



# SciFinder<sup>®</sup>

Essential content. Proven results.<sup>™</sup>

## SciFinder Web使用介绍

CAS中国代表处

培训专员：祁晶晶

2011.10.13



SciFinder<sup>®</sup>

CAS is a division of the American Chemical Society

# 提纲

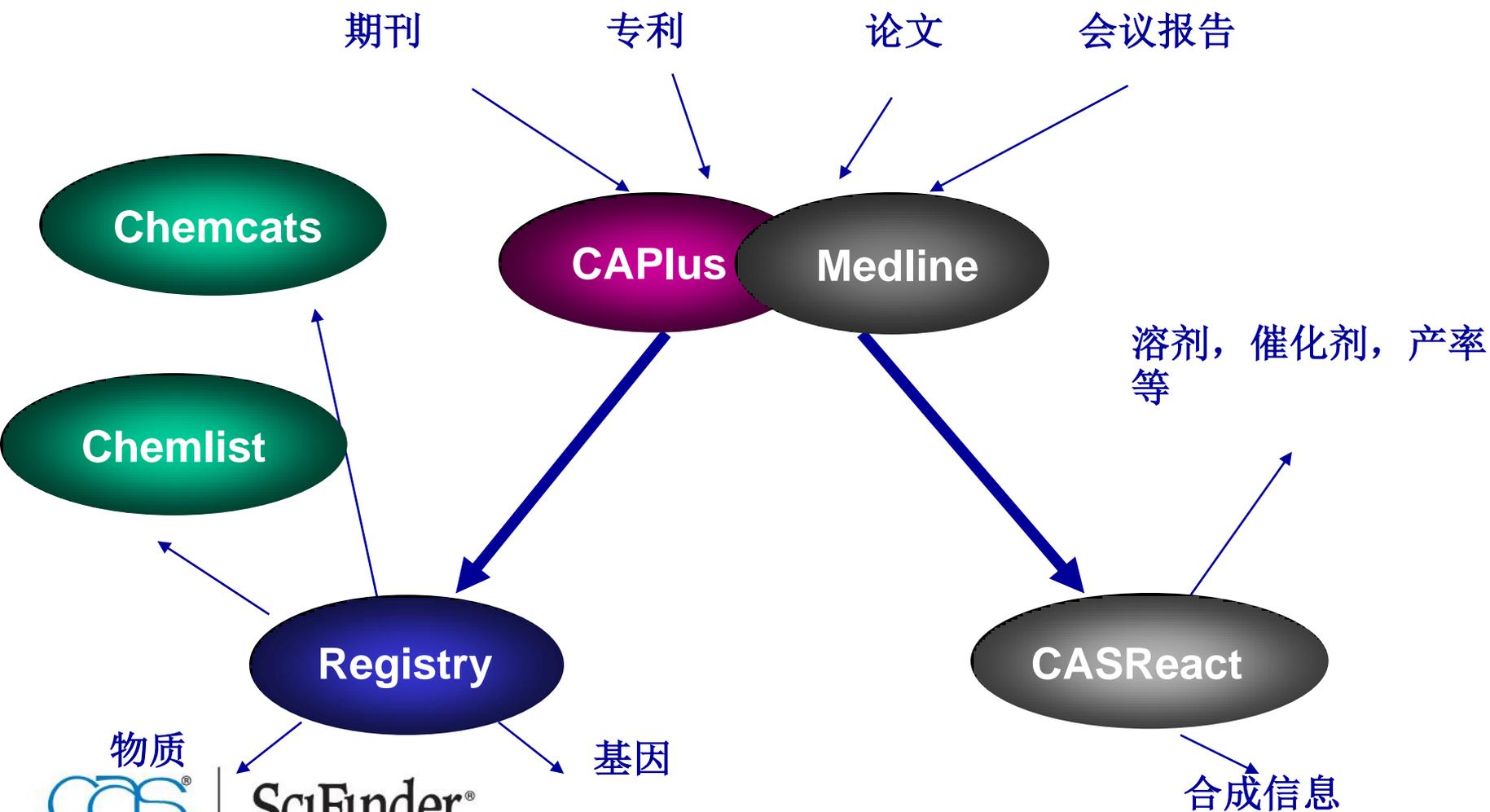
- 介绍
  - SciFinder 中的内容
  - SciFinder 的注册和登陆
- **SciFinder 中的检索和后处理**
  - SciFinder 中的文献检索
  - SciFinder 中的物质检索
  - SciFinder 中的Markush检索
  - SciFinder 中的反应检索
- **SciFinder 特色功能**
- **SciFinder网络资源平台**

## 美国化学文摘社—Chemical Abstract Service

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



# SciFinder中的内容



## SciFinder中的内容—文献数据库

### ➤CAPlus (Pre 1907—)

覆盖化学相关众多学科领域的参考文献。

3400万条文献信息。

上万种期刊和61个专利发行机构的专利（含专利族）。

会议录、技术报告、图书、学位论文、评论、会议摘要

日更新4500条以上的记录

### ➤Medline

美国国立医学图书馆出品

生命科学医学相关

毒理，病理学报告

期刊、临床报告

## SciFinder中的内容—反应数据库

### ➤CAS React (1840—)

源自61专利机构和上万种期刊

包含有机、有机金属、无机、生化反应。

3650万单步，多步反应。

1400万制备信息

每周更新3-5万条单步、多步反应。

## SciFinder中的内容—物质数据库

### ➤Registry (Pre 1957—)

世界上最大的物质数据库

6300万个物质、序列

无机物、有机物、聚合物、混合物、合金、核酸蛋白质序列等

所有具有CAS No 物质

日更新1.2万个物质

### ➤ChemList

查询备案/管控化学信息的工具。

### ➤Chemcats

4000万化学物质提供商的联系信息

包含价格情况、运送方式、质量等级等信息。

# 提纲

- 介绍
  - SciFinder 中的内容
  - SciFinder 的注册和登陆
- **SciFinder 中的检索和后处理**
  - SciFinder 中的文献检索
  - SciFinder 中的物质检索
  - SciFinder 中的Markush检索
  - SciFinder 中的反应检索
- **SciFinder 特色功能**
- **SciFinder网络资源平台**

# SciFinder的注册和登陆

**SciFinder Web**的系统要求

**Windows**用户支持**IE 8.x**或者**FireFox 2.x**

**Mac** 用户支持 **Firefox** 和 **Safari**

**Java** 安装（初次使用结构时自动安装）



在图书馆相关页面上找到**SciFinder Web**注册用的网址



# 东南大学SFweb注册地址



东南大学图书馆  
SOUTHEAST UNIVERSITY LIBRARIES

繁體版 旧版入口 馆长信箱

[首页](#) | [新闻资讯](#) | [查找资料](#) | [电子资源](#) | [服务指南](#) | [本馆概况](#) | [咨询中心](#) | [网站地图](#) | [Mylibrary](#)

电子资源

- 版权公告
- 电子期刊导航(试用)
- 电子图书
- 数字资源/数据库
- 学术站点推荐
- 试用数据库
- 培训课件
- 本校最新WoS收录
- 教参信息系统
- 校外访问

首页 >> 电子资源 >> 数字资源/数据库 >> SciFinder Scholar (美国《化学文摘》网络版)

| 数字资源 / 数据库

---

SciFinder Scholar (美国《化学文摘》网络版)

◆ <https://scifinder.cas.org>

◆ 客户端安装说明

访问方式 美国《化学文摘》简介 SciFinder Scholar各数据库简介 检索方法 参考文献

### 访问方式

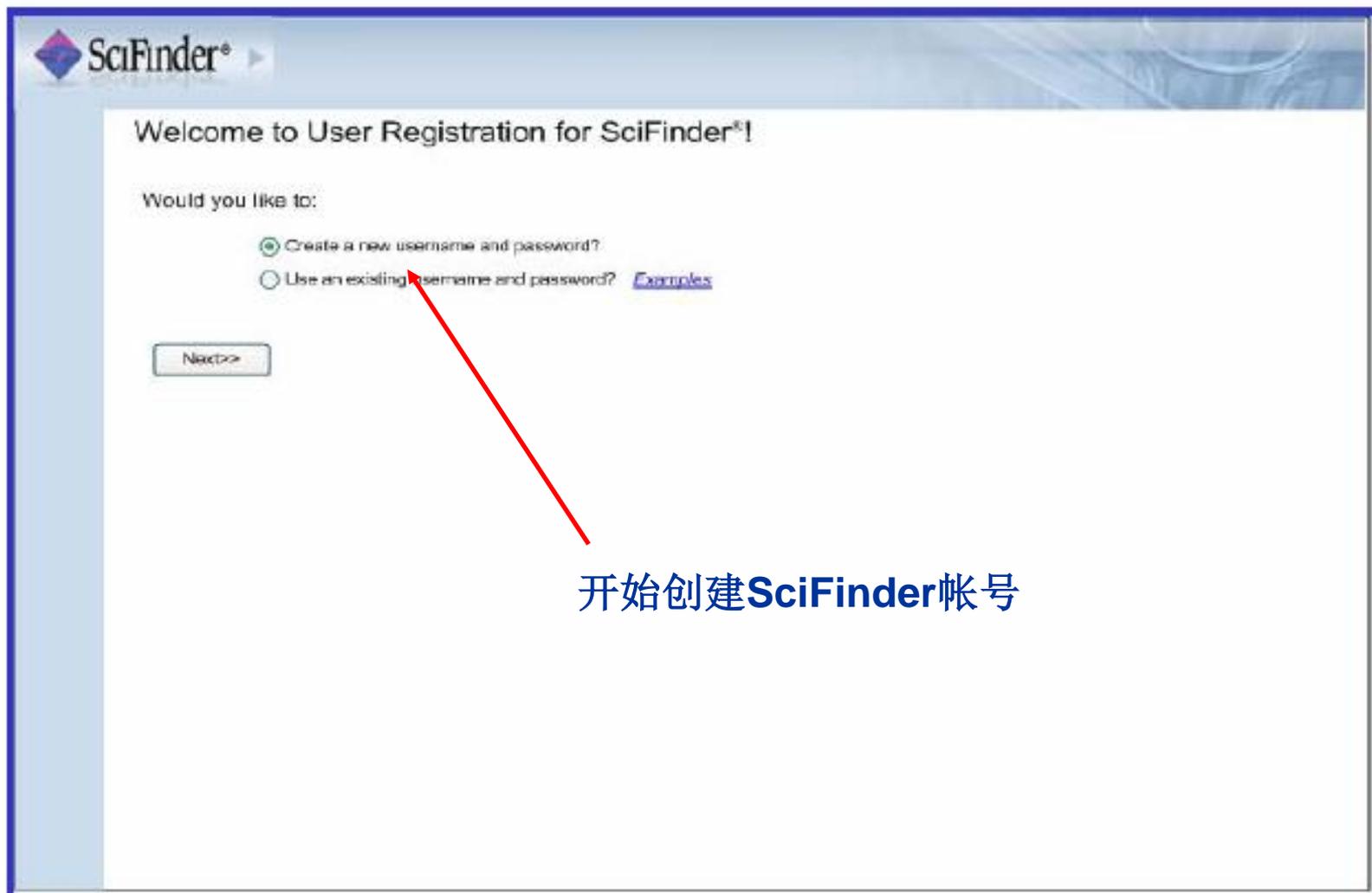
与其他数据库不同，提供两种访问方式：

1、Web访问方式：不用下载客户端软件，直接通过网页形式访问。首次使用时必须以东南大学邮件地址（含有“seu.edu.cn”）注册（注册后您将拥有自己的SciFinder用户名和密码），注册网址为[https://scifinder.cas.org/registration/index.html?](https://scifinder.cas.org/registration/index.html?corpKey=406031ACX86F35055X2E430FB61E6E029549)[corpKey=406031ACX86F35055X2E430FB61E6E029549](https://scifinder.cas.org/registration/index.html?corpKey=406031ACX86F35055X2E430FB61E6E029549)，按照提示操作即可。以后直接通过<https://scifinder.cas.org>，输入用户名、密码访问数据库。

2、客户端访问方式：需要安装客户端软件，通过软件访问数据库。不支持Windows 7操作系统。安装说明请访问<http://58.192.117.2/ca>。

以上两种版本所检索的数据库内容完全一致，功能上略有差别。SciFinder客户端版本功能不再增加，SciFinder Web版本功能会不断增加。（但客户端版本仍可使用客户端版本）

## 点击URL创建SciFinder账号



SciFinder®

Welcome to User Registration for SciFinder®!

Would you like to:

- Create a new username and password?
- Use an existing username and password? [Examples](#)

Next>>

开始创建SciFinder帐号

# 每个用户必须输入各自信息

用大学后缀名的邮箱注册

seu.edu.cn

**SciFinder®**

Please provide the following information:  
(bold\* = required)

**CONTACT INFORMATION**

First Name\*:

Last Name\*:

E-mail\*:

Confirm E-mail\*:

Phone Number:

Fax number:

Area of Research:

Job Title:

**USERNAME AND PASSWORD**

Username\*:  [Tip](#)

Password\*:

Re-enter Password\*:

**SECURITY INFORMATION**

Security Question\*:  [Why?](#)

Answer\*:

**Callout Box 1:** Email domain must match valid domain(s) and the entire address must be unique.

**Callout Box 2:** Username and password must meet minimum requirements and be unique.

**Callout Box 3:**

- What is your favorite color?
- What is the name of the city where you grew up?
- What is the name of your favorite pet?
- What is your favorite musical instrument?
- What is your ideal vacation location?

## 设置用户名及密码注意事项

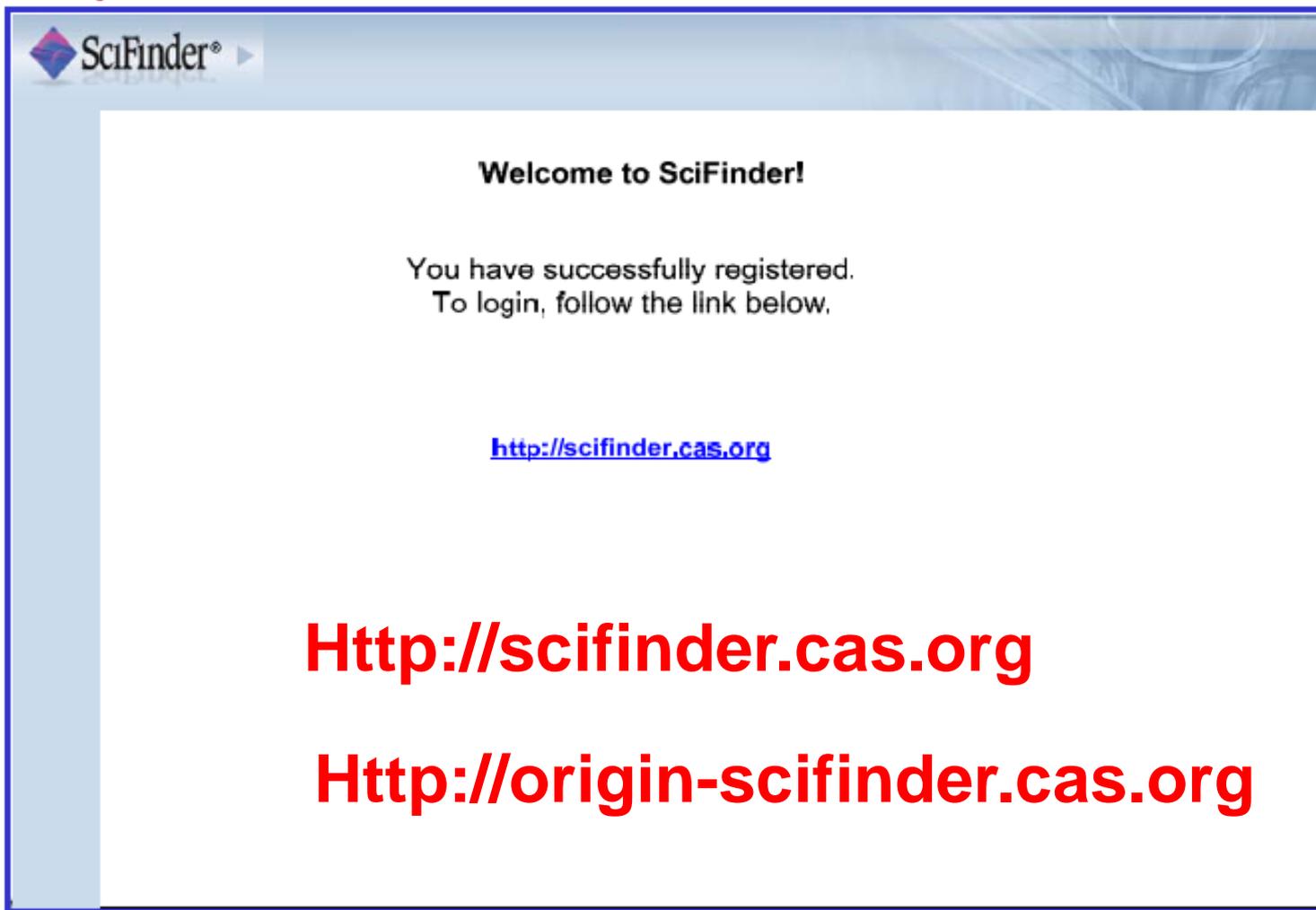
**用户名：**必须是唯一的，且包含 **5-15** 个字符。它可以只包含字母或字母组合、数字和/或以下特殊字符：

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

**密码：**必须包含 **7-15** 个字符，并且至少包含三个以下字符：

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

## 使用这个链接登陆SciFinder



The screenshot shows the SciFinder registration confirmation page. At the top left is the SciFinder logo. The main text reads: "Welcome to SciFinder! You have successfully registered. To login, follow the link below." Below this is a blue underlined link: <http://scifinder.cas.org>. At the bottom of the screenshot, two red links are displayed: [Http://scifinder.cas.org](http://scifinder.cas.org) and [Http://origin-scifinder.cas.org](http://origin-scifinder.cas.org).

