

**SciFinder Web**

**源于化学，超越化学**

## **SciFinder Web使用介绍**

**----上海工程技术大学**

**SciFinder产品专员 朱传娴**

**2013.11.**

# 提 纲

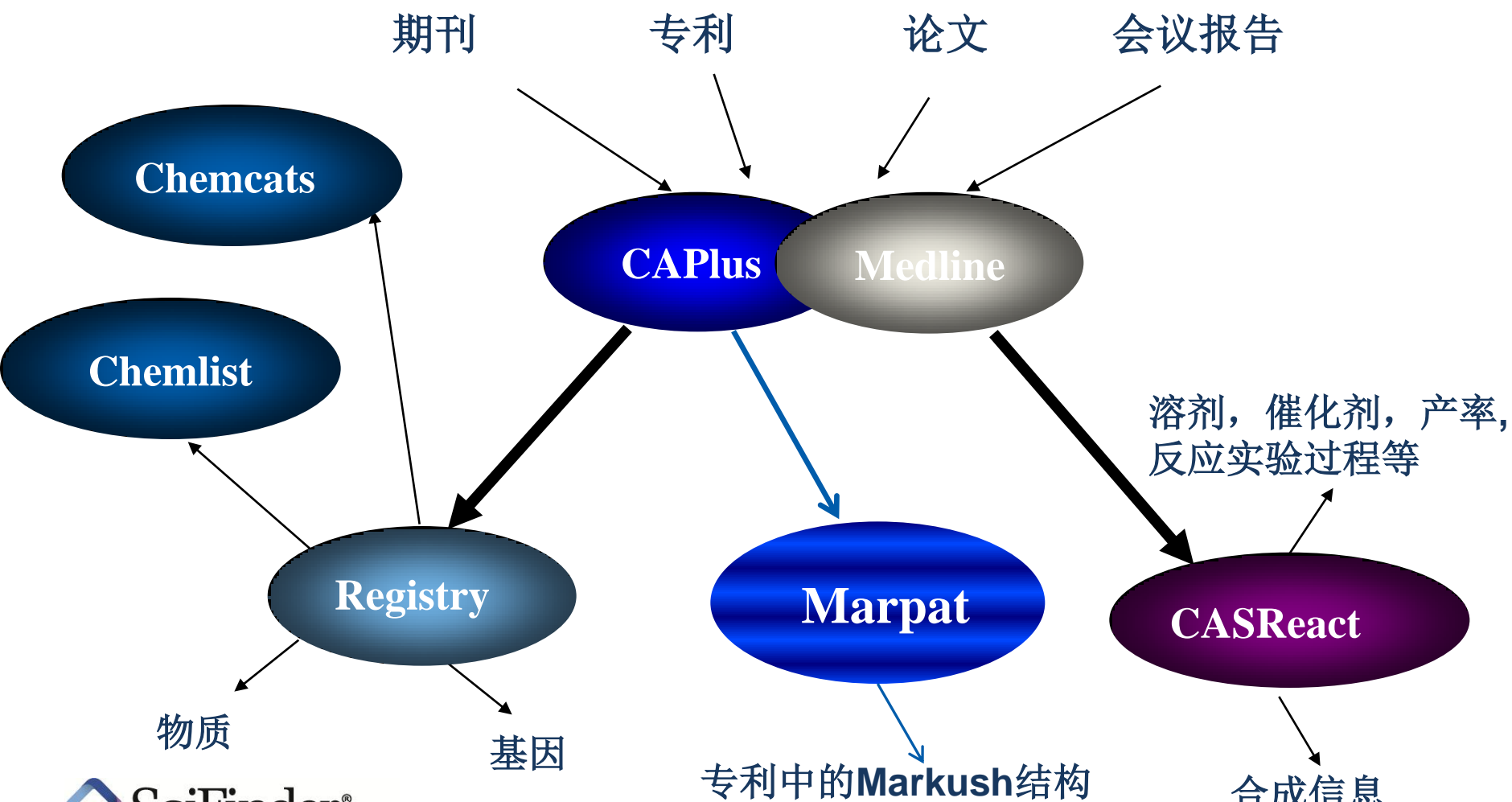
- 介绍
  - SciFinder Web中的内容
  - SciFinder Web的注册和登陆
- **SciFinder Web中的检索和后处理**
  - SciFinder Web中的文献检索
  - SciFinder Web中的物质检索
  - SciFinder Web中的Markush检索
  - SciFinder Web中的反应检索
- **SciFinder Web使用常见问题和网络资源**

# 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 Web中的内容



# SciFinder Web中的内容

## CAS REGISTRY<sup>SM</sup>

>7300万有机无机物质

>6400生物序列

每天更新约12000新物质

物质报道文献，回溯到1802年

物质信息包含了大量的实验数据，预测数据，以及物质标签和谱图

## CASREACT<sup>®</sup>

>5350万单步和多步反应

>1360万物质合成制备信息

源自专利和期刊文献

每首更新3-5万条单步多步反应

反应回溯到1840年

## CAS Databases

## CAplus<sup>SM</sup>

>3700万专利和期刊信息

>10000种期刊的覆盖

63个专利发行机构

每天更新3000条记录

文献回溯到19世纪初

引文信息回溯到1997年之前，超过3亿条引文信息

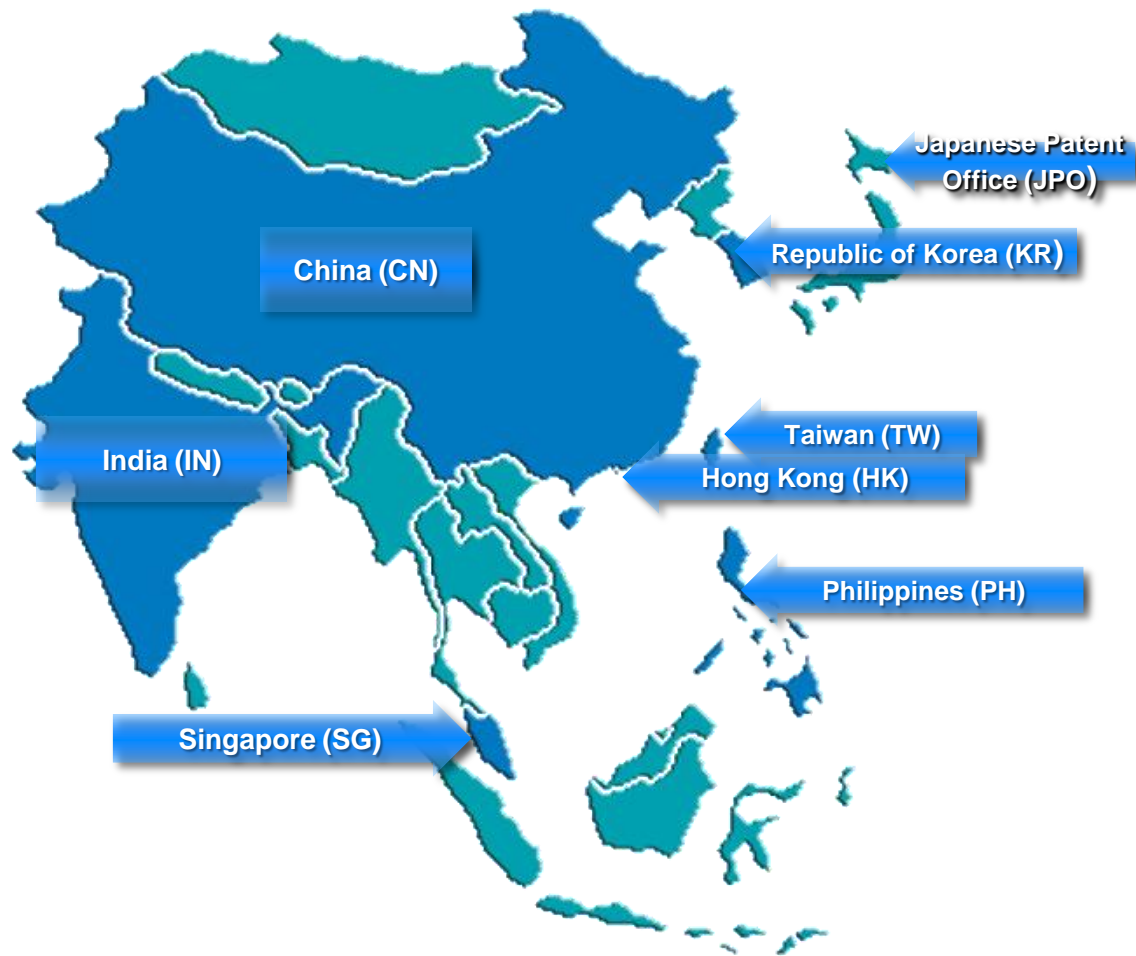
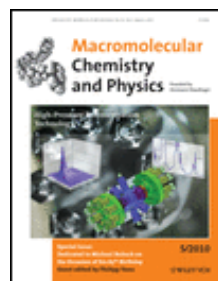
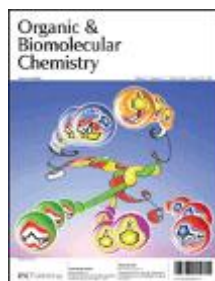
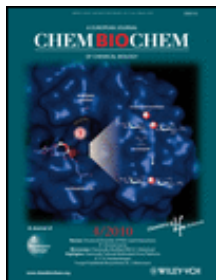
## CHEMCATS<sup>®</sup>

>6800万条商业购买信息

>1,098 供应商

>1,222 化学产品目录

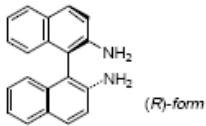
# CAplus<sup>SM</sup> + Medline 涵盖上万种期刊及63个专利发行机构专利





# CAS REGISTRY<sup>SM</sup> 是化学物质信息的“黄金标准”

Entry name → **2,2'-Diamino-1,1'-binaphthyl**

Structural formula and stereochemical description →  (R)-form

Alternative names → [1,1'-Binaphthalene]-2,2'-diamine, 9CI, 2,2'-Diamino-1,1'-dinaphthyl, 1,1'-Bi[2-naphthylamine]

CAS Registry Number → **FNCT6-Y [4488-22-6]**

Molecular Formula → **C<sub>20</sub>H<sub>16</sub>N<sub>2</sub>** Molecular weight → **M 284.360** RTECS® Number → **Intermediate for chiral auxiliaries.**

Use → **Exp. tumourigen by skin contact. Dec. with emission of toxic fumes. DU3090000**

Hazard alert symbol and description of hazards → (R)-form: FNCT6-A [18741-55-0] Mp 242.5-243°, [α]<sub>D</sub><sup>25</sup> + 155.5° (c. 1 in Py), [α]<sub>D</sub><sup>25</sup> + 46.8° (2M HCl). Supplier: Aldrich 38242-6; Fluka 32787. N,N-Di-Me: MNMCH-A [93713-30-5] Cryst. (EtOH). Mp 143-144° [α]<sub>D</sub><sup>25</sup> + 182° (c. 1.09 in C<sub>6</sub>H<sub>6</sub>). N,N,N',N'-Tetra-Me: MNMCH-A [135029-77-5] Cryst. (EtOH/C<sub>6</sub>H<sub>6</sub>). Mp 216-218°.

Supplier information → (S)-form: FNCT6-A [18531-95-8] Cryst. Mp 243° (235-239°), [α]<sub>D</sub><sup>25</sup> - 149° (Py), [α]<sub>D</sub><sup>25</sup> - 46° (2M HCl). Supplier: Aldrich 38243-4; Fluka 32788.

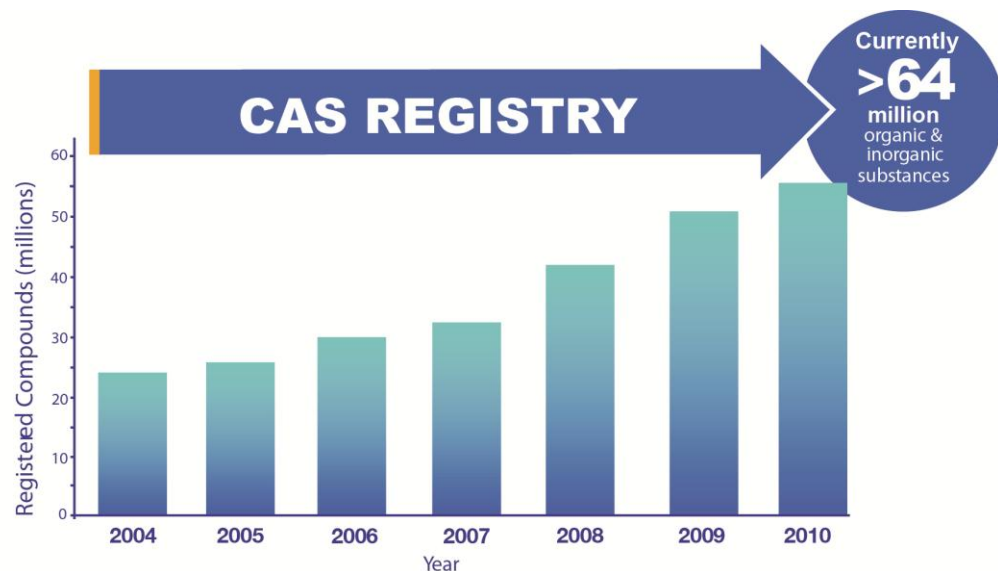
Stereoisomer heading → N,N-Di-Ac: FNCHV-Y C<sub>24</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub> M 368.434. Prisms (C<sub>6</sub>H<sub>6</sub>). Mp 226-227°. [α]<sub>D</sub><sup>25</sup> + 10.8° (c. 1 in THF). (±)-form: FNCHV-W [79082-81-8] Silvery plates (EtOH). Mp 193.2-194.5° (191°). Picrate: FNCHV-Z Brownish-yellow plates (C<sub>6</sub>H<sub>6</sub>). Mp 185° (dec.). N,N-Di-Ac: FNCHV-X Cubes (EtOH). Mp 235-236°. N,N-Dibenzoyl: FNCHV-Y C<sub>28</sub>H<sub>20</sub>N<sub>2</sub>O<sub>2</sub> M 492.576. Prisms (PhNO<sub>2</sub>). Mp 235°.

