

朱传娴

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hzhu@acsi.info

# 如何使用SciFinder获取科技信息

华东理工大学

2016.11.10



# 提纲

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

# 美国化学文摘社—Chemical Abstracts Service

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

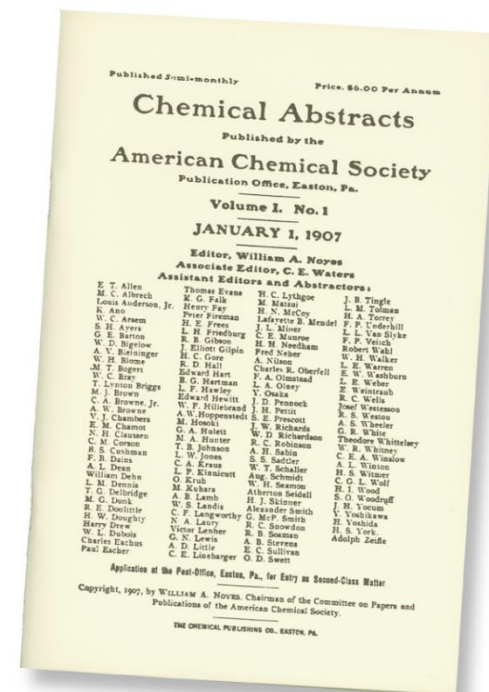


# 1907年，信息的汇集、管理发生了重大的变化



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



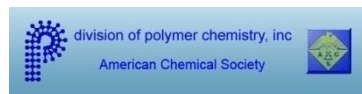
arXiv.org

Aldrichimica ACTA

ACS  
chemical  
biology



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OF ORGANIC CHEMISTRY



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

ACS Chemical  
Neuroscience



THE JOURNAL OF  
PHYSICAL CHEMISTRY  
Letters

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# CAS——构建最高质量的化学数据库



# CAS数据库——源于化学，超越化学

## 生物化学：

农化产品管控信息,生化遗传学,发酵,免疫化学,药理学

## 有机化学各领域：

氨基酸,生物分子,碳水化合物,有机金属化合物,类固醇

## 大分子化学各领域：

纤维素、木质素、造纸;涂料、墨水

染料、有机颜料;合成橡胶;纺织品、纤维

## 应用化学各领域：

大气污染,陶瓷,精油、化妆品,化石燃料,黑色金属、合金

## 物理、无机、分析化学各领域：

表面化学,催化剂,相平衡,核现象,电化学

# CAS数据库最具价值的内容——人工索引


## 4. Process for preparation of novel sofosbuvir crystal

By: Zhou, Haohui; Lin, Guoliang; Wu, Yao; Zou, Wenjuan; Chan, Yunxia

Assignee: Beijing Winsunny Pharmaceutical Co., Ltd., Peop. Rep. China

The invention relates to a novel sofosbuvir crystal having high stability and soly. The novel sofosbuvir crystal is prepd. through crystg. sofosbuvir in pos. solvent and neg. solvent. The method has high repeatability, easy control, high yield, and high product purity.

### Patent Information

Patent No.	Kind	Language	Date	Application No.	Date
CN 105732751  PATENTPAK	A		Jul 6, 2016	CN 2014-10742897	Dec 9, 2014

### Priority Application

CN 2014-10742897	Dec 9, 2014
------------------	-------------

### Indexing


Carbohydrates (Section33-9)

Section cross-reference(s): 34, 63

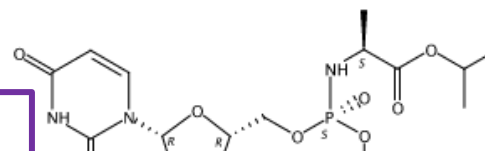
### Concepts

Crystallization	Drug bioavailability
Hepatitis C	Hepatitis C virus
Homo sapiens	Human
Pharmaceutical coated tablets	

### Substances

**1190307-88-0P Sofosbuvir**   
Absolute stereochemistry.

Page 2 in **PATENTPAK**



### Tips:

1. 98%以上的文献，都经过人工索引
2. 用Index Term标引文献中的重要技术术语
3. 用CAS RN标引出文献中的重要物质
4. 用CAS Role标引文献中重要物质的研究领域



# CAS人工标引解决的问题

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

# CAS最新动向—解决方案

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# CAS最新动向—解决方案

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

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

Quick View PATENTPAK

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

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

Patent No.	Kind	Language
WO 2016100441	A1	English

Patent Family

Patent No.	Kind	Language
US 20160176911	A1	English

atkina, Natalia  
Language: English, Database: CAPLUS

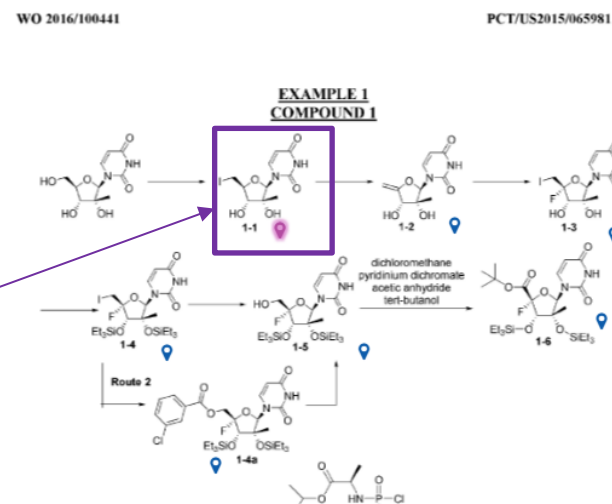
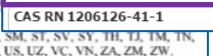
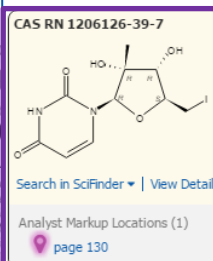
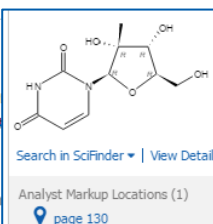
B is substituted purine and pyrimidine nucleobase; dashed bond between R and R' is absent, then R is H, substituted each R<sup>6</sup> and R<sup>7</sup> are independently hydrogen or deuterium; R<sup>5</sup> is -OH or F; methods of synthesizing nucleotide analogs and as a HCV infection with one or more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

7. Process for preparation of sofosbuvir

Quick View PATENTPAK

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

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



# 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

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Reaction Structure substructure > reactions (9)
Save   Print   Export

**REACTIONS** 1

Analyze Surface

Analyze by: 1

Report

Et<sub>3</sub>N 9

K<sub>2</sub>CO<sub>3</sub> 6

EDM(Ph)<sub>2</sub> 2

[Show Photo](#)

Get References Tools ▾

Group by: No Grouping   Sort by: Relevance ▾

1 of 9 reactions Selected

☐ 1. [View Reaction Detail](#) [Link](#) [Send to SciFinder](#)

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

**Overview**

**MethodNow™**

**Procedure**

1. Stir the mixture of 7-ethyl-4-methyl-2-methyl-2H-chromen-3-one (400 mg, 1.65 mmol), 1-iododecane (308 mg, 1.82 mmol), copper(II) sulfate pentahydrate (42 mg, 0.17 mmol), (+)-sodium-L-ascorbate (360 mg, 1.82 mmol) in t-BuOH/water (15 mL/25 mL) at room temperature for 4 hours.

[View more...](#)

**Available Experimental Data**

<sup>1</sup>H NMR, <sup>13</sup>C NMR, IR, HRMS, Mass Spec, MP

[View with MethodNow](#)

## 嵌在SciFinder中的合成模块

**METHODS**

Return to Home

- Analyte
  - Atorvastatin (227)
  - Atorvastatin calcium (211)
  - Ezetimibe (80)
  - Amlodipine besylate (56)
  - Fenofibrate (46)
  - [View All](#)
- Matrix
  - Pharmaceutical tablets (293)
  - Blood plasma (60)
  - Tablets (49)
  - Pharmaceutical capsules (34)
  - Garcinia atroviridis (20)
  - [View All](#)
- Method Category
  - Technique
    - Reversed-phase HPLC (152)
    - Spectrophotometry (101)
    - UV-visible spectroscopy (71)
    - HPLC (57)
    - Liquid chromatographic UV detectors (43)
    - [View All](#)

Results (528)

Sort Relevance

☐ ☐

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

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

## 单独的分析界面

# 提纲

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

# SciFinder覆盖的数据库



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

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(Do not use on a shared computer)

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SciFinder® is a research discovery application that provides integrated access to the world's most comprehensive and authoritative source of references, substances and reactions in chemistry and related sciences.

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### News & Updates

**Welcome to SciFinder**

**Did you notice our new look?**  
Our new branding will also be phased into training and other support materials in the coming months. If you are a Key Contact and have questions, or need assistance updating logos on any of your organization's websites, please contact the [CAS Customer Center](#).

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**New Commercial Source Logos**

# SciFinder主界面

检索完，请点击退出

工具栏

The screenshot shows the SciFinder web interface. At the top, there is a header bar with the SciFinder logo and navigation links. Below this is a secondary bar with tabs for 'Explore', 'Saved Searches', and 'SciPlanner'. The main content area is titled 'REFERENCES: RESEARCH TOPIC' and features a search input field with example text and a 'Search' button. On the left, a sidebar lists various search categories under 'REFERENCES', 'SUBSTANCES', and 'REACTIONS'. On the right, there is a section for 'SAVED ANSWER SETS' showing a list of saved searches and a 'KEEP ME POSTED' section.

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Explore | Saved Searches | SciPlanner

**REFERENCES**

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

**SUBSTANCES**

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

**REACTIONS**

- Reaction Structure

REFERENCES: RESEARCH TOPIC

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

[Search](#)

[Advanced Search](#)

**SAVED ANSWER SETS**

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

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已保存的结果集

检索入口

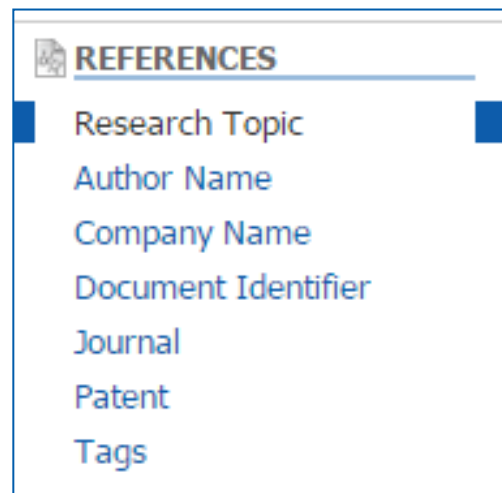
定题追踪



# SciFinder检索——文献检索

## ■ 文献检索方法

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



## ■ 检索策略推荐

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

# 文献检索——主题

主题检索：三维石墨烯的制备

检索式：prepare of 3D graphene

The screenshot displays the SciFinder web interface. At the top, the 'CAS Solutions' logo and 'SciFinder A CAS SOLUTION' are visible. Below the navigation bar (Explore, Saved Searches, SciPlanner), the breadcrumb trail reads: 'Research Topic "prepare of 3D graphene" > references (767) > Facile Synthesis of 3D Graphen...'. On the left sidebar, under the 'REFERENCES' section, various search criteria are listed: Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, Tags, and SUBSTANCES (Chemical Structure, Markush). The main search area on the right shows the input 'prepare of 3D graphene' in a text box. Below this, 'Examples:' are provided: 'The effect of antibiotic residues on dairy products' and 'Photocyanation of aromatic compounds'. A blue 'Search' button is positioned below the examples, followed by a link to 'Advanced Search'.

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Explore ▼ Saved Searches ▼ SciPlanner

Research Topic "prepare of 3D graphene" > references (767) > Facile Synthesis of 3D Graphen...

**REFERENCES**

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

**SUBSTANCES**

- Chemical Structure
- Markush

**REFERENCES: RESEARCH TOPIC ?**

prepare of 3D graphene

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

**Search**

Advanced Search

关键词之间用介词连接：in, with, of...

# 主题检索的候选项

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Explore ▾ Saved Searches ▾ SciPlanner

Research Topic "prepare of 3D graphene"

REFERENCES ?

Select All Deselect All

1 of 8 Research Topic Candidates Selected

	References
<input type="checkbox"/> 1 reference was found containing "prepare of 3D graphene" as entered.	1
<input checked="" type="checkbox"/> 910 references were found containing the two concepts "prepare" and "3D graphene" closely associated with one another.	910
<input type="checkbox"/> 1603 references were found where the two concepts "prepare" and "3D graphene" were present anywhere in the reference.	1603
<input type="checkbox"/> 58400 references were found containing the concept "prepare", and either the concept "3D" or the concept "graphene". The concepts found were closely associated with one another.	58400
<input type="checkbox"/> 102301 references were found containing the concept "prepare", and either the concept "3D" or the concept "graphene". The concepts found were present anywhere (perhaps widely separated) within the reference.	102301
<input type="checkbox"/> 11876585 references were found containing the concept "prepare".	11876585
<input type="checkbox"/> 2881 references were found containing the concept "3D graphene".	2881
<input type="checkbox"/> 421680 references were found containing either the concept "3D" or the concept "graphene".	421680

Get References

“Concepts”表示对主题词做了同义词的扩展；

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

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

# 按被引次数排序— Citing References

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Research Topic "prepare of 3D graphene" > references (767)

REFERENCES

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Analyze | Refine | Categorize

Sort by: Citing References

Analyze by: Author Name

Wei Wei 13

Huang Wei 11

Hu Yun Hang 10

Ma Jie 10

Yu Fei 10

Dong Xiaochen 9

Chen Peng 8

Zhang Hua 8

Qu Liangti 7

Shi Gaoquan 7

1. **Cobalt Oxide Electrode for High-Performance Supercapacitor and Enzymeless Glucose Detection**

By Dong, Xiao-Chen; Xu, Hang; Wang, Xue-Wan; Huang, Yin-Xi; Chan-Park, Mary B.; Zhang, Hua; Wang, Lian-Hui; Huang, Wei; Chen, Peng  
From ACS Nano (2012), 6(4), 3206-3213. | Language: English, Database: CAPLUS

Using a simple hydrothermal procedure, cobalt oxide (Co<sub>3</sub>O<sub>4</sub>) nanowires were in situ **synthesized** on three-dimensional (3D) **graphene** foam grown by chem. vapor deposition. The structure and morphol. of the resulting 3D **graphene**/Co<sub>3</sub>O<sub>4</sub> composites were characterized by SEM, TEM, x-ray diffraction, and Raman spectroscopy. The 3D **graphene**/Co<sub>3</sub>O<sub>4</sub> composite was used as the monolithic free-standing electrode for supercapacitor application and for enzymeless electrochem. detection of glucose. The authors demonstrate that it is capable of delivering high specific capacitance of ~1100 F g<sup>-1</sup> at a c.d. of 10...

2. **A Three-Dimensional Carbon Nanotube/Graphene Sandwich and Its Application as Electrode in Supercapacitors**

By Fan, Zhuangjun; Yan, Jun; Zhi, Linjie; Zhang, Qiang; Wei, Tong; Feng, Jing; Zhang, Milin; Qian, Weizhong; Wei, Fei  
From Advanced Materials (Weinheim, Germany) (2010), 22(33), 3723-3728. | Language: English, Database: CAPLUS

A 3D CNT/graphene sandwich structures with CNT pillars grown in between the **graphene** layers had been **prepd.** by CVD. The unique structure endows the high rate transportation of electrolyte ions and electrons throughout the electrode matrix and comprehensive utilization of pseudo and double-layer capacitance, resulting in excellent electrochem. performances. The supercapacitor based on CGS exhibits 1'00 a specific capacitance of 385 F g<sup>-1</sup> at 10 mV s<sup>-1</sup> in 6 M KOH 1600 2000 soln. After 2000 cycles, a capacitance increase of ca. 20 % of the initial capacitance is obsd., indicating excellent elec...

