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SciFinder Web使用介绍

俞靓

SciFinder培训专员

2014.12

提纲

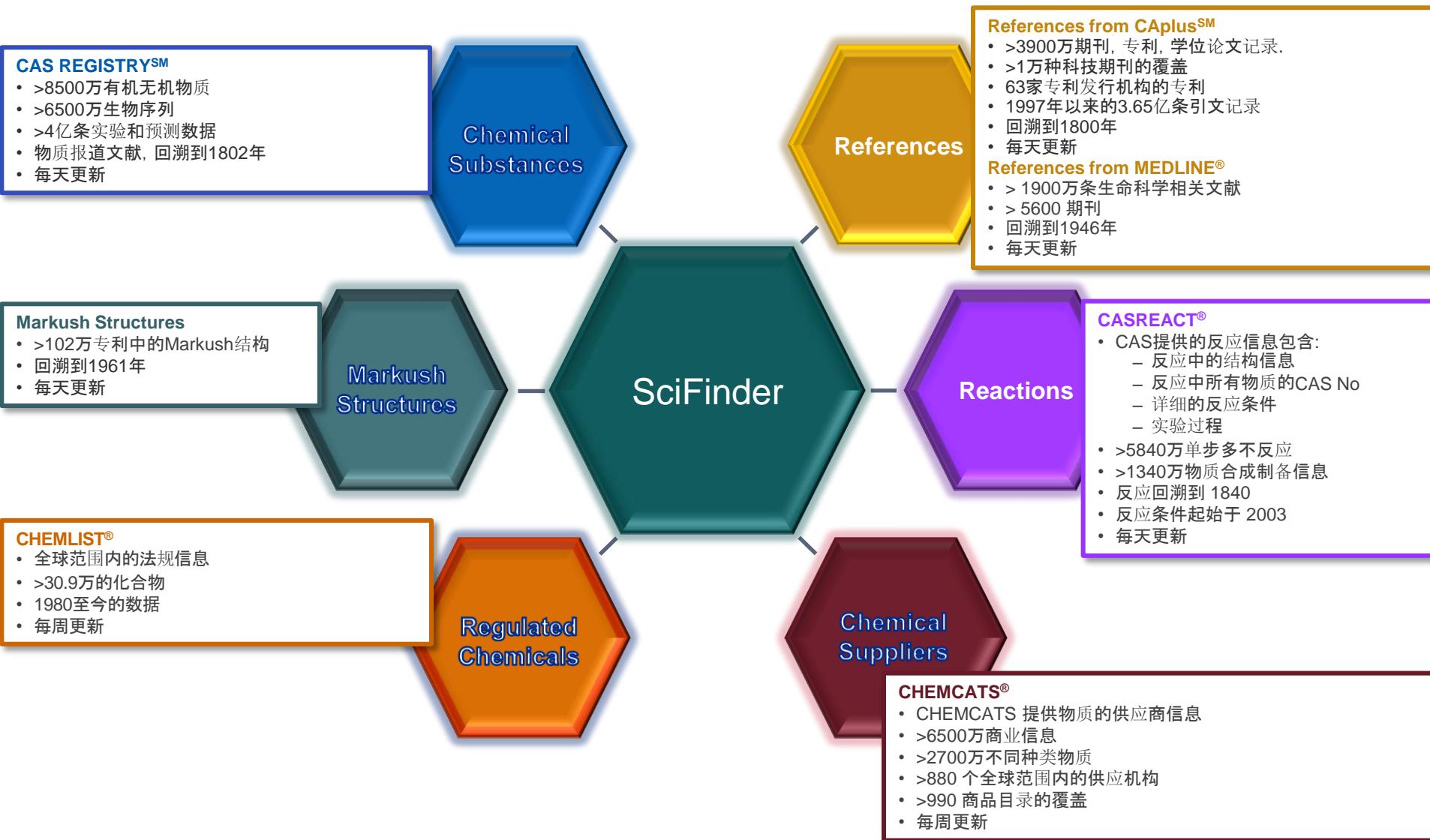
- 介绍
 - SciFinder Web中的内容
- **SciFinder Web中的检索和后处理**
 - SciFinder Web中的文献记录及主题检索
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 - SciFinder Web中的反应记录及反应检索
- **SciFinder Web的注册**

美国化学文摘社—Chemical Abstracts Service

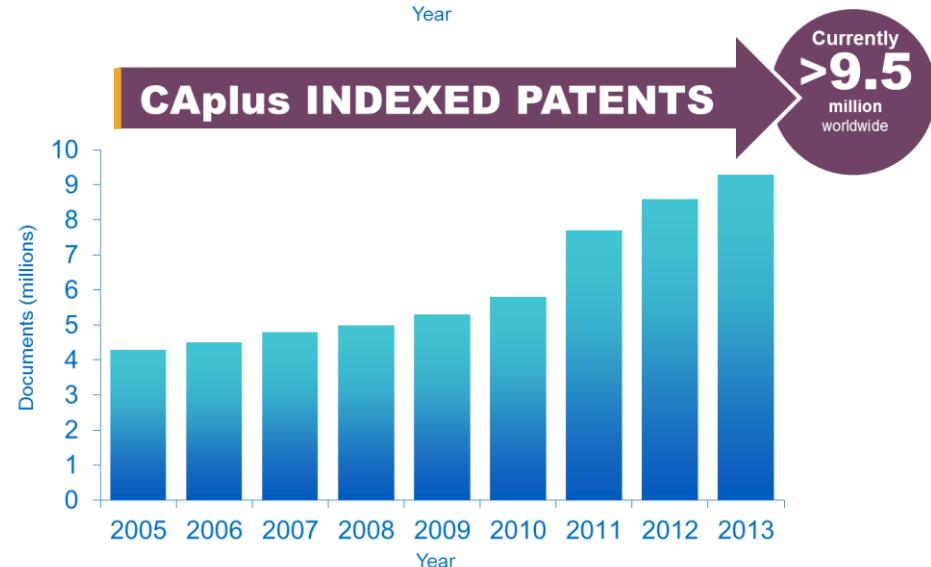
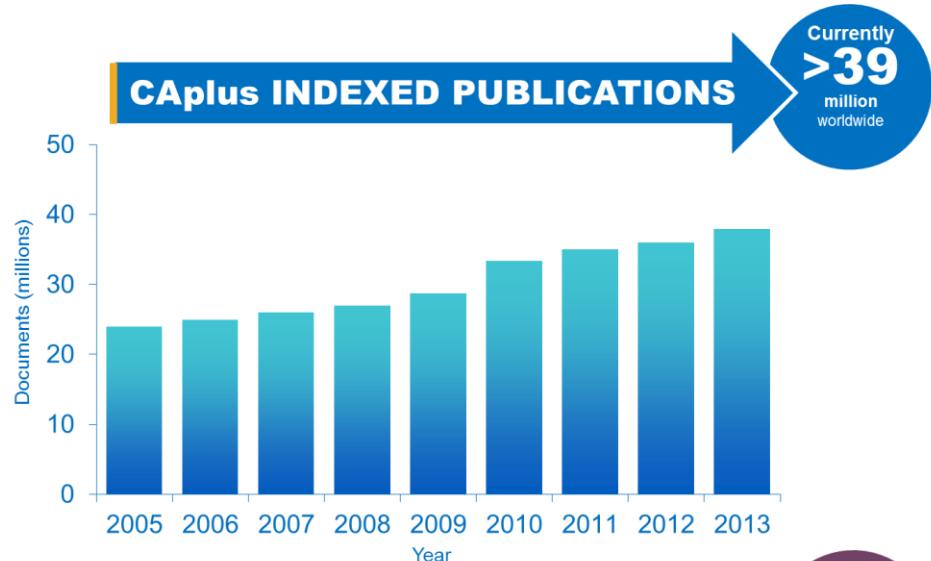
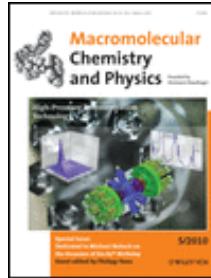
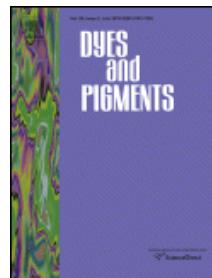
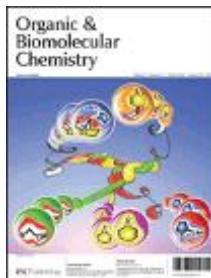
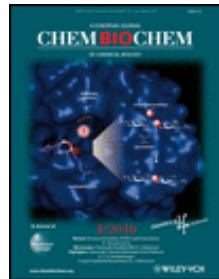
- 创建于1907年
- ACS的分支机构
- 密切关注，索引和提炼着全球化学相关的文献和专利
- 最早创立了《化学文摘》
- 总部坐落于俄亥俄州的哥伦布市



SciFinder的覆盖内容

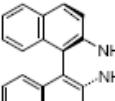


CAplusSM 涵盖上万种期刊及63个专利发行机构专利



CAS REGISTRYSM 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'-Diamo-1,1'-dimaphthyl, 1,1'-Bi[2-naphthylamine]

CAS Registry Number → FNCG-Y [4488-22-6]

Molecular Formula → C₂₀H₁₈N₂

Use → Intermediate for chiral auxiliaries.
 Hazard alert symbol and description of hazards → Exp. numourous by skin contact. Dsc. with emission of toxic fumes. DU3090000

Supplier information → Mp 242.5-243°. [α]_D²⁴ + 155.5° (c, 1 in Py). [α]_D²⁸ + 46.8° (2M HCl).
 Supplier: Aldrich 38242-6, Fluka 32787.

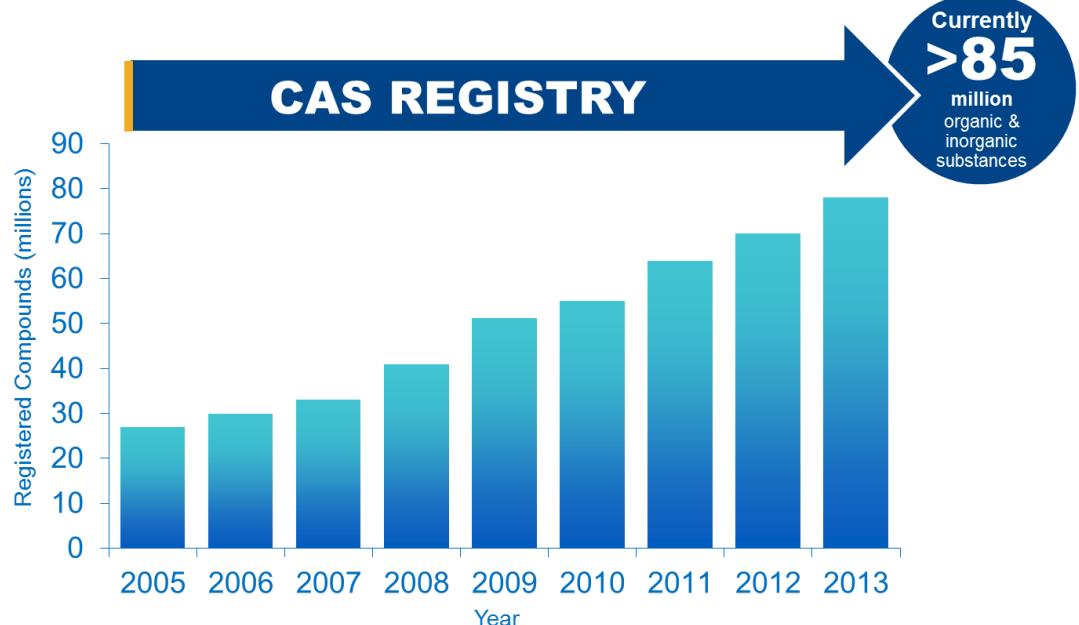
Stereoisomer heading → (R)-form: FNCG-Z [18741-85-0]
 Mp 242.5-243°. [α]_D²⁴ + 155.5° (c, 1 in Py). [α]_D²⁸ + 46.8° (2M HCl).
 (S)-form: FNCG-W [18531-95-8]
 Cryst. Mp 243° (235-239°). [α]_D²⁰ - 149° (Py). [α]_D²⁸ - 46° (2M HCl).
 Supplier: Aldrich 38243-4, Fluka 32788.

Derivative Subheading → N,N-Di-Ac: FNCH-X C₂₂H₂₀N₂O₂ M 368.434. Prisms (C₆H₆). Mp 226-227°. [α]_D²⁵ + 10.8° (c, 1 in THF).
 (±)-form FNCH-W [79082-81-8]
 Silvery plates (Et₂OH). Mp 193.2-194.5° (191°).
 Picrate: FNCH-Z Brownish-yellow plates (C₆H₆). Mp 185° (dec.).
 N,N-Di-Ac: FNCH-X Cubes (Et₂OH). Mp 235-236°.
 N,N-Dibenzoyl: FNCH-Y C₃₄H₃₀N₂O₄ M 492.576. Prisms (PhNO₂). Mp 235°.