Derivative Subheading → Physical data

Additional CAS Registry Numbers → [93621-61-5] [97644-73-0]

Bibliographic references → Kuhn, R. et al., *Annalen*, 1929, 470, 183 (*synth, resolu*)  
 Cumming, WM et al., *J.C.S.*, 1932, 528 (*synth*)  
 Clarno, GR et al., *J.C.S.*, 1939, 1114 (*synth*)  
 Mislow, K et al., *J.C.S.*, 1962, 84, 1455 (*rev, oral*)  
 Akimoto, H et al., *Tetrahedron*, 1971, 27, 5999 (*resolu, abs config*)  
 Miyano, S et al., *Bull. Chem. Soc. Jpn.*, 1984, 57, 2171 (*pmr, ir, deriv*)  
 Brown, KJ et al., *J.O.C.*, 1985, 50, 4345 (*synth, resolu*)  
 Benson, SC et al., *J.O.C.*, 1988, 53, 5335 (*synth, N-tetramethyl*)  
 Fieser and Fieser's *Reagents for Organic Synthesis*, Wiley, 1989, 14, 32 (*use*)  
 Franzini, L et al., *Acta Cryst. C*, 1991, 47, 1259 (*cryst struct, N-tetra-Me*)  
 Surcine, M et al., *J.O.C.*, 1992, 57, 1917 (*synth, resolu, bbb*)  
 Levin, RJ et al., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, BGB750

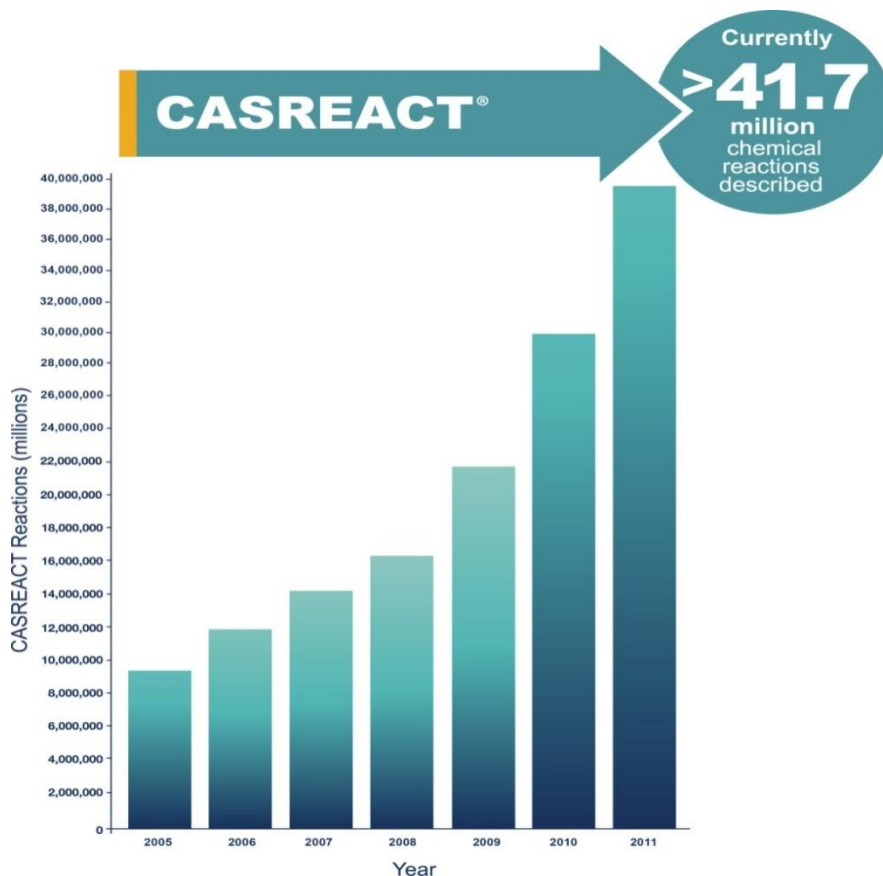
Reference contents



# CASREACT® 是检索化学反应最权威的来源

The screenshot displays the CASREACT web interface. At the top, there are navigation tabs: Reactions, Get References, Tools, and Send to SciFinder. Below this, a search bar shows '3 Reactions' and '0 Selected'. A dropdown menu for 'Sort by' is set to 'Accession Number'. The main content area shows a chemical reaction scheme for a Suzuki coupling. The reactants are a poly(5-iodo-1,2,3-triazole) chain and a phenylboronic acid derivative. The reaction is labeled '[Step 2.1]' and 'reaction products with polytriazoles'. Below the reaction scheme, there is an 'Overview' section with 'Steps/Stages' and 'Notes'. The 'Steps/Stages' section lists three steps: 1.1 C:862678-56-6, C:CuI, S:CH<sub>2</sub>Cl<sub>2</sub>, 15 min, rt; 1.2 S:CH<sub>2</sub>Cl<sub>2</sub>, 3 h, rt; 2.1 R:K<sub>2</sub>CO<sub>3</sub>, C: Pd, C: Pd(OAc)<sub>2</sub>, S:DMF, overnight, 80°C. The 'Notes' section provides additional context: '1) in-situ generated catalyst; 2) Suzuki coupling. Reactants: 2, Reagents: 1, Catalysts: 4, Solvents: 2, Steps: 2, Stages: 3, Most stages in any one step: 2'. A 'References' section at the bottom cites 'Synthesis and Postpolymerization Functionalization of Poly(5-iodo-1,2,3-triazole)s' by Schwartz, Erik et al. from Macromolecules (Washington, DC, United States), 44(12), 4735-4741; 2011.

CASREACT是世界上最大的，  
更新速度最快的反应数据库





# MARPAT®—全球专利文献中的Markush结构库

L1 ANSWER 1 OF 1 MARPAT COPYRIGHT 2007 ACS on STN

Full  
Text

AN 142:204619 MARPAT

TI Bioactive compositions for enhancement of drug comprising triazines  
IN Sahouani, Hassan; Scherrer, Robert A.; Jumaa, Mouhannad; Zarraga, Isidro  
Angelo Eleazar; Vogel, Kim M.; Vogel, Dennis E.; Zou, Wei

PA 3M Innovative Properties Company, USA

SO PCT Int. Appl., 28 pp.

CODEN: PIXXD2

DT Patent

LA English

IC ICM A61K009-00

CC 63-5 (Pharmaceuticals)

FAN.CNT 2

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2005011629	A1	20050210	WO 2004-US24515	20040729

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZH, ZW

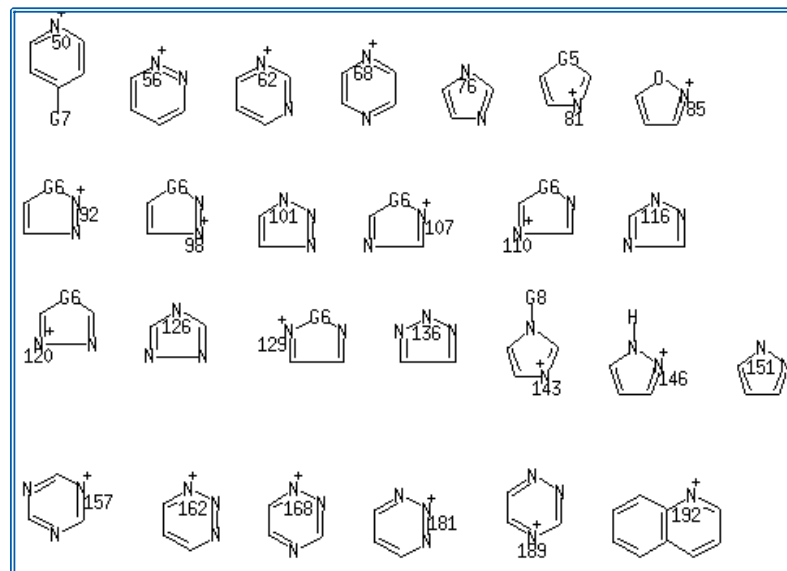
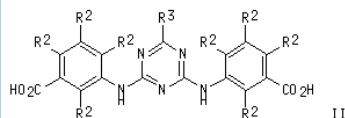
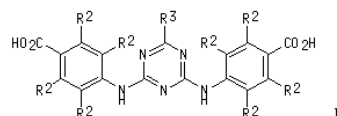
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AU 2004261243	A1	20050210	AU 2004-261243	20040729
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CA 2533128	A1	20050210	CA 2004-2533128	20040729
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EP 1651185	A1	20060503	EP 2004-779530	20040729
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⋮



MARPAT帮助最大程度的  
找到结构相关专利文献

# 提 纲

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  - SciFinder Web中的内容
  - SciFinder Web的注册和登陆
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  - SciFinder Web中的文献检索
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# SciFinder Web的注册和登陆

SciFinder Web的系统要求:

Windows用户支持IE 8.x或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, [www.java.com](http://www.java.com)）

在图书馆相关页面上找到  
SciFinder Web注册用的网址



The screenshot shows the 'SciFinder数据库使用指南' (SciFinder Database Usage Guide) page. The header is green with navigation links: 首页, 书目检索, 学科导航, 本校论文, 读者论坛, FAQ, 科技查新, 联系我们, English. The date '今天是: 2013年10月29日 星期二' is on the right. The main content area has a title 'SciFinder数据库使用指南' and a subtitle '发布时间: 2013-10-18 浏览次数: 222'. Below this is the SciFinder logo with the tagline 'The choice for chemistry research.' and an illustration of laboratory glassware. The text describes the database's history and features. At the bottom, it provides instructions on how to register and use the database, with a red box highlighting the link to the '注册指南.pdf' (Registration Guide.pdf).

SciFinder数据库使用指南

发布时间: 2013-10-18 浏览次数: 222

SciFinder®  
The choice for chemistry research.™

经过一系列的调研、试用和培训活动, 图书馆正式引进SciFinder数据库, 欢迎广大师生使用。SciFinder的前身是美国《化学文摘》(Chemical Abstracts, 简称CA)。CA是世界最大的化学文摘库, 也是目前世界上应用最广泛, 最为重要的化学、化工及相关学科的检索工具。CA创刊于1907年, 由CAS编辑出版, 被誉为“打开世界化学化工文献的钥匙”。CA的内容几乎涉及了化学家感兴趣的所有领域。随着网络技术的发展, 1995年CAS推出了SciFinder联机检索数据库。自推出以来, SciFinder一直都是全世界的科学家进行化学课题研究、成果查阅、学术期刊浏览、以及把握科技发展前沿的最得力工具。与CA相比, SciFinder具有更丰富的内容和更强大的功能。SciFinder数据库收录的文献资料来自全球200多个国家和地区的60多种语言, 包括1万 multiple 份期刊、63家专利机构的专利、评论、会议录、论文、技术报告和图书中的各种化学研究成果。SciFinder 比其他科学资源有更多的期刊和专利链接, 能够帮助您在研究过程中更有效率, 更有创意。

**数据库使用方式:** 学生及教师使用我校邮箱地址注册个人账号及密码。注册成功后, 在校园网IP范围内用个人账号和密码登录和使用化学文摘网页版。

**使用步骤:**

- 1、请点击进行账号注册, 注册流程可参考 [注册指南.pdf](#)。

# 点击URL创建SciFinder Web账号



Welcome to User Registration for SciFinder®!

Would you like to:

☒ Create a new username and password?

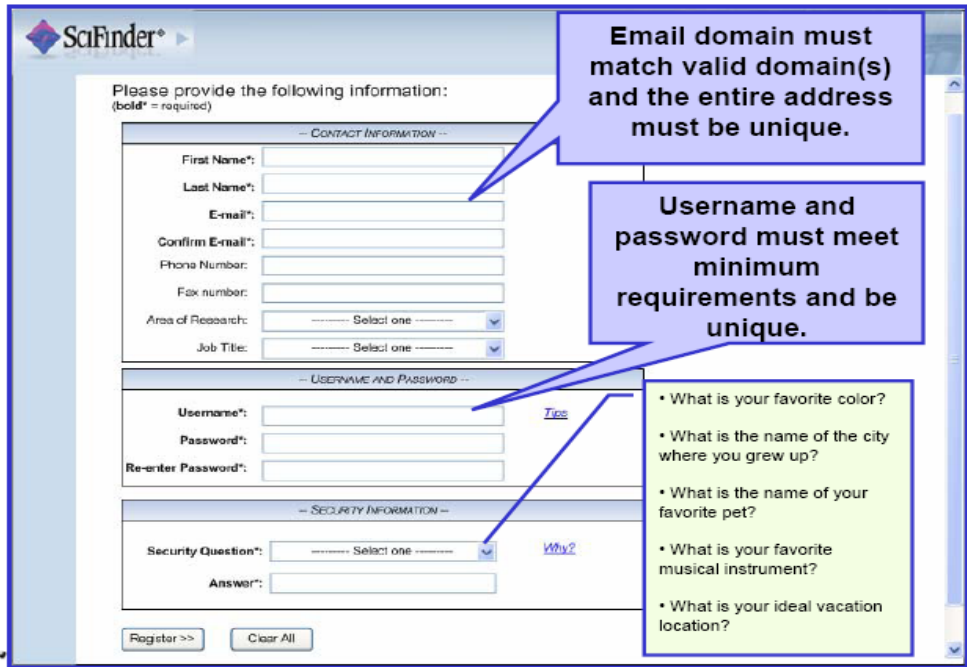
☐ Use an existing username and password? [Examples](#)

[Next](#)

开始创建SciFinder Web帐号

创建ID不能用代理服务器的IP地址

一人只能注册一个账号



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:  Select one

Job Title:  Select one

--- USERNAME AND PASSWORD ---

Username\*:

Password\*:

Re-enter Password\*:

--- SECURITY INFORMATION ---

Security Question\*:  Select one

Answer\*:

[Tip](#)

[Why?](#)

[Register >>](#) [Clear All](#)

Email domain must match valid domain(s) and the entire address must be unique.

Username and password must meet minimum requirements and be unique.

- 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：

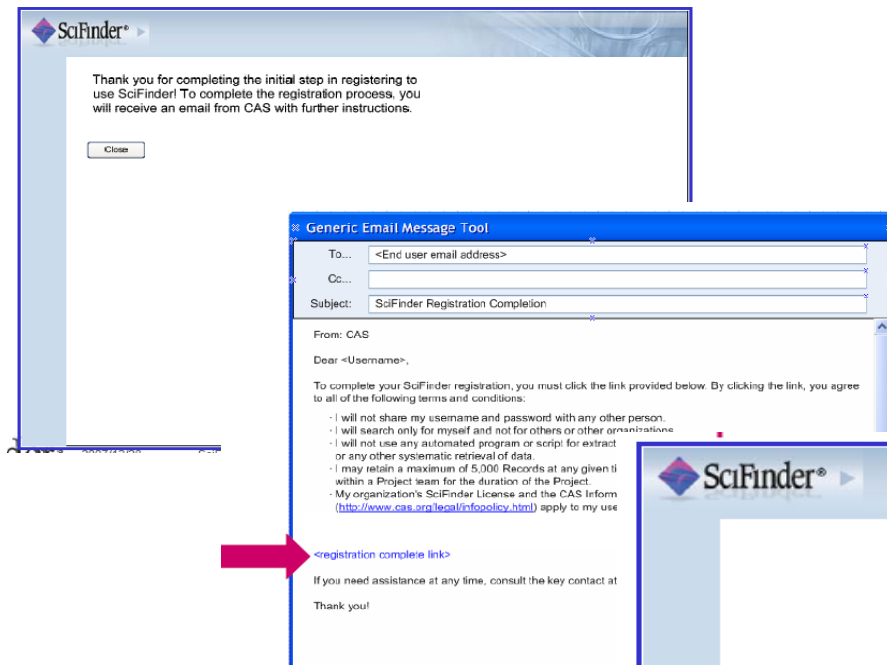
必须包含 7-15 个字符，并且至少包含三个以下字符：

字母、数字、非字母数字的字符（例如 @、#、%、&、\*）

## 密码设置小技巧：

- 1：不要和账号中有重复的字符
- 2：密码格式最好是abc@123

# 对新ID的Email确认



40分钟内查收邮件，注意垃圾邮箱  
48小时内点击邮件中的确认链接





# SciFinder Web登陆界面

**SciFinder®**  
The choice for chemistry research.™

## Sign In

输入SciFinder帐号和密码

Username

Password

NEW

☐ Remember me for two weeks unless I sign out  
(Do not use on a shared computer)

Sign In

[Forgot Username or Password?](#)

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



## News & Updates

### Welcome to SciFinder

**A New Non-Java Structure Editor is Now Available in SciFinder**

SciFinder now features a non-Java version of the CAS Structure Editor, a new option for your substance and reaction searching! Start searching with the new editor today. Plus, we've added a new option to Analyze reaction answer sets by reagent, along with other enhancements. See [all that's new](#) in the latest release.

**Learn about this year's Nobel Prize-winning chemistry research with SciFinder**

By now you've heard that Martin Karplus, Michael Levitt and Arieh Warshel were awarded the 2013 Nobel Prize in Chemistry. But did you know that much of their Nobel Prize-winning research can be found in SciFinder? Check out a few examples of their [most highly cited articles](#).

**Watch Part 3 of Our New Science in the News Podcast on Molecular Gastronomy**

In part 3 of our Science in the News podcast on molecular gastronomy, find out why SciFinder is essential to food chemistry research. [Watch it now](#) and don't forget to catch all three parts of

# SciFinder Web主界面

检索完，请点击退出

工具栏

The screenshot shows the SciFinder Web main interface. At the top is the SciFinder logo and navigation links: Preferences, SciFinder Help, and Sign Out. Below this is a toolbar with Explore, Saved Searches, and SciPlanner. On the left is a sidebar with three main sections: REFERENCES, SUBSTANCES, and REACTIONS. The REFERENCES section is expanded, showing options like Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, and Tags. The SUBSTANCES section shows Chemical Structure, Markush, Molecular Formula, Property, and Substance Identifier. The REACTIONS section shows Reaction Structure. The main content area is titled 'REFERENCES: RESEARCH TOPIC' and contains a search box with examples: 'The effect of antibiotic residues on dairy products' and 'Photocyanation of aromatic compounds'. Below the search box is a 'Search' button and a link to 'Advanced Search'. On the right side of the interface, there are two panels. The top panel is 'SAVED ANSWER SETS' and lists several saved sets: 'all', '聚芳醚', '1', 'HFUT', 'yanghua', 'pyrazole', 'Wuhan Institute of Tech', 'modification of chemical fiber', 'organosilicon', 'Ba', 'Autosaved Substance Set', and 'View All | Import'. The bottom panel is 'KEEP ME POSTED' and states 'You have no profiles. Learn how to: Create Keep Me Posted'.

