

朱传娴

客户顾问

hzhu@acs-i.org

# 如何使用SciFinder获取科技信息

东南大学

2018.10.11



# 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

# 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



# CAS——构建最高质量的化学数据库



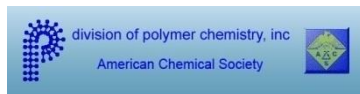
arXiv.org

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BEILSTEIN JOURNAL  
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Letters

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

# CAS——构建最高质量的化学数据库



# CAS数据库——源于化学，超越化学

## 生物化学：

农化产品管控信息,生化遗传学,发酵,免疫化学,药理学

## 有机化学各领域：

氨基酸,生物分子,碳水化合物,有机金属化合物,类固醇

## 大分子化学各领域：

纤维素、木质素、造纸;涂料、墨水

染料、有机颜料;合成橡胶;纺织品、纤维

## 应用化学各领域：

大气污染,陶瓷,精油、化妆品,化石燃料,黑色金属、合金

## 物理、无机、分析化学各领域：

表面化学,催化剂,相平衡,核现象,电化学




# CAS数据库最具价值的内容——人工索引

## 4. Process for preparation of novel sofosbuvir crystal

By: Zhou, Haohui; Lin, Guoliang; Wu, Yao; Zou, Wenjuan; Chan, Yunxia  
Assignee: Beijing Winsunny Pharmaceutical Co., Ltd., Peop. Rep. China

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

### Patent Information

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

### Priority Application

CN 2014-10742897	Dec 9, 2014
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### Indexing


Carbohydrates (Section33-9)

Section cross-reference(s): 34, 63

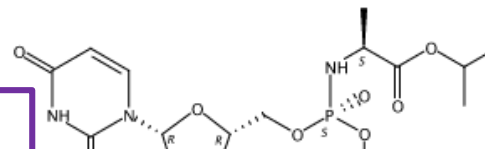
### Concepts

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

### Substances

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

Page 2 in PATENTPAK



### Tips:

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

# CAS人工标引解决的问题

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



# 提纲

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  - 文献检索
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  - 反应检索
  - 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/>



## Sign In

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Your SciFinder username and password are assigned to you alone and may not be shared with anyone else.

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### What is SciFinder?

SciFinder<sup>®</sup> 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.



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

[New Commercial Source Logos](#)

输入SciFinder帐号和密码

# SciFinder主界面

检索完，请点击退出

工具栏

The screenshot shows the SciFinder main interface. At the top, there is a navigation bar with the SciFinder logo and a 'Sign Out' button. Below this is a secondary navigation bar with 'Explore', 'Saved Searches', and 'SciPlanner' options. The main content area is titled 'REFERENCES: RESEARCH TOPIC' and features a search input field with a 'Search' button and an 'Advanced Search' link. On the left, a sidebar lists search categories: REFERENCES (Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, Tags), SUBSTANCES (Chemical Structure, Markush, Molecular Formula, Property, Substance Identifier), and REACTIONS (Reaction Structure). On the right, a 'SAVED ANSWER SETS' panel lists various saved search results like 'CSF1R', 'jmc', and 'EP 19870107847'. A 'KEEP ME POSTED' section is also visible at the bottom right.

已保存的结果集

检索入口

定题追踪

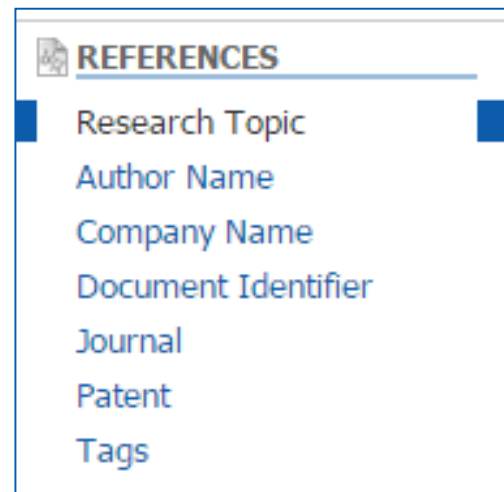
# SciFinder检索——文献检索

## ■ 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：离子液体催化剂

检索式：ionic liquid with catalysis

The screenshot displays the SciFinder web interface. At the top, there is a navigation bar with 'Explore', 'Saved Searches', and 'SciPlanner' tabs. Below this, the search topic 'ionic liquid with catalysis' is entered. On the left side, there are two main categories: 'REFERENCES' and 'SUBSTANCES'. Under 'REFERENCES', there is a list of search criteria including 'Research Topic', 'Author Name', 'Company Name', 'Document Identifier', 'Journal', 'Patent', and 'Tags'. Under 'SUBSTANCES', there are 'Chemical Structure' and 'Markush'. The main search area on the right shows the search term 'ionic liquid with catalysis' in a text box, with 'Examples:' listed below it: 'The effect of antibiotic residues on dairy products' and 'Photocyanation of aromatic compounds'. A blue 'Search' button is positioned below the text box. At the bottom of the search area, there is a link for 'Advanced Search'.

关键词之间用介词连接：in, with, of...



# 主题检索的候选项

Explore ▼ Saved Searches ▼ SciPlanner

Research Topic "ionic liquid with catalysis"

REFERENCES ⓘ

Select All Deselect All

1 of 5 Research Topic Candidates Selected

	References
<input type="checkbox"/> 74 references were found containing "ionic liquid with catalysis" as entered.	74
<input checked="" type="checkbox"/> 16803 references were found containing the two concepts "ionic liquid" and "catalysis" closely associated with one another.	16803
<input type="checkbox"/> 20983 references were found where the two concepts "ionic liquid" and "catalysis" were present anywhere in the reference.	20983
<input type="checkbox"/> 91371 references were found containing the concept "ionic liquid".	91371
<input type="checkbox"/> 3150688 references were found containing the concept "catalysis".	3150688

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

CAS Solutions | Preferences | SciFinder Help | Sign Out

SciFINDER  
A CAS SOLUTION

Welcome Helen Zhu

Explore | Saved Searches | SciPlanner | Save | Print | Export

Research Topic "ionic liquid with catalysis" > references (16803)

REFERENCES | Get Substances | Get Reactions | Get Related Citations | Tools

Create Keep Me Posted Alert | Send to SciPlanner

Analyze | Refine | Categorize

Sort by: Citing References

Display Options

Page: 1 of 841

Analyze by: Author Name

Author Name	Citing References
Wasserscheid Peter	170
Zhang Suojiang	146
Dupont Jairton	132
Li Huaming	97
Yu Shitao	96
Deng Youquan	91
Wang Jun	78
Chen Jing	76
Dyson Paul J	76
Fang Dong	75

1. **Ionic Liquids. Solvents for Synthesis and Catalysis**  
By Welton, Thomas  
From Chemical Reviews (Washington, D. C.) (1999), 99(8), 2071-2083. | Language: English, Database: CAPLUS  
A review with 124 refs. covering org. **reactions** in alkylhalo- and haloaluminate **ionic liqs.** ~9577

2. **Ionic liquids - new "solutions" for transition metal catalysis**  
By Wasserscheid, Peter; Keim, Wilhelm  
From Angewandte Chemie, International Edition (2000), 39(21), 3772-3789. | Language: English, Database: CAPLUS  
A review with 98 refs. **Ionic liqs.** are **salts** that are **liq.** at low **temp.** (<100°C), which represent a new class of solvents with nonmol., **ionic** character. Even though the first representative has been known since 1914, **ionic liqs.** have only been investigated as solvents for transition metal **catalysis** in the past ten years. Publications to date show that replacing an org. solvent by an **ionic liq.** can lead to remarkable improvements in well-known processes. **Ionic liqs.** form biphasic systems with many org. product mixts. This gives rise to the possibility of a multiphase **reaction** procedure wit... ~4015

3. **Ionic Liquid (Molten Salt) Phase Organometallic Catalysis**  
By Dupont, Jairton; de Souza, Roberto F.; Suarez, Paulo A. Z.  
From Chemical Reviews (Washington, DC, United States) (2002), 102(10), 3667-3691. | Language: English, Database: CAPLUS  
A review including **ionic liqs.**; oligomerization and polymn.; hydrogenation; dimerization and telomerization of dienes; carbonylation; oxidn. and radical **reactions**; Heck, Suzuki, Stille, Sonogashira, Negishi, and Ullmann coupling **reactions**; allylation; olefin metathesis; and mechanistic aspects of **reactions** in **ionic liqs.** ~3235

Citing Reference: 帮助找到最重要的文献



# 文献检索结果

CAS Solutions | SciFinder | A CAS SOLUTION

Preferences | SciFinder Help | Sign Out

Welcome Helen Zhu

Explore | Saved Searches | SciPlanner | Save | Print | Export

Research Topic "ionic liquid with catalysis" > referen

REFERENCES

Substances | Reactions | Citations | Tools

Analyze | Refine | Categorize

Sort by: Accession Number

0 of 16803 References Selected

Page: 1 of 841

1. Significant effect of 1,10,15,20-meso-tetraarylporphyrinatoiron(III) chloride/triflate and acidic/neutral/basic imidazolium ionic liquids in catalytic oxidation of phenols

By Ahmad, Sohail; Gautam, Renu; Singhal, Anchal; Chauhan, S. M. S.  
From Journal of Molecular Liquids (2018), 260, 292-303. | Language: English, Database: CAPLUS

The influence of acidic, neutral and basic ionic liqs. and their binary mixt. with dichloromethane on the reactivity of iron(III)porphyrins was investigated during oxidn. of phenols with hydrogen peroxide catalyzed by 5,10,15,20-tetraarylporphyrinatoiron(III) chloride and 5,10,15,20-tetraarylporphyrinatoiron(III) triflate. The generation of different intermediates of iron(III) porphyrin in different ILs was studied through viscosity, d., UV-Vis and <sup>1</sup>H NMR spectroscopy. The heterolytic cleavage efficiency of (TAP) Fe<sup>III</sup>-OOH and formation of quinone using iron(III)porphyrin (TAP)Fe<sup>III</sup>Cl with Cl...