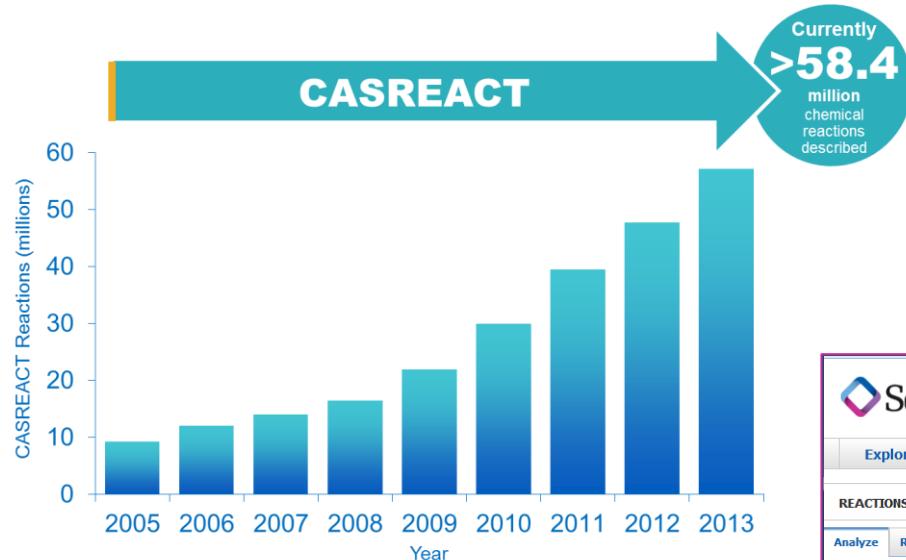
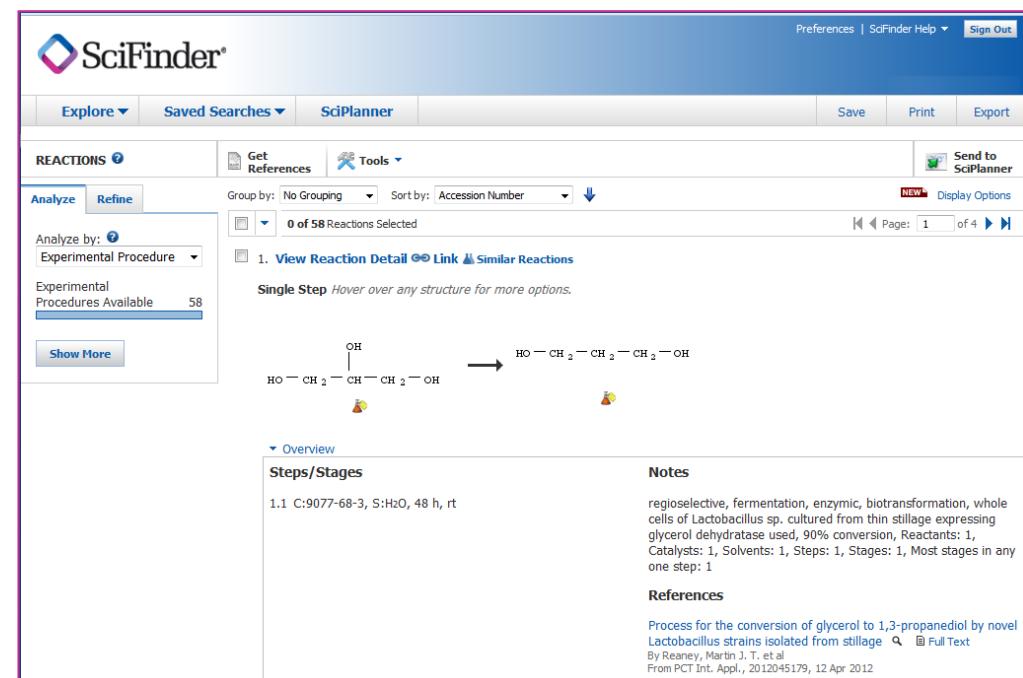
Additional CAS Registry Numbers → [93621-61-5] [97644-73-0]

Bibliographic references → Kuhn, R et al., Annalen, 1929, 470, 183 (*synth, resolv*)
 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 (*inv, ord*)
 Akimoto, H et al., Tetrahedron, 1971, 27, 5999 (*resolv, 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, resolv*)
 Benson, SC et al., J.O.C., 1988, 53, 5335 (*synth, N-tetramethyl*)
 Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1999, 14, 32 (*use*)
 Franzini, L et al., Acta Cryst. C, 1991, 47, 1259 (*cryst struct, N-tetra-Me*)
 Smircic, M et al., J.O.C., 1992, 57, 1917 (*synth, resolv, bbb*)
 Lewis, RJ et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, BGB750

Reference contents →



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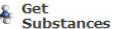
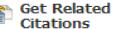
The screenshot displays the SciFinder software interface. The top navigation bar includes "Explore", "Saved Searches", "SciPlanner", "Sign Out", and "Display Options". The main search area is titled "REACTIONS" with tabs for "Analyze" (selected) and "Refine". It shows "0 of 58 Reactions Selected" and a single reaction step: OCC(O)C(O)C(O) >> O=C(O)CH2CH2CH2O. Below this is an "Overview" section with "Steps/Stages" (1.1 C:9077-68-3, S:H₂O, 48 h, rt), "Notes" (regioselective, fermentation, enzymic, biotransformation, whole cells of *Lactobacillus* 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), and "References" (Process for the conversion of glycerol to 1,3-propanediol by novel *Lactobacillus* strains isolated from stillage, By Reaney, Martin J. T., et al, From PCT Int. Appl., 2012045179, 12 Apr 2012).

CASREACT是世界上最大的，更新速度最快的反应数据库

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中的文献记录

REFERENCE DETAIL   

 [Return](#)  

1. Selective oxidation of light alkanes: interaction between the catalyst and the gas phase on different classes of catalytic materials

By: Cavani, F.; Trifiro, F.

A review, with 202 refs., on the selective oxidn. of light ($C \leq 6$) 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 oxides 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.

Indexing

Fossil Fuels, Derivatives, and Related Products (Section51-0)
Section cross-reference(s): 35, 45

Concepts

Redox reaction catalysts	
catalyst-gas phase interactions in selective oxidn. of light alkanes to bulk and industrial chems.	
Alkaline earth oxides	Rare earth oxides
catalysts contg.; catalyst-gas phase interactions in selective oxidn. of light alkanes to bulk and industrial chems.	
Catalyst use; Properties; Uses	

Substances

12026-66-3  58834-75-6 
catalyst-gas phase interactions in selective oxidn. of light alkanes to bulk and industrial chems.
Catalyst use; Uses
1303-86-2 Boron oxide, uses  1332-29-2 Tin oxide  7631-86-9 Silica, uses 

QUICK LINKS
0 Tags, 0 Comments

SOURCE
Catalysis Today
Volume51
Issue3-4
Pages561-580
Journal; General Review
1999
CODEN:CATTEA
ISSN:0920-5861
DOI:10.1016/S0920-5861(99)00041-3

COMPANY/ORGANIZATION
Dipartimento di Chimica
Industriale e dei Materiali
Bologna, Italy 40136

ACCESSION NUMBER
1999:340014
CAN131:159478
CAPLUS

PUBLISHER
Elsevier Science B.V.

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 
- Vedrine, J; Catal Today 1997, 33, 3 
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- 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

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- 功能方面

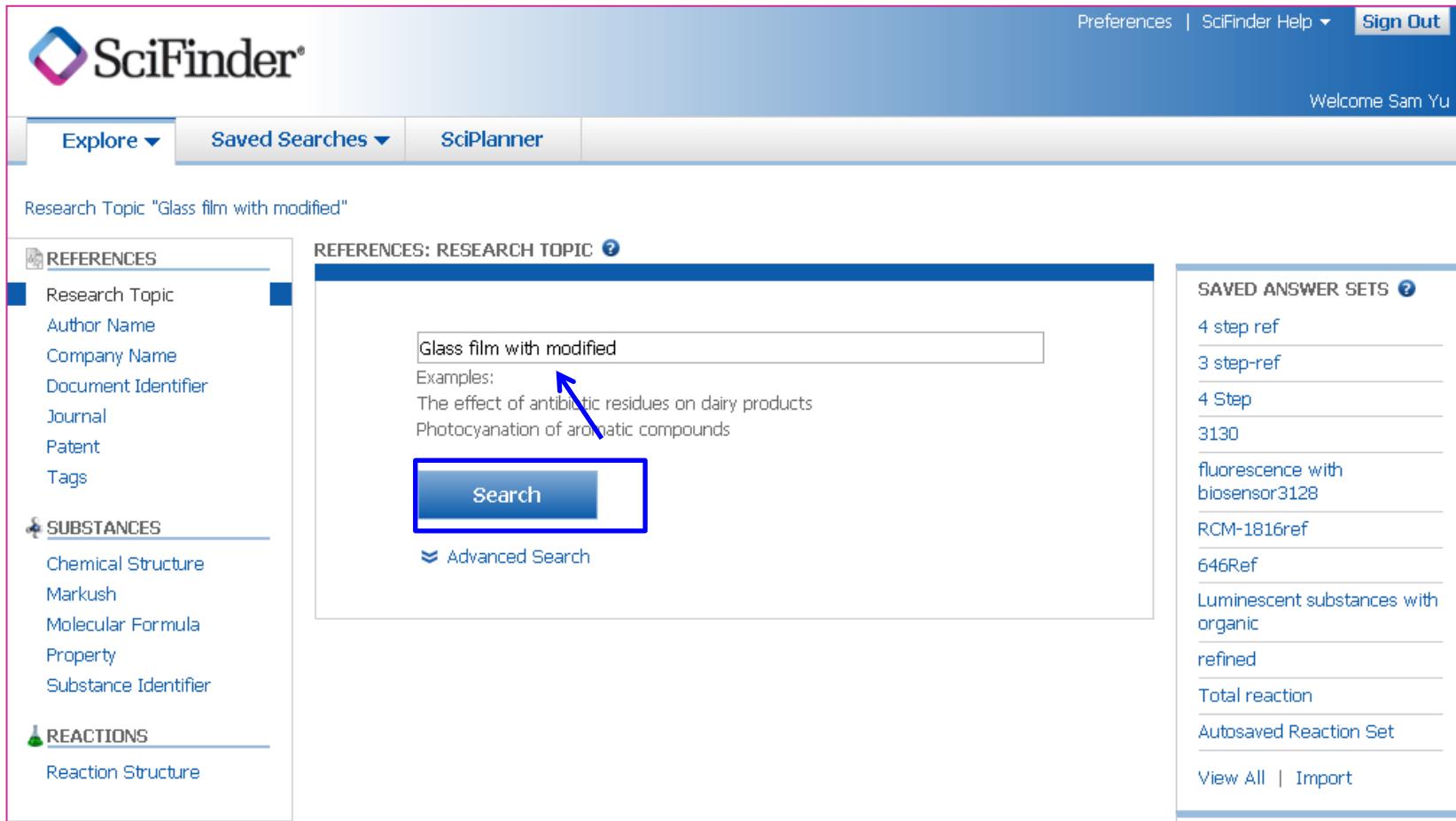
- 主题检索
- 作者名检索
- 机构名检索
- 文献标示符检索
- 从物质，反应获得文献

- 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: glass film with modified (玻璃贴膜的改进)



The screenshot shows the SciFinder Web interface with a search results page for the topic "Glass film with modified".

Top Navigation: Preferences | SciFinder Help ▾ | Sign Out | Welcome Sam Yu

Left Sidebar:

- REFERENCES**
 - Research Topic
 - Author Name
 - Company Name
 - Document Identifier
 - Journal
 - Patent
 - Tags
- SUBSTANCES**
 - Chemical Structure
 - Markush
 - Molecular Formula
 - Property
 - Substance Identifier
- REACTIONS**
 - Reaction Structure

Search Results:

REFERENCES: RESEARCH TOPIC

Glass film with modified

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

Search

Advanced Search

SAVED ANSWER SETS

- 4 step ref
- 3 step-ref
- 4 Step
- 3130
- fluorescence with biosensor3128
- RCM-1816ref
- 646Ref
- Luminescent substances with organic
- refined
- Total reaction
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主题检索的候选项

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Explore ▾ Saved Searches ▾ SciPlanner

Research Topic "Glass film with modified"

REFERENCES ?		References
Select All Deselect All 1 of 4 Research Topic Candidates Selected		
<input checked="" type="checkbox"/>	4461 references were found containing the two concepts "Glass film" and "modified" closely associated with one another.	4461
<input type="checkbox"/>	10712 references were found where the two concepts "Glass film" and "modified" were present anywhere in the reference.	10712
<input type="checkbox"/>	139072 references were found containing the concept "Glass film".	139072
<input type="checkbox"/>	2361190 references were found containing the concept "modified".	2361190
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

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

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Research Topic "Glass film with modified" > references (4461)

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Analyze Refine Categorize

Analyze by: Author Name

Author Name	Count
Chen Shen Ming	82
Dong Shaojun	48
Hu Shengshui	44
Ye Baoxian	32
Yuan Ruo	31
Lin Xinhua	27
Chai Yaqin	24
Huang Ke Jing	24

Sort by: Accession Number ▾

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1. Non-enzymatic glucose biosensor based on copper oxide-reduced graphene oxide nanocomposites synthesized from water-isopropanol solution

By Wang, Xiaolin; Liu, Enli; Zhang, Xiaoli
From Electrochimica Acta (2014), 130, 253-260. | Language: English, Database: CAPLUS

A novel, stable and sensitive non-enzymic glucose biosensor based on nanocomposites of copper oxide (CuO) and the reduced graphene oxide (rGO) was developed. A facile, green and effective chem. method was employed to synthesize the CuO-rGO nanocomposites in a mixt. soln. of water-isopropanol. During the synthesis process, isopropanol acted as both solvent and reductant. oxide (GO) sheets through electrostatic force and rGO without any addn. of strong redn. agents...

2. Direct electrochemistry and electrocatalysis of poly(ethylene glycol diglycidyl ether) and gold na hydrogen peroxide and nitric oxide

By Li, Fangping; Nie, Mingzhe; He, Xiulan; Fei, Junjie; Di From Microchimica Acta (2014), Ahead of Print. | Lan

Create Keep Me Posted Profile ?

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Title: * Glass film

Description:

Characters Remaining: 1024

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Explore references by research topic: Glass film with modified

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Display Options

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1. **Crystalline diamond thin-films as stable, biologically active substrates**

By Yang, Venkata; Ruicchio, Orlando; Butler, James E.; Cai, Wei; Carlisle, John A.; Gerbi, Jennifer E.; Gruen, Dieter M.; Knickerbocker, Tanya; Lasseter, Tami L.; Russell, John N.; et al
From Nature Materials (2002), 1(4), 253-257. | Language: English, Database: CAPLUS

Diamond, because of its elec. and chem. properties, may be a suitable material for integrated sensing and signal processing. But methods to control chem. or biol. **modifications** on diamond surfaces have not been established. Here, we show that nanocryst. diamond **thin-films** covalently **modified** with DNA oligonucleotides provide an extremely stable, highly selective platform in subsequent surface hybridization processes. We used a photochem. **modification** scheme to chem. **modify** clean, H-terminated nanocryst. diamond surfaces grown on silicon substrates, producing a homogeneous layer of amine gro...