# SciFinder登陆界面

**SciFinder**® Essential content. Proven results.™

**Sign In**

Username

Password

Remember my username

[Forgot Username or Password?](#)

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

**输入SciFinder帐号和密码**

**Welcome to SciFinder!**

**Are you an outstanding PhD Chemistry student?**

**We want to hear from you with our SciFinder Academic Exchange Program!**

This extraordinary opportunity is for outstanding PhD chemistry students to exchange ideas about chemical informatics with CAS senior management, editorial scientists, and technical specialists in Columbus, Ohio.

Participants are also invited to join their chemistry colleagues at the 242nd ACS National Meeting and Exposition, to be held in Denver, Colorado, in August 2011. All expenses are paid for this unique experience, and participants receive a \$1,000 stipend.

Don't miss out on your chance to apply - **all application materials are due April 30, 2011.**

**SciFinder Mobile**

With no need to download a special app, the new SciFinder Mobile platform allows researchers to use web-enabled smartphones to access CAS databases through SciFinder, the preferred research tool for chemical and related sciences. SciFinder Mobile is available to all SciFinder subscribers in commercial, academic, and government organizations and can be accessed at [scifinder.cas.org/mobile](http://scifinder.cas.org/mobile) with most mobile devices.

**What is SciFinder?**

SciFinder is a research discovery tool that allows you to explore the CAS databases containing literature from many scientific disciplines including biomedical sciences, chemistry, engineering, materials science, agricultural science, and more!

# SciFinder登陆后主界面

文献，物质，反应检索入口，默认文献检索入口

Explore References   Explore Substances   Explore Reactions

Welcome Sam Yu   **Sign Out**

**检索完，请点击退出**

Explore References

Research Topic *i*

Research Topic *i*

Search

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

**可用的检索方法**

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

**保存过的结果集**

**邮件提醒结果集**

Saved Answer Sets *i*

- pyridine
- Substructure-20100909
- Markush-20100908
- exa-markush
- sss-markush
- Total reaction -20100820
- Demo File
- End-reaction
- Total Reaction--20100518
- Xie ke Chang
- Autosaved Reaction Set

View All

**Import**

Keep Me Posted Results *i*

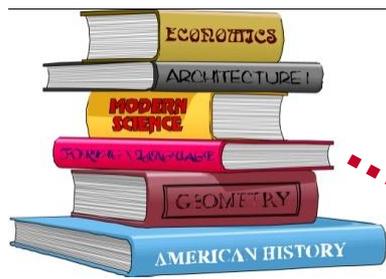
China -bone tissue engineering scaffold

- Apr 09, 2011 (23)
- Mar 05, 2011 (25)
- Jan 29, 2011 (33)

View All

16

# 课题研究中各个阶段的信息需求



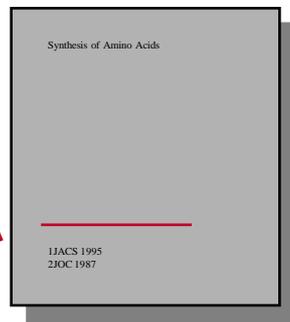
问题？选题：现有的研究条件、背景、能力。。



实验：实验方法，活性评价方法。。。。



信息检索、分析、精选。。。。



课题申报、开题论证：国内外研究前景。。



课题总结：期刊、专利、会议报告。。

## 提纲

- 介绍
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  - SciFinder 中的物质检索
  - SciFinder 中的Markush检索
  - SciFinder 中的反应检索
- **SciFinder 特色功能**
- **SciFinder网络资源平台**

## 选题、课题申报、开题论证。。。。。

- 课题的国际发展现状是什么？（有哪些国家参与？发展趋势是什么？）
- 课题的国内外的研究成果有哪些？（研究方法是什么？存在的问题？）
- 课题在国内的核心研究人员是谁？核心研究机构有哪些？
- 本课题的研究都涉及到哪些交叉学科？（是否有重大研究进展？）
- 课题未来可能的应用领域涉及哪些方面？
- 本课题的研究适合在哪些期刊投稿？

## **Scifinder** 中强大的文献检索功能

# Explore References 文献检索

SciFinder®

Welcome Sam Yu | Sign Out

Explore References | Explore Substances | Explore Reactions

Saved Answer Sets | Help  
Keep Me Posted Results | History  
**NEW** SciPlanner | Preferences  
My Connections

### Explore References

**Research Topic** Research Topic ⓘ  **Search**

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

**Research Topic** (Dropdown Menu):  
 Author Name  
 Company Name  
 Document Identifier → 可用的检索方法  
 Journal  
 Patent  
 Tags

**Publication Year(s)** ⓘ   
 Examples: 1995, 1995-1999, 1995-, -1995

**Document Type(s)** ⓘ

<input type="checkbox"/> Biography	<input type="checkbox"/> Dissertation	<input type="checkbox"/> Patent
<input type="checkbox"/> Book	<input type="checkbox"/> Editorial	<input type="checkbox"/> Preprint
<input type="checkbox"/> Clinical Trial	<input type="checkbox"/> Historical	<input type="checkbox"/> Report
<input type="checkbox"/> Commentary	<input type="checkbox"/> Journal	<input type="checkbox"/> Review
<input type="checkbox"/> Conference	<input type="checkbox"/> Letter	

**Saved Answer Sets** ⓘ

pyridine  
 Substructure-20100909  
 Markush-20100908  
 exa-markush  
 sss-markush  
 Total reaction -20100820  
 Demo File  
 End-reaction  
 Total Reaction--20100518  
 Xie ke Chang  
 Autosaved Reaction Set

View All

**Import**

**Keep Me Posted Results** ⓘ

China -bone tissue engineering scaffold  
**Apr 09, 2011 (23)**  
**Mar 05, 2011 (25)**  
**Jan 29, 2011 (33)**

View All

# SciFinder中的文献检索

磁性纳米复合材料的制备 **magnetic nanocomposites**、 **preparation**

The screenshot displays the SciFinder search interface. At the top, there are navigation links for "Explore References", "Explore Substances", and "Explore Reactions". The user is logged in as "Sam Yu". The main search area is titled "Explore References" and contains a search bar with the query "magnetic nanocomposites with preparation". A red arrow points to the word "with" in the query, indicating the use of a connector. To the right of the search bar is a "Search" button. Below the search bar, there are several filter sections: "Publication Year(s)", "Document Type(s)", and "Language(s)". Each filter section has a dropdown arrow and a list of options with checkboxes. The "Document Type(s)" section is highlighted with a red box, and a text box with the Chinese text "提前限定出版年限、文献类型等" is overlaid on it. The "Language(s)" section also has a red box around it.

Research Topic

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

Research Topic ▾

Author Name

Company Name

Document Identifier

Journal

Patent

Tags

Publication Year(s) ▾   
Examples: 1995, 1995-1999, 1995-, -1995

Document Type(s) ▾

Biography  Dissertation  Patent

Book  Journal  Review

Clinical Trial  Letter

Commentary

Conference

Language(s) ▾

Chinese  German  Polish

English  Italian  Russian

提前限定出版年限、文献类型等

# 主题检索的候选项

SciFinder® Explore References Explore Substances Explore Reactions

Welcome Sam Yu | Sign Out

Add KMP Alert Research Topic "magnetic nanocomposites with p..."

### Research Topic Candidates

5 Topics 1 Selected  
Select All Deselect All

Research Topic Candidates	References
<input type="checkbox"/> 3 references were found containing "magnetic nanocomposites with preparation" as entered.	3
<input checked="" type="checkbox"/> 3586 references were found containing the two concepts "magnetic nanocomposites" and "preparation" closely associated with one another.	3586
<input type="checkbox"/> 5897 references were found where the two concepts "magnetic nanocomposites" and "preparation" were present anywhere in the reference.	5897
<input type="checkbox"/> 9934 references were found containing the concept "magnetic nanocomposites".	9934
<input type="checkbox"/> 8936168 references were found containing the concept "preparation".	8936168

Get References

“Concept”表示做了同意词的扩展

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

“were present anywhere in the reference”  
表示同时出现在一段话中

# 如何在大量文献中发现最关键信息？

## 文献的分析工具

SciFinder® Explore References Explore Substances Explore Reactions

Welcome Sam Yu | Sign Out

Add KMP Alert Research Topic "magnetic nanocomposites with p..." > references (3416)

References Get Substances Get Reactions Get Related Tools Send to SciPlanner

3416 References 0 Selected

170 duplicates were automatically removed.

Select All Deselect All Sort by: Accession Number

1. **Synthesis of  $\gamma$ -Fe2O3/SiO2/Au magnetic composites for immobilization of bovine serum albumin**  
 By Li, ZhiXia; Peng, MingLi; Jin, YanYan; Wang, XiaoFang; Cui, YaLi; Chen, Chao  
 From Chinese Science Bulletin (2011), 56(27), 2911-2915. Language: English, Database: CAPLUS  
 A method for the two-step **synthesis of magnetic composites** with a  $\gamma$ -Fe2O3 core, silica inner layer and numerous gold nanoparticles (AuNPs) on the surface of silica ( $\gamma$ -Fe2O3/SiO2/Au) is described. First, thiol-functionalized  $\gamma$ -Fe2O3/SiO2 **composites** and gold colloids are prepared by mercaptosilane and redn. of Au3+ to Au0 with citrate, resp. Gold **nanoparticles** are then assembled on the surface of the silica-coated  $\gamma$ -Fe2O3/SiO2 **composites**. The structure of the **composite** particles is confirmed by transmission electron microscopy (TEM).

2. **A novel bienzyme glucose biosensor based on three-layer Au-Fe3O4 iO2 magnetic nanocomposite**  
 By Chen, Xiaojun; Zhu, Jinwei; Chen, Zixuan; Xu, Chenbin; Wang, Yan; Yao, Cheng  
 From Sensors and Actuators, B: Chemical (2011), 159(1), 220-228. Language: English, Database: CAPLUS  
 The **magnetic** core-shell Au-Fe3O4 iO2 **nanocomposite** was prepared by layer-by-layer assembly technique and was used as a glucose oxidase (GOD) and horseradish peroxidase (HRP) immobilization matrix. Glucose oxidase (GOD) and horseradish peroxidase (HRP) were simply mixed with Au-Fe3O4 iO2 **nanocomposite** and casted on nafion (Nf) and glutaraldehyde (GA). The modified electrode was designated as Nf-GOD-HRP/Au-Fe3O4 iO2/ITO. The electrocatalytic activity of the modified electrode towards glucose was investigated in phosphate buffered saline (PBS) containing supporting electrolyte, enzyme loading, the concn. of the mediator methylene blue (MB) and the applied potential were investigated.

Analysis Refine

Analyze by: Author Name

Click bar to view only those references within the current answer set

Jiang Jing	19
Liu Wei	19
Du Youwei	15
Niihara Koichi	15
Sekino Tohru	15
Hadjipanayis G C	14
Li Yaogang	14
Wang Hao	14

# Index Term——索引词分析

**Analysis** Refine

Analyze by: 

**Index Term** ▼

*Click bar to view only those references within the current answer set*

Nanocomposites	1941
Nanoparticles	1306
Magnetization	1186
Coercive force (magnetic)	709
Magnetic particles	609
Magnetic hysteresis	602
Microstructure	549
Magnetic materials	432
Particle Size	432
Composites	335

**Show More**

## Index Term帮助分析文献中重要的概念

**Analysis - Index Term** 

Only 1,000 Terms are displayed. [close](#)

**2416 Items** 0 Selected [Export](#)

Sort by: Frequency ▼ **1 2 3 4 5 6 ... 20** ▶

Select bars to view only those references within the current answer set.

<input type="checkbox"/> Nanocomposites	1941
<input type="checkbox"/> Nanoparticles	1306
<input type="checkbox"/> Magnetization	1186
<input type="checkbox"/> Coercive force (magnetic)	709
<input type="checkbox"/> Magnetic particles	609
<input type="checkbox"/> Magnetic hysteresis	602
<input type="checkbox"/> Microstructure	549
<input type="checkbox"/> Magnetic materials	432
<input type="checkbox"/> Particle Size	432
<input type="checkbox"/> Composites	335

**Apply** **Cancel**

## 本课题的核心研究人员是谁？核心研究机构有哪些？



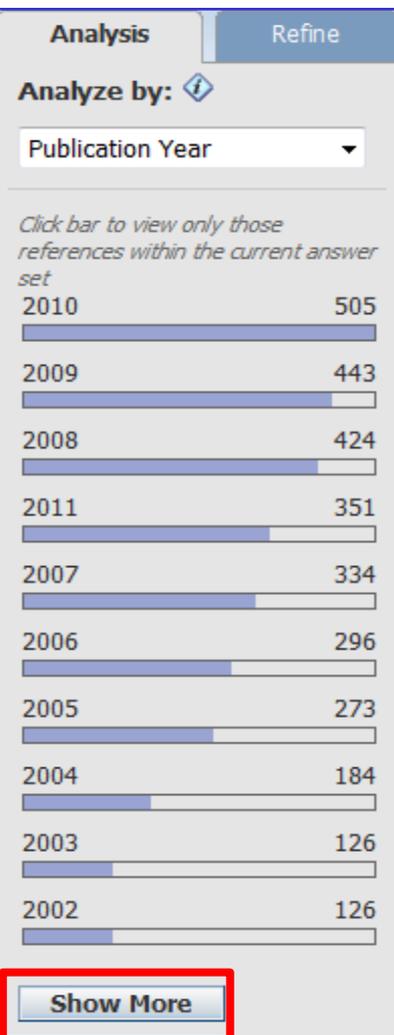
**Author Name** 作者  
名分析，了解本领域的主要研究人员



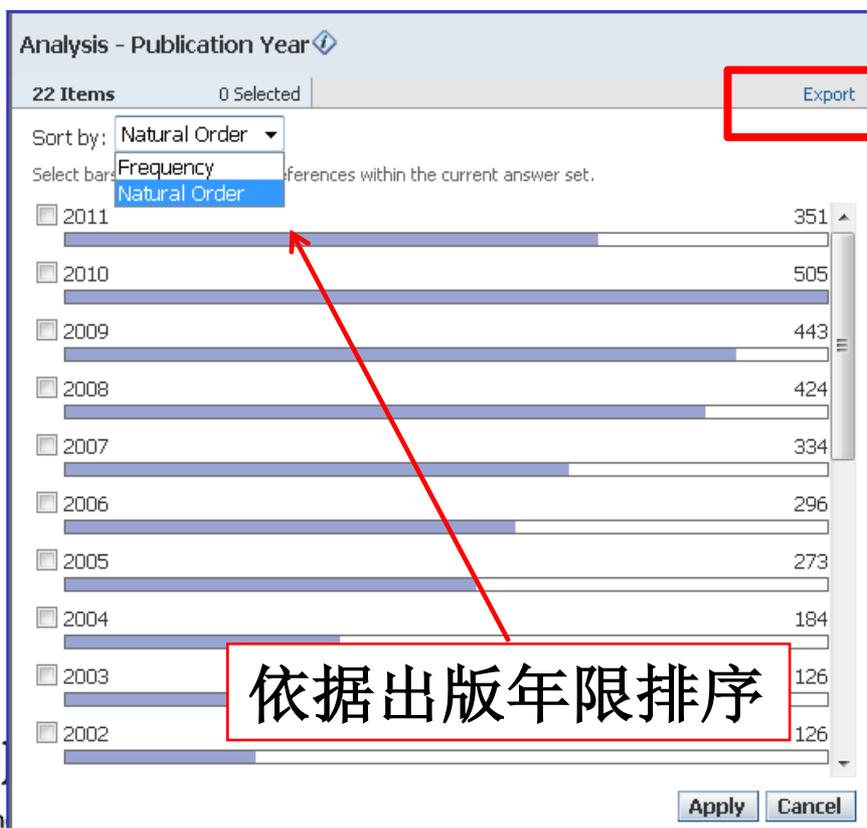
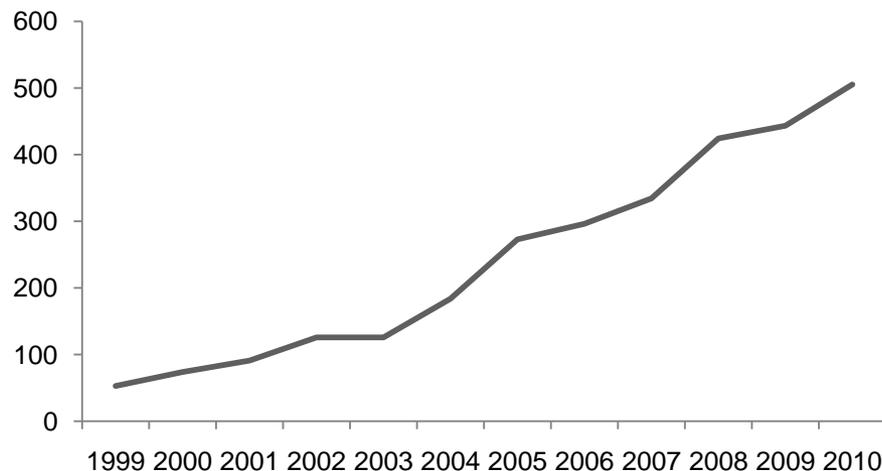
### Company-Organization