2. Supported ionic liquid phase (SILP) facilitated gas-phase enzyme catalysis - CALB catalyzed transesterification of vinyl propionate

By Lee, Changhee; Sandig, Bernhard; Buchmeiser, Michael R.; Haumann, Marco  
From Catalysis Science & Technology (2018), Ahead of Print. | Language: English, Database: CAPLUS

The supported ionic liq. phase (SILP) technol. has been used to immobilize Candida Antarctica Lipase B (CALB) within a hybrid monolith. The monolith was synthesized in-situ inside a Teflon cartridge via the 4-(dimethylamino)pyridine-catalyzed polyaddn. of 1,1,1-tris(hydroxymethyl)propane to 4,4'-methylenebis(phenylisocyanate) in the presence of porous cellulose-2.5-acetate beads. An ionic liq. contg. small amts. of CALB was impregnated into these beads and the resulting enzyme-SILP (e-SILP) catalyst was tested in the continuous gas-phase transesterification of vinyl propionate and 2-propanol...

3. A Phosphine-mediated Synthesis of 2,3,4,5-tetra-substituted Nhydroxypyrroles from α-oximino Ketones and Dialkyl Acetylenedicarboxylates Under Ionic Liquid Green-media

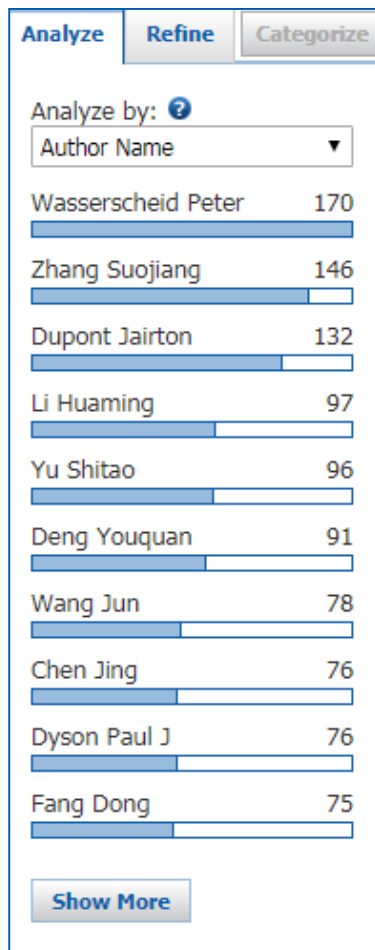
By Shahvelayati, Ashraf S.; Ghazvini, Maryam; Yadollahzadeh, Khadijeh; Delbari, Akram S.  
From Combinatorial Chemistry & High Throughput Screening (2018), 21(1), 14-18. | Language: English, Database: CAPLUS

Author Name	Count
Wasserscheid Peter	170
Zhang Suojiang	146
Dupont Jairton	132
Li Huaming	97
Yu Shitao	96
Deng Youquan	91
Wang Jun	78
Chen Jing	76
Dyson Paul J	76
Fang Dong	75

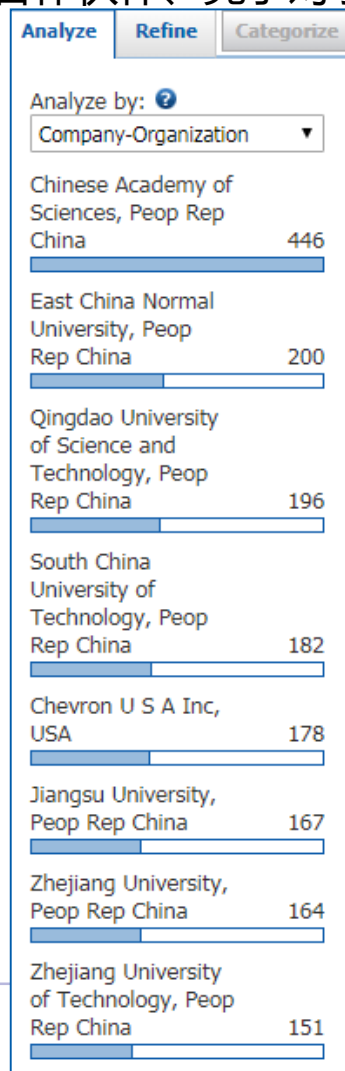
SciFinder提供强大的文献处理工具，帮助处理文献

# 文献检索结果的Analyze

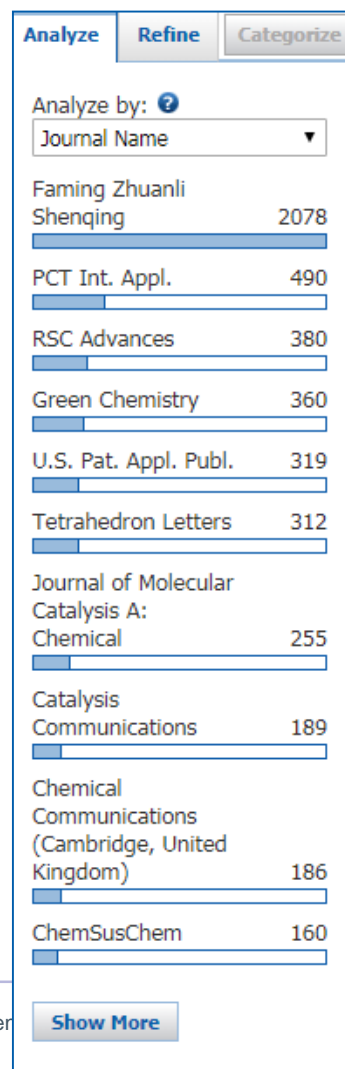
## 本领域研究人员



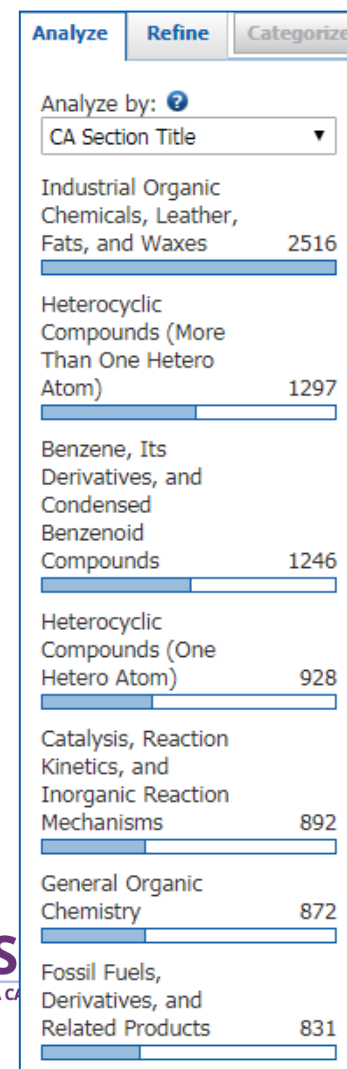
## 本领域研究机构、 合作伙伴、竞争对手



## 期刊



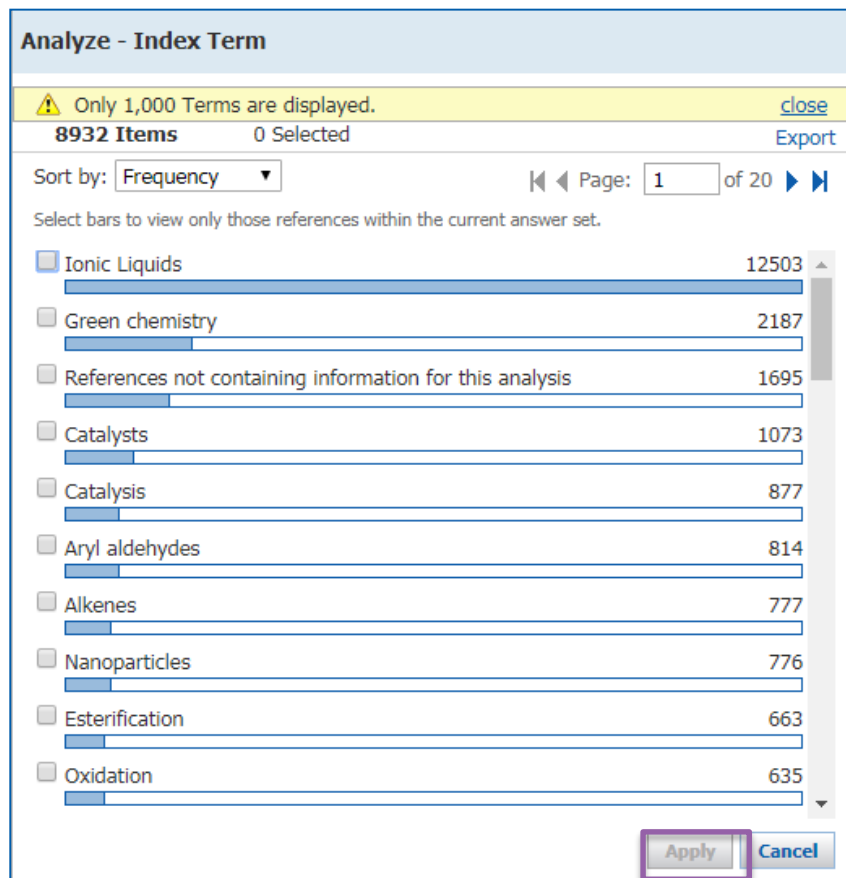
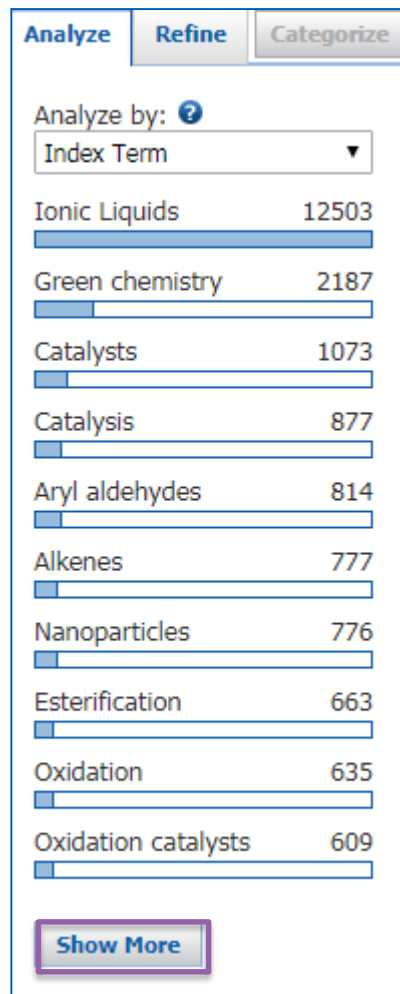
## 涉及学科领域



# 文献检索结果的Analyze

Index Term :