工具栏

SciFinder®

Explore Saved Searches SciPlanner

REFERENCES: RESEARCH TOPIC

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

Search

Advanced Search

已保存的结果集

检索页面

检索入口

邮件提醒结果集

SAVED ANSWER SETS

- all
- 聚芳醚
- 1
- HFUT
- yanghua
- pyrazole
- Wuhan Institute of Tech
- modification of chemical fiber
- organosilicon
- Ba
- Autosaved Substance Set
- View All | Import

KEEP ME POSTED

You have no profiles.  
Learn how to:  
Create Keep Me Posted

# 在线帮助

Contents Search - Search - Go

Getting Started  
Searching for References  
Searching for Substances  
Searching for Reactions  
Finding Commercial Sources  
Using Keep Me Posted (KMP) Alerts  
Organizing Information in SciPlanner  
Viewing Session History  
Transitioning to the Web version of SciFinder  
SciFinder Preferences  
System Information  
Terminology  
日本語 (Japanese)

**SciFinder®**

Getting Started : Introduction

## Introduction

To help you get started, see the suggested workflows for:

**Working with References** **Working with Substances** **Working with Reactions**

Because the information in SciFinder is uniquely integrated, you can start your exploration with a search for references, substances, or reactions, and then easily retrieve related information from any of the other areas.

### What's New in SciFinder

The June 2013 release features a new, streamlined interface that was created in close collaboration with scientists. See the [Quick Tour](#) for a brief, 10-minute presentation of the new design.

**SciFinder Quick Tour**

See [CAS Content at a Glance](#) for the most recent database statistics.

### Learning resources

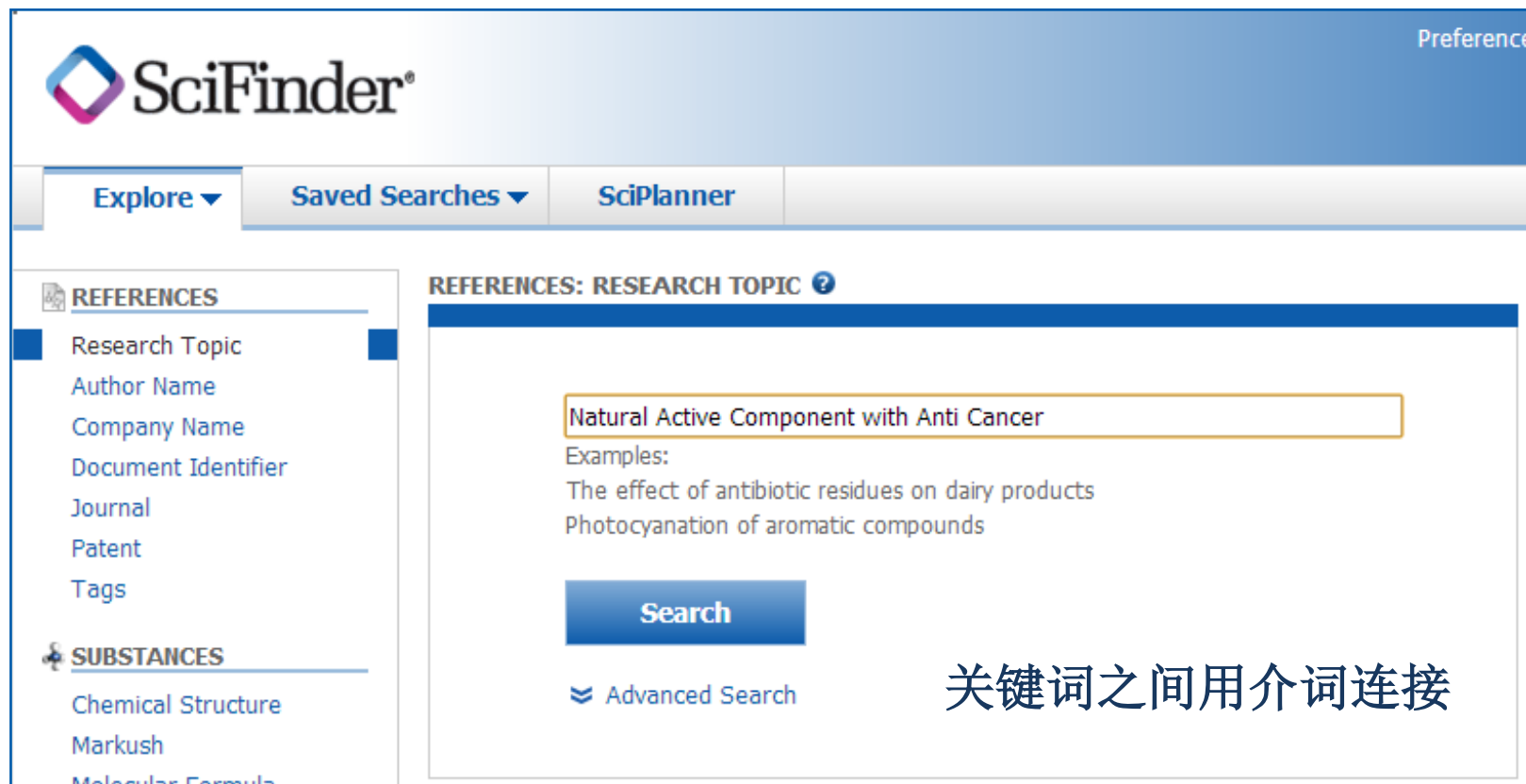
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# 文献检索—主题

主题检索： 具有抗癌作用的天然活性成分

关键词： **Natural Active Component** 、 **Anti Cancer**



The screenshot displays the SciFinder web interface. At the top, the SciFinder logo is visible on the left, and a 'Preference' link is on the right. Below the logo, there are three tabs: 'Explore' (selected), 'Saved Searches', and 'SciPlanner'. On the left side, there is a sidebar with two main sections: 'REFERENCES' and 'SUBSTANCES'. Under 'REFERENCES', there are links for 'Research Topic', 'Author Name', 'Company Name', 'Document Identifier', 'Journal', 'Patent', and 'Tags'. Under 'SUBSTANCES', there are links for 'Chemical Structure', 'Markush', and 'Molecular Formula'. The main content area is titled 'REFERENCES: RESEARCH TOPIC'. It features a search input field containing the text 'Natural Active Component with Anti Cancer'. Below the input field, there are two example sentences: 'The effect of antibiotic residues on dairy products' and 'Photocyanation of aromatic compounds'. A blue 'Search' button is positioned below the examples. At the bottom of the main content area, there is a link for 'Advanced Search'.

SciFinder®

Preference

Explore ▼ Saved Searches ▼ SciPlanner

REFERENCES

Research Topic

Author Name

Company Name

Document Identifier

Journal

Patent

Tags

SUBSTANCES

Chemical Structure

Markush

Molecular Formula

REFERENCES: RESEARCH TOPIC ?

Natural Active Component with Anti Cancer

Examples:

The effect of antibiotic residues on dairy products

Photocyanation of aromatic compounds

Search

Advanced Search

关键词之间用介词连接

# 主题检索的候选项

SciFinder® Preferences | SciFinder Help ▾ Sign Out

Welcome Sam Yu

Explore ▾ Saved Searches ▾ SciPlanner

Research Topic "Natural Active Component with ..."

只有104篇文献吗?

REFERENCES ?

Select All Deselect All

1 of 4 Research Topic Candidates Selected

		References
<input checked="" type="checkbox"/>	104 references were found containing the two concepts "Natural Active Component" and "Anti Cancer" closely associated with one another.	104
<input type="checkbox"/>	235 references were found where the two concepts "Natural Active Component" and "Anti Cancer" were present anywhere in the reference.	235
<input type="checkbox"/>	2840 references were found containing the concept "Natural Active Component".	2840
<input type="checkbox"/>	968272 references were found containing the concept "Anti Cancer".	968272

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



# 文献检索结果

文献  
分析  
工具

SciFinder®

Preferences | SciFinder Help | Sign Out

Welcome Sam Yu

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

Research Topic "Natural Active Component with ..." > references (104)

REFERENCES ?

Get Substances | Get Reactions | Get Related Citations | Get Full Text | Tools

Create Keep Me Posted Alert | Send to SciPlanner

Analyze | Refine | Categorize

Sort by: Accession Number

Answers per Page [20] Display: — = ≡

0 of 104 References Selected

1. **A method for preparing dandelion tea [Machine Translation].** Full Text  
By Fu, Zunan  
From Faming Zhuanli Shenqing (2013), CN 103330035 A 20131002. | Language: Chinese, Database: CAPLUS  
[Machine Translation of Descriptors]. The invention discloses a method for prepg. Dandelion Tea, comprises the following steps: (1) selecting materials for use; (2) after cleaning and drying, cut into pieces for use; (3) sterilizing at high temp.; (4) de-enzyming; (5) baking, baking **component** in two stages; (6) kneading, completed by mech. kneading twice; (7) loosing, mech. loosing; (8) fine selecting and packaging. the invention due to the adoption of pure **natural** Dandelion Leaf tea as raw materials, adding other adjuvants, Dandelion in pharmacol. provided thereon with antibacterial, endogen...

2. **Composition capable of reducing human blood sugar with natural product extract as effective component** Full Text  
By Zhao, Shijun  
From Faming Zhuanli Shenqing (2013), CN 103284045 A 20130911. | Language: Chinese, Database: CAPLUS  
The invention discloses a compn. capable of **reducing** human blood sugar with **natural** product ext. as effective

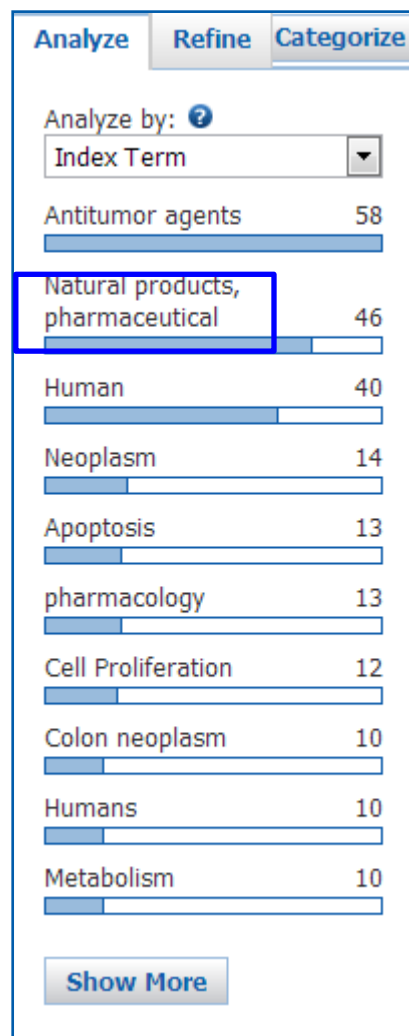
# 文献检索结果的Analyze

Analyze Refine Categorize

Analyze by: ?

Index Term ▼

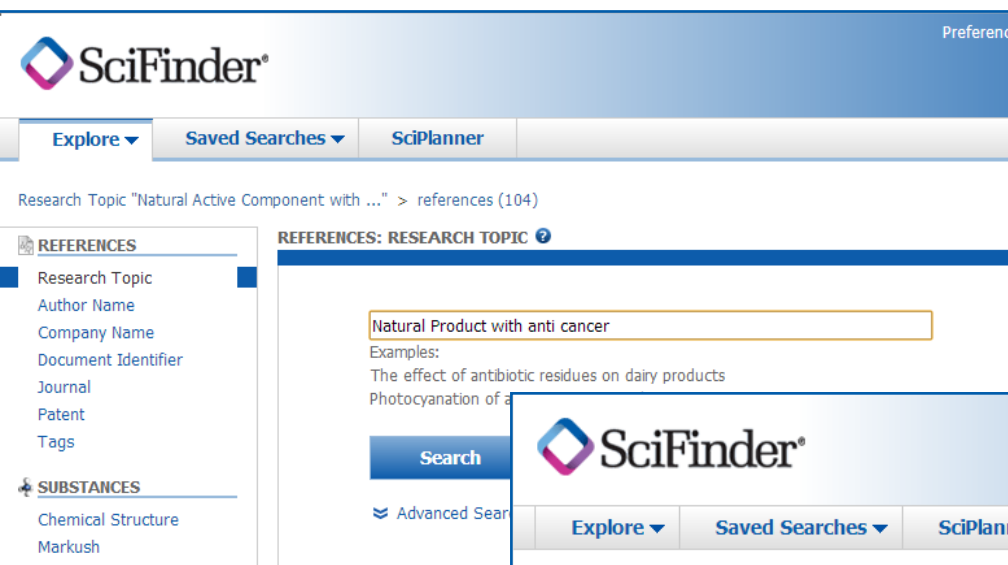
- Author Name
- CAS Registry Number
- CA Section Title
- Company-Organization
- Database
- Document Type
- Index Term
- CA Concept Heading
- Journal Name
- Language
- Publication Year
- Supplementary Terms



**Index Term**基于内容的分析工具，发现 **natural products, Pharmaceutical** 这个和天然活性成分很相关的词

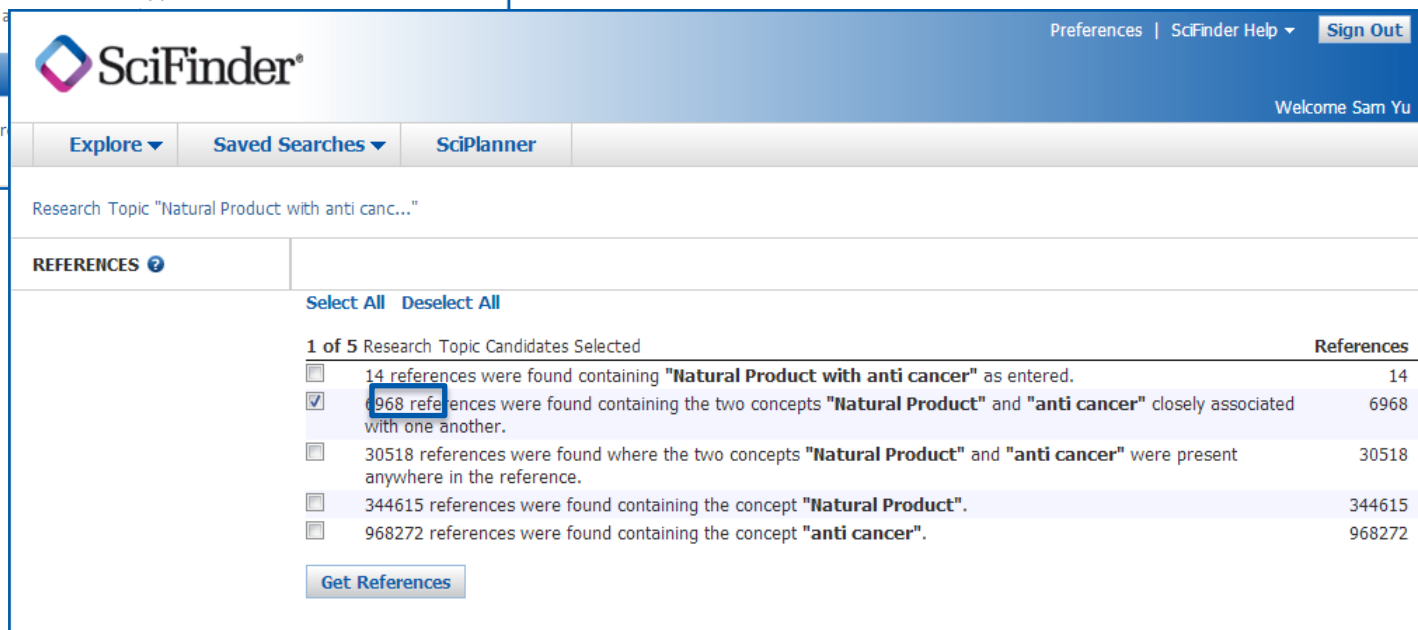
是否用这个词去检索，效果会更好？

# 尝试新的检索



新的检索式:  
**Natural Product with anti cancer**

更换检索词后,  
结果放大了70倍



# SciFinder中的结果

SciFinder®

Preferences | SciFinder Help | Sign Out

Welcome Sam Yu

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

Research Topic "Natural Product with anti canc..." > references (6968)

REFERENCES

Get Substances | Get Reactions | Get Related Citations | Get Full Text | Tools

Analyze | Refine | Categorize

Sort by: Accession Number | Answers per Page [20] Display: [List Icon]

0 of 6968 References Selected | Page: 1 of 349

Analyze by:

Author Name

Liu Li	46
Newman David J	41
Cheng Yiyu	39
Ge Zhiwei	39
Shui Wenbo	37

5. **Advances in research on the effects of traditional Chinese medicines on platinum antitumor drugs** | Full Text

By Zhang, Pei; Lu, Mengying; Liu, Quan; Bai, Ruizhen; Zhang, Zunjian; Xu, Fengguo  
From Yaoxue Jinzhan (2013), 37(5), 207-214. | Language: Chinese, Database: CAPLUS

Platinum complexes had a broad spectrum of **antitumor** activity and played an important role in the chemotherapy of malignant **tumors**. However, their clin. applications were limited due to the serious toxic and side effects such as nephrotoxicity, gastrointestinal toxicity, ototoxicity, hematopoietic system toxicity, nervous system toxicity, etc. Recently, some Traditional Chinese Medicines showed great potentials to enhance the efficacy and diminish the side effects when used in combination with platinum **antitumor** drugs. The advances in research on the effects of Traditional Chinese Medicines...