2. **An ESCA study of the termination of the passivation of elemental metals**

By Barr, Terry L.
From Journal of Physical Chemistry (1978), 82(16), 1801-10. | Language: English, Database: CAPLUS

A detailed ESCA study was made of the passivation of 16 metals which were allowed to oxidize (passivate) to completion in room-temp. air. Particular attention was paid to the characteristics of the final (satn.) layer that terminates the rapid oxidn. and provides the initial barrier to corrosion and other forms of metallic degrdn. The passivation of some of these metals (A) terminates with a micro thin (few Å) layer of the metal in its highest oxidn. state, whereas the bulk of the passivation **film** is largely composed of an oxide of a lower oxidn. state. On the other

~528

~321

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Analyze by: Author Name Chen Shen Ming 82 Dong Shaojun 48 Hu Shengshui 44 Ye Baoxian 32 Yuan Ruo 31 Lin Xinhua 27 Chai Yaqin 24 Huang Ke Jing 24 John S Abraham 24 Li Jing 24

1. Non-enzymatic glucose biosensor based on copper oxide-reduced graphene oxide nanocomposites synthesized from water-isopropanol solution
[Quick View](#) [Full Text](#)
 By Wang, Xiaolin; Liu, Enli; Zhang, Xiaoli
 From *Electrochimica Acta* (2014), 130, 253-260. | Language: English, Database: CAPLUS
 A novel, stable and sensitive non-enzymatic glucose biosensor based on nanocomposites of copper oxide (CuO) and the reduced graphene oxide (rGO) was developed. A facile, green and effective chem. method was employed to synthesize the CuO-rGO nanocomposites in a mixt. soln. of water-isopropanol. During the synthesis process, isopropanol acted as both solvent and reductant. CuO nanoparticles were successfully decorated onto the graphene oxide (GO) sheets through electrostatic force and hydrolysis reaction. Meantime, GO could be partly reduced to the rGO without any addn. of strong redn. agents...

2. Direct electrochemistry and electrocatalysis of hemoglobin on a glassy carbon electrode modified with poly(ethylene glycol diglycidyl ether) and gold nanoparticles on a quaternized cellulose support. A sensor for hydrogen peroxide and nitric oxide
[Quick View](#) [Full Text](#)
 By Li, Fangping; Nie, Mingzhe; He, Xiulan; Fei, Junjie; Ding, Yonglan; Feng, Bo
 From *Microchimica Acta* (2014), Ahead of Print. | Language: English, Database: CAPLUS
 A **glassy** carbon electrode was **modified** with gold nanoparticles (Au-NPs) on a quaternized cellulose support in a **film** composed of poly(ethylene glycol diglycidyl ether) (PEGDGE), and Hb was immobilized on the Au-NPs. The sensor **film** was characterized by UV-vis spectra, SEM, and electrochem. impedance spectroscopy. Cyclic voltammetry of the Hb in

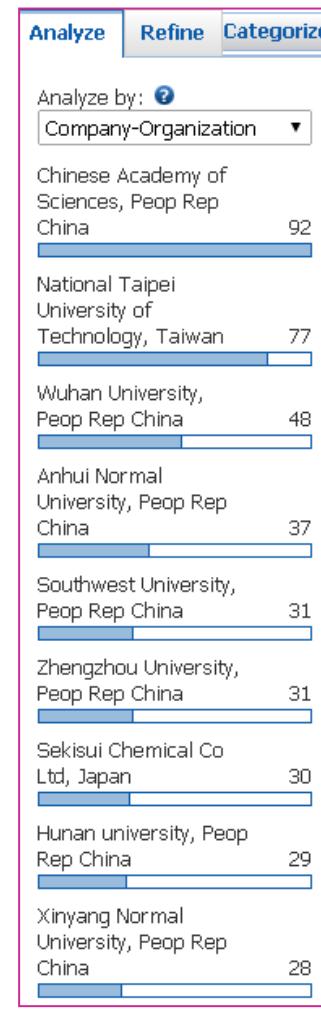
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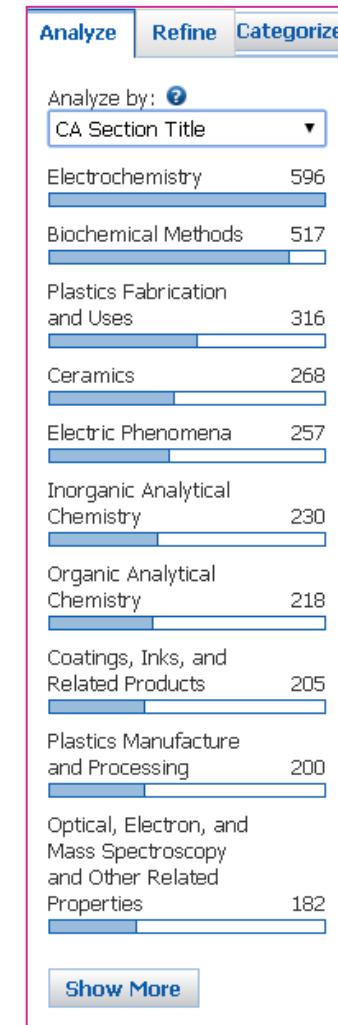
领域内主要研究
人员，专家



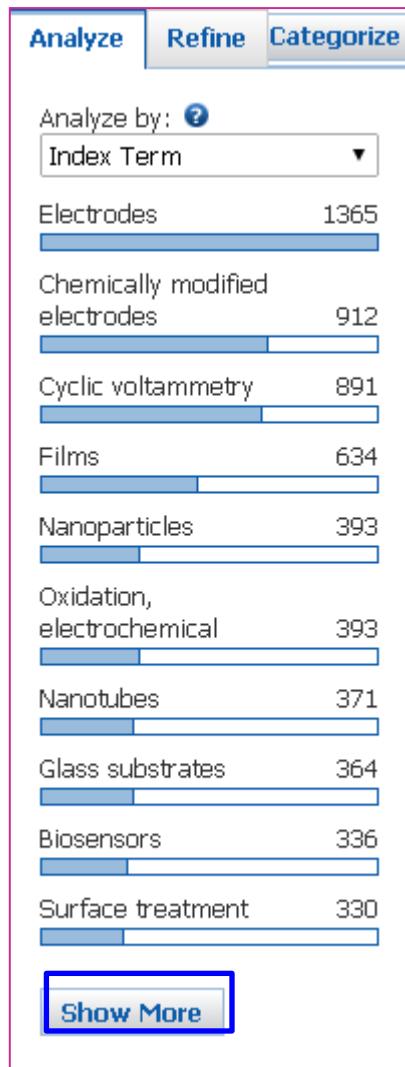
主要研究机构，合
作伙伴，竞争对手



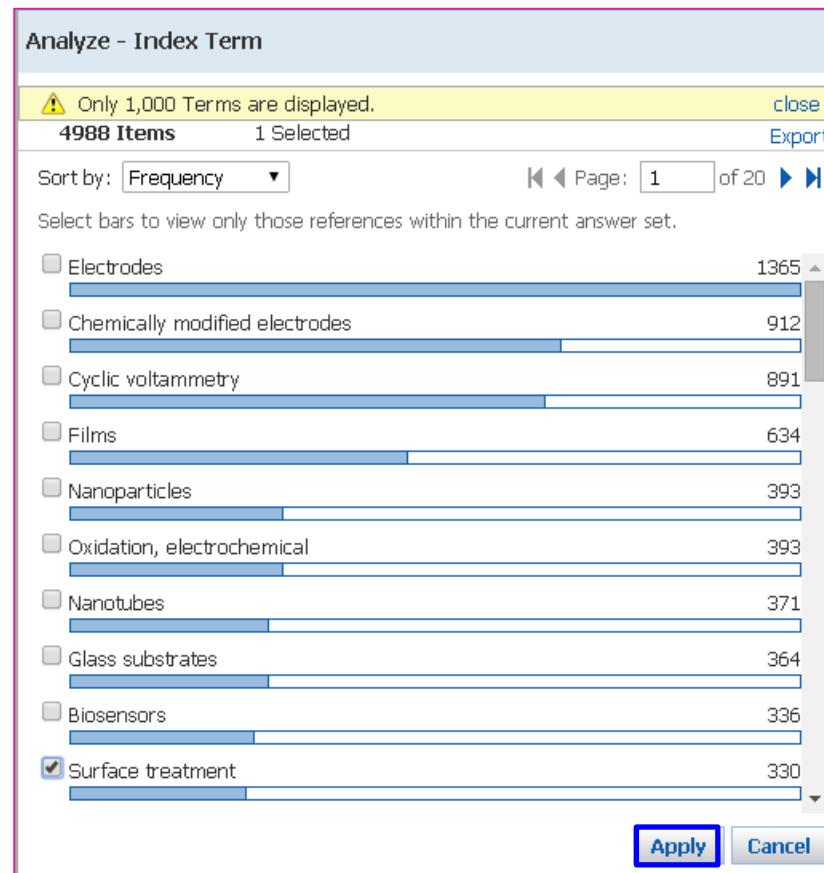
主要的学科领域



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- Company Name
- Document Type
- Publication Year
- Language
- Database

Company Name
3m

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3M
DuPont

Refine

Refine : 帮助用户迅速获得需要的文献

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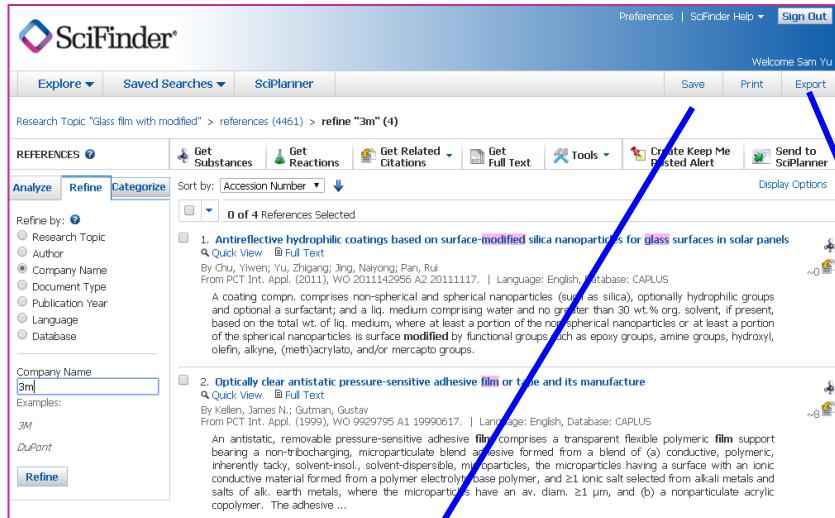
Sort by: Accession Number ▾

0 of 4 References Selected

1. **Antireflective hydrophilic coatings based on surface-modified silica nanoparticles for glass surfaces in solar panels**
[Quick View](#) [Full Text](#)
 By Chu, Yiwen; Yu, Zhigang; Jing, Naiyong; Pan, Rui
 From PCT Int. Appl. (2011), WO 2011142956 A2 20111117. | Language: English, Database: CAPLUS
 A coating compn. comprises non-spherical and spherical nanoparticles (such as silica), optionally hydrophilic groups and optional a surfactant; and a liq. medium comprising water and no greater than 30 wt.% org. solvent, if present, based on the total wt. of liq. medium, where at least a portion of the non-spherical nanoparticles or at least a portion of the spherical nanoparticles is surface **modified** by functional groups such as epoxy groups, amine groups, hydroxyl, olefin, alkyne, (meth)acrylate, and/or mercapto groups.

2. **Optically clear antistatic pressure-sensitive adhesive film or tape and its manufacture**
[Quick View](#) [Full Text](#)
 By Kellen, James N.; Gutman, Gustav
 From PCT Int. Appl. (1999), WO 9929795 A1 19990617. | Language: English, Database: CAPLUS
 An antistatic, removable pressure-sensitive adhesive **film** comprises a transparent flexible polymeric **film** support bearing a non-tribocharging, microparticulate blend adhesive formed from a blend of (a) conductive, polymeric, inherently tacky, solvent-insol., solvent-dispersible, microparticles, the microparticles having a surface with an ionic conductive material formed from a polymer electrolyte base polymer, and ≥ 1 ionic salt selected from alkali metals and salts of alk. earth metals, where the microparticles have an av. diam. ≥ 1 μm , and (b) a nonparticulate acrylic copolymer. The adhesive ...

结果集的保存



SciFinder

Explore Saved Searches SciPlanner

Welcome Sam Yu

Research Topic "Glass film with modified" > references (4461) > refine "3m" (4)

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

Analyze Refine Categorized Sort by: Accession Number

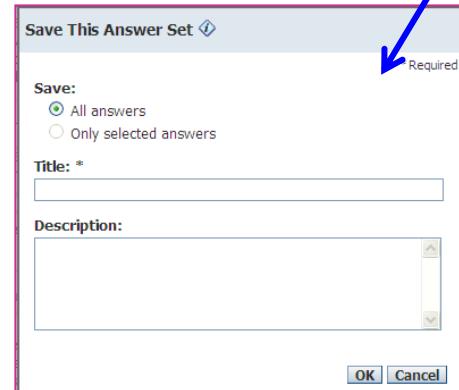
Refine by: Research Topic Author Company Name Document Type Publication Year Language Database

Company Name: 3M Examples: DuPont Refine

0 of 4 References Selected

1. Antireflective hydrophilic coatings based on surface-modified silica nanoparticles for glass surfaces in solar panels
 Quick View Full Text By Chu, Yiwen; Yu, Zhiqiang; Jing, Naiyong; Pan, Ruil From PCT Int. Appl. (2011), WO 2011142956 A2 20111117. | Language: English, Database: CAPLUS A coating compn. comprises non-spherical and spherical nanoparticles (such as silica), optionally hydrophilic groups and optional a surfactant; and a liq. medium comprising water and no greater than 30 wt % org. solvent, if present, based on the total wt. of liq. medium, where at least a portion of the non-spherical nanoparticles or at least a portion of the spherical nanoparticles is surface modified by functional groups such as epoxy groups, amine groups, hydroxyl, olefin, alkyne, (meth)acrylate, and/or mercapto groups.