Citing Reference: 帮助找到最重要的文献

# 文献检索结果

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Research Topic "prepare of 3D graphene" > references

REFERENCES

Get Substances Reactions Citations Tools

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Analyze Refine Categorize

Sort by: Accession Number

0 of 767 References Selected

Analyze by: Author Name

Wei Wei	13
Huang Wei	11
Hu Yun Hang	10
Ma Jie	10
Yu Fei	10
Dong Xiaochen	9
Chen Peng	8
Zhang Hua	8
Qu Liangti	7
Shi Gaoquan	7

1. Edge-rich and (N, S)-doped 3D porous graphene as efficient metal-free electrocatalyst for ORR

Quick View Other Sources

By Wu, Xiaobo; Xie, Zhiyong; sun, min; lei, tin; zuo, zhenming; Xie, Xiangmin; li, liangyi; Huang, Qizhong  
From RSC Advances (2016), Ahead of Print. | Language: English, Database: CAPLUS

A novel edge-rich and (N, S)-doped 3D porous graphene was synthesized by Chem. Vapor Deposition (CVD) and chem. corrosion. The hybrid material as a metal-free electrocatalyst exhibited a four-electron pathway, stronger alk. tolerance and excellent catalytic activity for oxygen redn. reaction due to the edge effect and heteroatom synergistic effect.

2. Facile Synthesis of 3D Graphene Flowers for Ultrasensitive and Highly Reversible Gas Sensing

Quick View Other Sources

By Wu, Jin; Feng, Shuanglong; Wei, Xingzhan; Shen, Jun; Lu, Wenqiang; Shi, Haoqi; Tao, Kai; Lu, Shirong; Sun, Tai; Yu, Leyong; et al  
From Advanced Functional Materials (2016), Ahead of Print. | Language: English, Database: CAPLUS

Fabrication of nanostructured graphene (Gr) for gas sensing applications has become increasingly attractive. For the first time, 3D graphene flowers (GF) cluster patterns are grown directly on an Ni foam substrate by inexpensive homebuilt microwave plasma-enhanced chem. vapor deposition (MPCVD) using the gas mixt.  $H_2/C_2H_4O_2@Ar$  as a precursor. The interim morphologies of the synthesized GF are investigated and the growth mechanism of the GF film is proposed. The GF are decompd. to few-layer Gr sheets by ultrasonication in ethanol. For the first time, MPCVD-synthesized Gr is exploited to fab...

3. N-P-O co-doped high performance 3D graphene prepared through red phosphorous-assisted "cutting-thin" technique: A universal synthesis and multifunctional applications

Quick View Other Sources

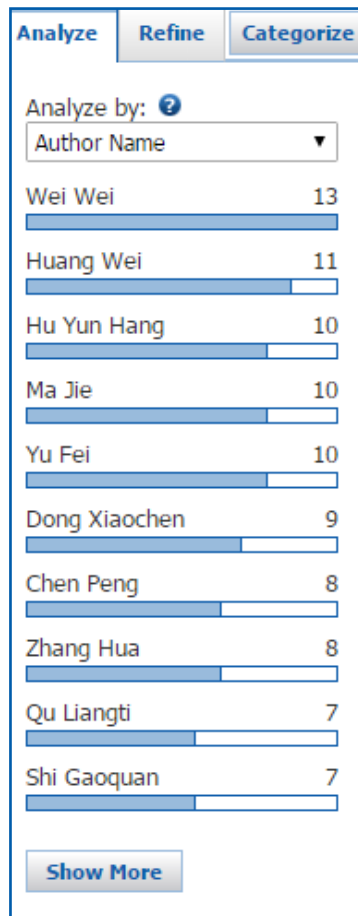
By Zhao, Yufeng; Huang, Shifei; Xia, Meirong; Rehman, Sarish; Mu, Shichun; Kou, Zongkui; Zhang, Zhi; Chen, Zhaoyang; Gao, Faming; Hou, Yanglong  
From Nano Energy (2016), 28, 346-355. | Language: English, Database: CAPLUS

Large scale prodn. of three dimensional (3D) graphene materials with high d. and low degree of defects stands for the main challenge hindering their practical applications.

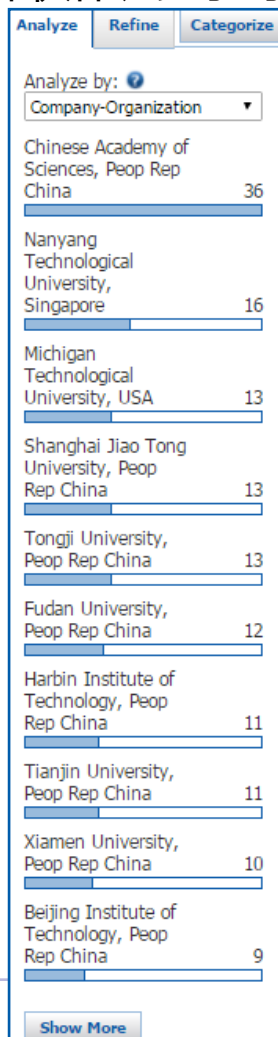
SciFinder提供强大的文献处理工具，帮助处理文献

# 文献检索结果的Analyze

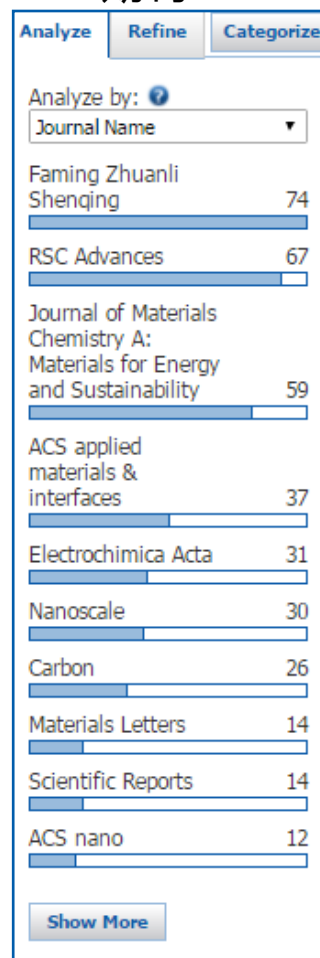
## 本领域研究人员



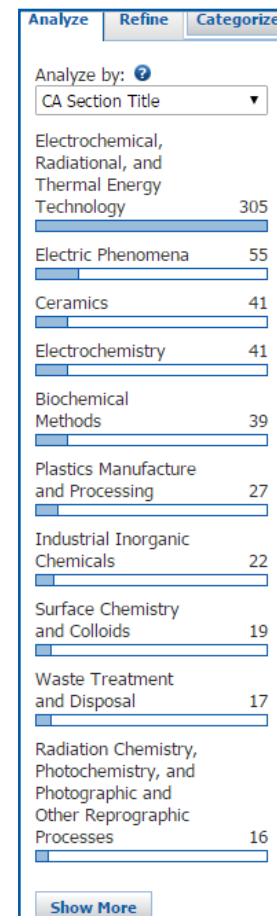
## 本领域研究机构、 合作伙伴、竞争对手



## 期刊



## 涉及学科领域

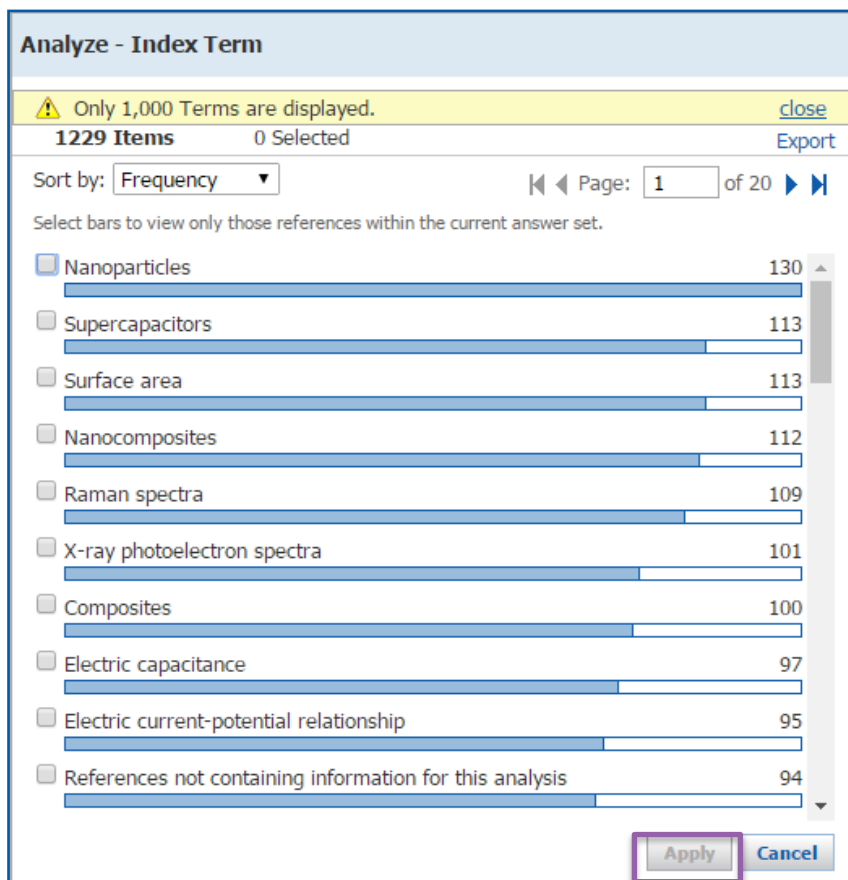
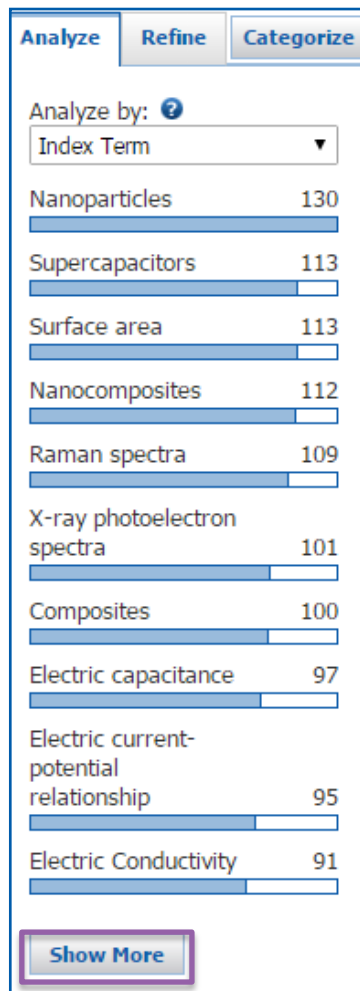


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# 文献检索结果的Analyze

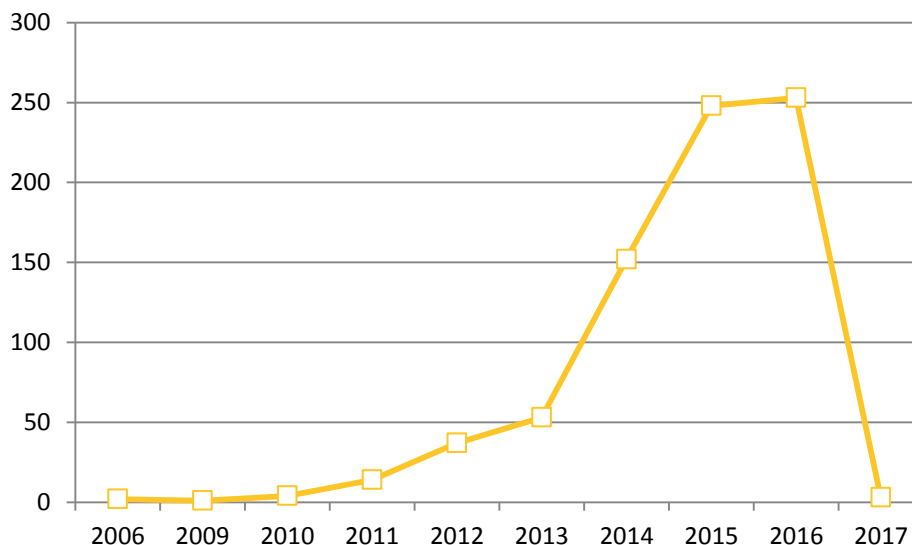
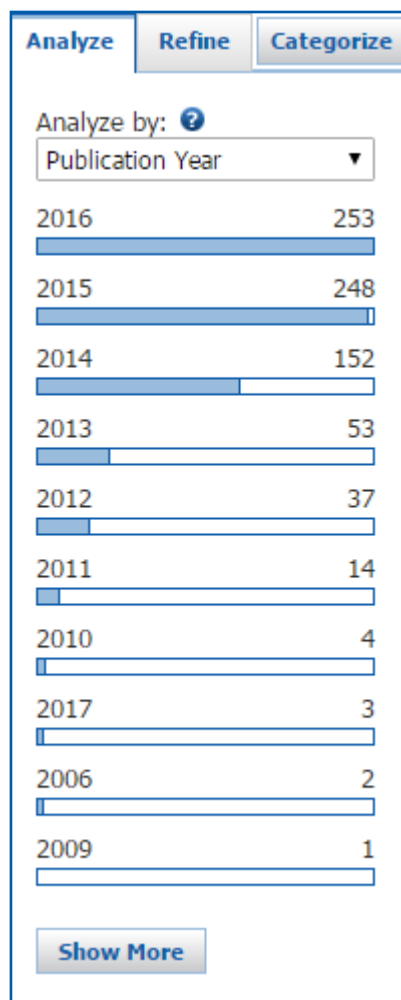
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# 文献检索结果的Analyze



Publication Year: 分析领域发展趋势



# 文献检索结果的Refine

AnalyzeRefineCategorize

Refine by: ?

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

Company Name  
china

Examples:  
3M  
DuPont

Refine

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Sort by: Accession Number

0 of 534 References Selected

Display Options

1. N-P-O co-doped high performance 3D graphene prepared through red phosphorous-assisted "cutting-thin" technique: A universal synthesis and multifunctional applications

Quick ViewOther Sources

By Zhao, Yufeng; Huang, Shifei; Xia, Meirong; Rehman, Sarish; Mu, Shichun; Kou, Zongkui; Zhang, Zhi; Chen, Zhaoyang; Gao, Faming; Hou, Yanglong

From Nano Energy (2016), 28, 346-355. | Language: English, Database: CAPLUS

Large scale prodn. of three dimensional (3D) graphene materials with high d. and low degree of defects stands for the main challenge hindering their practical applications. Herein, we report a universal and readily scalable strategy to produce an N-P-O co-doped free standing 3D graphene through a one-pot red phosphorus-assisted "cutting-thin" technique. The solid carbon precursor is gradually exfoliated through the slowly released gases (e.g.  $\text{PH}_3$ ,  $\text{H}_2$ ,  $\text{CO}_2$ ) and metallic K during the reaction, which allows the formation of dominant amt. nanopores, and ensures the high d. of the products. The ...

2. Rational construction of graphene oxide with MOF-derived porous NiFe@C nanocubes for high-performance microwave attenuation

Quick ViewOther Sources

By Yang, Zhihong; Lv, Hualiang; Wu, Renbing

From Nano Research (2016), Ahead of Print. | Language: English, Database: CAPLUS

Exploring lightwt. microwave attenuation materials with strong and tunable wideband microwave absorption is highly desirable but remains a significant challenge. Herein, three-dimensional (3D) porous hybrid composites consisting of NiFe nanoparticles embedded within carbon nanocubes decorated on graphene oxide (GO) sheets (NiFe@C nanocubes@GO) as high-performance microwave attenuation materials have been rationally synthesized. The 3D porous hybrid composites are fabricated by a simple method, which involves one-step pyrolysis of NiFe Prussian blue analog nanocubes in the presence of GO shee...