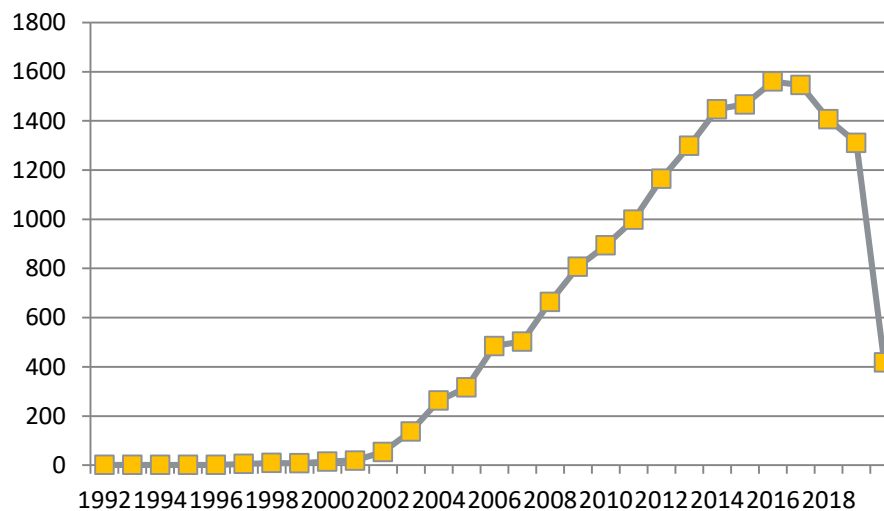
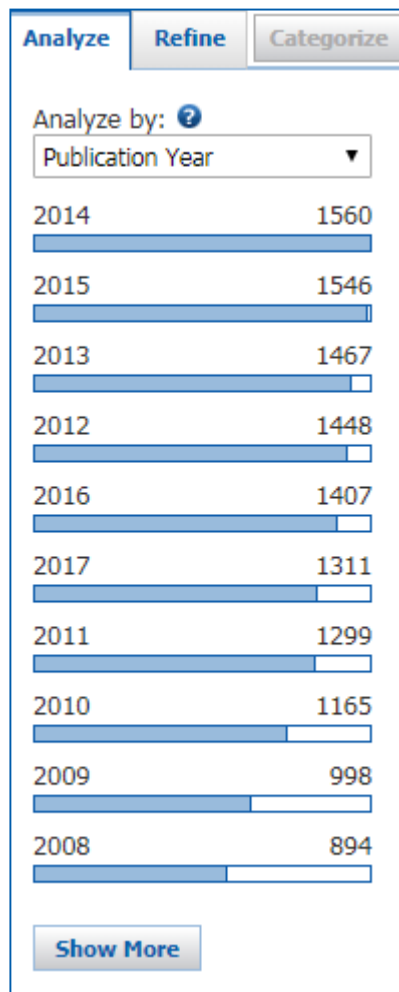
帮助用户了解涉及到的重要技术术语，并修正检索词



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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

Analyze Refine Categorize

Refine by: ?

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

Document Type(s)

- Biography
- Book
- Clinical Trial
- Commentary
- Conference
- Dissertation
- Editorial
- Historical
- Journal
- Letter
- Patent
- Preprint
- Report
- Review

Refine

Get Substances Get Reactions Get Related Citations Tools

Create Keep Me Posted Alert Send to SciPlanner

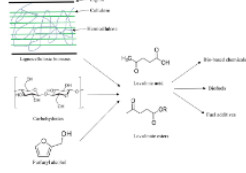
Sort by: Accession Number

0 of 1224 References Selected Page: 1 of 62

1. Conversion of Biomass and Its Derivatives to Levulinic Acid and Levulinic Esters via **Ionic Liquids**

Quick View Other Sources

By Tiong, Yong Wei; Yap, Chiew Lin; Gan, Suyin; Yap, Winnie Soo Ping  
From Industrial & Engineering Chemistry Research (2018), 57(14), 4749-4766. | Language: English, Database: CAPLUS



A review. Biomass has emerged as an abundant and relatively low cost carbon resource alternative to fossil fuel resources in the sustainable prodn. of specialty chems. and biofuel. Levulinic acid is an attractive platform chem. Upgrading of levulinic acid produces levulinic esters, which serve as a transportation fuel and fuel additive. The present review focuses on the development of sustainable conversion of biomass into levulinic acid and levulinic esters via **ionic liqs.** dual solvent-catalysts. The synthesis routes of levulinic acid and levulinic esters and the corresponding **ionic l...**

2. Recent Advances in Pd-Catalyzed Cross-Coupling Reaction in **Ionic Liquids**

Quick View Other Sources

By Li, Jianxiao; Yang, Shaorong; Wu, Wanqing; Jiang, Huanfeng  
From European Journal of Organic Chemistry (2018), 2018(11), 1284-1306. | Language: English, Database: CAPLUS

A review. **Ionic liqs. (ILs)** can behave as green solvents in comparison with conventional org. solvents, but more often they also act as ligands, co-catalysts, and stabilizing agents both for metal active species and for intermediates of **catalytic** systems. In this review we have mainly summarized the recent achievements (2013 to the present) in Pd-catalyzed cross-coupling in **ILs** for the assembly of structurally diverse and highly functionalized org. mols., with the focus on cascade **reactions** triggered by nucleopalladation, Suzuki coupling, Sonogashira coupling, allylic functionalization, and ...

3. Acid-Catalyzed Conversion of Carbohydrates into Value-Added Small Molecules in Aqueous Media and **Ionic Liquids**

Quick View Other Sources

By Bodachivskiy, Iurii; Kuzhiumparambil, Unnikrishnan; Williams, D. Bradley G.  
From ChemSusChem (2018), 11(4), 642-660. | Language: English, Database: CAPLUS

A review. Biomass is the only realistic major alternative source (to crude oil) of hydrocarbon substrates for the com. synthesis of bulk and fine chems. Within biomass, terrestrial sources are the most accessible, and therein lignocellulosic materials are most abundant. Although lignin shows promise for the delivery of certain types of org. mols., cellulose is a biopolymer with significant potential for conversion into high-vol. and high-value chems. This review covers the acid-catalyzed conversion of lower value (poly) carbohydrates into valorized org. building-block chems. (platform mols....

Refine : 帮助用户迅速获得需要的文献

# 文献检索结果的Categorize

学科领域  
主分类

学科领域  
副分类

Index Term

选中的Index Term

**Categorize** ?

1. Select a heading and category.      2. Select index terms of interest.

Category Heading	Category	Index Terms	Selected Terms
All	Catalysis (162)	Page: 1 of 4 Select All   Deselect All	Click 'x' to remove the category from 'Selected Terms'
Synthetic chemistry	<b>Catalysts (328)</b>	<input type="checkbox"/> Enzymes 46	<input checked="" type="checkbox"/> Catalysis > Catalysts (1 Terms)
General chemistry		<input checked="" type="checkbox"/> Imidazolium compounds 32	
<b>Catalysis</b>		<input type="checkbox"/> Transition metal complexes 31	
Physical chemistry		<input type="checkbox"/> Palladium 28	
Environmental chemistry		<input type="checkbox"/> Lewis acids 25	
Technology		<input type="checkbox"/> Transition metals 25	
Genetics & protein chemistry		<input type="checkbox"/> Heteropoly acids 24	
Polymer chemistry		<input type="checkbox"/> Zeolites, synthetic 21	
Biotechnology		<input type="checkbox"/> Lipase 20	
Biology		<input type="checkbox"/> Bronsted acids 17	
Analytical chemistry		<input type="checkbox"/> Ruthenium 17	
		<input type="checkbox"/> Metals 16	
		<input type="checkbox"/> Oxides (inorganic) 16	
		<input type="checkbox"/> Quaternary ammonium compounds 16	

Catalysis > Catalysts > 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

The screenshot shows the SciFinder search results page. At the top, there are navigation buttons for 'Save', 'Print', and 'Export'. Below the search bar, there are options for 'Get Substances', 'Get Reactions', 'Get Related Citations', and 'Tools'. The search results are sorted by 'Accession Number' and show 0 of 32 references selected. The first three results are listed, with the first one highlighted. A purple box highlights the title 'Chiral Ionic Liquids: Synthesis and Role as Efficient Green Catalyst in Asymmetric Synthesis' and another purple box highlights the text '文献详细信息' (Literature Detailed Information) with an arrow pointing to the first result's abstract.

Save : 保存在服务器上, 方便以后登陆查看, 每次可存1万条记录。

Export : 导出至本地电脑。

Print : 打印成PDF格式

Citation manager: 保存成RIS等格式, 可导入EndNote 等文献管理工具

Offline Review : 保存成PDF, RTF等格式, 用于脱机浏览

The screenshot shows the 'Export' dialog box in SciFinder. It has three main sections: 'Export:', 'For:', and 'Details:'. The 'Export:' section has radio buttons for 'All', 'Selected', and 'Range', with 'All' selected. The 'For:' section has radio buttons for 'Citation Manager', 'Offline review', and 'Saving locally', with 'Citation Manager' selected. The 'Details:' section has a 'File Name:' field with the value 'Reference\_06\_19\_2012\_100848' and radio buttons for 'Summary without abstracts', 'Summary with partial abstracts', 'Summary with full abstracts', and 'Detail (full record)', with 'Summary with full abstracts' selected. There are 'Export' and 'Cancel' buttons at the bottom right.

# 文献信息—题录、摘要、索引

获得引文及参考文献

REFERENCE DETAIL Get Substances Get Related Citations Link to Other Sources Send to SciFinder

Return

Previous Next

## 4. The Partial Hydrogenation of 1,3-Dienes Catalyzed by Soluble Transition-Metal Nanoparticles

By: Luza, Leandro; Gual, Aitor; Dupont, Jairton

A review. The partial hydrogenation of a 1,3-dienes is a structure sensitive reaction that is typically catalyzed by classical heterogeneous (heterotopic) or homogeneous (homotopic) catalysts. Recently, sol. transition-metal nanoparticles (M-NPs), particularly palladium and gold-based systems, have emerged as an efficient alternative. Here, the authors review the current state of the techniques for the partial hydrogenation of 1,3-dienes by M-NPs and conclude that, from the reactivity point of view, these materials possess heterotopic-like and homotopic-like characteristics. They are heterotopic-like because the relative concn. of the monoalkene with respect to the diene does not affect the product selectivity and their catalytic performance is affected by their phys. properties (such as size and shape). Furthermore, they are easily recoverable, with long catalytic lifetimes. Addnl., as homotopic systems, their reactivity can be tuned by using an appropriate org. stabilizer, which displays substrate-selective levels that are not obsd. for classical heterotopic catalysts.

