



# SciFinder Web

源于化学，超越化学的一站式检索平台

## SciFinder Web使用介绍

曾小雅

SciFinder客户顾问

2014.4



A division of the American Chemical Society

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

# 提纲

- 介绍

- SciFinder Web中的内容

- **SciFinder Web中的检索和后处理**

- SciFinder Web中的文献记录及主题检索
  - SciFinder Web中的物质结果及物质检索方法
  - SciFinder Web中的反应记录及反应检索

- **SciFinder Web的注册**

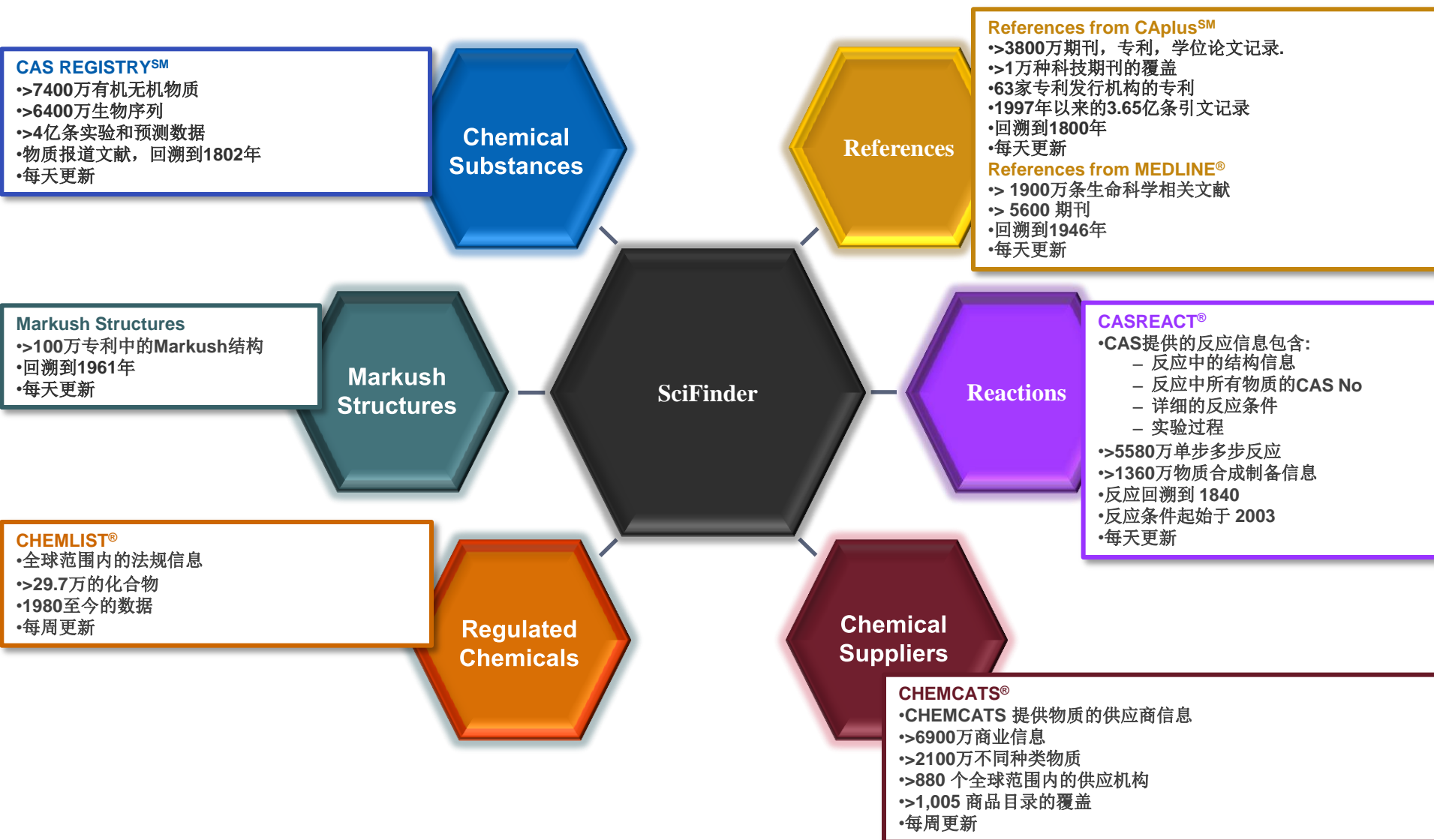
# 美国化学文摘社—Chemical Abstract Service

- ACS的分支机构，创立于1907年
- 致力于跟踪、索引并提炼全球化学相关的科技文献信息
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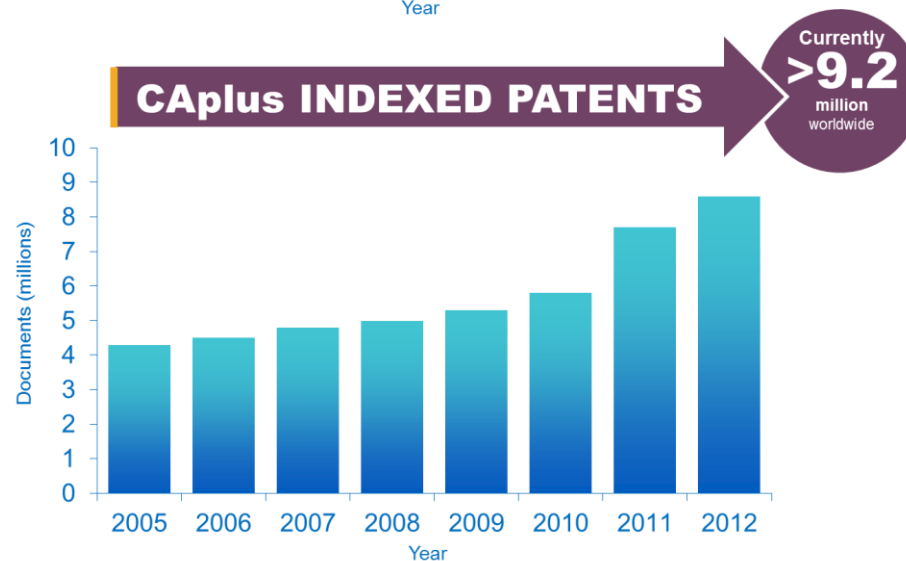
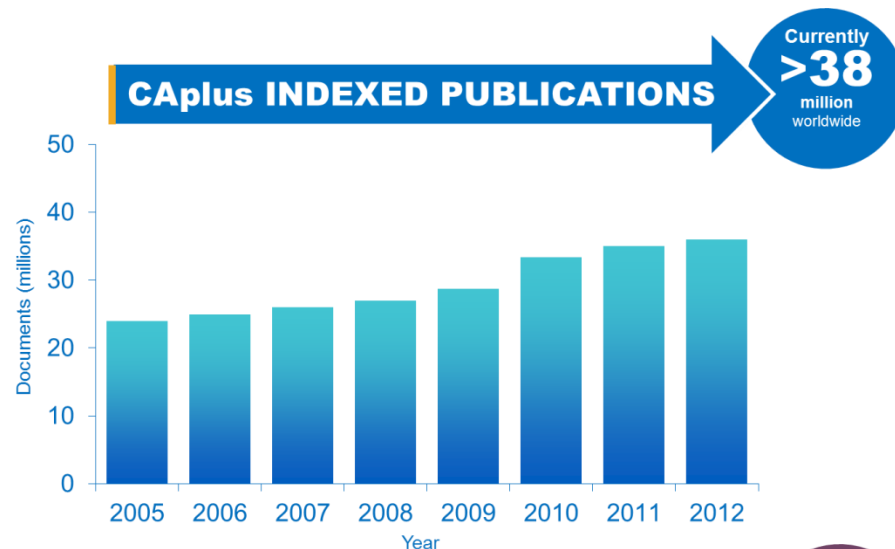
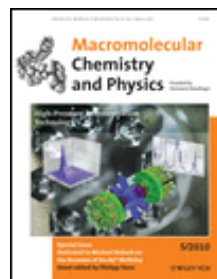
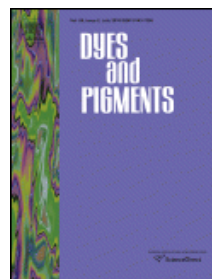
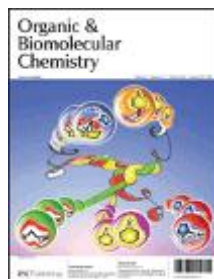
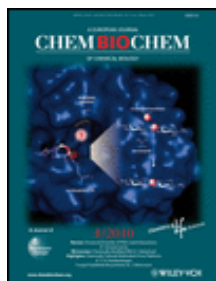


- 1300名员工，精通50多种语言。
- 关注索引上万种期刊和63家专利
- 客户覆盖全球1900所高校、500强公司以及所有主要的专利局。

# SciFinder的覆盖内容

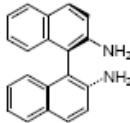


# CAPLUS<sup>SM</sup> 涵盖了上万种期刊及63个专利发行机构专利



# 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 → **DU3090000**

Use → **Intermediate for chiral auxiliaries.**

Hazard alert symbol and description of hazards → **Exp. tumorigen by skin contact. Dec. with emission of toxic fumes. DU3090000**

Supplier Information → **(R)-form: FNCT6-Z [18741-85-0] 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: MMX3-Z [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: MMX3-A [135029-77-5] Cryst. (EtOH/C<sub>6</sub>H<sub>6</sub>). Mp 216-218°. (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. N,N'-Di-Ac: FNCH-V C<sub>24</sub>H<sub>20</sub>N<sub>2</sub>O<sub>2</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). (S)-form: FNCH-W [79082-81-8] Silvery plates (EtOH). Mp 193.2-194.5° (191°). Picrate: FNCH-Z Brownish-yellow plates (C<sub>6</sub>H<sub>6</sub>). Mp 185° (dec.). N,N'-Di-Ac: FNCH-X Cubes (EtOH). Mp 235-236°. N,N'-Dibenzoyl: FNCH-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°.**

Stereoisomer heading →

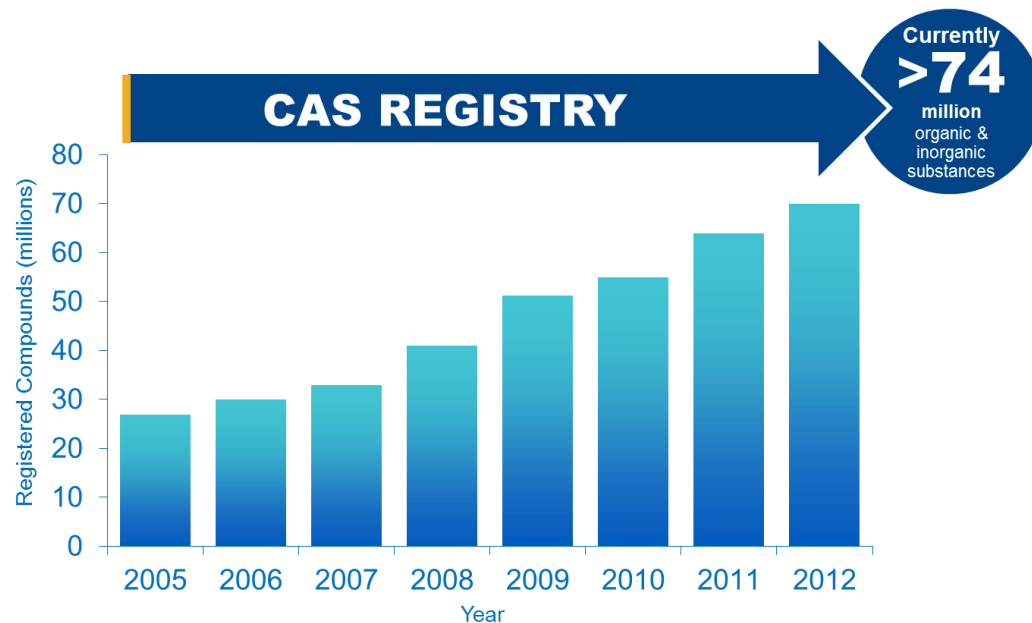
Derivative Subheading →

Additional CAS Registry Numbers → **[93621-61-1] [97644-73-0]**

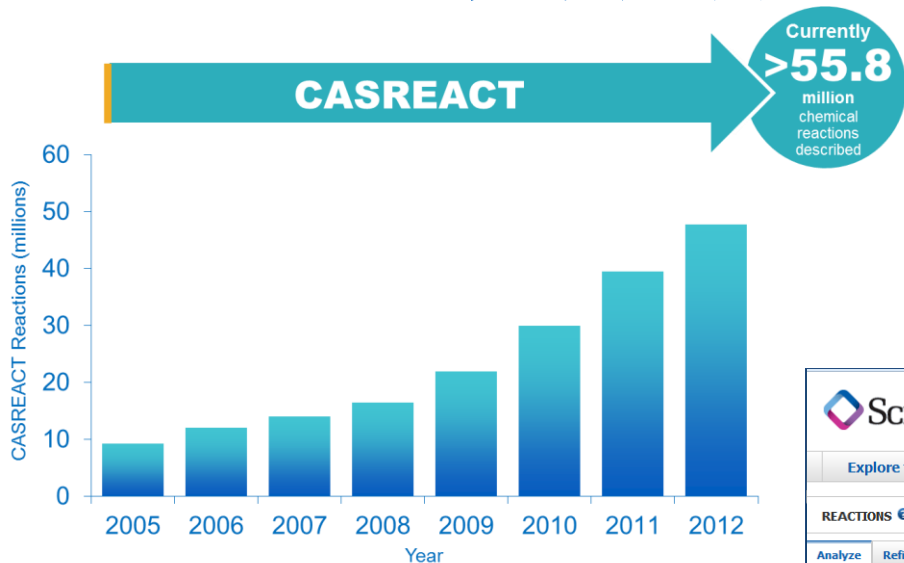
Bibliographic references → **Kuhn, R. et al., *Annalen*, 1929, 470, 183 (*synth, resoln*)  
Cumming, WM. et al., *J.C.S.*, 1932, 528 (*synth*)  
Clemo, GR. et al., *J.C.S.*, 1939, 1114 (*synth*)  
Mislow, K. et al., *J.A.C.S.*, 1962, 84, 1455 (*rev, ora*)  
Akimoto, H. et al., *Tetrahedron*, 1971, 27, 5999 (*resoln, abs config*)  
Miyano, S. et al., *Bull. Chem. Soc. Jpn.*, 1984, 57, 2171 (*pmr, ir, deriv*)  
Brown, KI. et al., *J.O.C.*, 1985, 50, 4345 (*synth, resoln*)  
Beason, 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*)  
Frizzini, L. et al., *Acta Cryst. C*, 1991, 47, 1259 (*cryst struct, N-tetra-Me*)  
Suzcins, M. et al., *J.O.C.*, 1992, 57, 1917 (*synth, resoln, bibl*)  
Lewis, RJ. et al., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, BGS750**

