*J*]-1,2-benzodioxepin-10(3*H*)-one,
octahydro-3,6,9-trimethyl-, [3*R*-(3*a*,5a*B*,6*B*,8a*B*,9*O*,12*B*,12a*R*^{*})]-
(3*R*,5a*S*,6*R*,8a*S*,9*R*,12*S*,12a*R*)-Octahydro-3,6,9-trimethyl-3,12-epoxy-
12*H*-pyrano[4,3-*J*]-1,2-benzodioxepin-10(3*H*)-one
(+)-Arteannuin
(+)-Artemisinin
(+)-Qinghaosu
[View more...](#)

由物质获得文献，反应，供应商等信息



A chemical structure diagram of a complex polycyclic compound. It features a central benzodioxepin ring system with an epoxide group at position 3. Attached to the ring are a pyranose ring, a cyclohexene ring, and a cyclohexane ring. Various substituents are shown with stereochemistry indicated by 'R' and 'S' labels and dashed lines. A '»' icon is in the top right corner of the box.

Absolute stereochemistry.

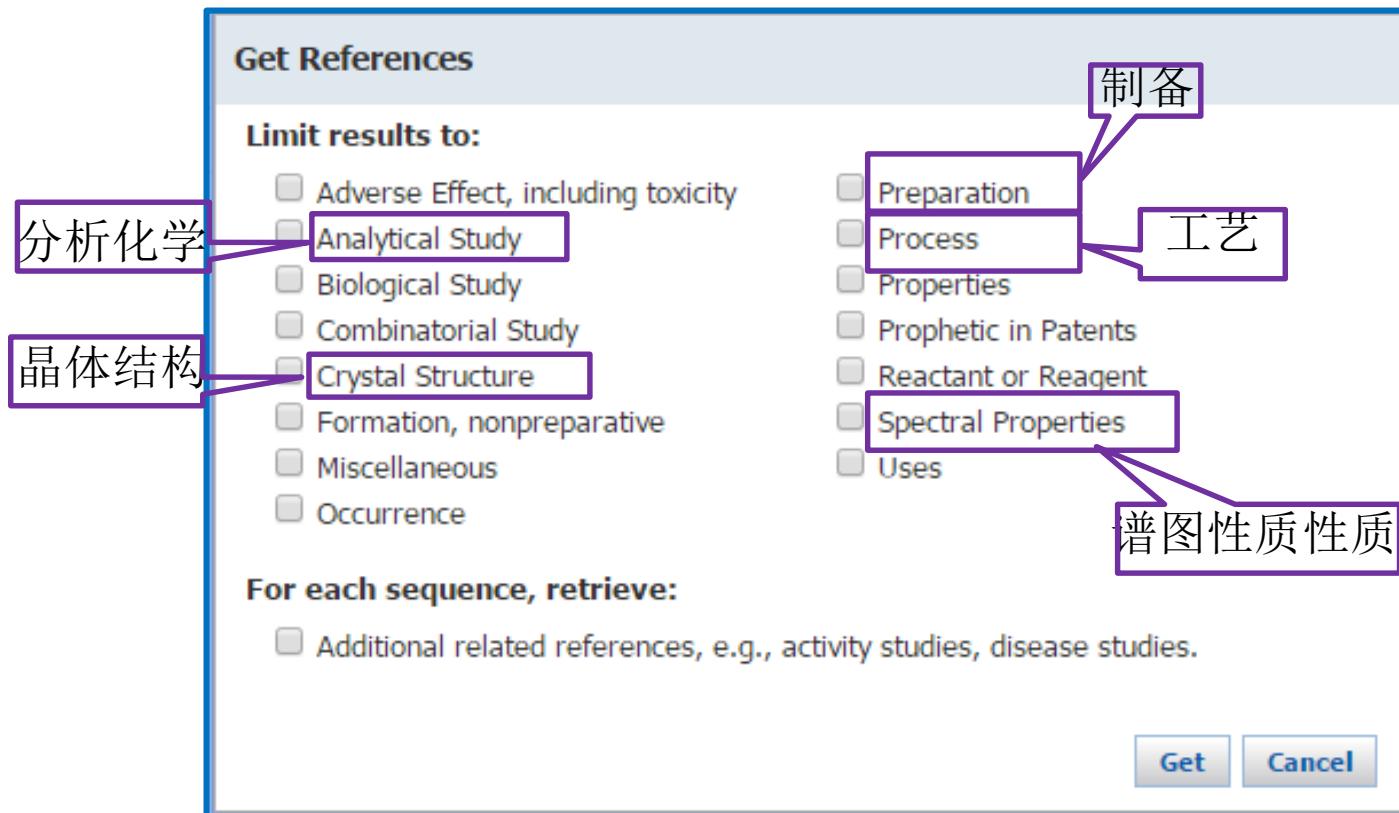
物质详情

 **SCI-FINDER**[®]
A CAS SOLUTION

ACS / Proprietary and Confidential / Do Not Distribute

43

通过物质获得文献



EXPERIMENTAL PROPERTIES

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

Structure Related Properties

	Value	Note
Bond Angle	See full text	(2)CAS
Bond Length	See full text	(2)CAS
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

EXPERIMENTAL SPECTRA

¹H NMR ¹³C NMR Hetero NMR IR Mass Raman

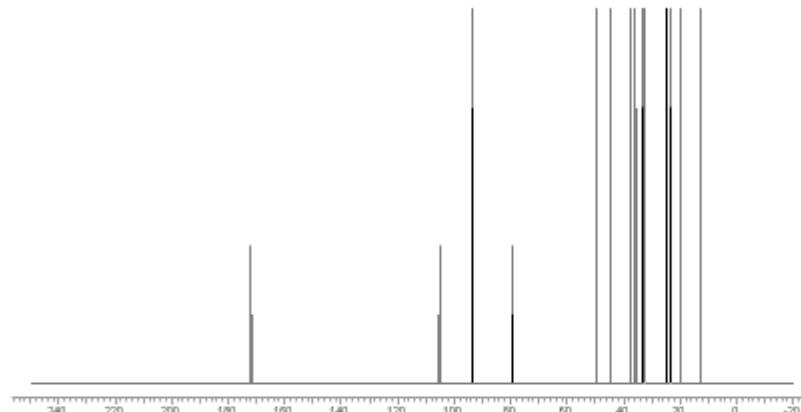
¹³C NMR Properties

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

实验数据与实验谱图

1 of 4

Carbon-13 NMR Spectrum

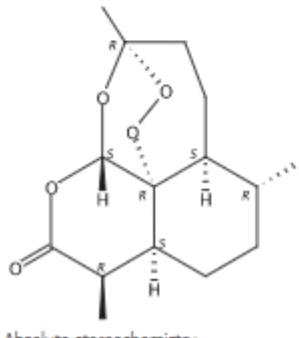


FORMULA
C15H22O5

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

NUCLEUS
¹³C

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



Absolute stereochemistry

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 (μ B)

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

Searches

SUBSTANCES

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...

v.ip138.com—IP

Search

SCI-FINDER®
A CAS SOLUTION

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  

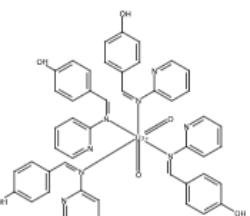
Analyze by:  Substance Role 

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

0 of 241 Substances Selected  Page: 1 of 17 

1. 1260101-12-9 

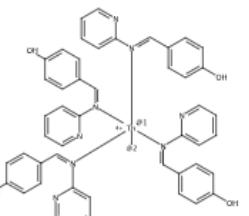
1260101-11-8   C48H40N8O6U



14797-73-0  ClO4

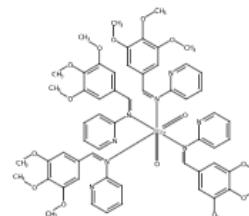
2. 1260101-08-3 

1260101-07-2   C72H60N12O6Th



3. 1260101-01-6 

1260101-00-5   C60H64N8O14U



14797-73-0  ClO4

通过分析/限定工具筛选结果

SUBSTANCES ?

Analyze Refine

Analyze by: Elements

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

Show More

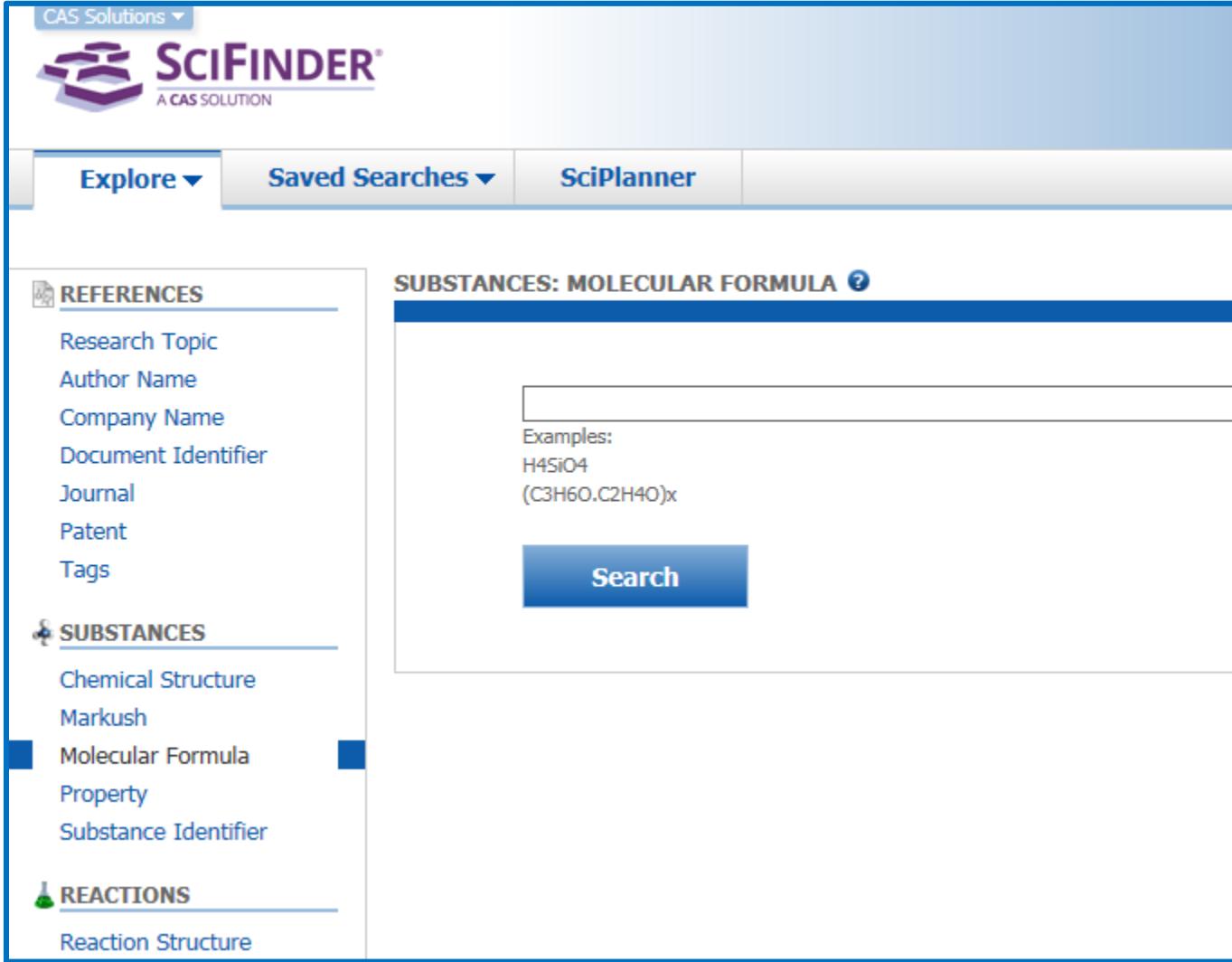
Get References Get Reactions Get Commercial Sources Tools

Create Keep Me Posted Alert Send to SciPlanner

Display Options

Page: 1 of 3

分子式检索



The screenshot shows the SciFinder interface with a blue header bar. The header includes the "CAS Solutions" dropdown, the SciFinder logo with "A CAS SOLUTION" text, and navigation tabs: "Explore" (selected), "Saved Searches", and "SciPlanner".

The main content area is titled "SUBSTANCES: MOLECULAR FORMULA" with a help icon. It features a search input field with examples: H4SiO4 and (C3H6O.C2H4O)x, and a large blue "Search" button.

The left sidebar, titled "REFERENCES", lists: Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, and Tags.

The sidebar also includes a "SUBSTANCES" section with "Molecular Formula" selected, and "Chemical Structure", "Markush", "Property", and "Substance Identifier".