### Indexing

General Organic Chemistry (Section 21.0)

#### Concepts

重要概念

Hydrogenation  
Ionic liquids  
Polymer-supported catalysts  
Hydrogenation catalysts  
Nanoparticles  
Surfactants

#### Substances

重要物质

7439-89-6 Iron (nanoparticles), uses  
7440-05-3 Palladium (nanoparticles), uses  
7440-16-6 Rhodium (nanoparticles), uses  
7440-18-8 Ruthenium (nanoparticles), uses

advances in development of methods for synthesis of alkene derivs. by transition-metal catalyst hydrogenation of alkadienes

Catalyst use; Uses

592-57-4 1,3-Cyclohexadiene

advances in development of methods for synthesis of alkene derivs. by transition-metal catalyst hydrogenation of alkadienes

Reactant; Reactant or reagent

### QUICK LINKS

0 Tags, 0 Comments

### SOURCE

ChemCatChem  
Volume6  
Issue3  
Pages702-710  
Journal; General Review;  
Online Computer File  
2014  
CODEN:CHEMK3  
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### COMPANY/ORGANIZATION

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CAPLUS

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Co. KGaA

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
- 根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
  - 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



### SUBSTANCES

Chemical Structure

Markush

Molecular Formula

Property

Substance Identifier

## ■ 物质检索策略推荐

—有机化合物，天然产物：结构检索

—无机物，合金：分子式检索

—高分子化合物：分子式检索和结构检索

# 物质检索——标识符检索

Explore ▾ Saved Searches ▾ SciPlanner

Research Topic "ionic liquid with catalysis" > references (16803) > refine "Review" (1224) > refine by c

**REFERENCES**

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

**SUBSTANCES**

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

**SUBSTANCES: SUBSTANCE IDENTIFIER** ⓘ

UHMWPE

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

The screenshot displays the SciFinder interface. At the top, it shows "0 of 1 Substance Selected". Below this, a search bar contains the CAS Registry Number "9002-88-4". A callout box points to this number with the text "点击CAS RN 获得物质详细信息". Below the search bar, there are icons for "359876" and "112". The main content area shows the substance record for Ethene, with the CAS Registry Number "74-85-1" and the chemical formula  $C_2H_4$ . The chemical structure  $CH_2=CH_2$  is displayed. Below the structure, the name "(C<sub>2</sub>H<sub>4</sub>)<sub>x</sub>" and "Ethene, homopolymer" are listed. A section titled "Key Physical Properties" includes links for "Regulatory Information", "Spectra", and "Experimental Properties". A context menu is open over the substance record, listing the following options: "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", and "Send to SciPlanner".

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

# SciFinder中的物质记录

**SUBSTANCE DETAIL** ?

Get References   Get Reactions   Get Commercial Sources

Return

**CAS Registry Number** 9002-88-4

~359,876   ~112

**(C<sub>2</sub>H<sub>4</sub>)<sub>x</sub>**  
Ethene, homopolymer  
Polymer

**Polymer Class Terms**  
Polyolefin

**Melting Point (Experimental)**  
Value: 100-120 °C

**Boiling Point (Experimental)**  
Value: 48-110 °C | Condition: Press: 9 Torr

**Density (Experimental)**  
Value: 0.9745 g/cm<sup>3</sup> | Condition: Temp: 25 °C

**Other Names**  
Ethylene, polymers (8CI)  
0017ZSK  
0100F  
0134M  
030S  
[View more...](#)

74-85-1  
C<sub>2</sub>H<sub>4</sub>  
C=C

物质详情

由物质获得文献，反应，供应商等信息

# 通过物质获得文献

**Get References**

**Retrieve references for:**

All substances  
 Selected substances

**Limit results to:**

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

**For each sequence, retrieve:**

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

分析化学

生物研究

制备

工艺

谱图数据

用途



**SCIFINDER**  
A CAS SOLUTION

▼ EXPERIMENTAL PROPERTIES

Biological Chemical Density Electrical Electronic Flow and Diffusion Interface Magnetic Mechanical Nuclear Optical and Scattering Structure Related Thermal

Interface Properties	Value	Condition	Note
Contact Angle	See full text	1 of 31	(12)CAS
Surface Tension	See full text	1 of 12	(872)CAS

Notes

(12) Choi, Woo-Zin; Geosystem Engineering 2004, V7(3), P57-62 CAPLUS 🔍  
(872) Sanchis, M. R.; European Polymer Journal 2006, V42(7), P1558-1568 CAPLUS 🔍

实验数据与实验谱图

▼ EXPERIMENTAL SPECTRA

<sup>1</sup>H NMR <sup>13</sup>C NMR Hetero NMR IR Mass Raman UV and Visible X-Ray Additional Spectra

<sup>1</sup> H NMR Properties	Value	Condition	Note
Proton NMR Spectrum	See full text	1 of 15	(1313)CAS

Notes

(1313) Kemmere, Maartje; DECHEMA Monographien 2004, V138(8th International Workshop on Polymer Reaction Engineering, 2004), P189-195 CAPLUS 🔍

▶ REGULATORY INFORMATION

▶ CAS REFERENCE ROLES

▶ ADDITIONAL DETAILS



# 物质检索——Property explore

CAS Solutions ▾

**SciFINDER**  
A CAS SOLUTION

Explore ▾ Saved Searches ▾ SciPlanner

Substance Identifier "UHMWPE" > substances (1) > 9002-88-4

**REFERENCES**

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

**SUBSTANCES**

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

**SUBSTANCES: PROPERTY** ?

Experimental

Electric Resistance (ohm) ▾ >125  
Examples: 44, 25-35, >125

Predicted

Select Property... ▾  
Examples: 44, 25-35, >125

**Search**

寻找电阻率大于125ohm的含铁物质

# 物质结果集的筛选——Refine

SUBSTANCES ?

Get References

Get Reactions

Get Commercial Sources

Tools v

Create Keep Me Posted Alert

Send to SciPlanner

---

Analyze ?

Refine

Sort by: CAS Registry Number v

Display Options

Analyze by: ?

Elements v

O	73
C	37
H	30
Fe	19
N	19
Mg	16
Ca	13
Cr	13
Se	13
In	12

Show More

0 of 137 Substances Selected

Page: 1 of 3

1. 1360099-47-3 ?

~250

Component	Component Ratio
Te	x
Cd	x
Hg	x

Cd . Hg . Te

Cadmium mercury telluride  
Experimental Properties

2. 1262894-47-2 ?

~2

Double bond geometry as shown.,Relative stereochemistry.

C<sub>25</sub> H<sub>20</sub> N<sub>4</sub> O

3. 1160936-40-2 ?

~1

Component	Component Ratio
Te	1.8
Se	0.2
In	0.1
Cu	0.1
Cd	1.8

Cd . Cu . In . Se . Te

4. 1160936-38-8 ?

~1

Component	Component Ratio
Te	1.6
Se	0.4
In	0.2
Cu	0.2
Cd	1.6

Cd . Cu . In . Se . Te

5. 1160936-37-7 ?

~1

Component	Component Ratio
Te	1.4
Se	0.6
In	0.3
Cu	0.3
Cd	1.4

Ca . Fe . Mg . O

Calcium iron magnesium oxide  
(Ca<sub>0.02</sub>Fe<sub>1.8</sub>Mg<sub>0.2</sub>O<sub>2.82</sub>)  
Experimental Properties

1. 775325-57-0 ?

~1

Component	Component Ratio
O	2.82
Ca	0.02
Mg	0.1
Fe	1.8

Ca . Fe . Mg . O

Calcium iron magnesium oxide  
(Ca<sub>0.14</sub>Fe<sub>1.8</sub>Mg<sub>0.2</sub>O<sub>2.74</sub>)  
Experimental Properties

2. 775325-56-9 ?

~1

Component	Component Ratio
O	2.74
Ca	0.14
Mg	0.2
Fe	1.6

Ca . Fe . Mg . O

Calcium iron magnesium oxide  
(Ca<sub>0.07</sub>Fe<sub>1.6</sub>Mg<sub>0.2</sub>O<sub>2.67</sub>)  
Experimental Properties

3. 775325-55-8 ?

~1

Component	Component Ratio
O	2.67
Ca	0.07
Mg	0.2
Fe	1.6

Ca . Fe . Mg . O

Calcium iron magnesium oxide  
(Ca<sub>0.04</sub>Fe<sub>1.6</sub>Mg<sub>0.2</sub>O<sub>2.64</sub>)  
Experimental Properties

4. 775325-54-7 ?

~1

Component	Component Ratio
O	2.64
Ca	0.04
Mg	0.2
Fe	1.6

Ca . Fe . Mg . O

Calcium iron magnesium oxide  
(Ca<sub>0.14</sub>Fe<sub>1.3</sub>Mg<sub>0.35</sub>O<sub>2.44</sub>)  
Experimental Properties

5. 775325-53-6 ?

~1

Component	Component Ratio
O	2.44
Ca	0.14
Mg	0.35
Fe	1.3

Ca . Fe . Mg . O

Calcium iron magnesium oxide  
(Ca<sub>0.07</sub>Fe<sub>1.3</sub>Mg<sub>0.35</sub>O<sub>2.37</sub>)  
Experimental Properties

6. 775325-52-5 ?

~1

Component	Component Ratio
O	2.37
Ca	0.07
Mg	0.35
Fe	1.3

Ca . Fe . Mg . O

Calcium iron magnesium oxide  
(Ca<sub>0.04</sub>Fe<sub>1.3</sub>Mg<sub>0.35</sub>O<sub>2.34</sub>)  
Experimental Properties

7. 775325-51-4 ?

~1

Component	Component Ratio
O	2.34
Ca	0.04
Mg	0.35
Fe	1.3

Ca . Fe . Mg . O

Calcium iron magnesium oxide  
(Ca<sub>0.14</sub>FeMg<sub>0.2</sub>O<sub>2.14</sub>)  
Experimental Properties

8. 775325-50-3 ?