Physical data →

Reference contents →



# CASREACT<sup>®</sup> 是检索化学反应最权威的来源



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**REACTIONS** Get References Tools | Send to SciPlanner

Analyze Refine Group by: No Grouping Sort by: Accession Number

0 of 58 Reactions Selected

1. View Reaction Detail Link Similar Reactions

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

OCC(O)CO >> OCCOCCO

**Overview**

Steps/Stages	Notes
1.1 C:9077-68-3, S:H <sub>2</sub> O, 48 h, rt	regioselective, fermentation, enzymic, biotransformation, whole cells of <i>Lactobacillus</i> sp. cultured from thin stillage expressing glycerol dehydratase used, 90% conversion, Reactants: 1, Catalysts: 1, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

**References**

Process for the conversion of glycerol to 1,3-propanediol by novel *Lactobacillus* strains isolated from stillage Full Text  
By Reaney, Martin J. T. et al  
From PCT Int. Appl., 2012045179, 12 Apr 2012

# 提纲

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- **SciFinder Web中的检索和后处理**

- SciFinder Web中的文献记录及主题检索
  - SciFinder Web中的物质结果及物质检索方法
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- **SciFinder Web的注册**

# SciFinder中的文献记录

REFERENCE DETAIL	Get Substances	Get Related Citations	Get Full Text	Send to SciPlanner
Return				
<p><b>1. Selective oxidation of light alkanes: interaction between the catalyst and the gas phase on different classes of catalytic materials</b></p> <p>By: Cavani, F.; Trifiro, F.</p> <p>A review, with 202 refs., on the selective oxidn. of light (C<sub>5</sub>-6) alkanes to bulk and industrial chems., with emphasis on catalyst-gas phase interactions. Attention was given mainly to: (1) the role of the redox properties of transition metal oxide-based systems, and (2) the contribution of radical-type, homogeneous and heterogeneously-initiated homogeneous reactions over nonreducible metal oxide and noble metal catalysts. Other topics included: (1) key factors in selective oxidn. of light alkanes, (2) bulk and surface properties of catalysts, (3) oxidative dehydrogenation, (4) control of oxygen supply to the catalyst, (5) non-redox-type metal oxides (e.g., alk. earth oxides, rare earth oxides, boron oxides, tin oxides, and silica). Some research examples are: (1) oxidn. of propane to acrylic acid and isobutane to methacrylic acid over Keggin-type heteropolymolybdates, (2) oxidative dehydrogenation of alkanes to alkenes over vanadium oxide-based catalysts, and (3) oxidn. of butane and pentane over vanadyl pyrophosphate.</p>				
<p><b>Indexing</b></p> <p>Fossil Fuels, Derivatives, and Related Products (Section51-0)</p> <p>Section cross-reference(s): 35, 45</p>				
<p><b>Concepts</b></p> <p>Redox reaction catalysts</p> <p>catalyst-gas phase interactions in selective oxidn. of light alkanes to bulk and industrial chems.</p> <p>Alkaline earth oxides      Rare earth oxides</p> <p>catalysts contg.; catalyst-gas phase interactions in selective oxidn. of light alkanes to bulk and industrial chems.</p> <p>Catalyst use; Properties; Uses</p>				
<p><b>Substances</b></p> <p>12026-66-3      58834-75-6</p> <p>catalyst-gas phase interactions in selective oxidn. of light alkanes to bulk and industrial chems.</p> <p>Catalyst use; Uses</p> <p>1303-86-2 Boron oxide, uses      1332-29-2 Tin oxide      7631-86-9 Silica, uses</p>				
<p><b>QUICK LINKS</b></p> <p>0 Tags, 0 Comments</p>				
<p><b>SOURCE</b></p> <p><i>Catalysis Today</i> Volume51 Issue3-4 Pages561-580 Journal; General Review 1999 CODEN:CATTEA ISSN:0920-5861 DOI:10.1016/S0920-5861(99)00041-3</p>				
<p><b>COMPANY/ORGANIZATION</b></p> <p>Dipartimento di Chimica Industriale e dei Materiali Bologna, Italy 40136</p>				
<p><b>ACCESSION NUMBER</b></p> <p>1999:340014 CAN131:159478 CAPLUS</p>				
<p><b>PUBLISHER</b></p> <p>Elsevier Science B.V.</p>				

## Citations

Bielanski, A; Oxygen in Catalysis 1991  
 Haber, J; ACS Symp Series 1996, 638, 20  
 Oyama, S; ACS Symp Series 1996, 638, 2  
 Lee, J; Catal Rev-Sci Eng 1988, 30, 249  
 Kung, H; Adv Catal 1994, 40, 1  
 Viedrine, J; Catal Today 1997, 33, 3  
 Viedrine, J; Catal Today 1996, 32, 115  
 Busca, G; Catal Today 1996, 32, 133  
 Cavani, F; Catalysis 1994, 11, 246  
 Albonetti, S; Catal Rev-Sci Eng 1996, 38, 413  
 Sokolovskii, V; Catal Rev-Sci Eng 1990, 32, 1  
 Delmon, B; Catalysts in Petroleum Refining and Petrochemical Industries 1995 1996  
 Burch, R; J Mol Catal A 1995, 100, 13  
 Schmidt, L; Chem Eng Sci 1994, 49, 3981  
 Kung, H; ACS Symp Series 1993, 523, 387  
 Trifiro, F; Selective Partial Oxidation of Hydrocarbons and Related Oxidations 1994  
 Trifiro, F; Oxidative dehydrogenation and alternative dehydrogenation processes 1993  
 Cavani, F; Catal Today 1995, 24, 307

一篇完整的文献界面包括:

1. 题录信息
2. 摘要信息
3. 文献中重要的概念
4. 文献中重要的物质
5. 书目信息
6. 获得文献中的物质, 反应, 引文等
7. 文献中的引文信息

# SciFinder中的文献检索方法

## 功能方面

- 主题检索
- 作者名检索
- 机构名检索
- 文献标示符检索
- 从物质，反应获得文献

## 检索方法推荐

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

# SciFinder Web中的主题检索

主题: **VEGFR inhibitor with anticancer**(VEGFR抑制剂在抗肿瘤方面的研究进展)

The screenshot displays the SciFinder web interface. At the top, the SciFinder logo is visible. Below it, there are navigation tabs: 'Explore', 'Saved Searches', and 'SciPlanner'. The 'Explore' tab is selected. Under 'Explore', there is a breadcrumb trail: 'Research Topic "VEGFR Inhibitor with anticanc..." > references (618)'. 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', 'Molecular Formula', 'Property', and 'Substance Identifier'. The main content area is titled 'REFERENCES: RESEARCH TOPIC'. It contains a search input field with the text 'VEGFR inhibitor with anticancer'. Below the input field, there are examples: 'The effect of antibiotic residues on dairy products' and 'Photocyanation of aromatic compounds'. A blue 'Search' button is located below the examples. At the bottom of the main content area, there is a link for 'Advanced Search'.

Research Topic "VEGFR Inhibitor with anticanc..." > references (618)

REFERENCES

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

SUBSTANCES

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

REFERENCES: RESEARCH TOPIC

VEGFR inhibitor with anticancer

Examples:

- The effect of antibiotic residues on dairy products
- Photocyanation of aromatic compounds

Search

Advanced Search

使用介词 (of, with, in)  
来连接关键词

# 主题检索的候选项

Explore ▼	Saved Searches ▼	SciPlanner
Research Topic "VEGFR inhibitor with anticanc..."		
REFERENCES ?		
Select All Deselect All		
1 of 5 Research Topic Candidates Selected		References
<input type="checkbox"/>	6 references were found containing <u>"VEGFR inhibitor with anticancer" as entered.</u>	6
<input checked="" type="checkbox"/>	618 references were found containing the two <u>concepts "VEGFR inhibitor" and "anticancer" closely associated with one another.</u>	618
<input type="checkbox"/>	2888 references were found where the two <u>concepts "VEGFR inhibitor" and "anticancer" were present anywhere in the reference.</u>	2888
<input type="checkbox"/>	5255 references were found containing the concept <u>"VEGFR inhibitor".</u>	5255
<input type="checkbox"/>	1001993 references were found containing the concept "anticancer".	1001993
Get References		

- ◆ “as entered” 表示完全匹配
- ◆ “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
- ◆ “present anywhere in the reference” 表示同时出现在一段话中

# SciFinder 中的文献检索结果及后处理

文献分析、  
限定工具 系统分类工具

Research Topic "VEGFR inhibitor with anticanc..." > **references (618)**

**REFERENCES** ?

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**Analyze** **Refine** **Categorize** Sort by: Accession Number

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Author Name

Ciardello Fortunato	15
Troiani Teresa	11
Myers Jeffrey N	9
Fontanini Gabriella	8
Jiang Yuyang	8
Tan Chunyan	8
Tan Yuting	8
Tortora Giampaolo	8
Zhang Shixi	8

- Evidence for G-quadruplex in the promoter of *vegfr-2* and its targeting to inhibit tumor angiogenesis**  
 Quick View Full Text  
 By Salvati, Erica; Zizza, Pasquale; Rizzo, Angela; Iachettini, Sara; Cingolani, Chiara; D'Angelo, Carmen; Porru, Manuela; Randazzo, Antonio; Pagano, Bruno; Novellino, Ettore; et al  
 From Nucleic Acids Research (2014), 42(5), 2945-2957. | Language: English, Database: CAPLUS  

Tumor angiogenesis is mainly mediated by vascular endothelial growth factor (VEGF), a pro-angiogenic factor produced by **cancer** cells and active on the endothelium through the VEGF receptor 2 (**VEGFR-2**). Here we identify a G-rich sequence within the proximal promoter region of *vegfr-2*, able to form an antiparallel G-quadruplex (G4) structure. This G4 structure can be efficiently stabilized by small mols. with the consequent **inhibition** of *vegfr-2* expression. Functionally, the G4-mediated redn. of **VEGFR-2** protein causes a switching off of signaling components that, converging on actin cytoskele...
- Icrucumab, a fully human monoclonal antibody against the vascular endothelial growth factor receptor-1, in the treatment of patients with advanced solid malignancies: a Phase 1 study**  
 Quick View Full Text  
 By Lo Russo, Patricia M.; Krishnamurthi, Smitha; Youssoufian, Hagop; Hall, Nancy; Fox, Floyd; Dontabhaktuni, Aruna; Grebennik, Dmitri; Remick, Scot  
 From Investigational New Drugs (2014), 32(2), 303-311. | Language: English, Database: CAPLUS  

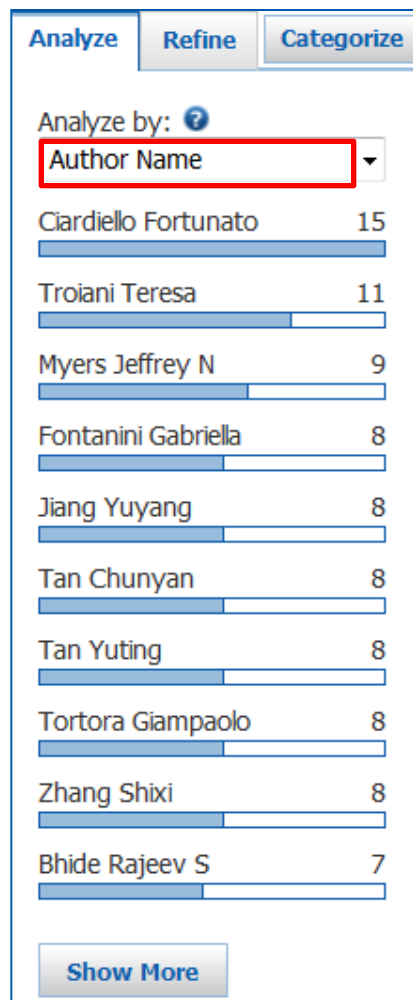
Background IMC-18F1 (icrucumab), a human monoclonal antibody against vascular endothelial growth factor receptor-1 (**VEGFR-1**), potently **inhibits** ligand-dependent phosphorylation of **VEGFR-1** and downstream signaling, making icrucumab an attractive candidate for **antitumor** activity. Objectives The primary objective was to det. the safety profile and max. tolerated dose of icrucumab in patients with advanced solid **tumors** that were previously unresponsive to std. therapy or for which no std. therapy was available. Methods In this open-label, dose-escalation, Phase 1 study, patients received icrucum...