2. Optically clear antistatic pressure-sensitive adhesive film or tape and its manufacture
 Quick View Full Text By Kellam, James N.; Gutman, Gustav From PCT Int. Appl. (1999), WO 9929795 A1 19990617. | Language: English, Database: CAPLUS An antistatic, removable pressure-sensitive adhesive film comprises a transparent flexible polymeric film support bearing a non-triobcharging, microparticulate blend adhesive formed from a blend of (a) conductive, polymeric, inherently tacky, solvent-insol., solvent-dispersible, microparticles, the microparticles having a surface with an ionic conductive material formed from a polymer electrolyte base polymer, and ≥ 1 ionic salt selected from alkali metals and salts of alk. earth metals, where the microparticles have an av. diam. $\geq 1 \mu\text{m}$, and (b) a nonparticulate acrylic copolymer. The adhesive ...



Save This Answer Set

Save:
 All answers
 Only selected answers

Title: *

Description:

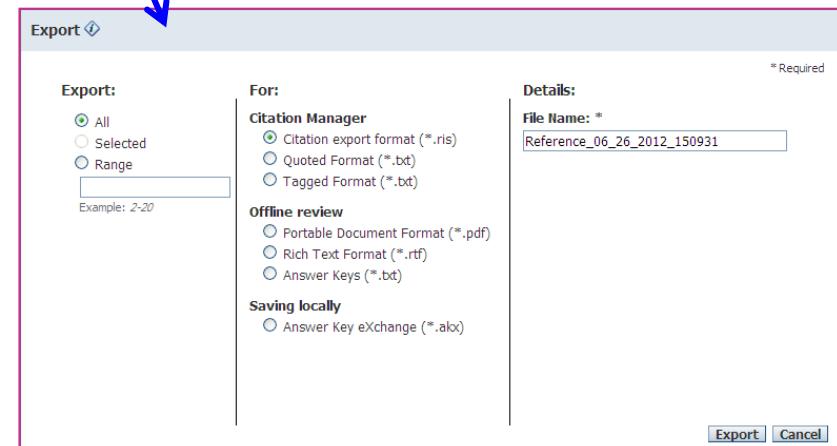
OK Cancel

Required

Save:
 保存在服务器上，可登陆后查看

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



Export

Export:
 All
 Selected
 Range
 Example: 2-20

For:
Citation Manager
 Citation export format (*.ris)
 Quoted Format (*.txt)
 Tagged Format (*.bt)

Details:
 File Name: * Reference_06_26_2012_150931

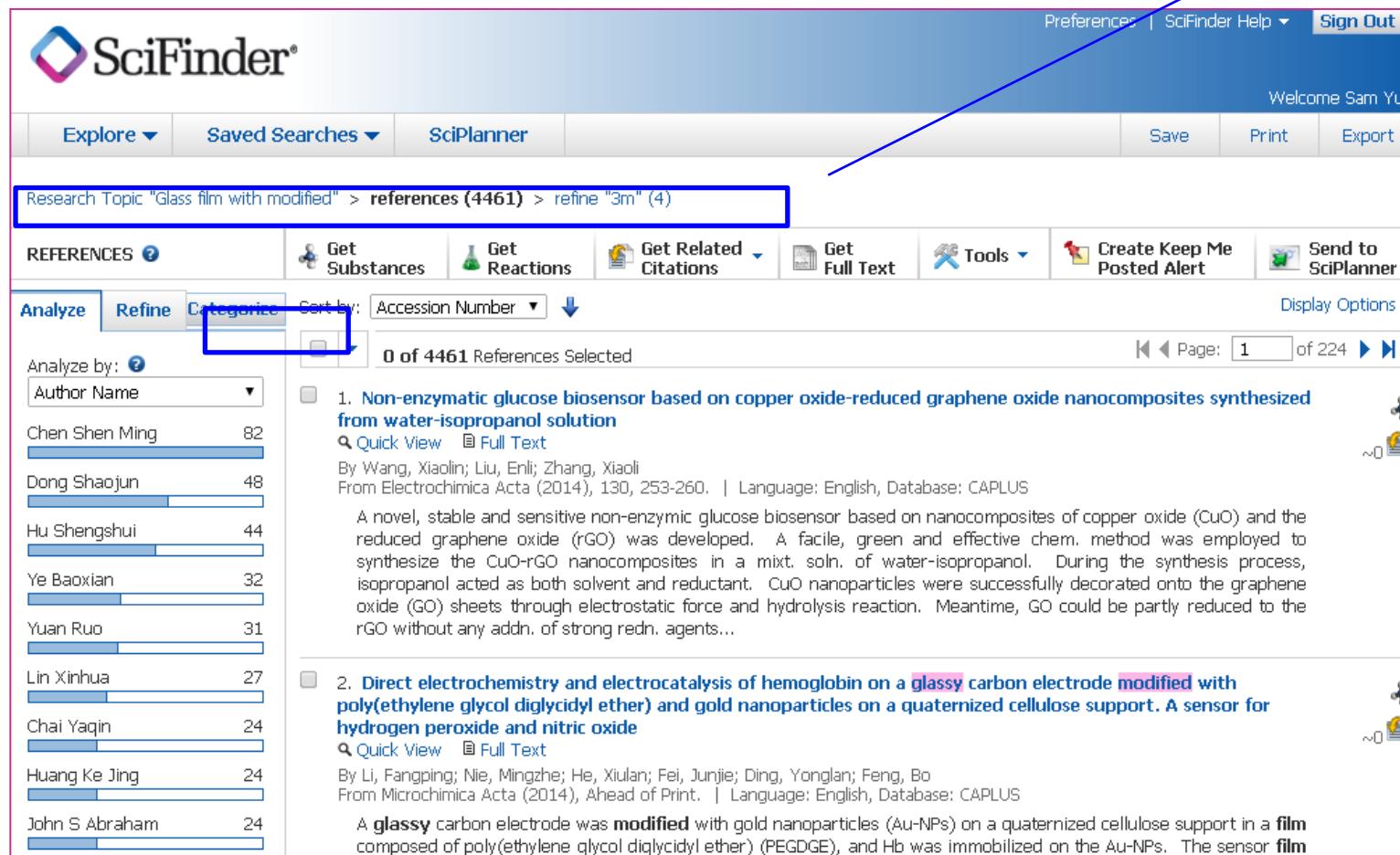
Offline review
 Portable Document Format (*.pdf)
 Rich Text Format (*.rtf)
 Answer Keys (*.txt)

Saving locally
 Answer Key eXchange (*.alex)

Export Cancel

SciFinder 中的Categorize

通过历史导航条回到任一检索界面



SciFinder

Explore ▾ Saved Searches ▾ SciPlanner Preferences | SciFinder Help ▾ Sign Out Welcome Sam Yu

Research Topic "Glass film with modified" > references (4461) > refine "3m" (4)

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 ▾ Display Options

Analyze by: ? Author Name Chen Shen Ming 82 Dong Shaojun 48 Hu Shengshui 44 Ye Baoxian 32 Yuan Ruo 31 Lin Xinhua 27 Chai Yaqin 24 Huang Ke Jing 24 John S Abraham 24

0 of 4461 References Selected Page: 1 of 224

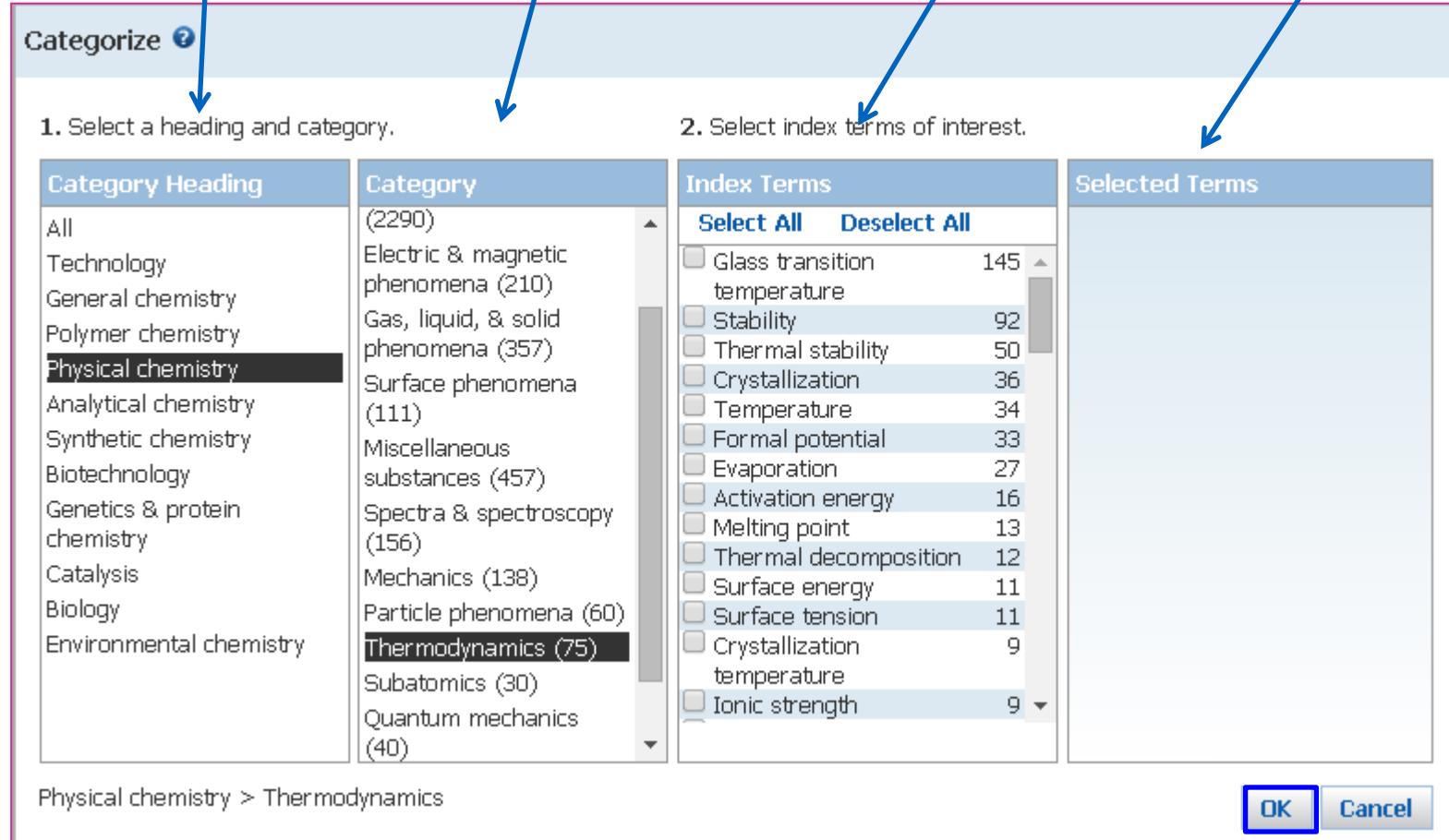
1. Non-enzymatic glucose biosensor based on copper oxide-reduced graphene oxide nanocomposites synthesized from water-isopropanol solution
 Quick View Full Text
 By Wang, Xiaolin; Liu, Enli; Zhang, Xiaoli
 From *Electrochimica Acta* (2014), 130, 253-260. | Language: English, Database: CAPLUS
 A novel, stable and sensitive non-enzymic glucose biosensor based on nanocomposites of copper oxide (CuO) and the reduced graphene oxide (rGO) was developed. A facile, green and effective chem. method was employed to synthesize the CuO-rGO nanocomposites in a mixt. soln. of water-isopropanol. During the synthesis process, isopropanol acted as both solvent and reductant. CuO nanoparticles were successfully decorated onto the graphene oxide (GO) sheets through electrostatic force and hydrolysis reaction. Meantime, GO could be partly reduced to the rGO without any addn. of strong redn. agents...

2. Direct electrochemistry and electrocatalysis of hemoglobin on a glassy carbon electrode modified with poly(ethylene glycol diglycidyl ether) and gold nanoparticles on a quaternized cellulose support. A sensor for hydrogen peroxide and nitric oxide
 Quick View Full Text
 By Li, Fangping; Nie, Mingzhe; He, Xiulan; Fei, Junjie; Ding, Yonglan; Feng, Bo
 From *Microchimica Acta* (2014), Ahead of Print. | Language: English, Database: CAPLUS
 A **glassy** carbon electrode was **modified** with gold nanoparticles (Au-NPs) on a quaternized cellulose support in a **film** composed of poly(ethylene glycol diglycidyl ether) (PEGDGE), and Hb was immobilized on the Au-NPs. The sensor **film**

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



The screenshot shows the 'Categorize' dialog box with the following steps:

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

Category Heading	Category	Index Terms	Selected Terms
All	(2290)	<input type="checkbox"/> Glass transition temperature 145	
Technology	Electric & magnetic phenomena (210)	<input type="checkbox"/> Stability 92	
General chemistry	Gas, liquid, & solid phenomena (357)	<input type="checkbox"/> Thermal stability 50	
Polymer chemistry	Surface phenomena (111)	<input type="checkbox"/> Crystallization 36	
Physical chemistry	Miscellaneous substances (457)	<input type="checkbox"/> Temperature 34	
Analytical chemistry	Spectra & spectroscopy (156)	<input type="checkbox"/> Formal potential 33	
Synthetic chemistry	Mechanics (138)	<input type="checkbox"/> Evaporation 27	
Biotechnology	Particle phenomena (60)	<input type="checkbox"/> Activation energy 16	
Genetics & protein chemistry	Thermodynamics (75)	<input type="checkbox"/> Melting point 13	
Catalysis	Subatomic (30)	<input type="checkbox"/> Thermal decomposition 12	
Biology	Quantum mechanics (40)	<input type="checkbox"/> Surface energy 11	
Environmental chemistry		<input type="checkbox"/> Surface tension 11	
		<input type="checkbox"/> Crystallization temperature 9	
		<input type="checkbox"/> Ionic strength 9	