6. **Progress in research of the natural product Oroxylin A** | Full Text

By Guo, Ying; Qu, Jing-tian; Zhao, Xin; Wang, Hong  
From Liaoning Zhongyi Zazhi (2012), 39(12), 2512-2515. | Language: Chinese, Database: CAPLUS

The **natural product** Oroxylin A has a wide range of biol. activities, such as **anti-tumor**, neuroprotective, **anti-inflammatory**, tocolytic and **anti-pruritic** activity. Currently it has evoked great interests in the world. In this paper, it reviewed the researches on the extrn., synthesis, biol. activities and mol. mechanism of Oroxylin A in recent years.

7. **Nucleoside analogue as an anticancer compound** | Full Text

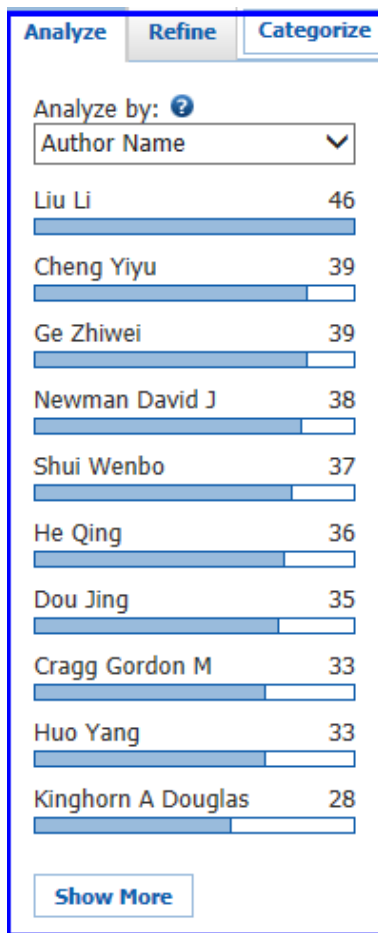
By Kate, Abhijeet Sudhir; George, Saji David; Sonawane, Shailendra; Periyasamy, Giridharan  
From PCT Int. Appl. (2013), WO 2013144894 A1 20131003. | Language: English, Database: CAPLUS

The invention relates to a compd. of I. The invention includes all isomeric forms and tautomeric forms I and pharmaceutically acceptable salts and derivs. such as esters and ethers. The invention further relates to the processes for isolation and prodn. of the compd. of formula (1) by fermn. of the marine actinomycetes strain PM0895117/MTCC 5675. The invention also relates to the pharmaceutical compns. contg. I as an active ingredient and use in medicines for the treatment of **cancer**.

一些相关词同时被检索出来

# 文献检索结果的Analysis

## 领域内主要专家



## 主要研究机构，合作伙伴，竞争对手



## 主要出版杂志



# 文献检索结果的Refine

## Refine Document Type:

可以帮助我们迅速获得特定文献类型的文献

AnalyzeRefineCategorize

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

SciFinder®

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

Research Topic "Natural Product with anti canc..." > references (6298) > refine "Review" (1539)

REFERENCES | Get Substances | Get Reactions | Get Related Citations | Get Full Text | Tools | Create Keep Me Posted Alert | Send to SciPlanner

AnalyzeRefineCategorize

Sort by: Accession Number | 0 of 1539 References Selected | Answers per Page [20] | Display: | Page: 1 of 77

Analyze by: ?

Journal Name

Current Medicinal Chemistry34

Zhongcaoyao32

Anti Cancer Agents in Medicinal Chemistry31

Natural Product Reports24

Mini Reviews in Medicinal Chemistry21

Current Drug Targets19

Journal of Natural Products18

☐ 1. Advances in research on the effects of traditional Chinese medicines on platinum antitumor drugs

By Zhang, Pei; Lu, Mengying; Liu, Quan; Bai, Ruizhen; Zhang, Zunjian; Xu, Fengguo  
From Yaoxue Jinzhan (2013), 37(5), 207-214. | Language: Chinese, Database: CAPLUS

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☐ 2. Progress in research of the natural product Oroxylin A

By Guo, Ying; Qu, Jing-tian; Zhao, Xin; Wang, Hong  
From Liaoning Zhongyi Zazhi (2012), 39(12), 2512-2515. | Language: Chinese, Database: CAPLUS

The **natural product** Oroxylin A has a wide range of biol. activities, such as **anti-tumor**, neuroprotective, **anti-inflammatory**, tocolytic and **anti-pruritic** activity. Currently it has evoked great interests in the world. In this paper, it reviewed the researches on the extrn., synthesis, biol. activities and mol. mechanism of Oroxylin A in recent years.

☐ 3. Advances in studies on application of polymer-supported reagents in synthesis of chiral drugs

By Zhang, Wei-guang; Cai, Zhi-qiang; Xu, Wei-ren; Tang, Li-da; Liu, Hong-qiang



# 引文排序

SciFinder®

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Explore ▾ Saved Searches ▾ SciPlanner Save Print Export

Research Topic "Natural Product with anti canc..." > references (6298) > refine "Review" (1539)

REFERENCES ?

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

Analyze Refine **Categorize**

Analyze by: ?  
Journal Name ▾

Current Medicinal Chemistry 34  
Zhongcaoyao 32  
Anti Cancer Agents in Medicinal Chemistry 31  
Natural Product Reports 24  
Mini Reviews in Medicinal Chemistry 21  
Current Drug Targets 19  
Journal of Natural Products 18

Sort by: Citing References ▾  
Accession Number  
Author Name  
**Citing References**  
Publication Year  
Title

Answers per Page [20] Display: — = ≡

Page: 1 of 77

1. **as Sources of New Drugs over the Last 25 Years** Full Text  
By Newman, David J.; Cragg, Gordon M.  
From Journal of Natural Products (2007), 70(3), 461-477. | Language: English, Database: CAPLUS

1291

2. **P-glycoprotein: from genomics to mechanism** Full Text  
By Ambudkar, Suresh V.; Kimchi-Sarfaty, Chava; Sauna, Zuben E.; Gottesman, Michael M.  
From Oncogene (2003), 22(47), 7468-7485. | Language: English, Database: CAPLUS

481

引文排序功能帮助查找重要的、有影响力的文章

# 文献检索结果的Categorize

一级目录

二级目录

和二级目录相关的Index Term

选中的Index Term

Categorize ?

1. Select a heading and category.

Category Heading	Category
All	Substances in biology (1023)
Biotechnology	<b>Organisms (525)</b>
General chemistry	Animal pathology (117)
<b>Biology</b>	Processes & systems (105)
Genetics & protein chemistry	Anatomy (101)
Synthetic chemistry	Immunology (60)
Technology	Endocrinology (44)
Physical chemistry	Substances in adverse effects (50)
Polymer chemistry	
Analytical chemistry	
Environmental chemistry	
Catalysis	

2. Select index terms of interest.

Index Terms	
Page: 1 of 6	
Select All Deselect All	
<input type="checkbox"/> Plant (Embryophyta)	72
<input type="checkbox"/> Fungi	37
<input checked="" type="checkbox"/> Marine animal	30
<input type="checkbox"/> Microorganism	24
<input type="checkbox"/> Sponge (Porifera)	23
<input type="checkbox"/> Animal	17
<input type="checkbox"/> Bacteria (Eubacteria)	17
<input type="checkbox"/> Marine invertebrate	17
<input type="checkbox"/> Plant (Embryophyta), medicinal	17
<input type="checkbox"/> Vegetable	16
<input type="checkbox"/> Human immunodeficiency virus 1	15
<input type="checkbox"/> Curcuma longa	14
<input type="checkbox"/> Eubacterium	14
<input type="checkbox"/> Ganoderma lucidum	14

Selected Terms

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

☒ Biology > Organisms (1 Terms)

Biology > Organisms > 1 Index Term(s) Selected

OK

Cancel

Categorize系统分类功能，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

SciFinder®

Preferences | SciFinder Help | Sign Out

Welcome Helen Zhu

Explore | Saved Searches | SciPlanner

Save | Print | Export

0 duplicates were automatically removed.

Research Topic "Natural Product with anti cancer..." > references (6298) > refine "Review" (1539) > refine by categories

REFERENCES

Analyze | Refine | Categorize

Sort by: Citing References

0 of 30 References Selected

1. Marine Natural Products and Related Compounds in Clinical and Advanced Preclinical Trials

By Newman, David J.; Cragg, Gordon M.

From Journal of Natural Products (2004), 67(8), 1216-1238. | Language: English, Database: CAPLUS

A review. The marine environment has proven to be a very rich source of extremely potent compds. that have demonstrated significant activities in antitumor, antiinflammatory, analgesia, immunomodulation, allergy, and antiviral assays. Although the case can and has been made that the nucleosides such as Ara-A and Ara-C are derived from knowledge gained from investigations of bioactive marine nucleosides, no drug directly from marine sources (whether isolated or by total synthesis) has yet made it to the com. sector in any disease. However, as shown in this review, there are now significant ...

2. Drug development from marine natural products

By Molinski, Tadawa F.; Dalisay, Dorelyne C.; Liawens, Sarah L.; Caludes, Joel D.

From Nature Reviews Drug Discovery (2009), 8(1), 69-85. | Language: English, Database: CAPLUS

A review. Drug discovery from marine natural products has enjoyed a renaissance. Ziconotide (Prialt; Elan Pharmaceuticals), a peptide originally discovered in a tropical marine-derived compd. to be approved in the United States in Dec. 2004 for the treatment of severe chronic pain. In 2007, trabectedin (Yondelis; PharmaMar) became the first marine anticancer drug to be approved in the Union. Here, we review the history of drug discovery from marine natural products, and ...

文献详细信息

**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

Export

Export:

All  
Selected  
Range

Example: 2-20

For:

Citation Manager

Citation export format (\*.ris)  
Quoted Format (\*.bt)  
Tagged Format (\*.bt)

Offline review

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

Saving locally

Answer Key eXchange (\*.aex)

Details:

File Name: \*

Reference\_06\_19\_2012\_100848

Format:

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

Include:

Task History  
Tags  
Comments

Export Cancel

**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

# 文献信息—题录、摘要、索引

REFERENCE DETAIL ⓘ

Get Substances

Get Related Citations

Get Full Text

Send to SciFinder

[Return](#) [Previous](#) [Next](#)

## 2. Drug development from marine natural products

By: Molinski, Tadeusz F.; Dalisay, Doralyn S.; Lievens, Sarah L.; Saludes, Jonel P.

A review. Drug discovery from marine natural products has enjoyed a renaissance in the past few years. Ziconotide (Prialt; Elan Pharmaceuticals), a peptide originally discovered in a tropical cone snail, was the first marine-derived compd. to be approved in the United States in Dec. 2004 for the treatment of pain. Then, in Oct. 2007, trabectedin (Yondelis; PharmaMar) became the first marine anticancer drug to be approved in the European Union. Here, we review the history of drug discovery from marine natural products, and by describing selected examples, we examine the factors that contribute to new discoveries and the difficulties assocd. with translating marine-derived compds. into clin. trials. Providing an outlook into the future, we also examine the advances that may further expand the promise of drugs from the sea.

### Indexing

Pharmacology (Section1-0)

Concepts 重要概念

Antitumor agents

antimitotic; drug development from marine natural products

Drug design

Human

Natural products, pharmaceutical

Drug discovery

Marine animal

Neoplasm

Snail

drug development from marine natural products

Substances 重要物质

114899-77-3 Yondelis 🔍

drug development from marine natural products

Natural product occurrence; Pharmacological activity; Therapeutic use; Biological study; Occurrence; Uses

107452-89-1 Prialt 🔍

ziconotide; drug development from marine natural products

Natural product occurrence; Pharmacological activity; Therapeutic use; Biological study; Occurrence; Uses

### QUICK LINKS

0 Tags, 0 Comments

### SOURCE

*Nature Reviews Drug Discovery*  
Volume8  
Issue1  
Pages69-85  
Journal; General Review  
2009  
CODEN:NRDDAG  
ISSN:1474-1776  
DOI:10.1038/nrd2487

### COMPANY/ORGANIZATION

Department of Chemistry and Biochemistry and Skaggs School of Pharmacy and Pharmaceutical Sciences  
University of California, San Diego  
La Jolla, CA, USA 92093

### ACCESSION NUMBER

2009:9244  
CAN150:113584  
CAPLUS

# 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**Concept**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，请参考[www.igroup.com.cn/cas](http://www.igroup.com.cn/cas)

# 提 纲

- 介绍
  - SciFinder Web中的内容
  - SciFinder Web的注册和登陆
- **SciFinder Web中的检索和后处理**
  - SciFinder Web中的文献检索
  - SciFinder Web中的物质检索
  - SciFinder Web中的Markush检索
  - SciFinder Web中的反应检索
- **SciFinder Web使用常见问题和网络资源**



# 物质检索--标识符检索

在SciFinder 中查找AZD7545（AstraZeneca公司开发的治疗糖尿病的前药）

The screenshot displays the SciFinder web interface. At the top, the SciFinder logo is on the left, and navigation links for 'Preferences', 'SciFinder Help', and 'Sign Out' are on the right. Below the header, a navigation bar includes 'Explore', 'Saved Searches', and 'SciPlanner'. The main content area shows a breadcrumb trail: 'Research Topic "potassium channel with antican..." > references (262) > get substances (10746) > keep analysis "Bioactivity Indicators" (529)'. On the left sidebar, the 'SUBSTANCES' section is active, listing options like 'Chemical Structure', 'Markush', 'Molecular Formula', 'Property', and 'Substance Identifier'. The central search area is titled 'SUBSTANCES: SUBSTANCE IDENTIFIER' and features a text input field containing 'AZD 7545'. Below the input field, it says 'Enter one per line. Examples: 50-00-0, 999815, Acetaminophen'. A blue arrow points to the input field with the text '输入CAS RN或名称'. A 'Search' button is located below the input field. On the right sidebar, the 'SAVED ANSWER SETS' section lists various saved sets, and the 'KEEP ME POSTED' section shows a message about profiles.


提示:

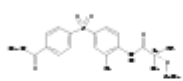
1. 一次最多可输入25个物质。
2. 每行一个物质标示符。

物质标示符包括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

1. **Substance Detail**  
**1084955-47-4**

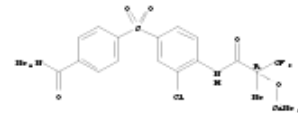
~13 




Absolute stereochemistry.