SciFinder提供强大的文献处理工具，帮助处理文献

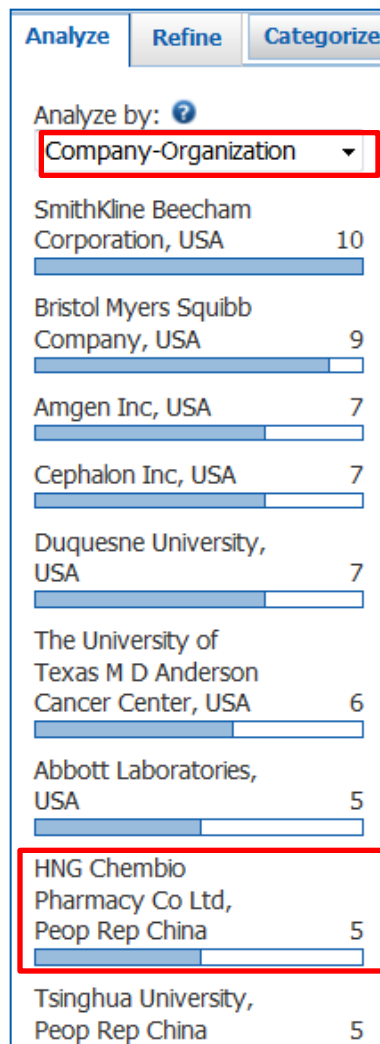
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# SciFinder中的Analyze

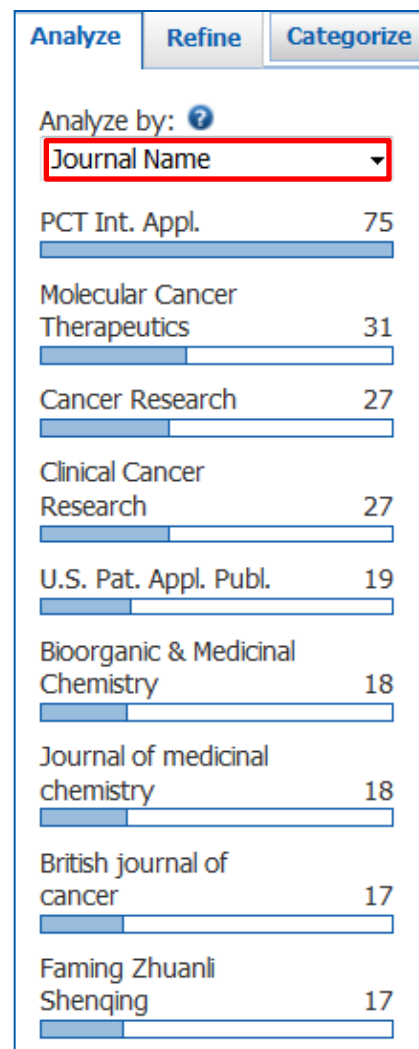
领域内主要研究人员，专家



主要研究机构，合作伙伴，竞争对手

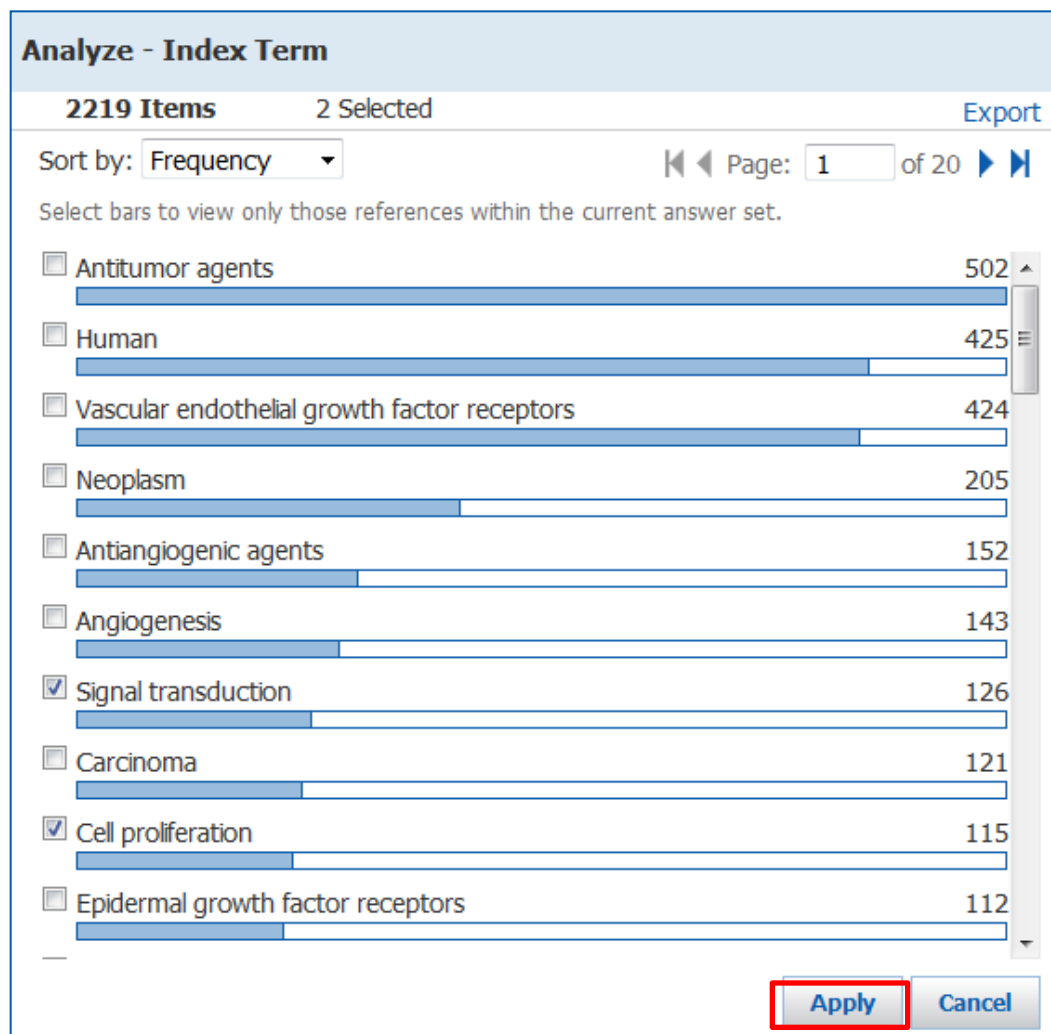
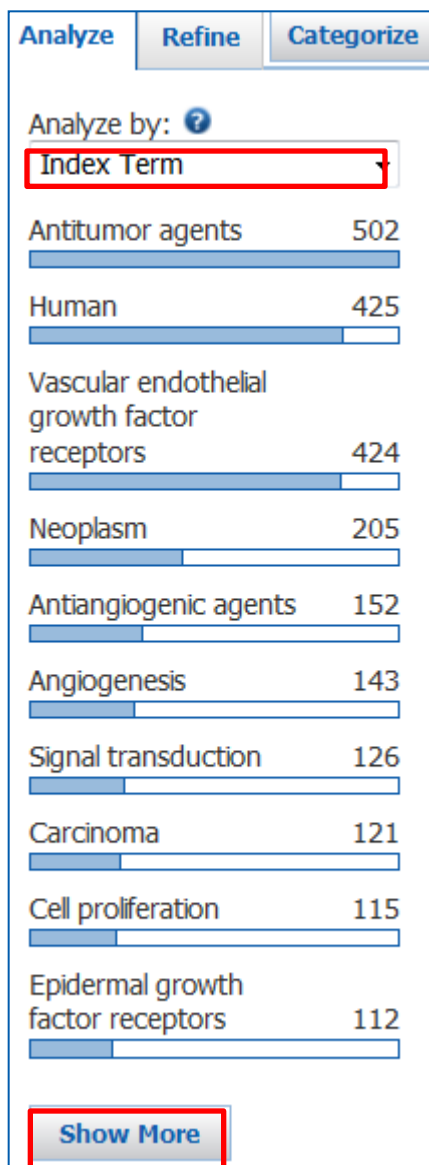


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# SciFinder中的Analyze- Index Term

索引词 (Index Term)：可以帮助我们大致了解文献的内容



# SciFinder中的Refine

文献类型限定：获得最新综述类文献

Analyze
Refine
Categorize

Refine by: ?

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

Document Type(s)

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

Refine

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- VEGF Signal System: The Application of Antiangiogenesis**  
[Quick View](#) [Full Text](#)  
 By Liang, Xuewu; Xu, Fuming; Li, Xiaoguang; Ma, Chunhua; Zhang, Yingjie; Xu, Wenfang  
 From Current Medicinal Chemistry (2014), 21(7), 894-910. | Language: English, Database: CAPLUS  

A review. Among the numerous endogenous promoters of angiogenesis, vascular endothelial growth factor (VEGF) plays a leading role in angiogenesis, which has huge impact on proliferation, survival, migration and permeability of **tumor** cells. VEGF signal system also becomes remarkable **anticancer** targets, including VEGF, vascular endothelial growth factor receptor (**VEGFR**), and VEGF downstream signal pathways. So far, there has been many clin. or approved **anticancer** drugs that directly or indirectly interfere with VEGF signal system applied in the treatment of various **tumors** and other diseases as...
- Clinical Pharmacology of Axitinib**  
[Quick View](#) [Full Text](#)  
 By Chen, Ying; Tortorici, Michael A.; Garrett, May; Hee, Brian; Klamers, Karen J.; Pithavala, Yazdi K.  
 From Clinical Pharmacokinetics (2013), 52(9), 713-725. | Language: English, Database: CAPLUS  

A review. Axitinib is a potent and selective second-generation **inhibitor** of vascular endothelial growth factor receptors 1, 2, and 3 that is approved in the US and several other countries for treatment of patients with advanced renal cell **carcinoma** after failure of one prior systemic therapy. The recommended clin. starting dose of axitinib is 5 mg twice daily, taken with or without food. Dose increase (up to a max. of 10 mg twice daily) or redn. is permitted based on individual tolerability. Axitinib pharmacokinetics are dose-proportional within 1-20 mg twice daily, which includes the clin...
- BIBF 1120/nintedanib: a new triple angiokinase inhibitor-directed therapy in patients with non-small cell lung cancer**  
[Quick View](#) [Full Text](#)  
 By Rolfo, Christian; Raez, Luis E.; Bronte, Giuseppe; Santos, Edgardo S.; Papadimitriou, Kostantinos; Buffoni, Lucio; van Meerbeeck, Jan P.; Russo, Antonio  
 From Expert Opinion on Investigational Drugs (2013), 22(8), 1081-1088. | Language: English, Database: CAPLUS  

A review. Introduction: Several new targeted agents with **anti**-angiogenic properties have been developed recently, including vandetanib, sunitinib, sorafenib, bevacizumab and others. **Tumor** development, progression, metastasis are strongly linked to angiogenesis. Targeted agents like bevacizumab, a monoclonal antibody which targets VEGF, have been fully developed in several solid **tumors**. These new agents strongly advocate that targeting angiogenesis is one of the best approaches for **cancer** therapy. Areas covered: Those agents that target addnl. pro-angiogenic intracellular signaling pathways...

# SciFinder 中的Categorize

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Tan Chunyan	8
Tan Yuting	8
Tortora Giampaolo	8
Zhang Shixi	8
Bhide Rajeev S	7

1. Evidence for G-quadruplex in the promoter of vegfr-2 and its targeting to inhibit tumor angiogenesis

Quick View Full Text

By Salvati, Erica; Zizza, Pasquale; Rizzo, Angela; Iachettini, Sara; Cingolani, Chiara; D'Angelo, Carmen; Porru, Manuela; Randazzo, Antonio; Pagano, Bruno; Novellino, Ettore; et al  
From Nucleic Acids Research (2014), 42(5), 2945-2957. | Language: English, Database: CAPLUS

Tumor angiogenesis is mainly mediated by vascular endothelial growth factor (VEGF), a pro-angiogenic factor produced by cancer cells and active on the endothelium through the VEGF receptor 2 (VEGFR-2). Here we identify a G-rich sequence within the proximal promoter region of vegfr-2, able to form an antiparallel G-quadruplex (G4) structure. This G4 structure can be efficiently stabilized by small mols. with the consequent inhibition of vegfr-2 expression. Functionally, the G4-mediated redn. of VEGFR-2 protein causes a switching off of signaling components that, converging on actin cytoskele...

2. Icrucumab, a fully human monoclonal antibody against the vascular endothelial growth factor receptor-1, in the treatment of patients with advanced solid malignancies: a Phase 1 study

Quick View Full Text

By Lo Russo, Patricia M.; Krishnamurthi, Smitha; Youssoufian, Hagop; Hall, Nancy; Fox, Floyd; Dontabhaktuni, Aruna; Grebennik, Dmitri; Remick, Scot  
From Investigational New Drugs (2014), 32(2), 303-311. | Language: English, Database: CAPLUS

Background IMC-18F1 (icrucumab), a human monoclonal antibody against vascular endothelial growth factor receptor-1 (VEGFR-1), potentially inhibits ligand-dependent phosphorylation of VEGFR-1 and downstream signaling, making icrucumab an attractive candidate for antitumor activity. Objectives The primary objective was to det. the safety profile and max. tolerated dose of icrucumab in patients with advanced solid tumors that were previously unresponsive to std. therapy or for which no std. therapy was available. Methods In this open-label, dose-escalation, Phase 1 study, patients received icrucum...

3. Use of neural stem cells for treatment of malignancy using a biocompatible adhesive at the post-surgical site to inhibit angiogenesis

Quick View Full Text PDF

By Crawford, Susan E.