Physical chemistry > Thermodynamics

OK Cancel

主题检索小结

- 关键词之间用介词链接，With, Of, In, On
- 建议2-3个关键词，最多不超过5个
- 候选项选择包含Concept和Closed associated with的选项
- 可以使用KMP时时跟踪文献
- 可以使用Citing Reference排序获得被引次数最多的文献
- 尽可能多的使用Analyze, Refine, 功能对文献进行处理
- 使用Categorize对文献进行系统分类
- 可以使用历史导航条返回任意检索界面

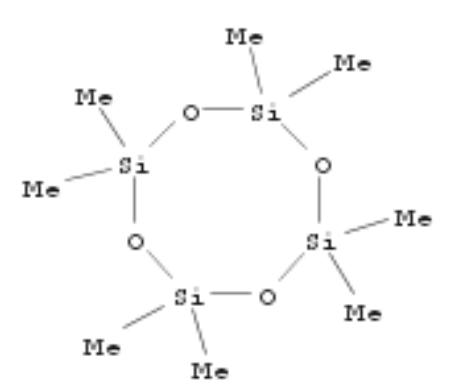
提纲

- 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

1. 556-67-2

~5137 ~77



C₈H₂₄O₄Si₄
 Cyclotetrasiloxane, 2,2,4,4,6,6,8,8-octamethyl-

[Regulatory Information](#)
[Spectra](#)
[Experimental Properties](#)

一个完整的物质结果
界面向包含：

- 物质详情连接
- 文献连接
- 反应连接
- 商品信息连接
- 管制品信息连接
- 谱图连接
- 实验性质连接

SciFinder中的物质详情界面

CAS Registry Number 556-67-2



C₈H₂₄O₄Si₄

Cyclotetrasiloxane, 2,2,4,4,6,6,8,8-octamethyl-

Molecular Weight

296.62

Melting Point (Experimental)

Value: 17.5 °C

Boiling Point (Experimental)

Value: 175 °C

Density (Experimental)

Value: 0.9558 g/cm³

Other Names

Cyclotetrasiloxane, octamethyl- (8CI,9CI)

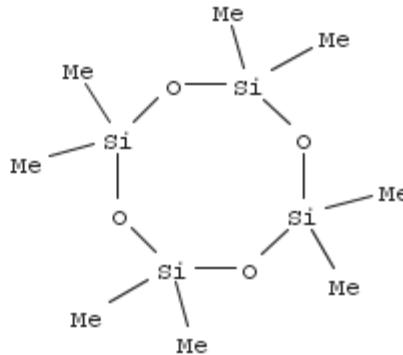
Abil K 4

Cyclic dimethylsiloxane tetramer

D 4

DC 244

[View more...](#)



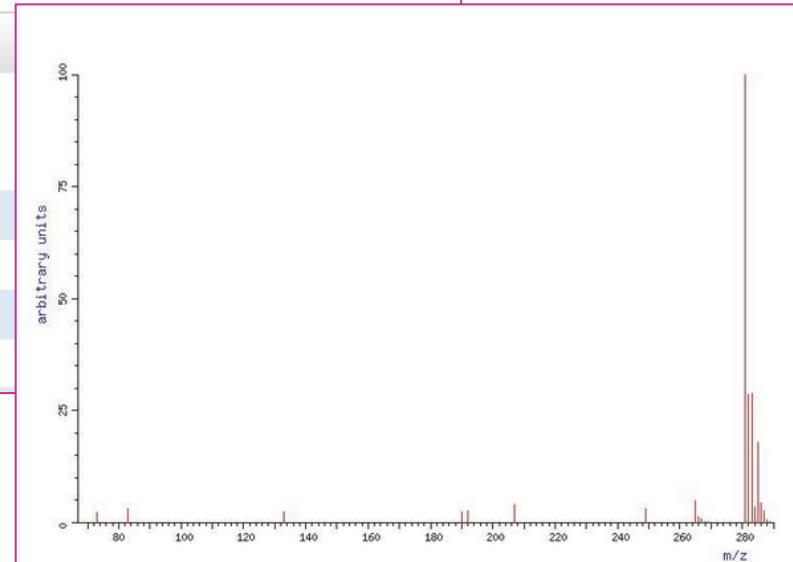
SciFinder中的实验性质和实验谱图

EXPERIMENTAL PROPERTIES

Biological	Chemical	Density	Flow and Diffusion	Interface	Lipinski	Optical and Scattering	Thermal
Density Properties		Value			Condition		Note
Density		1.06 g/cm ³					(28)CAS
Density		0.96 g/cm ³					(22)NIOSH
Density		0.9561 g/cm ³		Temp: 20 °C			(4)CAS
Density		0.9561 g/cm ³		Temp: 420 °C			(15)CAS
Density		0.956 g/cm ³					(8)GELEST

EXPERIMENTAL SPECTRA

¹ H NMR	¹³ C NMR	Hetero NMR	IR	Mass	Raman	UV and Visible
Mass Properties		Value			Condition	
Mass Spectrum		See spectrum				
Mass Spectrum		See spectrum				
Mass Spectrum		See spectrum				
Mass Spectrum		See spectrum				
Mass Spectrum		See spectrum				



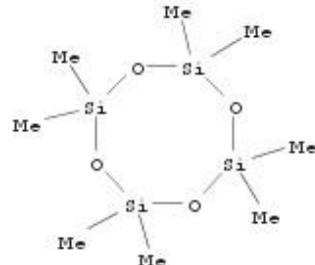
SciFinder中依据物质角色所作的文献分类

▼ CAS REFERENCE ROLES

Roles	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	✓	✓	✓	✓

物质有关的反应

1. Substance Detail
556-67-2



~4816



C₈H₂₄O₄Si₄
Cyclotetrasiloxane, 2,2,4,4,6,6,8,8-octamethyl-

Get Reactions 

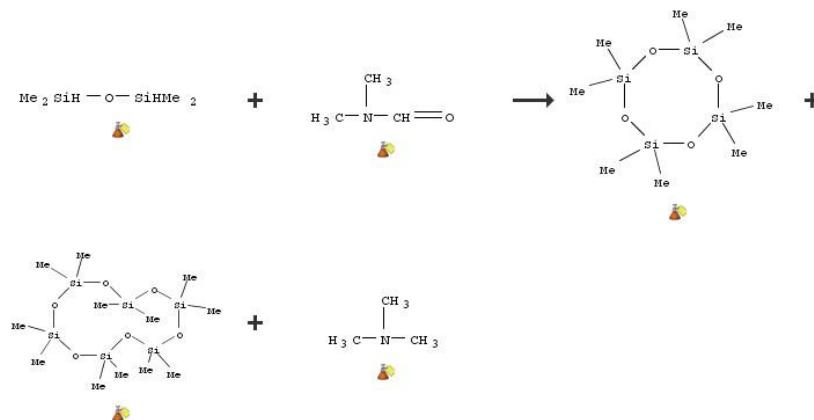
Limit results by reaction role:

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

Get **Cancel**

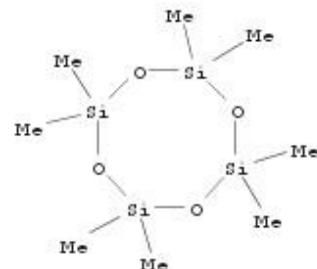
1. View Reaction Detail 

2 Steps Hover over any structure for more options.



物质有关的文献信息

1. Substance Detail
556-67-2



C₈H₂₄O₄Si₄

Cyclotetrasiloxane, 2,2,4,4,6,6,8,8-octamethyl-

Experimental P

4816



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"/> Prophetic 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:

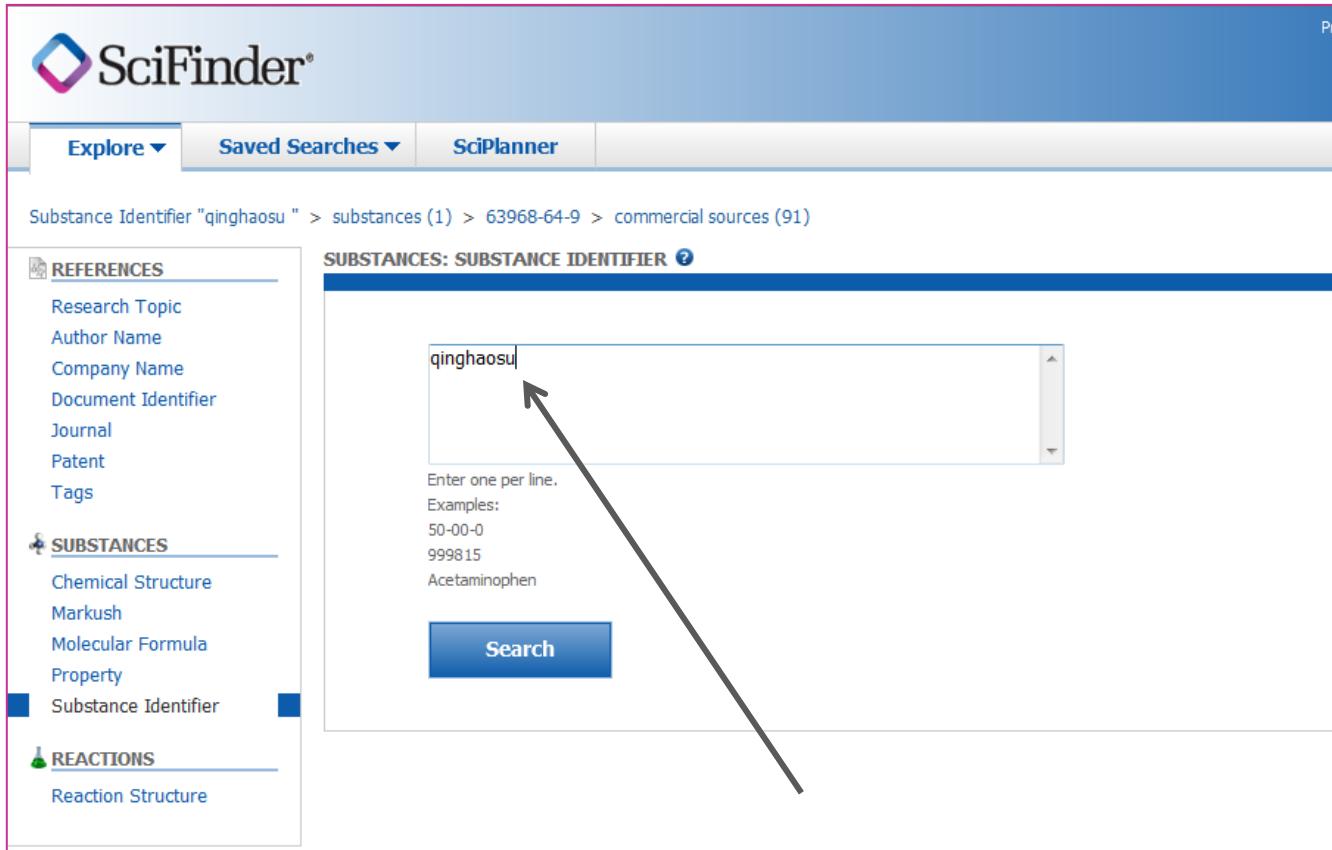
- Additional related references, e.g., activity studies, disease studies.

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 ---结构比较方便
 - 无机物 ---分子式比较方便
 - 高分子化合物 ---首先分子式, 其次结构