~1

Component	Component Ratio
O	2.14
Ca	0.14
Mg	0.5
Fe	1

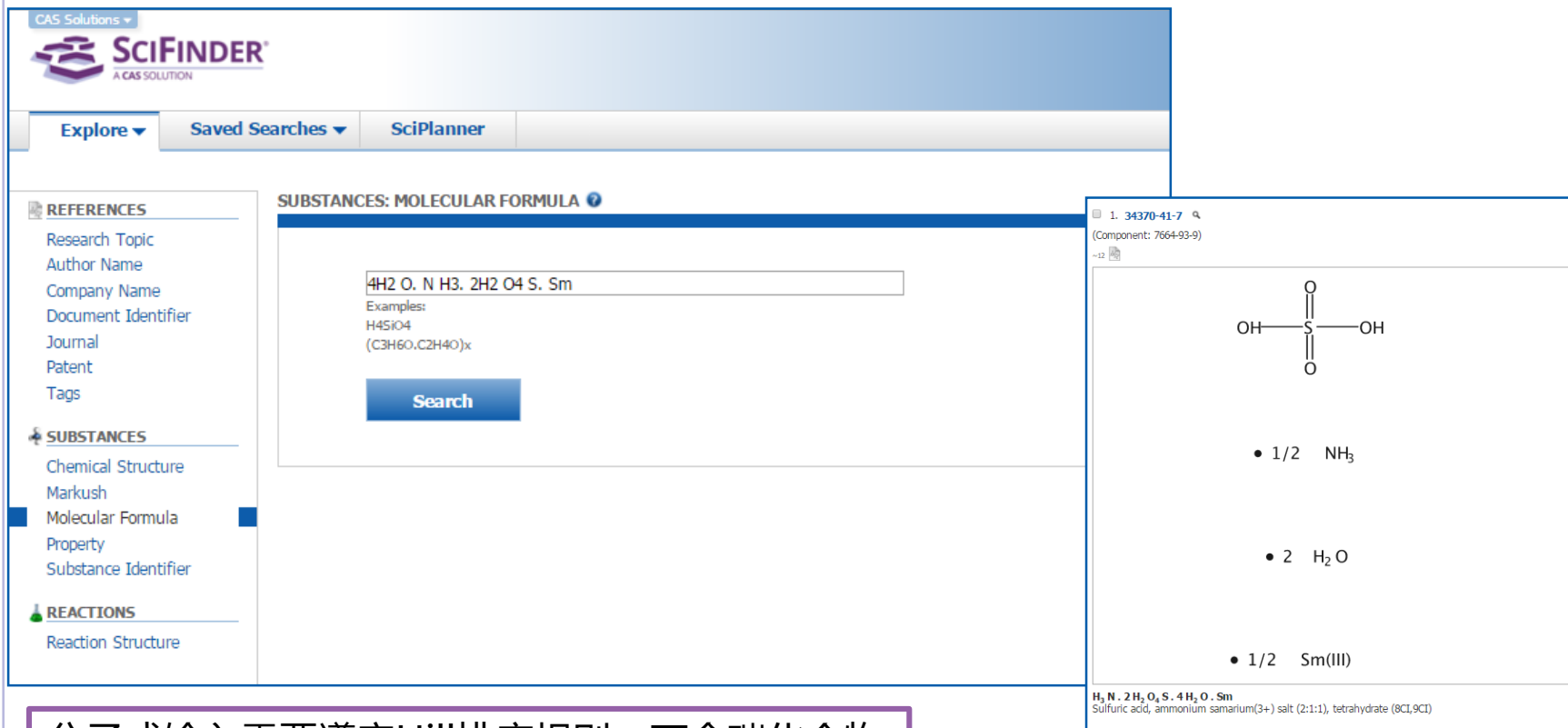
Ca . Fe . Mg . O

Calcium iron magnesium oxide  
(Ca<sub>0.14</sub>FeMg<sub>0.2</sub>O<sub>2.14</sub>)  
Experimental Properties

## 如何筛选含铁物质？

# 物质检索——分子式

检索(N H4) Sm (S O4)2 (H2 O)4, Ammonium Samarium Bis(sulfate(VI)) Tetrahydrate



CAS Solutions

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

Explore Saved Searches SciPlanner

REFERENCES

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

SUBSTANCES

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

REACTIONS

- Reaction Structure

SUBSTANCES: MOLECULAR FORMULA

4H2 O. N H3. 2H2 O4 S. Sm

Examples:  
H4SiO4  
(C3H6O.C2H4O)x

Search

1. 34370-41-7  
(Component: 7664-93-9)

OH—S(=O)<sub>2</sub>—OH

- 1/2 NH<sub>3</sub>
- 2 H<sub>2</sub>O
- 1/2 Sm(III)

H<sub>3</sub>N · 2 H<sub>2</sub>O<sub>4</sub>S · 4 H<sub>2</sub>O · Sm  
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

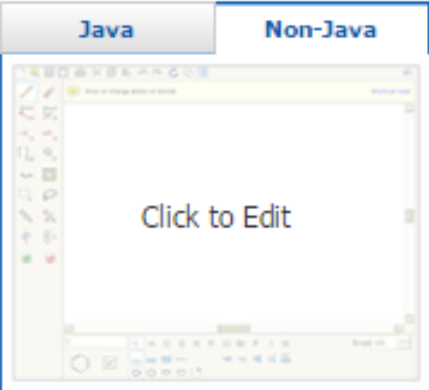
**REACTIONS**

- 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 a screenshot of the 'Structure Editor' software interface. The interface includes a toolbar on the left with various drawing and editing tools, a central workspace for drawing chemical structures, and a 'Drawing Editor' panel on the right. The 'Drawing Editor' panel has radio buttons for 'Structure', 'Reaction', and 'Markush', and search options for 'Exact search', 'Substructure search', and 'Similarity search'. The interface also features a command line at the bottom with a chemical formula 'C H O S N P Cl Br F I Si' and a 'Scale' dropdown set to '100'. The labels point to the following features:

- 橡皮 (Eraser)
- 结构和反应切换功能 (Structure and Reaction Switching Function)
- 铅笔 (Pencil)
- 元素周期表 (Periodic Table)
- 可变基团 (Variable Group)
- 重复基团工具 (Repeat Group Tool)
- 碳链工具 (Carbon Chain Tool)
- 选择工具 (Selection Tool)
- 环锁定工具 (Ring Locking Tool)
- 旋转工具 (Rotation Tool)
- 正电子 (Positive Charge)
- 负电子 (Negative Charge)
- 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 (Lasso Selection Tool)
- 原子锁定工具 (Atom Locking Tool)
- 镜面旋转工具 (Mirror Rotation Tool)
- 结构检索选择 (Structure Search Selection)
- 单双键, RS构型, 不确定键定义工具 (Single/Double Bond, RS Configuration, Uncertain Bond Definition Tool)
- 常见环, 多元环工具 (Common Rings, Poly-ring Tools)

# 物质检索——精确结构检索

Structure Editor

Draw or change atoms or bonds. Shortcut Keys

Sm

H  
|  
H—N—H  
|  
H

O  
||  
O=S=O  
|  
O

H  
|  
O—H

Sm . H<sub>4</sub>N . H<sub>2</sub>O . S . H<sub>2</sub>O

150.36 . 18.04 . 98.08 . 18.02

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 倒序排列 Display Options

0 of 5 Substances Selected

<p>1. 34370-41-7 <span style="float: right;">Q</span></p> <p>(Component: 7664-93-9)</p> <p>~12 </p> <ul style="list-style-type: none"> <li>• 1/2 NH<sub>4</sub><sup>+</sup></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 <span style="float: right;">Q</span></p> <p>(Component: 7664-93-9)</p> <p>~1 </p> <ul style="list-style-type: none"> <li>• NH<sub>4</sub><sup>+</sup></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 <span style="float: right;">Q</span></p> <p>(Component: 7664-93-9)</p> <p>~1 </p> <ul style="list-style-type: none"> <li>• 1/2 NH<sub>4</sub><sup>+</sup></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 <span style="float: right;">Q</span></p> <p>~1 </p> <div style="border: 1px solid black; padding: 5px;"> <p>49856-58-8 (Component: 736080-59-4) H<sub>8</sub>O<sub>11</sub>S<sub>2</sub>Sm · H<sub>4</sub>N · H<sub>2</sub>O</p> <ul style="list-style-type: none"> <li>• NH<sub>4</sub><sup>+</sup></li> <li>• H<sub>2</sub>O</li> </ul> </div> <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, homopolymer (9CI)</p>
<p>5. 49856-58-8 <span style="float: right;">Q</span></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

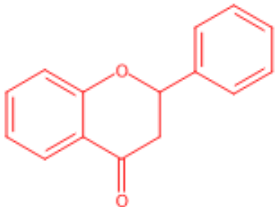
The screenshot displays the 'Structure Editor' window. The central workspace shows a chemical structure of a benzofuran derivative with a phenyl group at the 2-position and a carbonyl group at the 3-position. The structure is O=C1CCc2ccccc2O1. The interface includes a toolbar on the left with various drawing tools, a top toolbar with file operations, and a right-hand panel with search options. The search options are: 'Exact search', 'Substructure search' (which is selected and highlighted with a purple box), and 'Similarity search'. Below the search options are 'OK' and 'Cancel' buttons. At the bottom of the window, the molecular formula  $C_{15}H_{12}O_2$  and the molecular weight 224.26 are displayed.

# 物质检索——亚结构检索

0 of 23824 Substances Selected

1. 487-26-3

~2093

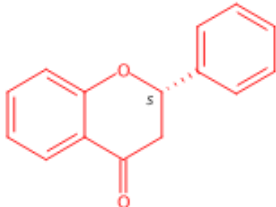


$C_{15}H_{12}O_2$   
4-phenyl-4H-1-benzopyran-4-one, 2,3-dihydro-2-phenyl-

▶ Key Physical Properties  
Regulatory Information  
Spectra  
Experimental Properties

2. 17002-31-2

~244



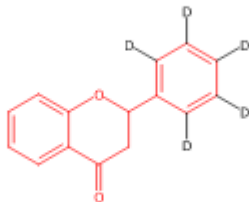
Absolute stereochemistry...Rotation (-).