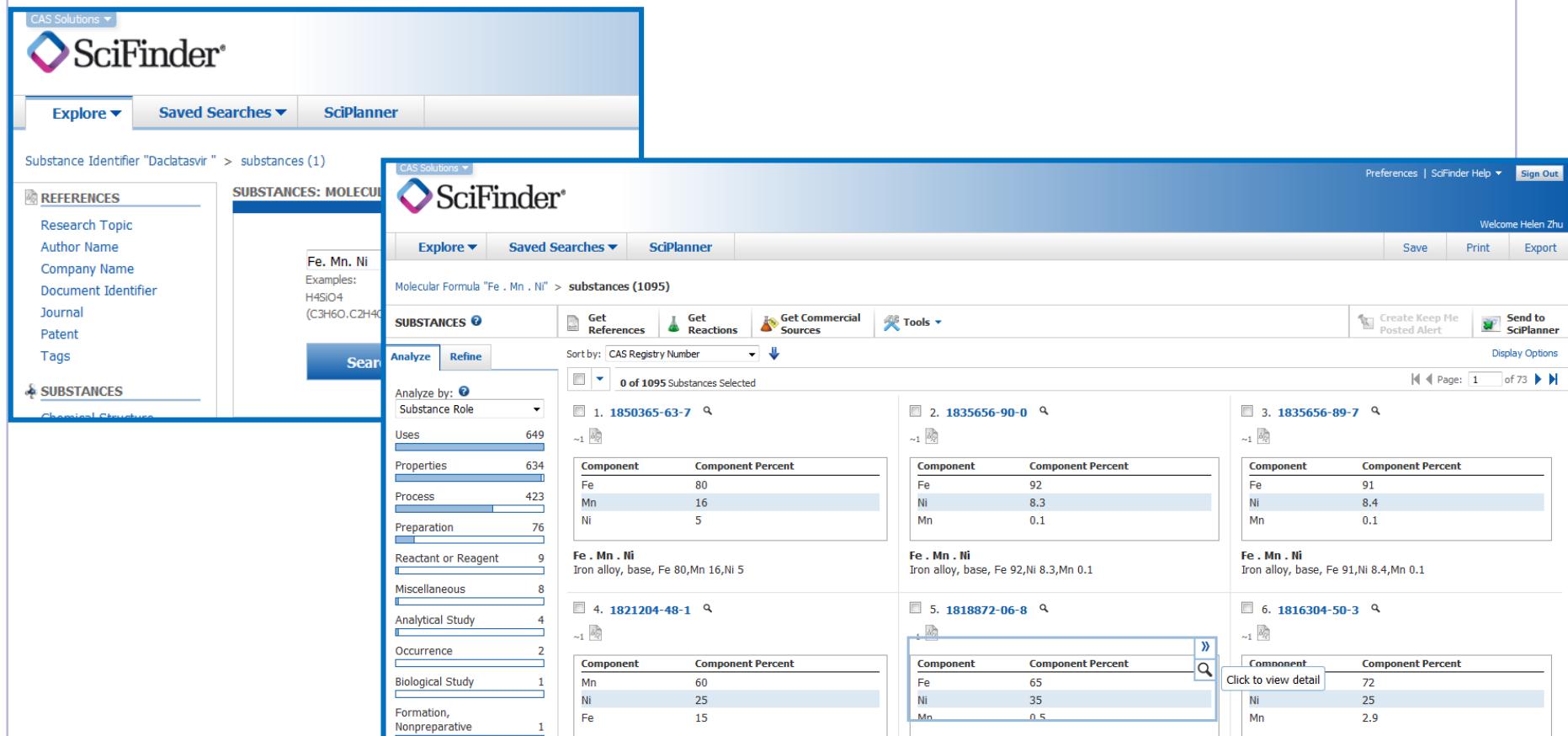
The bottom of the sidebar has a "REACTIONS" section with "Reaction Structure".

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 shows the SciFinder interface with a search results page for substances containing Fe, Mn, and Ni. The search bar at the top contains the molecular formula "Fe . Mn . Ni". The results page displays 1095 substances, with the first six listed below:

Substance ID	Component	Component Percent
1. 1850365-63-7	Fe	80
	Mn	16
	Ni	5
2. 1835656-90-0	Fe	92
	Ni	8.3
	Mn	0.1
3. 1835656-89-7	Fe	91
	Ni	8.4
	Mn	0.1
4. 1821204-48-1	Mn	60
	Ni	25
	Fe	15
5. 1818872-06-8	Fe	65
	Ni	35
	Mn	0.5
6. 1816304-50-3	Click to view detail	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 interface for searching chemical substances. On the left, a 'Structure Editor' window is open, showing a chemical structure with atoms Fe, Mn, and Ni. The main window shows search results for substances containing these elements. The results are listed in a grid, with each entry showing a substance ID, a preview icon, and a detailed component analysis table.

Sample Analysis:

- Substance Role: 0 of 205650 Substances Selected
- Uses: ≥ 14737
- Properties: ≥ 9165
- Process: ≥ 8141
- Preparation: ≥ 1757
- Reactant or Reagent: ≥ 355
- Miscellaneous: ≥ 182
- Analytical Study: ≥ 123
- Biological Study: ≥ 112
- Formation, Nonpreparative: ≥ 22
- Occurrence: ≥ 21

Component Percent Tables:

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

Component	Component Percent
Fe	98
Mn	0.7
Ni	0.6
C	0.1

Component	Component Percent
Fe	96
Ni	2.2
Mn	1.3
Si	0.3

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

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

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

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

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

Import CXF

Search

Advanced Search Always Show

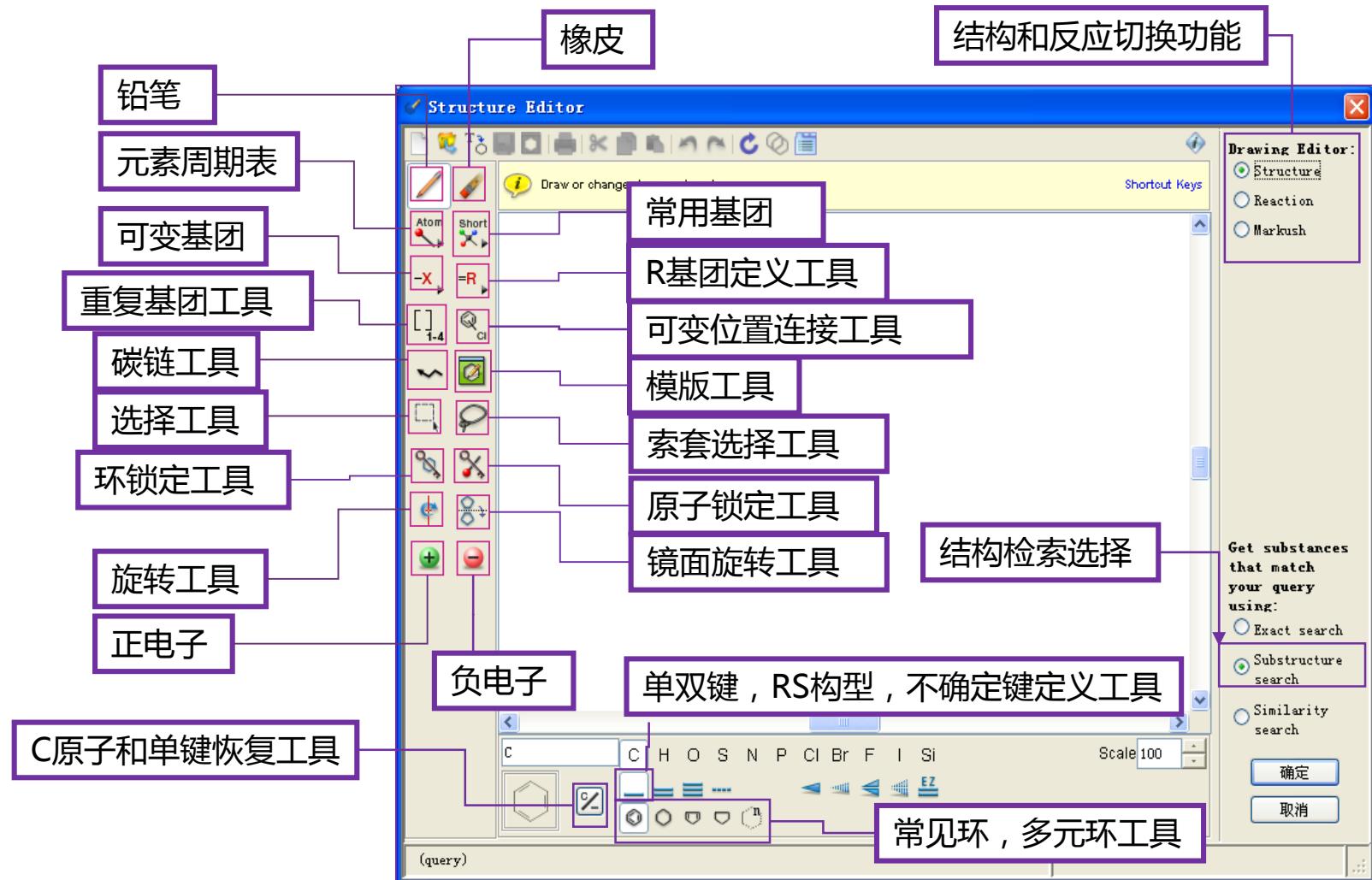
Search Type:

- Exact Structure
- Substructure
- Similarity

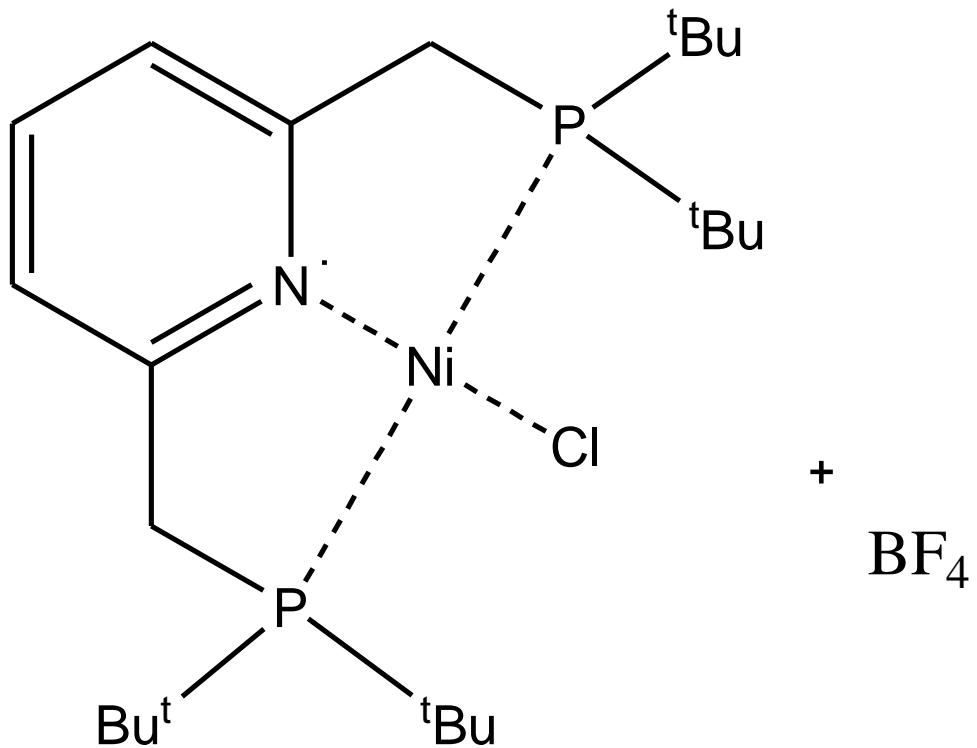
Show precision analysis

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

物质检索——结构



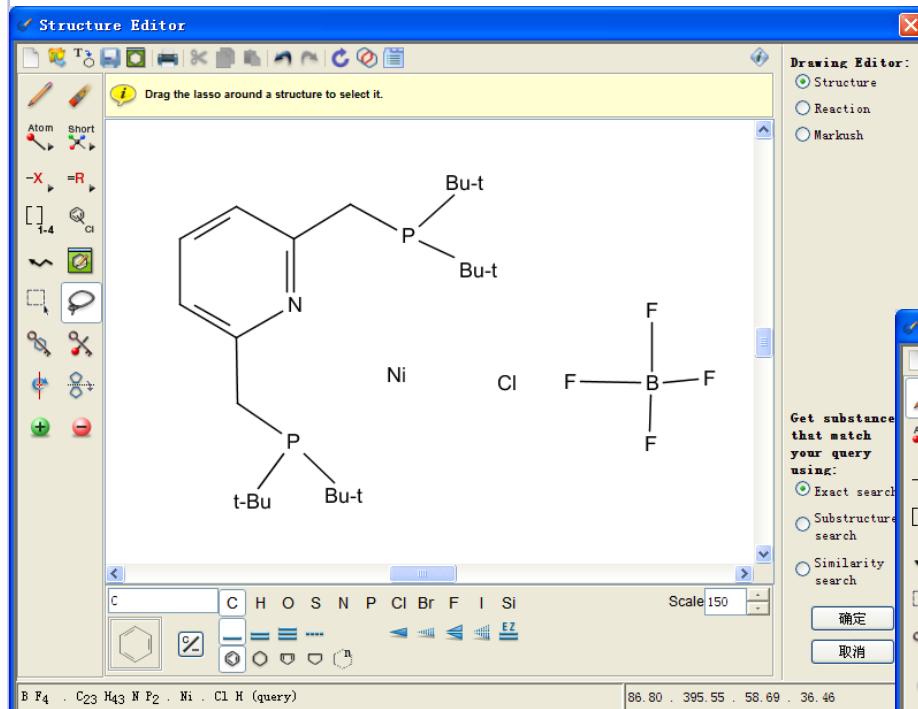
物质检索——精确结构检索



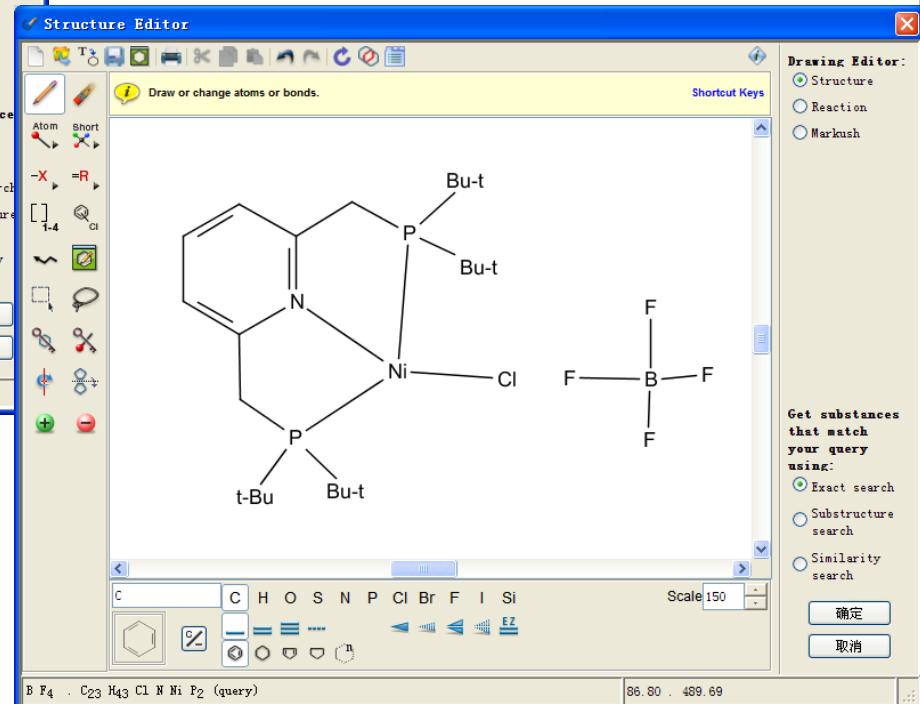
该结构中包含：

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 

Sort by: CAS Registry Number 

Analyze by:  Substance Role 

Preparation 1

Properties 1

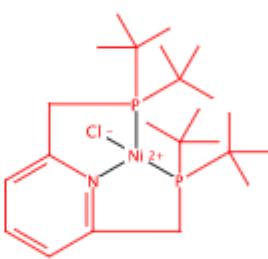
Reactant or Reagent 1

Show More

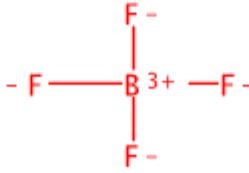
0 of 1 Substance Selected

1. 1136166-99-8 

 1136166-98-7  C₂₃H₄₃ClN Ni P₂



14874-70-5 

B F₄ 

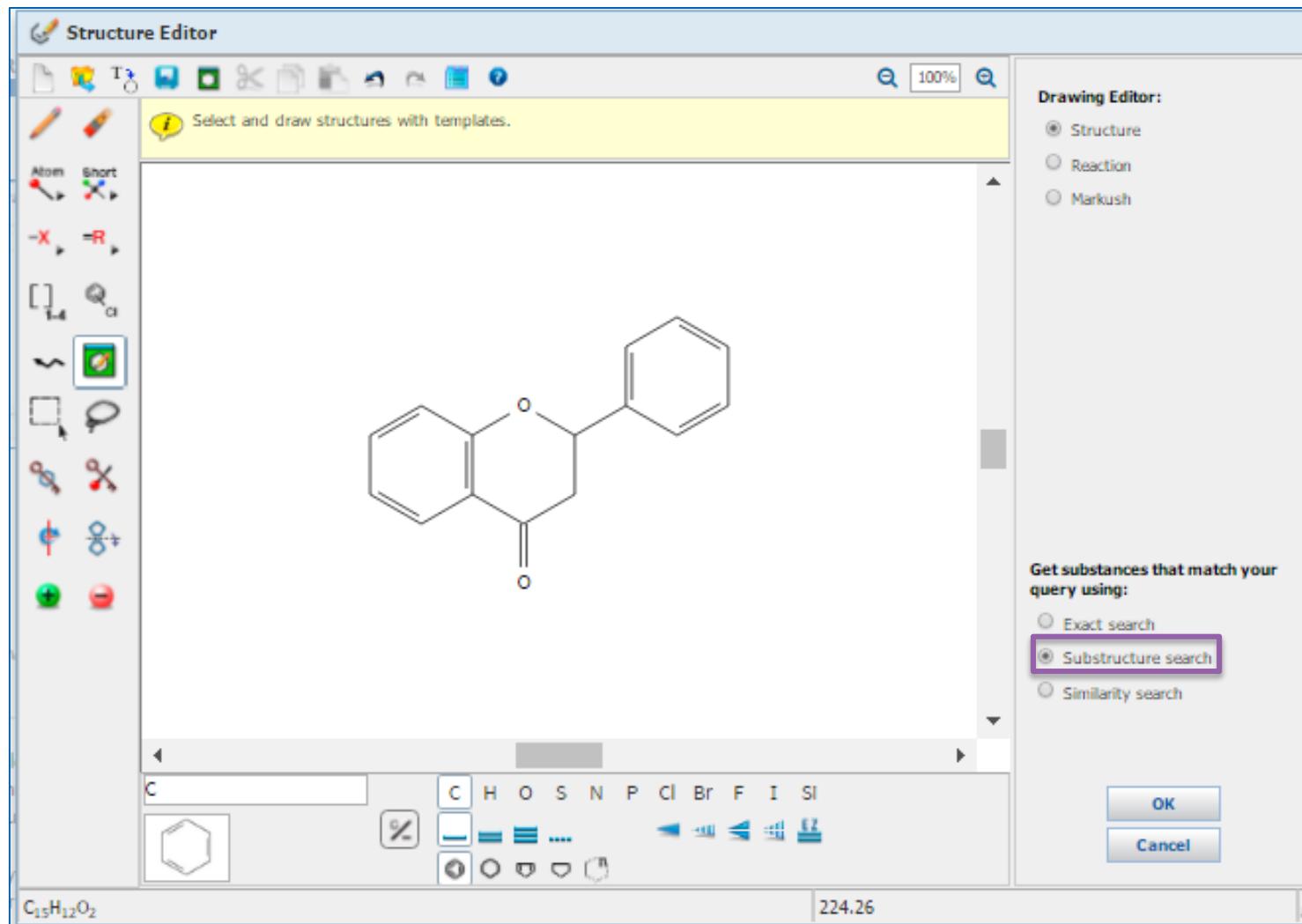
C₂₃H₄₃ClN Ni P₂ · BF₄
Nickel(1+), [2,6-bis[[bis(1,1-dimethylethyl)phosphino- κ P]methyl]pyridine- κ N]
chloro-, (5 P -4-3)-, tetrafluoroborate(1-) (1:1)

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

C₁₅ H₁₂ O₂
4H-1-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 (-).

C₁₅ H₁₂ O₂
4H-1-Benzopyran-4-one, 2,3-dih

Key Physical Properties
Experimental Properties

10. 146196-91-0

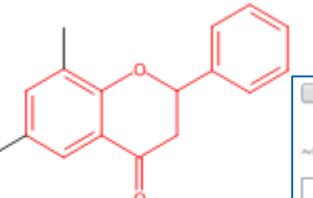
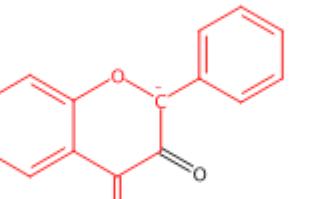
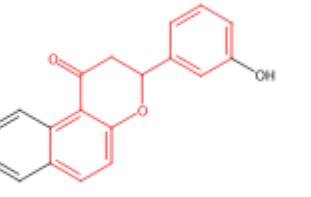
~1 ~5

C₁₅ H₇ D₅ O₂
4H-1-Benzopyran-4-one, 2,3-dihydro-2-(phenyl-d₃)- (9CI)

Spectra

同位素

亚结构检索结果

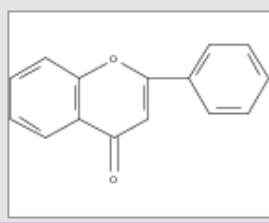
<p>281. 123251-10-5 </p> <p>~3  ~1 </p> <p>取代物</p> 	<p>295. 780723-19-5 </p> <p>~0 </p> <p>离子</p> 	<p>284. 136116-23-9 </p> <p>~2 </p> <p>稠环物质</p> 
<p>C₁₇ H₁₆ O₂ 4H-1-Benzopyran-4-one, 2,3-dihydro-6,8-dimethyl</p> <p>► Key Physical Properties Experimental Properties</p>	<p>C₁₅ H₉ O₃ 2H-1-Benzopyran-3,4-dione, 2-phenyl-, ion(1-)</p>	<p>C₁₉ H₁₄ O₃ 1H-Naphtho[2,1-b]pyran-1-one, 2,3-dihydro-3-(3-hydroxyphenyl)-</p> <p>► Key Physical Properties</p>

亚结构检索结果的限定

Analysis Refine

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

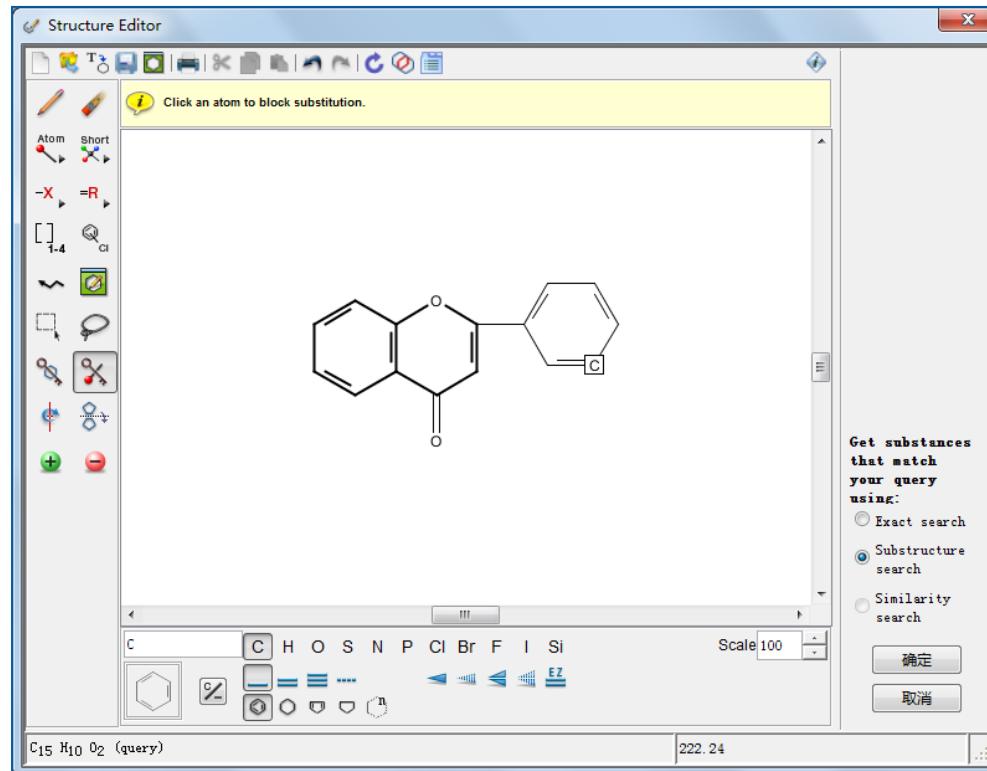
Chemical Structure:



Click image to change structure or view detail

Search type: **Substructure**

化学结构的再次限定



环锁定

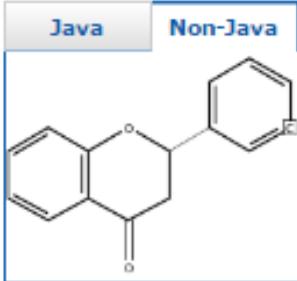


原子锁定

亚结构检索结果的限定

Structure Editor:

Java **Non-Java**



Click image to change structure or view detail.

Search type: **Substructure**

Only retrieve substances that:

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

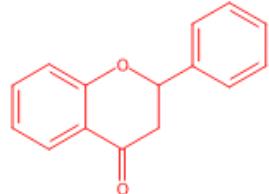
Refine

Get References Get Reactions Get Commercial Sources Tools

Sort by: Relevance 0 of 13826 Substances Selected

1. 487-26-3

~2093



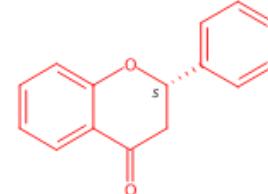
C₁₅H₁₂O₂
4H-1-Benzopyran-4-one, 2,3-dihydro-2-phenyl-