物质名称检索



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: SUBSTANCE IDENTIFIER

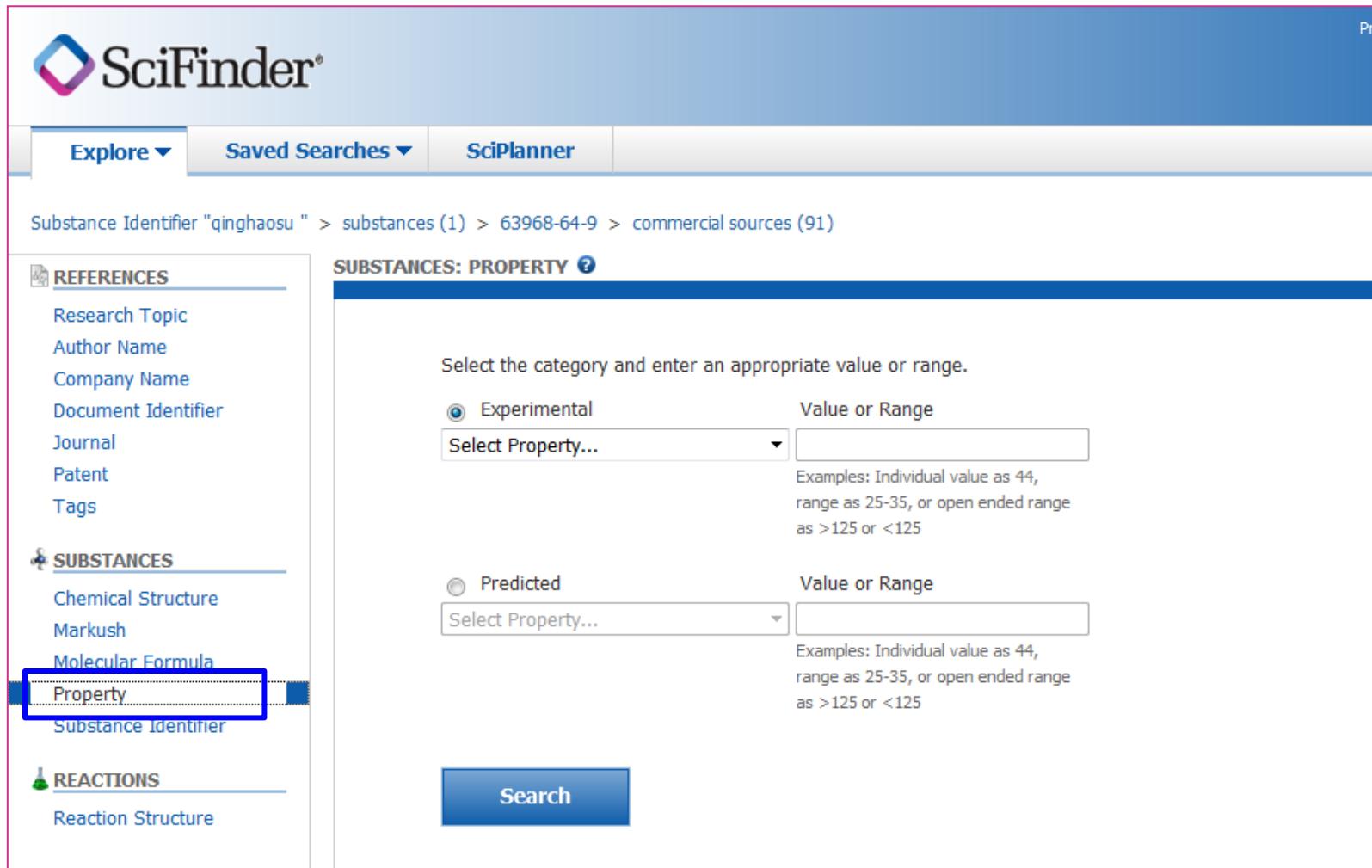
qinghaosu

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

Search

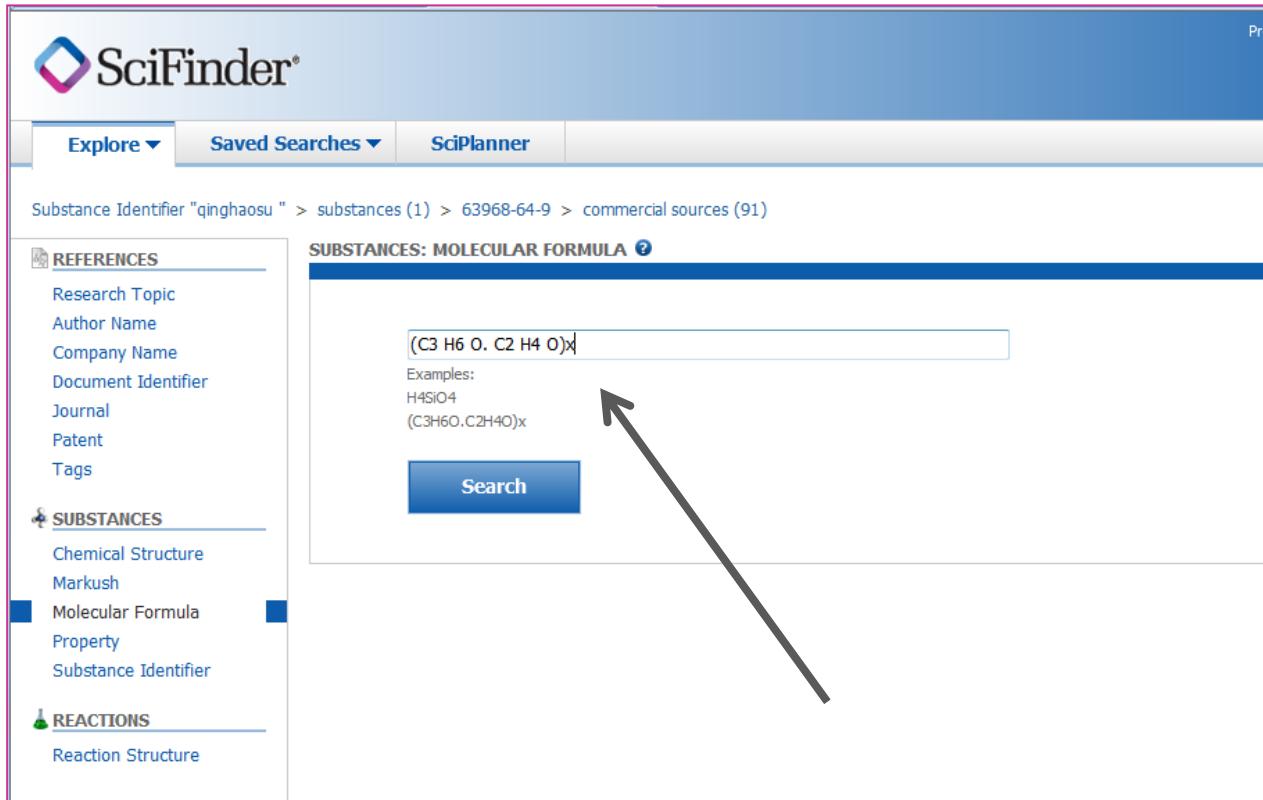
直接输入物质的名称，CAS No，俗名，都能检索，一次最多检索25个物质，用换行换开

理化性质检索



The screenshot shows the SciFinder interface with a blue header bar. The top left contains the SciFinder logo. The top right has a "Pre" button. Below the header is a navigation bar with "Explore ▾", "Saved Searches ▾", and "SciPlanner". The main content area shows the search path: Substance Identifier "qinghaosu" > substances (1) > 63968-64-9 > commercial sources (91). On the left, there's a sidebar with sections for "REFERENCES", "SUBSTANCES", and "REACTIONS". The "SUBSTANCES" section has options for "Chemical Structure", "Markush", "Molecular Formula", "Property" (which is highlighted with a red box), and "Substance Identifier". The "REACTIONS" section has an option for "Reaction Structure". The main search area is titled "SUBSTANCES: PROPERTY ?" and contains two sets of input fields. The first set is for "Experimental" properties, with a dropdown menu "Select Property..." and a "Value or Range" input field. A note says: "Examples: Individual value as 44, range as 25-35, or open ended range as >125 or <125". The second set is for "Predicted" properties, with a similar structure. A large blue "Search" button is at the bottom of the search area.

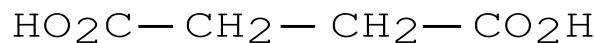
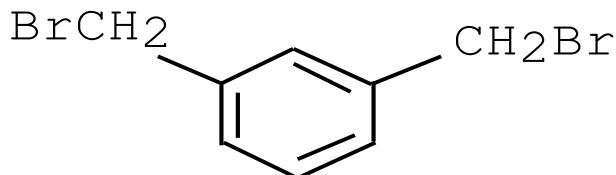
分子式检索



The screenshot shows the SciFinder search interface. The top navigation bar includes 'Explore', 'Saved Searches', and 'SciPlanner'. The main search area is titled 'SUBSTANCES: MOLECULAR FORMULA' with a question mark icon. A search input field contains the formula '(C3 H6 O. C2 H4 O)x'. Below the input field are examples: H4SiO4 and (C3H6O.C2H4O)x. A large blue 'Search' button is positioned below the examples. A black arrow points from the text '(C3 H6 O. C2 H4 O)x' in the input field towards the 'Search' button.

分子式的检索，需要按照HILL排序进行

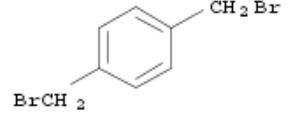
只知道起始原料的聚合物



(C₈H₈Br₂ . C₄H₆O₄)_x

1. Substance Detail
176516-41-9

623-24-5
C₈H₈Br₂



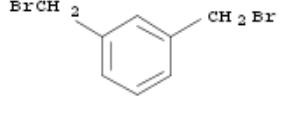
110-15-6
C₄H₆O₄

HO2C-CH2-CH2-CO2H

(C₈H₈Br₂ . C₄H₆O₄)_x
Butanedioic acid, polymer with 1,4-bis (bromomethyl)benzene (9CI)

2. Substance Detail
132010-54-9

626-15-3
C₈H₈Br₂

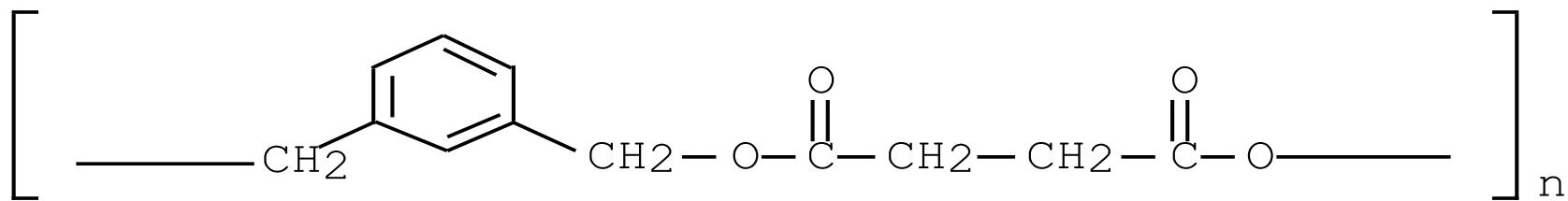


110-15-6
C₄H₆O₄

HO2C-CH2-CH2-CO2H

(C₈H₈Br₂ . C₄H₆O₄)_x
Butanedioic acid, polymer with 1,3-bis (bromomethyl)benzene (9CI)

知道最终SRU的检索



(C₁₂ H₁₂ O₄)_n

合金的检索

- 检索铁镍锰合金
- Fe.Mn.Ni

SUBSTANCES: MOLECULAR FORMULA ?

Examples:
H4SiO4
(C3H6O.C2H4O)x

Search

Sort by: CAS Registry Number		Display Options																								
<input type="checkbox"/> 0 of 1068 Substances Selected																										
<p><input type="checkbox"/> 1. 1621605-56-8 </p> <table border="1" style="width: 100%; border-collapse: collapse; text-align: center;"> <thead> <tr> <th>Component</th> <th>Component Percent</th> </tr> </thead> <tbody> <tr> <td>Fe</td> <td>90</td> </tr> <tr> <td>Ni</td> <td>9</td> </tr> <tr> <td>Mn</td> <td>0.5</td> </tr> </tbody> </table> <p>Fe . Mn . Ni Iron alloy, base, Fe 90,Ni 9,Mn 0.5</p>	Component	Component Percent	Fe	90	Ni	9	Mn	0.5	<p><input type="checkbox"/> 2. 1609450-43-2 </p> <table border="1" style="width: 100%; border-collapse: collapse; text-align: center;"> <thead> <tr> <th>Component</th> <th>Component Percent</th> </tr> </thead> <tbody> <tr> <td>Fe</td> <td>98</td> </tr> <tr> <td>Mn</td> <td>1.5</td> </tr> <tr> <td>Ni</td> <td>0.2</td> </tr> </tbody> </table> <p>Fe . Mn . Ni Steel, Fe 98,Mn 1.5,Ni 0.2</p>	Component	Component Percent	Fe	98	Mn	1.5	Ni	0.2	<p><input type="checkbox"/> 3. 1609284-41-4 </p> <table border="1" style="width: 100%; border-collapse: collapse; text-align: center;"> <thead> <tr> <th>Component</th> <th>Component Percent</th> </tr> </thead> <tbody> <tr> <td>Fe</td> <td>100</td> </tr> <tr> <td>Mn</td> <td>0.3 - 0.4</td> </tr> <tr> <td>Ni</td> <td>0.1</td> </tr> </tbody> </table> <p>Fe . Mn . Ni Steel, Fe 100,Mn 0.3-0.4,Ni 0.1</p>	Component	Component Percent	Fe	100	Mn	0.3 - 0.4	Ni	0.1
Component	Component Percent																									
Fe	90																									
Ni	9																									
Mn	0.5																									
Component	Component Percent																									
Fe	98																									
Mn	1.5																									
Ni	0.2																									
Component	Component Percent																									
Fe	100																									
Mn	0.3 - 0.4																									
Ni	0.1																									
<p><input type="checkbox"/> 4. 1522325-36-5 </p> <table border="1" style="width: 100%; border-collapse: collapse; text-align: center;"> <thead> <tr> <th>Component</th> <th>Component Percent</th> </tr> </thead> <tbody> <tr> <td>Fe</td> <td>68</td> </tr> <tr> <td>Ni</td> <td>30</td> </tr> <tr> <td>Mn</td> <td>1.5</td> </tr> </tbody> </table> <p>Fe . Mn . Ni Iron alloy, base, Fe 68,Ni 30,Mn 1.5</p>	Component	Component Percent	Fe	68	Ni	30	Mn	1.5	<p><input type="checkbox"/> 5. 1521111-49-8 </p> <table border="1" style="width: 100%; border-collapse: collapse; text-align: center;"> <thead> <tr> <th>Component</th> <th>Component Percent</th> </tr> </thead> <tbody> <tr> <td>Fe</td> <td>96</td> </tr> <tr> <td>Ni</td> <td>3.6</td> </tr> <tr> <td>Mn</td> <td>0.6</td> </tr> </tbody> </table> <p>Fe . Mn . Ni Iron alloy, base, Fe 96,Ni 3.6,Mn 0.6</p>	Component	Component Percent	Fe	96	Ni	3.6	Mn	0.6	<p><input type="checkbox"/> 6. 1497308-48-1 </p> <table border="1" style="width: 100%; border-collapse: collapse; text-align: center;"> <thead> <tr> <th>Component</th> <th>Component Percent</th> </tr> </thead> <tbody> <tr> <td>Fe</td> <td>68</td> </tr> <tr> <td>Ni</td> <td>29</td> </tr> <tr> <td>Mn</td> <td>3.1</td> </tr> </tbody> </table> <p>Fe . Mn . Ni Iron alloy, base, Fe 68,Ni 29,Mn 3.1</p>	Component	Component Percent	Fe	68	Ni	29	Mn	3.1
Component	Component Percent																									
Fe	68																									
Ni	30																									
Mn	1.5																									
Component	Component Percent																									
Fe	96																									
Ni	3.6																									
Mn	0.6																									
Component	Component Percent																									
Fe	68																									
Ni	29																									
Mn	3.1																									

Tabular Inorganic Substance的检索

- 检索 Al0.33 Fe0.07 Mg0.67 (CO₃)0.02 (CN)0.43 (OH)2
- 使用以下的分子式检索： CN . CO₃ . Al . Fe . HO . Mg

SUBSTANCES: MOLECULAR FORMULA ?