Categorize系统分类功能，基于Index Term，对文献依学科方向进行分类

# SciFinder中的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 medicine (8704)
General chemistry	Medicine (323)
<b>Biotechnology</b>	Substances in biological uses (1035)
Synthetic chemistry	Substances in adverse effects (165)
Genetics & protein chemistry	Toxicology & forensics (23)
Biology	Agriculture (22)
Physical chemistry	Food (6)
Polymer chemistry	
Analytical chemistry	
Technology	
Environmental chemistry	
Catalysis	

2. Select index terms of interest.

Index Terms	
Page: 1 of 88	
Select All Deselect All	
<input type="checkbox"/> ZD6474	54
<input checked="" type="checkbox"/> Sorafenib	46
<input type="checkbox"/> Antitumor agents	36
<input type="checkbox"/> Antibodies and Immunoglobulins	34
<input type="checkbox"/> Bevacizumab	33
<input checked="" type="checkbox"/> Paclitaxel	33
<input type="checkbox"/> Sunitinib	33
<input type="checkbox"/> Gefitinib	28
<input type="checkbox"/> Vascular endothelial growth factor receptors	27
<input type="checkbox"/> Erlotinib	22
<input type="checkbox"/> 5-Fluorouracil	21
<input type="checkbox"/> Cetuximab	21
<input type="checkbox"/> Cisplatin	21
<input type="checkbox"/> Carboplatin	20

Selected Terms

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

✖ Biotechnology > Substances in medicine (2 Terms)

索拉菲尼  
紫杉醇

Biotechnology > Substances in medicine > 2 Index Term(s) Selected

OK Cancel

# SciFinder中的KMP

随时跟踪科研最新进展

The screenshot shows the SciFinder web interface. At the top, there are navigation tabs: 'Get Substances', 'Get Reactions', 'Get Related Citations', 'Get Full Text', and 'Tools'. A red box highlights the 'Create Keep Me Posted Alert' button. Below the navigation bar, there is a 'Sort by: Citing References' dropdown and a 'Display Options' link. The main content area displays search results for '0 of 485 References Selected'. Two results are visible:

- 1. Stability of food allergens to digestion in vitro**  
By Astwood, James D.; Leach, John N.; Fuchs, Roy L.  
From Nature Biotechnology (1996), 14(10), 1269-1273. | Language: English, Database: CAPLUS  
An integral part of the **safety** assessment of **genetically modified** plants is consideration of possible human health effects, esp. **food** allergy. Prospective testing for allergenicity of proteins obtained from sources with no prior history of causing allergy has been difficult because of the absence of valid methods and models. **Food** allergens may share physicochem. properties that distinguish them from nonallergens, properties that may be used as a tool to predict the inherent allergenicity of proteins newly introduced into the **food** supply by **genetic** engineering. One candidate property is stab...
- 2. The feeding value of soybeans fed to rats, chickens, catfish and dairy cattle is not altered by genetic incorporation of glyphosate tolerance**  
By Hammond, Bruce G.; Vicini, John L.; Hartnell, Gary F.; Naylor, Mark W.; Knight, Christopher D.; Robinson, Edwin H.; Fuchs, Roy L.; Padgett, Stephen R.  
From Journal of Nutrition (1996), 126(3), 717-27. | Language: English, Database: CAPLUS  
Animal **feeding** studies were conducted with rats, broiler chickens, catfish and dairy cattle fed diets containing **genetically modified** to tolerate in-season application of glyphosate. The **feeding** value of the diets of glyphosate-tolerant soybeans (GTS) to the **feeding** value of the parent soybeans was compared. The diets at the same concns. as used com.; dairy cows were fed 10 g/...

The 'Create Keep Me Posted Profile' dialog box is shown, with the following fields and options:

- Title:** \* Required (Annotation: 题目)
- Description:** (Annotation: 设置有效期)
- Duration:** Expires On: Mar 07, 2015 (Change)
- Frequency:** Send updates once every Week (Annotation: 设置提醒频率)
- ☐ Exclude previously retrieved references.
- Search:** Explore references by research topic: **Genetically Modified Food with safety**
- Candidates Selected:** References which contain the two concepts "Genetically Modified Food" and "safety" closely associated with one another
- Create** and **Cancel** buttons.

# 结果集的保存

SciFinder®

Preferences | SciFinder Help | Sign Out

Welcome Sam Yu

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

Research Topic "gold nanoparticles with modifi..." > references (5792) > refine "China" (2270)

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: Citing References | 0 of 2270 References Selected | Page: 1 of 114

1. **Graphene/AuNPs/chitosan nanocomposites film for glucose biosensing** | Full Text  
 By Shan, Changsheng; Yang, Hualong; Han, Dongxue; Zhang, Qilang; Ivaska, Art; Niu, Li  
 From Biosensors & Bioelectronics (2010), 25(5), 1070-1074. | Language: English, Database: CAPLUS  
 ~212

2. **CdS Nanocrystal-Based Electrochemiluminescence Biosensor for the Detection of Low-Density Lipoprotein by Increasing Sensitivity with Gold Nanoparticle Amplification** | Full Text  
 By Jie, Guifeng; Liu, Bo; Pan, Hongcheng; Zhu, Jun-Jie; Chen, Hong-Yuan  
 From Analytical Chemistry (Washington, DC, United States) (2007), 79(15), 5574-5581. | Language: English, Database: CAPLUS  
 ~172

Chinese Academy of Sciences, Peop Rep China 160  
 Southwest University, Peop Rep China 94  
 Nanjing University, Peop Rep China 71  
 Hunan University, Peop Rep China 65  
 Anhui Normal University, Peop Rep China 58

**Export:**

**Citation manager:** 保存成RIS格式，用于导入EndNote等文献管理工具

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

**Save This Answer Set** ⓘ

\* Required

**Save:**

☒ All answers

☐ Only selected answers

**Title: \***

**Description:**

OK Cancel

**Save:**

保存在服务器上，可登陆后查看

**Export** ⓘ

\* Required

**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 (\*.alox)

**Details:**

**File Name: \***

Export Cancel

## 练习

- 检索和转基因食品安全评估的文献，获得近5年的综述文献
  
- 检索策略：
  - Topic Search: Genetically Modified Food with safety
  - Refine publish year: 2009-
  - Refine document type: Review

## 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

更多细节化内容，请参考

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

# 提纲

- 介绍

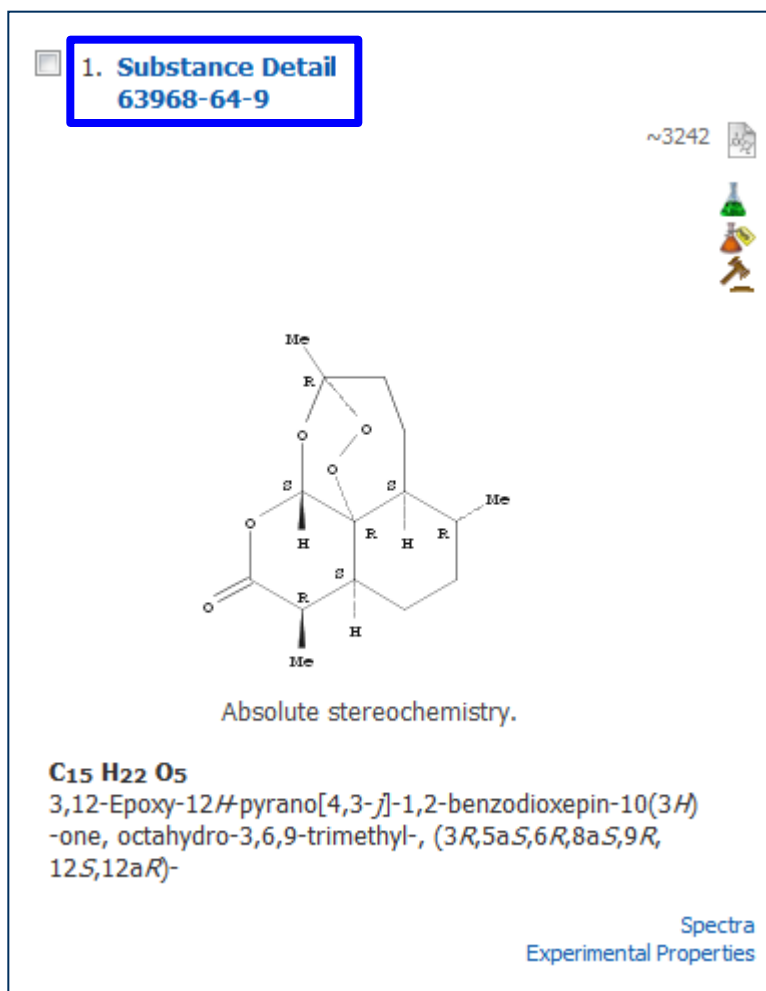
- SciFinder Web中的内容

- **SciFinder Web中的检索和后处理**

- SciFinder Web中的文献记录及主题检索
  - SciFinder Web中的物质结果及物质检索方法
  - SciFinder Web中的反应记录及反应检索

- **SciFinder Web的注册**

# SciFinder中的物质结果界面



一个完整的物质结果界面包含：

- 物质详情链接
- 文献链接
- 反应链接
- 商品信息链接
- 管制品信息链接
- 谱图链接
- 实验性质链接

# Substance Detail—查看物质详细信息

SciFinder®

Explore ▾ Saved Searches ▾ SciPlanner

Substance Identifier "qinghaosu" > substances (1) > 63968-64-9

SUBSTANCE DETAIL ⓘ

Get References Get Reactions Get Commercial Sources Get Regulatory Information

Return

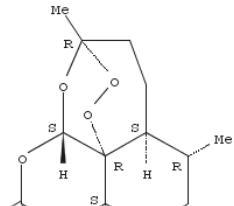
**CAS Registry Number:** 63968-64-9

C<sub>15</sub> H<sub>22</sub> O<sub>5</sub>

3,12-Epoxy-12H-pyrano[4,3-*f*]-1,2-benzodioxepin-10(3*H*)-one, octahydro-3,6,9-trimethyl-, (3*R*,5*a*,5,6*R*,8*a*,5,9*R*,12*S*,12*a**R*)-

3,12-Epoxy-12H-pyrano[4,3-*j*]-1,2-benzodioxepin-10(3*H*)-one, octahydro-3,6,9-trimethyl-, [3*R*-(3*a*,5*a*β,6β,8*a*β,9*a*,12β,12*a**R*\*)]-; (+)-Arteannuin; (+)-Artemisinin; (+)-Qinghaosu; Arteannuin; Artemef; Artemisine; Artemisinin; Artemisinine; Huanghuahaosu; NSC 369397; QHS; Qing Hau Sau; Qing Hau Su; Qinghaosu; Qinghosu

**Deleted CAS Registry Numbers:** 91487-93-3



物质的CAS号、分子式、结构式、化学名、别名

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。

Document Types: Book, Conference, Dissertation, Journal, Patent, Report

CAS Role	Patents	Nonpatents	Nonspecific Derivatives from Patents	Nonspecific Derivatives from Nonpatents
Analytical Study	✓	✓	✓	✓
Biological Study	✓	✓	✓	✓
Formation, Nonpreparative		✓	✓	✓
Miscellaneous	✓	✓		
Occurrence	✓	✓		✓
Preparation	✓	✓	✓	✓
Process	✓	✓	✓	✓
Properties	✓	✓	✓	✓
Prophetic in Patents	✓			
Reactant or Reagent	✓	✓	✓	✓
Uses	✓	✓	✓	✓

# Substance Detail—查看物质详细信息

▼ Bioactivity Indicators <small>NEW</small>		References
Anti-infective agents (all) >>> Antimalarials		805
Anti-infective agents (all) >>> Antiviral agents		34
Anti-infective agents (all) >> Parasitocides		43
Anti-inflammatory agents (all) > Anti-inflammatory agents		41
Antitumor agents (all) > Antitumor agents		169
Natural products MD pharmaceutical		108

▼ Target Indicators <small>NEW</small>		References
Cytokines (all) >> Chemokines		13
Cytokines (all) >> Tumor necrosis factors		11
DNA-binding proteins (all) >>> Transcription factor NF- $\kappa$ B		21
Enzymes (all) >>>> Adenosine triphosphatase		15
Enzymes (all) >>>> 26S proteasome		15
Enzymes (all) >>>>>> Src kinase		13
Glycoproteins (all) >> P-glycoproteins		15
Hemoproteins (all) >>> Cytochrome P 450		12
Hemoproteins (all) >>> Cytochrome P 450 3A4		12
Phosphoproteins (all) >> P-glycoproteins		15
Proteins		19
Receptors (all) > Toll-like receptors		13
RNA formation factors (all) >>>		21
Transcription factors (all) >>>		21
Transporters (all) >>>		21
Transposons (all) >>>		21
Endoplasmic reticulum (all) >>>		21

物质的生物活性和靶点信息，  
直接点击，获得相关文献

SciFinder®

Preferences | SciFinder Help | Sign Out

Welcome Sam Yu

Explore ▼ Saved Searches ▼ SciPlanner Save Print Export

Substance Identifier "qinghaosu" > substances (1) > 63968-64-9 > get references (24)

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 ↓

0 of 24 References Selected

1. **Enhanced IL-12p40 production in LPS-stimulated macrophages by inhibiting JNK activation by artemisinin** ⓘ Full Text  
By Cho, Young-Chang; Lee, Sung Ho; Lee, Mina; Kim, Hyun Jung; Oak, Min-ho; Lee, Ik-Soo; Kang, Bok Yun  
From Archives of Pharmacol Research (2012), 35(11), 1961-1968. | Language: English, Database: CAPLUS

Artemisinin can be isolated from *Artemisia annua* L. In addn. to its well-known anti-malarial activity, artemisinin has antitumor and anti-microbial effects. In this study, we investigated the effect of artemisinin on the prodn. of IL-12p40, which is important in the generation of T helper 1 responses. Artemisinin significantly induced IL-12p40 prodn. in LPS-stimulated RAW264.7 macrophage cells. To elucidate the signaling mols. regulated by artemisinin in induced IL-12p40 prodn., the DNA-binding activity of several transcription factors and activation of mitogen-activated protein kinase (MA...

2. **Artemisinin attenuates post-infarct myocardial remodelling by down-regulating the NF- $\kappa$ B pathway** ⓘ Full Text  
By Gu, Yongwei; Wang, Xi; Wang, Xin; Yuan, Mingjie; Wu, Gang; Hu, Juan; Tang, Yanhong; Huang, Congxin  
From Tohoku Journal of Experimental Medicine (2012), 227(3), 161-170. | Language: English, Database: CAPLUS

Myocardial infarction (MI) leads to progressive left ventricular (LV) dilatation and is assocd. with interstitial fibrosis in the non-infarcted myocardium. The NF- $\kappa$ B signaling pathway plays an important role in ventricular remodeling after MI. Recent studies have indicated that the anti-malarial agent artemisinin can inhibit NF- $\kappa$ B activation, which may attenuate post-infarct myocardial remodeling. In this study, we investigated the effect of artemisinin on post-infarct myocardial remodeling using a rat model of MI. Adult male Sprague Dawley rats were divided into a sham group (n = 10) and ...