Key Physical Properties

Regulatory Information
Spectra
Experimental Properties

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

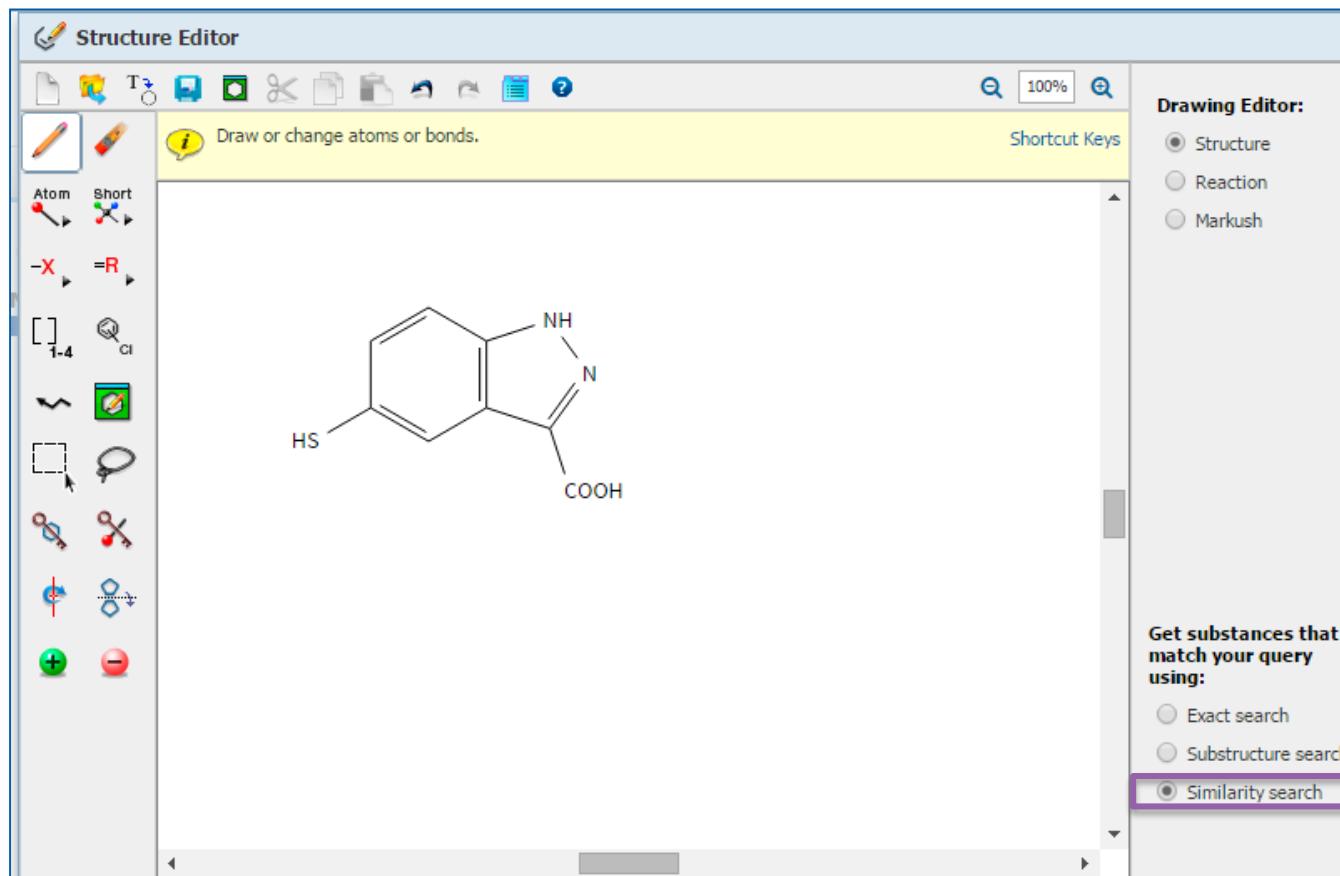
~2

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

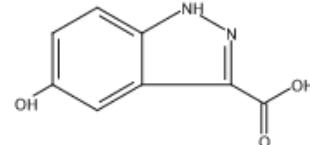
评分越高，相似度越高，结构越相似

Score: 88

1. 885518-94-5



~1



C₈ H₆ N₂ O₃

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

► Key Physical Properties

取代基变化

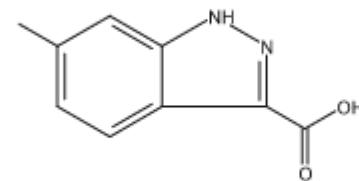
Score: 86

5. 858227-12-0

取代基位置变化



~7



C₉ H₈ N₂ O₂

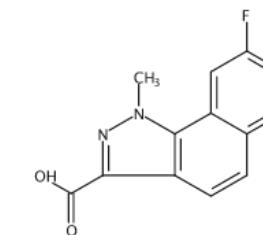
1H-Indazole-3-carboxylic acid, 6-methyl-

► Key Physical Properties

Score: 65

541. 1100422-

母体结构变化



C₁₃ H₉ FN₂ O₂

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

► Key Physical Properties



SCI-FINDER®
A CAS SOLUTION

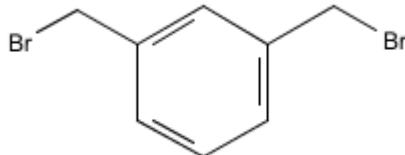
物质检索——相似结构检索

- 相似结构检索：

获得片段或整体结构与被检索结构相似的结果，母体结构可以被取代，也可以被改变

聚合物的检索

已知起始原料的聚合物



$(C_8H_8Br_2 \cdot C_4H_6O_4)_x$

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

623-24-5
 $C_8H_8Br_2$

110-15-6
 $C_4H_6O_4$

$(C_8H_8Br_2 \cdot C_4H_6O_4)_x$
Butanedioic acid, polymer with 1,4-bis(bromomethyl)benzene (9CI)

2. 132010-54-9

626-15-3
 $C_8H_8Br_2$

110-15-6
 $C_4H_6O_4$

$(C_8H_8Br_2 \cdot C_4H_6O_4)_x$
Butanedioic acid, polymer with 1,3-bis(bromomethyl)benzene (9CI)

分子式检索后会得到同分异构体

SCI-FINDER®
A CAS SOLUTION

聚合物的检索

Structure Editor

Draw or change atoms or bonds.

Atom Short

Structure Editor

Structure

Reaction

Markush

Br

Br

HOOC

COOH

Get substances that match your query using:

Exact search (radio button selected)

Substructure search

Similarity search

OK

Cancel

C₈H₈Br₂ · C₄H₆O₄ (query)

263.96 · 118.09

Characteristics

- Single component
- Commercially available
- Included in references

Classes

- Alloys
- Coordination compounds
- Incompletely defined
- Mixtures
- Polymers
- Organics, and others not listed

Studies

- Analytical
- Biological
- Preparation
- Reactant or reagent

单一组分
聚合物

0 of 1 Substance Selected

1. 132010-54-9

~2

626-15-3

C₈H₈Br₂

Br

110-15-6

C₄H₆O₄

OH

O

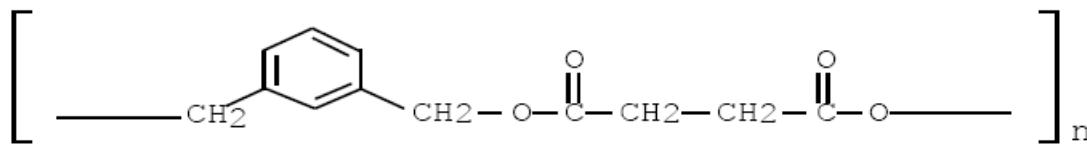
O

(C₈H₈Br₂ · C₄H₆O₄)_x

Butanedioic acid, polymer with 1,3-bis(bromomethyl)benzene (9CI)

聚合物的检索

已知重复单元的聚合物



(C12 H12 O4)n

SciFinder®

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

SUBSTANCES 2

Analyze Refine

Analyze by: Substance Role

- Preparation 34
- Properties 27
- Uses 24
- Process 14
- Reactant or Reagent 13
- Biological Study 7
- Analytical Study 3
- Prophetic in Patents 3
- Combinatorial Study 1
- Formation, Nonpreparative 1

Get References Get Reactions Get Commercial Sources Tools

Sort by: CAS Registry Number

0 of 45 Substances Selected

1. 1801551-81-4

2. 1637772-98-5

3. 1421756-46-8

4. 1392419-56-5

5. 1353713-96-8

6. 1341223-97-9

Click to view detail

(C12 H12 O4)n INDEX NAME NOT YET ASSIGNED

(C12 H8 D4 O4)n Poly[oxy-1,4-butanediyl oxycarbonyl(1,4-phenylene-2,3,5,6-d4) carbonyl]

(C12 H12 O4)n Poly[oxy-((R)-phenyl-1,2-ethanediyl)oxy(1,4-dioxo-1,4-butanediyl)]

Substance Image Cannot Be Displayed 1421756-46-8

Substance Image

Substance Image

聚合物的检索

Analyze Refine

Refine by: [?](#)

Chemical Structure

Isotope-Containing

Metal-Containing

Commercial Availability

Property Availability

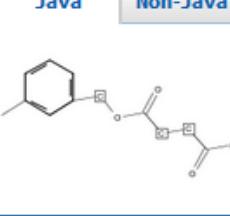
Property Value

Reference Availability

Atom Attachment

Structure Editor:

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



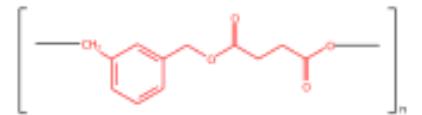
Click image to change structure or view detail.

Search type: **Substructure**

0 of 1 Substance Selected

1. [132010-11-8](#) 

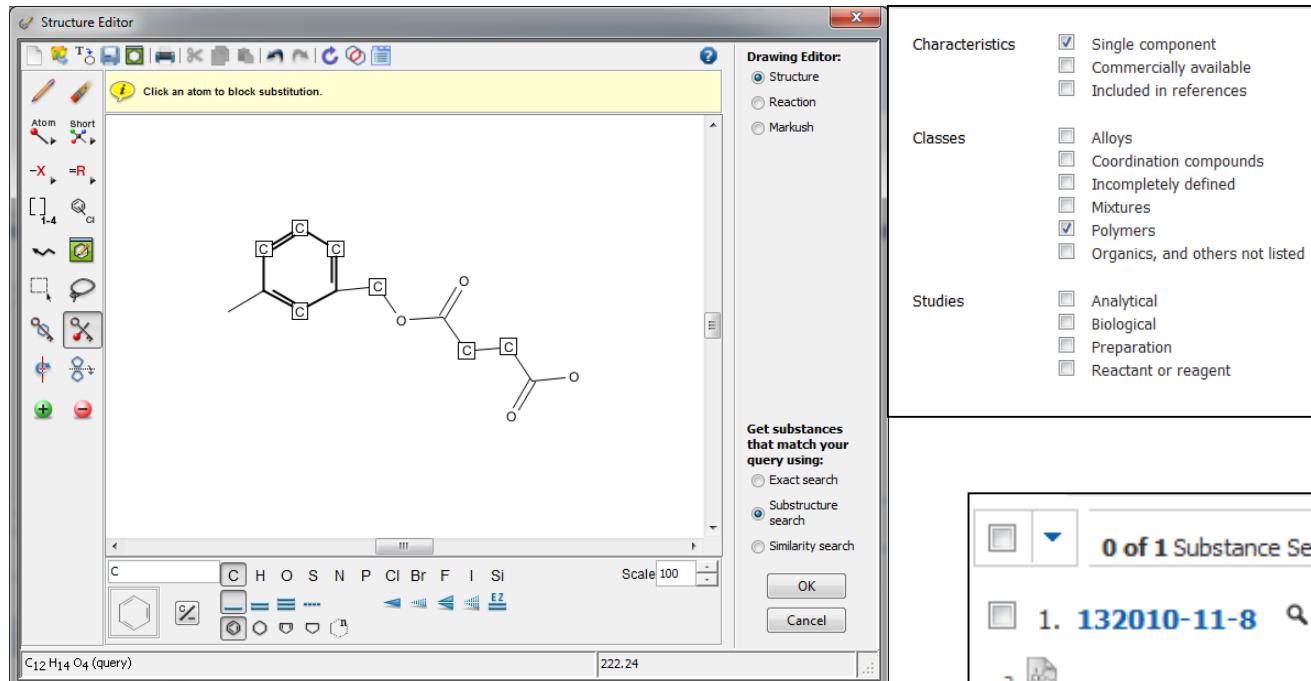
~2 



(C₁₂ H₁₂ O₄)_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

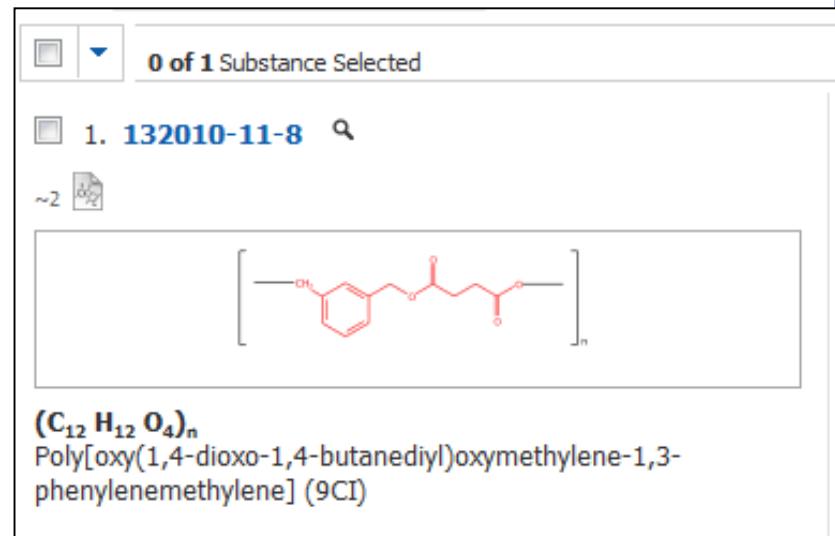
聚合物检索



单一组分

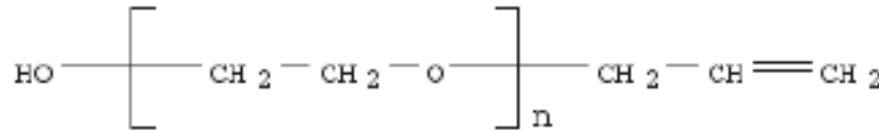
聚合物

绘制好SRU后用亚结构检索
因为两段为开放状态



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

SUBSTANCES: MOLECULAR FORMULA ?

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

Examples:
 H_4SiO_4
 $(\text{C}_3\text{H}_6\text{O}.\text{C}_2\text{H}_4\text{O})_x$

Search

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

↑
SRU部分 ↑
两端部分

0 of 4 Substances Selected

1. 1500029-22-0 ?

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

Poly(oxy-1,2-ethanediyl), α -(1-methylethylene)- ω -hydroxy-

2. 191403-44-8 ?

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

Poly(oxy-1,2-ethanediyl), α -1-propen-1-yl- ω -hydroxy-

3. 50856-25-2 ?

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

Poly(oxy-1,2-ethanediyl), α -ethenyl- ω -methoxy-

4. 27274-31-3 ?