组织机构分析，了解本领域的核心研究机构，有哪些国际机构参与，寻找国际合作伙伴

# 课题的发展趋势是什么？

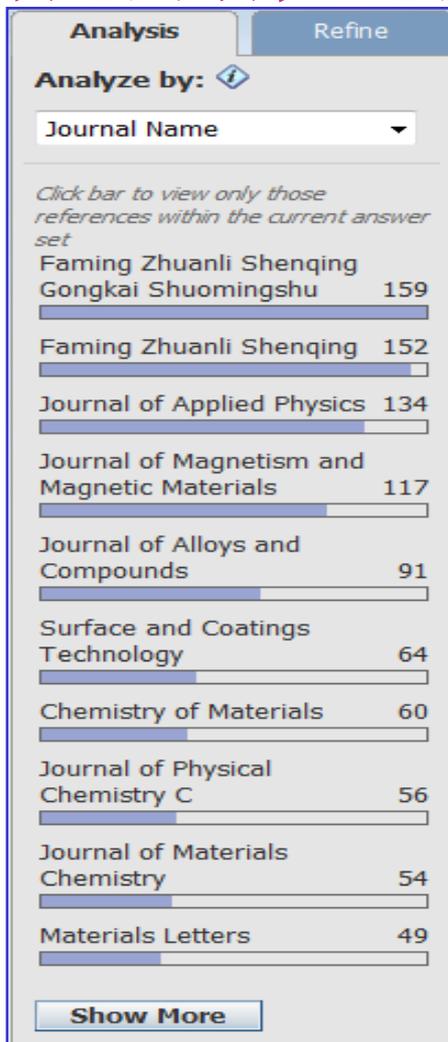


出版年限分析，了解近年来的发展趋势



依据出版年限排序

## 本课题的研究适合在哪些期刊投稿？



**Journal Name** 期刊名分析，  
了解本课题研究成果发表在  
哪些期刊、会议、报告上

# 如何获得课题相关的综述文献？

## Refine限定工具

Document Type(s)

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

Refine

Refine by:

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

Research Topic

Examples:

The effect of antibiotic residues on dairy products

Photocyanation of aromatic compounds

Refine

文献类型分析，通过综述文献快速了解国内外的研究进展



# 历史导航——返回原先的检索界面

SciFinder® Explore References Explore Substances Explore Reactions

Welcome Sam Yu | Sign Out

Add KMP Alert Research Topic "magnetic nanocomposites with p..." **references (3416)** refine "Review" (108)

References Get Substances Get Reactions Get Related Tools Send to SciPlanner

3416 References 0 Selected Save Print Export

Select All Deselect All Sort by: Accession Number Answers per Page [20] 1 2 3 4 5 6 ... 171 Display: [icon]

1. **Synthesis of  $\gamma$ -Fe<sub>2</sub>O<sub>3</sub>/SiO<sub>2</sub>/Au magnetic composites for immobilization of bovine serum albumin**  
 By Li, ZhiXia; Peng, MingLi; Jin, YanYan; Wang, XiaoFang; Cui, YaLi; Chen, Chao  
 From Chinese Science Bulletin (2011), 56(27), 2911-2915. Language: English, Database: CAPLUS  
 A method for the two-step **synthesis of magnetic composites** with a  $\gamma$ -Fe<sub>2</sub>O<sub>3</sub> core, silica inner layer and numerous gold **nanoparticles** supported on the surface of the silica ( $\gamma$ -Fe<sub>2</sub>O<sub>3</sub>/SiO<sub>2</sub>/Au) is described. First, thiol-functionalized  $\gamma$ -Fe<sub>2</sub>O<sub>3</sub>/SiO<sub>2</sub> **composites** and gold colloids are **prepd.** by modifying  $\gamma$ -Fe<sub>2</sub>O<sub>3</sub>/SiO<sub>2</sub> **composites** with mercaptosilane and redn. of Au<sup>3+</sup> to Au<sup>0</sup> with citrate, resp. Gold **nanoparticles** are then assembled on the surface of the thiol-functionalized  $\gamma$ -Fe<sub>2</sub>O<sub>3</sub>/SiO<sub>2</sub> **composites** to form  $\gamma$ -Fe<sub>2</sub>O<sub>3</sub>/SiO<sub>2</sub>/Au **composites**. The structure of the **composite** particles is confirmed by transmission el...

2. **A novel bienzyme glucose biosensor based on three-layer Au-Fe<sub>3</sub>O<sub>4</sub> iO<sub>2</sub> magnetic nanocomposite**  
 By Chen, Xiaojun; Zhu, Jinwei; Chen, Zixuan; Xu, Chenbin; Wang, Yan; Yao, Cheng  
 From Sensors and Actuators, B: Chemical (2011), 159(1), 220-228. Language: English, Database: CAPLUS  
 The **magnetic** core-shell Au-Fe<sub>3</sub>O<sub>4</sub> iO<sub>2</sub> **nanocomposite** was **prepd.** by layer-by-layer assembly technique and was used to fabricate a novel bienzyme glucose biosensor. Glucose oxidase (GOD) and horseradish peroxidase (HRP) were simply mixed with Au-Fe<sub>3</sub>O<sub>4</sub> iO<sub>2</sub> **nanocomposite** and cross-linked on the ITO **magnetism**-electrode with nafion (NF) and glutaraldehyde (GA). The modified electrode was designated as Nf-GOD-HRP/Au-Fe<sub>3</sub>O<sub>4</sub> iO<sub>2</sub>/ITO. The effects of some exptl. variables such as the pH of supporting electrolyte, enzyme loading, the concn. of the mediator methylene blue (MB) and the applied potential wer...

Analysis Refine

Analyze by: Database

Click bar to view only those references within the current answer set

CAPLUS	3396
MEDLINE	20

Show More

Categorize

More detailed analysis based on CAS indexing

Categorize

本课题的研究都涉及到哪些交叉学科？

# Categorize系统分析工具

一级目录

二级目录

和二级目录有关的  
Index Term

**Categorize**

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

Category Heading	Category	Index Terms	Selected Terms
All	Polymers (793)	<input checked="" type="checkbox"/> Coating materials 192	Click 'x' to remove the category from 'Selected Terms'
Technology	Modifiers & additives (449)	<input type="checkbox"/> Conducting polymers 64	<input checked="" type="checkbox"/> Polymer chemistry >
General chemistry	Processes & apparatus (35)	<input type="checkbox"/> Polyelectrolytes 21	Applications & phenomena (1 Terms)
Physical chemistry	Applications & phenomena (33)	<input type="checkbox"/> Polydispersity 17	
Synthetic chemistry	Miscellaneous substances (48)	<input type="checkbox"/> Membranes, nonbiological 16	
<b>Polymer chemistry</b>		<input type="checkbox"/> Electrodeposits 11	
Biotechnology		<input type="checkbox"/> Reinforced plastics 10	
Environmental chemistry		<input type="checkbox"/> Synthetic polymeric fibers 9	
Catalysis		<input type="checkbox"/> Binders 6	
Genetics & protein chemistry		<input type="checkbox"/> Plastics 6	
Analytical chemistry		<input type="checkbox"/> Latex 5	
Biology		<input type="checkbox"/> Plastic films 5	
		<input type="checkbox"/> Plastic foams 5	
		<input type="checkbox"/> Inks 4	
		<input type="checkbox"/> Polyamide fibers 4	
		<input type="checkbox"/> Polypropene fibers 4	
		<input type="checkbox"/> Liquid crystals, polymeric 2	

Polymer chemistry > Applications & phenomena > 1 Index Term(s) Selected

OK Cancel

这里可以选择感兴趣的内容，用于文献的筛选

# 点击文献标题，查看、获取文献更多的详细信息

SciFinder®

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Research Topic "magnetic nanocomposites with p..." > references (3416) > refine by categories

References | Get Substances | Get Reactions | Get Related | Tools | Send to SciPlanner

192 References | 0 Selected

Select All | Deselect All | Sort by: Accession Number

Answers per Page [20] | 1 | 2 | 3 | 4 | 5 | 6 | ... | 10

Display: [icon]

- 1. Microstructure, mechanical and tribological properties of Ti(C,N)/a-C gradient composite films**

By Li, Bin; Zhang, Guojun; Zhang, Peng; Liu, Gang

From Thin Solid Films (2011), 519(19), 6246-6251. Language: English, Database: CAPLUS

Titanium carbonitride/amorphous carbon (Ti(C,N)/a-C) composite films with compositional gradient from Ti-TiN-Ti(C,N) to TiC nanocrystal-contg. a-C layers have been prepd. by closed-field unbalanced magnetron sputtering. Within the composite films, the carbon contents gradually increase and achieve max. in the a-C layer by increasing the power applied to the graphite targets, the nitrogen contents gradually decrease to zero from Ti(C,N) layer of the interface to a-C layer of the films. To achieve a good combination of the mech. and tribol. properties in the composite films, a designed exptl. ...

+ Substances | Reactions | Citings | Full Text | Link | Comments | Tags
- 2. The structure and tribological properties of aluminum/carbon nanocomposite thin films synthesized by reactive magnetron sputtering**

By Zhou, Shengguo; Wang, Liping; Xue, Qunj

From Surface and Interface Analysis (2011), 43(7), 1057-1063. Language: English, Database: CAPLUS

Hydrogenated nanocomposite aluminum/carbon thin films (Al/a-C:H) were fabricated on stainless steel and silicon wafer substrates via unbalanced reactive magnetron sputtering from an Al target in CH<sub>4</sub>/Ar plasma. The compn. and structure of Al/a-C:H films were investigated by high-resoln. transmission electron microscope (HRTEM), XPS and micro-Raman spectroscopy. Nanoindenter, interferometer, and ball-on-disk tribometer were carried out to evaluate the hardness, internal stress and tribol. properties of Al/a-C:H films. HRTEM observations confirmed that the metallic Al nanocrystallites were uni...

+ Substances | Reactions | Citings | Full Text | Link | Comments | Tags

## 摘要信息

## Tribological properties of aluminum/carbon nanocomposite thin films synthesized by reactive magnetron sputtering

By: Zhou, Shengguo; Wang, Liping; Xue, Qunji

Hydrogenated nanocomposite aluminum/carbon thin films (Al/a-C:H) were fabricated on stainless steel and silicon wafer substrates via unbalanced reactive magnetron sputtering from an Al target in CH<sub>4</sub>/Ar plasma. The compn. and structure of Al/a-C:H films were investigated by high-resoln. transmission electron microscope (HRTEM), XPS and micro-Raman spectroscopy. Nanoindenter, interferometer, and ball-on-disk tribometer were carried out to evaluate the hardness, internal stress and tribol. properties of Al/a-C:H films. HRTEM observations confirmed that the metallic Al nanocrystallites were uniformly dispersed in the amorphous carbon matrix. XPS and Raman analyses indicated that the sp<sup>2</sup> content increased with the increase of Al content in the films. Nanoindenter and interferometer tests exhibited that the uniform incorporation of Al nanocrystallites can diminish drastically the magnitude of internal stress with maintaining the higher hardness of as-deposited films. Esp., the ball-on-disk tribometer measurements revealed that the nanocomposite film with 2.3 at.% Al content exhibited relatively better wear resistance and self-lubrication performance with a friction coeff. of 0.06 and wear rate of  $3.1 \times 10^{-16}$  m<sup>3</sup>/(N m) under ambient air, which can be attributed to the relatively higher hardness, the formation of continuous graphitized transfer film on counterface, and the reduced reaction of oxygen with carbon.

## Source

Surface and Coatings Technology  
Volume 43  
Issue 7  
Pages 1057-1062  
Journal  
2011  
CODEN: SIANDQ  
ISSN: 0142-2421  
DOI: 10.1002/sia.3691

## Company/Organization

State Key Laboratory of Solid Lubrication, Lanzhou Institute of Chemical Physics  
Chinese Academy of Sciences  
Lanzhou, Peop. Rep. China  
730000

## Accession Number

2011:709221  
CAN 155:102047  
CAPLUS

## Publisher

John Wiley &amp; Sons Ltd.

## Language

English

文献详细  
著录信息

## Concepts

## Coating materials

antifricition; structure and tribol. properties of aluminum/carbon nanocomposite thin films *prepd.* by reactive magnetron sputtering

## Graphitization

on counterface; structure and tribol. properties of aluminum/carbon nanocomposite thin films *prepd.* by reactive magnetron sputtering

## Stress, mechanical

residual; structure and tribol. properties of aluminum/carbon nanocomposite thin films *prepd.* by reactive magnetron sputtering

## Wear

resistance; structure and tribol. properties of aluminum/carbon nanocomposite thin films *prepd.* by reactive magnetron sputtering

## Lubrication

self-lubrication; structure and tribol. properties of aluminum/carbon nanocomposite thin films *prepd.* by reactive magnetron sputtering

## 重要概念索引

## Substances

## 7440-44-0DP Carbon, hydroge

amorphous; structure and tribol. properties of aluminum/carbon nanocomposite thin films *prepd.* by reactive magnetron sputtering

Properties; Synthetic preparation; Preparation

## 7429-90-5 Aluminum, processes

structure and tribol. properties of aluminum/carbon nanocomposite thin films *prepd.* by reactive magnetron sputtering

Physical, engineering or chemical process; Properties; Process

## 74-82-8 Methane, processes

structure and tribol. properties of aluminum/carbon nanocomposite thin films *prepd.* by reactive magnetron sputtering

Physical, engineering or chemical process; Process

## 7440-21-3 Silicon, uses

## 12597-68-1 Stainless steel, uses

substrate; structure and tribol. properties of aluminum/carbon nanocomposite thin films *prepd.* by reactive magnetron sputtering

Other use, unclassified; Uses

## 物质链接

## 保存

## 使用Export将结果输出

References **Get Substances** **Get Reactions** **Get Related** **Tools** **Send to SciPlanner**

192 References 0 Selected Save Print **Export**

Select All Deselect All Sort by: Accession Number ↓ Answers per Page [20] 1 2 3 4 5 6 7 8 9 10 11 12 Display: [icon]

1. **Microstructure, mechanical and tribological properties of Ti(C,N)/a-C gradient composite films**  
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 Substances Reactions Citings Full Text Link Comments Tags

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 Substances Reactions Citings Full Text Link Comments Tags

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- Range

Example: 2-20

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- Quoted Format (\*.txt)
- Tagged Format (\*.txt)

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- Portable Document Format (\*.pdf)
- Rich Text Format (\*.rtf)
- Answer Keys (\*.txt)

**Saving locally**

- Answer Key eXchange (\*.akx)

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Reference\_09\_09\_2011\_111619

**Format:**

- Summary without abstracts
- Summary with partial abstracts
- Summary with full abstracts
- Detail (full record)

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- Task History
- Tags
- Comments

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**Offline Review:** 保存过成 PDF, RTF格式，用于脱机浏览

## 文献检索小结

- 主题检索时，使用介词作为连接
- 尽量选择包含**Concepts**和**Closed Associated with**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
- 更多细节化内容，请参考
- [www.igroup.com.cn/cas](http://www.igroup.com.cn/cas)

## 提纲

- 介绍
  - SciFinder 中的内容
  - SciFinder 的注册和登陆
- **SciFinder 中的检索和后处理**
  - SciFinder 中的文献检索
  - SciFinder 中的物质检索
  - SciFinder 中的Markush检索
  - SciFinder 中的反应检索
- **SciFinder 特色功能**
- **SciFinder网络资源平台**

# 物质检索

SciFinder®

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Explore References | Explore Substances | Explore Reactions

Explore Substances

Chemical Structure

Markush

Molecular Formula

Substance Identifier

Click to Edit

Search

四种物质检索方式：  
 结构检索  
 Markush检索  
 分子式检索  
 物质标示符检索

Characteristic(s)

- Single component
- Commercially available
- Included in reference(s)

Class(es)

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

Studies

- Analytical
- Biological
- Preparation
- Reactant or reagent

## 分子式检索

- 检索聚合物、金属配合物
- 举例检索二茂铁 (**C<sub>10</sub>H<sub>10</sub>Fe**)



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Welcome Amy Qi | Sign Out

Explore References | Explore Substances | Explore Reactions

Explore Substances

Chemical Structure | **Molecular Formula** | Substance Identifier

Molecular Formula

Examples:  
*H4SiO4*  
*H4O4Si*  
*H4SiO4*

**CH**写在前面，其他的按照字母顺序排列：  
 聚合物：(C<sub>12</sub> H<sub>12</sub> O<sub>4</sub>)<sub>n</sub>、(C<sub>8</sub> H<sub>8</sub> Br<sub>2</sub> . C<sub>4</sub> H<sub>6</sub> O<sub>4</sub>)<sub>x</sub>  
 用点将不同的组分分开：  
 醋酸钠：C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>.Na