# Substance Detail—查看物质详细信息

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

Biological Properties	Value	Condition	Note	Top
Bioconcentration Factor	31.2	pH 1 Temp: 25 °C	(26)	
Bioconcentration Factor	31.2	pH 2 Temp: 25 °C	(26)	
Bioconcentration Factor	31.2	pH 3 Temp: 25 °C	(26)	
Bioconcentration Factor	31.2	pH 4 Temp: 25 °C	(26)	
Bioconcentration Factor	31.2	pH 5 Temp: 25 °C	(26)	
Bioconcentration Factor	31.2	pH 6 Temp: 25 °C	(26)	
Bioconcentration Factor	31.2	pH 7 Temp: 25 °C	(26)	
Bioconcentration Factor	31.2	pH 8 Temp: 25 °C	(26)	
Bioconcentration Factor	31.2	pH 9 Temp: 25 °C	(26)	
Bioconcentration Factor	31.2	pH 10 Temp: 25 °C	(26)	

Lipinski and Related Properties	Value	Condition	Note	Top
Freely Rotatable Bonds	0		(26)	
H Acceptors	5		(26)	
H Donors	0		(26)	
H Donor/Acceptor Sum	5		(26)	
logP	2.269±0.680	Temp: 25 °C	(26)	
Molecular Weight	282.33		(26)	
Spectra Properties	Value	Condition	Note	Top
Carbon-13 NMR Spectrum	See spectrum		(27)	
Proton NMR Spectrum	See spectrum		(27)	

# Substance Detail—查看物质详细信息

**Experimental Properties:** Biological Chemical Density Flow and Diffusion Lipinski and Related Optical and Scattering Spectra Structure-related Thermal

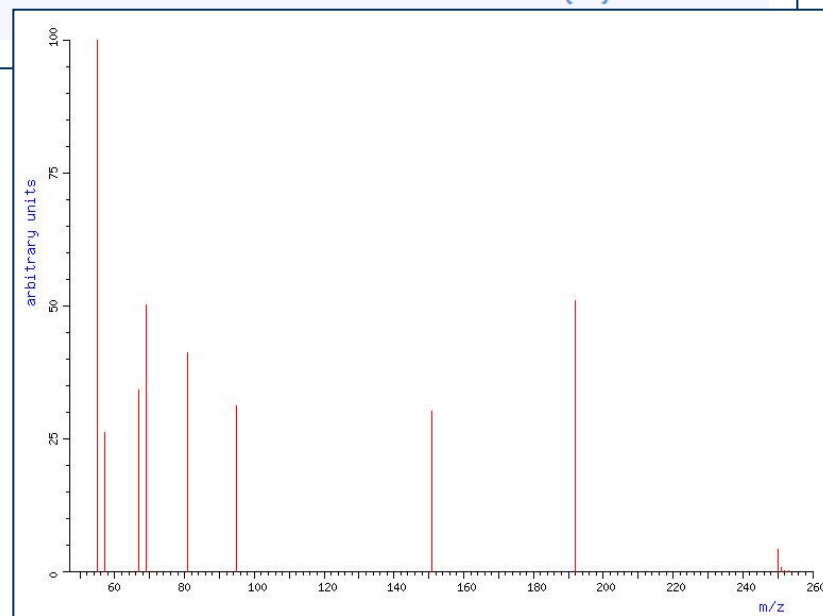
Biological Properties	Value	Condition	Note	Top
ADME (Absorption, Distribution, Metabolism, Excretion)	See full text		(1)CAS	
Half-Life (Biological)	See full text	1 of 2	(9)CAS	
Median Lethal Dose(LD50)	5576 mg/kg	Organism: rat Route: oral	(14)APC	
Median Lethal Dose(LD50)	5105 mg/kg	Organism: mouse Route: oral	(14)APC	
Median Lethal Dose(LD50)	2800 mg/kg	Organism: mouse Route: intramuscular	(14)APC	
Median Lethal Dose(LD50)	2571 mg/kg	Organism: rat Route: intramuscular	(14)APC	
Median Lethal Dose(LD50)	1558 mg/kg	Organism: mouse Route: intraperitoneal	(14)APC	
Minimum Inhibitory Concentration	See full text	1 of 2	(18)CAS	

Lipinski and Related Properties	Value	Condition	Note	Top
logP	See full text	1 of 2	(12)CAS	
Optical and Scattering Properties	Value	Condition	Note	Top
Optical Rotatory Power	+87.9 °	Solv: 1,4-dioxane (123-91-1); Wavlen: 589.3 nm	(20)CAS	
Optical Rotatory Power	+75-+78 °	Conc: 1.0 g/100mL; Solv: ethanol (64-17-5); Wavlen: 589.3 nm; Temp: 20 °C	(12)CAS	
Optical Rotatory Power	+68.2 °	Conc: 0.97 g/100mL; Solv: chloroform (67-66-3); Temp: 25 °C	(16)IC	

# Substance Detail—查看物质详细信息

Spectra Properties	Value	Condition	Note	Top
Carbon-13 NMR Spectrum	See full text	1 of 8	(3)CAS	
Circular Dichroism Spectrum	See full text	1 of 2	(4)IC	
IR Absorption Spectrum	See full text	1 of 11	(11)CAS	
Mass Spectrum	<a href="#">See spectrum</a>		(13)WSS	
Mass Spectrum	<a href="#">See spectrum</a>		(13)WSS	
Mass Spectrum	See full text	1 of 10	(1)CAS	
Proton NMR Spectrum	See full text	1 of 10	(15)CAS	
Raman Spectrum	See full text	1 of 2	(5)CAS	
Two-Dimensional NMR Spectrum	See full text	1 of 2	(24)CAS	
UV and Visible Absorption Spectrum	See full text		(22)CAS	
UV and Visible Emission/Luminescence Spectrum	See full text		(25)CAS	

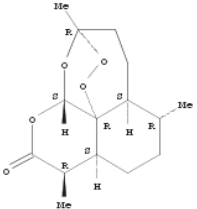
## 物质的实验谱图



# 物质有关的反应

1. Substance Detail  
63968-64-9

~3242



Absolute stereochemistry.

**C<sub>15</sub>H<sub>22</sub>O<sub>5</sub>**  
3,12-Epoxy-12H-pyrano[4,3-j]-1,2-benzodioxepin-10(3H)-one, octahydro-3,6,9-trimethyl-, (3R,5aS,6R,8aS,9R,12S,12aR)-


## Get Reactions

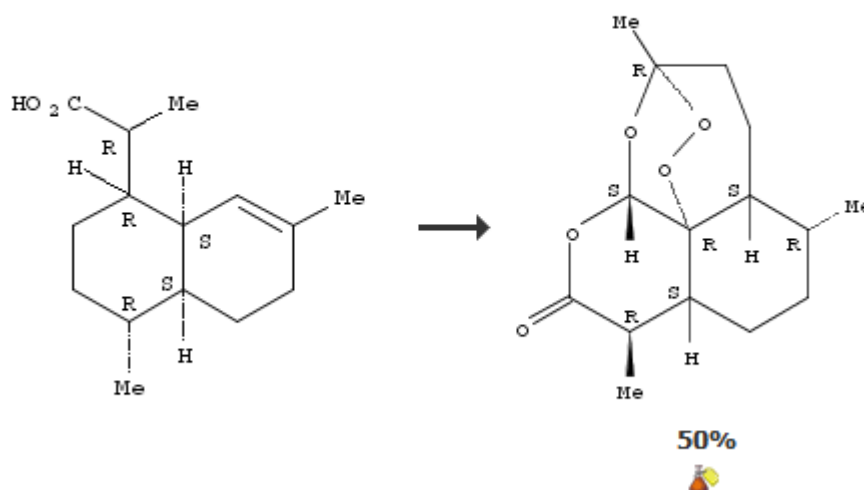
Limit results by reaction role:

☒ Product

- ☐ Reactant
- ☐ Reagent
- ☐ Reactant or reagent
- ☐ Catalyst
- ☐ Solvent
- ☐ Any role

Get Cancel

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




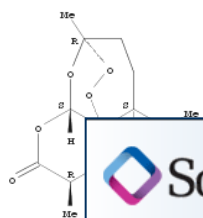
► Overview

# 物质有关的商业来源

可以直接Export到Excel中，又或者使用分析工具，对商业信息进行处理

1. Substance Detail  
63968-64-9

~3242 



Absolute

**C<sub>15</sub> H<sub>22</sub> O<sub>5</sub>**  
3,12-Epoxy-12H-pyrano[3,4-b:4',5'-d]pyridine, octahydro-3,6,9-trimethyl-12,5,12aH-

[Preferences](#) | [SciFinder Help](#) | [Sign Out](#)

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Explore ▾
Saved Searches ▾
SciPlanner

⚠ This chemical supplier information is provided on an "as is" basis. Please consult the suppliers for current information regarding pricing, regional availability, available quantities, purities, etc. THERE ARE NO WARRANTIES OF ANY KIND, EITHER EXPRESSED OR IMPLIED. ACS is not liable for any loss of profit, goodwill or any other damages arising out of the use of this information.

Substance Identifier "qinghaosu" > substances (1) > 63968-64-9 > **commercial sources (91)**

**COMMERCIAL SOURCES** ?

Analyze by: ?

Catalog Name ▾

Accel Pharmtech Product List 2

AK Scientific Product Catalog 2

Chemieliva Pharmaceutical Product List 2

ChemPacific Product

Sort by: Catalog Name ▾ ↑
Answers per Page [20]

0 of 91 Commercial Sources Selected
Page: 1 of 5

1. **3B Scientific Corporation Product List**

Supplier Name: 3B Scientific Corporation, Catalog Publication Date: 12 Jul 2012

Order Number: 3B2-3802

Quantity: 1g

63968-64-9 Artemisinin

[Link](#)

2. **A Chemtek Product List**

Supplier Name: A Chemtek, Catalog Publication Date: 13 Mar 2013

Order Number: 031-18967

Quantity: N/A

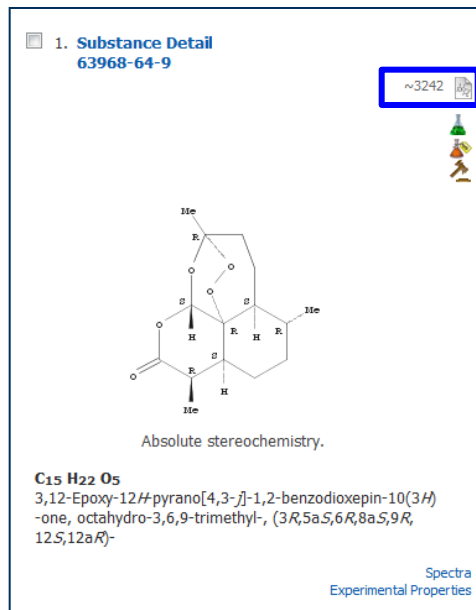
63968-64-9 Artemisinin

CAS is a division of the American Chemical Society.

32

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# 物质有关的文献信息



一键获得文献，可以获得全部，也可以勾选特别感兴趣的内容，不勾选，默认获得全部

**Get References**

**Limit results to:**

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

**For each sequence, retrieve:**

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

**Get Cancel**

# SciFinder中的物质检索方法

## ■ 功能方面

- 物质名称, CAS No
- 分子式
- 结构式
- 理化性质

## ■ 推荐的物质检索功能

- 有机物, 天然产物及衍生物
- 无机物
- 高分子化合物

---结构比较方便

---分子式比较方便


---首先分子式, 其次结构

# 物质名称检索

The screenshot displays the SciFinder web application. At the top, the SciFinder logo is visible. Below the logo, there are navigation tabs: 'Explore', 'Saved Searches', and 'SciPlanner'. The 'Explore' tab is selected. The breadcrumb trail indicates the search path: 'Substance Identifier "qinghaosu" > substances (1) > 63968-64-9 > commercial sources (91)'. On the left side, there is a sidebar with three main categories: 'REFERENCES', 'SUBSTANCES', and 'REACTIONS'. Under 'SUBSTANCES', the 'Substance Identifier' option is highlighted. The main search area is titled 'SUBSTANCES: SUBSTANCE IDENTIFIER'. It features a large text input field containing the text 'qinghaosu'. Below the input field, there is a small text prompt: 'Enter one per line. Examples: 50-00-0, 999815, Acetaminophen'. A blue 'Search' button is located below the input field. A black arrow points from the bottom right towards the 'Search' button.

直接输入物质的名称，**CAS No**，俗名，都能检索，一次最多检索**25**个物质，用换行换开

# 理化性质检索

Pre

Explore ▾ Saved Searches ▾ SciPlanner

Substance Identifier "qinghaosu " > substances (1) > 63968-64-9 > commercial sources (91)

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

Value or Range

Select Property... ▾

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

☐ Predicted

Value or Range

Select Property... ▾

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

Search

# 分子式检索

The screenshot displays the SciFinder web interface. At the top, the SciFinder logo is visible. Below it, there are navigation tabs: "Explore", "Saved Searches", and "SciPlanner". A breadcrumb trail indicates the current path: "Substance Identifier 'qinghaosu' > substances (1) > 63968-64-9 > commercial sources (91)".

On the left side, there is a sidebar with three main sections: "REFERENCES", "SUBSTANCES", and "REACTIONS". Under "SUBSTANCES", the "Molecular Formula" option is selected and highlighted.

The main content area is titled "SUBSTANCES: MOLECULAR FORMULA". It features a search input field containing the text "(C3 H6 O. C2 H4 O)x". Below the input field, there are examples of molecular formulas: "H4SiO4" and "(C3H6O.C2H4O)x". A blue "Search" button is positioned below the examples. A large black arrow points from the bottom right towards the search input field.