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

Poly(oxy-1,2-ethanediyl), α -2-propen-1-yl- ω -hydroxy-

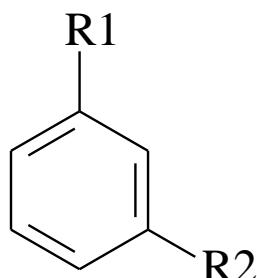
Regulatory Information

提纲

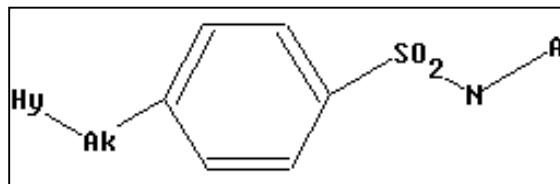
- 美国化学文摘社简介
- SciFinder简介及检索方式
 - 文献检索 (PatentPak)
 - 物质检索
 - **Markush检索**
 - 反应检索 (MethodsNow Synthesis)
 - SciPlanner
 - MethodsNow Analysis
- SciFinder常见问题及解决

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



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



Markush检索



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



Display Options

0 of 1969 References Selected

Page: 1 of 99

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

全部是专利

1. Compounds and methods for anticoagulation therapy

[Quick View](#) PATENTPAK

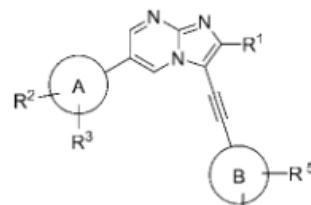
By Allende Rodriguez, Mikel; Hermida Santos, Jose; Montes Diaz, Ramon; Oyarzabal Santamarina, Julen
From PCT Int. Appl. (2016), WO 2016120432 A1 20160804. | Language: English, Database: CAPLUS

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

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

[Quick View](#) PATENTPAK

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



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

提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
 - 文献检索 (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

 **REACTIONS**
Reaction Structure

- 常用获取方法

- 已知物质：由物质获取反应

- 已知文献：从文献中获取反应

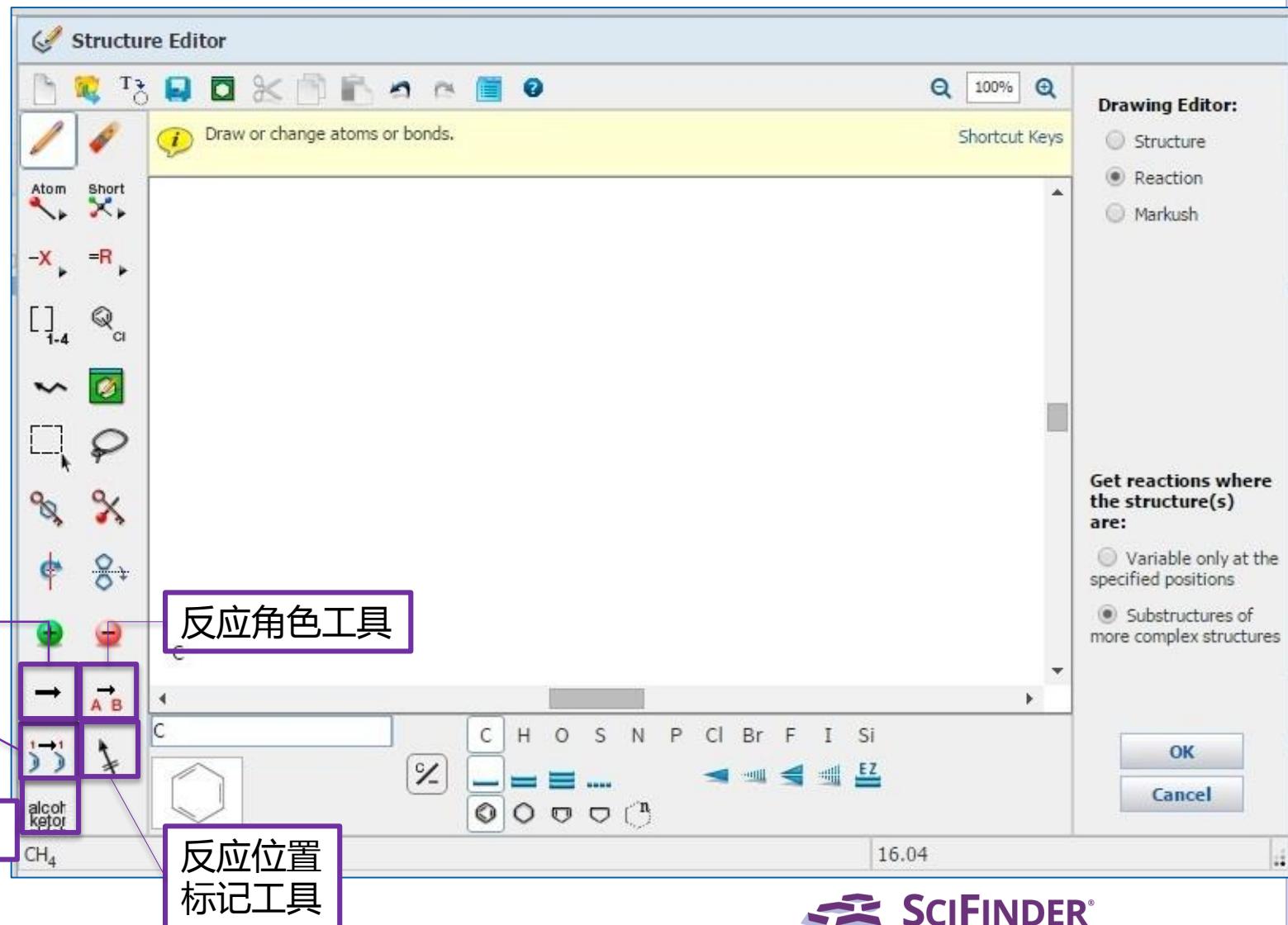
- 精确结构反应检索

- 亚结构反应检索

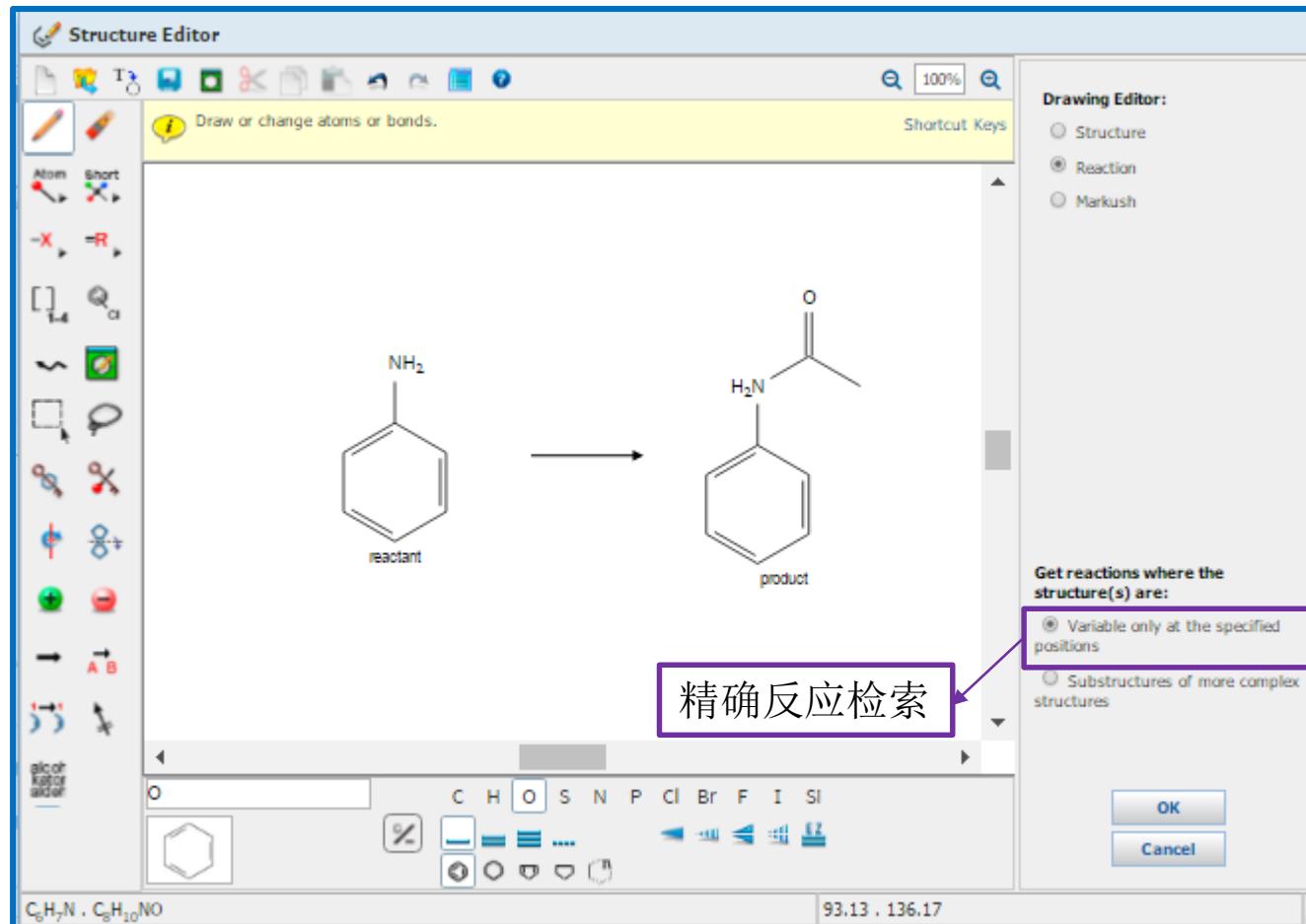
**Get reactions where
the structure(s)
are:**

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

反应绘制工具



SciFinder反应检索——精确反应检索



反应检索结果

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

Group by: No Grouping ▾ Sort by: Relevance ▾

No Grouping
Document
Transformation

1. View Reaction Detail 获取相似反应

Single Step Hover over any structure for more options.

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

选择相似反应的相似限制：

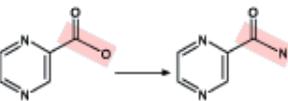
- Broad : 仅反应中心相似
- Miedum : 反应中心及附属原子和键
- Narrow : 反应中心及扩展的原子和键

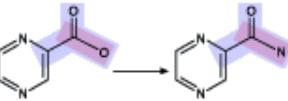
Get Similar Reactions ?

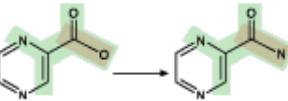
Retrieve similar reactions from:

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 Dicarbonates
188 Reactions

2. Acylation of Nitrogen Nucleophiles by Carboxylic Acids
81 Reactions

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

Y = O, S, NR'

更精确的查找需要的反应

反应检索结果的筛选

Analyze Refine

Group by: No Grouping Sort by: Relevance

Analyze by: Solvent

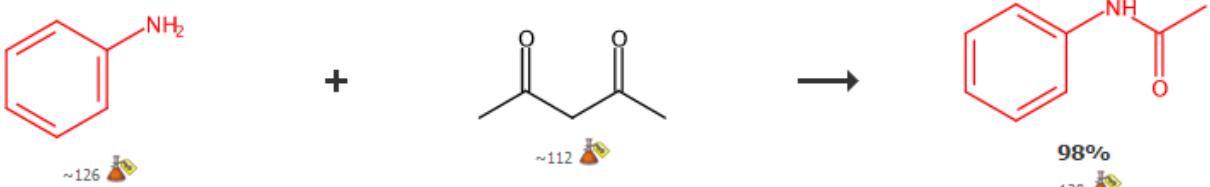
H ₂ O	99
CH ₂ Cl ₂	65
MeCN	55
THF	27
PhMe	26
AcOH	25
CHCl ₃	22
DMF	15
DMSO	15
Me ₂ CO	15

0 of 606 Reactions Selected

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

Single Step Hover over any structure for more options.

筛选用水作溶剂的反应



98%
~128

▼ Overview

Steps/Stages

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

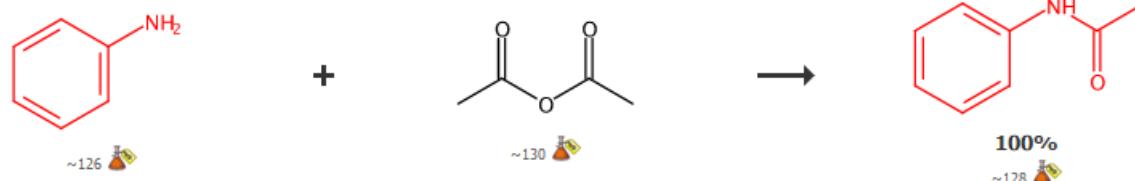
Notes

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

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(PPh_3)₄, S:BuNH₂, 21 h, 100°C
- 2.1 R:DMSO, R:Cl(O=)CC(=O)Cl, S:CH₂Cl₂, 15 min, -78°C
- 2.2 S:CH₂Cl₂, -78°C; 2 h, -78°C
- 2.3 R:Et₃N, 30 min, -78°C; -78°C → rt
- 2.4 R:LiCl, 20 min, 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: 5
- 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

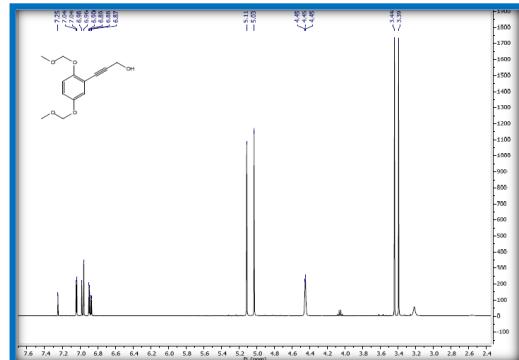
NATURAL PRODUCTS

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(Ph_3)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 H_2O (80 mL). The product was extracted with EtOAc (3 × 80 mL). The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4 , and evaporated under reduced pressure. The crude product was purified by silica gel column chromatography (EtOAc/hexanes, 10–50%). β -[2,5-Bis(methoxymethoxy)phenyl]prop-2-yn-1-ol² (**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 μL , 3.12 mmol) in dry CH₂Cl₂ (9 mL) was added to a stirred solution of DMSO (332 μL , 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 Na_2SO_4 , and evaporated under reduced pressure. β -[2,5-Bis(methoxymethoxy)phenyl]prop-2-ynal⁹ (**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-1a), 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), 95.58 (C-1a), 110.70 (C-2), 116.72 (C-6), 122.0 (C-5), 122.09 (C-3), 151.85 (C-4), 154.88 (C-1), 176.92 (C-9); HRESIMS m/z 273.0741 [M + Na]⁺ (calcd for C₁₃H₁₄O₅ 273.0739).