3. Facile self-assembly N-doped graphene quantum dots/graphene for oxygen reduction reaction

Quick ViewOther Sources

By Fan, Mengmeng; Zhu, Chunlin; Yang, Jiazhi; Sun, Dongping

From Electrochimica Acta (2016), 216, 102-109. | Language: English, Database: CAPLUS

Nitrogen doping carbon nanomaterial has become an important metal-free electrocatalyst for oxygen redn. reaction (ORR) in fue cells. N-doped graphene quantum dots (N-GQDs) are one of the most promising nanomaterials due to abundant electrocatalytic edging and N doping active sites, but low yield, high dispersity and no forming efficient percolative conductive network hinder their direct application as the electrocatalyst. Hydrothermal method is an effective route for prepg. high-quality N-GQDs and meanwhile, overcomes the drawbacks of complicated prepg. progress and low yield. We further hy...

4. High performance agar/graphene oxide composite aerogel for methylene blue removal

Quick ViewOther Sources

By Chen, Long; Li, Yanhui; Du, Qiuju; Wang, Zonghua; Xia, Yanzhi; Yedinak, Emily; Lou, Jun; Ci, Lijie

From Carbohydrate Polymers (2017), 155, 345-353. | Language: English, Database: CAPLUS

Refine : 帮助用户迅速获得需要的文献

# 文献检索结果的Categorize

学科领域  
主分类

学科领域  
副分类

Index Term

选中的Index Term

**Categorize** ?

1. Select a heading and category.

Category Heading	Category
All	Substances in technology (716)
<b>Technology</b>	<b>Materials &amp; products (203)</b>
General chemistry	Processes & apparatus (202)
Physical chemistry	Metallurgy (52)
Synthetic chemistry	Power & fuel topics (25)
Polymer chemistry	Formed, removed, & other substances (106)
Catalysis	Construction (11)
Biotechnology	Imaging & recording (12)
Analytical chemistry	Ceramics (8)
Environmental chemistry	
Genetics & protein chemistry	
Biology	

2. Select index terms of interest.

Index Terms	
Page: 1 of 3	
Select All Deselect All	
<input type="checkbox"/> Graphene	427
<input type="checkbox"/> Nanocomposites	86
<input type="checkbox"/> Composites	85
<input type="checkbox"/> Graphite	83
<input type="checkbox"/> Platinum	31
<input type="checkbox"/> Hydrogen	26
<input type="checkbox"/> Carbon black	21
<input type="checkbox"/> Oxygen	20
<input checked="" type="checkbox"/> Nanostructured materials	19
<input type="checkbox"/> Porous materials	16
<input type="checkbox"/> Adsorbents	13
<input type="checkbox"/> Solar cells	12
<input type="checkbox"/> Nanowires	11
<input type="checkbox"/> Sulfur	11
<input type="checkbox"/> Argon	10

Selected Terms

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

\* Technology > Materials & products (1 Terms)

Technology > Materials & products > 1 Index Term(s) Selected

OK Cancel

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

# 结果集的保存— Save, Print, Export

Searches ▾ SciPlanner Save Print Export

ally removed.

aphene" > references (767) > refine "china" (534) > refine by categories

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Sort by: Accession Number ▾ Display Options

0 of 19 References Selected

1. A green and simple strategy to prepare graphene foam-like three-dimensional porous carbon/Ni nanoparticles for glucose sensing

Quick View Other Sources

By Wang, Li; Zhang, Yayun; Yu, Jie; He, Juan; Yang, Han; Ye, Yihan; Song, Yonghai

From Sensors and Actuators, B: Chemical (2017), 239, 172-179. | Language: English, Database: CAPLUS

A green and simple strategy to prep. graphene foam-like three-dimensional (3D) porous carbon/Ni nanoparticles (NINPs) nanocomposites was developed for glucose detection. The discarded sponge-like natural product, pomelo peel, was employed as novel supporting materials. The pomelo peel was carbonized to construct the graphene foam-like 3D porous carbon/NINPs nanocomposites. The nanocomposites were carefully characterized by SEM, transmission electron microscopy, N<sub>2</sub> adsorption/desorption isotherms, X-ray powder...

2. Facile synthesis of flower-like platinum nanostructures as an efficient electrocatalyst for methanol electro-oxidation

Quick View Other Sources

By Zhang, Jie; Chen, Jinwei; Jiang, Yiwu; Zhou, Feilong; Zhong, Jing; Wang, Gang; Kiani, Maryam; Wang, Rulin

From Journal of Colloid and Interface Science (2016), 479, 64-70. | Language: English, Database: CAPLUS

This paper presents a facile approach for the synthesis of a novel Pt/graphene-nickel foam (Pt/GNF) electrode composed of flower-like Pt nanoparticles (NPs) and 3D graphene. The fabrication process involved the chem. vapor deposition of graphene onto Ni foam as a substrate and the subsequent growth of Pt NPs via a galvanic replacement reaction without using any seed and org. solvent. The surface morphol. and compn. of the prepd. materials were characterized. Meanwhile, cyclic voltammetry and electrochem. impedance spectroscopy were employed to confirm their typical electrochem. characterist...

3. Extremely Weak van der Waals Coupling in Vertical ReS<sub>2</sub> Nanowalls for High-Current-Density Lithium-Ion Batteries

Quick View Other Sources

By Zhang, Qin; Tan, Shuangjie; Mendes, Rafael G.; Sun, Zhongti; Chen, Yongting; Kong, Xin; Xue, Yinghui; Ruenmell, Mark H.; Wu, Xiaojun; Chen, Shengli; et al

From Advanced Materials (Weinheim, Germany) (2016), 28(13), 2616-2623. | Language: English, Database: CAPLUS

In addn. to the weak interlayer coupling, ReS<sub>2</sub> possesses the highest anisotropic ratio along its two principle axes as compared to all exptl. investigated 2D layered materials. As shown in early studies, the direction of the Re-Re at. chain is more conductive than other cryst. orientations. However, 2D layered materials, including ReS<sub>2</sub>, are oriented in a conventional stacked geometry. Therefore, we first synthesized ultrauniformly distributed vertical ReS<sub>2</sub> nanowalls (V-ReS<sub>2</sub>) grown on 3D carbon foam...

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Reference\_06\_19\_2012\_100848

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☐ Summary with partial abstracts  
☒ Summary with full abstracts  
☐ Detail (full record)

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☐ Task History  
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☐ Comments

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# 文献信息一题录、摘要、索引

## 3. Extremely Weak van der Waals Coupling in Vertical ReS<sub>2</sub> Nanowalls for High-Current-Density Lithium-Ion Batteries

By: Zhang, Qin; Tan, Shuangjie; Mendes, Rafael G.; Sun, Zhongti; Chen, Yongting; Kong, Xin; Xue, Yinghui; Ruemmel, Mark H.; Wu, Xiaojun; Chen, Shengli; Fu, Lei

In addn. to the weak interlayer coupling, ReS<sub>2</sub> possesses the highest anisotropic ratio along its two principle axes as compared to all exptl. investigated 2D layered materials. As shown in early studies, the direction of the Re-Re at. chain is more conductive than other cryst. orientations. However, 2D layered materials, including ReS<sub>2</sub>, are always randomly oriented in a conventional stacked geometry. Therefore, we first synthesized ultrauniformly distributed vertical ReS<sub>2</sub> nanowalls (V-ReS<sub>2</sub>) grown on 3D graphene foam (3DGF) by chem. vapor deposition with Re-Re sites adjacent to the graphene for the purpose of enhancing the cond. Meanwhile, the ReS<sub>2</sub> nanowalls expose more active sulfur edge sites, which improves easy lithium intercalation and deintercalation. To enhance the cond. of the whole electrode material, 3DGF was selected as template due to its high cond. and high-sp. surface area. Moreover, this favorable vertical structure shortens the pathways and facilitates fast diffusion of both Li<sup>+</sup> and electrolyte ions. As expected, the V-ReS<sub>2</sub>/3DGF composite demonstrated good cycling stability at high-current-densities when serving as anode material for LIBs. At the high c.d. of 1000 mA/g, the capacity of our ReS<sub>2</sub>/3DGF anodes still maintained over 200 mAh/g even after 500 cycles. The extremely weak vdW coupling material of ReS<sub>2</sub> holds great promise for practical applications in LIBs. In addn., it broadens the material choice of anode materials for other alk.-ion batteries.

### Indexing

Electrochemistry / Energy Technology (Section52-2)

#### Concepts

### 重要概念

Battery anodes  
Delithiation  
Lithiation  
Nanostructured materials  
Current density  
Intercalation  
Lithium-ion secondary batteries

extremely weak van der Waals coupling in vertical ReS<sub>2</sub> nanowalls for high-current-d. lithium-ion batteries

#### Substances

### 重要物质

12038-63-0P Rhenium sulfide

extremely weak van der Waals coupling in vertical ReS<sub>2</sub> nanowalls for high-current-d. lithium-ion batteries

Synthetic preparation; Technical or engineered material use; Preparation; Uses

7439-93-2 Lithium, uses  
1034343-98-0 Graphene

extremely weak van der Waals coupling in vertical ReS<sub>2</sub> nanowalls for high-current-d. lithium-ion batteries

Technical or engineered material use; Uses

#### QUICK LINKS

0 Tags, 0 Comments

#### SOURCE

*Advanced Materials*  
(Weinheim, Germany)  
Volume28  
Issue13  
Pages2616-2623  
Journal; Online Computer File  
2016  
CODEN:ADVMEW  
ISSN:0935-9648  
DOI:10.1002/adma.201505498

#### COMPANY/ORGANIZATION

College of Chemistry and Molecular Science  
Wuhan University  
Wuhan, Peop. Rep. China  
430072

#### ACCESSION NUMBER

2016:170829  
CAN164:397211  
CAPLUS

#### PUBLISHER

Wiley-VCH Verlag GmbH & Co. KGaA

#### LANGUAGE

English

文献详情界面包括：

1. 标题
2. 摘要
3. 文献中重要的技术术语
4. 文献中重要的物质
5. 书目信息
6. 获得文献中的物质，反应
7. 参考文献
8. 链接原文

# 文献检索小结

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

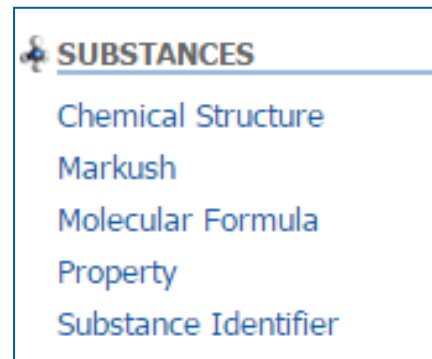
# 提纲

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

# SciFinder检索选项——物质检索

## ■ 物质检索方法


- 结构式检索
- 分子式检索
- 理化性质检索
- 物质标识符检索：化学名称，CAS RN



## ■ 物质检索策略推荐

- 有机化合物，天然产物：结构检索
- 无机物，合金：分子式检索
- 高分子化合物：分子式检索和结构检索

# 物质检索——标识符检索

 **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 ?**

sudan red

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

Search

提示：

1. 一次最多可输入25个物质。
2. 每行一个物质标识符。

物质标识符包括CAS RN和化学名称，化学名称可以是通用名称、商品名、俗名。

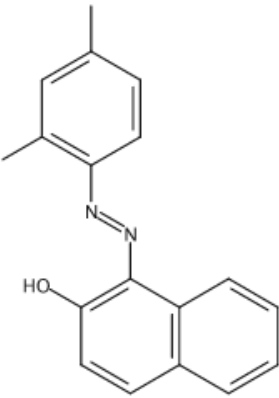


# SciFinder中的物质记录

点击CAS RN 获得物质详细信息

1 3118-97-6

~894 ~58



**C<sub>18</sub> H<sub>16</sub> N<sub>2</sub> O**  
2-Naphthalenol, 1-[2-(2,4-dimethylphenyl)diazenyl]-

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

CAS Registry Number: 3118-97-6

- » View Substance Detail
- » Explore by Structure
- Synthesize this...
- Get Reactions where Substance is a
- Get Commercial Sources
- Get Regulatory Information
- Get References
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# SciFinder中的物质记录

**SUBSTANCE DETAIL** ?

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**CAS Registry Number** 3118-97-6

~894 ~58

**C<sub>18</sub> H<sub>16</sub> N<sub>2</sub> O**  
2-Naphthalenol, 1-[2-(2,4-dimethylphenyl)diazenyl]-

**Molecular Weight**  
276.33

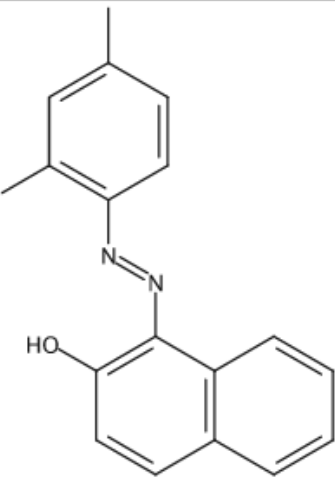
**Melting Point (Experimental)**  
Value: 166 °C

**Boiling Point (Predicted)**  
Value: 476.7±40.0 °C | Condition: Press: 760 Torr

**Density (Predicted)**  
Value: 1.14±0.1 g/cm<sup>3</sup> | Condition: Temp: 20 °C Press: 760 Torr

**pKa (Predicted)**  
Value: 13.52±0.50 | Condition: Most Acidic Temp: 25 °C

**Other Names**  
2-Naphthalenol, 1-[(2,4-dimethylphenyl)azo]- (9CI)  
C.I. Solvent Orange 7 (7CI,8CI)  
Sudan Red (6CI)  
1-[2-(2,4-Dimethylphenyl)diazenyl]-2-naphthalenol  
AF Red No. 5  
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物质详情

# 通过物质获得文献

分析化学  
生物研究

### Get References

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<input type="checkbox"/> Biological Study	<input type="checkbox"/> Properties
<input type="checkbox"/> Combinatorial Study	<input type="checkbox"/> Prophetic in Patents
<input type="checkbox"/> Crystal Structure	<input type="checkbox"/> Reactant or Reagent
<input type="checkbox"/> Formation, nonpreparative	<input type="checkbox"/> Spectral Properties
<input type="checkbox"/> Miscellaneous	<input type="checkbox"/> Uses
<input type="checkbox"/> Occurrence	

**For each sequence, retrieve:**

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

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工艺

谱图数据  
用途



**SCIFINDER®**  
A CAS SOLUTION

**EXPERIMENTAL PROPERTIES****EXPERIMENTAL SPECTRA****实验数据与实验谱图****<sup>1</sup>H NMR** IR Mass Raman UV and Visible

<sup>1</sup> H NMR Properties	Value	Condition	Note
Proton NMR Spectrum	See spectrum		(13)BIORAD
<b>Notes</b>			
(13) BIORAD: Copyright Bio-Rad Laboratories. All Rights Reserved.			

**PREDICTED PROPERTIES**

Biological Chemical Density Lipinski Structure Related Thermal

Lipinski Properties	Value	Condition	Note
Freely Rotatable Bonds	3		(21)
H Acceptors	3		(21)
H Donors	1		(21)
H Donor/Acceptor Sum	4		(21)
logP	5.471±1.252	Temp: 25 °C	(21)
Molecular Weight	276.33		(21)
<b>Notes</b>			
(21) Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994-2015 ACD/Labs)			

**预测数据与预测谱图****PREDICTED SPECTRA**

# 物质检索——Property explore

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Opened saved answer set "c-c bond formation" (693) > Formation Mechanism of the Fir...

**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: PROPERTY**

Experimental

Electric Conductivity (S/cm) ▾ > 353400

Select Property...