C N . C O₃ . A l . F e . H O . M g |

Examples:
H₄SiO₄
(C₃H₆O.C₂H₄O)_x

Search

Sort by: CAS Registry Number ▾

0 of 12 Substances Selected

Component	Component Ratio
HO	2
Mg	0.83
Fe	0.02
Al	0.17
CO ₃	0.05
CN	0.12

1. 156348-99-1

~1

Component	Component Ratio
HO	2
Mg	0.57
Fe	0.09
Al	0.43
CO ₃	0.03
CN	0.55

C N . C O₃ . A l . F e . H O . M g
Aluminum iron magnesium carbonate cyanide hydroxide ($\text{Al}_{0.17}\text{Fe}_{0.02}\text{Mg}_{0.83}(\text{CO}_3)_{0.05}(\text{CN})_{0.12}(\text{OH})_2$)

2. 154948-24-0

~1

Component	Component Ratio
HO	2
Mg	0.67
Fe	0.07
Al	0.33
CO ₃	0.02
CN	0.43

C N . C O₃ . A l . F e . H O . M g
Aluminum iron magnesium carbonate cyanide hydroxide ($\text{Al}_{0.43}\text{Fe}_{0.09}\text{Mg}_{0.57}(\text{CO}_3)_{0.05}(\text{CN})_{0.55}(\text{OH})_2$)

3. 154948-23-9

~1

Component	Component Ratio
HO	2
Mg	0.67
Fe	0.07
Al	0.33
CO ₃	0.02
CN	0.43

C N . C O₃ . A l . F e . H O . M g
Aluminum iron magnesium carbonate cyanide hydroxide ($\text{Al}_{0.33}\text{Fe}_{0.07}\text{Mg}_{0.67}(\text{CO}_3)_{0.02}(\text{CN})_{0.43}(\text{OH})_2$)

Display Options

结构式检索—精确检索

Preferences
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REFERENCES

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[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 ?

- [4 step ref](#)
- [3 step-ref](#)
- [4 Step](#)
- [3130](#)
- [fluorescence with biosensor3128](#)
- [RCM-1816ref](#)
- [646Ref](#)
- [Luminescent substances with organic](#)
- [refined](#)
- [Total reaction](#)
- [Autosaved Substance Set](#)

[View All](#) | [Import](#)

KEEP ME POSTED ?

You have no profiles.

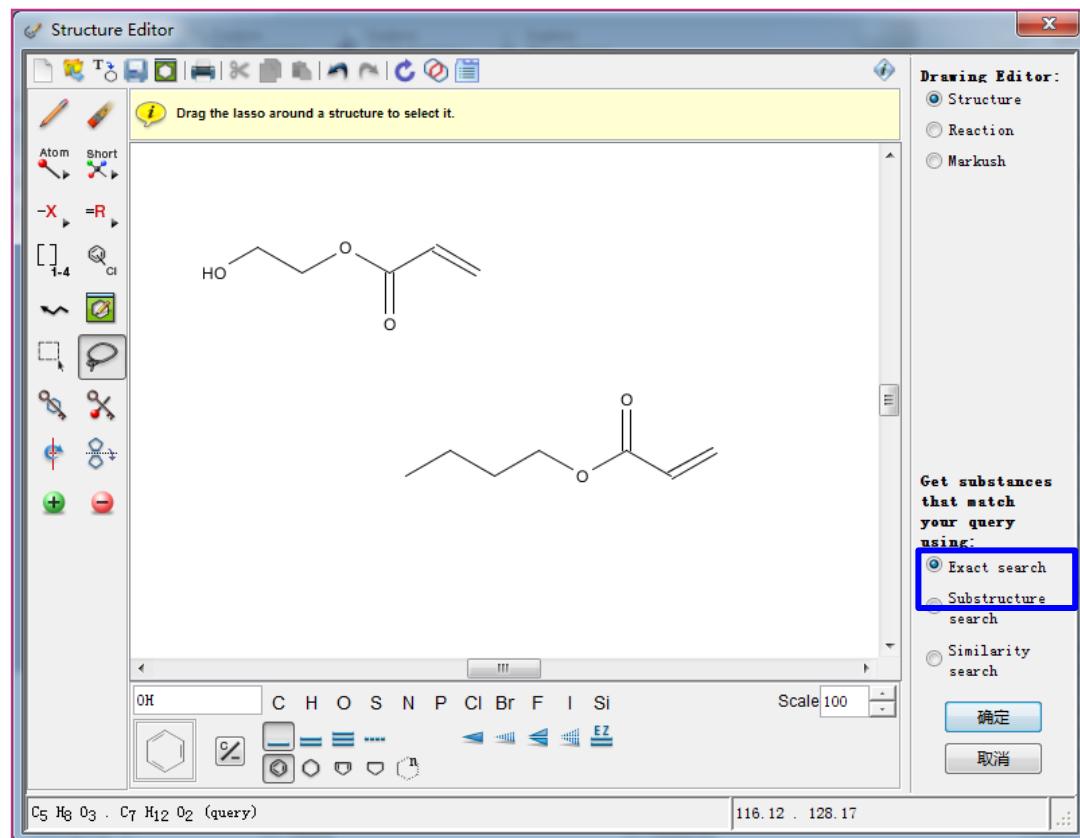
CAS is a division of the American Chemical Society.

38

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知道起始原料的聚合物检索

- 检索由丙烯酸丁酯 (Butyl acrylate) 和丙烯酸羟乙酯 (2-hydroxyethyl acrylate) 聚合产生的聚合物
- 只绘制单体，精确结构



使用精确结构检索

检索结果—看名字得到区别

1. Substance Detail 1041101-23-8

818-61-1 C₅H₈O₃

HO—CH₂—CH₂—O—C(=O)CH=CH₂

141-32-2 C₇H₁₂O₂

n-BuO—C(=O)CH=CH₂

(C₇H₁₂O₂ · C₅H₈O₃)_x
2-Propenoic acid, butyl ester, polymer with
2-hydroxyethyl 2-propenoate, triblock

2. Substance Detail 830358-94-6

818-61-1 C₅H₈O₃

HO—CH₂—CH₂—O—C(=O)CH=CH₂

141-32-2 C₇H₁₂O₂

n-BuO—C(=O)CH=CH₂

(C₇H₁₂O₂ · C₅H₈O₃)_x
2-Propenoic acid, butyl ester, polymer with
2-hydroxyethyl 2-propenoate, graft

3. Substance Detail 765276-02-6

818-61-1 C₅H₈O₃

HO—CH₂—CH₂—O—C(=O)CH=CH₂

141-32-2 C₇H₁₂O₂

n-BuO—C(=O)CH=CH₂

(C₇H₁₂O₂ · C₅H₈O₃)_x
2-Propenoic acid, butyl ester, polymer with
2-hydroxyethyl 2-propenoate, diblock

4. Substance Detail 121264-61-7

818-61-1 C₅H₈O₃

HO—CH₂—CH₂—O—C(=O)CH=CH₂

141-32-2 C₇H₁₂O₂

n-BuO—C(=O)CH=CH₂

(C₇H₁₂O₂ · C₅H₈O₃)_x
2-Propenoic acid, butyl ester, polymer with
2-hydroxyethyl 2-propenoate, block

5. Substance Detail 32409-50-0

818-61-1 C₅H₈O₃

HO—CH₂—CH₂—O—C(=O)CH=CH₂

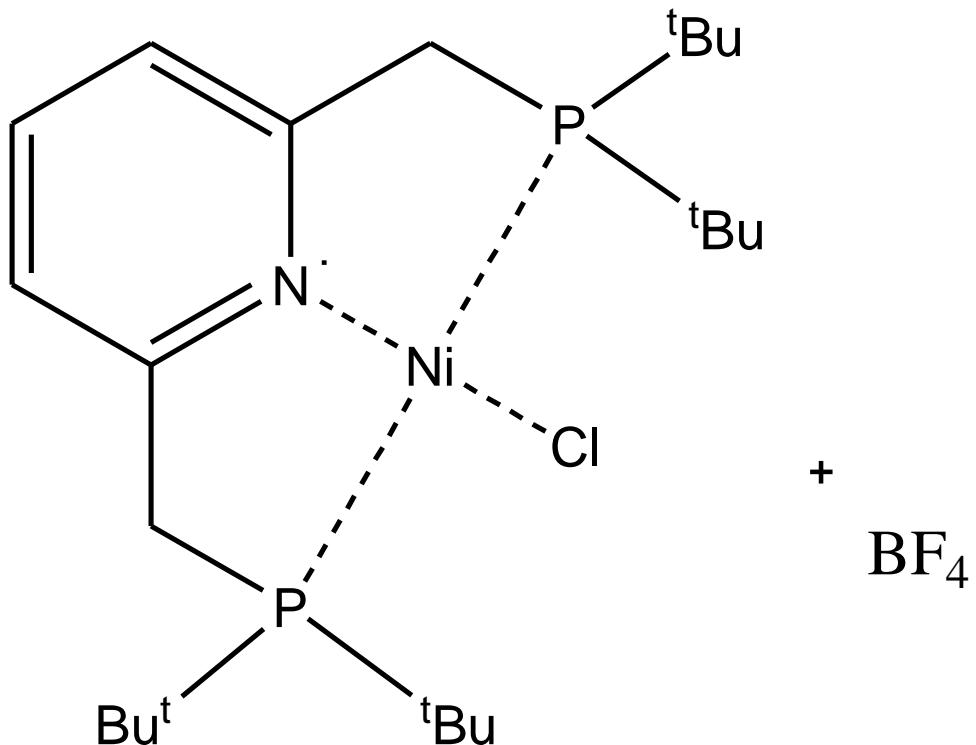
141-32-2 C₇H₁₂O₂

n-BuO—C(=O)CH=CH₂

(C₇H₁₂O₂ · C₅H₈O₃)_x
2-Propenoic acid, butyl ester, polymer with
2-hydroxyethyl 2-propenoate