**C<sub>22</sub> H<sub>26</sub> Cl F<sub>3</sub> N<sub>2</sub> O<sub>5</sub> S Si**  
Benzamide, 4-[[[3-chloro-4-[[[(2R)-3,3,3-trifluoro-2-methyl-1-oxo-2-[(trimethylsilyl)oxy]propyl]amino]phenyl]sulfonyl]-N,N-dimethyl-

**Substance Detail**  
获得和物质有关的所有信息



» 

**CAS Registry Number:** 108-78-1

- 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
- Send to SciPlanner

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

# Substance Detail—物质详情

SUBSTANCE DETAIL ?

Get References

Get Reactions

Get Commercial Sources

Return

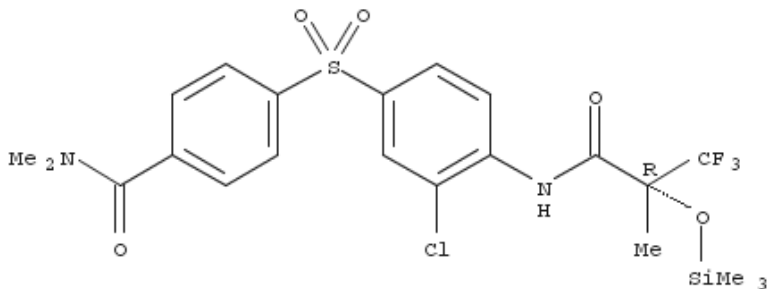
CAS Registry Number: 1084955-47-4

C<sub>22</sub> H<sub>26</sub> Cl F<sub>3</sub> N<sub>2</sub> O<sub>5</sub> S Si

Benzamide, 4-[[[3-chloro-4-[[[(2*R*)-3,3,3-trifluoro-2-methyl-1-oxo-2-[(trimethylsilyl)oxy]propyl]amino]phenyl]sulfonyl]-*N,N*-dimethyl-

AZD 7545

Deleted CAS Registry Numbers: 670276-04-7



Absolute stereochemistry.

CAS号、分子式、结构式、化学名、别名

Source of Registration: CA

~13 References

物质信息来源

Document Types: Journal, Patent

CAS Role	Patents	Nonpatents	Nonspecific Derivatives from Patents	Nonspecific Derivatives from Nonpatents
Biological Study	✓	✓	✓	✓
Preparation		✓		
Properties		✓		✓
Uses	✓	✓	✓	

Target Indicators

Enzymes (all) >>>> Pyruvate dehydrogenase kinase	References
	4

按照CAS Role分类的专利、非专利文献列表。对某类文献感兴趣，仅需点击交叉处的 ✓ 即可方便快捷地获取。

# 预测数据与实验数据

## Predicted Properties: Biological Chemical Density Lipinski and Related Spectra Structure-related Thermal

Biological Properties	Value	Condition	Note	Top
Bioconcentration Factor	104	pH 1 Temp: 25 °C	(1)	
Bioconcentration Factor	104	pH 2 Temp: 25 °C	(1)	
Bioconcentration Factor	104	pH 3 Temp: 25 °C	(1)	
Bioconcentration Factor	104	pH 4 Temp: 25 °C	(1)	
Bioconcentration Factor	104	pH 5 Temp: 25 °C	(1)	
Bioconcentration Factor	104	pH 6 Temp: 25 °C	(1)	
Bioconcentration Factor	104	pH 7 Temp: 25 °C	(1)	
Bioconcentration Factor	104	pH 8 Temp: 25 °C	(1)	
Density Properties	Value	Condition	Note	Top
Bioconcentration Density	1.314±0.06 g/cm3	Temp: 20 °C Press: 760 Torr	(1)	
Molar Volume	419.1±3.0 cm3/mol	Temp: 20 °C Press: 760 Torr	(1)	
Chemical Properties	Value	Condition	Note	Top
Koc				
Koc				
Lipinski and Related Properties	Value	Condition	Note	Top
Freely Rotatable Bonds	7		(1)	
H Acceptors	7		(1)	
H Donors	1		(1)	
H Donor/Acceptor Sum	8		(1)	
logP	2.956±0.651	Temp: 25 °C	(1)	
Molecular Weight	551.05		(1)	
Spectra Properties	Value	Condition	Note	Top
Carbon-13 NMR Spectrum	See spectrum		(2)	
Proton NMR Spectrum	See spectrum		(2)	
Structure-related Properties	Value	Condition	Note	Top
Polar Surface Area	101 A2		(1)	
Thermal Properties	Value	Condition	Note	Top
Boiling Point	630.3±55.0 °C	Press: 760 Torr	(1)	
Enthalpy of Vaporization	93.23±3.0 kJ/mol	Press: 760 Torr	(1)	

# 物质检索--Property explore

Explore ▼

Saved Searches ▼

SciPlanner

Research Topic "Natural Product with anti canc..." > references (6305)

REFERENCES

Research Topic

Author Name

Company Name

Document Identifier

Journal

Patent

Tags

SUBSTANCES

Chemical Structure

Markush

Molecular Formula

Property

Substance Identifier

REACTIONS

Reaction Structure

SUBSTANCES: PROPERTY ?

Select the category and enter an appropriate value or range.

☐ Experimental

Select Property... ▼

Value or Range

Examples: Individual value as 44, range as 25-35, or open ended range as >125 or <125

☒ Predicted

Molecular Weight ▼

Value or Range

250-400 ✕

Examples: Individual value as 44, range as 25-35, or open ended range as >125 or <125

Search

寻找分子量在250-400之间的黄酮类物质

# 物质结果集的筛选--Refine

Explore ▾ Saved Searches ▾ SciPlanner Save Print Export

Property "Predicted - Molecular Weight, ..." > substances (23893644)

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

Analyze Refine Sort by: CAS Registry Number ▾

0 of 23893644 Substances Selected

Answers per Page [15] View: ||| ||| |||

Page: 1 of 1592910

Refine by: ?

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

Structure Editor:

Java Non-Java

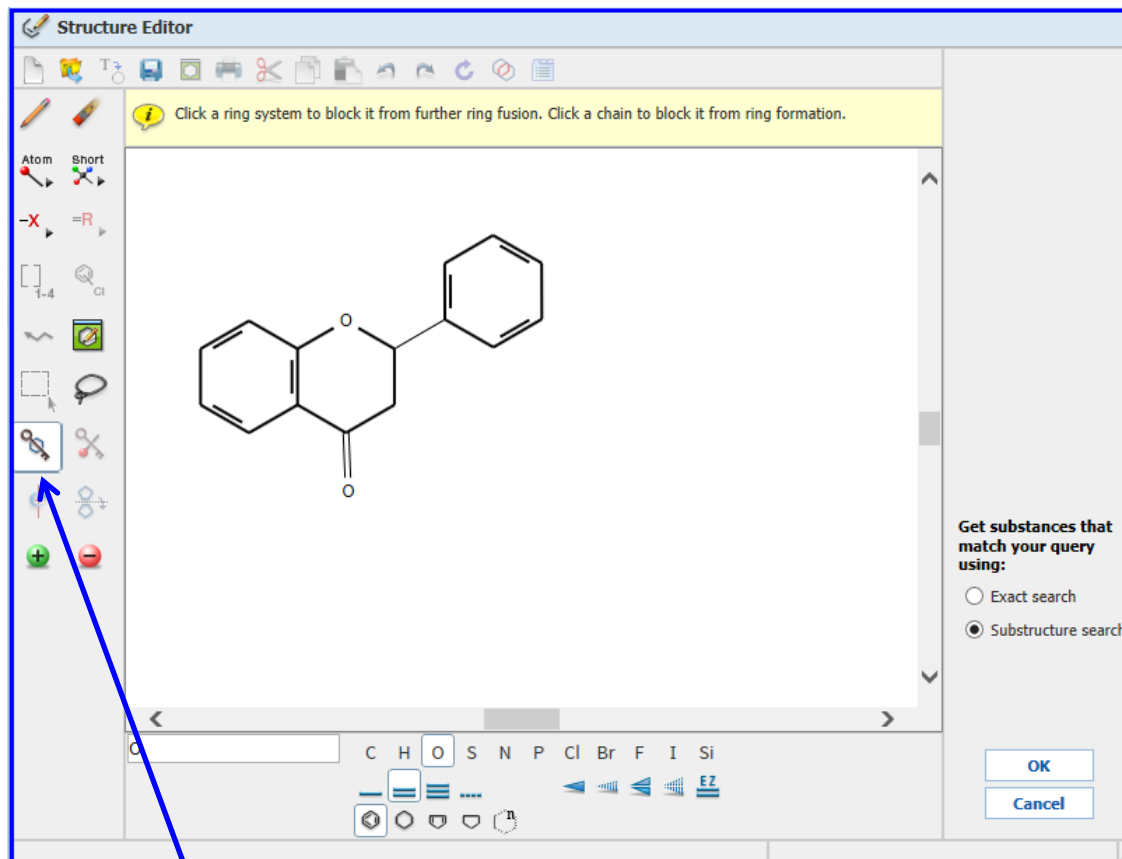
Click to Edit

Search type: Exact Structure

Only retrieve substances

<input type="checkbox"/> 1. <b>Substance Detail</b> 1462241-01-5 ~0	<input type="checkbox"/> 2. <b>Substance Detail</b> 1462241-00-4 ~0	<input type="checkbox"/> 3. <b>Substance Detail</b> 1462240-99-8 ~0	<input type="checkbox"/> 4. <b>Substance Detail</b> 1462240-97-6 ~0
 <b>C<sub>12</sub> H<sub>14</sub> N<sub>4</sub> S<sub>2</sub></b> 3-Pyridinecarbothioamide, 6-[[1-(2-thiazolyl)propyl]amino]	 <b>C<sub>13</sub> H<sub>16</sub> Br N O<sub>2</sub></b> Benzenepropanamide, 3-bromo-N-(3-hydroxycyclobutyl)-	 <b>C<sub>15</sub> H<sub>20</sub> N<sub>4</sub> S</b> 4-Piperidinemethanamine, N-cyclopropyl-1-thieno[2,3-d]pyrimidin-4-yl-	 <b>C<sub>13</sub> H<sub>15</sub> Br N<sub>2</sub> O<sub>3</sub></b> Ethanone, 1-[1-(5-bromo-2-nitrophenyl)-3-piperidinyl]-
<input type="checkbox"/> 5. <b>Substance Detail</b> 1462240-95-5	<input type="checkbox"/> 6. <b>Substance Detail</b> 1462240-95-5	<a href="https://scifinder.cas.org/scifinder/substances/answers/E992D17AX86F350AFX2FAD5C7519FA...">https://scifinder.cas.org/scifinder/substances/answers/E992D17AX86F350AFX2FAD5C7519FA...</a>	

# 物质结果集的筛选--Refine



原子锁工具避免找到环结构变化的物质

Analyze Refine

Refine by: ?

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

Structure Editor:

Java Non-Java

Click image to change structure or view detail.

Search type: **Substructure**

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



# 物质结果集的筛选--Refine

Explore ▾ Saved Searches ▾ SciPlanner Save Print Export

Property "Predicted - Molecular Weight, ..." > substances (23893644) > refine "substructure" (6879)

SUBSTANCES

Get References Get Reactions Get Commercial Sources Tools ▾

Create Keep Me Posted Alert Send to SciPlanner

Analyze Refine

Sort by: Relevance ▾

Answers per Page [15] View:

0 of 6879 Substances Selected

Page: 1 of 459

Analyze by:

Substance Role ▾

Preparation 5256

Biological Study 2892

Uses 1857

Properties 1615

Reactant or Reagent 1574

Occurrence 805

Analytical Study 436

Process 308

Formation, Nonpreparative 172

Prophetic in Patents 40

Show More

<input type="checkbox"/> 1. <b>Substance Detail</b> 958734-07-1  ~1 <b>C<sub>15</sub> H<sub>12</sub> O<sub>4</sub></b> 4'-Hydroxy-2,3-dihydro-4H-1-benzopyran-4-one	<input type="checkbox"/> 2. <b>Substance Detail</b> 1438763-28-0  ~1 Absolute stereochemistry. <b>C<sub>17</sub> H<sub>16</sub> O<sub>2</sub></b> 4-Ethyl-2,3-dihydro-4H-1-benzopyran-4-one	<input type="checkbox"/> 3. <b>Substance Detail</b> 21785-09-1  ~133 <b>C<sub>16</sub> H<sub>14</sub> O<sub>3</sub></b> 7-Methoxy-2-phenyl-2,3-dihydro-4H-1-benzopyran-4-one Spectra Experimental Properties	<input type="checkbox"/> 4. <b>Substance Detail</b> 72984-48-6  ~20 Absolute stereochemistry., Rotation (-). <b>C<sub>16</sub> H<sub>14</sub> O<sub>3</sub></b> 7-Methoxy-2-phenyl-2,3-dihydro-4H-1-benzopyran-4-one Experimental Properties
<input type="checkbox"/> 5. <b>Substance Detail</b> 725263-73-0  ~14 Absolute stereochemistry., Rotation (+). <b>C<sub>16</sub> H<sub>14</sub> O<sub>3</sub></b> 7-Methoxy-2-phenyl-2,3-dihydro-4H-1-benzopyran-4-one	<input type="checkbox"/> 6. <b>Substance Detail</b> 62252-06-6  ~7 <b>C<sub>15</sub> H<sub>12</sub> O<sub>4</sub></b> 4-Ethyl-2,3-dihydro-4H-1-benzopyran-4-one	<input type="checkbox"/> 7. <b>Substance Detail</b> 138474-12-1  ~2 Absolute stereochemistry. <b>C<sub>15</sub> H<sub>12</sub> O<sub>4</sub></b> 4-Ethyl-2,3-dihydro-4H-1-benzopyran-4-one	<input type="checkbox"/> 8. <b>Substance Detail</b> 1256571-17-1  ~2 Absolute stereochemistry. <b>C<sub>15</sub> H<sub>12</sub> O<sub>4</sub></b> 4-Ethyl-2,3-dihydro-4H-1-benzopyran-4-one

这些物质的结构特点？

# 物质结果集的筛选--Refine

Analyze Refine

Refine by: ?

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

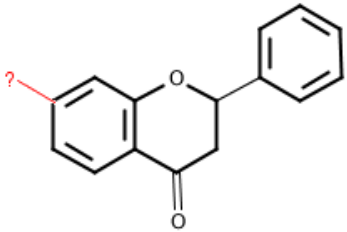
Select Attachments

**Atom Attachment:**  
了解结构中原子修饰情况。

Refine by Atom Attachment ?