Boiling Point (°C)

Density (g/cm<sup>3</sup>)

Electric Conductance (S)

Electric Conductivity (S/cm)

Electric Resistance (ohm)

Electric Resistivity (ohm\*cm)

Glass Transition Temp. (°C)

Magnetic Moment (μB)

Median Lethal Dose (LD50) (mg/kg)

Melting Point (°C)

Optical Rotatory Power (degrees)

Refractive Index

Tensile Strength (MPa)

Examples: 44, 25-35, >125

寻找导电率比铜的60%大的非金属材料

# 物质结果集的筛选——Refine

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Property "Experimental - Electric Conduc..." > substances (39) > refine "exclude metal-containing" (14)

SUBSTANCES

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Analyze | Refine

Sort by: CAS Registry Number

0 of 39 Substances Selected

Refine by:

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

Select One:

- Include only metal-containing substances
- Exclude metal-containing substances**

Refine

1. 1044804-35-4

~929

Substance  
Image  
Cannot Be  
Displayed  
1044804-35-4

Editor Note: A sulfonated polystyrene-doped PEDOT (H.C. Starck)

Unspecified  
Clevios P-VP-AI 4083  
Experimental Properties

2. 943433-94-1

~2

210531-45-6 (Component: 625392-06-5)  
C<sub>13</sub> H<sub>8</sub> F<sub>2</sub> O<sub>7</sub> S<sub>2</sub> · 2 Na

Click to view detail

0 of 14 Substances Selected

1. 1044804-35-4

~929

Substance  
Image  
Cannot Be  
Displayed  
1044804-35-4

Editor Note: A sulfonated polystyrene-doped PEDOT (H.C. Starck)

Unspecified  
Clevios P-VP-AI 4083  
Experimental Properties

2. 868628-72-2

~2

C<sub>18</sub> H<sub>32</sub> B N<sub>2</sub>  
Boron, tributyl(1-(2-propen-1-yl)-1H-imidazole-κN<sup>2</sup>), (7-4)-

Key Physical Properties  
Experimental Properties

3. 868628-71-1

~2

4. 866023-23-6

~3

120120-58-3  
C<sub>10</sub> H<sub>6</sub> O<sub>4</sub> S<sub>4</sub>

如何筛选非金属物质？

# 物质检索——分子式

检索(N H<sub>4</sub>) Sm (S O<sub>4</sub>)<sub>2</sub> (H<sub>2</sub> O)<sub>4</sub>, Ammonium Samarium Bis(sulfate(VI)) Tetrahydrate

The screenshot displays the SciFinder web interface. On the left, there is a sidebar with navigation options: REFERENCES, SUBSTANCES, and REACTIONS. The SUBSTANCES section is expanded, showing options like Chemical Structure, Markush, Molecular Formula, Property, and Substance Identifier. The main area is titled 'SUBSTANCES: MOLECULAR FORMULA'. A search box contains the formula '4H2 O. N H3. 2H2 O4 S. Sm'. Below the search box, there are examples: 'H4SiO4' and '(C3H6O.C2H4O)x'. A blue 'Search' button is positioned below the examples. To the right of the search results, a detailed view of the first result is shown. It includes the CAS number '1. 34370-41-7', the component name '(Component: 7664-93-9)', and the chemical structure of sulfuric acid (H2SO4). Below the structure, the formula 'H3 N . 2 H2 O4 S . 4 H2 O . Sm' is listed, followed by the description 'Sulfuric acid, ammonium samarium(3+) salt (2:1:1), tetrahydrate (8CI,9CI)'.

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

# 物质检索——结构

**REFERENCES**

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

**SUBSTANCES**

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

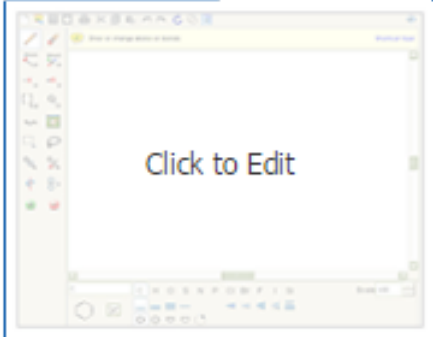
**REACTIONS**

- Reaction Structure

## SUBSTANCES: CHEMICAL STRUCTURE ?

Structure Editor:


Java Non-Java



Search Type:


- ☐ Exact Structure
- ☒ Substructure
- ☐ Similarity

☐ Show precision analysis

 **ChemDraw**  
Launch a SciFinder substance or reaction

Import CXF

**Search**

 Advanced Search ☒ Always Show



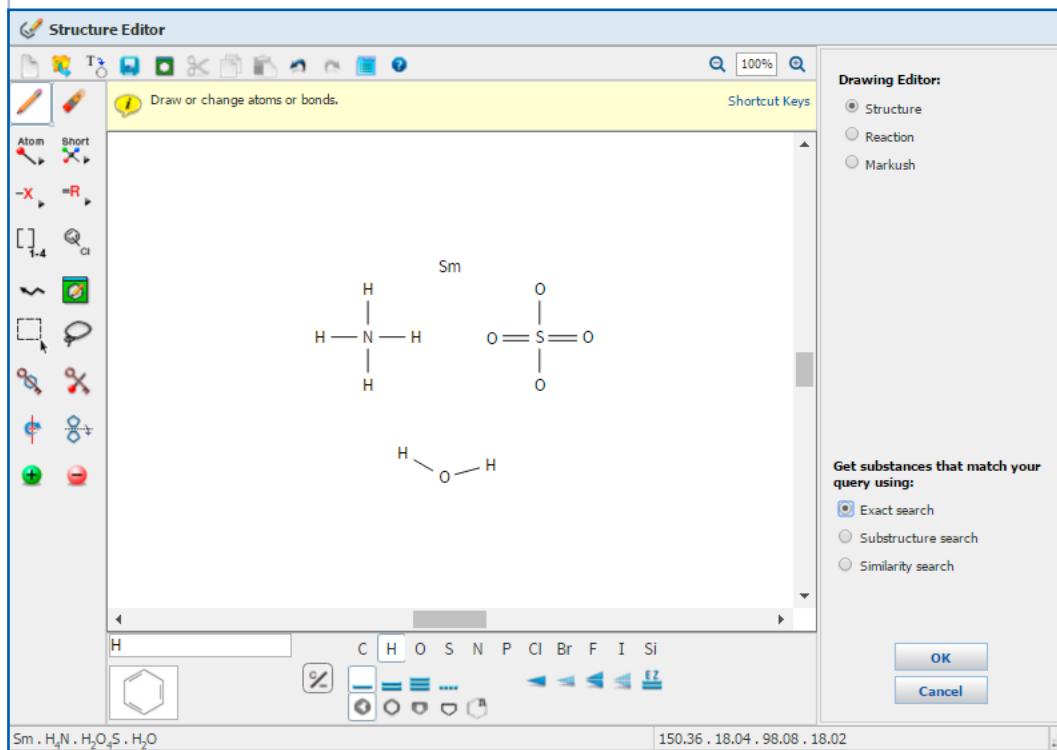
# 物质检索——结构

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

- 橡皮** (Eraser)
- 结构和反应切换功能** (Structure and Reaction Switching Function)
- 铅笔** (Pencil)
- 元素周期表** (Periodic Table)
- 可变基团** (Variable Group)
- 重复基团工具** (Repeat Group Tool)
- 碳链工具** (Carbon Chain Tool)
- 选择工具** (Select Tool)
- 环锁定工具** (Ring Locking Tool)
- 旋转工具** (Rotate Tool)
- 正电子** (Positron)
- 负电子** (Electron)
- C原子和单键恢复工具** (C Atom and Single Bond Restoration Tool)
- 常用基团** (Common Groups)
- R基团定义工具** (R Group Definition Tool)
- 可变位置连接工具** (Variable Position Connection Tool)
- 模版工具** (Template Tool)
- 索套选择工具** (Snare Selection Tool)
- 原子锁定工具** (Atom Locking Tool)
- 镜面旋转工具** (Mirror Rotation Tool)
- 结构检索选择** (Structure Search Selection)
- 单双键，RS构型，不确定键定义工具** (Single/Double Bond, RS Configuration, Uncertain Bond Definition Tool)
- 常见环，多元环工具** (Common Rings, Polycyclic Rings Tool)

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

# 物质检索——精确结构检索



- 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

限定为单一组分




精确结构检索

# 物质检索——精确结构检索

Sort by: CAS Registry Number ↑

0 of 5 Substances Selected

**倒序排列**

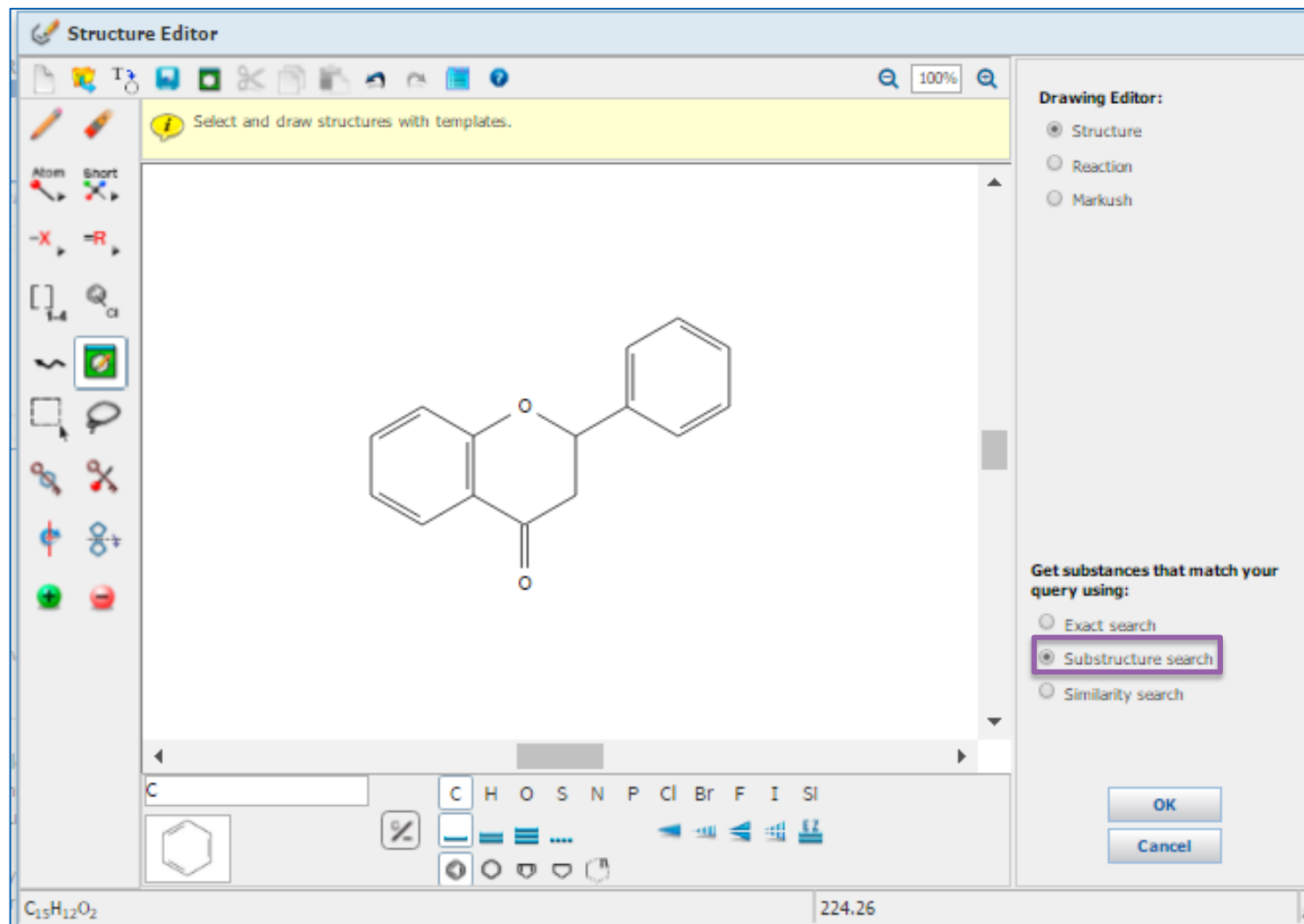
<p>1. 34370-41-7</p> <p>(Component: 7664-93-9)</p> <p>~12</p>  <ul style="list-style-type: none"> <li>• 1/2 NH<sub>3</sub></li> <li>• 2 H<sub>2</sub>O</li> <li>• 1/2 Sm(III)</li> </ul> <p><b>H<sub>3</sub>N · 2 H<sub>2</sub>O<sub>4</sub>S · 4 H<sub>2</sub>O · Sm</b> Sulfuric acid, ammonium samarium(3+) salt (2:1:1), tetrahydrate (8CI,9CI)</p>	<p>2. 40148-71-8</p> <p>(Component: 7664-93-9)</p> <p>~1</p>  <ul style="list-style-type: none"> <li>• NH<sub>3</sub></li> <li>• 1/3 H<sub>2</sub>O</li> <li>• 1/3 Sm(III)</li> </ul> <p><b>H<sub>3</sub>N · H<sub>2</sub>O<sub>4</sub>S · 1/3 H<sub>2</sub>O · 1/3 Sm</b> Sulfuric acid, ammonium samarium(3+) salt (3:3:1), monohydrate (9CI)</p>	<p>3. 40148-74-1</p> <p>(Component: 7664-93-9)</p> <p>~1</p>  <ul style="list-style-type: none"> <li>• 1/2 NH<sub>3</sub></li> <li>• H<sub>2</sub>O</li> <li>• 1/2 Sm(III)</li> </ul> <p><b>H<sub>3</sub>N · 2 H<sub>2</sub>O<sub>4</sub>S · 2 H<sub>2</sub>O · Sm</b> Sulfuric acid, ammonium samarium(3+) salt (2:1:1), dihydrate (9CI)</p>	<p>4. 42949-48-4</p> <p>(Component: 736080-59-4)</p> <p>~1</p>  <ul style="list-style-type: none"> <li>• NH<sub>4</sub><sup>+</sup></li> <li>• H<sub>2</sub>O</li> </ul> <p><b>(H<sub>8</sub>O<sub>11</sub>S<sub>2</sub>Sm · H<sub>4</sub>N · H<sub>2</sub>O)<sub>n</sub></b> Samarate(1-), triaquabis[sulfato(2-)-O,O']-, ammonium monohydrate, homopolymer (9CI)</p>
<p>5. 49856-58-8</p> <p>(Component: 736080-59-4)</p> <p>~0</p>  <ul style="list-style-type: none"> <li>• NH<sub>4</sub><sup>+</sup></li> <li>• H<sub>2</sub>O</li> </ul> <p><b>H<sub>8</sub>O<sub>11</sub>S<sub>2</sub>Sm · H<sub>4</sub>N · H<sub>2</sub>O</b> Samarate(1-), triaquabis[sulfato(2-)-O,O']-, ammonium monohydrate (9CI)</p>			

# 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

**C<sub>15</sub>H<sub>12</sub>O<sub>2</sub>**  
4-phenyl-4H-benzopyran-4-one, 2,3-dihydro-2-phenyl-

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

2. **17002-31-2**

~244 ~4

Absolute stereochemistry...Rotation (-).