# 得到27个符合C<sub>10</sub>H<sub>10</sub>Fe的物质

Substances Get References Get Reactions Tools Send to SciPlanner

27 Substances 0 Selected Save Print Export

Select All Deselect All Sort by: CAS Registry Number ↓ Answers per Page [15] 1 2

View: ■ ■ ■ ■ ■

1. Substance Detail  
866919-52-0

**C<sub>10</sub> H<sub>10</sub> Fe**  
Iron, (η10-1,3,5,7,9-cyclodecapentaene)- (9CI)

~1 References  
Reactions  
Commercial Sources  
Regulatory Information  
Link

检索到很多同分异构体，  
利用**Refine**进行结构的再次  
限定

2. Substance Detail

**C<sub>10</sub> H<sub>10</sub> Fe**  
Ferrocene-56Fe (9CI)

3. Substance Detail

**C<sub>10</sub> H<sub>10</sub> Fe**  
Ferrocene-56Fe (9CI)

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 draw or import structure

**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**

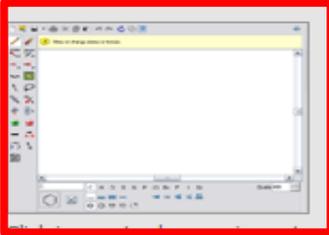
# 金属配合物的分子式检索

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 draw or import structure

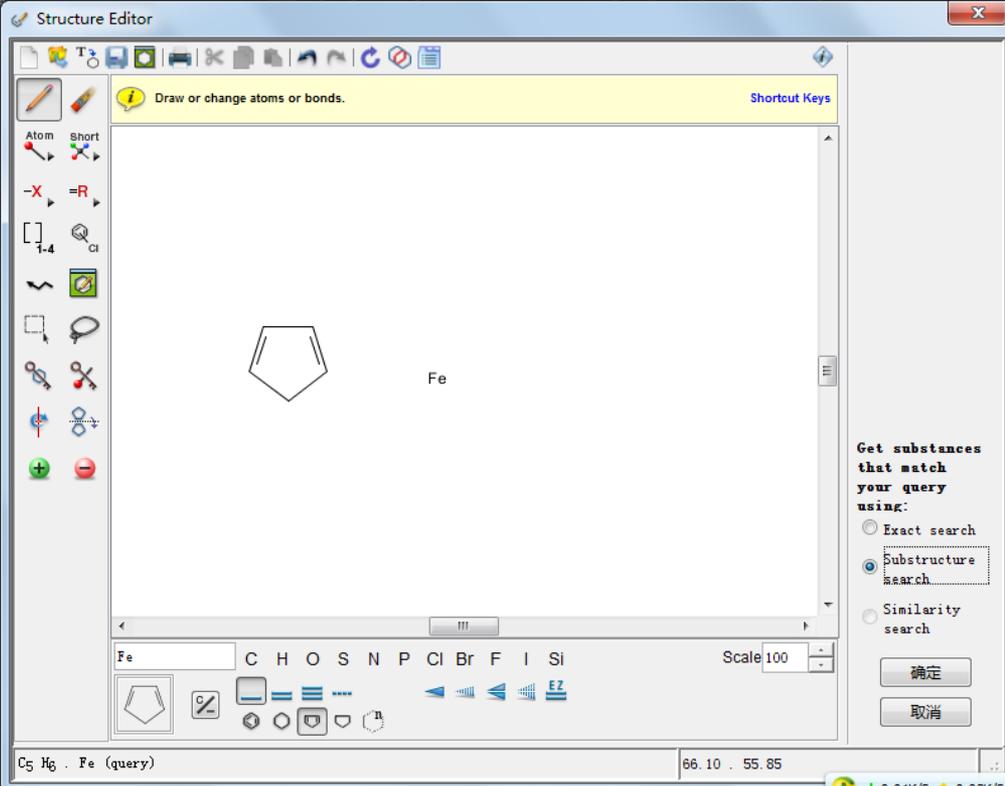
**Only retrieve substances that:**

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

- 利用结构限定
- 选择单一组分物质

Structure Editor

Draw or change atoms or bonds. Shortcut Keys



Atom Short

-X =R

[ ] 1-4 Cl

Scale 100

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

Get substances that match your query using:

- Exact search
- Substructure search
- Similarity search

确定 取消

C<sub>5</sub>H<sub>6</sub> · Fe (query) 66.10 · 55.85

# 精选到19个物质

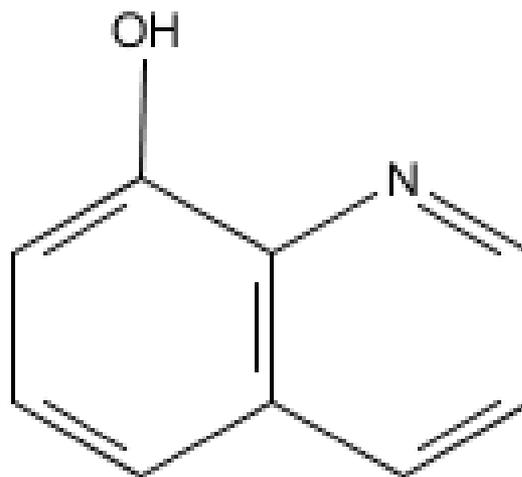
检索到二茂铁的很多同位素，利用**Refine**去除同位素

The screenshot shows the SciFinder interface with the following details:

- Substances:** 19 Substances, 0 Selected. Sort by: CAS Registry Number.
- Substance 1:** Substance Detail 774583-14-1. Structure: C10H10Fe (Ferrocene).
- Substance 2:** Substance Detail 548770-67-8. Structure: C10H9D9Fe (Ferrocene-d9).
- Refine Dialog:**
  - Refine by:**  Isotope-Containing
  - Select One:**  Exclude isotope-containing substances
- Refine Panel (Right):**
  - Refine by:**  Chemical Structure
  - Chemical Structure:**  Isotope-Containing,  Metal-Containing,  Commercial Availability,  Property Availability,  Property Value,  Reference Availability,  Atom Attachment.
  - Only retrieve substances that:**  Have references,  Are commercially available,  Are a single component,  Are in specific substance.

# 化学结构式检索

查找**8-羟基喹啉**  
衍生物为配体的  
金属化合物



配体

# SciFinder结构绘制工具

The image shows the SciFinder Structure Editor interface with various tools and features labeled in Chinese. The labels are as follows:

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

The interface includes a toolbar on the left with icons for drawing and editing, a central workspace for the chemical structure, and a right-hand panel for search options (Exact, Substructure, Similarity) and drawing editor settings (Structure, Reaction). The bottom of the window shows a search bar with a query and a scale control.

Structure Editor

Draw or change atoms or bonds. Shortcut Keys

Atom Short

-X

1-4 Cl

OH

N

M

Variables

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

Close

Drawing Editor:

- Structure
- Reaction
- Markush

Get substances that match your query using:

- Exact search
- Substructure search
- Similarity search

确定

取消

Formula not available

可变基团

亚结构检索，  
可以查找特定母  
核结构的一类物  
质

## 物质检索结果

SciFinder® Explore References Explore Substances Explore Reactions

Welcome Bruce Peng | Sign Out

Add KMP Alert Chemical Structure substructure > substances (14606)

Get References Get Reactions Tools Send to SciPlanner

14606 Substances 0 Selected

Select All Deselect All Sort by: CAS Registry Number

Save Print Export

Answers per Page [15] 1 2 3 4 5 6 ... 974

View: [Icons]

Analysis Refine

Analyze by: Substance Role

Click bar to view only those substances within the current answer set

Preparation	8658
Properties	4658
Uses	2680
Reactant or Reagent	1630
Biological Study	1574
Process	1113
Formation, Nonpreparative	535
Analytical Study	262
Prophetic in Patents	155
Occurrence	12

1. Substance Detail 1333419-24-1

2. Substance Detail 1333320-37-8

3. Substance Detail 1333320-36-7

C<sub>38</sub> H<sub>30</sub> N<sub>4</sub> O<sub>5</sub> Th

C<sub>33</sub> H<sub>21</sub> Al F<sub>9</sub> N<sub>3</sub> O<sub>3</sub>

C<sub>30</sub> H<sub>21</sub> Al F<sub>3</sub> N<sub>3</sub> O<sub>3</sub>

~1 References

Reactions

Commercial Sources

Regulatory Information

~1 References

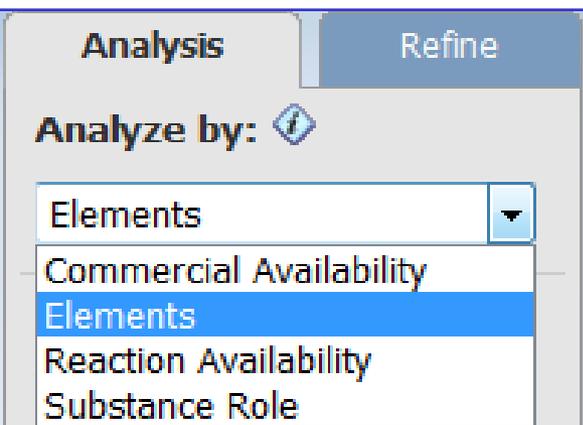
Reactions

Commercial Sources

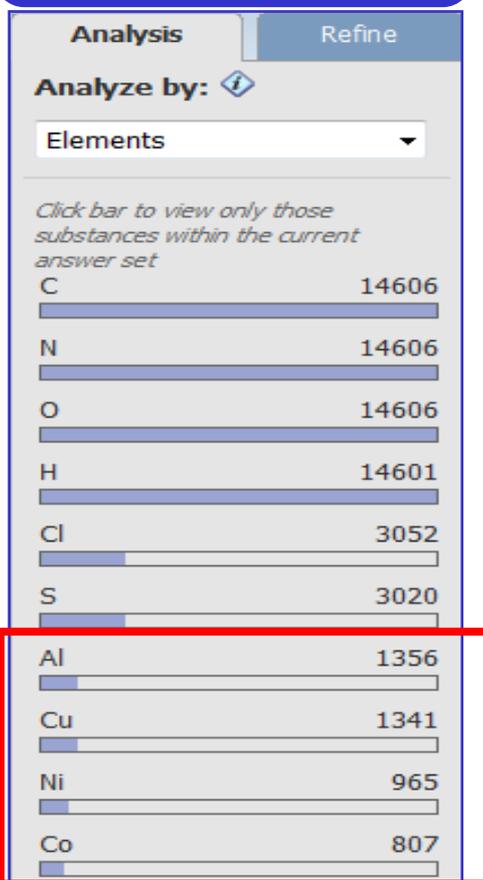
获得与物质相关的文献、反应、商品信息

分析和限定工具

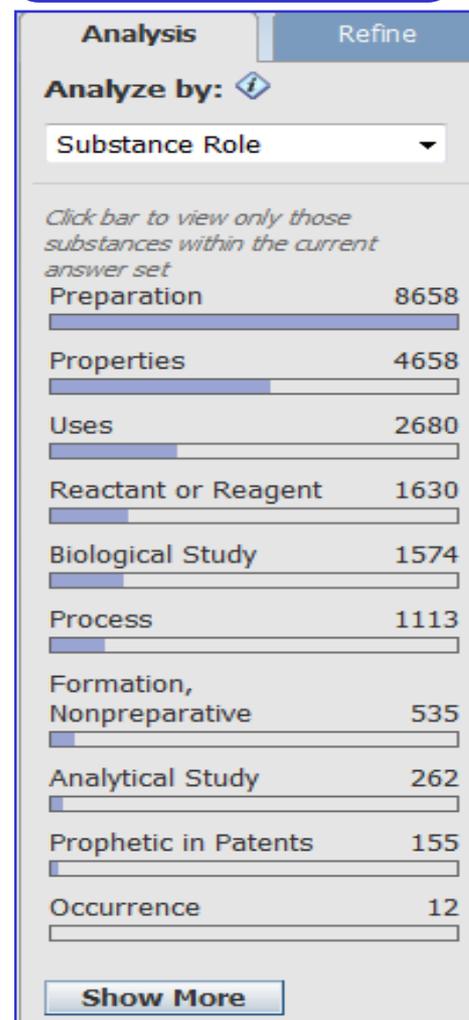
# 物质检索的分析工具



了解配体与哪些金属螯合



了解物质的应用领域



一共4种分析工具：  
商业来源分析  
元素分析  
反应分析  
物质角色分析

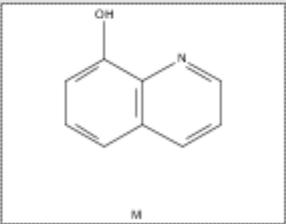
# 物质检索的限定工具

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**

七种限定功能:

- 1 结构修饰
- 2 同位素包含
- 3 金属包含
- 4 商业来源
- 5 理化性质
- 6 文献来源
- 7 原子附属性

精选对PH、熔点、沸点等理化性质有特殊要求的物质

Refine by Property Value

Select a property on the left, and specify values or limits on the right. Repeat for multiple properties.

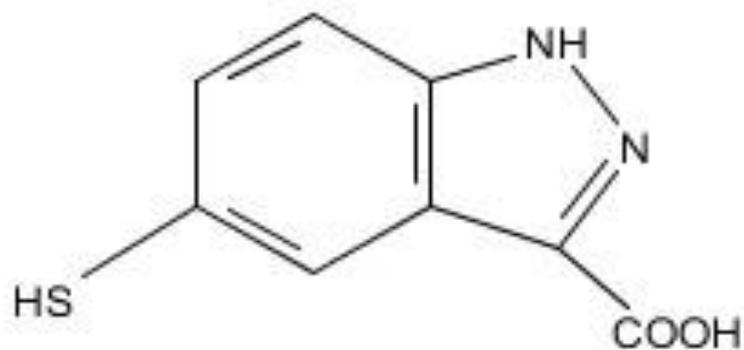
Properties - 1 selected	Values - Predicted pKa
<input type="checkbox"/> H Acceptors	Specify range:
<input type="checkbox"/> H Donors	0.0 to 14.0
<input type="checkbox"/> Molecular Weight	Min: Max:
<input type="checkbox"/> logP	Limit by:
<input type="checkbox"/> Freely Rotatable Bonds	<input type="checkbox"/> Most acidic
<input type="checkbox"/> Bioconcentration Factor	<input type="checkbox"/> Most basic
<input type="checkbox"/> Boiling Point	
<input type="checkbox"/> Density	
<input type="checkbox"/> Enthalpy of Vaporization	
<input type="checkbox"/> Flash Point	
<input type="checkbox"/> H Acceptor/Donor Sum	
<input type="checkbox"/> Koc	
<input type="checkbox"/> logD	
<input type="checkbox"/> Mass Intrinsic Solubility	
<input type="checkbox"/> Mass Solubility	
<input type="checkbox"/> Molar Intrinsic Solubility	
<input type="checkbox"/> Molar Solubility	
<input type="checkbox"/> Molar Volume	
<input checked="" type="checkbox"/> pKa	
<input type="checkbox"/> Polar Surface Area	
<input type="checkbox"/> Vapor Pressure	

Include substances with no values for selected properties.

Reset Refine Cancel

# 新设计的化合物，如何预测其理化性质？

- **Scifinder**化学结构检索



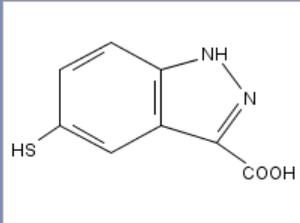
The screenshot displays the 'Explore Substances' interface in Scifinder. The main area is titled 'Chemical Structure' and contains a list of options: 'Markush', 'Molecular Formula', and 'Substance Identifier'. To the right, there is a 'Click to Edit' button. The interface is designed for users to interact with and edit chemical structures.

# 化学结构检索

Explore Substances

Chemical Structure Chemical Structure

Markush  
Molecular Formula  
Substance Identifier



Click image to change structure or view detail

Search type: 

- Exact Structure
- Substructure
- Similarity

Show precision analysis

**Search**

**Exact 精确结构检索**  
**Substructure 亚结构检索**

SciFinder®

Explore References Explore Substances Explore Reactions

Welcome Sam Yu | Sign Out

Create Keep Me Posted Chemical Structure Substructure Substances (0)

Substances

0 Substances 0 Selected

Explore Substances resulted in 0 substances [Return](#)

**新物质, 无检索记录**

# Similarity 相似结构检索

Structure Editor

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

Atom Short

-X =R

[ ] 1-4 Cl

HS

NH

COOH

Get substances that match your query using:

Exact search

Substructure search

Similarity search

确定

取消

COOH C H O S N P Cl Br F I Si Scale 100

C<sub>8</sub> H<sub>6</sub> N<sub>2</sub> O<sub>2</sub> S (query) 194.21

Explore Substances

Chemical Structure Chemical Structure ↕

Markush

Molecular Formula

Substance Identifier

Search

Click image to change structure or view detail

Search type:  Exact Structure  Substructure  Similarity

Show precision analysis

# Similarity 相似结构检索

Similarity Candidates

6 Candidates 3 Selected

Select All Deselect All

Similarity Candidates	Substances
<input type="checkbox"/> ≥ 99 (most similar)	0
<input type="checkbox"/> 95-98	0
<input type="checkbox"/> 90-94	0
<input checked="" type="checkbox"/> 85-89	9
<input checked="" type="checkbox"/> 80-84	26
<input checked="" type="checkbox"/> 75-79	45
<input type="checkbox"/> 70-74	147
<input type="checkbox"/> 65-69	311
<input type="checkbox"/> 0-64 (least similar)	649

相似度越高，结构越相近

Get Substances

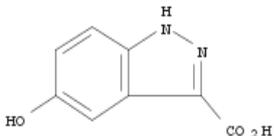
# 获得相似度75分以上的物质

Substances [Get References](#) [Get Reactions](#) [Tools](#) [NEW Send to SciPlanner](#)

80 Substances 0 Selected Save Print Export

Select All Deselect All Sort by: Similarity Score Answers per Page [15] 1 2 3 4 5 6 View:

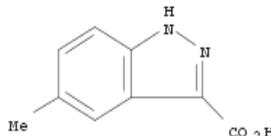
1. **Substance Detail**  
885518-94-5 Score: 88



**C<sub>8</sub> H<sub>6</sub> N<sub>2</sub> O<sub>3</sub>**  
1H-Indazole-3-carboxylic acid, 5-hydroxy-

- ~1 References
- Reactions
- Commercial Sources
- Regulatory Information
- Link

2. **Substance Detail**  
1201-24-7 Score: 87

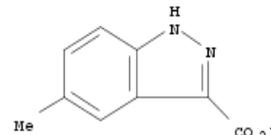


**C<sub>9</sub> H<sub>8</sub> N<sub>2</sub> O<sub>2</sub>**  
1H-Indazole-3-carboxylic acid, 5-methyl-

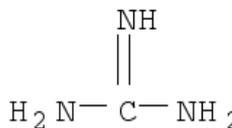
- ~17 References
- Reactions
- Commercial Sources
- Regulatory Information
- Link

3. **Substance Detail**  
108259-82-1 Score: 87

1201-24-7  
C<sub>9</sub> H<sub>8</sub> N<sub>2</sub> O<sub>2</sub>



113-00-8  
C<sub>5</sub> H<sub>5</sub> N<sub>3</sub>



**C<sub>9</sub> H<sub>8</sub> N<sub>2</sub> O<sub>2</sub> · C<sub>5</sub> H<sub>5</sub> N<sub>3</sub>**  
1H-Indazole-3-carboxylic acid, 5-methyl-, compd. with guanidine (1:1)

**Analysis** Refine

Analyze by:

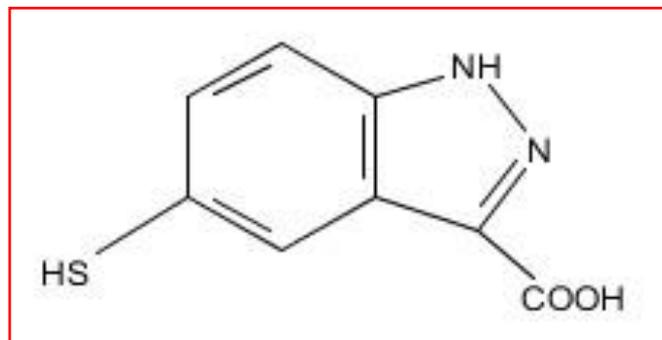
Substance Role ▼

*Click bar to view only those substances within the current answer set*

Reactant or Reagent	43
Preparation	38
Uses	8
Process	4
Properties	3
Prophetic in Patents	3
Biological Study	2
Analytical Study	1
Combinatorial Study	1
Formation, Nonpreparative	1

**Show More**

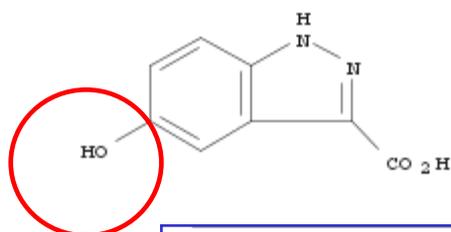
# 与原结构存在的区别



取代基不同

1. Substance Detail  
885518-94-5

Score: 88

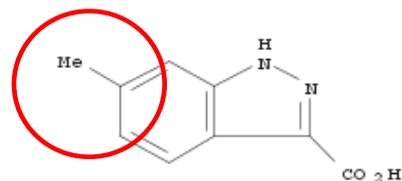


$C_8 H_6 N_2 O_3$

1H-Indazole-3-carboxylic acid

4. Substance Detail  
858227-12-0

Score: 86



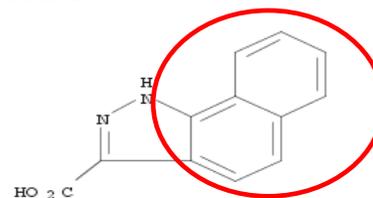
$C_9 H_8 N_2 O_2$

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

取代基位置不同

63. Substance Detail  
665020-19-9

Score: 76



$C_{12} H_8 N_2 O_2$

1H-Benz[g]indazole-3-carboxylic acid

母核结构不同

# 如何获得有参考价值的反应信息？

Substances Get References **Get Reactions** Tools NEW Send to SciPlanner

80 Substances 0 Selected Save Print Export

Select All Deselect All Sort by: Similarity Score Answers per Page [15] 1 2 3 4 5 6

1. **Substance Detail** Score: 88  
**885518-94-5**

C8 H6 N2 O3  
 1H-Indazole-3-carboxylic acid, 5-hydroxy-

~1 References  
 Reactions  
 Commercial Sources  
 Regulatory Information  
 Link

**Get Reactions** ⓘ

Retrieve reactions for:

All substances  
 Selected substances

Limit results by reaction role:

**Product**  
 Reactant  
 Reagent  
 Reactant or reagent  
 Catalyst  
 Solvent  
 Any role

Get Cancel

**定义为产物，  
获得合成信息**

C9 H8 N2 O2 . C H5 N3  
 1H-Indazole-3-carboxylic acid, 5-methyl-, compd. with guanidine (1:1)

**Analysis** Refine

Analyze by: ⓘ

Substance Role

*Click bar to view only those substances within the current answer set*

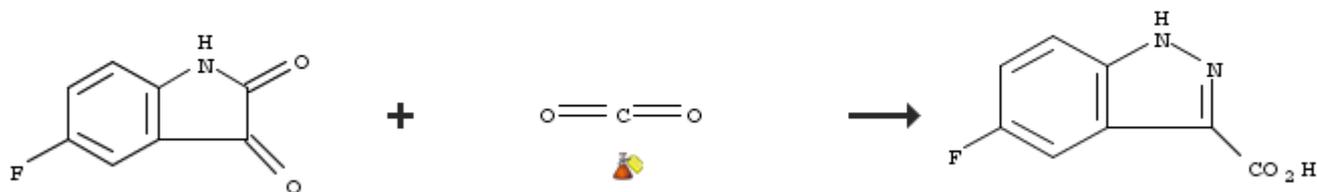
Reactant or Reagent	43
Preparation	38
Uses	8
Process	4
Properties	3
Prophetic in Patents	3
Biological Study	2
Analytical Study	1
Combinatorial Study	1
Formation, Nonpreparative	1

Show More

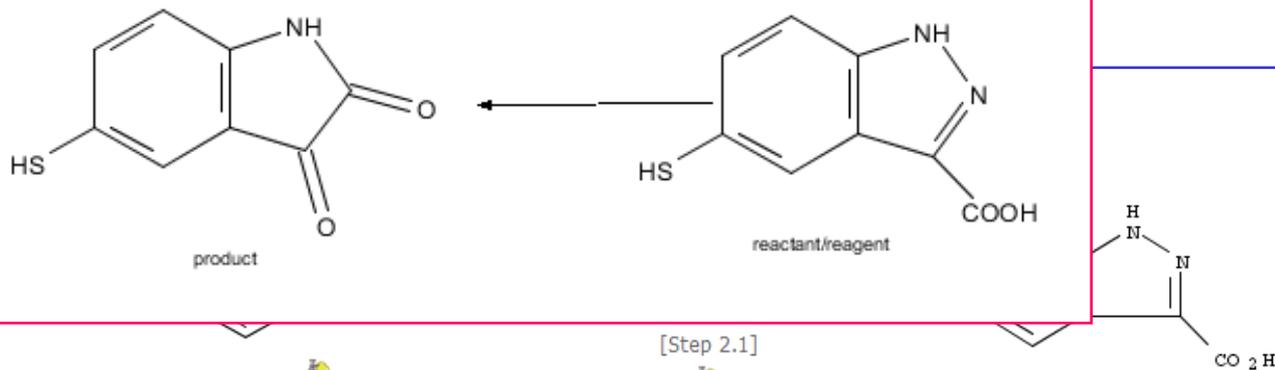
# 获得有帮助的反应信息

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

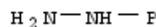
Single Step *Hover over any structure for more options.*



## 逆合成分析



3. View Reaction Detail  
3 Steps *Hover over any structure for more options.*



## 结构检索小结

- 精确结构检索：  
获得物质的盐，聚合物，混合物，配合物等，母体结构不能修改，不能修饰
- 亚结构检索：  
所画的结构必须存在，母体结构不能修改，但可以被修饰
- 相似结构检索：  
相似度越高结构越相近，母体结构可以修改，也可以被修饰，用相似度来控制获得的结果

# 化学结构检索

Explore Substances

Chemical Structure Chemical Structure

Markush  
Molecular Formula  
Substance Identifier

**那么能否申请专利?**



Click image to change structure or view detail

Search type:  Exact Structure  
 Substructure  
 Similarity

Show precision analysis

**Exact 精确结构检索**  
**Substructure 亚结构检索**

Search

SciFinder®

Explore References Explore Substances Explore Reactions

Welcome Sam Yu | Sign Out

Create Keep Me Posted Chemical Structure substructure > substances (0)

Substances  Combine Answer Sets

0 Substances 0 Selected

Explore Substances resulted in 0 substances Return

**无检索记录，意味着我们设计的化合物就是新结构**

## 提纲

- 介绍
  - SciFinder 中的内容
  - SciFinder 的注册和登陆
- **SciFinder 中的检索和后处理**
  - SciFinder 中的文献检索
  - SciFinder 中的物质检索
  - SciFinder 中的Markush检索
  - SciFinder 中的反应检索
- **SciFinder 特色功能**
- **SciFinder网络资源平台**

# Markush检索——初步的专利评估

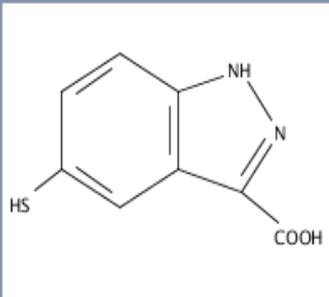
Explore Substances

Chemical Structure Markush 

**Markush**

Molecular Formula

Substance Identifier



Click image to change structure or view detail

Search type:   Allow variability only as specified  Substructure

**Search**

# Markush检索直接返回保护了该结构的专利

References Get Substances Get Reactions Get Related Tools Send to SciPlanner

23 References 0 Selected Save Print Export

Select All Deselect All Sort by: Accession Number Answers per Page [20] 1 2

Display:

**1. Bicyclic heteroaryl compounds for the treatment of cancer**  
 By Sun, Chung-Ming; Kuo, Min-Liang  
 From U.S. Pat. Appl. Publ. (2011), US 20110082143 A1 20110407. Language: English, Database: CAPLUS  
 The invention discloses bicyclic heteroaryl compds. I, (X1, X2, X3= C, N, where at least 2 of X1, X2, X3= N; R1, R3= H, alkyl, alkenyl, alkynyl, etc.; R2= heterocycloalkenyl, aryl, heteroaryl; R4, R5, R6, R7= H, alkyl, alkenyl, alkynyl, cycloalkyl, etc), eg. Me 2-(3,3-diphenyl-propyl)-2H-indazole-6-carboxylate. Also disclosed are the prepn. of compds. of the invention and the treatment of cancer with these compds.  
 Substances Reactions ~0 Citings **Full Text** Link 0 Comments 0 Tags

**2. Method for manufacturing a boronic acid ester compound**  
 By Miki, Takashi; Shimasaki, Yasuharu; Babu, Srinivasan; Cheng, Zhigang; Reynolds, Mark E.; Tian, Qingping  
 From PCT Int. Appl. (2010), WO 2010110782 A1 20100930. Language: English, Database: CAPLUS  
 The present invention relates to a method for manufg. a boronic acid ester compd. I (Ar = substituted arom. hydrocarbon group, substituted arom. heterocyclic group; R = divalent org. group), characterized by reacting an aryl halide compd. and a diboron ester compd. in the presence of a nitrogen-contg. org. base, a nickel catalyst, a phosphine compd. and a solvent. According to the manufg. method of the present invention, even if a nickel catalyst is used as the catalyst, a desired boronic acid ester compd. can be obtained in a sufficiently high yield. Furthermore, even if aryl chloride or ar...  
 Substances Reactions ~0 Citings Full Text Link 0 Comments 0 Tags

获得专利原文

# 查看专利权利要求说明书



Europäisches Patentamt  
European Patent Office  
Office européen des brevets

## Espacenet

Patent search

Deutsch English Français

Contact

Change country ▼

◀ About Espacenet Other EPO online services ▼

Search Result list **★ My patents list (0)** Query history Settings

US 2011082143 (A1)

Bibliographic data

Description

**Claims**

Mosaics

Original document

INPADOC legal status

---

Quick help —

- [What happens if I click on "In my patents list"?](#)
- [What happens if I click on the "Register" button?](#)
- [What happens if I click on the button "Translate this text"?](#)
- [How can I view the claim structure?](#)
- [Why are the claims sometimes in French or German, or some other language?](#)

### Claims: US 2011082143 (A1)

★ In my patents list → Report data error

#### Bicyclic Heteroaryl Compounds

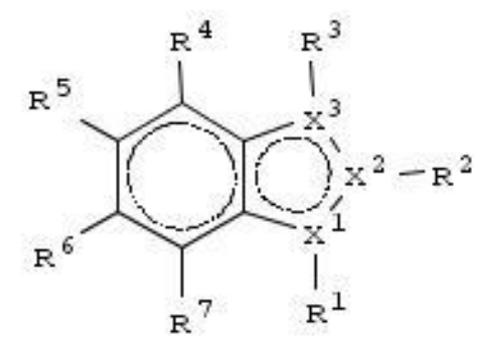
#### Claims of US 2011082143 (A1)

[Translate this text](#) [Claims tree](#)

The EPO does not accept any responsibility for the accuracy of data and information originating from other authorities than the EPO; in particular, the EPO does not guarantee that they are complete, up-to-date or fit for specific purposes.

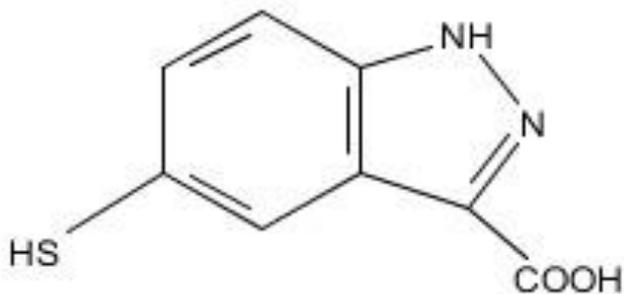
1. What is claimed is: 1. A compound of formula (I):

wherein  
each of X1, X2, and X3, independently, is C or N, and at least two of X1, X2, and X3 are each N;  
each of R1 and R3, independently, is deleted, H, alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkenyl, heterocycloalkyl, heterocycloalkenyl, aryl, heteroaryl, halo, CN, NO2, ORa, COORa, OC(O)Ra, C(O)Ra, C(O)NRaRb, C(O)N(Ra)N(Rb)C(O)Rc, NRaRb, N(Rc)SO2NRaRb, SO2NRaRb, or SRa, in which each of Ra, Rb, and Rc, independently, is H, alkyl, cycloalkyl, heterocycloalkyl, aryl, or heteroaryl, or Ra and Rb together with the nitrogen atom to which they are attached form heterocycloalkyl or heteroaryl;

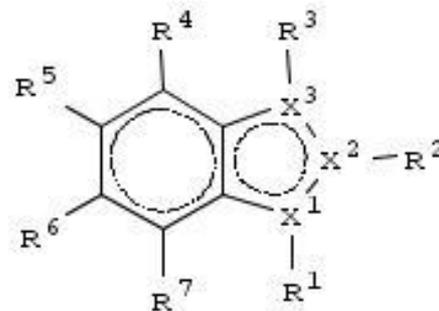


I

Print



## 设计的目标化合物



I

## 专利原文中保护的结构

1. What is claimed is: 1. A compound of formula (I):

**X1, X2, X3为C、N原子, 至少有两个是N原子**  
**R1包括COOH基团, R6包括SH基团**  
**保护了我们设计的目标化合物**

wherein

each of X1, X2, and X3, independently, is C or N, and at least two of X1, X2, and X3 are each N;

each of R1 and R3, independently, is deleted, H, alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkenyl, heterocycloalkyl, heterocycloalkenyl, aryl, heteroaryl, halo, CN, NO<sub>2</sub>, ORa, COORa, OC(O)Ra, C(O)Ra, C(O)NRaRb, C(O)N(Ra)N(Rb)C(O)Rc, NRaRb, N(Rc)SO<sub>2</sub>NRaRb, SO<sub>2</sub>NRaRb, or SRa, in which each of Ra, Rb, and Rc, independently, is H, alkyl, cycloalkyl, heterocycloalkyl, aryl, or heteroaryl, or Ra and Rb together with the nitrogen atom to which they are attached form heterocycloalkyl or heteroaryl;

R2 is heterocycloalkenyl, aryl, or heteroaryl;

each of R4, R5, R6, and R7, independently, is H, alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkenyl, heterocycloalkyl, heterocycloalkenyl, aryl, heteroaryl, halo, CN, NO<sub>2</sub>, ORd, COORd, OC(O)Rd, C(O)Rd, C(O)NRdRe, C(O)N(Rd)N(Re)C(O)Rf, NRdRe, N(Rf)SO<sub>2</sub>NRdRe, SO<sub>2</sub>NRdRe, or SRd, in which each of Rd, Re, and Rf, independently, is H, alkyl, cycloalkyl, heterocycloalkyl, aryl, or heteroaryl, or Rd and Re together with the nitrogen atom to which they are attached form heterocycloalkyl or heteroaryl.

## 提纲

- 介绍
  - SciFinder 中的内容
  - SciFinder 的注册和登陆
- **SciFinder 中的检索和后处理**
  - SciFinder 中的文献检索
  - SciFinder 中的物质检索
  - SciFinder 中的Markush检索
  - SciFinder 中的反应检索
- **SciFinder 特色功能**
- **SciFinder网络资源平台**

# SciFinder中的反应定义工具

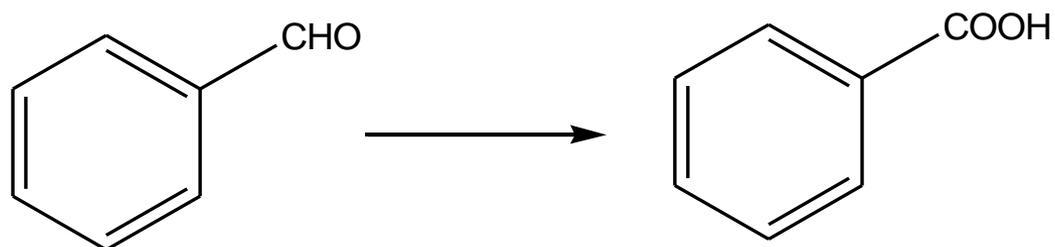
The image shows the Reaction Editor window in SciFinder. The interface includes a toolbar on the left with various drawing and editing tools, a central workspace for drawing reactions, and a right-hand panel for drawing editor settings. Red boxes with Chinese labels point to specific tools in the toolbar:

- 反应箭头** (Reaction Arrow): Points to the arrow tool in the toolbar.
- 反应原子标记工具** (Reaction Atom Labeling Tool): Points to the tool that adds atom labels (A, B) to a reaction arrow.
- 反应官能团列表** (Reaction Functional Group List): Points to the list of functional groups (retro, ketone, aldol) at the bottom of the toolbar.
- 反应角色工具** (Reaction Role Tool): Points to the tool that adds a role (R) to a reaction arrow.
- 反应位置标记工具** (Reaction Position Labeling Tool): Points to the tool that adds a position label (1) to a reaction arrow.

The right-hand panel, titled "Drawing Editor:", has radio buttons for "Structure", "Reaction" (which is selected), and "Markush". Below this, there 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" (which is selected). At the bottom right of the panel are "确定" (OK) and "取消" (Cancel) buttons.