SciFinder中的分子式的检索，需要按照HILL排序方式输入，简单来说，**CH**写前面，其他的按照字母顺序写

# 结构式检索—精确检索

The screenshot displays the SciFinder web interface. At the top, the SciFinder logo is visible. Below it, a navigation bar includes 'Explore', 'Saved Searches', and 'SciPlanner'. The left sidebar contains a list of search categories: REFERENCES, SUBSTANCES, and REACTIONS. Under SUBSTANCES, 'Chemical Structure' is selected. The main content area is titled 'SUBSTANCES: CHEMICAL STRUCTURE'. It features a 'Structure Editor' with 'Java' and 'Non-Java' tabs, a 'Search Type' section with radio buttons for 'Exact Structure', 'Substructure' (selected), and 'Similarity', and a checkbox for 'Show precision analysis'. A 'Non-Java Structure Editor' box provides additional information. At the bottom, there is an 'Import CXF' button, a 'Search' button, and a link to 'Advanced Search'.

SciFinder®

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: CHEMICAL STRUCTURE ?

Structure Editor:

Java Non-Java

Click to Edit

Search Type:

- ☐ Exact Structure
- ☒ Substructure
- ☐ Similarity

☐ Show precision analysis

Non-Java Structure Editor

This editor lets you draw structures without having to resolve Java issues. To switch between editors, click the tabs above the structure editor box.

Import CXF

Search

Advanced Search

# SciFinder结构绘制工具

The image shows the SciFinder Structure Editor interface with various tools labeled in Chinese. The labels are connected to the corresponding tools in the software interface by red lines.

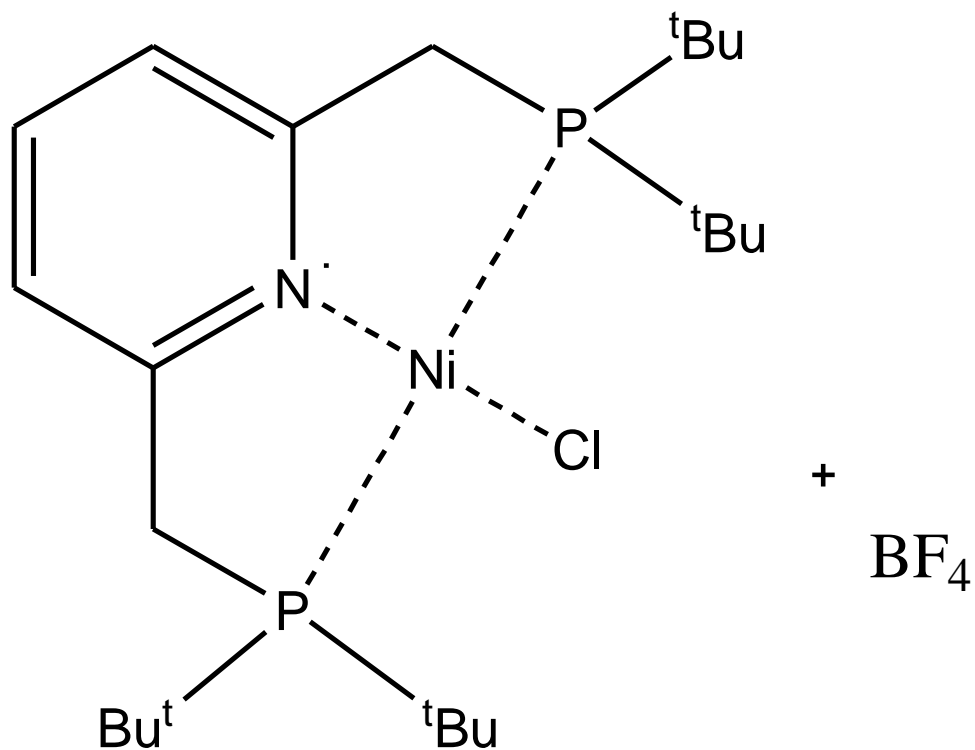
**Tools and Labels:**

- 铅笔 (Pencil)
- 橡皮 (Eraser)
- 结构 and 反应切换功能 (Structure and Reaction Switching Function)
- 元素周期表 (Periodic Table)
- 常用基团 (Common Groups)
- R基团定义工具 (R Group Definition Tool)
- 可变基团 (Variable Groups)
- 可变位置连接工具 (Variable Position Connection Tool)
- 重复基团工具 (Repeat Group Tool)
- 模版工具 (Template Tool)
- 碳链工具 (Carbon Chain Tool)
- 索套选择工具 (Lasso Selection Tool)
- 选择工具 (Selection Tool)
- 原子锁定工具 (Atom Locking Tool)
- 环锁定工具 (Ring Locking Tool)
- 镜面旋转工具 (Mirror Rotation Tool)
- 旋转工具 (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)
- 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 Rings Tool)

**Structure Editor Interface Details:**

- Structure Editor window title bar.
- Draw or change atoms or bonds. (Yellow bar)
- Shortcut Keys (Right side)
- Drawing Editor: Structure (Selected), Reaction, Markush.
- Get substances that match your query using: Exact search, Substructure search (Selected), Similarity search.
- Scale 100 (Bottom right)
- Bottom bar: C, H, O, S, N, P, Cl, Br, F, I, Si.
- Bottom bar: (query)

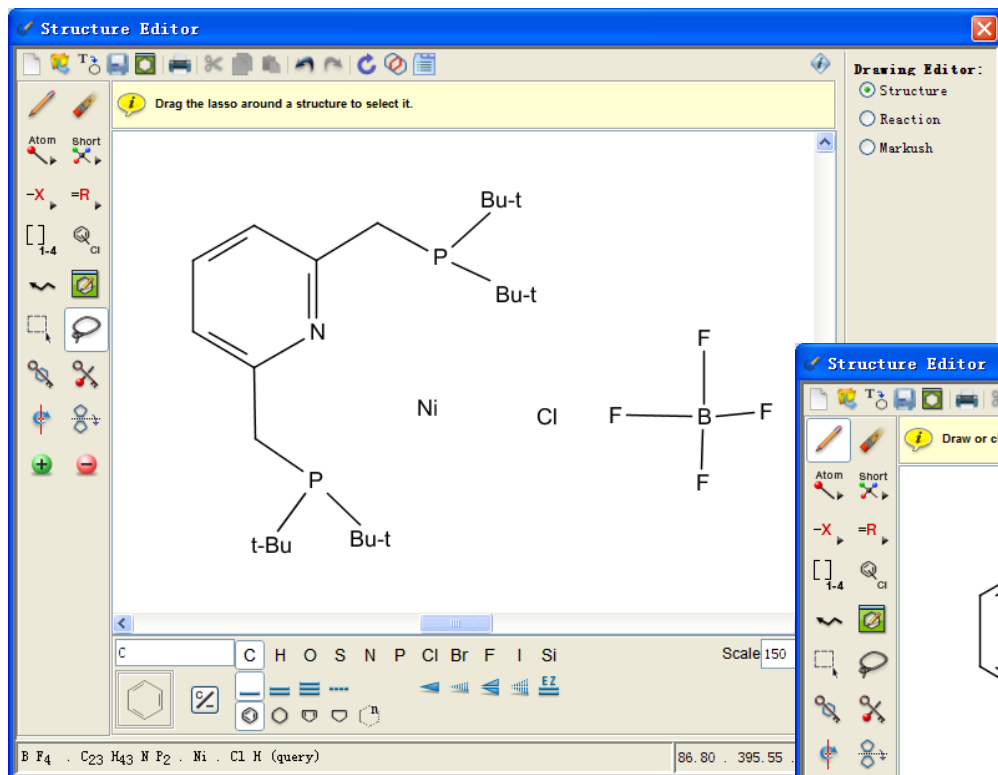
## 精确结构检索—检索金属配合物



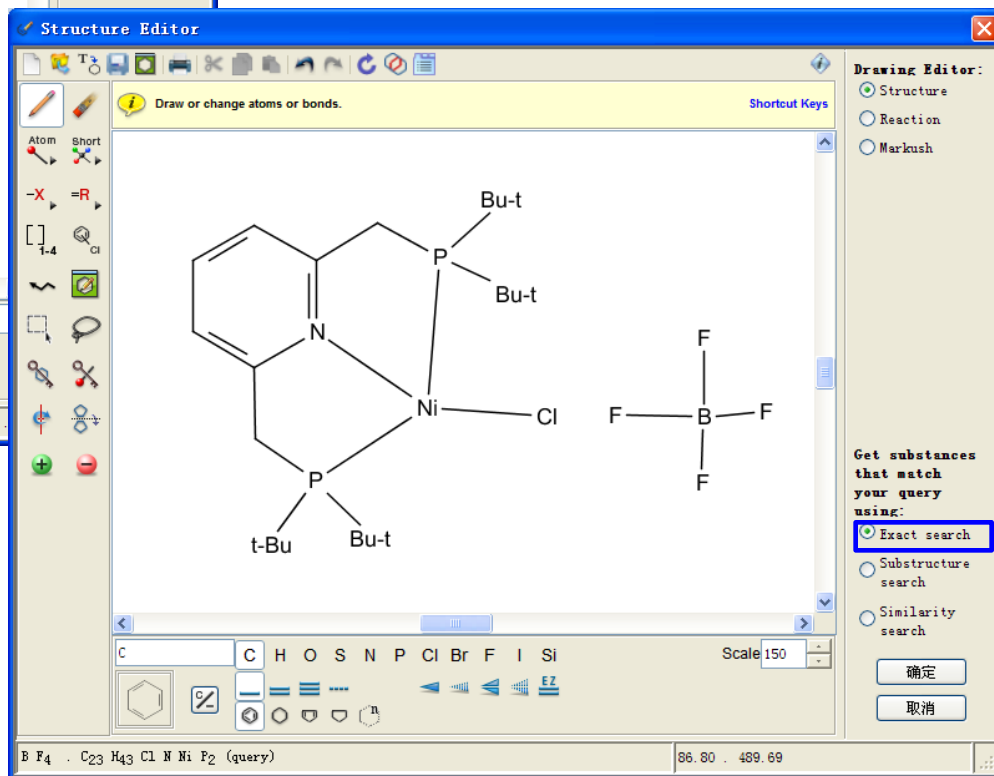
该结构中包含：

配体  
金属  
阳离子  
阴离子

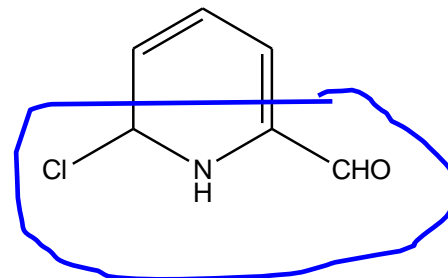
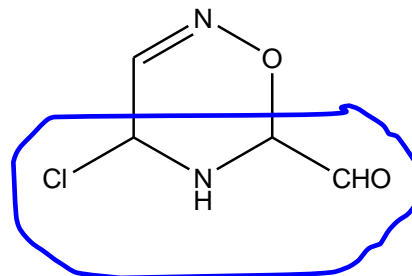
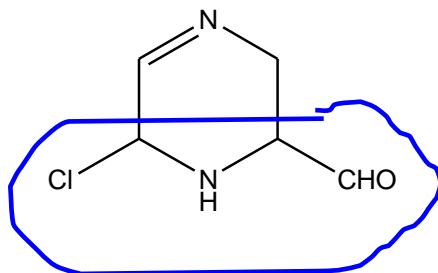
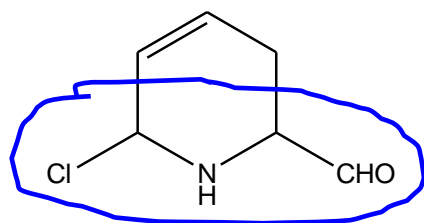
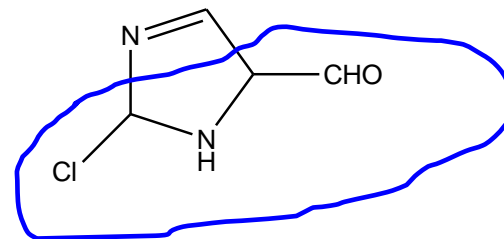
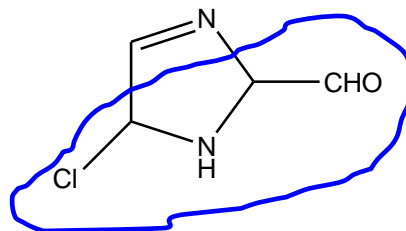
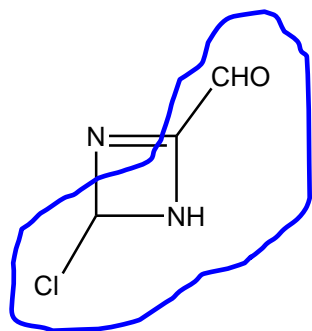
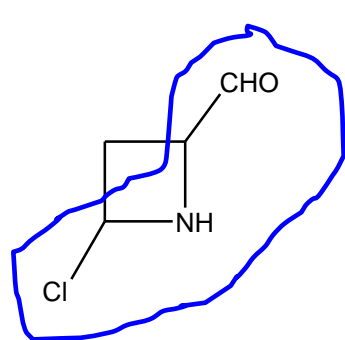
# 检索界面