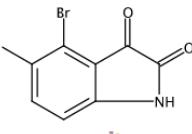
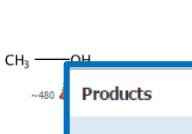
MethodsNow Synthesis

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

 ~106 	 ~480 	1
		Products Benzoic acid, 6-amino-2-bromo-3-methyl-, methyl ester, 84%, CAS RN: 147149-88-0
		Reactants 1-/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 $K_2S_2O_8$ (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 $K_2S_2O_8$ by aqueous 5% $Na_2S_2O_4$ solution (450 mL).6. After rotary evaporation under a reduced pressure at 55 °C, Leave a brown liquid.7. Mix the mixture with CH_2Cl_2 (6 L) and H_2O (4 L).8. Separate the organic phase.9. Extract the aqueous phase with CH_2Cl_2 (4 L).10. Dry the combined organic phases over Na_2SO_4.11. Concentrate the combined organic phases with a rotavapor.12. Distill the resulted brown liquid under high vacuum.
		Scale milligram
		1H NMR $CDCl_3$; δ 2.8 (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} : ν 3472, 3382, 2953, 2924, 1716, 1622, 1480, 1277, 816.

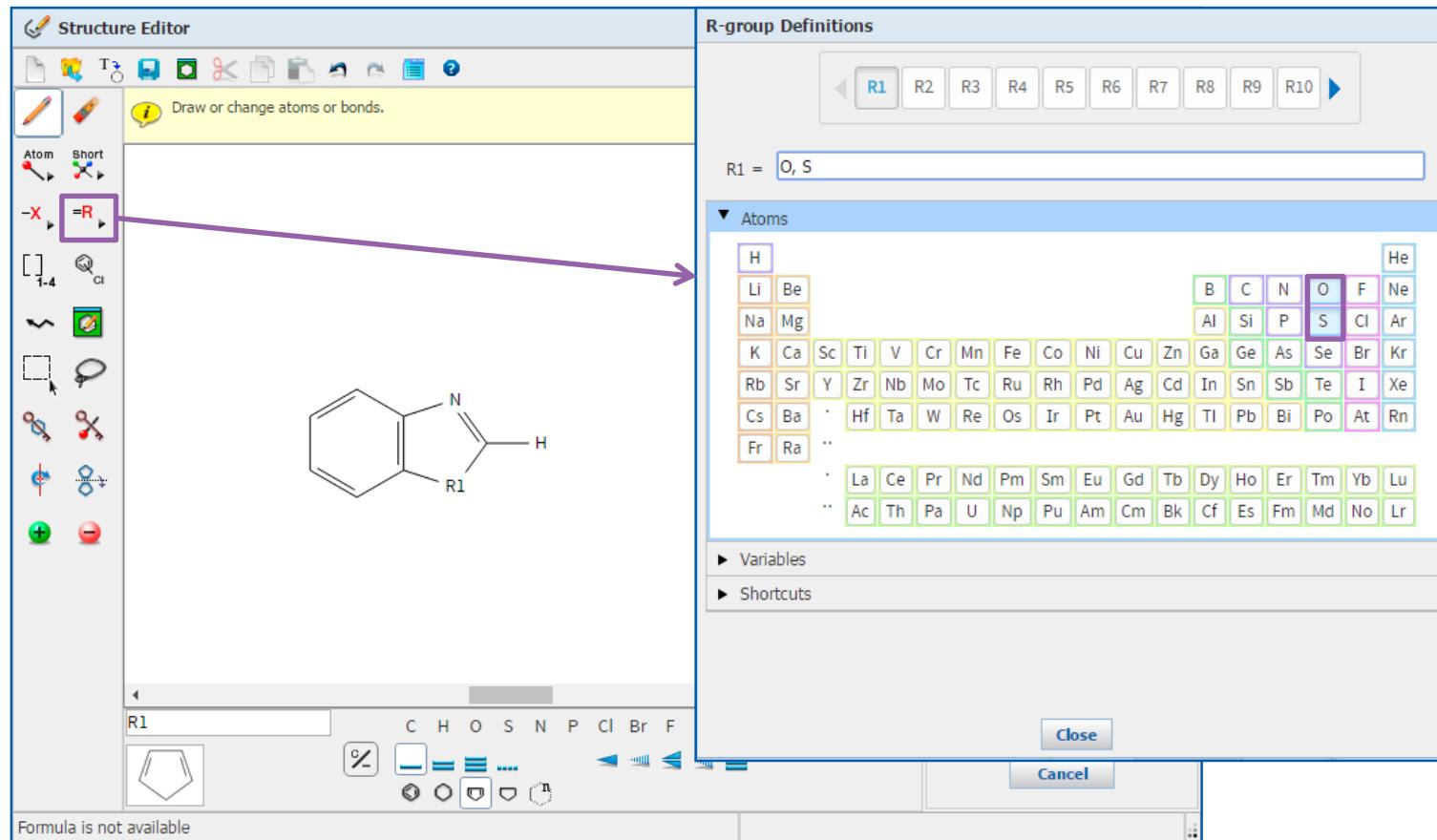
物质信息

实验过程

图谱信息

亚结构反应检索

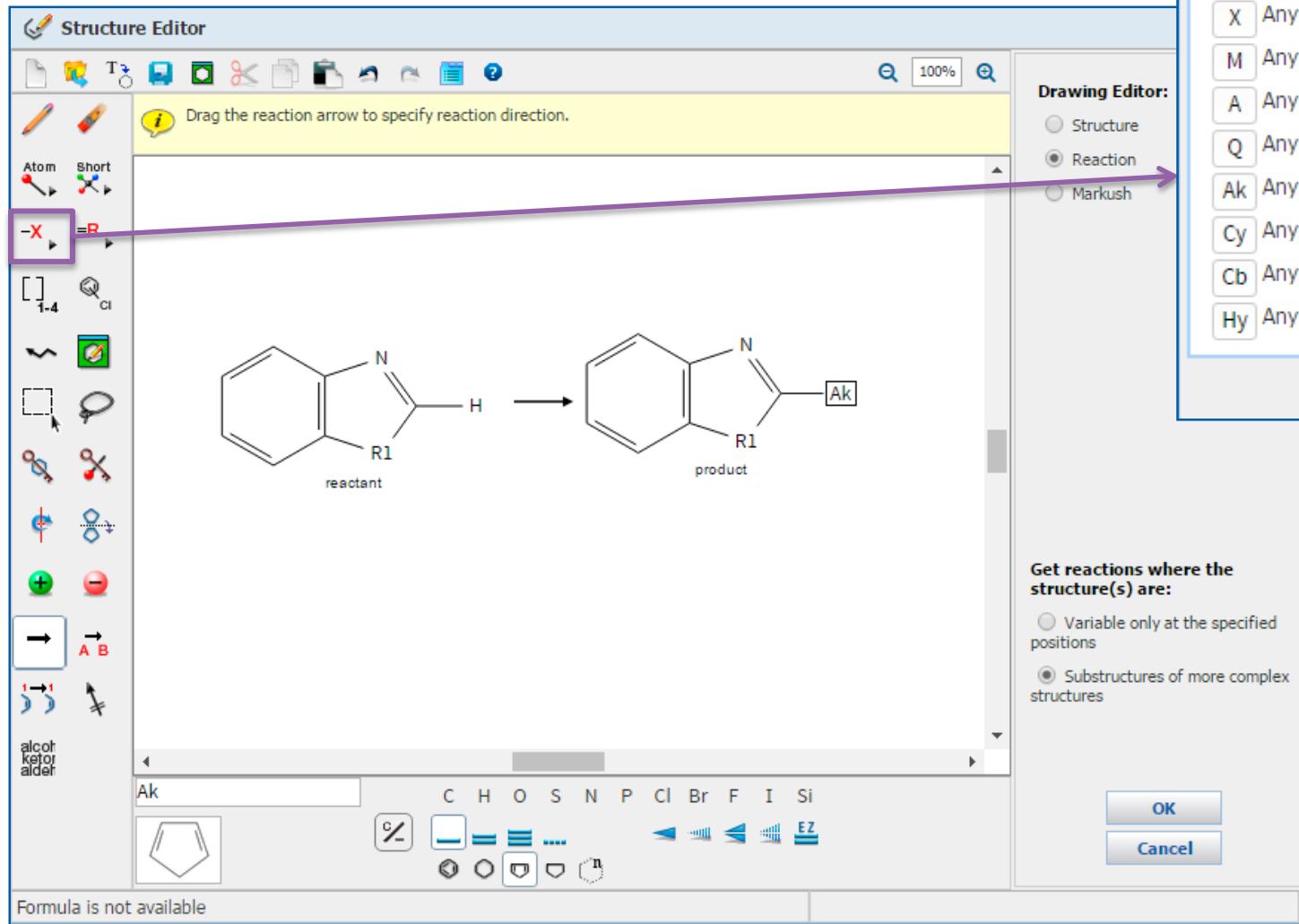
通过C-H活化对苯并噻唑或者恶唑进行烷基化



ACS / Proprietary and Confidential / Do Not Distribute

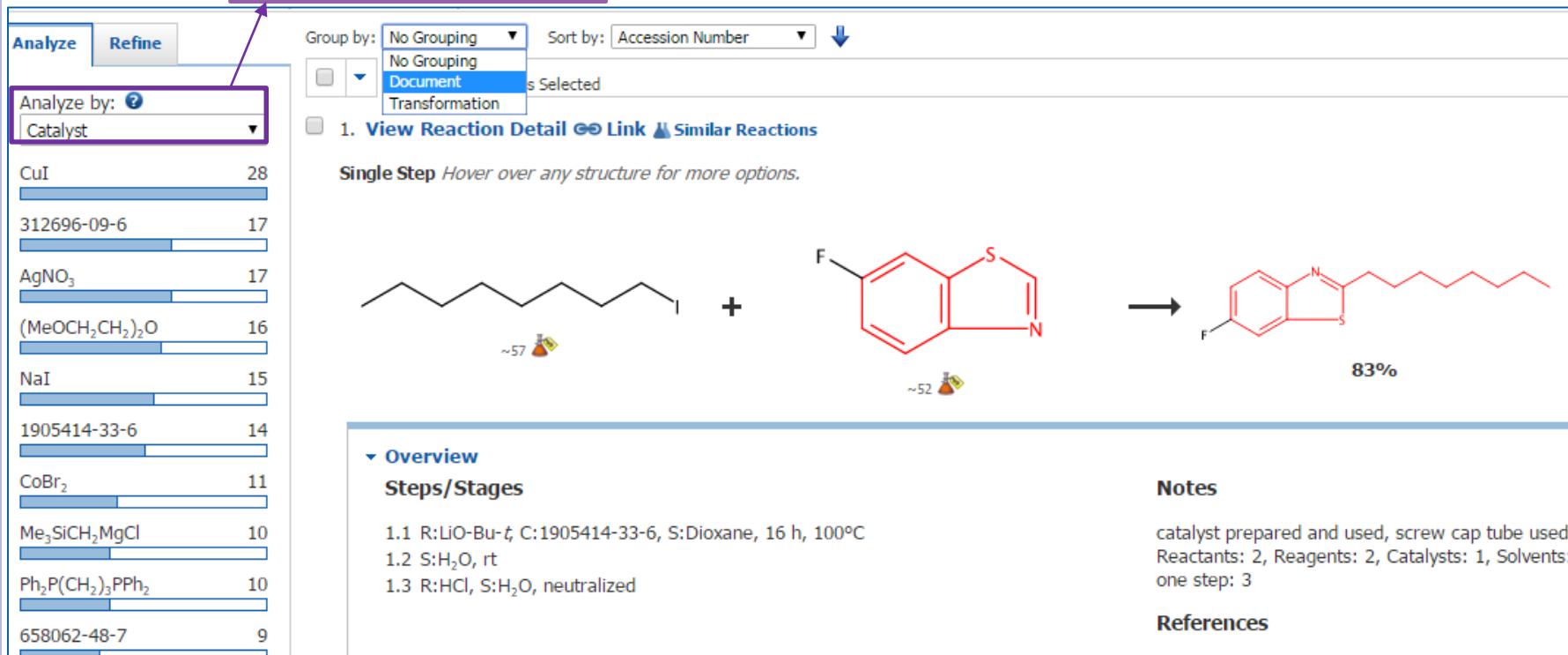
SCI-FINDER
A CAS SOLUTION

亚结构反应检索



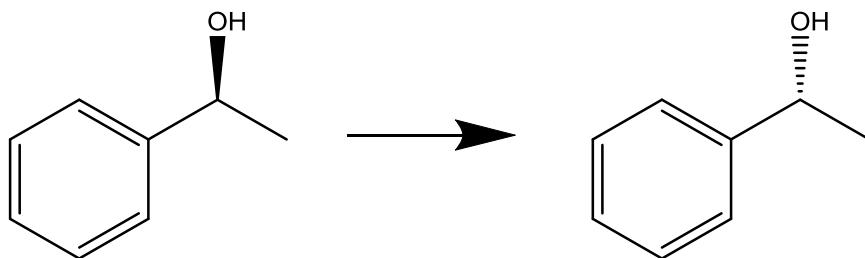
通过后处理工具筛选反应--Analyze

通过催化剂筛选反应



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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.



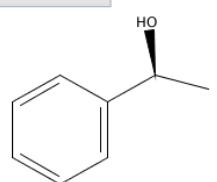
案例：如何获取手性翻转反应

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。

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

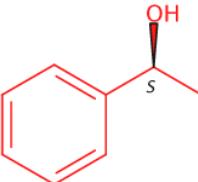
Show precision analysis

ChemDraw®
Launch a SciFinder substance search

1 of 52 Substances Selected

1. 1445-91-6 

~3499  ~90 



Absolute stereochemistry, Rotation (-).