**C<sub>15</sub>H<sub>12</sub>O<sub>2</sub>**  
4-phenyl-4H-benzopyran-4-one, 2,3-dihydro-

▶ **Key Physical Properties**  
Experimental Properties

10. **146196-91-0**

~1 ~5

**C<sub>15</sub>H<sub>7</sub>D<sub>5</sub>O<sub>2</sub>**  
4-(2,3,4,5-tetradeuteriophenyl)-4H-benzopyran-4-one, 2,3-dihydro- (9CI)

Spectra

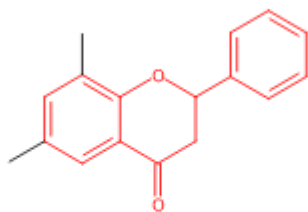
同位素

# 亚结构检索结果

281. 123251-10-5

~3 ~1

取代物



$C_{17}H_{16}O_2$

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

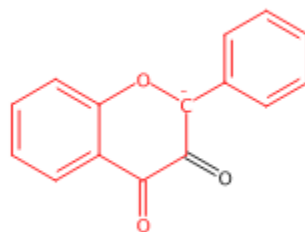
Key Physical Properties

Experimental Properties

295. 780723-19-5

~0

离子



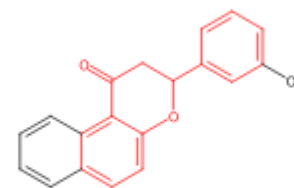
$C_{15}H_9O_3$

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

284. 136116-23-9

~2

稠环物质



$C_{19}H_{14}O_3$

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

Key Physical Properties

# 亚结构检索结果的限定

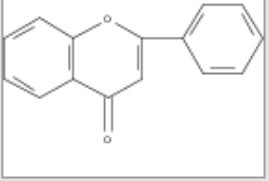
## 化学结构的再次限定

Analysis Refine

Refine by: ⓘ

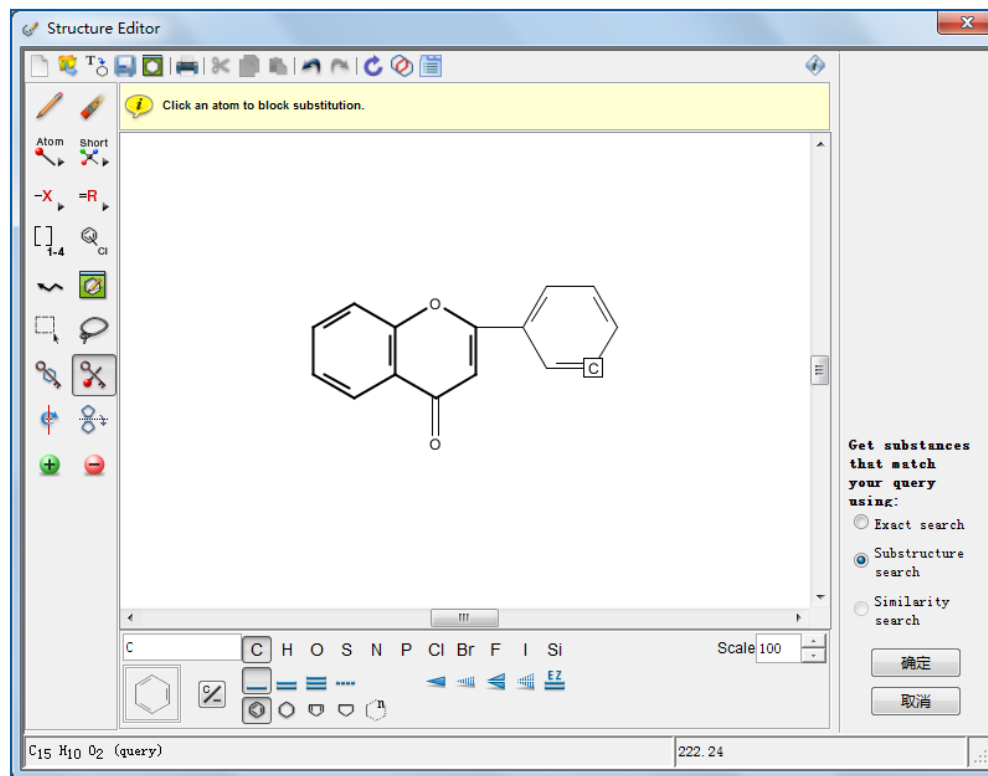
- ☒ Chemical Structure
- ☐ Isotope-Containing
- ☐ Metal-Containing
- ☐ Commercial Availability
- ☐ Property Availability
- ☐ Property Value
- ☐ Reference Availability
- ☐ Atom Attachment

Chemical Structure:



Click image to change structure or view detail

Search type: **Substructure**



环锁定



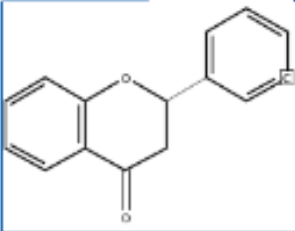
原子锁定



# 亚结构检索结果的限定

Structure Editor:

Java Non-Java



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

Only retrieve substances that:

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

**Refine**

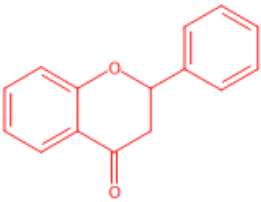
Get References Get Reactions Get Commercial Sources Tools

Sort by: Relevance

0 of 13826 Substances Selected

1. **487-26-3**

~2093

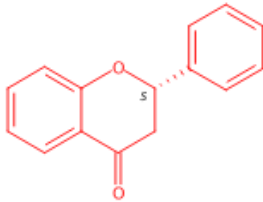


**C<sub>15</sub>H<sub>12</sub>O<sub>2</sub>**  
4*H*-1-Benzopyran-4-one, 2,3-dihydro-2-phenyl-

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

2. **17002-31-2**

~244



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

▶ **Key Physical Properties**  
Experimental Properties

Absolute stereochemistry, Rotation (-).

4. **104550-32-5**

~3

5. **75524-43-5**

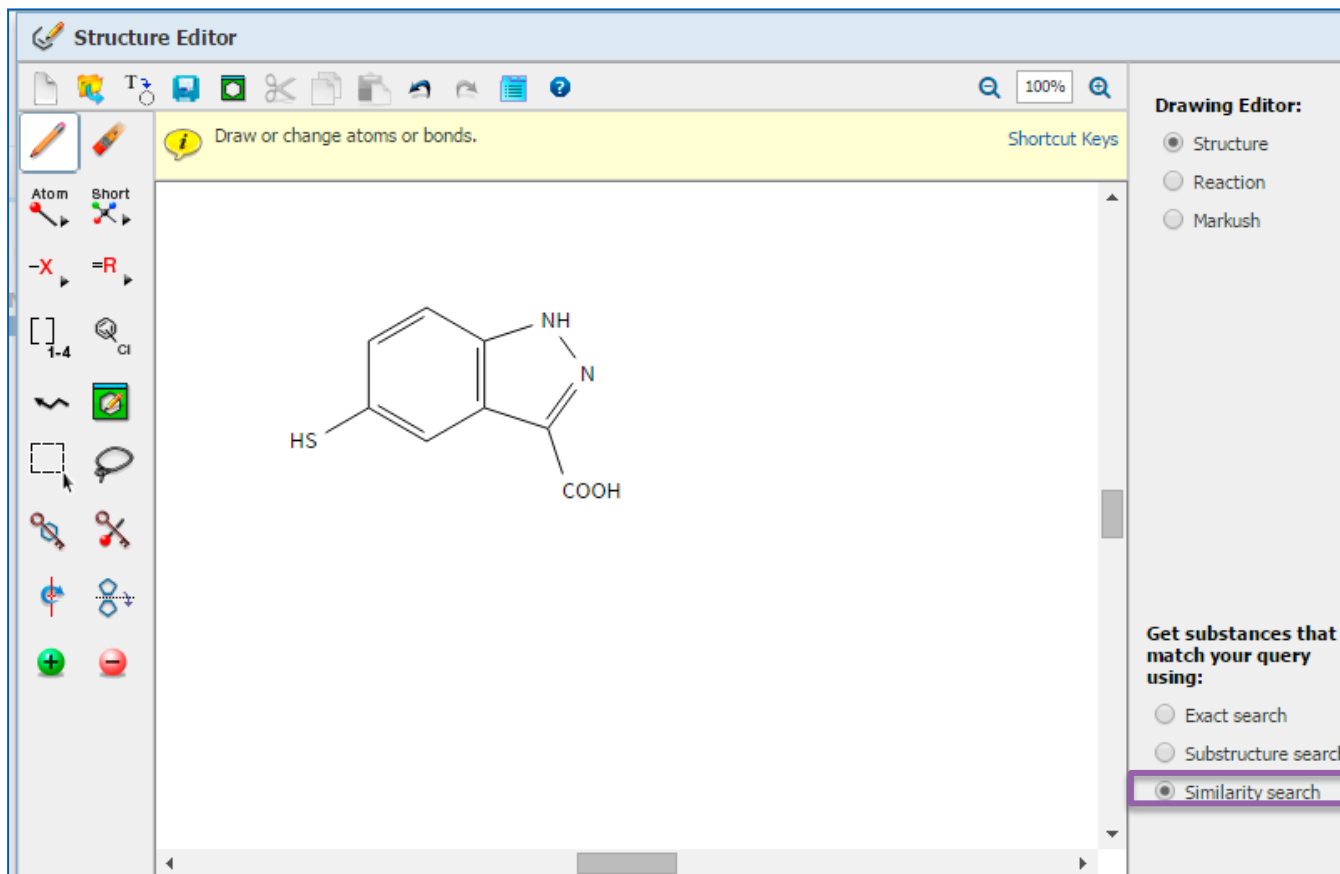
~2

# 物质检索——亚结构检索

- 亚结构检索：

包括精确结构检索结果，及被检索结构的修饰结构

# 物质检索——相似结构检索



# 相似结构检索结果

Select All Deselect All

0 of 6 Similarity Candidates Selected

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

Get Substances

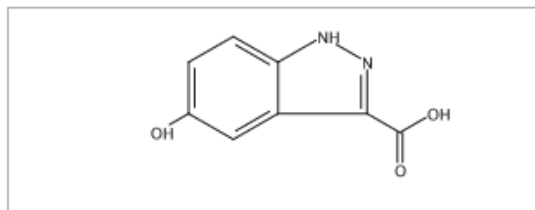
评分越高，相似度越高，结构越相似

Score: 88

☐ 1. 885518-94-5

取代基变化

~1 ~35



$C_8H_6N_2O_3$

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

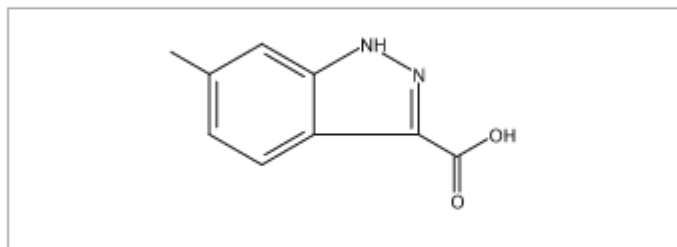
► Key Physical Properties

Score: 86

☐ 5. 858227-12-0

取代基位置变化

~7 ~41



$C_9H_8N_2O_2$

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

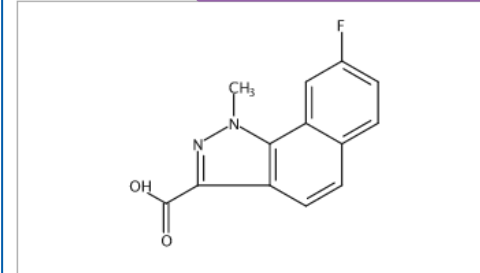
► Key Physical Properties

Score: 65

☐ 541. 1100422-

母体结构变化

~1



$C_{13}H_9FN_2O_2$

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

► Key Physical Properties



**SCIFINDER®**  
A CAS SOLUTION

# 物质检索——相似结构检索

- 相似结构检索：

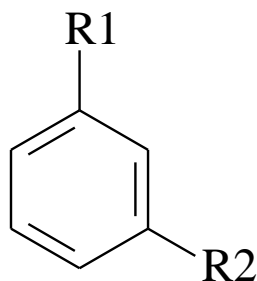
获得片段或整体结构与被检索结构相似的结果，母体结构可以被取代，也可以被改变

# 提纲

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

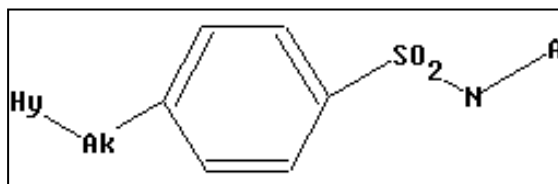
# Markush检索

- 具体物质[Specific Substance] :
  - 以具体化学结构陈述的特定物质，会被分配CAS RN
- 预测性物质[Prophetic Substance] :
  - 使用Markush结构陈述的预测物质，一个Markush可以陈述上百或上千个化学物质
  - 专利中所陈述的预测物质，不会被分配CAS RN
  - Markush检索，能检索到通过结构检索检不到的专利



R1 = H, Br, Cl, I

R2 = Br, Cl, I, —CH<sub>2</sub>—halogen, —CH(CH<sub>3</sub>)—halogen,



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

Structure Editor

Draw or change atoms or bonds. [Shortcut Keys](#)

100%

Atom Short

-X =R

1-4 Cl

Hy-Ak

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

Drawing Editor:

- ☐ Structure
- ☐ Reaction
- ☒ Markush

Get Markush patents where the structure(s) are:


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

OK Cancel

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



# Markush检索


**SCIFINDER**  
 A CAS SOLUTION

Welcome Helen Zhu

Explore ▼
 Saved Searches ▼
 SciPlanner
 Save
 Print
 Export

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

REFERENCES ⓘ
 Get Substances
 Get Reactions
 Get Related Citations ▼
 Tools ▼
 Create Keep Me Posted Alert
 Send to SciPlanner

Analyze
 Refine
 Categorize

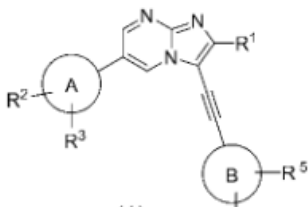
Sort by: Accession Number ▼
 0 of 1969 References Selected
 Page: 1 of 99

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

**1. Compounds and methods for anticoagulation therapy**  
 PATENTPAK  
 By Allende Rodriguez, Mikel; Hermida Santos, Jose; Montes Diaz, Ramon; Oyarzabal Santamarina, Julen  
 From PCT Int. Appl. (2016), WO 2016120432 A1 20160804. | Language: English, Database: CAPLUS

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

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



The title imidazo[1,2-a]pyrimidine derivs. I [R<sup>1</sup> = H or halogen; ring A Ph or pyridyl; R<sup>2</sup>, R<sup>3</sup> (same or different) = hydrogen, halogen, C<sub>1-4</sub> alkyl or C<sub>1-4</sub> alkoxy each optionally substituted with 1-5 halogen atoms; or in case where R<sup>2</sup> and R<sup>3</sup> are at the adjacent substitution position, R<sup>2</sup> and R<sup>3</sup> together with ring A form C<sub>5-8</sub> carbocyclic ring (optionally substituted with 1-5 halogen or 1-2 hydroxy group) or 5- or 6-membered satd. heterocyclic ring; ring B = Ph or pyridyl; R<sup>4</sup>, R<sup>5</sup> (same or different) = H, halogen, hydroxy, amino, -C(O)OR<sup>a</sup>, -C(O)NR<sup>a</sup>R<sup>b</sup>, SO<sub>3</sub>H, SO<sub>2</sub>NR<sup>a</sup>R<sup>b</sup>, SO<sub>2</sub>R<sup>b</sup>, or NR<sup>a</sup>SO<sub>2</sub>R<sup>b</sup>; R<sup>a</sup>, R<sup>b</sup> (same...