任何一种结构,使用精确结构都可以检索到

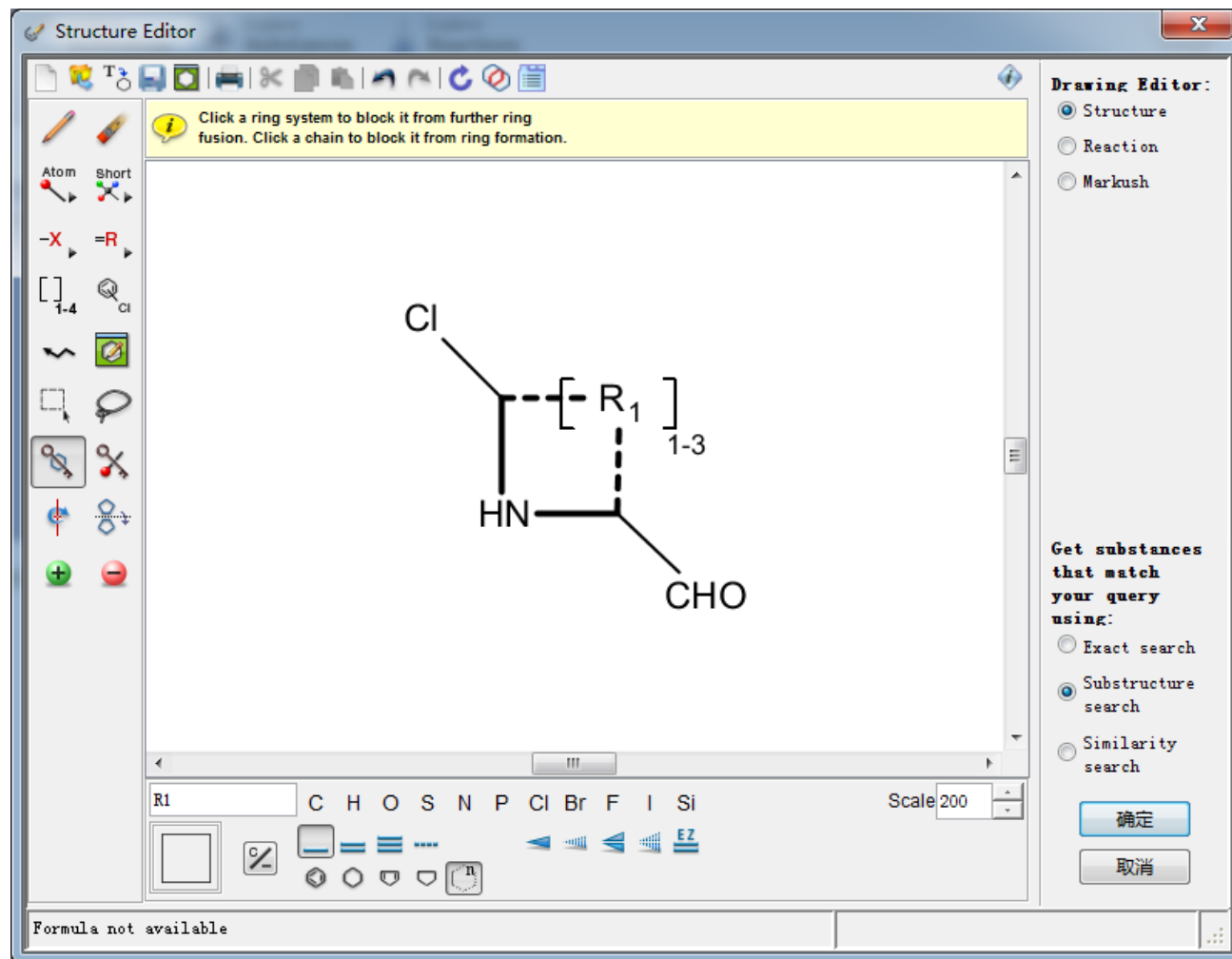


# 我想获得以下的一系列物质



o o o o o o

# 结构定义



用亚结构检索获得所有的物质

# 亚结构检索结果

SciFinder®

Preferences | SciFinder Help | Sign Out

Welcome Sam Yu

Explore ▾ Saved Searches ▾ SciPlanner Save Print Export

Chemical Structure substructure > substances (469)

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

Analyze Refine

Sort by: Number of References ▾

Answers per Page [50] View: ||| ||| |||

0 of 469 Substances Selected

Page: 1 of 10

Analyze by: ? Substance Role

Preparation 155

Reactant or Reagent 123

Biological Study 15

Uses 11

Prophetic in Patents 8

Properties 6

Formation, Nonpreparative 2

Analytical Study 1

1. Substance Detail 54087-03-5 ~33

C5H4ClNO

2. Substance Detail 1757-28-4 ~19

C4H2Cl2N2O

3. Substance Detail 81293-97-2 ~11

C5H4ClNO

Experimental Properties

# 练习

- 用结构检索二茂铁
- 检索策略
  - 绘制两个环戊二烯
  - 绘制一个铁
  - 精确检索，选择配位化合物

# 提纲

- 介绍

- SciFinder Web中的内容

- **SciFinder Web中的检索和后处理**

- SciFinder Web中的文献记录及主题检索
  - SciFinder Web中的物质结果及物质检索方法
  - SciFinder Web中的反应记录及反应检索

- **SciFinder Web的注册**

# SciFinder Web中的反应记录

SciFinder®

Preferences | SciFinder Help | Sign Out

Welcome Sam Yu

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

Opened saved answer set "total reaction" (817)

REACTIIONS

Analyze | Refine

Get References | Tools

Group by: No Grouping | Sort by: Experimental Procedure

Send to SciPlanner

Display Options

0 of 817 Reactions Selected

Page: 1 of 41

1. View Reaction Detail | Link | Similar Reactions

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

$\text{HS}-\text{CH}_2-\text{CH}_2-\text{SH}$  + 
  $\text{OHC}-\text{CH}(\text{Me})-(\text{CH}_2)_8-\text{Me}$ 
 $\rightarrow$

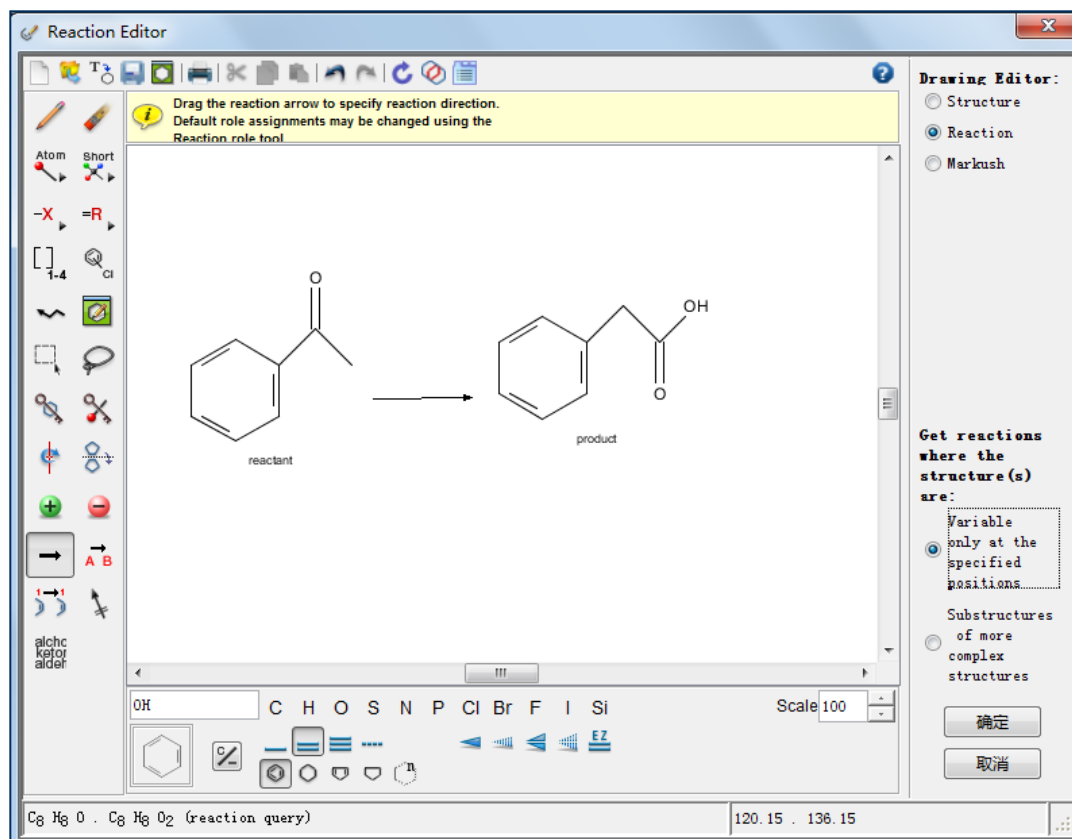
94%

Overview

Experimental Procedure

1. 反应分组功能
2. 反应排序功能
3. 反应后处理功能
4. 反应全景及实验过程
5. SciPlanner


# SciFinder反应检索



**Allow variability only as specified:** 仅在特定位点发生变化

**Substructure:** 亚结构检索，允许有更多取代情况

# 反应检索界面



Preferences | SciFinder Help | Sign Out

Welcome Tony Liu

Explore | Saved Searches | SciPlanner

REFERENCES

Research Topic  
Author Name  
Company Name  
Document Identifier  
Journal  
Patent  
Tags

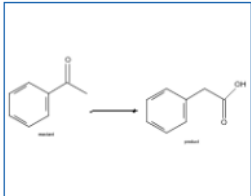
SUBSTANCES

Chemical Structure  
Markush  
Molecular Formula  
Property  
Substance Identifier

REACTIONS

Reaction Structure

REACTIONS: REACTION STRUCTURE ?



Click image to change structure or view detail.

Import CXF

**Search**

Advanced Search

Search Type:

- ☒ Allow variability only as specified
- ☐ Substructure

SAVED ANSWER SETS ?

1

Autosaved Reference Set

View All | Import

KEEP ME POSTED ?

You have no profiles.

Learn how to:  
Create Keep Me Posted

# 精确反应检索结果

Reaction Structure structure variable only at spe... > reactions (9)

**REACTIONS**

Get References Tools Send to SciPlanner

Analyze **Refine**

Analyze by: Catalyst

HSO<sub>3</sub>F 2

BF<sub>3</sub>·Et<sub>2</sub>O 1

SeO<sub>2</sub> 1

TEBAC 1

[Show More](#)

Group by: No Grouping Sort by: Relevance

0 of 9 Reactions Selected

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

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

**Overview**

Steps/Stages	Notes
1.1 R:S, R:Morpholine, R: <i>p</i> -MeC <sub>6</sub> H <sub>4</sub> SO <sub>3</sub> H, 8 h, 120-130°C	<b>Notes</b> Reactants: 1, Reagents: 6, Catalysts: 1, Solvents: 2, Steps: 1, Stages: 7, Most stages in any one step: 7  <b>References</b> A facile synthesis of phenylacetic acids via Willgerdt-Kindler reaction under PTC condition By Alam, M. Mujahid and Adapa, Srinivas R. From <i>Synthetic Communications</i> , 33(1), 59-63; 2003
1.2 R:NaOH, C:TEBAC, S:H <sub>2</sub> O, 5 h, 100°C	
1.3 R:HCl, S:H <sub>2</sub> O, pH 6	
1.4 R:HCl, S:H <sub>2</sub> O, pH 2	
1.5 R:NaHCO <sub>3</sub> , S:H <sub>2</sub> O	
1.6 S:AcOEt	
1.7 R:HCl, S:H <sub>2</sub> O	

# Group by Document 按照出处文献分类显示

Reaction Structure structure variable only at spe... > reactions (9)

REACTIIONS

Get References Tools

Send to SciPlanner

Analyze Refine

Analyze by: Catalyst

HSO<sub>3</sub>F 2

BF<sub>3</sub>·Et<sub>2</sub>O 1

SeO<sub>2</sub> 1

TEBAC 1

Show More

Group by: Document Sort by: Relevance

No Grouping

Document

Transformation

Selected

1. A facile synthesis of phenylacetic acids via Willgerdt-Kindler reaction under PTC condition Full Text

1 Reaction Similar Reactions

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

Overview


Steps/Stages	Notes
1.1 R:S, R:Morpholine, R:p-MeC <sub>6</sub> H <sub>4</sub> SO <sub>3</sub> H, 8 h, 120-130°C	Reactants: 1, Reagents: 6, Catalysts: 1, Solvents: 2, Steps: 1, Stages: 7, Most stages in any one step: 7
1.2 R:NaOH, C:TEBAC, S:H <sub>2</sub> O, 5 h, 100°C	
1.3 R:HCl, S:H <sub>2</sub> O, pH 6	
1.4 R:HCl, S:H <sub>2</sub> O, pH 2	
1.5 R:NaHCO <sub>3</sub> , S:H <sub>2</sub> O	
1.6 S:AcOEt	

References

A facile synthesis of phenylacetic acids via Willgerdt-Kindler reaction under PTC condition Full Text

来自同一篇文献的反应都被整合到一起并集中显示

# Group by Transformation 按照反应类型分类显示

Get References  Tools

Group by: Transformation Sort by: Frequency

0 of 9 Reactions Selected

☐ 1. Reduction of Carbonyl to Methylene in Aldehydes and Ketones/ Clemmensen Reduction/ Wolff-Kishner Reduction  
4 Reactions

$$\text{R}-\overset{\text{O}}{\parallel}{\text{C}}-\text{R}^1 \longrightarrow \text{R}-\text{CH}_2-\text{R}^1$$

☐ 2. Willgerodt/ Willgerodt-Kindler Reactions  
4 Reactions

$$\text{R}-\overset{\text{O}}{\parallel}{\text{C}}-\text{Y} \xrightarrow{(\text{NH}_4)_2\text{S}_n} \text{R}-\text{CH}_2-\overset{\text{NH}_2}{\parallel}{\text{C}}-\text{Y}$$

Y = O, S

☐ 3. Arylation at a Carbon Containing an Active Hydrogen/ Hurlley Reaction  
1 Reaction

$$\text{Ar}-\text{Y} + \text{Z}-\text{CH}_2-\text{R} \longrightarrow \text{Ar}-\text{CH}(\text{Z})-\text{R}$$