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

▶ Key Physical Properties  
Experimental Properties

10. 146196-91-0

~1 ~5



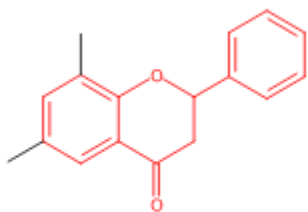
$C_{15}H_7D_5O_2$   
4-(phenyl-d<sub>5</sub>)-4H-1-benzopyran-4-one, 2,3-dihydro-2-(phenyl-d<sub>5</sub>)- (9CI)

Spectra

同位素

# 亚结构检索结果

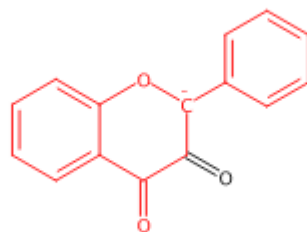
取代物



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

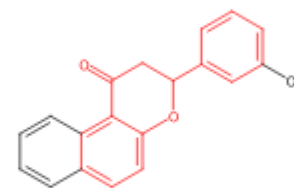
▶ **Key Physical Properties**  
Experimental Properties

离子



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

稠环物质



$C_{19}H_{14}O_3$   
1*H*-Naphtho[2,1-*b*]pyran-1-one, 2,3-dihydro-3-(3-hydroxyphenyl)-

▶ **Key Physical Properties**

# 亚结构检索结果的限定

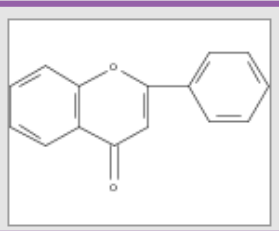
## 化学结构的再次限定

Analysis Refine

Refine by: ⓘ

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

**Chemical Structure:**

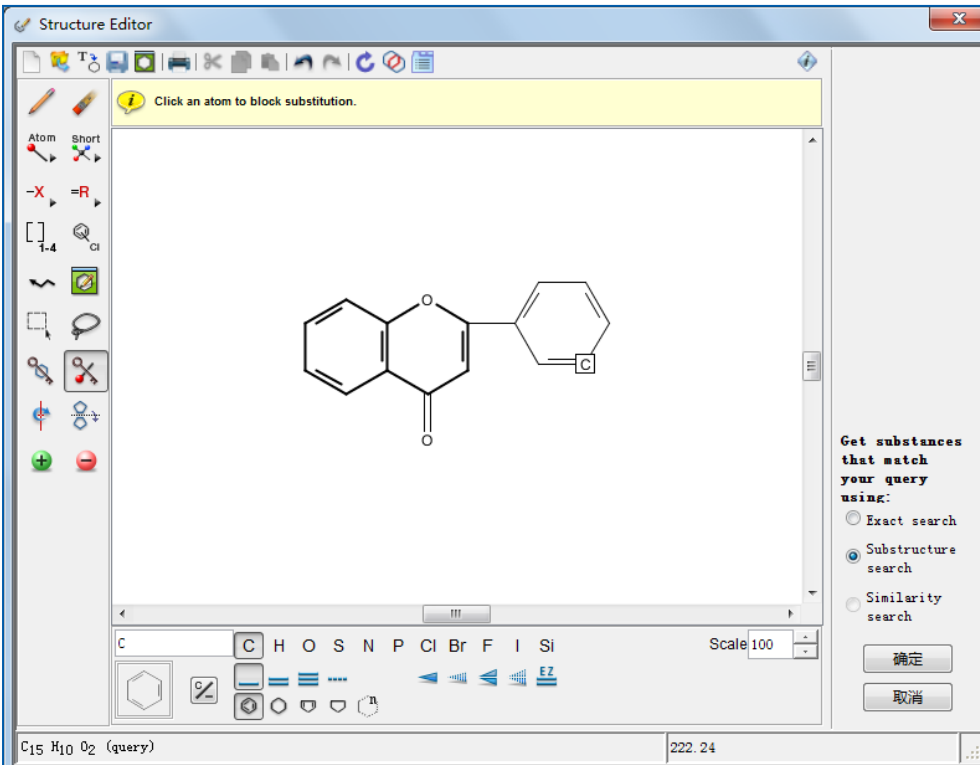


Click image to change structure or view detail

Search type: **Substructure**

Structure Editor

Click an atom to block substitution.



Get substances that match your query using:

- Exact search
- Substructure search
- Similarity search

确定 取消

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



环锁定

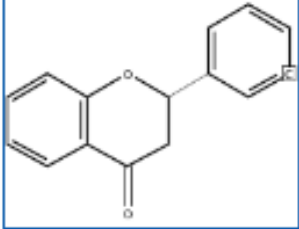


原子锁定

# 亚结构检索结果的限定

Structure Editor:

Java Non-Java



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

Only retrieve substances that:

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

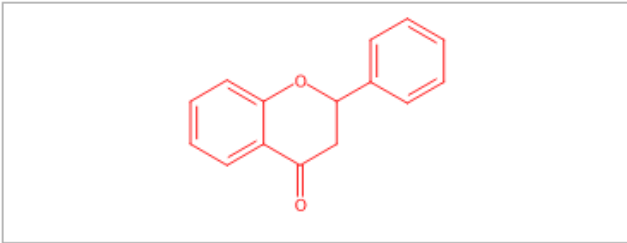
**Refine**

Get References Get Reactions Get Commercial Sources Tools

Sort by: Relevance

0 of 13826 Substances Selected

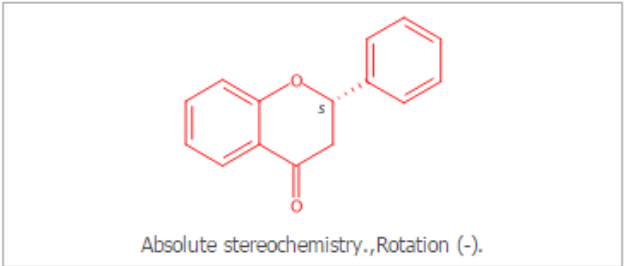
1. 487-26-3  
~2093



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

Key Physical Properties  
Regulatory Information  
Spectra  
Experimental Properties

2. 17002-31-2  
~244



Absolute stereochemistry., Rotation (-).