1. Click an atom to display the attachments present at that site. 2. Select attachment(s) of interest.

Substructure



Atom Attachments

Select All Deselect All

<input type="checkbox"/> H or None	3048
<input type="checkbox"/> O	3410
<input type="checkbox"/> C	261
<input type="checkbox"/> N	56
<input type="checkbox"/> Cl	46
<input type="checkbox"/> F	38
<input type="checkbox"/> Br	15
<input type="checkbox"/> I	4
<input type="checkbox"/> S	1
<input type="checkbox"/> A - Any (not H)	3831
<input type="checkbox"/> Q - Any (not C,H)	3570
<input type="checkbox"/> Ak - Alkyl chain	256
<input type="checkbox"/> X - Halogen	103
<input type="checkbox"/> Hy - Heterocycle	4
<input type="checkbox"/> Cb - Carbocycle	4

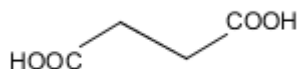
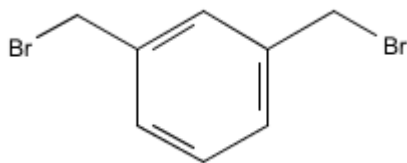
? =

Refine Cancel

鼠标放在任意原子上，  
显示“？”，右侧列出该原子修饰基团。

# 物质检索—分子式

## 已知起始原料的聚合物



**$(C_8 H_8 Br_2 . C_4 H_6 O_4) x$**

Explore ▾ Saved Searches ▾ SciPlanner

REFERENCES

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

SUBSTANCES

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

REACTIONS

- Reaction Structure

SUBSTANCES: MOLECULAR FORMULA ⓘ

Examples:  
H4SiO4  
(C3H6O.C2H4O)x

Search

☐ 1. Substance Detail  
176516-41-9

~3

623-24-5  
C<sub>8</sub> H<sub>8</sub> Br<sub>2</sub>

110-15-6  
C<sub>4</sub> H<sub>6</sub> O<sub>4</sub>

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

☐ 2. Substance Detail  
132010-54-9

~2

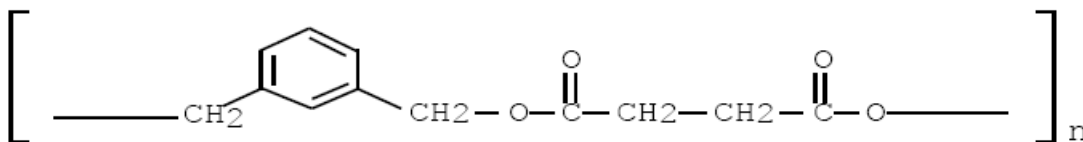
626-15-3  
C<sub>8</sub> H<sub>8</sub> Br<sub>2</sub>

110-15-6  
C<sub>4</sub> H<sub>6</sub> O<sub>4</sub>

**$(C_8 H_8 Br_2 . C_4 H_6 O_4)_x$**   
Butanedioic acid, polymer with  
1,3-bis(bromomethyl)benzene  
(9CI)

# 物质检索—分子式

## 已知重复单元的聚合物



(C<sub>12</sub> H<sub>12</sub> O<sub>4</sub>)<sub>n</sub>

Explore ▾ Saved Searches ▾ SciPlanner Save Print Export

Molecular Formula "(C<sub>12</sub> H<sub>12</sub> O<sub>4</sub>)<sub>n</sub>" > substances (43)

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

Analyze Refine

Sort by: CAS Registry Number ▾

0 of 43 Substances Selected

Answers per Page [15] View: ▢ ▢ ▢ ▢

Page: 1 of 3

Substance	Image	Cannot Be	Displayed
1. Substance Detail 1421756-46-8		~1	1421756-46-
2. Substance Detail 1392419-56-5		~1	1353713-96-
3. Substance Detail 1353713-96-8		~1	1341223-97-9
4. Substance Detail 1341223-97-9		~1	
5. Substance Detail 1287722-74-0		~1	
6. Substance Detail 1284217-62-4		~2	
7. Substance Detail 863506-77-8		~8	
8. Substance Detail 272113-34-5		~1	

**Analyze** **Refine**

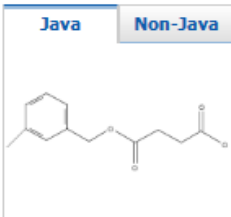
Refine by: ?

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

---

Structure Editor:

Java **Non-Java**



Click image to change structure or view detail.

Search type: **Substructure**

---

Only retrieve substances that:

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

**SUBSTANCES** ?


Get References Get Reactions Get Commercial Sources Tools ▾


**Analyze** **Refine**

Sort by: CAS Registry Number ▾

☐ ▾ 0 of 1 Substance Selected

☐ 1. **Substance Detail**  
**132010-11-8**

~2 



**(C<sub>12</sub> H<sub>12</sub> O<sub>4</sub>)<sub>n</sub>**  
Poly[oxy(1,4-dioxo-1,4-butanediyl)  
oxymethylene-1,3-phenylenemethylene]  
(9CI)

Analyze by: ?  
Substance Role ▾

Preparation 1

Properties 1

**Show More**

利用结构特征进行**Refine**，迅速查找需要的物质

# 物质检索--结构

The screenshot displays the SciFinder web interface. At the top, there's a navigation bar with 'SciFinder' logo, 'Preferences', 'SciFinder Help', and 'Sign Out'. Below this, a secondary bar shows 'Explore', 'Saved Searches', and 'SciPlanner'. The main content area is titled 'SUBSTANCES: CHEMICAL STRUCTURE'. On the left, a sidebar lists search criteria under 'REFERENCES' (Research Topic, Author Name, etc.) and 'SUBSTANCES' (Chemical Structure, Molecular Formula, etc.). The 'Chemical Structure' option is highlighted. The main panel shows a 'Structure Editor' with 'Java' and 'Non-Java' tabs. An arrow points to the 'Non-Java' tab with the text '无需安装Java版' (No need to install Java version). Below the editor, there are search type options: 'Exact Structure', 'Substructure' (selected), and 'Similarity'. A 'Search' button is at the bottom. On the right, there's a 'SAVED ANSWER SETS' section with a list of saved sets and a 'KEEP ME POSTED' section.

SciFinder®

Preferences | SciFinder Help | Sign Out

Welcome Helen Zhu

Explore | Saved Searches | SciPlanner

Author Name "yan, d" > references (1019)

REFERENCES

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

SUBSTANCES

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

REACTIONS

- Reaction Structure

SUBSTANCES: CHEMICAL STRUCTURE ?

Structure Editor:

Java Non-Java

Click to Edit

Search Type:

- ☐ Exact Structure
- ☒ Substructure
- ☐ Similarity

☐ Show precision analysis

Import CXF

Search

Advanced Search

SAVED ANSWER SETS ?

- all
- 聚芳醚
- 1
- HFUT
- yanghua
- pyrazole
- Wuhan Institute of Tech
- modification of chemical fiber
- organosilicon
- Ba
- Autosaved Reference Set

View All | Import

KEEP ME POSTED ?

You have no profiles.

Learn how to:

点击画图版来进行结构输入，初次使用时需要安装Java插件

64位系统：需同时安装32位和64位Java

# SciFinder结构绘制工具

The image shows the SciFinder Structure Editor interface with various tools 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)
- 选择工具 (Selection tool)
- 索套选择工具 (Lasso selection 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 recovery tool)
- 负电子 (Electron)
- 单双键, RS构型, 不确定键定义工具 (Single/double bond, RS configuration, uncertain bond definition tool)
- 结构检索选择 (Structure search selection)
- 常见环, 多元环工具 (Common rings, polycyclic tools)



Structure Editor

Add to Editor

Enter CAS Registry Number, SMILES, or InChI:

196618-13-0

Examples:  
50-00-0  
CCCC  
InChI=1S/C3H8O/c1-2-3-4/h4H, 2-3H2, 1H3

达非的CAS No.

Drawing Editor:  
☒ Structure  
☐ Reaction  
☐ Markush

Structure Editor

Save As Template...

Please enter a template name

dafei

确定 取消

存为模板

调用模板

Templates

- Polycyclic
- O-containing
- Nucleic Acid
- NOS-containing
- W-containing
- Monocyclic
- Misc
- Cycloalkane
- Coordination
- Carbohydrate
- Bicarbocyclic
- Amino Acid
- Alkaloid
- User Defined

dafei

Close

Get substances that match your query using:  
☐ Exact search  
☒ Substructure search  
☐ Similarity search

确定 取消

Scale 100

312.41

# 精确结构检索

精确结构检索：  
获得结构本身、盐及混合物

Explore ▾ Saved Searches ▾ SciPlanner

Substance Identifier "AZD 7545" > substances (1) > 1084955-47-4

**REFERENCES**

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

**SUBSTANCES: CHEMICAL STRUCTURE**

Search Type:

- ☒ Exact Structure
- ☐ Substructure
- ☐ Similarity

Click image to change structure or view detail.

Import CFX

**Search**

Advanced Search

**Stereo Candidates**

5 Candidates 1 Selected

Select All Deselect All

**Stereo Candidates**

- ☒ Absolute stereo match
- ☐ Absolute stereo mirror image
- ☐ Relative stereo match
- ☐ Stereo that doesn't match query
- ☐ No stereo in answer structure

**Get Substances**

Sort by: Relevance ▾

0 of 25 Substances Selected

Answers per Page [15] View: ▮ ▮ ▮

Page: 1 of 2

☐ 1. **Substance Detail**  
**196618-13-0**

~1245

Absolute stereochemistry.,Rotation (-).

**C<sub>16</sub> H<sub>28</sub> N<sub>2</sub> O<sub>4</sub>**

1-Cyclohexene-1-carboxylic acid, 4-(acetylamino)-5-amino-3-(1-ethylpropoxy)-, ethyl ester, (3R,4R,5S)-

Experimental Properties

☐ 2. **Substance Detail**  
**204255-11-8**

~552

Absolute stereochemistry.,Rotation (-).

**C<sub>16</sub> H<sub>28</sub> N<sub>2</sub> O<sub>4</sub> · H<sub>3</sub> O<sub>4</sub> P**

1-Cyclohexene-1-carboxylic acid, 4-(acetylamino)-5-amino-3-(1-ethylpropoxy)-, ethyl ester, (3R,4R,5S)-, phosphate (1:1)

☐ 3. **Substance Detail**  
**756819-03-1**

~4

Absolute stereochemistry.,Rotation (-).

**C<sub>16</sub> H<sub>28</sub> N<sub>2</sub> O<sub>4</sub> · x H<sub>2</sub> O<sub>4</sub> S**

1-Cyclohexene-1-carboxylic acid, 4-(acetylamino)-5-amino-3-(1-ethylpropoxy)-, ethyl ester, (3R,4R,5S)-, sulfate

☐ 4. **Substance Detail**  
**204255-09-4**  
(Component: 196618-13-0)

~3

Absolute stereochemistry.,Rotation (-).

**C<sub>16</sub> H<sub>28</sub> N<sub>2</sub> O<sub>4</sub> · Cl H**

1-Cyclohexene-1-carboxylic acid, 4-(acetylamino)-5-amino-3-(1-ethylpropoxy)-, ethyl ester, hydrochloride (1:1), (3R,4R,5S)-

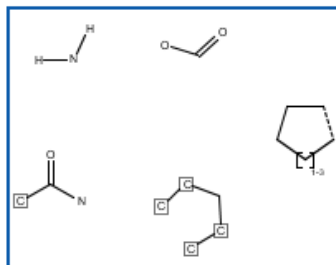
# 亚结构检索

## 作用机理

[编辑本段](#)

帕拉米韦是Babu等在分析**唾液酸**、**扎那米韦**、奥司他韦与NA的互相作用机制及构效关系的基础上设计并合成的环戊烷衍生物，与环连接的基团有亲水的羧基和胍基以及疏水的异戊基和乙酰氨基，4个极性不同的基团分别作用于流感病毒NA结构中不同的活性位点区域。羧基部分与NA活性位点的3个精氨酸残基Arg118, Arg292,

## SUBSTANCES: CHEMICAL STRUCTURE ?



Click image to change structure or view detail.

Import CXF

Search

[Advanced Search](#) ☐ Always Show

Search Type:

- ☐ Exact Structure  
☒ Substructure  
☐ Similarity

☐ Show precision analysis

Formula Weight

☐ Return only substances in this formula weight range:

Min:  Max:

Characteristics

- ☒ Single component  
☐ Commercially available  
☐ Included in references

单组分物质

Classes

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

有机物质

# 亚结构检索

0 of 704 Substances Selected

1. Substance Detail  
127971-59-9

C<sub>15</sub> H<sub>21</sub> N<sub>3</sub> O<sub>5</sub>

Benzoic acid, 5-(acetylamino)-4-[(1-ethylpropyl)amino]-2-methyl-3-nitro-

Experimental Properties

2. Substance Detail  
127971-80-6

C<sub>17</sub> H<sub>25</sub> N<sub>3</sub> O<sub>4</sub>

Benzoic acid, 3,5-bis(acetylamino)-4-[(1-ethylpropyl)amino]-2-methyl-

3. Substance Detail  
182367-45-9

C<sub>14</sub> H<sub>22</sub> N<sub>4</sub> O<sub>4</sub>

1-Cyclohexene-1-carboxylic acid, 4-(acetylamino)-5-azido-3-(1-ethylpropoxy)-, (3a,4β,5α)-(9CI)

Relative stereochemistry.

4. Substance Detail  
182367-47-1

C<sub>16</sub> H<sub>28</sub> N<sub>2</sub> O<sub>4</sub>

1-Cyclohexene-1-carboxylic acid, 4-(acetylamino)-5-amino-3-(1-ethylpropoxy)-, ethyl ester, (3a,4β,5α)-(9CI)

5. Substance Detail  
182367-71-1

C<sub>14</sub> H<sub>24</sub> N<sub>2</sub> O<sub>4</sub>

1-Cyclohexene-1-carboxylic acid, 4-(acetylamino)-5-amino-3-(1-ethylpropoxy)-, (3R,4R,5S)-rel

Relative stereochemistry.

6. Substance Detail  
182367-73-3

C<sub>17</sub> H<sub>30</sub> N<sub>4</sub> O<sub>4</sub>

1-Cyclohexene-1-carboxylic acid, 4-(acetylamino)-5-[(aminoiminomethyl)amino]-3-(1-ethylpropoxy)-, ethyl ester, (3R,4R,5S)-rel

Relative stereochemistry.

7. Substance Detail  
182367-74-4

182367-73-3  
C<sub>17</sub> H<sub>30</sub> N<sub>4</sub> O<sub>4</sub>

Relative stereochemistry.

76-05-1  
C<sub>2</sub> H F<sub>3</sub> O<sub>2</sub>

1. Substance Detail  
330600-85-6

C<sub>15</sub> H<sub>28</sub> N<sub>4</sub> O<sub>4</sub>

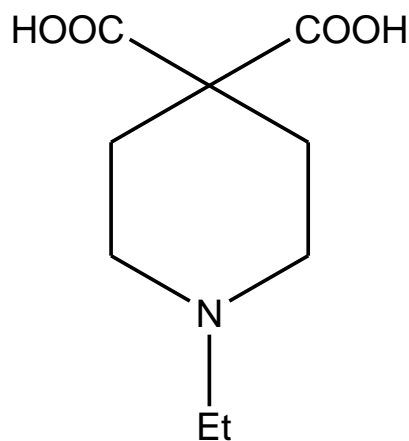
Cyclopentanecarboxylic acid, 3-[(1S)-1-(acetylamino)-2-ethylbutyl]-4-[(aminoiminomethyl)amino]-2-hydroxy-, (1S,2S,3R,4R)-

亚结构检索：获得包含全部片段结构的所有物质

SciFinder®  
The choice for chemistry research.™

50

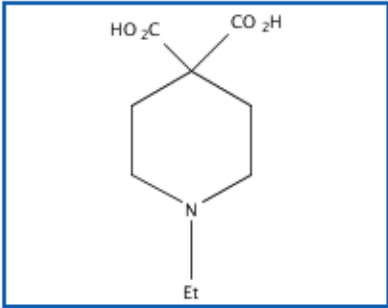
# 结构检索—结构相似的检索



Chemical Structure exact > **substances (0)**

SciFinder中的相似结构检索，帮助获得在结构上存在相似的物质。

SUBSTANCES: CHEMICAL STRUCTURE ?



Click image to change structure or view detail.

Import CXF

**Search**

≡ Advanced Search

Search Type:

- ☐ Exact Structure
- ☐ Substructure
- ☒ **Similarity**

☐ Show precision analysis

# 相似结构检索

Select All Deselect All

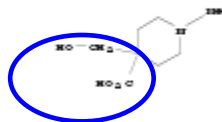
1 of 6 Similarity Candidates Selected

	Substances
<input type="checkbox"/> $\geq 99$ (most similar)	0
<input type="checkbox"/> 95-98	0
<input type="checkbox"/> 90-94	0
<input checked="" type="checkbox"/> 85-89	11
<input type="checkbox"/> 80-84	30
<input type="checkbox"/> 75-79	127
<input type="checkbox"/> 70-74	435
<input type="checkbox"/> 65-69	1287
<input type="checkbox"/> 0-64 (least similar)	4617

Get Substances

Score: 88

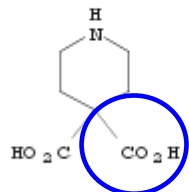
☐ 1. Substance Detail  
1267985-98-7



**C<sub>8</sub> H<sub>15</sub> N O<sub>3</sub>**  
4-Piperidinecarboxylic acid, 4-(hydroxymethyl)-1-methyl-

Score: 83

☐ 13. Substance Detail  
121880-27-1



**C<sub>7</sub> H<sub>11</sub> N O<sub>4</sub>**  
4,4-Piperidinedicarboxylic acid

Score: 78

☐ 17. Substance Detail  
1027511-99-4



**C<sub>10</sub> H<sub>17</sub> N O<sub>3</sub>**  
1-Azepine-4-carboxylic acid, 1-acetylhexahydro-4-methyl-

相似结构检索:

取代基位置变化  
取代基变化  
母体结构变化

# 无文献的物质

Score: 78

17. Substance Detail  
1027511-99-4

C10H17NO3  
1H-Azepine-4-carboxylic acid, 1-acetylhexahydro-4-methyl-



17.