Y = OSO<sub>2</sub>R', Halogen  
Z = Electron withdrawing group

☐ 4. Multi-Step Reactions  
4 Reactions

同一类反应被整合到一起并以通式结构集中显示；  
仅适用于单步反应，未被分类的反应显示在结果集最后

# 获得有实验步骤的反应结果集

**REACTIONS**

Get References Tools

Analyze Refine

Analyze by: Author Name

Khosrowshahi, Jaffar S. 2

Moriarty, Robert M. 2

Prakash, Om 2

Adapa, Srinivas R. 1

Alam, M. Mujahid 1

Andersch, Joerg 1

Chandalia, Sampatraj B. 1

Ghaffarzadeh, Mohammad 1

Haiss, Peter 1

Li, Jin-lian 1

Show More

Group by: No Grouping Sort by: Experimental Procedure

0 of 9 Reactions Selected

Experimental Procedure

1. View Reaction Detail Product Yield Publication Year

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

Overview

**Steps/Stages**

1.1 R:S, R:Morpholine, R:*p*-MeC<sub>6</sub>H<sub>4</sub>SO<sub>3</sub>H, 8 h, 120-130°C  
 1.2 R:NaOH, C:TEBAC, S:H<sub>2</sub>O, 5 h, 100°C  
 1.3 R:HCl, S:H<sub>2</sub>O, pH 6  
 1.4 R:HCl, S:H<sub>2</sub>O, pH 2  
 1.5 R:NaHCO<sub>3</sub>, S:H<sub>2</sub>O  
 1.6 S:AcOEt  
 1.7 R:HCl, S:H<sub>2</sub>O

**Notes**

Reactants: 1, Reagents: 6, Catalysts: 1, Solvents: 2, Steps: 1, Stages: 7, Most stages in any one step: 7

Overview

**Steps/Stages**

1.1 R:S, R:Morpholine, R:*p*-MeC<sub>6</sub>H<sub>4</sub>SO<sub>3</sub>H, 8 h, 120-130°C  
 1.2 R:NaOH, C:TEBAC, S:H<sub>2</sub>O, 5 h, 100°C  
 1.3 R:HCl, S:H<sub>2</sub>O, pH 6  
 1.4 R:HCl, S:H<sub>2</sub>O, pH 2  
 1.5 R:NaHCO<sub>3</sub>, S:H<sub>2</sub>O  
 1.6 S:AcOEt  
 1.7 R:HCl, S:H<sub>2</sub>O

**Notes**

Reactants: 1, Reagents: 6, Catalysts: 1, Solvents: 2, Steps: 1, Stages: 7, Most stages in any one step: 7

**References**

A facile synthesis of phenylacetic acids via Willgerodt-Kindler reaction under PTC condition  
 Full Text  
 By Alam, M. Mujahid and Adapa, Srinivas R.  
 From Synthetic Communications, 33(1), 59-63; 2003

**Experimental Procedure**

**Typical procedure for the preparation of phenylacetic acid:** Acetophenone (1.20 g, 10 mmol), sulfur (0.64 g, 20 mmol), morpholine (3 mL, 30 mmol), *p*-toluene sulphonic acid (0.06 g, 0.35 mmol) were added and held at reflux under constant stirring in an oil bath at 120-130°C for 8 h. After completion of the reaction as indicated by TLC, the reaction mixture was allowed to cool and 20% NaOH and triethyl benzyl ammonium chloride (TEBA) (114 mg, 0.05 mmol) were added to the reaction mixture and continued hydrolysis for further 8 h at 100°C. After completion of the reaction as indicated by TLC; the reaction mixture was cooled and filtered, the filtrate was acidified with HCl to pH 6 and then filtered off. The filtrate was further acidified to pH 2 and thus crude phenylacetic acid was obtained. The acid was then taken into 10% NaHCO<sub>3</sub> solution and was washed with ethyl acetate (3 x 30 mL), separated the organic layer, and the aqueous layer was acidified with dilute HCl, to yield the pure phenylacetic acid as solid. In case of products from hydroxy acetophenones, the products were extracted into ethyl acetate. The dried organic layer was evaporated under reduced pressure to yield pure phenylacetic acid. Phenylacetic acid, yield 80%.

## 练习

- 检索从硝基吡啶还原成吡啶氨的反应，
- 检索策略
  - 分别绘制硝基吡啶和吡啶氨
  - 中间绘制箭头，确定反应物和产物

# 提纲

- 介绍

- SciFinder Web中的内容

- **SciFinder Web中的检索和后处理**

- SciFinder Web中的文献记录及主题检索
  - SciFinder Web中的物质结果及物质检索方法
  - SciFinder Web中的反应记录及反应检索

- **SciFinder Web的注册**

# SciFinder Web的注册和登陆

**SciFinder Web的系统要求**

**Windows用户支持IE 9.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，建议安装Java 7）**

**在图书馆相关页面上找到SciFinder Web注册用的网址**

# SciFinder Web 注册

内蒙古大学图书馆  
INNER MONGOLIA UNIVERSITY LIBRARY

首页 | 生命科学 | 数学 | 物理 | 化学/环境 | 计算机 | 电子/自动化 | 蒙古学 | 哲学 | 民族学/社会学 | 历史 | 文学 | 法律 | 管理 | 交通 | 外语

桃李搜索 | 馆藏书目 | 我的图书馆

所有字段 标题 作者 主题词 ISSN ISBN

外文资源 中文资源

资源导览 | 服务指南 | 本馆概况

电子资源

- 版权公告
- 资源发现服务
- 数据库导航
- 馆藏书刊检索
- 随书光盘

纸质资源

- 书刊报纸
- 学位论文
- 教学参考书

特色资源

- 本馆特色资源
- 蒙古学信息网
- 蒙古文期刊网

咨询台

内蒙古大学图书馆数据库试用专题

新闻公告 | 资源动态

公告内容	日期
《工作周志》参考样式	2014/03/12
图书馆升级随书光盘系统!	2014/01/15
图书馆2014年寒假开放时间	2014/01/14
图书馆2014年增加了很多新资源, 邀...	2014/01/10

# SciFinder Web 注册

RSC(英国皇家化学学会)	期刊	外文数据库	化学/环境 生命科学	详细信息
SAGE期刊全文数据库 (SAGE出版社)	期刊	外文数据库	综合	详细信息
Science(科学出版社)	期刊+新闻	外文数据库	综合	详细信息
SciFinderScholar(化学文摘)	多种文献	外文数据库	化学/环境	详细信息
SpringerProtocols实验室指南	——	外文数据库	化学/环境 生命科学	详细信息
Springer(Springer出版社)	期刊	外文数据库	综合	详细信息
SIAM (工业与应用数学学会) 全文电子期刊	期刊	外文数据库	数学	详细信息
Taylor & Francis ST科技&SSH人文期刊数据库	期刊	外文数据库	综合	详细信息
Transactions American Mathematical Society	期刊	外文数据库	数学	详细信息
天然产物词典	事实	外文数据库	化学/环境	详细信息
thieme化学电子期刊	期刊	外文数据库	化学/环境	详细信息
Wiley (含AGU) 电子期刊全文库	期刊	外文数据库	综合	详细信息
World eBook Library电子图书数据库	电子图书	外文数据库	综合	详细信息
剑桥大学电子期刊回溯库(国家图书馆授权)	期刊	外文数据库	综合	详细信息

注册地址: [https://scifinder.cas.org/registration/index.html?](https://scifinder.cas.org/registration/index.html?corpKey=9C7E58A2X86F35055X38B8612E5EB1079C05)  
corpKey=9C7E58A2X86F35055X38B8612E5EB1079C05

# 点击URL创建SciFinder Web账号



SciFinder®  
The choice for chemistry research.™

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**Welcome to User Registration for SciFinder®**

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Click Next to begin registration as a new user.

**Next >>**

开始创建SciFinder Web帐号

### License Agreement

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**SciFinder® is for Educational use ONLY.**

Commercial use of your University account is strictly prohibited.

By clicking the Accept button, **I agree to the terms below:**

1. I am a current faculty, staff member or officially registered student of the University.
2. I will use SciFinder® ONLY for my own academic research.
3. I will not use SciFinder® for commercial research or for organizations other than my University.
4. I will not share my unique username and password with any other individual.
5. I will not use an automated script.
6. I may store no more than 5,000 records in electronic form at any one time.

Violations of these terms may result in your University losing SciFinder® access.

*Contact your University's Key Contact for assistance or CAS Customer Care ([help@cas.org](mailto:help@cas.org)) for commercial licensing information.*

**Accept**   **Decline**

# 点击URL创建SciFinder Web账号

## Registration Information

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

### Contact Information

First Name\*:

Last Name\*:

Email\*:

Confirm Email\*:

Phone Number:

Fax Number:

Area of Research:

Job Title:

### Username and Password

Username\*:  [Tips](#)

Password\*:

Re-enter Password\*:

### Security Information

Security Question\*:

Answer\*:  [Why?](#)

- 1、带\*号的是必须要填写的内容
- 2、必须使用真实姓名
- 3、使用学校后缀邮箱或公共邮箱均可用于注册

# 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 @、#、%、&、*） |

## 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**



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

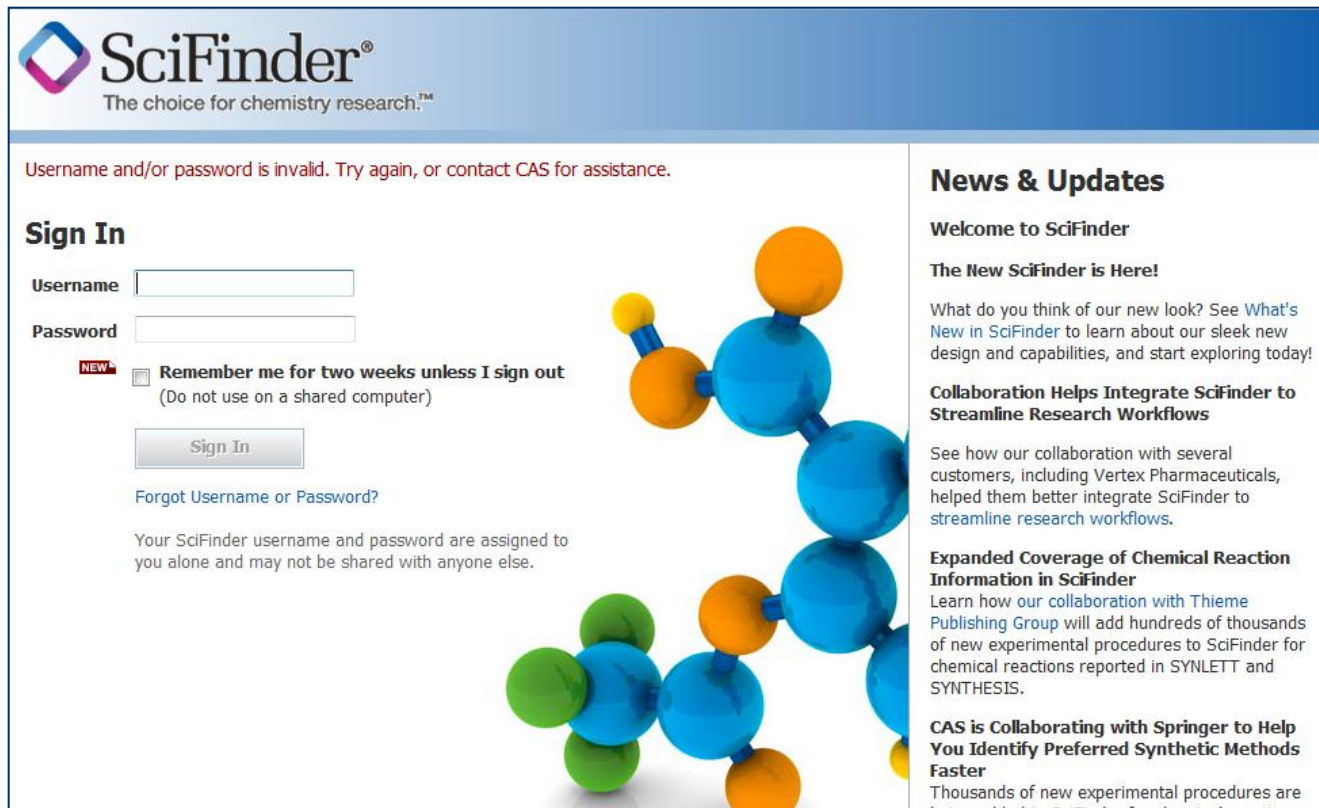
### **Registration for SciFinder<sup>®</sup> is Complete**

You have successfully completed the registration process. To sign in to SciFinder<sup>®</sup>, click the link below.

<https://scifinder.cas.org/scifinder>

**<http://scifinder.cas.org>**

# SciFinder Web 常见问题



The screenshot shows the SciFinder web 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." To the left of the main content area is a "Sign In" section with input fields for "Username" and "Password", a "Remember me for two weeks unless I sign out" checkbox, and a "Sign In" button. Below the button are links for "Forgot Username or Password?" and a note about account security. To the right is a "News & Updates" section with three articles: "Welcome to SciFinder", "The New SciFinder is Here!", "Collaboration Helps Integrate SciFinder to Streamline Research Workflows", "Expanded Coverage of Chemical Reaction Information in SciFinder", and "CAS is Collaborating with Springer to Help You Identify Preferred Synthetic Methods Faster". A 3D molecular model is positioned between the sign-in and news sections.

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

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)

[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

**The New SciFinder is Here!**

What do you think of our new look? See [What's New in SciFinder](#) to learn about our sleek new design and capabilities, and start exploring today!

#### Collaboration Helps Integrate SciFinder to Streamline Research Workflows

See how our collaboration with several customers, including Vertex Pharmaceuticals, helped them better integrate SciFinder to [streamline research workflows](#).

#### Expanded Coverage of Chemical Reaction Information in SciFinder

Learn how our [collaboration with Thieme Publishing Group](#) will add hundreds of thousands of new experimental procedures to SciFinder for chemical reactions reported in SYNLETT and SYNTHESIS.

#### CAS is Collaborating with Springer to Help You Identify Preferred Synthetic Methods Faster

Thousands of new experimental procedures are [being added to SciFinder](#) for chemical reactions.

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

将页面截图下来，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

**SciFinder QQ答疑群207211509**

**Comprehensive Content**

**Sophisticated Analysis**

**Unprecedented Results**



***Thank You***

曾小雅

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