全部是专利

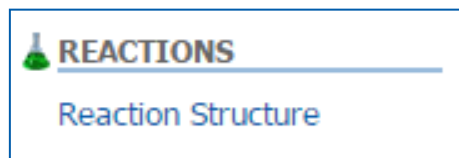
# 提纲

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

# SciFinder检索选项——反应检索

- 反应检索方法

结构式



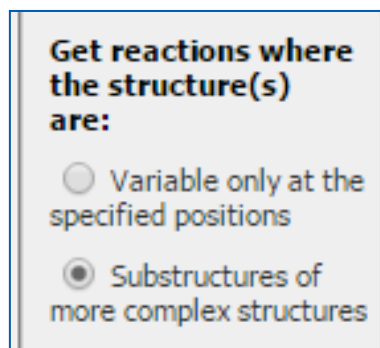
- 常用获取方法

已知物质：由物质获取反应

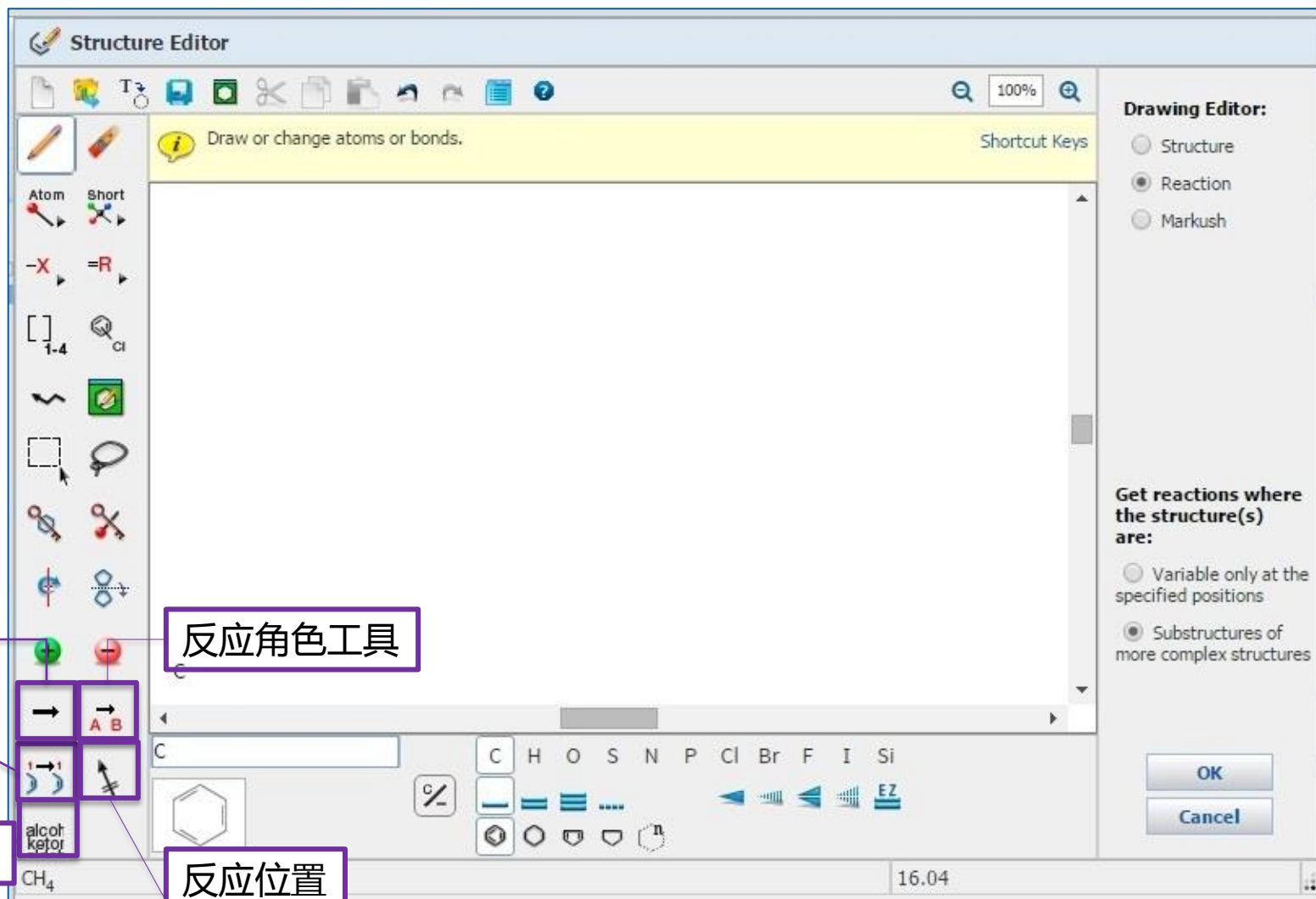
已知文献：从文献中获取反应

精确结构反应检索

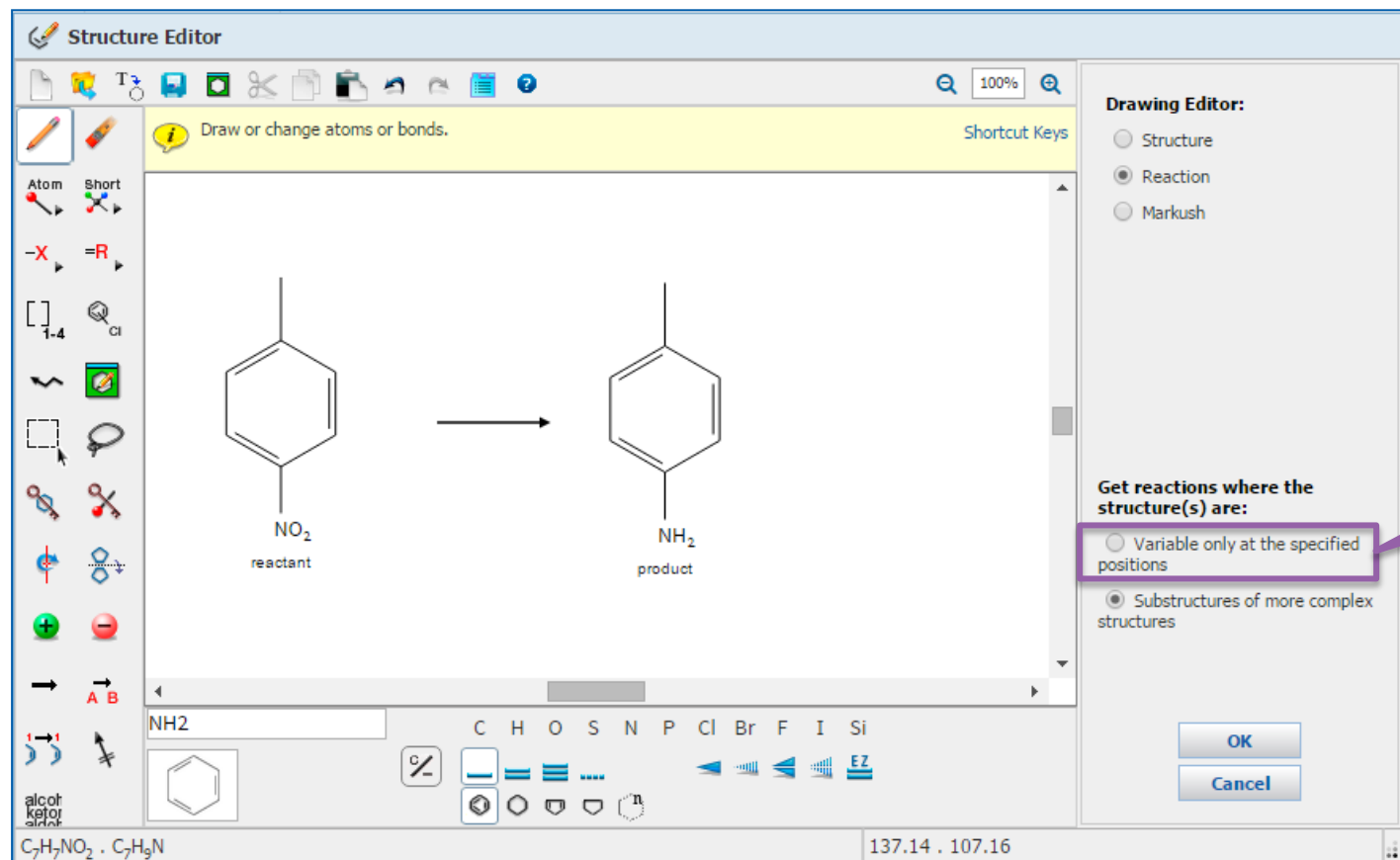
亚结构反应检索



# 反应绘制工具



# SciFinder反应检索——精确反应检索



精确反应检索

# 反应检索结果

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

获取相似反应

Get References Tools

Group by: **No Grouping** | Sort by: Relevance | Display Options

☐ **Document** Selected

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

Single Step Hover over any structure for more options.

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

### Overview

#### Steps/Stages

1.1 R:NaBH<sub>4</sub>, C:1832616-28-0, C:Ru, S:H<sub>2</sub>O, S:THF, 45 min, 25°C

#### Notes

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

#### References

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

# 获取相似反应

选择相似反应的相似限制：

Broad：仅反应中心相似

Medium：反应中心及附属原子和键

Narrow：反应中心及扩展的原子和键

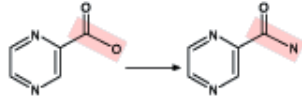
**Get Similar Reactions ?**

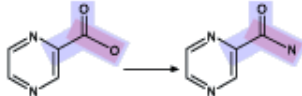
**Retrieve similar reactions from:**

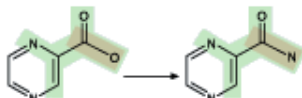
- ☒ All reactions
- ☐ Current answer set

**Include this level of similarity:**

- ☒ Broad - Reaction centers only (2934)


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


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



Get Reactions

Cancel

# 按照反应类型排序

Group by: Transformation ▼ Sort by: Frequency ▼

☐ 0 of 560 Reactions Selected

☐ 1. Reduction of Nitro Compounds to Amines  
538 Reactions

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

☐ 2. Reduction of Nitro to Azo Compounds  
11 Reactions

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

☐ 3. Reduction of Nitro to Azoxy Compounds  
11 Reactions

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

更精确的查找需要的反应



# 反应检索结果的筛选

获得特定物质做还原剂的反应

**REACTIONS** ?

Get References Tools

Analyze Refine

Analyze by: Reagent

H <sub>2</sub>	148
NaBH <sub>4</sub>	51
N <sub>2</sub> H <sub>4</sub> ·H <sub>2</sub> O	43
KOH	17
CO	16
HCO <sub>2</sub> H	16
NH <sub>4</sub> <sup>+</sup> ·HCO <sub>2</sub> <sup>-</sup>	16
H <sub>2</sub> O	14
N <sub>2</sub> H <sub>4</sub>	14
NaOH	14

Show More

Group by: No Grouping Sort by: Relevance

0 of 512 Reactions Selected

1. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.

Overview

Steps/Stages

1.1 R:NaBH<sub>4</sub>, C:1832616-28-0, C:Ru, S:H<sub>2</sub>O, S:THF, 45 min, 25°C

Notes

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

References

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

# SciFinder囊括最大的反应实验过程合集

Single Step Hover over any structure for more options.



## ▼ Overview

### Steps/Stages

1.1 R:H<sub>2</sub>, R:Cs<sub>2</sub>CO<sub>3</sub>, C:1610424-70-8, C:1034343-98-0 (oxide), S:PhMe, 2 h, 100°C, 1 atm

### Notes

solid-supported catalyst, palladium catalyst supported on graphene oxide prepared and used, reusable catalyst, Reactants: 1, Reagents: 2, Catalysts: 2, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

### References

Catalyst Enhancement and Recyclability by Immobilization of Metal Complexes onto Graphene Surface by Noncovalent Interactions

[Quick View](#) [Other Sources](#)

By Sabater, Sara et al

From ACS Catalysis, 4(6), 2038-2047; 2014

## ▼ Experimental Procedure

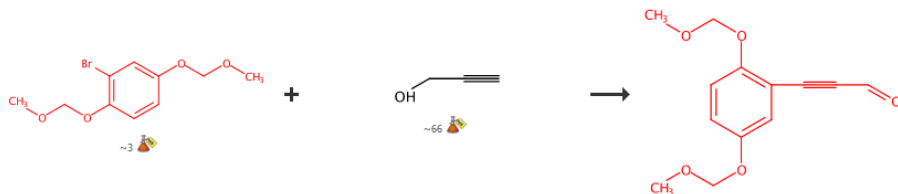


General/Typical Procedure: **General Procedure for Nitroarene Reductions.** Molecular hydrogen was added with a balloon filled with 1 atm of H<sub>2</sub> to a mixture of nitroarene (0.3 mmol), Cs<sub>2</sub>CO<sub>3</sub> (0.3 mmol), anisole as internal standard (0.3 mmol), and NHC-Pd-rGO (6 × 10<sup>-3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

不用阅读全文，直接获得包含实验过程的反应记录

# SciFinder囊括最大的反应实验过程合集

2 Steps Hover over any structure for more options.



## Overview

### Steps/Stages

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

### Notes

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

### References

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

## Experimental Procedure:

我们可以做得更好

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

## Experimental Procedure

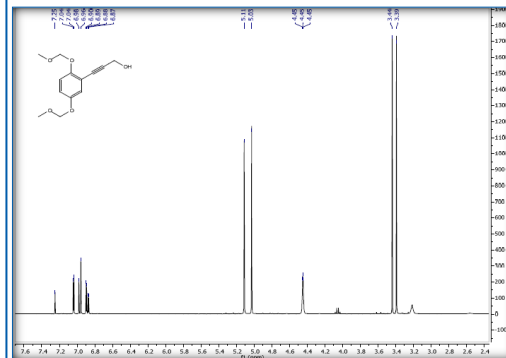


### Step 1

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

### Step 2

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



**SCIFINDER**  
 A CAS SOLUTION

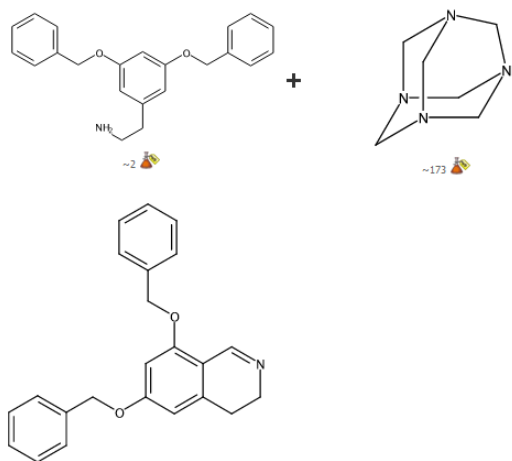
# MethodsNow Synthesis

## MethodsNow

### Asymmetric formal synthesis of schulzeines A and C

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

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



多步反应中，原文没有描述  
的实验过程以灰色标示

Products	Isoquinoline, 3,4-dihydro-6,8-bis(phenylmethoxy)-, 95%, CAS RN: 1384461-35-1
Reactants	Benzeneethanamine, 3,5-bis(phenylmethoxy)-, CAS RN: 188662-05-7 Hexamethylenetetramine, CAS RN: 100-97-0
Solvents	Trifluoroacetic acid, CAS RN: 76-05-1 Acetic acid, CAS RN: 64-19-7
Procedure	1. Add hexamethylenetetramine (3.1 g, 22.1 mmol) to the mixture of 2-(3,5-bis(benzyloxy)phenyl)ethanamine (2.0 g, 11.0 mmol), AcOH (12 mL) and TFA (3 mL) under argon. 2. Stir the mixture for 3 hours at 90°C. 3. Dilute the reaction mixture with H <sub>2</sub> O. 4. Basify with potassium carbonate and extract with CH <sub>2</sub> Cl <sub>2</sub> . 5. Wash the combined organic layers with brine. 6. Dry over MgSO <sub>4</sub> and concentrate in vacuo. 7. Purify the residue by column chromatography on silica gel (5 to 10% EtOAc in hexane) to obtain 6,8-bis(benzyloxy)-3,4-dihydroisoquinoline.
Scale	gram
<sup>1</sup> H NMR	(CDCl <sub>3</sub> , 400 MHz) δ 8.69 (s, 1H), 7.43 - 7.29 (m, 10H), 6.45 (d, <i>J</i> = 1.88 Hz, 2H), 6.36 (s, 1H), 5.05 (s, 2H), 5.04 (s, 2H), 3.67 (t, 2H), 2.65 (t, 2H)
<sup>13</sup> C NMR	(CDCl <sub>3</sub> , 100 MHz) δ 161.9, 157.7, 155.2, 140.0, 136.3, 128.6, 128.5, 128.1, 128.0, 127.4, 127.1, 111.9, 105.3, 98.5, 70.1, 46.5, 26.0
IR	(thin film, neat) ν <sub>max</sub> 3062, 3032, 2935, 1736, 1620, 1603, 1575, 1497, 1442, 1377, 1351, 1309 cm <sup>-1</sup>
HRMS	(FAB+) calcd for C <sub>23</sub> H <sub>22</sub> NO <sub>2</sub> (M+H <sup>+</sup> ) 344.1651; found 344.1658
Mass Spec	(FAB+) <i>m/z</i> 344 (M+H <sup>+</sup> )
State	yellow solid
CAS Method Number	3-614-CAS-200055