CAS Registry Number: 1027511-99-4

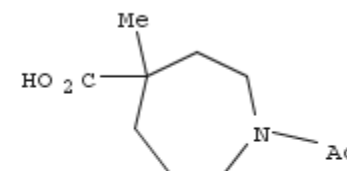
Score: 78

C10H17NO3

1H-Azepine-4-carboxylic acid, 1-acetylhexahydro-4-methyl-

Source of Registration: Chemical Catalog  
Supplier: AstaTech, Inc.

~0 References



很多无文献的物质是有试剂供应商提供给CAS申请登记号，并有证据表明其存在



# 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：  
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

# 提 纲

- 介绍
  - SciFinder Web中的内容
  - SciFinder Web的注册和登陆
- **SciFinder Web中的检索和后处理**
  - SciFinder Web中的文献检索
  - SciFinder Web中的物质检索
  - SciFinder Web中的Markush检索
  - SciFinder Web中的反应检索
- **SciFinder Web使用常见问题和网络资源**

➤ 具体物质[Specific Substance]：

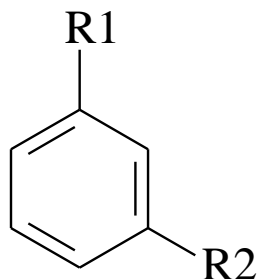
以具体化学结构所陈述的特定物质，会被标示CAS No.

➤ 预测性物质[Prophetic Substance]：

使用Markush结构所陈述的预测物质，一个Markush可以陈述上百或上千的化学物质

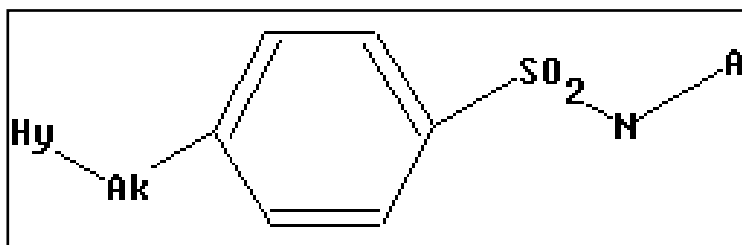
Patent 中所陈述的预测物质，不会被标示CAS No.

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>



SciFinder中的Markush检索  
能帮助做初步的专利评估。

Explore ▾ Saved Searches ▾ SciPlanner

Chemical Structure similarity > substances (127) > 1027511-99-4

**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: MARKUSH ?**

Click image to change structure or view detail.

Search Type:

- ☒ Allow variability only as specified
- ☐ Substructure

Import CXF

**Search**

# 全部是专利文献

Explore ▼ Saved Searches ▼ SciPlanner Save Print Export

Markush structure variable only at spe... > references (119)

REFERENCES ? Get Substances Get Reactions Get Related Citations Get Full Text Tools ▼

Analyze Refine Categorize

Analyze by: Document Type Patent 119 Show More

Sort by: Accession Number ↓

Answers per Page [20] Display: — = ≡

0 of 119 References Selected

1. Substituted piperidine derivatives as a GPR119 agonist useful in treatment of metabolism related diseases and their preparation Full Text

By Yang, Jin; Kim, Jinwoong; Lee, Hankyu; Kim, Jaehyun; Son, Changmo; Lee, Kyuhwan; Choi, Hyunghe; Kim, Daehoon; Choi, Hyosun; Rhee, Jaekool  
From PCT Int. Appl. (2013), WO 2013105753 A1 20130718. | Language: English, Database: CAPLUS

The invention is related to substituted piperidine derivs. of formula I as a GPR119 agonist useful in treatment of metab. related diseases such as diabetes or obesity and their prepn. The invention compds. I, wherein A is (un)substituted Ph or heterocyclic group; R<sup>1</sup> is COOR<sub>3</sub>, or a (un)substituted heterocyclic group; R<sup>2</sup> and R<sup>3</sup> are each independently a straight or branched chain, or a(un)substituted C<sub>1-5</sub> alkyl group; m is 0, 1, 2, 3; n is 1, 2, 3; their pharmaceutically acceptable salts are claimed. Compd. II was prepd. by multi-step procedure (procedure given). The invention compds. were eva...

2. Preparation of tricyclic heterocyclic compounds as JAK inhibitors Full Text

By Hayashi, Keishi; Watanabe, Tsuneo; Toyama, Koji; Kamon, Junji; Minami, Masataka; Uni, Miyuki; Nasu, Mariko  
From PCT Int. Appl. (2013), WO 2013024895 A1 20130221. | Language: English, Database: CAPLUS

Title compds. I [A<sup>a</sup> = 5- to 6-membered heteroaryl contg. one or two N atom; X<sup>a</sup> = H or CR<sup>9a</sup>; R<sup>1a</sup> = H, halo, alkyl or haloalkyl; ring B<sup>a</sup> = cycloalkane, cycloalkene, 3- to 14-membered nonarom. heterocycle, arom. carbocycle or 5- to 10-membered arom. heterocycle; R<sup>2a</sup> = H, halo, azido, cycloalkyl, etc.; L<sup>1a</sup> = single bond, alkylene, alkenylene or alkynylene; L<sup>2a</sup> = single bond, alkylene, alkenylene, or alkynylene; L<sup>3a</sup> = single bond, O, S, etc.; Y<sup>a</sup> = CR<sup>10a</sup>; n = 0, 1 or 2, R<sup>3a</sup> = hydroxy, amino, carboxy, carbamoyl, each of R<sup>9a</sup> and R<sup>10</sup> independently = H, halogen, cyano, carbamoyl, etc.], and their pharma...

# 提 纲

- 介绍
  - SciFinder Web中的内容
  - SciFinder Web的注册和登陆
- **SciFinder Web中的检索和后处理**
  - SciFinder Web中的文献检索
  - SciFinder Web中的物质检索
  - SciFinder Web中的Markush检索
  - SciFinder Web中的反应检索
- **SciFinder Web使用常见问题和网络资源**

# SciFinder 中反应定义工具

The image shows the 'Reaction Editor' window in SciFinder. The interface includes a toolbar on the left with various chemical drawing tools, a central workspace, and a right-hand panel with 'Drawing Editor' options and search filters. Red boxes with Chinese labels point to specific tools in the toolbar:

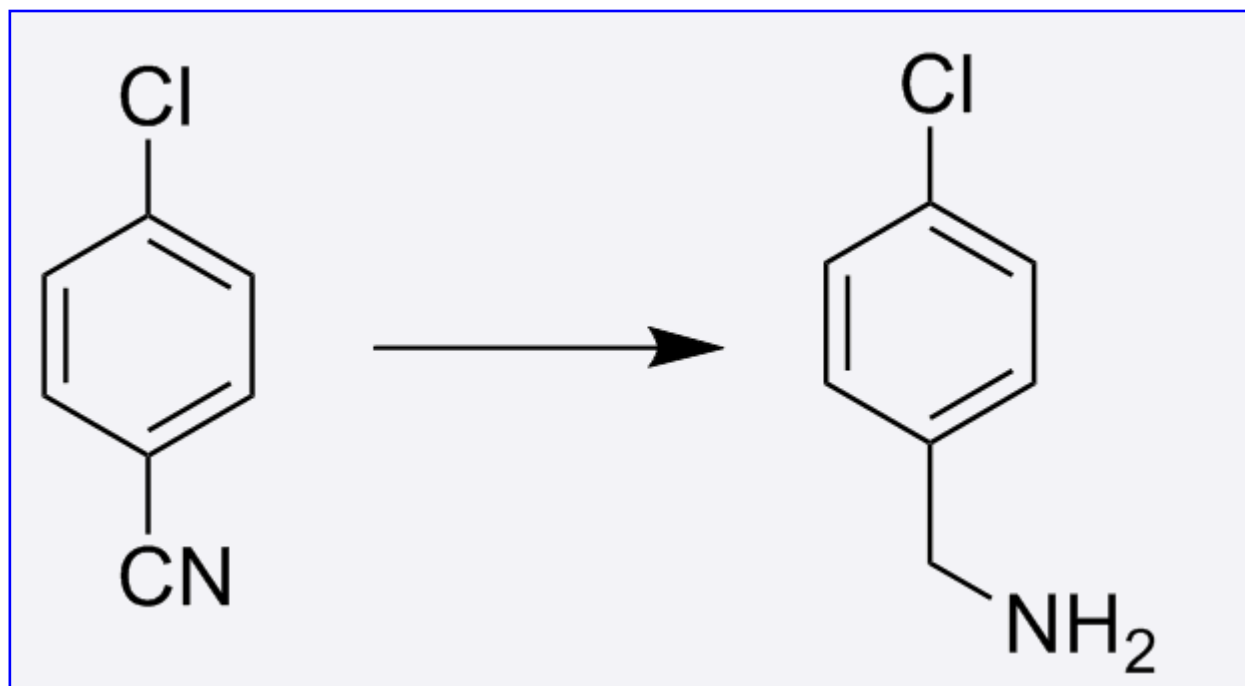
- 反应箭头 (Reaction Arrow): Points to the arrow tool in the toolbar.
- 反应原子标记工具 (Reaction Atom Labeling Tool): Points to the tool with a plus sign and a minus sign.
- 反应官能团列表 (Reaction Functional Group List): Points to the 'alchc ketor alder' button.
- 反应角色工具 (Reaction Role Tool): Points to the tool with 'A' and 'B' labels.
- 反应位置标记工具 (Reaction Position Labeling Tool): Points to the tool with a crosshair.

The right-hand panel includes the 'Drawing Editor' section with radio buttons for 'Structure', 'Reaction' (selected), and 'Markush'. Below this is a section for 'Get reactions where the structure(s) are:' with options for 'Variable' and 'Substructures of more complex structures'. At the bottom right are '确定' (OK) and '取消' (Cancel) buttons.

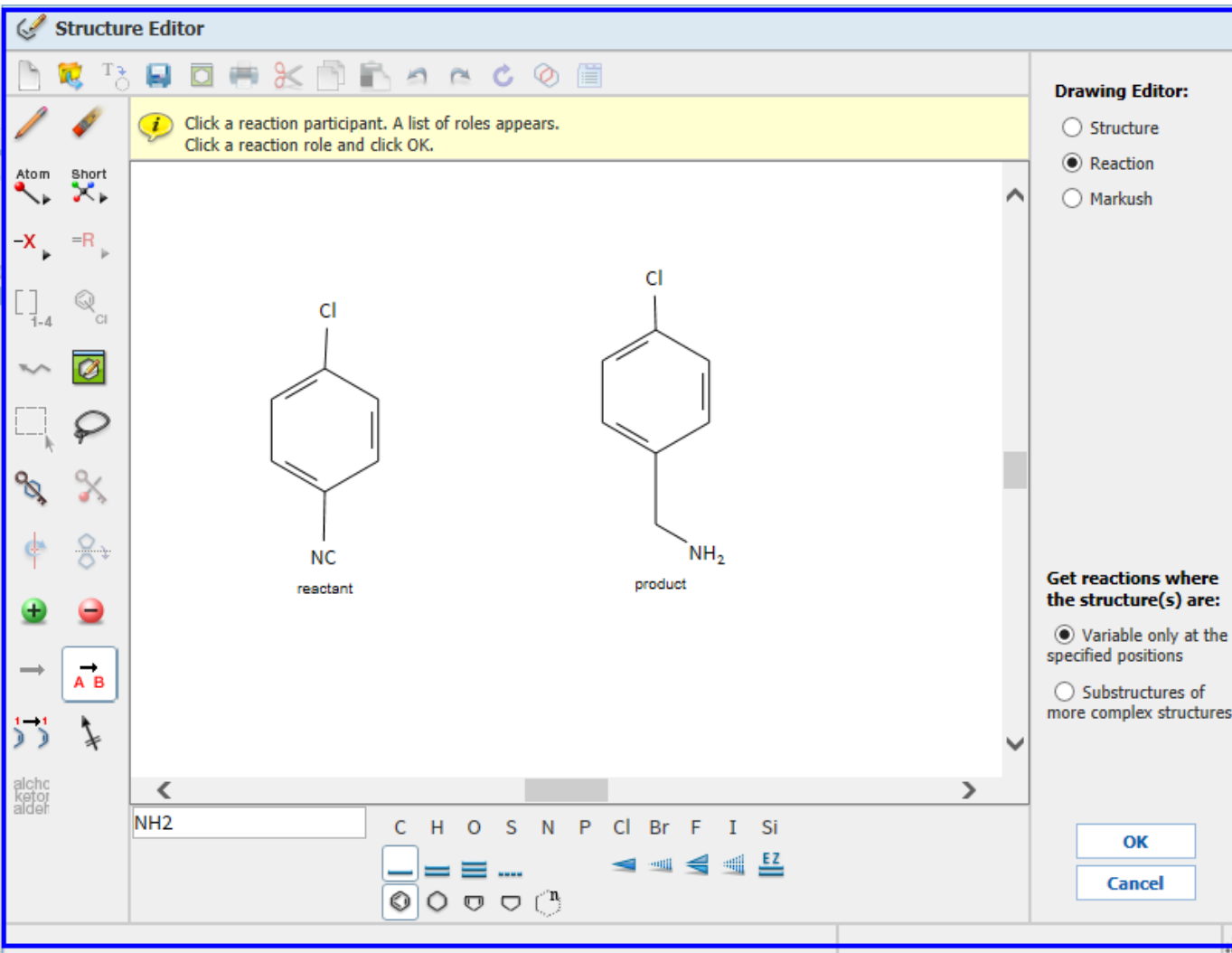


# 反应检索

检索：腈基的还原



# 反应检索



## 精确反应检索

# 反应检索结果

Explore ▾ Saved Searches ▾ SciPlanner Save Print Export

Reaction Structure structure variable only at spe... > reactions (20)

REACTIONS ? Get References Tools ▾ Send to SciPlanner

Analyze Refine

Group by: No Grouping ▾ Sort by: Relevance ▾ ↓

Answers per Page [50] Display: [Icons]

Analyze by: ?  
Reagent (New) ▾

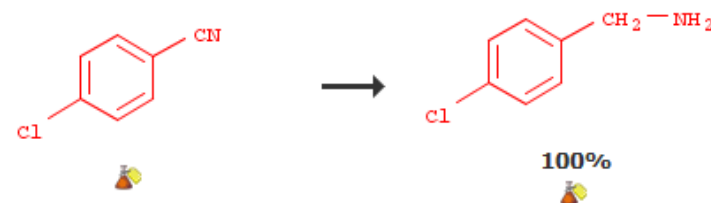
H <sub>2</sub>	5
HCl	5
NaOH	4
SmI <sub>2</sub>	3
F <sub>3</sub> CCO <sub>2</sub> H	2
H <sub>2</sub> O	2
KOH	2
NaBD <sub>4</sub>	2
NaBH <sub>4</sub>	2
NH <sub>3</sub>	2

Show More

☐ ▾  
No Grouping  
Document Selected  
Transformation

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


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



► Overview

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

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



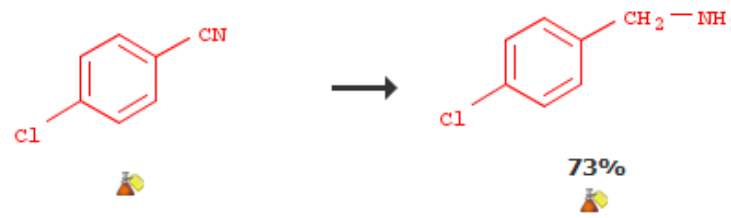
# 反应检索结果

文献题目

命中反应数

☐ 9. Selective Ruthenium-Catalyzed Transfer Hydrogenations of Nitriles to Amines with 2-Butanol 🔍 [Full Text](#)  
2 Reactions 🔍 Similar Reactions

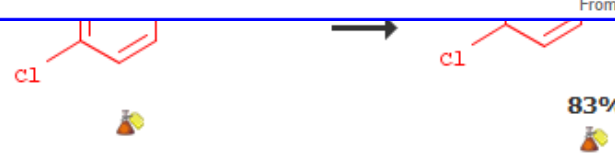
Single Step Hover over any structure for more options.