The bottom of the window shows a search bar with "(query)" and a list of elements: C, H, O, S, N, P, Cl, Br, F, I, Si. There is also a "Scale" control set to 100.

# 反应检索—特定物质之间的反应



精确反应检索帮助获得特定物质之间的反应，点击确定

# 可以提前设定反应溶剂和不参与反应的官能团

可以自定义一些反应溶剂以及不参与反应的官能团。

SciFinder®  
Welcome Sam Yu | Sign Out

Explore References | Explore Substances | Explore Reactions

Explore Reactions

Reaction Structure | Reaction Structure

Search

Click image to change structure or view detail

Search type:  Allow variability only as specified  
 Substructure

Solvent(s)

Non-participating Functional Group(s)

Solvent Hierarchy  
[View Solvent List]

0 Selected | Select All | Deselect All

- Inorganic solvents
  - Ammonia
  - Ammonia-15N
  - Ammonia-d3
  - Water
  - Water-17O
  - Water-18O
  - Water-d
  - Water-d2
  - Water-d2-18O
  - Water-t
  - Water-t2

Find:  Next Previous

View: All 217

0 Selected | Clear Selections

- Acetal
- Acetyl
- Acid Halide
- Acyclic Alkene
- Acyclic Ketone
- Acylmetal
- ALCOHOLS
- Aldehyde
- pi-Alkene
- ALKENES
- Alkyl Halide

Reactions must have  all selections  
 any selection

# 反应检索结果

点击**Overview**查看具体信息

Reactions Get References Find Additional Reactions Combine Answer Sets

292 Reactions 0 Selected Keep Selected Remove Selected Save Print Export

Select All Deselect All Sort by: Relevance (New) ↓ Answers per Page [15] 1 2 3 4 5 6 ... 20

Display:

1. View Reaction Detail Link Similar Reactions  
Single Step Hover over any structure for more options.

**Analysis**

Analyze by:

Catalyst

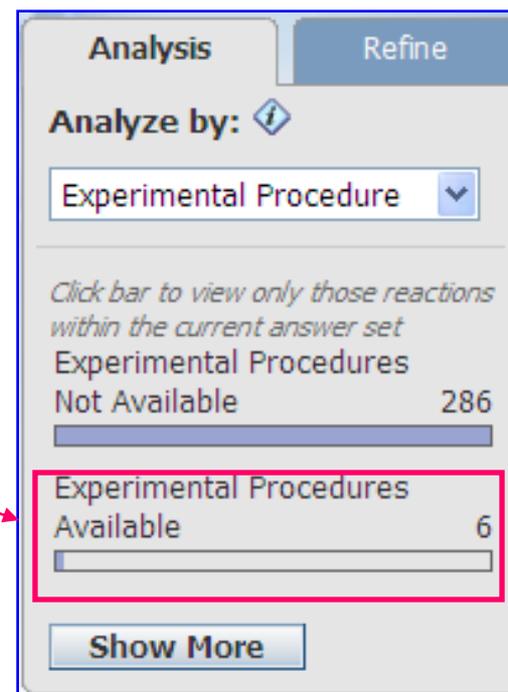
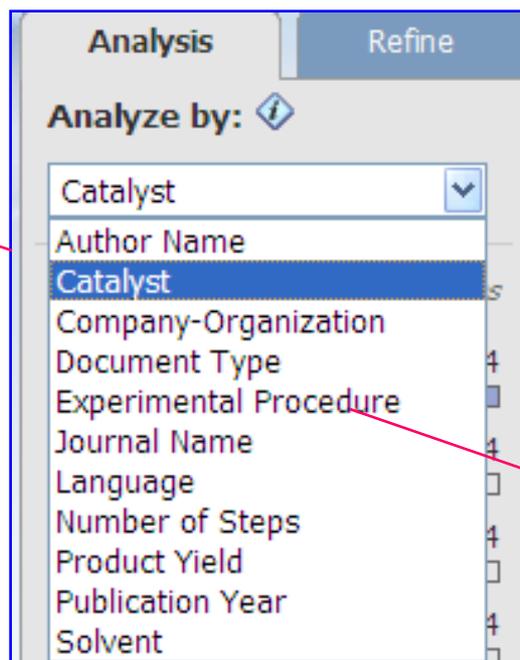
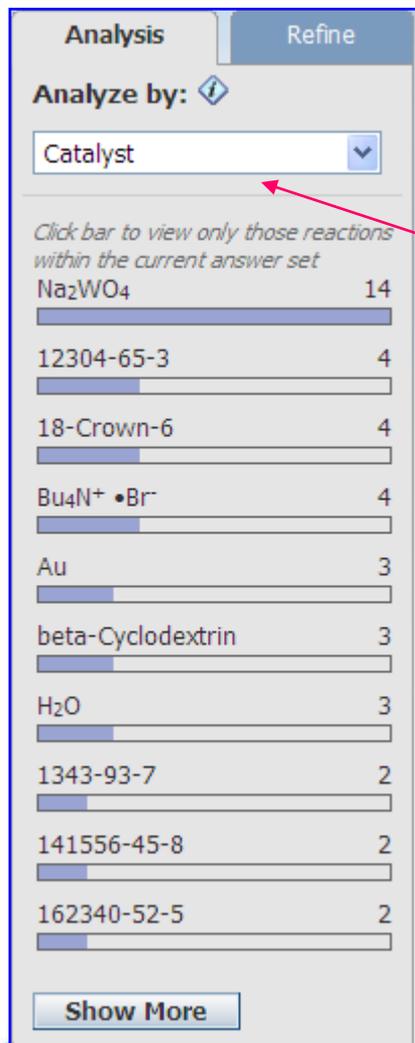
*Click bar to view only those reactions within the current answer set*

Na <sub>2</sub> WO <sub>4</sub>	14
12304-65-3	4
18-Crown-6	4
Bu <sub>4</sub> N <sup>+</sup> • Br <sup>-</sup>	4

**Overview**

Steps/Stages	Notes
1.1 R:O <sub>2</sub> , C:56396-12-4, S:CH <sub>2</sub> Cl <sub>2</sub> , S:MeCN, 72 h, rt	under visible light; Fluorescent Circular lamp used, photochemical, Reactants: 1, Reagents: 1, Catalysts: 1, Solvents: 2, Steps: 1, Stages: 1, Most stages in any one step: 1
	<b>References</b>
	A new and efficient aerobic oxidation of aldehydes to carboxylic acids with singlet oxygen in the presence of porphyrin sensitizers and visible light By Hajimohammadi, Mahdi et al From Tetrahedron Letters, 51(31), 4061-4065; 2010 <input type="checkbox"/> Full Text

# 反应结果分析



催化剂分析，用于找到经济型催化剂  
 实验过程分析，用于找到有实验过程描述的反应

## 查看实验过程

Reactions Get References Combine Answer Sets

6 Reactions 0 Selected Keep Selected Remove Selected Save Print Export

Select All Deselect All Sort by: Relevance (New) ↓ Answers per Page [15]

Display:

1. View Reaction Detail Link Similar Reactions  
Single Step *Hover over any structure for more options.*

► Overview

► Experimental Procedure **NEW**

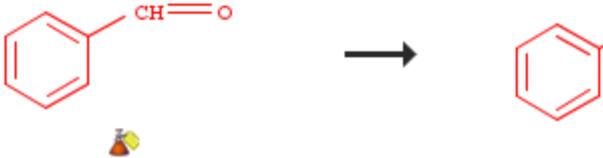
Experimental Procedure **NEW**

**JOC** The Journal of Organic Chemistry

General/Typical Procedure: Procedure A: Standard procedure for the oxidation of primary alcohols and aldehydes. A 500 mL flask was charged with NiCl<sub>2</sub> hexahydrate (0.27 g, 1.14 mmol) and water (5 mL) and allowed to dissolve. A primary alcohol or an aldehyde (45 mmol) was added followed by dichloromethane (15 mL). The reaction was cooled in an ice bath after reaching homogeneity and cold bleach (300 mL) was added in a steady stream over 5 minutes. Afine black precipitate formed immediately. The resulting slurry was stirred for 2 hours at 0°C and 2 hours at room temperature. The slurry was then acidified with 2 M hydrochloric acid until the aqueous layer was strongly acidic by pH paper. The aqueous layer was extracted with diethyl ether (3 x 100 mL). The combined organic extracts were dried over anhydrous MgSO<sub>4</sub> and filtered. Removal of the solvent by rotary evaporation and brief high vacuum gave the crude product. The purities could generally be improved to greater than 98% by distillation of the crude product or by recrystallization in the case of solids. Benzoic acid, yield 5.28 g, 96%. <sup>1</sup>H NMR(CDCl<sub>3</sub>): δ 7.49 (t, <sup>3</sup>J<sub>HH</sub> = 7.4 Hz, 2H), 7.63 (t, <sup>3</sup>J<sub>HH</sub> = 7.4 Hz, 1H), 8.14 (d, <sup>3</sup>J<sub>HH</sub> = 7.4 Hz, 2H), 12.02 (broad, 1H). <sup>13</sup>C NMR (CDCl<sub>3</sub>): δ 128.8, 129.5, 130.5, 134.1, 172.9. MS (ESI) m/z = 121 [M-H]<sup>-</sup>. CAS# [65-85-0].

# 获得反应中心相似的反应

1. **1 Hits in this Reference** **Similar Reactions**  
 Single Step *Hover over any structure for more options.*



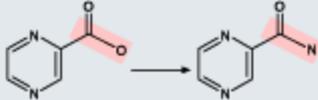
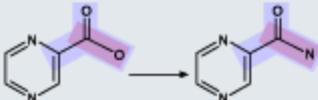
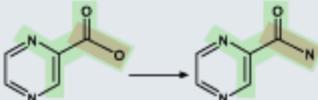
Overview

Get Similar Reactions ⓘ

Retrieve similar reactions from:

- All reactions
- Current answer set

Include this level of similarity:

- Broad - Reaction centers only (8045)
 
- Medium - Reaction centers plus adjacent atoms and bonds (3522)
 
- Narrow - Reaction centers plus extended atoms and bonds (2911)
 

Get Reactions Cancel

相似反应检索，依据和反应中心的相似程度，查询反应中心彼此相似的反应。

# 选择相似级别

Get Similar Reactions

Retrieve similar reactions from:

All reactions

Current answer set

Include this level of similarity:

Broad - Reaction centers only (8045)

Medium - Reaction centers plus adjacent atoms and bonds (3522)

Narrow - Reaction centers plus extended atoms and bonds (2911)

Get Reactions Cancel

对于选择是全部反应中检索相似反应，还是在当前结果集中检索相似反应

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

Reactions Get References Combine Answer Sets

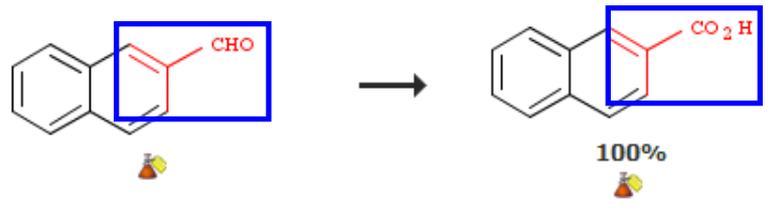
2911 Reactions 0 Selected Keep Selected Remove Selected Save Print Export

Select All Deselect All Sort by: Similarity Answers per Page [15] 1 2 3 4 5 6 ... 195

Display: [Icons]

1. View Reaction Detail Link Similar Reactions

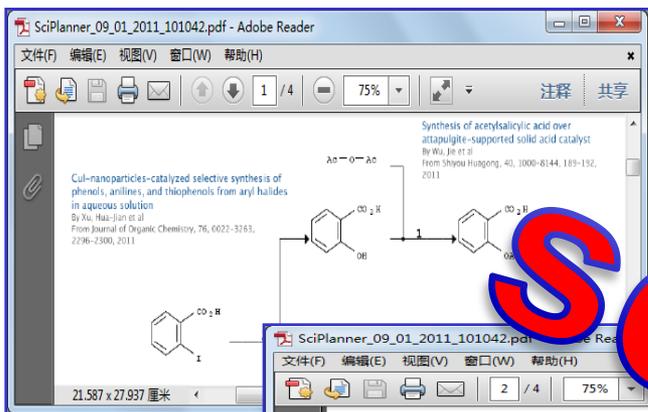
Single Step Hover over any structure for more options.



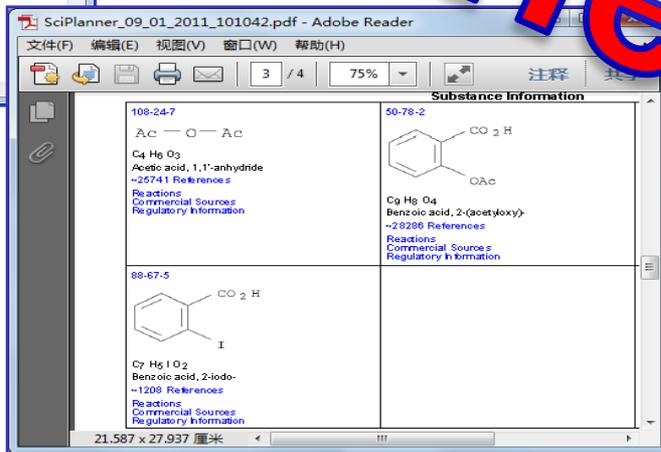
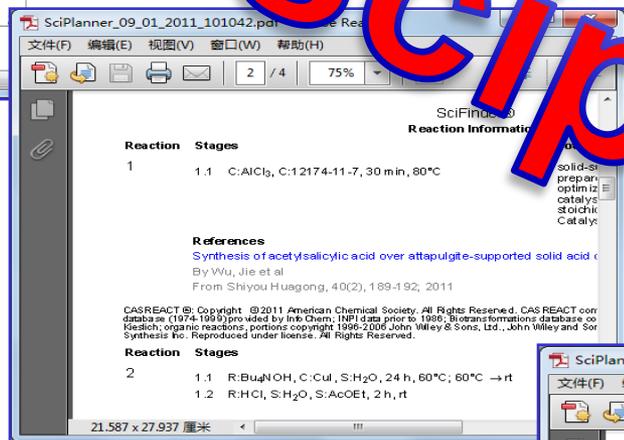
100%

Overview

# 如何加工整合得到一份完整的合成路线报告？

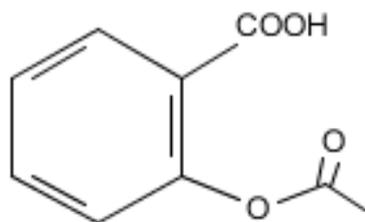


合成路线



中间体物质信息

# 阿司匹林的合成路线报告



阿司匹林

The screenshot shows the Reaction Editor interface. The main workspace displays the chemical structure of Aspirin with an arrow pointing to it from the left, indicating it is the product. A red box highlights the reaction arrow icon in the left-hand toolbar, with the text "定义为产物" (Defined as product) next to it. On the right side, the Drawing Editor panel is visible, with the "Reaction" radio button selected. Below it, the "Get reactions where the structure (s) are:" section has the "only at the specified positions" radio button selected, also highlighted with a red box. The bottom status bar shows the chemical formula "C<sub>9</sub>H<sub>8</sub>O<sub>4</sub> (reaction query)" and the molecular weight "180.16".

# SciPlanner—检索结果的智能编辑器

Reactions Get References Tools **Send to SciPlanner**

68 Reactions 1 Selected Save Print Export

1 Reaction sent to SciPlanner.

Select All Deselect All Sort by: Relevance Answers per Page [15] 1 2 3 4 5

Display:

1. [View Reaction Detail](#) [Link](#) [Similar Reactions](#)  
**Single Step** *Hover over any structure for more options.*

O=C(O)c1ccccc1.CC(=O)OC(=O)C>>CC(=O)Oc1ccccc1C(=O)O
  
 93%

- 勾选感兴趣的反应
- 点击**Send to SciPlanner**
- 可以看到有1条反应推送到**SciPlanner**

# SciPlanner—主面板

The screenshot displays the SciPlanner software interface. The title bar shows 'SciPlanner' and the file name 'SciPlanner\_08\_23\_2011\_171005'. The menu bar includes 'Workspace', 'Edit', 'View', and 'GoTo'. A toolbar on the left contains several icons, with the 'New' icon (a plus sign) highlighted by a red box. In the center of the workspace, the text '•创建一个新的SciPlanner文件' (Create a new SciPlanner file) is displayed. A 'New' dialog box is open, with the title field containing 'SciPlanner\_08\_23\_2011\_171005'. A red arrow points from the 'New' icon in the toolbar to the dialog box. On the right side, a 'Clear Reactions' panel is visible, showing a chemical reaction scheme with a red box around it. The reaction scheme depicts the conversion of a substituted benzene ring with a carboxylic acid group and an acetate group to a similar structure with a different substitution pattern.