$C_{15}H_{12}O_2$   
4H-1-Benzopyran-4-one, 2,3-dihydro-2-phenyl-, (2S)-

Key Physical Properties  
Experimental Properties

4. 104550-32-5  
~3

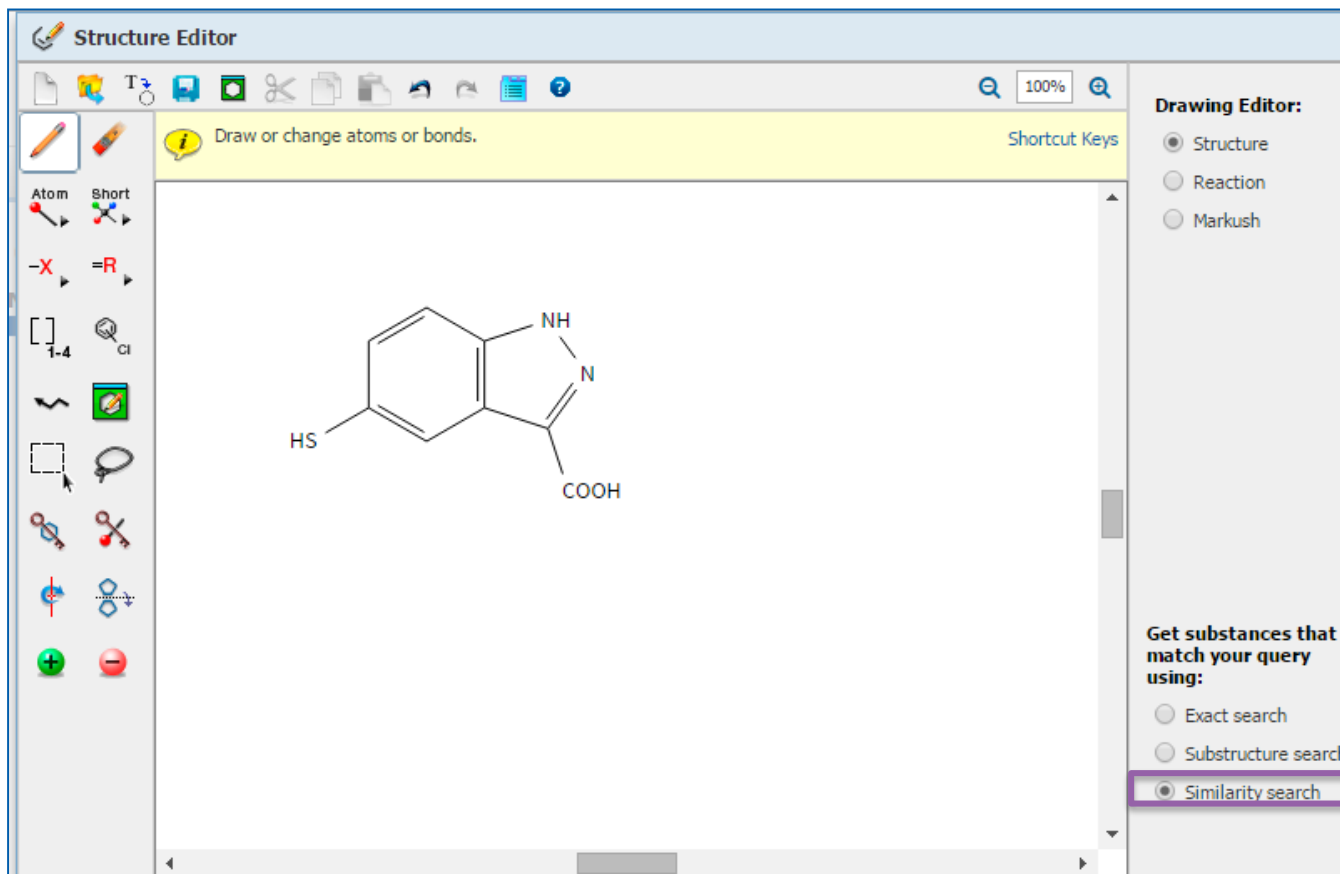
5. 75524-43-5  
~2

# 物质检索——亚结构检索

- 亚结构检索：

包括精确结构检索结果，及被检索结构的修饰结构

# 物质检索——相似结构检索



# 相似结构检索结果

Select All Deselect All

0 of 6 Similarity Candidates Selected

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

Get Substances

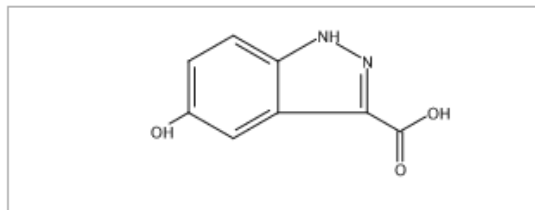
评分越高，相似度越高，结构越相似

Score: 88

1. 885518-94-5

取代基变化

~1 ~35



$C_8 H_6 N_2 O_3$

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

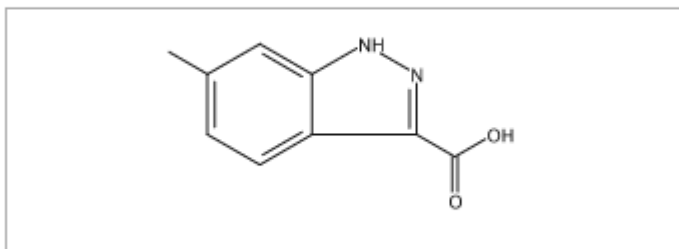
▶ Key Physical Properties

Score: 86

5. 858227-12-0

取代基位置变化

~7 ~41



$C_9 H_8 N_2 O_2$

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

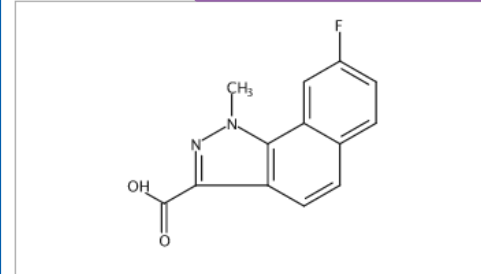
▶ Key Physical Properties

Score: 65

541. 1100422-

母体结构变化

~1



$C_{13} H_9 F N_2 O_2$

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

▶ Key Physical Properties



SCIFINDER®  
A CAS SOLUTION



# 物质检索——相似结构检索

- 相似结构检索：

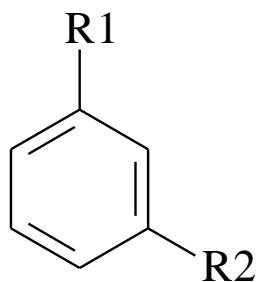
获得片段或整体结构与被检索结构相似的结果，母体结构可以被取代，也可以被改变

# 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
  - SciPlanner
- SciFinder常见问题及解决

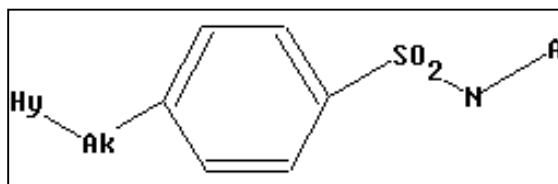
# Markush检索

- 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—halogen,  
|  
CH<sub>3</sub>



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

Structure Editor

Draw or change atoms or bonds. Shortcut Keys

100%

Atom Short

-X =R

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

**Drawing Editor:**

- Structure
- Reaction
- Markush


**Get Markush patents where the structure(s) are:**

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

OK Cancel

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

# Markush检索



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

Analyze by: Document Type ▾

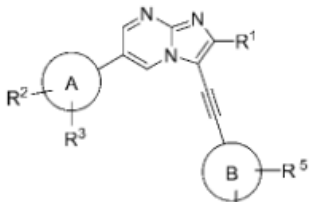
Patent	1969
Journal	1

Show More

全部是专利

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

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



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

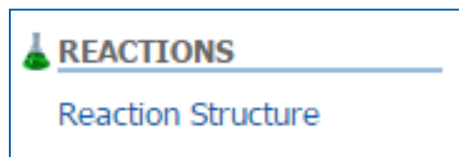
# 提纲

- 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



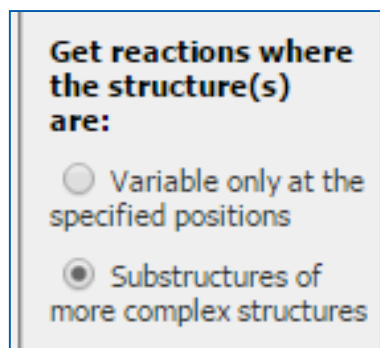
- 常用获取方法

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

The screenshot shows the Structure Editor window with various toolbars and a central canvas. The interface includes a top toolbar with icons for file operations and a search bar. Below this is a yellow status bar with the text "Draw or change atoms or bonds." and "Shortcut Keys". The main toolbar on the left is divided into "Atom" and "Short" sections, containing icons for drawing atoms, bonds, and functional groups. The right sidebar contains the "Drawing Editor" settings, with "Reaction" selected. Below this are options for "Get reactions where the structure(s) are:" with radio buttons for "Variable only at the specified positions" and "Substructures of more complex structures". The bottom of the window features a chemical formula input field (containing "CH<sub>4</sub>"), a list of elements (C, H, O, S, N, P, Cl, Br, F, I, Si), and a set of bond type icons. The status bar at the bottom right shows the version number "16.04".

Reaction arrow: 反应箭头

Reaction atom marking tool: 反应原子标记工具

Functional group list: 官能团列表

Reaction position marking tool: 反应位置标记工具

Reaction role tool: 反应角色工具



# SciFinder反应检索——精确反应检索

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

精确反应检索

# 反应检索结果

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

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

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

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

~102      100%  
~122

**Overview**  
**Steps/Stages**

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

**Notes**

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

**References**

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

# 获取相似反应

选择相似反应的相似限制：

Broad：仅反应中心相似

Medium：反应中心及附属原子和键

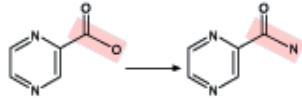
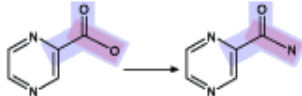
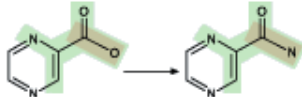
Narrow：反应中心及扩展的原子和键

### Get Similar Reactions ?

**Retrieve similar reactions from:**

- All reactions
- Current answer set

**Include this level of similarity:**

- Broad - Reaction centers only (2934)  

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

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


# 按照反应类型排序

Group by: Transformation ▼ Sort by: Frequency ▼ ↓

0 of 560 Reactions Selected

1. Reduction of Nitro Compounds to Amines  
538 Reactions

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

2. Reduction of Nitro to Azo Compounds  
11 Reactions

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

3. Reduction of Nitro to Azoxy Compounds  
11 Reactions

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

更精确的查找需要的反应

# 反应检索结果的筛选

获得特定物质做还原剂的反应

REACTIONS ? Get References Tools Send to SciPlann

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 Display Options Page: 1 of 11

**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

# 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

The screenshot displays the 'Structure Editor' interface. On the left, the 'Structure Editor' toolbar includes various drawing tools, with the '=R' button highlighted. A purple arrow points from this button to the 'R-group Definitions' dialog box on the right. The dialog box shows 'R1 = O, S' in the input field. Below this, the 'Atoms' section contains a periodic table where the element 'S' (Sulfur) is selected. The main window shows a chemical structure of a benzothiazole derivative with an R1 group attached to the C2 position. The status bar at the bottom left indicates 'Formula is not available'.

# 亚结构反应检索

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

**Structure Editor**

Drag the reaction arrow to specify reaction direction.

**Drawing Editor:**

- Structure
- Reaction
- Markush

**Variables**

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

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

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

Buttons: OK, Cancel, Close

Bottom status bar: Formula is not available



# 通过后处理工具筛选反应--Analyze

通过催化剂筛选反应

Analyze Refine

Analyze by: ?  
Catalyst

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

Group by: No Grouping Sort by: Accession Number

No Grouping  
Document  
Transformation

1. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.

~57 ~52 83%

Overview

Steps/Stages

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

Notes

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

References

ACS / Proprietary and Confidential / Do Not Distribute

# 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

# 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**

Overview

**Steps/Stages**

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

**Notes**

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

**References**

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

**进入SciPlanner 新建文件**

**将刚推送过来的反应拖至编辑面板**

SciPlanner SciPlanner\_11\_19\_2015\_112612

Workspace Edit View GoTo

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

Your Workspace is empty.

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

# SciPlanner使用简介

SciPlanner 11\_19\_2015\_112612

Workspace Edit View GoTo

CAS Registry Number: 13091-23-1

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

打开中间产物的标准菜单  
选择Synthesis this

1 2 3

Get References Tools

Send selected records to SciPlanner. Send to SciPlanner

Group by: No Grouping Sort by: Accession Number

1 of 34 Reactions Selected

1. View Reaction Detail

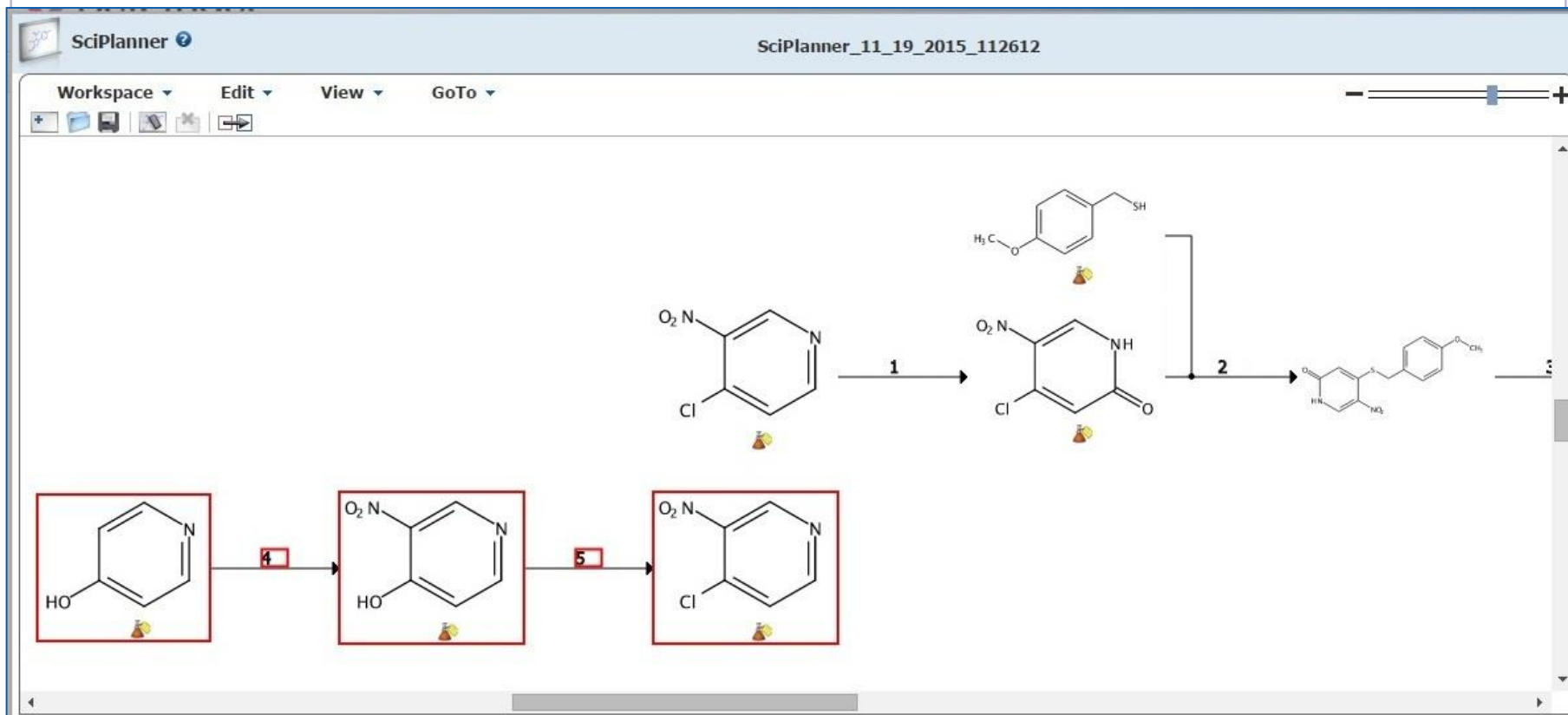
2 Steps Hover over any structure for more options.