物质信息

实验过程

图谱信息

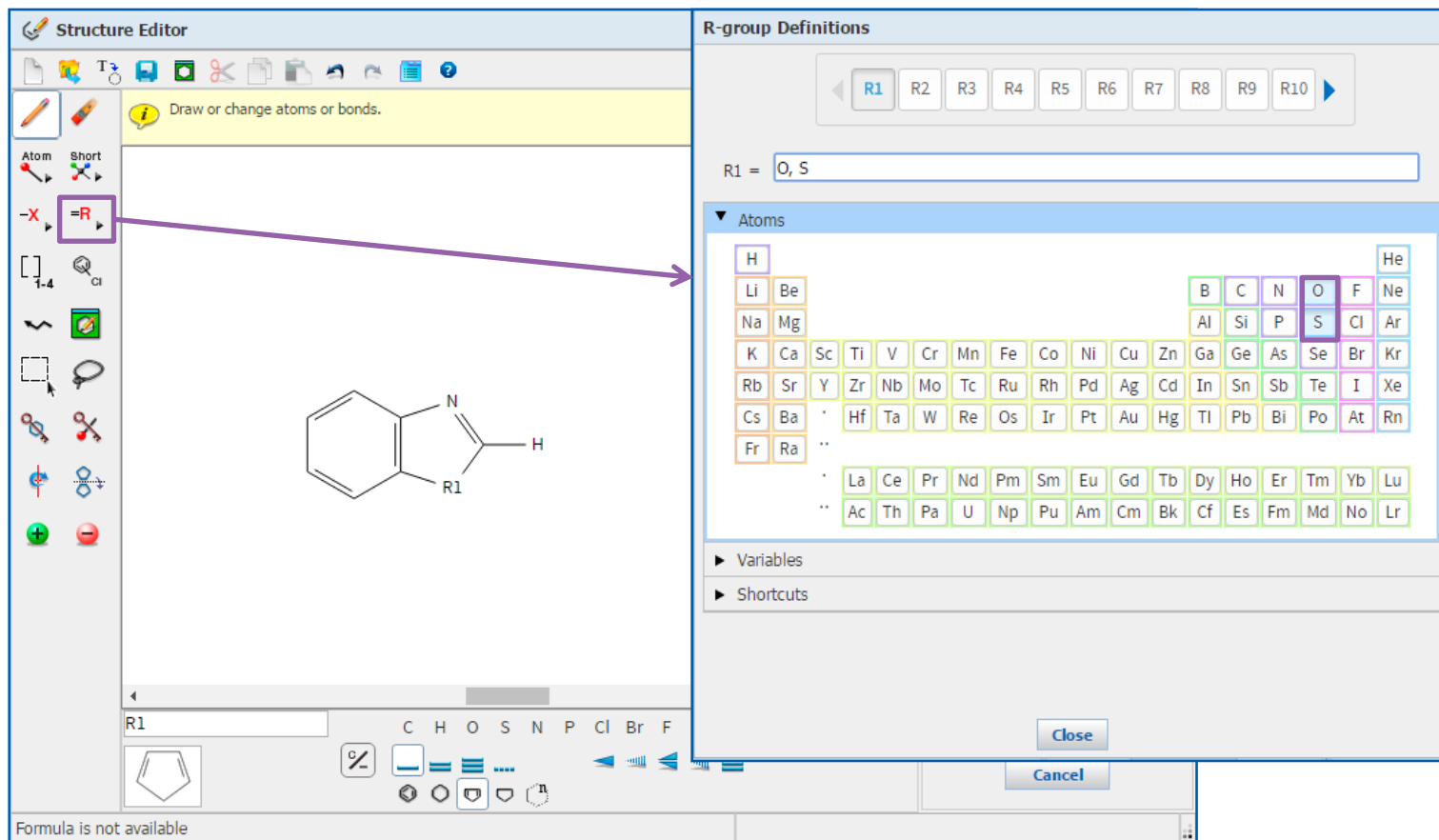
保存/导出方法

Print/Export

Close

# 亚结构反应检索

## 通过C-H活化对苯并噻唑或者恶唑进行烷基化



# 亚结构反应检索

**Structure Editor**

Drag the reaction arrow to specify reaction direction.

**Drawing Editor:**

- ☐ Structure
- ☒ Reaction
- ☐ Markush

**Variables**

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

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

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

**Chemical Reaction:**

Reactant: A benzimidazole ring with a substituent R1 and a hydrogen atom (H) at the 2-position.

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

**Formulas:**

Reactant: C1=CN=C2C=CC=CC=C2N1

Product: C1=CN=C2C=CC=CC=C2N1Ak

**Buttons:** OK, Cancel, Close

# 通过后处理工具筛选反应--Analyze

通过催化剂筛选反应

**Analyze** **Refine**

Analyze by: Catalyst

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

Group by: No Grouping Sort by: Accession Number

☐ No Grouping  
☒ Document  
☐ Transformation

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

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

**Overview**

**Steps/Stages**

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

**Notes**

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

**References**

ACS / Proprietary and Confidential / Do Not Distribute

# 提纲

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



# 案例分析

检索文献：

1. 去除N-甲基甲酰胺（123-39-7）的文献？
2. 用N-甲基甲酰胺（123-39-7）作洗脱剂的文献？

# 案例分析

## 去除N-甲基甲酰胺（123-39-7）

The screenshot displays the SciFinder web interface. At the top, there are tabs for 'Explore', 'Saved Searches', and 'SciPlanner'. On the left, a sidebar menu under 'REFERENCES' lists various search criteria: Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, and Tags. Below this, the 'SUBSTANCE' section is partially visible, showing 'Chemical' and 'Markush' options.

The main content area is titled 'REFERENCES: RESEARCH TOPIC'. It features a search input field containing the text 'remove of 123-39-7'. Below the input field, there are example sentences: 'The effect of antibiotic residues on dairy products' and 'Photocyanation of aromatic compounds'.

Below the main content area, there is a section titled 'Research Topic "remove of 123-39-7"'. It includes a 'REFERENCES' tab and a list of search results. The results are displayed in a table with columns for 'Select All', 'Deselect All', and '1 of 4 Research Topic Candidates Selected'. The table contains four rows of results, each with a checkbox and a description of the search results.

Select All	Deselect All	1 of 4 Research Topic Candidates Selected
<input checked="" type="checkbox"/>	<input type="checkbox"/>	49 references were found containing the two concepts "remove" and "123-39-7" closely associated with one another.
<input type="checkbox"/>	<input type="checkbox"/>	264 references were found where the two concepts "remove" and "123-39-7" were present anywhere in the reference.
<input type="checkbox"/>	<input type="checkbox"/>	2808271 references were found containing the concept "remove".
<input type="checkbox"/>	<input type="checkbox"/>	4512 references were found containing the concept "123-39-7".

At the bottom of the results section, there is a button labeled 'Get References'.

# 案例分析

## 1. Removal of gas phase dimethylamine and N,N-dimethylformamide using non-thermal plasma

By: Wang, Wenzheng; Fan, Xing; Zhu, Tianle; Wang, Haining; Ye, Daiqi; Hong, Xiaowei

Dimethylamine (DMA) and N,N-dimethylformamide (DMF) are typical N-VOCs exhausted from manufg. factories. In the present study, the behavior of non-thermal plasma (NTP) was systematically investigated for removal of gas-phase DMA and DMF in a link tooth wheel-cylinder plasma reactor. Exptl. results show that DMA is much easier to be decompd. by NTP than DMF. Coexisting DMF has no effect on DMA conversion while DMF conversion is significantly promoted by the addn. of DMA. Regardless of initial gas compns. as well as DMA and DMF concn., CO<sub>x</sub> selectivity increased monotonously with increasing ED. But CO<sub>x</sub> selectivity of 100% cannot be obtained even with ED higher than 70 J L<sup>-1</sup>, indicating the formation of org. intermediates during DMA and DMF decompn. Based on org. products anal. with GC-MS and mol. optimization results with d. functional theory calcn., possible mechanisms on DMA and DMF decompn. were proposed. The org. products from DMA and DMF decompn. by NTP were found to have great soly. and high biodegradability. Thus, NTP enhanced absorption/biol. method is suggested for complete removal of DMA and DMF.

### Indexing

Air Pollution and Industrial Hygiene (Section59-4)

### Concepts

Absorption	Air pollution control
Bond energy	Bond length
Decomposition	Decomposition catalysts
Plasma	Waste gas treatment








removal of gas phase dimethylamine and N,N-dimethylformamide using non-thermal plasma

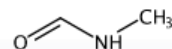
### Volatile organic compounds


removal of gas phase dimethylamine and N,N-dimethylformamide using non-thermal plasma

Removal or disposal; Process

### Substances

56-40-6 Glycine, formation (nonpreparative)   
64-18-6 Formic acid, formation (nonpreparative)   
75-12-7 Formamide, formation (nonpreparative)   
79-20-9 Methyl acetate   
105-37-3 Ethyl propionate   
107-31-3 Methyl formate   
123-39-7 N-Methyl formamide 



144-62-7 Oxalic acid, formation (nonpreparative) 

removal of gas phase dimethylamine and N,N-dimethylformamide using non-thermal plasma

Formation, unclassified; Formation, nonpreparative

## 需要的文献

# 案例分析

## 3. Removing agent containing alkylamide mixture

By: Li, Bo; Yu, Ran

Assignee: Qingdao Hui Cheng Petrochemical Technology Co., Ltd., Peop. Rep. China

The present invention relates to a kind of alkylamide removing agent. The removing agent comprises N-methylformamide 50-70 wt.%, N, N-dimethyl acetamide 30-50 wt.% and water as balance. The alkylamide removing agent of the present invention has water compatibility, and has no corrosivity for copper or copper alloy, and is generally nontoxic to mankind and environment. Because the constituent of alkylamide removing agent only comprises two main constituents, the removing agent after use can be easily by fractionation and recombine to original formula, and can be recycled to apply in the prepn. process to achieve the effect of reducing cost and environmental protection. The present invention also provides a method of using the removing agent of the present invention to remove photoresist.

### Patent Information

Patent No.	Kind	Language	Date	Application No.	Date
CN 104698775	PATENTPAK	A	Jun 10, 2015	CN 2013-10646205	Dec 4, 2013

### Priority Application

CN 2013-10646205	Dec 4, 2013
------------------	-------------

### Indexing

Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes (Section74-5)

### Concepts

Coating removers Photoresists

removing agent contg. alkylamide mixt.

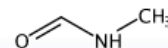
Amides

removing agent contg. alkylamide mixt.

Other use, unclassified; Physical, engineering or chemical process; Process; Uses

### Substances

123-39-7 N-Methylformamide 🔍



127-19-5 N, N-Dimethyl acetamide 🔍

removing agent contg. alkylamide mixt.

Other use, unclassified; Physical, engineering or chemical process; Process; Uses

## 噪音信息更多，如何去除？

# 案例分析

CAS Solutions
SciFINDER<sup>®</sup>  
A CAS SOLUTION

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Research Topic "remove of 123-39-7" > references (49) > Removing agent containing alky...

REFERENCES
Get Substances
Get Reactions
Get Related Citations
Tools

Create Keep Me Posted Alert
Send to SciPlanner

Analyze
Refine
Categorize

Sort by: Accession Number

0 of 49 References Selected

Analyze by:
Author Name

Egbe Matthew I	4
Hara Yasushi	4
Takahashi Fumiharu	4
Bang Sun Hong	2
Hong Heon Pyo	2
Legenza Michael Walter	2
Ward Irl E	2
Albrecht Herbert	1
Alsters Paul	1
Aoba Kazuhiro	1

1. Removal of gas phase dimethylamine and N,N-dimethylformamide using non-thermal plasma
Quick View Other Sources

By Wang, Wenzheng; Fan, Xing; Zhu, Tianle; Wang, Haining; Ye, Daiqi; Hong, Xiaowei  
From Chemical Engineering Journal (Amsterdam, Netherlands) (2016), 299, 184-191. | Language: English, Database: CAPLUS

Dimethylamine (DMA) and N,N-dimethylformamide (DMF) are typical N-VOCs exhausted from manufg. factories. In the present study, the behavior of non-thermal plasma (NTP) was systematically investigated for **removal** of gas-phase DMA and DMF in a link tooth wheel-cylinder plasma reactor. Exptl. results show that DMA is much easier to be decompd. by NTP than DMF. Coexisting DMF has no effect on DMA conversion while DMF conversion is significantly promoted by the addn. of DMA. Regardless of initial gas compns. as well as DMA and DMF concn., CO<sub>x</sub> selectivity increased monotonously with increasing E...

2. Stripping composition for removing photoresist and a method, for peeling photoresist, using same
Quick View PATENTPAK

By Park, Tae Moon; Jung, Dae Chul; Lee, Dong Hoon; Lee, Woo Ram; Lee, Hyun Jun; Kim, Ju Young  
From PCT Int. Appl. (2016), WO 2016027985 A1 20160225. | Language: Korean, Database: CAPLUS

The present invention relates to a stripping compn. for **removing** a photoresist and a method, for peeling a photoresist, using same, the stripping compn. comprising: one or more amine compds.; an amide-based compd. substituted with one or two of C1-5 straight or branched alkyl groups; a polar org. solvent; a particular triazole-based compd.; and a benzimidazole-based compd.

3. Removing agent containing alkylamide mixture
Quick View PATENTPAK

By Li, Bo; Yu, Ran  
From Faming Zhuanli Shenqing (2015), CN 104698775 A 20150610. | Language: Chinese, Database: CAPLUS

The present invention relates to a kind of alkylamide **removing** agent. The **removing** agent comprises N-methylformamide 50-70 wt.%, N, N-dimethyl acetamide 30-50 wt.%

# 案例分析

Categorize ?

1. Select a heading and category.

Category Heading	Category
All	Substances in technology (824)
<b>Technology</b>	Materials & products (76)
General chemistry	<b>Formed, removed, &amp; other substances (61)</b>
Physical chemistry	Metallurgy (45)
Biotechnology	Processes & apparatus (35)
Polymer chemistry	Imaging & recording (4)
Environmental chemistry	Power & fuel topics (5)
Synthetic chemistry	Ceramics (2)
Catalysis	Construction (2)
Genetics & protein chemistry	
Biology	
Analytical chemistry	

2. Select index terms of interest.

Index Terms		Selected Terms
Select All	Deselect All	
<input checked="" type="checkbox"/>	N-Methyl formamide 6	Click 'x' to remove the category from 'Selected Terms'  ✕ Technology > Formed, removed, & other substances (1 Terms)
<input type="checkbox"/>	N,N-Dimethylformamide 3	
<input type="checkbox"/>	Copper 2	
<input type="checkbox"/>	Copper alloy 2	
<input type="checkbox"/>	Dimethylamine 2	
<input type="checkbox"/>	Formamide 2	
<input type="checkbox"/>	Oxides (inorganic) 2	
<input type="checkbox"/>	Polyimides 2	
<input type="checkbox"/>	1-Fluoro-1,2,2-trichloroethane 1	
<input type="checkbox"/>	2,3-Dimethyl-1-butanol 1	
<input type="checkbox"/>	2,4-Di-tert-butylphenol 1	
<input type="checkbox"/>	2,6-Di-tert-butyl-1,4-benzoquinone 1	
<input type="checkbox"/>	2-(Methyl mercapto)benzothiazole 1	

Technology > Formed, removed, & other substances > 1 Index Term(s) Selected

OK

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# 提纲

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

# SciPlanner使用简介

3. View Reaction Detail [Link](#) **勾选想要的反应**

3 Steps Hover over any structure for more options.

**点击Send to SciPlanner**

**进入SciPlanner 新建文件**

**将刚推送过来的反应拖至编辑面板**

**Send to SciPlanner**  
Display Options

**Overview**

**Steps/Stages**

1.1 R: NH<sub>3</sub>, R: t-BuOK, R: t-BuOOH, S: THF  
2.1 R: NaH, S: THF  
3.1 R: POCl<sub>3</sub>, reflux

**Notes**

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

**References**

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

SciPlanner [SciPlanner\\_11\\_19\\_2015\\_112612](#)

**Workspace** Edit View GoTo

New  
Open  
Save  
Duplicate  
Import  
Export  
Print  
Close

Your Workspace is empty.