•创建一个新的SciPlanner文件

New ⓘ

Title:  
SciPlanner\_08\_23\_2011\_171005

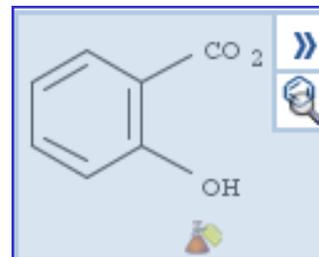
OK Cancel

Clear Reactions

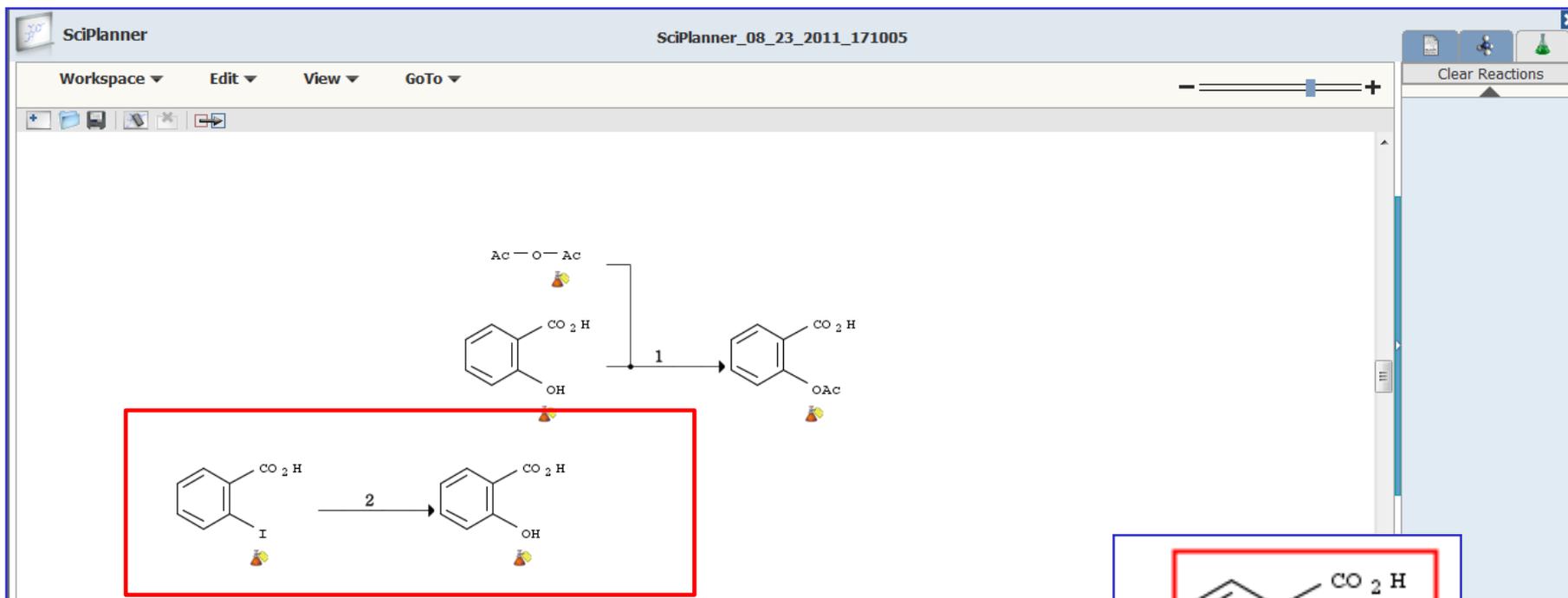
75

# SciPlanner—拖入反应，并尝试中间体的合成检索

- 将右侧的反应，拖入**SciPlanner**中
- 如对其中一个物质的合成很感兴趣，可以直接点击，使用物质标准菜单，获得它的合成方法

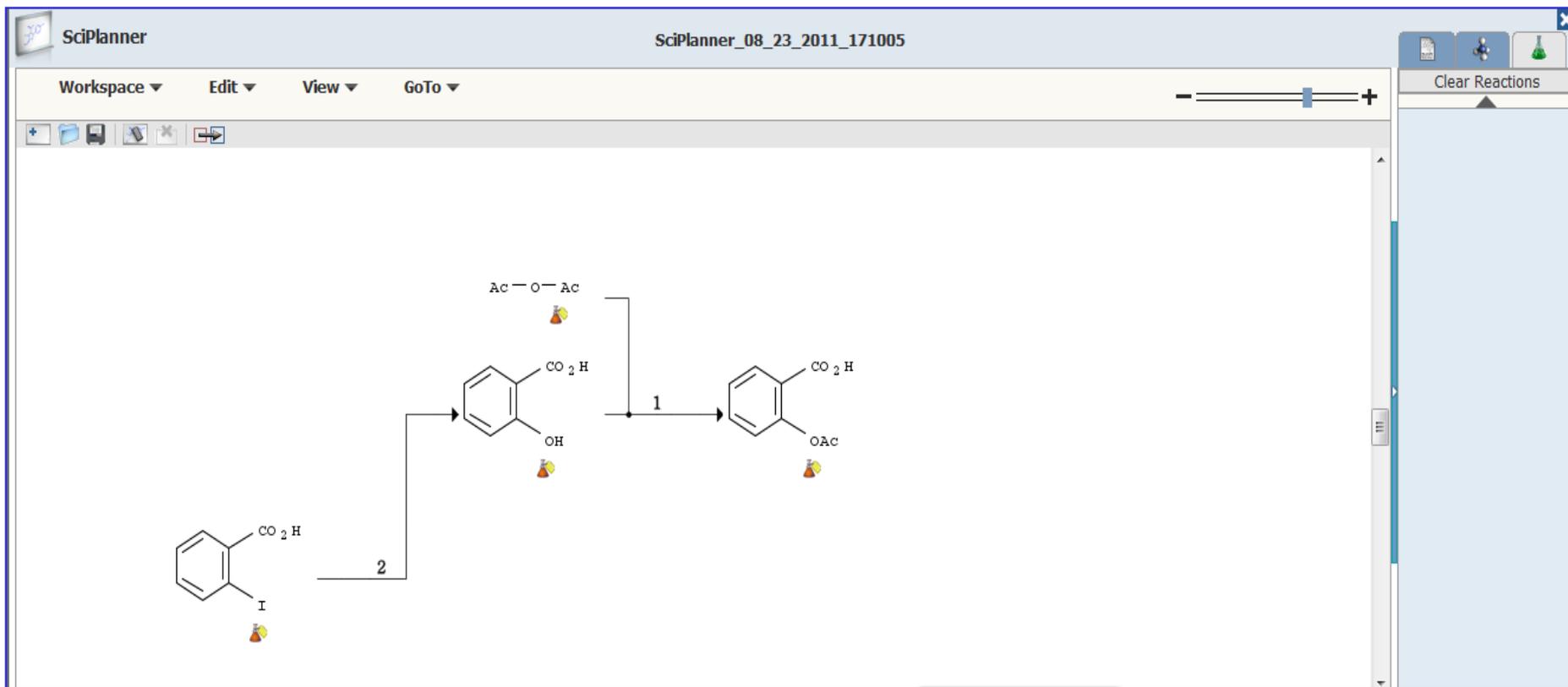


# SciPlanner—将中间体的合成路线添加至SciPlanner

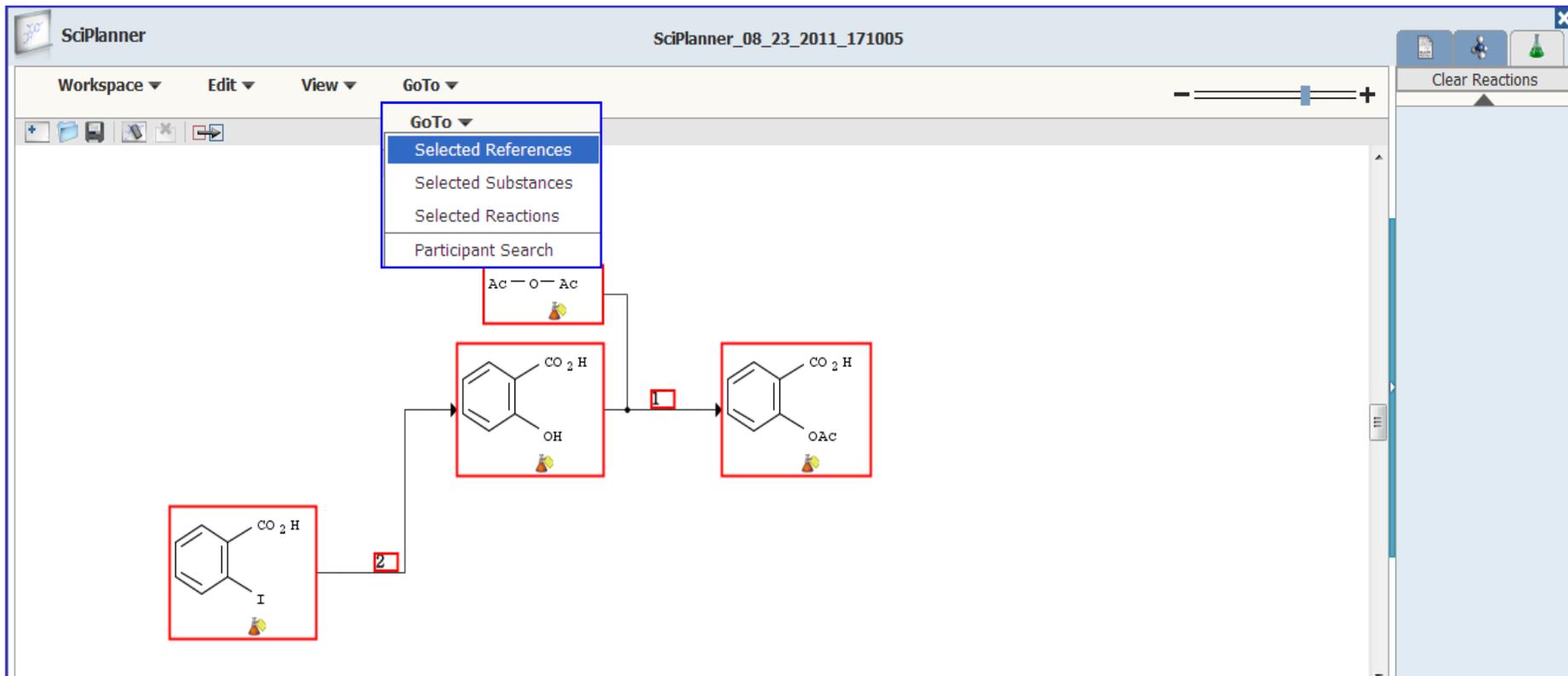


- 类似上述的步骤，将中间体的反应拖至**SciPlanner**中
- 可以看到这两条反应的产物和反应物是同样的
- 用鼠标将这两个结构拖至重贴状态

## 编辑为完整的反应路线



# SciPlanner—获得反应对应的文献



- 框选所有的反应，所有的结构都显示为红色
- 点击上面的**Goto**，选择**Selected References**

# SciPlanner—反应对应的文献

References Get Substances Get Reactions Get Related Tools **NEW** Send to SciPlanner

2 References 2 Selected Save Print Export

2 References sent to SciPlanner.

Select All Deselect All Sort by: Accession Number ↓

Answers per Page [20] Display:

1. **Synthesis of acetylsalicylic acid over attapulgite-supported solid acid catalyst**  
 by Wu, Jie; Jiang, Jinlong; Qian, Xiaomin  
 from *Shiyou Huagong* (2011), 40(2), 189-192. Language: Chinese, Database: CAPLUS  
 Attapulgite (ATP)-supported H<sup>+</sup> and AlCl<sub>3</sub> solid acid catalysts (H<sup>+</sup>/ATP and AlCl<sub>3</sub>/ATP) were sep. prepd. and their catalytic activities for synthesis of acetylsalicylic acid (I) from salicylic acid (II) and acetic anhydride (III) were compared with the free acids. The solid acid catalysts exhibited higher activity than those of the free acids, esp. AlCl<sub>3</sub>/ATP catalyst. The yield and the purity of I reached 92.5% and 99.5% resp., at AlCl<sub>3</sub>/ATP content of 5% (based on II), III/II of 2.0 mol, and 80° for 30. The synthesized I was characterized by means of FTIR and <sup>1</sup>H NMR. The I yield reached 89.2%...  
 Substances Reactions ~0 Citings Full Text Link 0 Comments 0 Tags

2. **CuI-nanoparticles-catalyzed selective synthesis of phenols, anilines, and thiophenols from aryl halides in aqueous solution**  
 by Xu, Hua-Jian; Liang, Yu-Feng; Cai, Zhen-Ya; Qi, Hong-Xia; Yang, Chun-Yan; Feng, Yi-Si  
 from *Journal of Organic Chemistry* (2011), 76(7), 2296-2300. Language: English, Database: CAPLUS  
 CuI-nanoparticles-catalyzed selective synthesis of phenols, anilines, and thiophenols from aryl halides was developed in the absence of both ligands and org. solvents. Anilines were formed selectively with ammonia competing with hydroxylation and thiophenols were generated selectively with sulfur powder after subsequent redn. competing with hydroxylation and amination.  
 Substances Reactions ~1 Citing Full Text Link 0 Comments 0 Tags

- 勾选文献
- Send to SciPlanner
- 2篇文献推送到SciPlanner中

# SciPlanner—自由组合文献和反应的排列

The screenshot displays the SciPlanner software interface. The main workspace shows a chemical reaction scheme for the synthesis of acetylsalicylic acid. The reaction involves the conversion of salicylic acid (2-hydroxybenzoic acid) to acetylsalicylic acid (aspirin) using acetic anhydride. The reaction is labeled with '1' and '2'. The workspace also contains a menu bar with 'Workspace', 'Edit', 'View', and 'GoTo' options. A 'Workspace' dropdown menu is open, showing options: 'New', 'Open', 'Save', 'Duplicate', 'Export', 'Print', and 'Close'. The 'Export' option is highlighted. An 'Export' dialog box is overlaid on the workspace, showing the following options:

- For:**
  - Offline review
  - Image (\*.png)
  - Citations (\*.ris)
  - Portable Document Format (\*.pdf)
- Details:**
  - File Name:** \* (Required) SciPlanner\_08\_23\_2011\_172215
  - Title:** (Empty field)
- Include:**
  - SciPlanner Image
  - Reaction Details
  - Substance Details
  - Reference Details

Buttons for 'Export' and 'Cancel' are visible at the bottom of the dialog box.

获得结果后，点击WorkPlace下的  
**Export**，将结果输出成PDF格式



获得完整的报告

## 提纲

- 介绍
  - SciFinder 中的内容
  - SciFinder 的注册和登陆
- **SciFinder 中的检索和后处理**
  - SciFinder 中的文献检索
  - SciFinder 中的物质检索
  - SciFinder 中的Markush检索
  - SciFinder 中的反应检索
- **SciFinder 特色功能**
- **SciFinder网络资源平台**

# SciFinder特色功能—KMP定题查询

设定Email提醒，一旦有新的记录，会发邮件通知

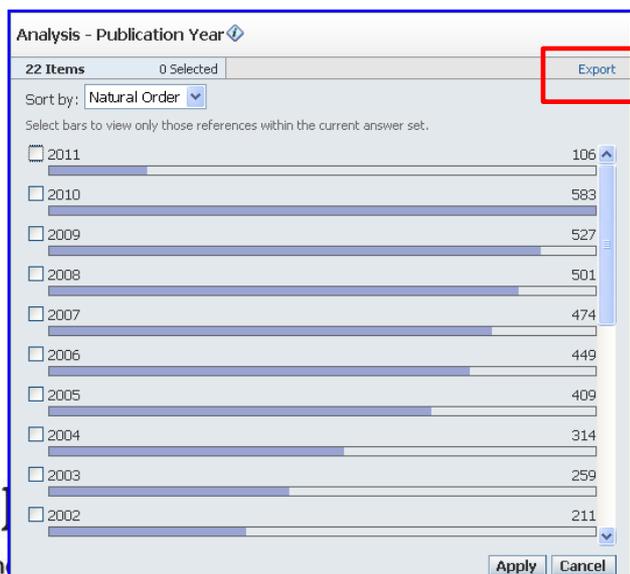
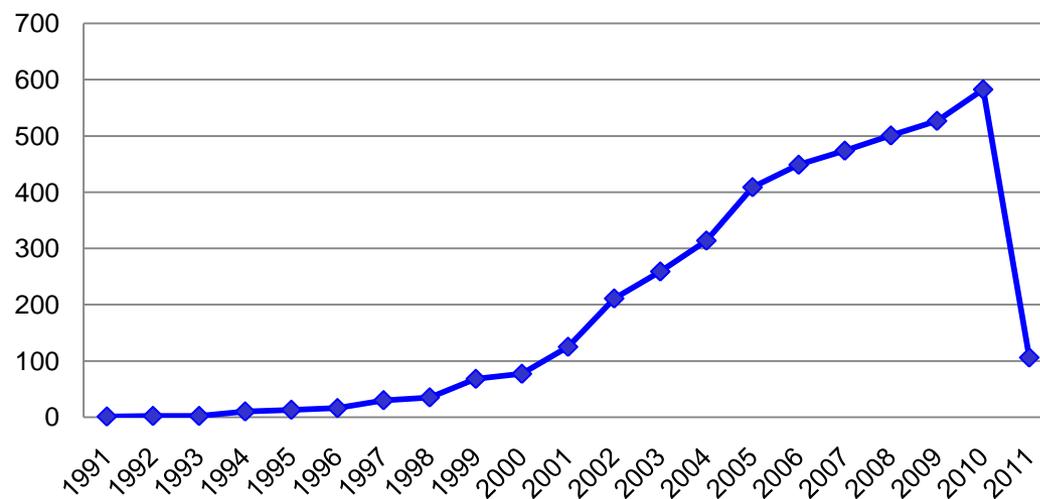
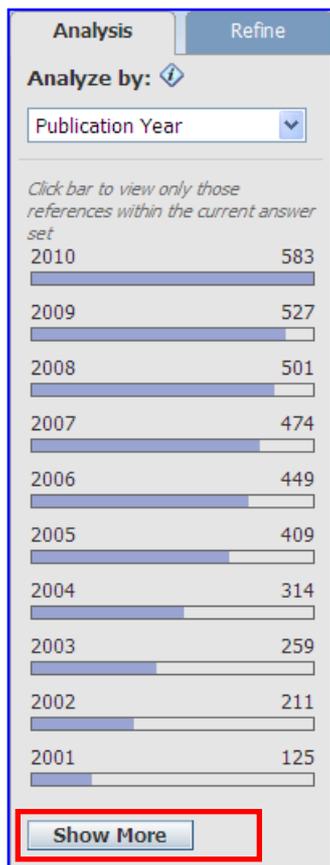
The screenshot displays the SciFinder interface for a search on "catalyst for suzuki reaction". The search results show 291 references, with the first three listed. A red box highlights the "Create Keep Me Posted" button in the top left. A modal window titled "Create Keep Me Posted Profile" is open, showing the following details:

- Title:** petroleum cracking
- Description:** (empty field)
- Duration:** Expires On: Mar 17, 2012
- Frequency:** Send updates once every **Week**
- Search Strategy:**
  - Explore references by research topic: petroleum cracking with catalyst
  - Reference refine by company name: china

A text box on the right side of the modal window contains the text: "设置提醒文件名和失效时间".