在检索到的反应中选择感兴趣的反应

继续推送到SciPlanner

~161 ~192

# SciPlanner使用简介



步骤同前，将推送过来的反应拖到编辑面板中，可以看到两条反应中存在同样的结构

# SciPlanner使用简介

The screenshot displays the SciPlanner software interface. The main workspace shows a chemical reaction sequence: a starting material (a pyridine ring with a nitro group and a hydroxyl group) reacts (step 4) to form a pyridine ring with a nitro group and a chlorine atom. This intermediate then reacts (step 5) to form another pyridine ring with a nitro group and a chlorine atom. Finally, this intermediate reacts (step 1) to form a pyridine ring with a nitro group and a chlorine atom, which is then converted to a pyridine ring with a nitro group and a chlorine atom, and finally to a pyridine ring with a nitro group and a chlorine atom.

Three callout boxes provide instructions:

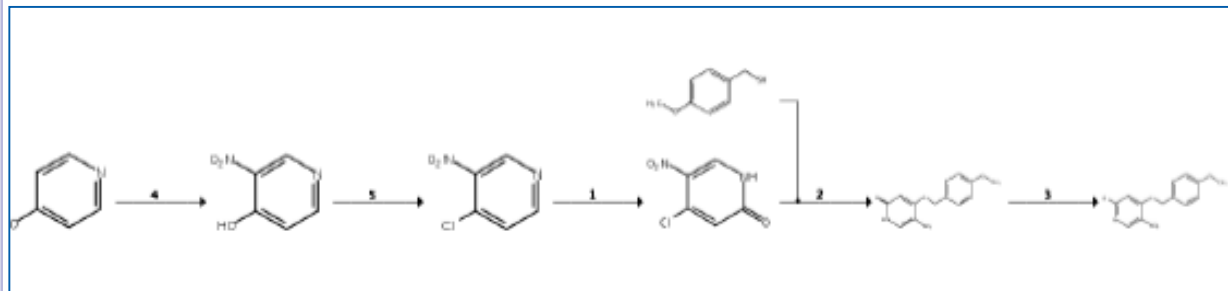
- Click Workspace, select Export to export results.
- Use the mouse to drag two identical structures to overlap, merging the two reactions.
- Select an appropriate output format to output results.

The 'Export' dialog box is open, showing the following options:

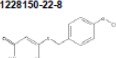
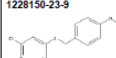
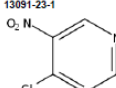
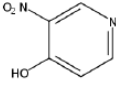
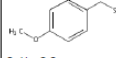
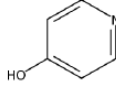
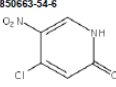
- For:**
  - Portable Document Format (\*.pdf)
  - Citations (\*.ris)
  - Image (\*.png)
- Saving Locally:**
  - SciPlanner eXchange (\*.pkx)
- Details:**
  - File Name:** SciPlanner\_11\_19\_2015\_112612
  - Title:**
- Include:**
  - SciPlanner Image
  - Reaction Details
  - Substance Details
  - Reference Details

Buttons: Export, Cancel

# SciPlanner导出结果



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

Substance Information		
<p>1228150-22-8</p>  <p>C<sub>13</sub>H<sub>12</sub>N<sub>4</sub>O<sub>4</sub>S 2-(1H)-Pyridinone, 4-[[[4-methoxyphenyl]methyl]thio]-5-nitro-</p> <p>Related Info: ~ 2 References Reactions</p>	<p>1228150-23-9</p>  <p>C<sub>13</sub>H<sub>11</sub>ClN<sub>4</sub>O<sub>3</sub>S Pyridine, 2-chloro-4-[[[4-methoxyphenyl]methyl]thio]-5-nitro-</p> <p>Related Info: ~ 2 References Reactions</p>	<p>13091-23-1</p>  <p>C<sub>5</sub>H<sub>3</sub>ClN<sub>2</sub>O<sub>2</sub> Pyridine, 4-chloro-3-nitro-</p> <p>Related Info: ~ 301 References Reactions ~ 100 Commercial Sources Regulatory Information</p>
<p>5435-54-1</p>  <p>C<sub>6</sub>H<sub>4</sub>N<sub>2</sub>O<sub>3</sub> 4-Pyridinol, 3-nitro-</p> <p>Related Info: ~ 113 References Reactions ~ 197 Commercial Sources Regulatory Information</p>	<p>6258-60-2</p>  <p>C<sub>8</sub>H<sub>10</sub>O S Benzenemethanethiol, 4-methoxy-</p> <p>Related Info: ~ 749 References Reactions ~ 71 Commercial Sources Regulatory Information</p>	<p>626-64-2</p>  <p>C<sub>5</sub>H<sub>5</sub>N O 4-Pyridinol</p> <p>Related Info: ~ 1351 References Reactions ~ 160 Commercial Sources Regulatory Information</p>
<p>850663-54-6</p>  <p>C<sub>6</sub>H<sub>3</sub>ClN<sub>2</sub>O<sub>3</sub> 2-(1H)-Pyridinone, 4-chloro-5-nitro-</p> <p>Related Info: ~ 22 References Reactions ~ 136 Commercial Sources</p>		

# 提纲

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



# SciFinder浏览器选择建议

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

# 如何获取SciFinder账号

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

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

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

请注意：

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

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

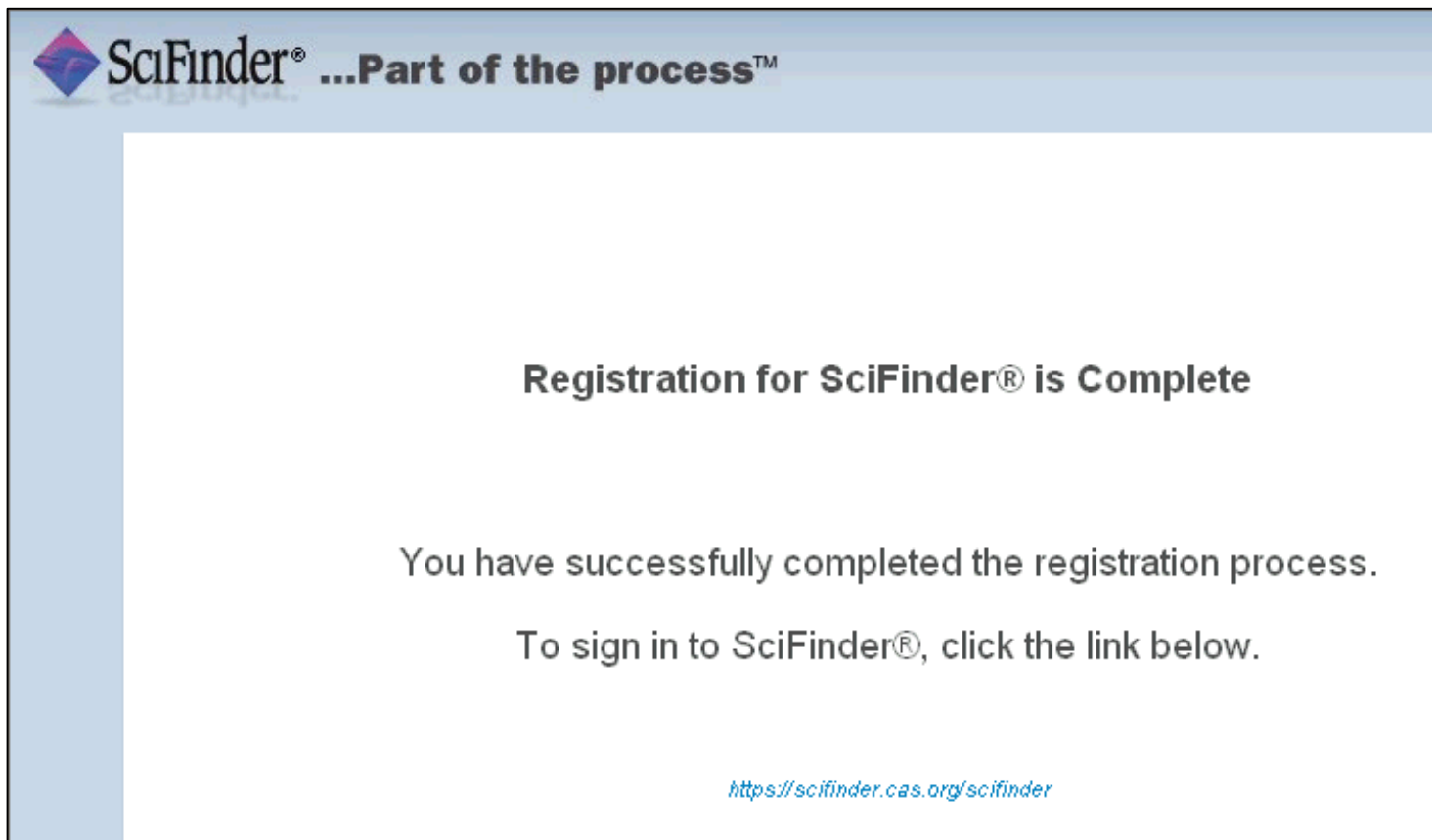
3. 密码必须包含 7-15 个字符，并且至少**包含三种以下字符**：

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

例：abc@123

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

# 如何获取SciFinder账号



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

# SciFinder使用注意事项

- 在校内完成注册（教学楼、图书馆、实验室）
- 一人注册一个帐号
- 请提供真实姓名信息
- 严禁过量下载
- 严禁账号分享
- 严禁将账号用于非学术研究

更多培训资料请访问

[www.cas-china.org](http://www.cas-china.org)

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