C₈H₁₀O
Benzinemethanol, α -methyl-, (S)-

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

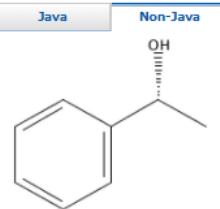
检索思路：

- 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

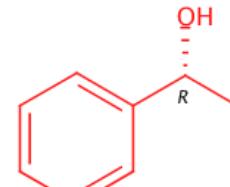
Show precision analysis

ChemDraw® Launch a SciFinder substance search

1 of 54 Substances Selected

1. 1517-69-7 

~3531  ~94 



Absolute stereochemistry,,Rotation (+).

C₈H₁₀O
Benzinemethanol, 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

Reactions (52) > get reactions (7938)

Get References Tools ▾

Group by: No Group

Find Additional Reactions

Combine Answer Sets

0 of 79. 1. View Reaction Details

4 Steps Hover over any structure for more options.

Send to SciPlanner

Display Options

Page: 1 of 530

Combine Answer Sets

2 of 50 Reaction A

2 (4185)
产物
Chemical Structure

1 (7938)
反应物
Chemical Structure

2 (3888)
Chemical Structure

1 (9519)
Chemical Structure

手性2 (172)

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

Combine Include all reactions from both sets

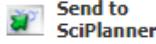
Intersect Include only reactions that appear in both sets

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 ▾ 

Group by: No Grouping Sort by: Accession Number  Display Options

 0 of 27 Reactions Selected  Page: 1 of 2 

1. [View Reaction Detail](#) 

Single Step Hover over any structure for more options.


Reaction scheme showing the conversion of 1-phenylethanol to (R)-1-phenylethanol. The reactant is 1-phenylethanol (a benzene ring attached to a CH₂OH group). The product is (R)-1-phenylethanol, where the hydroxyl group is shown with a wedge bond, indicating its absolute configuration. The yield is 100%.

 Overview

Steps/Stages

1.1 S:H₂O, 5:Me,  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

▲
▼

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

Search

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

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

Single Step Hover over any structure for more options.

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

3 Steps Hover over any structure for more options.

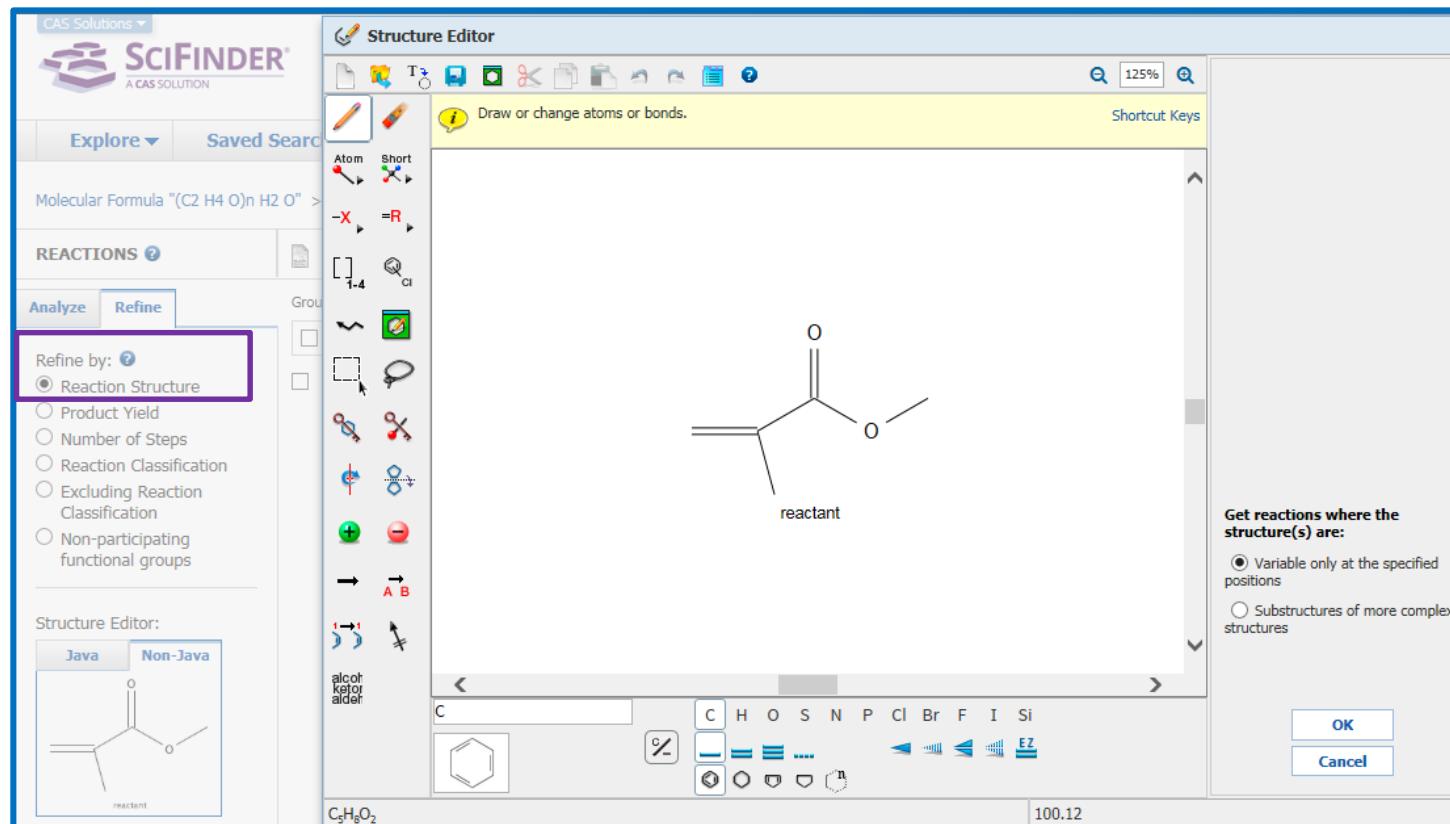
Overview

Steps/Stages

1.1 S:EtC(=O)
1.2 80°C

[Step 3.1]

限定反应：根据参与反应的甲基丙烯酸甲酯，限定反应结构



获得改性后的聚合物：获得甲基丙烯酸甲酯(MMA)接枝的PEG

Analyze Refine Group by: No Grouping Sort by: Relevance Display Options

Analyze by: Reagent

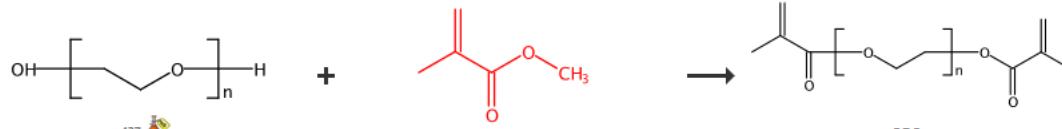
NaN ₃	23
DCC	17
NaOH	17
Et ₃ N	16
(NH ₄) ₂ S ₂ O ₈	12
NH ₃	11
NH ₄ Cl	11
MeOH	10
25190-89-0	8
9004-82-4	8

0 of 156 Reactions Selected

Page: 1 of 11

1. View Reaction Detail [Link](#)

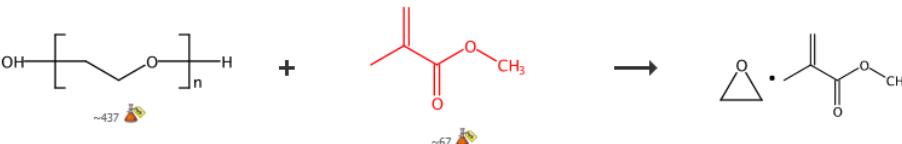
Single Step Hover over any structure for more options.



MMA封端的PEG

3. View Reaction Detail [Link](#)

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:Pheno

~437 

~67 

Overview Steps/Stages

1.1 C:(PhCO₂)₂, S:CH₂Cl₂, 6 h, 80°C

Notes

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

References

Chemistry modification of PMMA-g-PEG copolymer

Quick View  Other Sources

By Rosa, Juliana dos Santos et al
From Macromolecular Symposia, 343(1), 78-87; 2014

提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
 - 文献检索 (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

勾选想要的反应

3 Steps Hover over any structure for more options.

Send to SciPlanner

Display Options

进入Sciplanner 新建文件

将刚推送过来的反应拖至编辑面板

The screenshot shows the SciPlanner software interface. At the top, there is a reaction setup window with a checked checkbox for 'View Reaction Detail'. A pink box highlights the text '勾选想要的反应' (Check the reactions you want). Below this, a reaction scheme is shown with two reagents and a product. A pink box highlights the text '3 Steps Hover over any structure for more options.' and the 'Send to SciPlanner' button. Another pink box highlights the text '进入Sciplanner 新建文件' (Enter SciPlanner to create a new file). The main workspace below shows an empty 'Workspace' with a toolbar and a 'SciPlanner' menu bar. A pink box highlights the text '将刚推送过来的反应拖至编辑面板' (Drag the just-pushed reaction to the editing panel). On the right, there is a 'Reaction Library' panel with a reaction scheme and a 'Clear Reactions' button.

SciPlanner使用简介

打开中间产物的标准菜单
选择Synthesis this

在检索到的反应中选择感兴趣的反应

继续推送到SciPlanner

SciPlanner

Workspace Edit View GoTo

CAS Registry Number: 13091-23-1

View Substance Detail

Explore by Structure

Synthesize this...

Get Reactions where Substance is a

Get Commercial Sources

Get Regulatory Information

Get References

Export as Image

Export as molfile

1 → Cl → 2 → 3 →

Send selected records to SciPlanner.

Group by: No Grouping Sort by: Accession Number

1 of 34 Reactions Selected

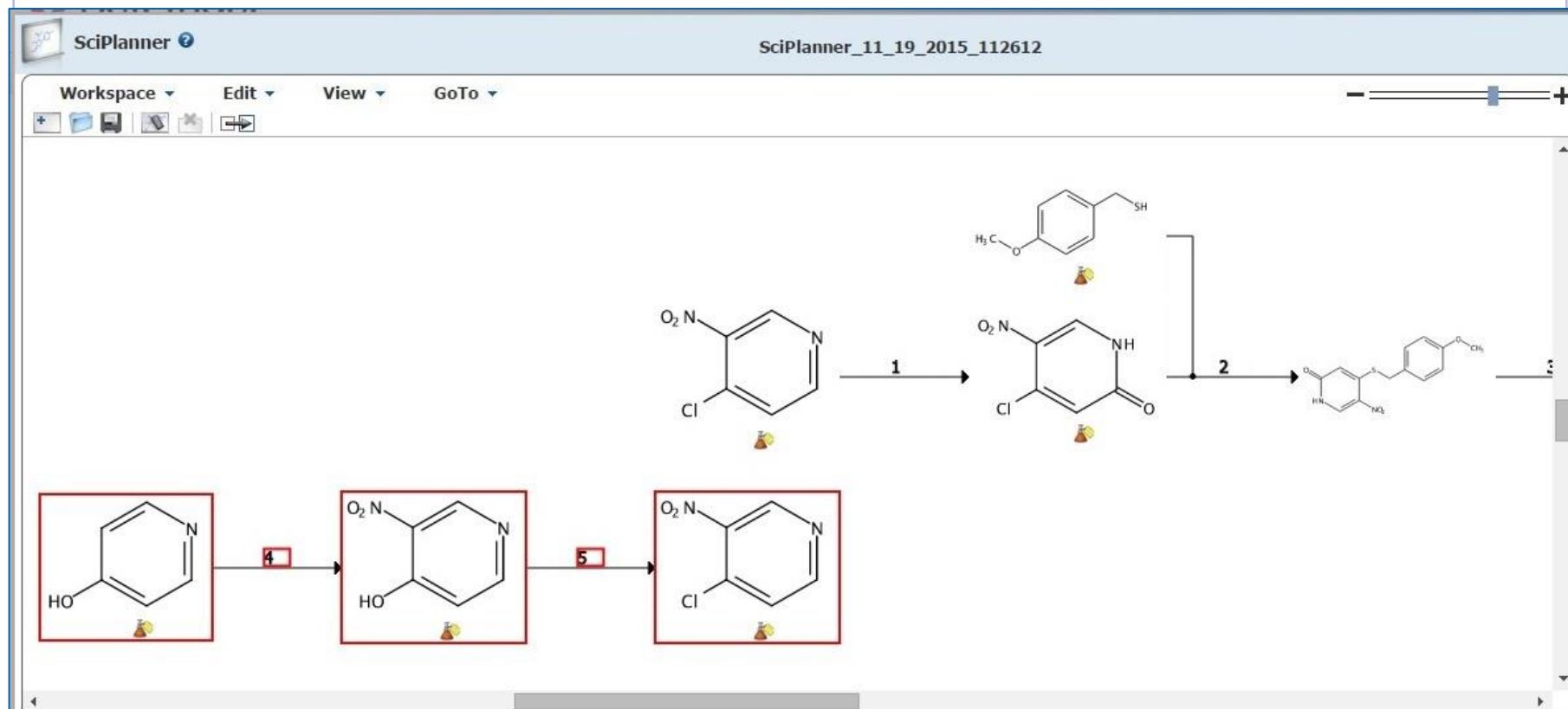
1. View Reaction Detail

2 Steps Hover over any structure for more options.

HO → O₂ N

~161 ~192

SciPlanner使用简介



步骤同前，将推送过来的反应拖到编辑面板中，可以看到两条反应中存在同样的结构

SciPlanner使用简介

SciPlanner ?