# SciFinder特色功能—分析结果的导出

## 年文献量



年文献量趋势图，帮助了解课题在全球范围内的研究状态。

## SciFinder 特色功能—物质标准菜单



在**SciFinder**中，鼠标滑过物质，可以打开物质的标准菜单，通过标准菜单，可以获得和物质有关的所有内容

# SciFinder特色功能---Markush检索

Welcome Sam Yu | Sign Out  
Create Keep Me Posted Opened saved answer set "RCM-1816ref" (1816)

Explore Substances

Chemical Structure **Markush**

Markush

Molecular Formula  
Substance Identifier

Search

Click image to change structure or view detail

Search type:  Allow  Subs

直接检索和结构有关的专利，用于做初步的专利评估

Welcome Sam Yu | Sign Out  
Create Keep Me Posted Markush substructure > references (1503)

References  Get Substances  Get Reactions  Get Related  Tools  Send to SciPlanner

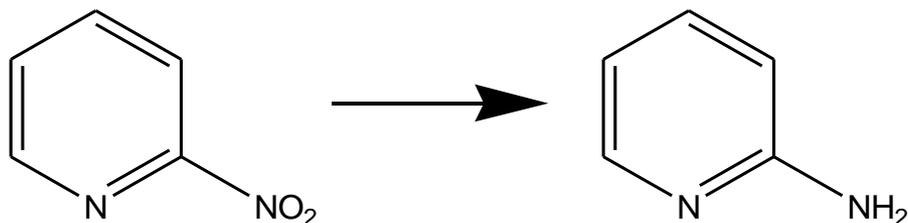
1503 References 0 Selected Save Print Export

Select All Deselect All Sort by: Accession Number Answers per Page [20] 1 2 3 4 5 6 ... 76 Display: [ ] [ ] [ ]

1. **Preparation of pyridinylpyrrole derivatives as tyrosine kinase modulators**  
By Guo, Xialing; Zhu, Zhen  
From U.S. Pat. Appl. Publ. (2011), US 20110053905 A1 20110303. Language: English, Database: CAPLUS  
Title compds. I [X = NR1, O, and S(O)n; n = 0-2; R1 = H, alkenyl, alkoxyalkyl, etc.; RI = H, halo, alkyl, etc.; m = 0-3; RII = H, alkoxy, alkoxyalkoxy, etc.; n = 0-2; Y = O, NH, CO, etc.; ring A = Ph, naphthyl, 5- to 6-membered monocyclic heteroaryl, etc.; RIII = alkyl, haloalkyl, alkoxy, etc.; Z = C(O)NH, NHS(O)2, S(O)2NHCH2, etc.; ring B = Ph, naphthyl, 5- to 6-membered monocyclic heteroaryl, etc.; RIV = alkoxy, alkoxyalkyl, alkoxy-carbonyl, etc.], and their pharmaceutically acceptable salts or prodrugs, are prepd. and disclosed. Thus, e.g., II was prepd. by amidation of 3-methyl-2-furoic ac...  
[Substances](#) [Reactions](#) [Citations](#) [Full Text](#) [Link](#) [Comments](#) [Tags](#)

2. **HIV integrase inhibitors**  
By Wai, John S.; Su, Dai-Shi; Wiscount, Catherine M.  
From PCT Int. Appl. (2011), WO 2011025683 A1 20110303. Language: English, Database: CAPLUS  
4-Pyridinone and 4-pyranone compds. of Formula I (X = O or N(R3); Y = CH(R4) or CH(R4)CH(R4); R1 is substituted alkyl; R2 = H, C1-6 alkyl, etc.; R3 = H, C1-6 alkyl, etc.; R4 = H or C1-6 alkyl) are inhibitors of HIV integrase and inhibitors of HIV replication. The compds. are useful for the prophylaxis or treatment of infection by HIV and the prophylaxis, treatment, or delay in the onset or progression of AIDS. The compds. are employed against HIV infection and AIDS as compds. per se (or as hydrates or solvates thereof) or in the form of pharmaceutically acceptable salts. The compds. and the...  
[Substances](#) [Reactions](#) [Citations](#) [Full Text](#) [Link](#) [Comments](#) [Tags](#)

## SciFinder 特色功能—反应关联度排序



4. **5 Hits in this Reference** **Single Step** *Hover over any structure for more options.*

Sort by: **Relevance (New)**

- Relevance (New)
- Accession Number
- Experimental Procedure
- Number of Steps
- Product Yield
- Publication Year

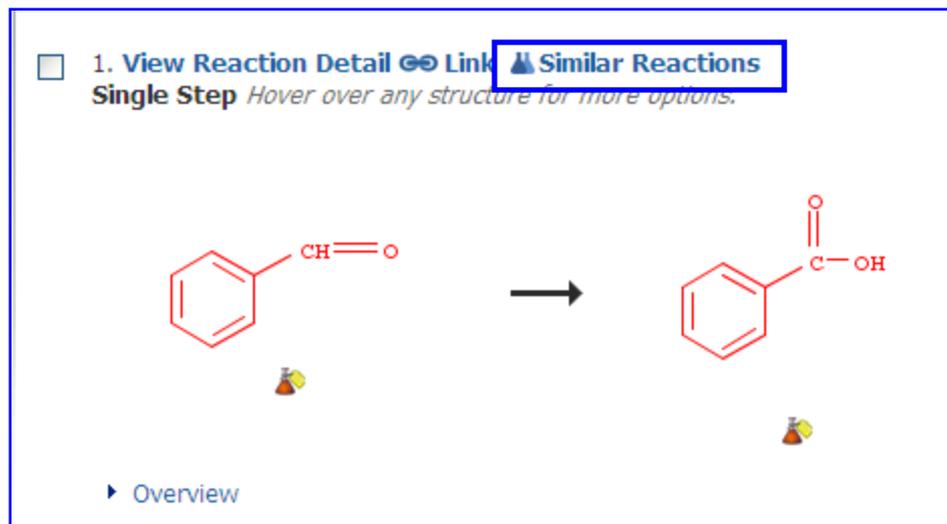
95%

提供按照关联度排序，在亚结构检索反应时，可以将和所画结构最相近的反应，排在前面

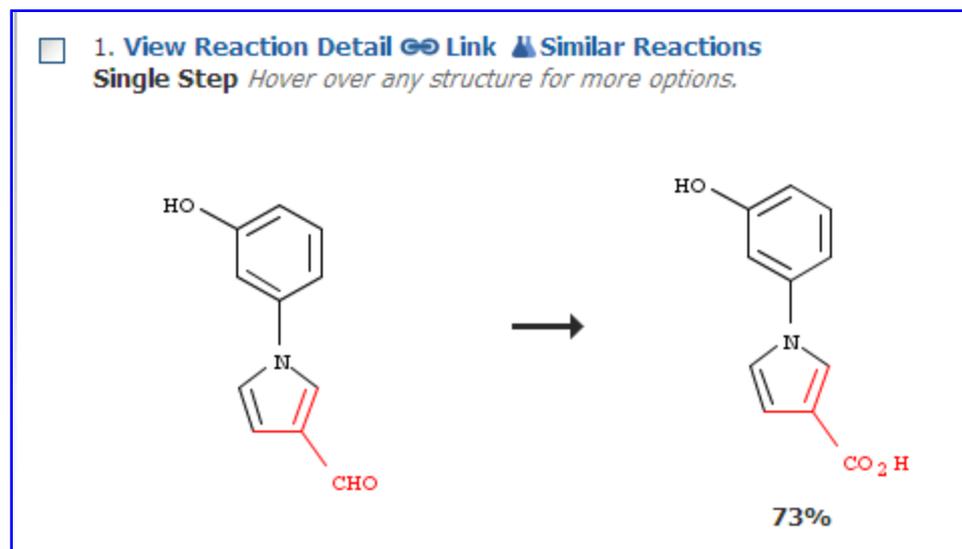
1. **1 Hits in this Reference** **Similar Reactions** **Single Step** *Hover over any structure for more options.*

95%

# SciFinder特色功能—相似反应检索

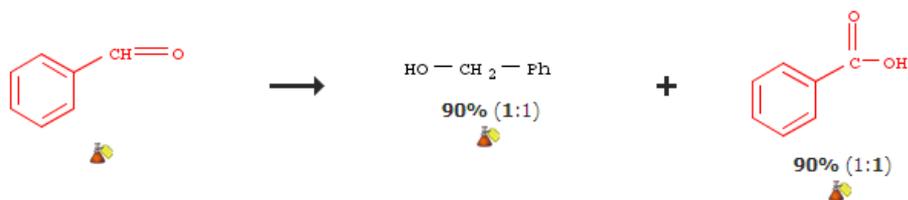


相似反应检索，依据相似级别的设定，帮助获取反应中心相同的反应



# SciFinder特色功能—反应过程的获取

1. View Reaction Detail [Link](#) [Similar Reactions](#)  
**Single Step** Hover over any structure for more options.



► Overview

► Experimental Procedure **NEW**

SciFinder中的部分源自期刊和专利中的反应，提供了反应过程信息，使得科研工作者不需要阅读原文，就可以获得对应的反应历程。

▼ Experimental Procedure **NEW**

*Organic*  
**LETTERS**

a ) LiBr catalyzed Cannizzaro reactions a ) LiBr catalyzed Cannizzaro reactions a ) LiBr catalyzed Cannizzaro reactions A mixture of LiBr (2 mmol), the aldehyde (4 mmol), and triethylamine (6 mmol) was stirred for 2 days at room temperature under inert atmosphere until complete consumption of the aldehyde was observed. Progress of the reaction was monitored by TLC and GC analyses. Then the mixture was stirred with excess H<sub>2</sub>O for 2 hours and subsequently was extracted by ether. The volatile portion of the organic phase was evaporated after being dried over Na<sub>2</sub>SO<sub>4</sub>. Analysis of the residue by <sup>1</sup>H NMR and GC-MS showed the formation of the corresponding alcohol and carboxylic acid in equal amounts. The alcohol portion was separated by bulb to bulb distillation or by basic separation of the acid portion.

# SciFinder特色功能—反应溶剂，不反应官能团设定

Reaction Structure

Click image to change structure or view detail

Search type:  Allow variability only as specified  
 Substructure

Solvent(s) **Select Solvents**

Non-participating Functional Group(s) **Select Groups**

Close

View: All 217

0 Selected Clear Selections

- Acetal
- Acetyl
- Acid Halide
- Acyclic Alkene
- Acyclic Ketone
- Acylmetal
- ALCOHOLS
- Aldehyde
- pi-Alkene
- ALKENES
- Alkyl Halide

Reactions must have  all selections  
 any selection

Close

Solvent Hierarchy  
 [View Solvent List]

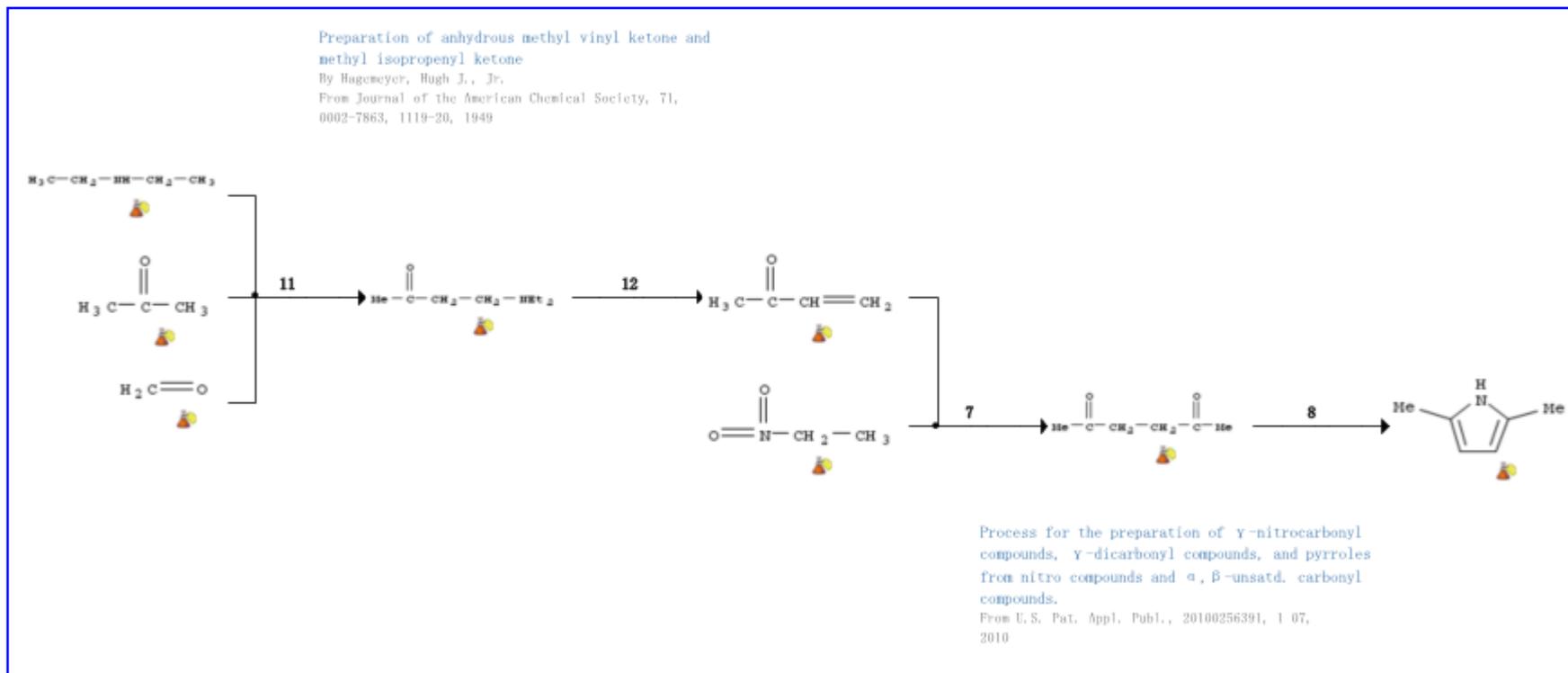
0 Selected Select All Deselect All

- Inorganic solvents
  - Ammonia
  - Ammonia-15N
  - Ammonia-d3
  - Water
  - Water-17O
  - Water-18O
  - Water-d
  - Water-d2
  - Water-d2-18O
  - Water-t
  - Water-t2

Find:  Next Previous

定义反应中的溶剂  
 定义反应中不参与反应的官能团

# SciFinder特色功能—SciPlanner



# 提纲

- 介绍
  - SciFinder 中的内容
  - SciFinder 的注册和登陆
- **SciFinder 中的检索和后处理**
  - SciFinder 中的文献检索
  - SciFinder 中的物质检索
  - SciFinder 中的Markush检索
  - SciFinder 中的反应检索
- **SciFinder 特色功能**
- **SciFinder网络资源平台**

# 网络在线资源平台

[www.igroup.com.cn/cas](http://www.igroup.com.cn/cas)



CAS 资源下载

- SciFinder Web 入门指南
- SciFinder Web 用户指南
- SciFinder 案例演示
- SciFinder 客户端用户指南
- 生物材料案例研究 **NEW**

资源下载: **PDF文件**

在线演示: **Flash演示**

网络培训: 不定期的网络专题培训

## Flash演示

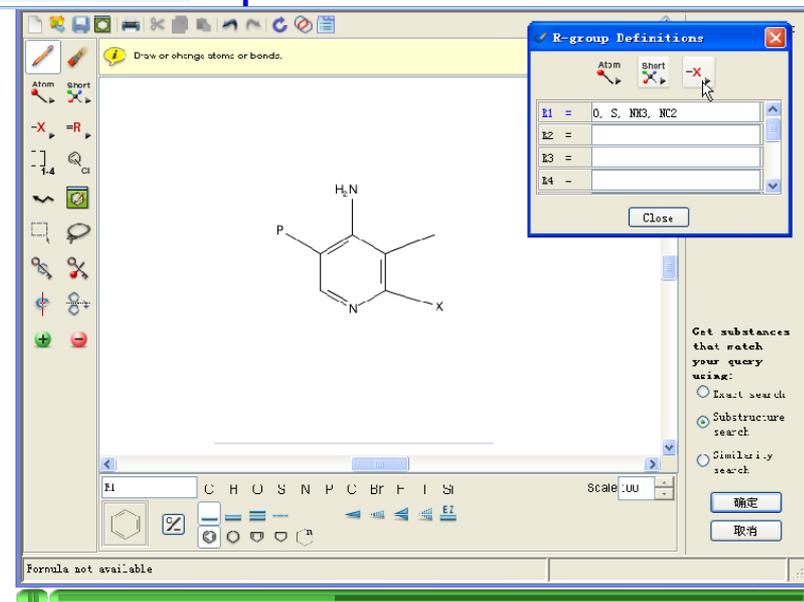


在线视频演示

SciFinder现在有2个版本，Client版和Web版，请根据你具体的情况，选择相应的版本点击观看。

Web版本	主题	人气
文献检索	Web版主题检索	756
文献检索	Web版作者名检索	
文献检索	Web版机构名检索	
结构物质检索	Web版结构检索	
结构物质检索	Web版结构绘制工具	
结构物质检索	Web版具体物质检索	
结构物质检索	Web版分子式检索	
反应检索	Web版反应检索	
反应检索	Web版反应设计	
反应检索	Web版反应工具	

在线演示，录制了不同检索类型下的检索步骤，帮助了解更加细节的内容。



Draw or change atoms or bonds.

Atom Short -X

K-group Definitions

E1 = O, S, NH3, NC2

E2 =

E3 =

E4 =

Close

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