73%

**Overview**

Steps/Stages	Notes
<input type="checkbox"/> 11 3 1.1 R: <i>s</i> -BuOH, C: 52462-29-0, C: (Ph <sub>2</sub> PCH <sub>2</sub> CH <sub>2</sub> ) <sub>2</sub> , 5 min, rt 1.2 R: NaOH, 5 min, rt Si 1.3 rt; 20 min, 120°C	GC yield; 2-butanol also used as solvent (stage 1), Reactants: 1, Reagents: 2, Catalysts: 2, Steps: 1, Stages: 3, Most stages in any one step: 3
	<b>References</b> Selective Ruthenium-Catalyzed Transfer Hydrogenations of Nitriles to Amines with 2-Butanol 🔍 <a href="#">Full Text</a> By Werkmeister, Svenja et al From Chemistry - A European Journal, 19(14), 4437-4440; 2013



83%

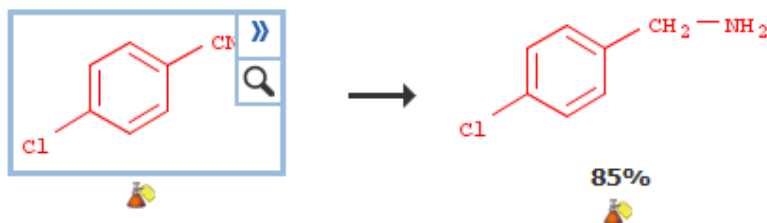
Overview

一篇文献只出现一条反应记录

# Experimental Procedure

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

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



► Overview

► Experimental Procedure



General/Typical Procedure: In a typical procedure, in a 100 ml conical flask mounted over a magnetic stirrer, fitted with reflux condenser and a mercury trap, was placed a mixture of nitrile (9.8 mmol), anhyd. nickel (II) chloride (9.8 mmol) and dry ethanol (20 ml). Sodium borohydride (29.4 mmol) was added very cautiously while stirring the solution vigorously. The progress of the reaction was monitored by TLC using benzene : ethyl acetate (90: 10, v/v) as eluent. After the complete disappearance of the nitrile (~5 min), the reaction mixture was filtered through a celite pad after ~ 15 min. The filtered nickel boride precipitate was washed with ethanol (2 x 10 ml). The combined filtrate was diluted with water (150 ml) and extracted with ethyl acetate (3 x 10 ml). The combined extract was dried over anhyd. MgSO<sub>4</sub>, filtered and concentrated on a rotary vacuum evaporator. After drying under vacuum, the product was purified by column chromatography over silica gel (20 x 2 cm; 100-200 mesh) using benzene: ethyl acetate as the eluent. Eluate was concentrated under reduced pressure to afford the products which were analysed by IR, NMR and mass spectra as most of these are known products.<sup>10</sup> **2d**, yield 85%

不用阅读全文，直接获得包含实验过程的反应记录

# 按照反应类型排序

Explore ▾ Saved Searches ▾ SciPlanner Save Print Export

Reaction Structure structure variable only at spe... > reactions (20)

REACTIONS ? Get References Tools ▾ Send to SciPlanner

Analyze Refine

Analyze by: ?  
 Reagent (New) ▾

H <sub>2</sub>	5
HCl	5
NaOH	4
SmI <sub>2</sub>	3
F <sub>3</sub> CCO <sub>2</sub> H	2
H <sub>2</sub> O	2
KOH	2
NaBD <sub>4</sub>	2

Group by: Transformation ▾ Sort by: Frequency ▾ ↓

☐ 0 of 20 Reactions Selected

- ☐ 1. Reduction of Nitriles to Amines  
20 Reactions  

$$\text{R}-\text{C}\equiv\text{N} \longrightarrow \text{R}-\text{CH}_2\text{NH}_2$$
- ☐ 2. Dehalogenation of Aromatic Compounds  
2 Reactions  


$$\text{Ar}-\text{X} \xrightarrow{\text{cat.}} \text{Ar}-\text{H}$$
- ☐ 3. Reduction of Alkyl Halides/ Dehalogenation  
2 Reactions  


$$\text{R}-\text{X} \longrightarrow \text{R}-\text{H}$$

更精确的查找需要的反应

# 反应检索结果的筛选


Analyze Refine


Analyze by: 


Reagent (New) 

H <sub>2</sub>	5
HCl	5
NaOH	4
SmI <sub>2</sub>	3
F <sub>3</sub> CCO <sub>2</sub> H	2
H <sub>2</sub> O	2
KOH	2
NaBD <sub>4</sub>	2
<b>NaBH<sub>4</sub></b>	<b>2</b>
NH <sub>3</sub>	2


Show More



REACTIONS 

Get References Tools 



Send to SciPlanner 

Analyze Refine

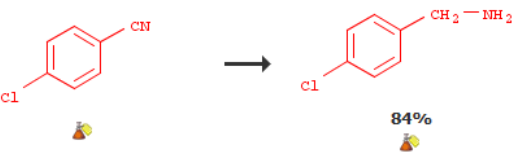
Group by: No Grouping Sort by: Relevance 

Answers per Page [50] Display:  



☐ 0 of 20 Reactions Selected

☐ 7. View Reaction Detail  Link  Similar Reactions

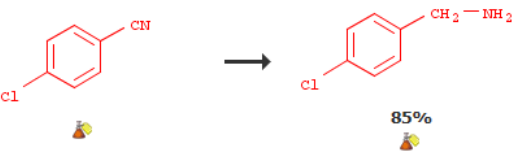
Single Step Hover over any structure for more options.



Overview

☐ 8. View Reaction Detail  Link  Similar Reactions

Single Step Hover over any structure for more options.



Overview

Experimental Procedure

获得特定物质做还原剂的反应

# 提 纲

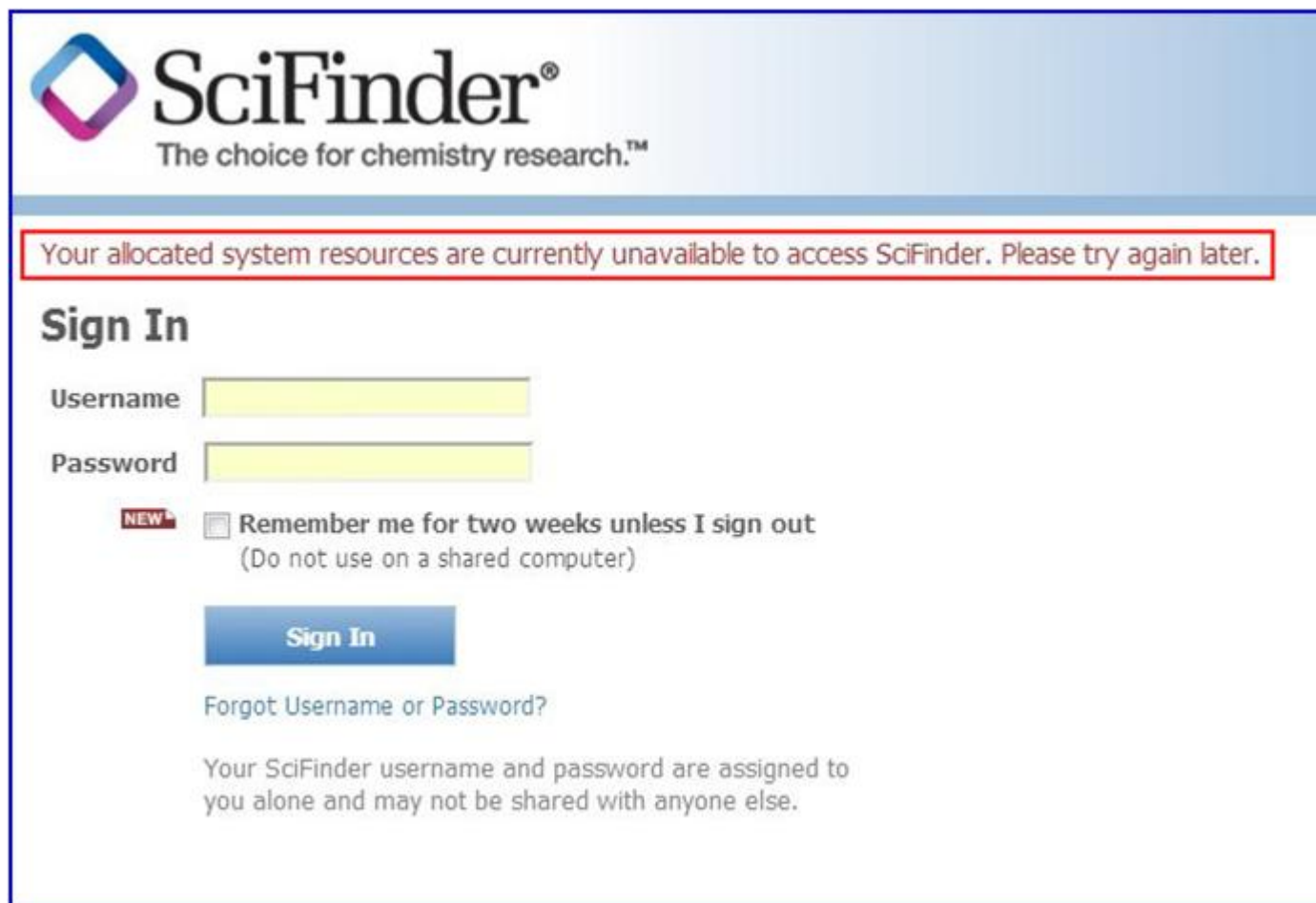
- 介绍
  - SciFinder Web中的内容
  - SciFinder Web的注册和登陆
- **SciFinder Web中的检索和后处理**
  - SciFinder Web中的文献检索
  - SciFinder Web中的物质检索
  - SciFinder Web中的Markush检索
  - SciFinder Web中的反应检索
- **SciFinder Web使用常见问题和网络资源**




# SciFinder Web使用注意事项

- 一人注册一个账号
- 严禁过量下载
- 严禁账号分享
- 严禁将账号用于非学术研究

# SciFinder Web 常见问题



 **SciFinder<sup>®</sup>**  
The choice for chemistry research.™

Your allocated system resources are currently unavailable to access SciFinder. Please try again later.

### Sign In

Username

Password

**NEW** ☐ Remember me for two weeks unless I sign out  
(Do not use on a shared computer)

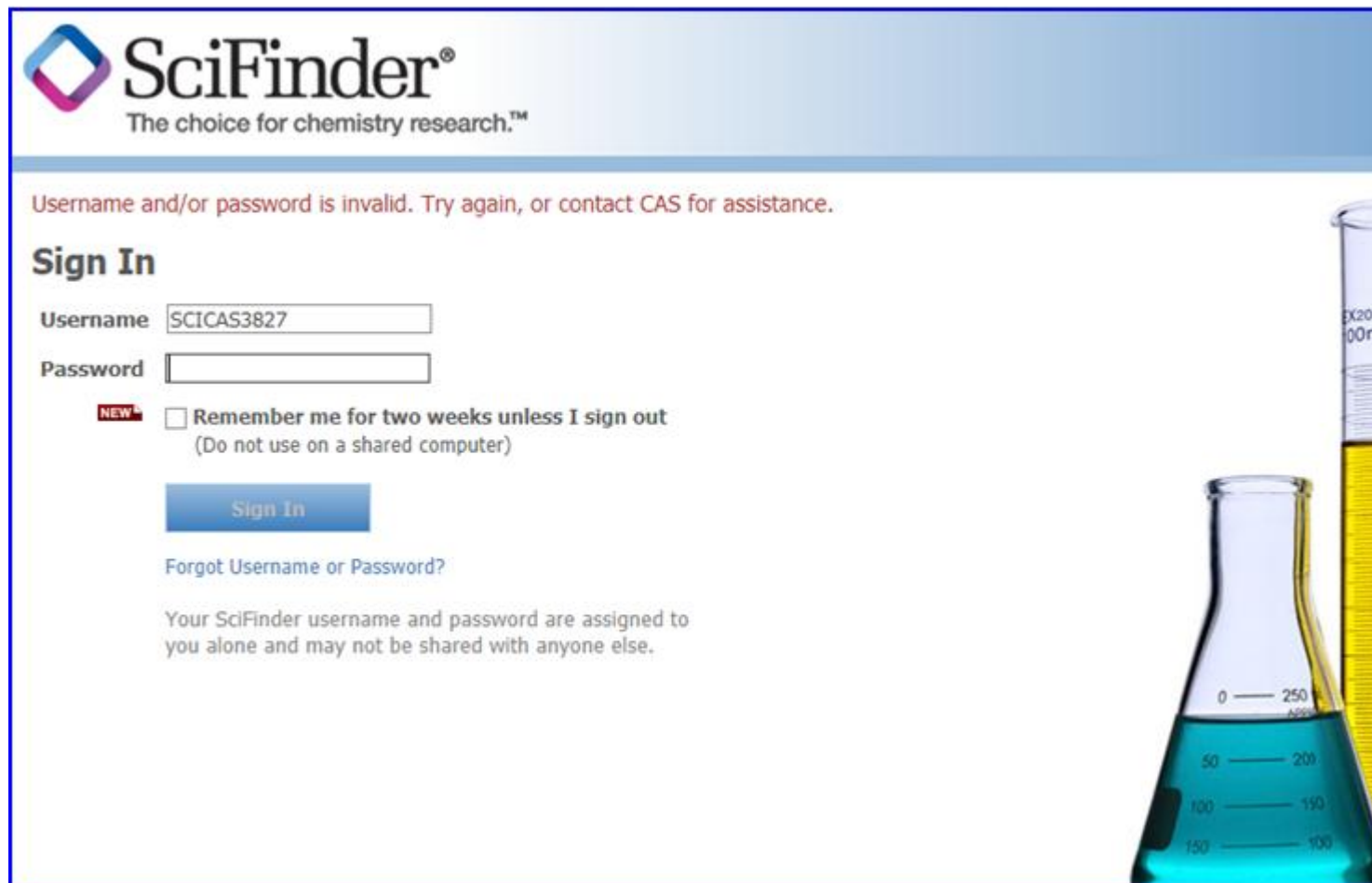
**Sign In**

[Forgot Username or Password?](#)

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

并发用户数已满，请稍后再试

# SciFinder Web 常见问题



The image shows the SciFinder login interface. At the top left is the SciFinder logo with the tagline "The choice for chemistry research.™". Below the logo, a red error message states: "Username and/or password is invalid. Try again, or contact CAS for assistance." The "Sign In" section contains a "Username" field with the text "SCICAS3827", an empty "Password" field, and a checkbox labeled "Remember me for two weeks unless I sign out (Do not use on a shared computer)". A blue "Sign In" button is positioned below the checkbox. A link for "Forgot Username or Password?" is located below the button. At the bottom of the login section, a note reads: "Your SciFinder username and password are assigned to you alone and may not be shared with anyone else." On the right side of the page, there is a vertical image of laboratory glassware, including a test tube and an Erlenmeyer flask, both containing yellow liquid.

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Username and/or password is invalid. Try again, or contact CAS for assistance.

**Sign In**

Username

Password

**NEW** ☐ Remember me for two weeks unless I sign out  
(Do not use on a shared computer)

**Sign In**

[Forgot Username or Password?](#)

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

账号或密码错误，请在username处填写，截图，并与图书馆联系

# SciFinder Web 常见问题

任何需要反馈给图书馆的问题，都请点击测试IP地址的链接

<http://www.cas.org/cgi-bin/casip>



Your IP address comes across to CAS as: 210.32.9.45

将页面做成截图，一并发给图书馆

# SciFinder Web网络在线资源平台

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



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

**Comprehensive Content**  
**Sophisticated Analysis**  
**Unprecedented Results**



***Thank You***

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