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

Reaction Diagram:

Reaction 1: 4-nitro-2-pyridine → 4-nitro-2-chloropyridine (step 5)

Reaction 2: 4-nitro-2-chloropyridine → 4-nitro-2,6-dichloropyridine (step 1)

Reaction 3: 4-nitro-2,6-dichloropyridine → 4-nitro-2,6-dichloro-3-((2-methoxybenzyl)thio)pyridine (step 4)

Export Dialog:

For: Offline Review

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

Saving Locally

SciPlanner eXchange (*.pkx)

Details:

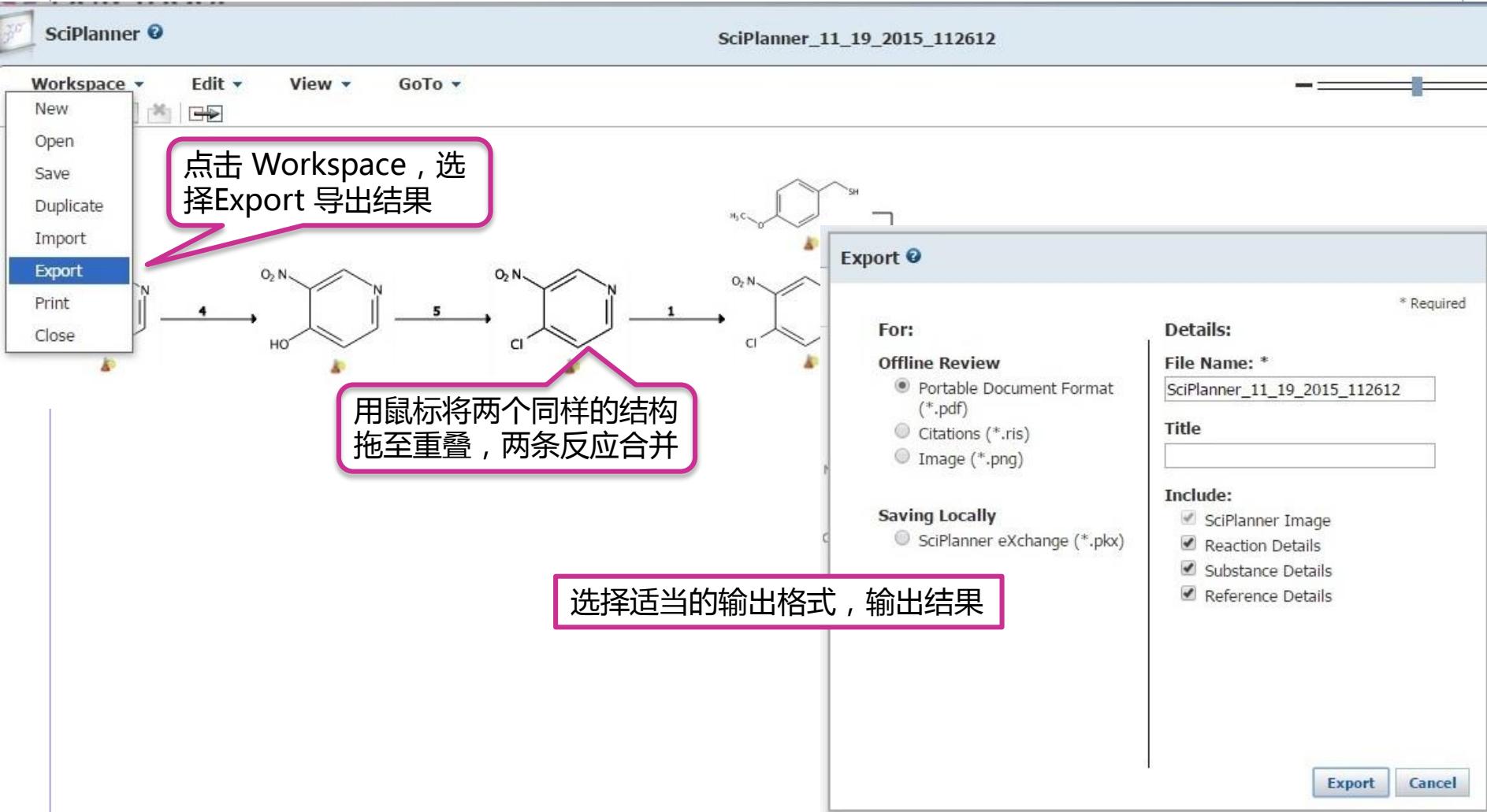
File Name: * SciPlanner_11_19_2015_112612

Title:

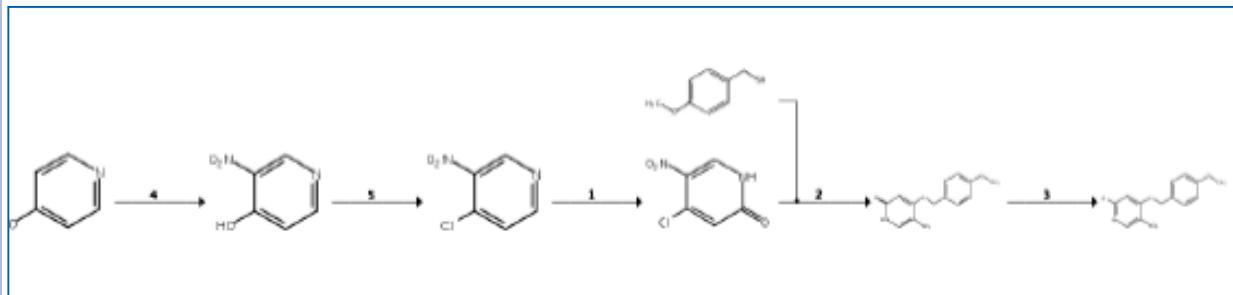
Include:

SciPlanner Image
 Reaction Details
 Substance Details
 Reference Details

Export Cancel



SciPlanner导出结果



Reaction	Stages	Notes	Yield
5	1.1 R:POCl ₃ , S:PhMe, 0°C → rt; 16 h, rt → 110°C 1.2 R:K ₂ CO ₃ , S:H ₂ O, cooled, pH 10	Reactants: 1, Reagents: 2, Solvents: 2, Steps: 1, Stages: 2 Transformation: 1. Formation of Alkyl Halides from Alcohols	90%
References			
<p>High color rendering index and color stable hybrid white efficient OLEDs with a double emitting layer structure using a single phosphorescence dopant of heteroleptic platinum complexes By Poloeck, Anurach et al From Journal of Materials Chemistry C: Materials for Optical and Electronic Devices, 2(48), 10343-10356; 2014</p>			

Substance Information		
1228150-22-8 C ₁₃ H ₁₂ N ₂ O ₄ S 2(1H)-Pyridinone, 4-[[4-methoxyphenyl]methyl]thio]-5-nitro-	1228150-23-9 C ₁₃ H ₁₁ ClN ₂ O ₄ S Pyridine, 2-chloro-4-[[4-methoxyphenyl]methyl]thio]-5-nitro-	13091-23-1 C ₆ H ₃ ClN ₂ O ₂ Pyridine, 4-chloro-3-nitro-
5435-54-1 C ₆ H ₄ N ₂ O ₃ 4-Pyridinol, 3-nitro-	6258-60-2 C ₈ H ₁₀ OS Benzenemethanethiol, 4-methoxy-	626-64-2 C ₆ H ₅ N ₂ O 4-Pyridinol
850663-54-6 C ₉ H ₇ ClN ₂ O ₃ 2(1H)-Pyridinone, 4-chloro-5-nitro-		

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
- 来自重要的全文信息资源：CAS高质量标引、全新的、增值的方法
- 满足合成和分析研究工作者的需求
- 分析与合成两个模块
- 逾百万的合成和分析方法合集——数量持续增加!



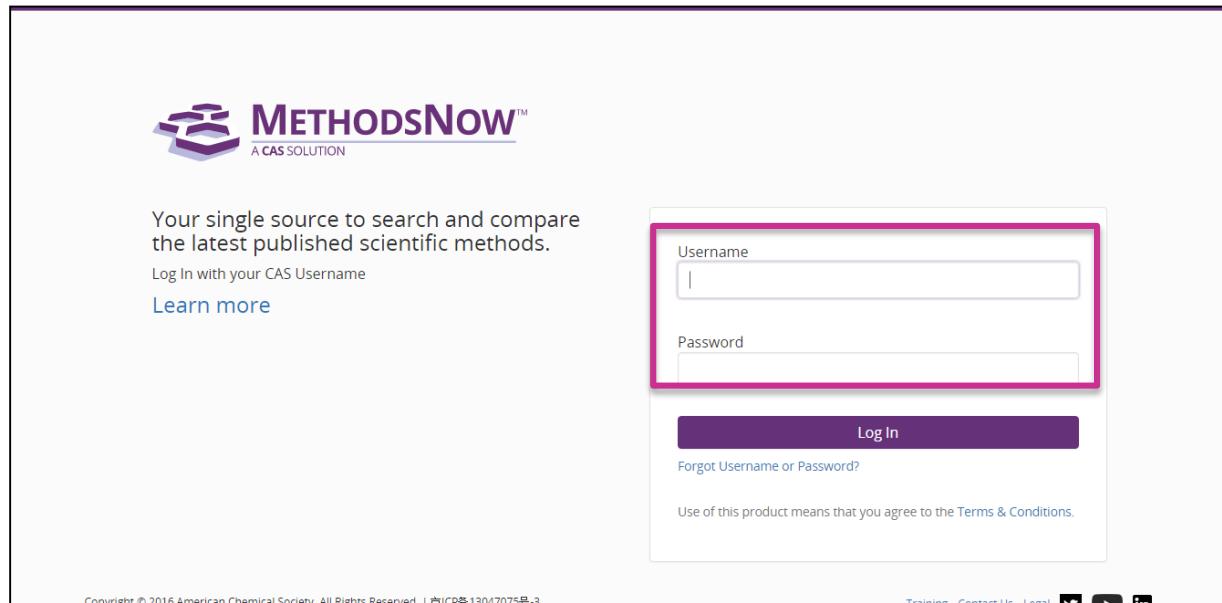
MethodsNow – Analysis(www.methodsnnow.com)

- 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，生物标记细胞实验，生物标记药物实验，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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输入SciFinder的账号密码



MethodsNow – Analysis(www.methodsnnow.com)

检索/高级检索



方法分类



历史检索



高级检索

The screenshot shows the METHODSNOW Advanced Search interface. The top navigation bar includes 'CAS Solutions', the METHODSNOW logo, 'Saved', and 'Account'. Below the navigation is a search bar with a 'Return to Home' link. The main search area is titled 'Advanced Search' and contains a 'Keyword' input field, an 'AND' dropdown menu with 'Matrix' selected, and another 'AND' dropdown menu with 'Analyte' selected. A 'Add Search Criteria' button is available. A search button with a magnifying glass icon is highlighted with a purple box and labeled '增加检索条件' (Add search criteria). A dropdown menu is open, showing options: 'Publication Name' (highlighted with a purple box and labeled '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, Publication Name)), 'Keyword', 'Analyte', 'Matrix', 'Method Category', 'Technique', 'CAS Method Number', and 'Publication Name'. A purple box labeled '逻辑运算符: and, or, not' (Logical operators: and, or, not) points to the 'AND' dropdowns. A purple box labeled '删除检索条件' (Delete search criteria) points to the 'X' button in the top right corner of the search bar. The bottom right corner features the SCI-FINDER logo.

案例：高效液相色谱法测定血液中罗红霉素的含量

CAS Solutions ▾

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Search

Enter keyword, matrix, analyte, etc.

roxithromycin

Advanced Search

Search

此处只需输入一个关键词即可

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

Analyte

- Roxithromycin (5)
- (+)-Cycloserine (1)
- (+)-Ethambutol (1)
- Ambroxol hydrochloride (1)
- 4-Aminosalicylic acid (1)

[View All](#)

Matrix

- Blood plasma (5)

Method Category

- Active Pharmaceutical Ingredient and Metabolite Analysis (5)
- Toxin Assay (1)

Technique

- HPLC-tandem mass spectrometry (3)
- Atmospheric precipitation (1)
- Electrospray ionization tandem mass spectrometry (1)
- High-performance liquid

Analysis of Roxithromycin in Blood plasma by HPLC-tandem mass spectrometry

CAS MN: 1-101-CAS-1241367

[View Details & Instructions](#) 查看方法详情

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Analyte: Roxithromycin; Ambroxol hydrochloride

Matrix: Blood plasma

Other Materials: Reagent: Methanol; Acetonitrile; Ammonium acetate; Heparin
Material: C₁₈ 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](#)

Abstract

结果显示

Method Detail (2 of 5)

实验材料

文献信息

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

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: JCBAAI | 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 μ L 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 μ L aliquots of acetonitrile and transfer the sample to a glass reaction vial.
2. Add a 100 μ L aliquots of a 2.5 mg/L 9-fluorenylmethyl chloroformate (FMOC-Cl) in acetonitrile and 100 μ L aliquots of a phosphate buffer, pH 7.5.
3. Incubate the sample at 40 °C for 40 min.
4. Inject an aliquot 100 μ L 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 μ L) using autosampler model G1313A.
5. Perform the separation on a 125 x 4.6 mm i.d. LiChrospher RP-18e column packed with 5 μ m particles, with a guard column (LiChrospher RP-18e), both from Merck.

实验步骤

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

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	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)
Analyte	Roxithromycin; Ambroxol hydrochloride	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
Matrix	Blood plasma	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
	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	Instrument: Detection- SIM mode. Chromatographic: Injection volume- 20 µL; mobile phase- (75:25, v/v) of View All
	Preparation Collection of plasma samples	Standards Preparation	Stochastic resonance is applied to quantitative analysis for weak chromatographic signal of View All
			Plasma samples



提纲

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 - 物质检索
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 - SciPlanner
 - MethodsNow Analysis
- SciFinder常见问题及解决

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 - . (句点)
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3. 密码必须包含 7-15 个字符，并且至少包含三种以下字符：
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 - 混合的大小写字母
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