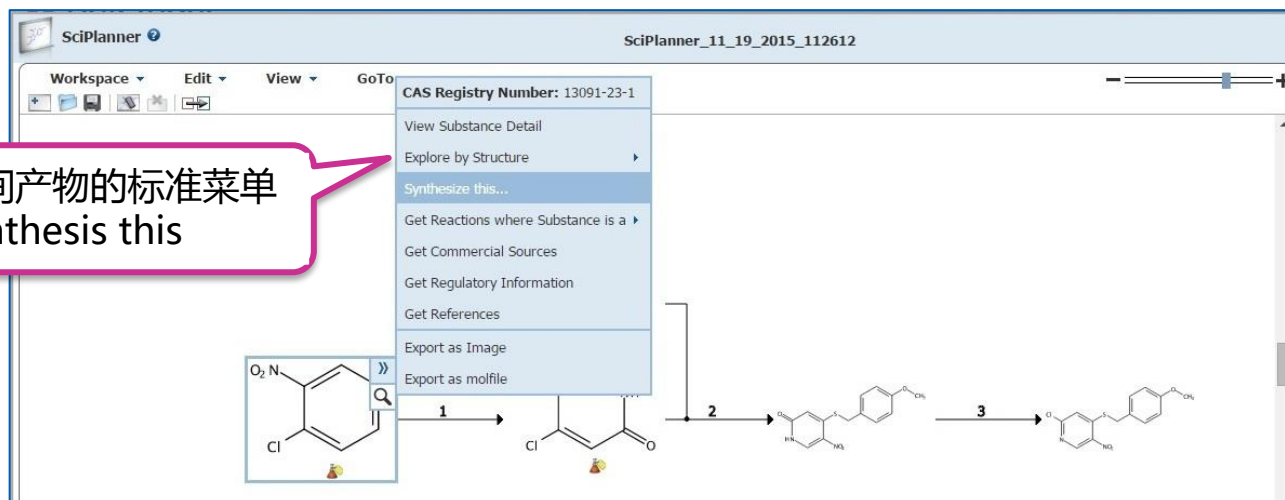
Drag items from the reference, substance, and reaction libraries (on the right) to this area.

Chemical reaction scheme showing the synthesis of a thiazolo[4,5-c]pyridine derivative from a pyridine derivative and a thiol derivative.



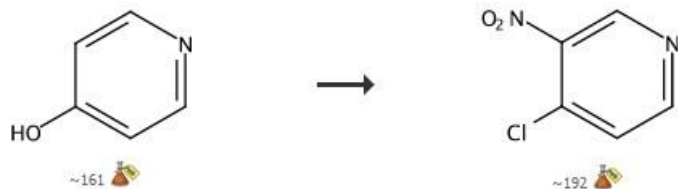
# SciPlanner使用简介

打开中间产物的标准菜单  
选择Synthesize this

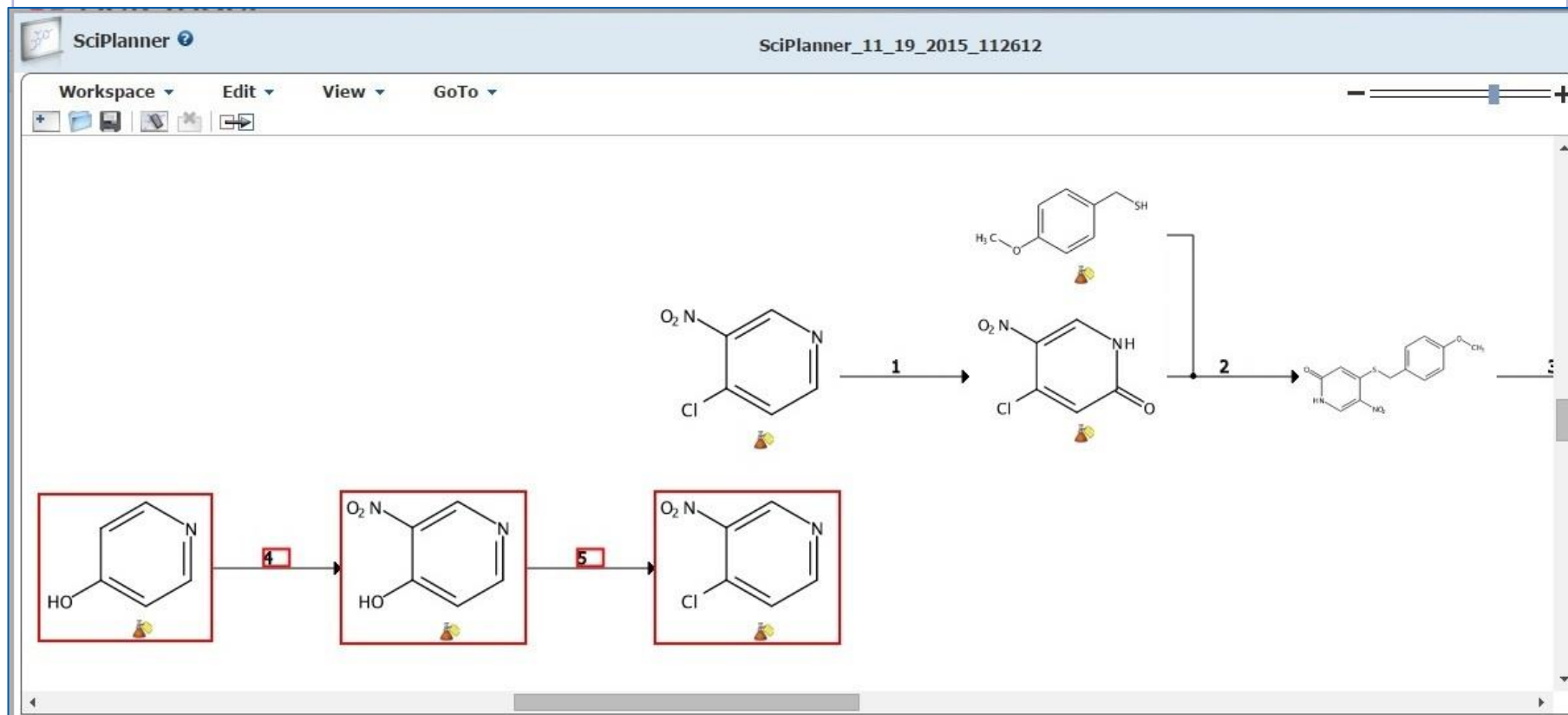


在检索到的反应中选择感兴趣的反应

继续推送到SciPlanner



# SciPlanner使用简介



步骤同前，将推送过来的反应拖到编辑面板中，可以看到两条反应中存在同样的结构

# SciPlanner使用简介

SciPlanner 11\_19\_2015\_112612

Workspace Edit View GoTo

New  
Open  
Save  
Duplicate  
Import  
**Export**  
Print  
Close

点击 Workspace, 选择 Export 导出结果

用鼠标将两个同样的结构拖至重叠, 两条反应合并

选择适当的输出格式, 输出结果

**Export**

**For:**

**Offline Review**

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- ☐ Citations (\*.ris)
- ☐ Image (\*.png)

**Saving Locally**

- ☐ SciPlanner eXchange (\*.pkx)

**Details:**

**File Name:** \*  
SciPlanner\_11\_19\_2015\_112612

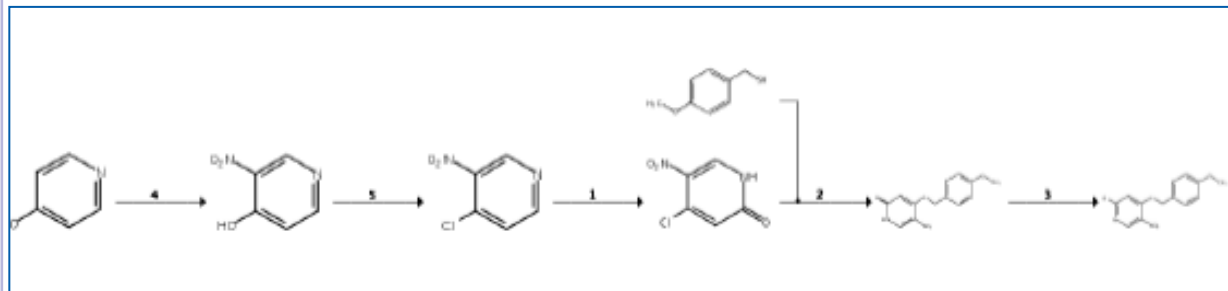
**Title**  
[Empty Field]

**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 <sub>3</sub> , S:PhMe, 0°C → rt; 16 h, rt → 110°C	Reactants: 1, Reagents: 2, Solvents: 2, Steps: 1, Stages: 2	90%
	1.2 R:K <sub>2</sub> CO <sub>3</sub> , S:H <sub>2</sub> O, cooled, pH 10	Transformation: 1. Formation of Alkyl Halides from Alcohols	

## References

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

By Poloek, Anurach et al

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

Substance Information		
<p>1228150-22-8</p> <p>C<sub>13</sub>H<sub>12</sub>N<sub>2</sub>O<sub>4</sub>S 2(1H)-Pyridone, 4-[[4-methoxyphenyl]methyl]thio-5-nitro- Related Info: ~ 2 References Reactions</p>	<p>1228150-23-9</p> <p>C<sub>13</sub>H<sub>11</sub>ClN<sub>2</sub>O<sub>4</sub>S Pyridine, 2-chloro-4-[[4-methoxyphenyl]methyl]thio-5-nitro- Related Info: ~ 2 References Reactions</p>	<p>13091-23-1</p> <p>C<sub>5</sub>H<sub>3</sub>ClN<sub>2</sub>O<sub>2</sub> Pyridine, 4-chloro-3-nitro- Related Info: ~ 391 References Reactions ~ 190 Commercial Sources Regulatory Information</p>
<p>5435-54-1</p> <p>C<sub>6</sub>H<sub>4</sub>N<sub>2</sub>O<sub>3</sub> 4-Pyridinol, 3-nitro- Related Info: ~ 113 References Reactions ~ 197 Commercial Sources Regulatory Information</p>	<p>6258-60-2</p> <p>C<sub>8</sub>H<sub>10</sub>O S Benzenemethanethiol, 4-methoxy- Related Info: ~ 749 References Reactions ~ 71 Commercial Sources Regulatory Information</p>	<p>626-64-2</p> <p>C<sub>5</sub>H<sub>5</sub>N O 4-Pyridinol Related Info: ~ 1351 References Reactions ~ 160 Commercial Sources Regulatory Information</p>
<p>850663-54-6</p> <p>C<sub>6</sub>H<sub>3</sub>ClN<sub>2</sub>O<sub>3</sub> 2(1H)-Pyridone, 4-chloro-5-nitro- Related Info: ~ 22 References Reactions ~ 138 Commercial Sources</p>		

# 提纲

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# SciFinder浏览器选择建议

- Windows 7以上用户建议升级IE到10以上
- Chrome和FireFox浏览器在所有系统上的表现都优于IE浏览器
- 不建议使用360浏览器检索SciFinder，会被自动拦截相关功能或插件

# 如何获取SciFinder账号



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EAST CHINA UNIVERSITY OF SCIENCE AND TECHNOLOGY LIBRARY

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使用SciFinder Web版是以互联网的用户形式注册, 允许您建立您自己的SciFinder用户名和密码。Web版的注册

地址是:[https://scifinder.cas.org/registration/index.html?](https://scifinder.cas.org/registration/index.html?corpKey=67260907X86F35055X146B276313514305D7)

[corpKey=67260907X86F35055X146B276313514305D7](https://scifinder.cas.org/registration/index.html?corpKey=67260907X86F35055X146B276313514305D7)在您提交表格之后, CAS为您发送电子邮件, 指导您完成注册过程。因此, 您必须有一个本校的电子邮件域的电子邮件地址。(如: [xxxx@ecust.edu.cn](mailto:xxxx@ecust.edu.cn)或是 [xxxx@mail.ecust.edu.cn](mailto:xxxx@mail.ecust.edu.cn))。

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# 如何获取SciFinder账号

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

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

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

请注意：

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

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

3.密码必须包含 7-15 个字符，并且至少**包含三种以下字符**：

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

例：abc@123

4.从下拉列表中选择一个密码提示问题并给出答案。  
单击 Register ( 注册 )。



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From: CAS

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

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

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

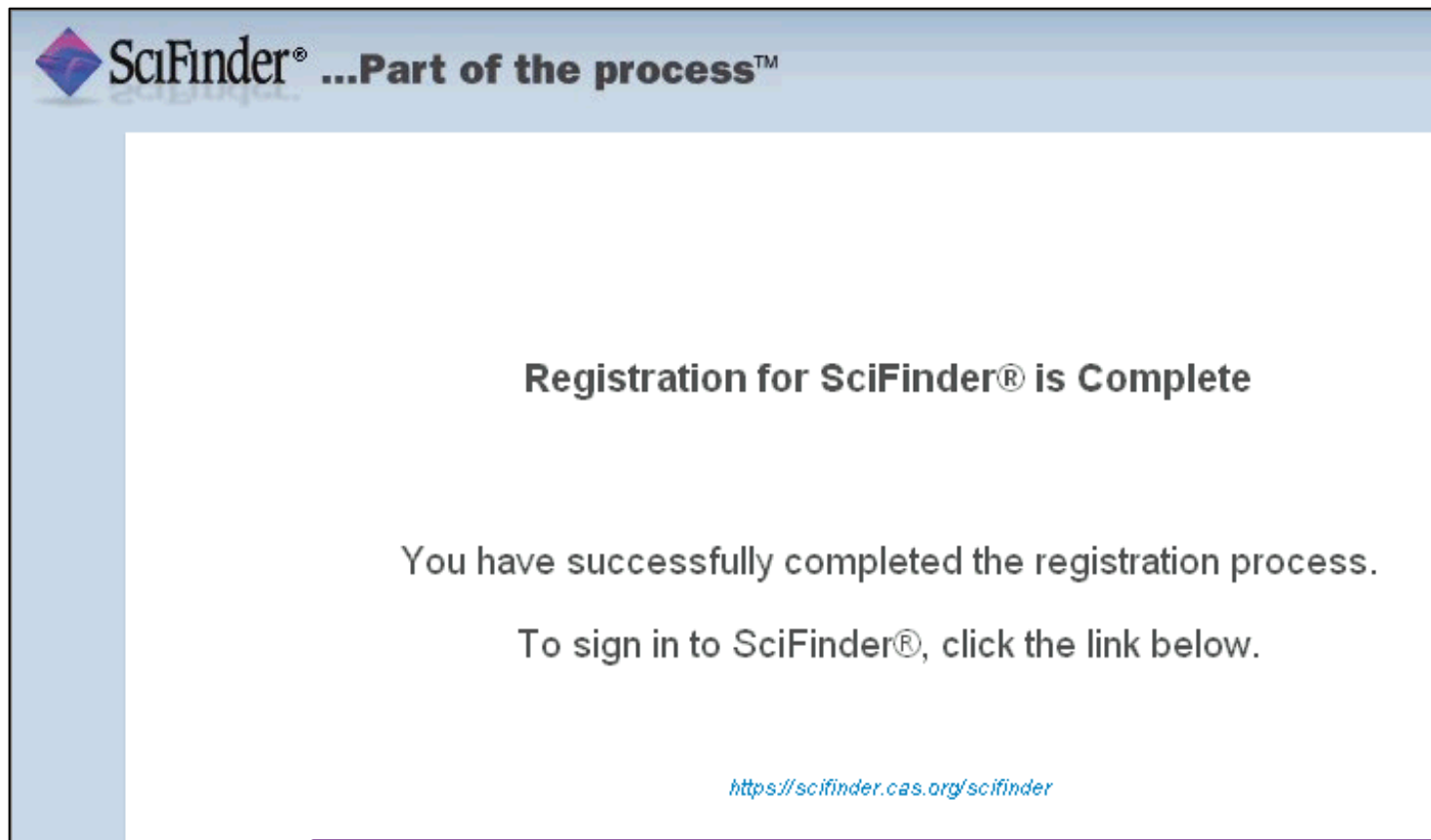
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- 严禁账号分享
- 严禁将账号用于非学术研究

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