Triblock, Graft, Diblock,
Block, 无序

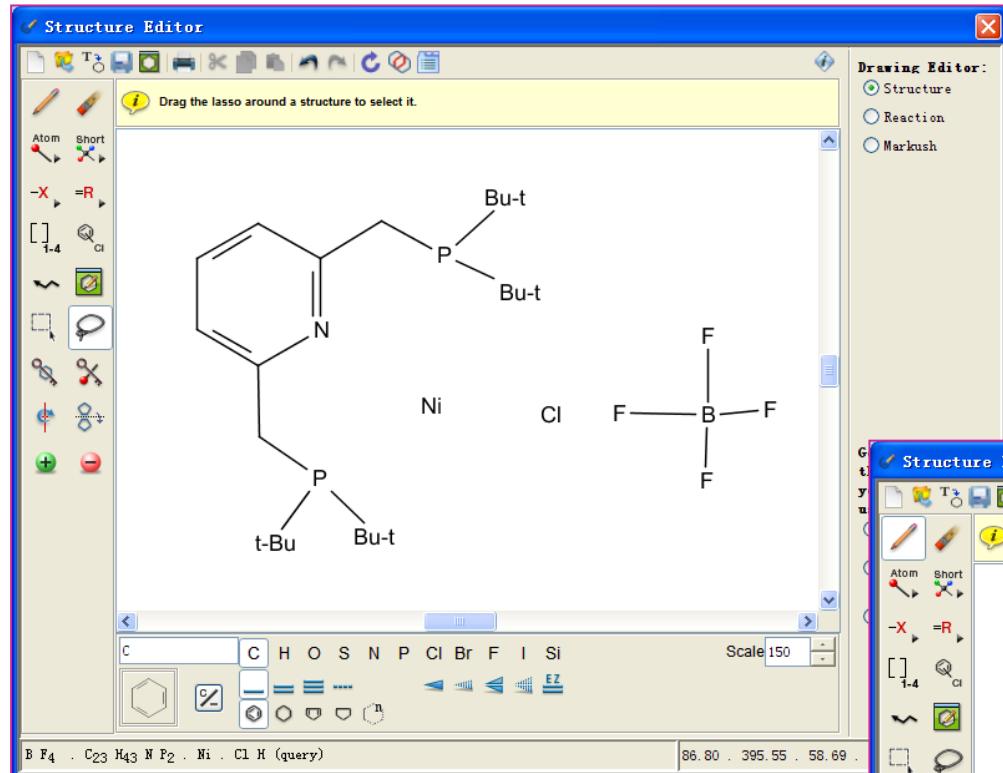
精确结构检索—检索金属配合物



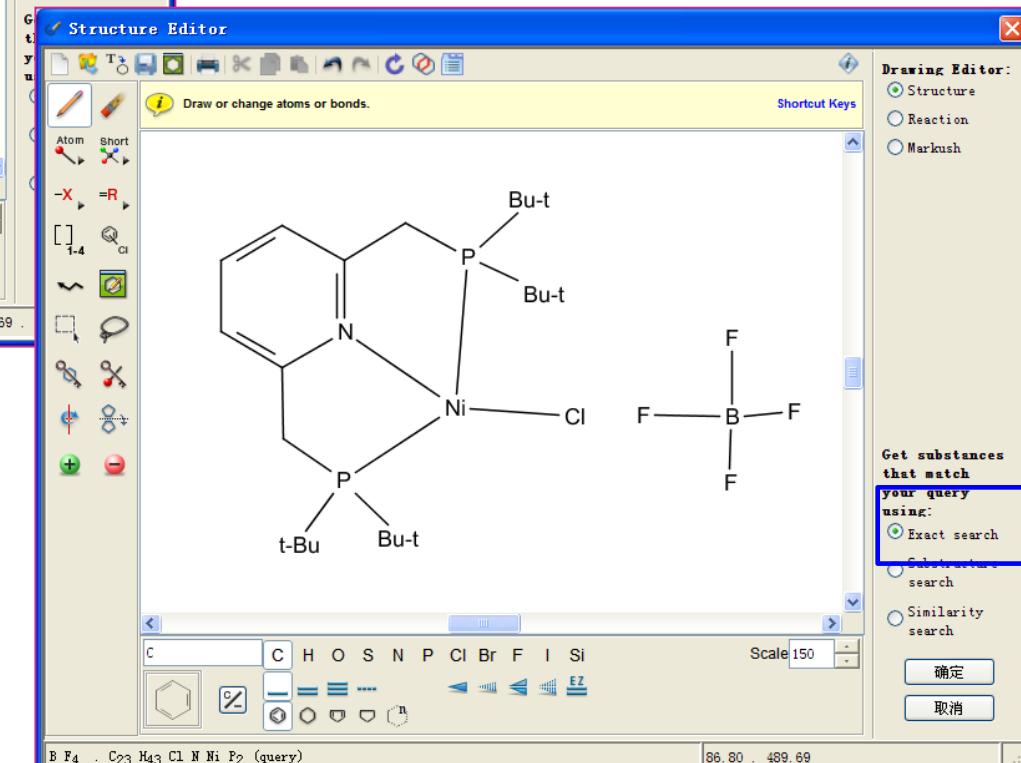
该结构中包含：

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

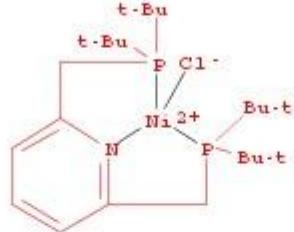


SciFinder中的结果

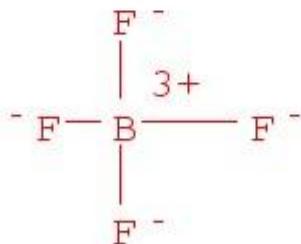
1. Substance Detail
1136166-99-8

~1 

1136166-98-7
C₂₃H₄₃ClN Ni P₂



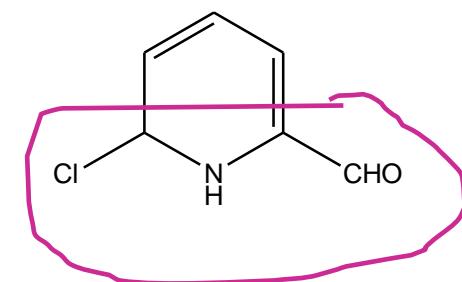
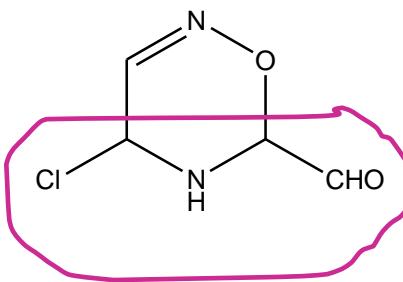
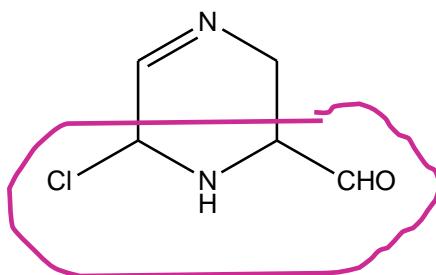
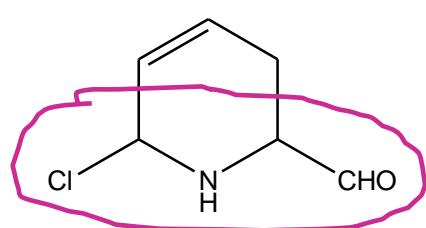
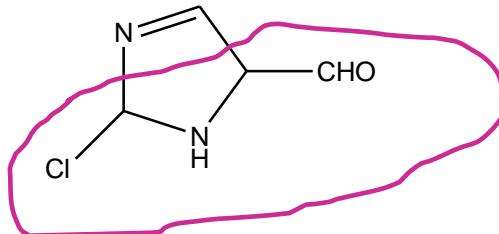
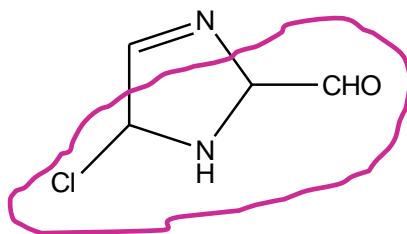
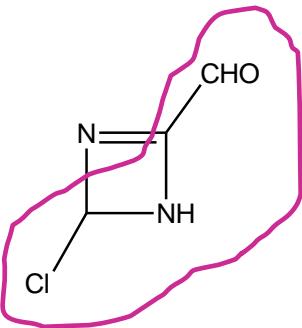
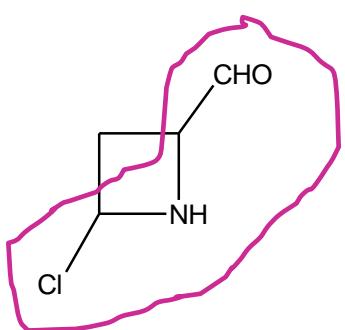
14874-70-5
BF₄



C₂₃H₄₃ClN Ni P₂ . BF₄

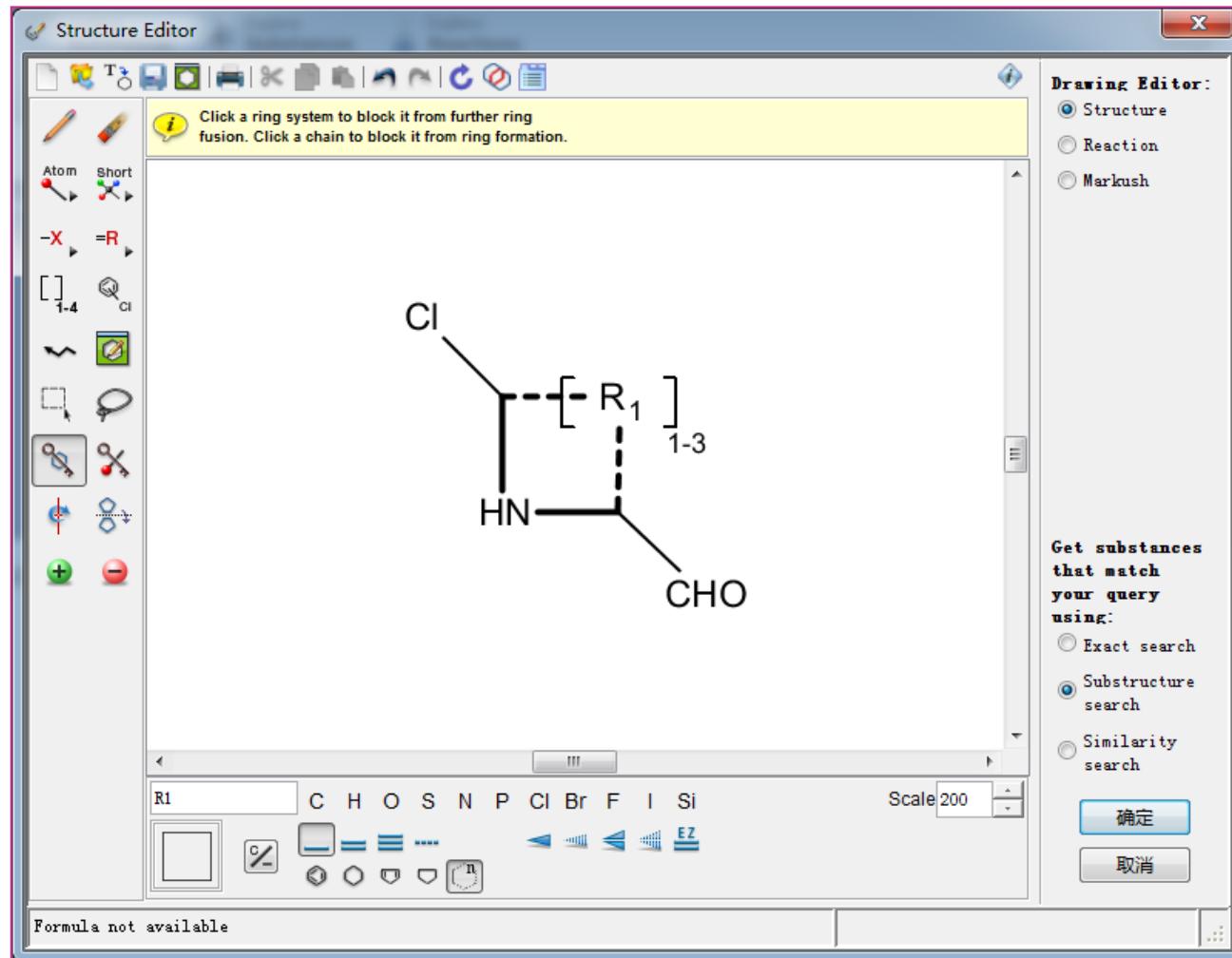
Nickel(1+), [2,6-bis[[bis(1,1-dimethylethyl)phosphino-κ^P]methyl]pyridine-κ^N]chloro-, (*S*^A-4-3)-, tetrafluoroborate(1-) (1:1)

我想获得以下的一系列物质



○ ○ ○ ○ ○ ○

结构定义



用亚结构检索获得所有的物质

亚结构检索结果

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Chemical Structure substructure > substances (469)

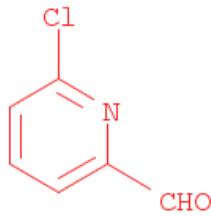
SUBSTANCES ? Get References Get Reactions Get Commercial Sources Tools ▾ Create Keep Me Posted Alert Send to SciPlanner

Analyze Refine Sort by: Number of References ▾ 0 of 469 Substances Selected Answers per Page [50] View: █ █ █ █ █

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

0 of 469 Substances Selected

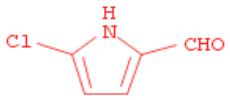
1. Substance Detail 54087-03-5 ~33 0 of 469 Substances Selected



C=CC1=C(Cl)C=CC(=O)N1

C₆H₄ClN₂O

2. Substance Detail 1757-28-4 ~19 0 of 469 Substances Selected



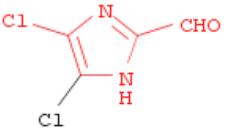
C=CC1=C(Cl)C=CN1=O

C₅H₄ClN₂O

1-(5-chloropyrrole-2-carbaldehyde)

Experimental Properties

3. Substance Detail 81293-97-2 ~11 0 of 469 Substances Selected



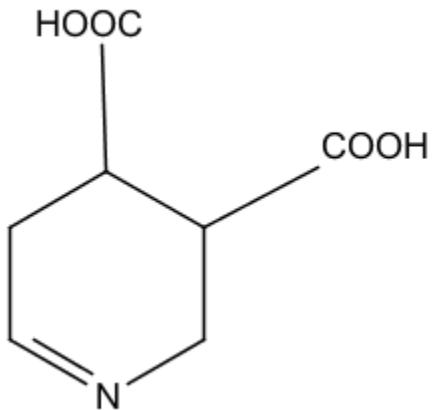
C=CC1=C(Cl)C=CC(=O)N1=CN2=CC=C(Cl)C2=O

C₄H₂Cl₂N₂O

1-(4,5-dichloro-2-formylimidazol-1-yl)butan-1-one

相似结构检索

这是一个不存在的化合物，有没有办法通过寻找类似物的方法，找到这个化合物的合成方法



Structure Editor

Draw or change atoms or bonds.

Shortcut Keys

Drawing Editor:
 Structure
 Reaction
 Markush

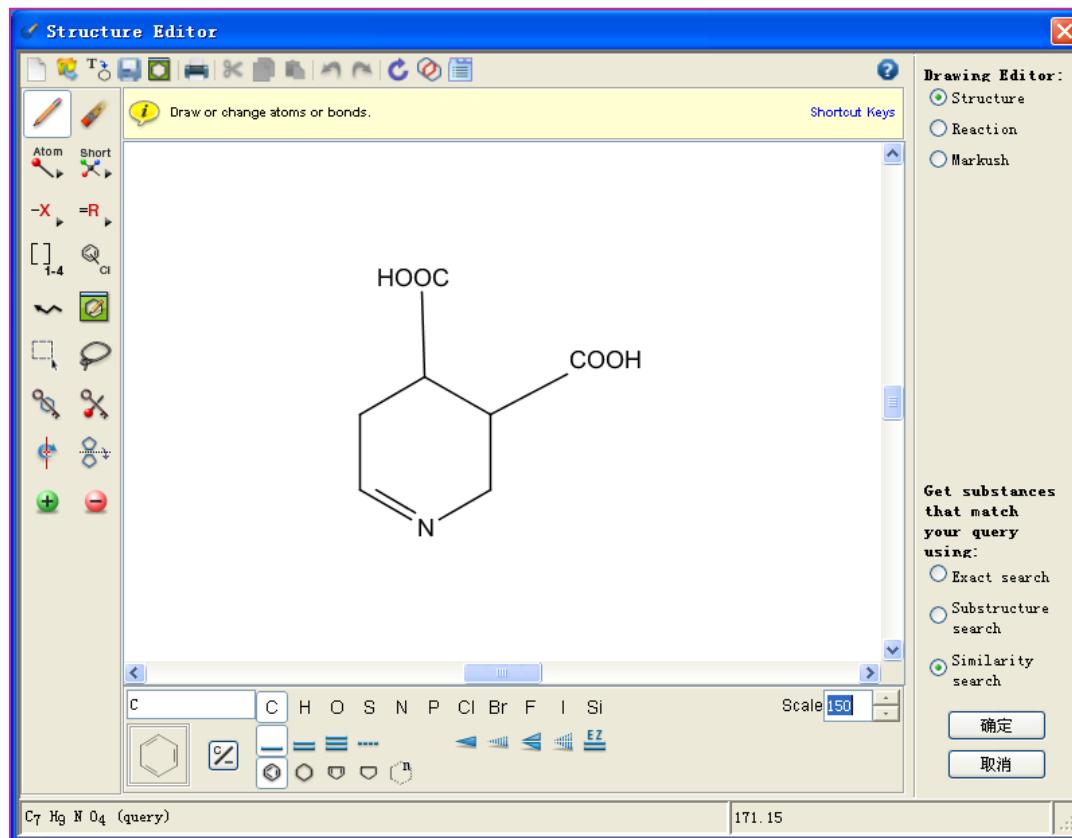
Get substances that match your query using:
 Exact search
 Substructure search
 Similarity search

确定 取消

Scale 150

C H O S N P Cl Br F I Si

C7 H9 N O4 (query) 171.15



相似结构检索

SciFinder

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Chemical Structure similarity > substances (55)

REFERENCES

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

SUBSTANCES

- Chemical Structure** (selected)
- Markush
- Molecular Formula
- Property
- Substance Identifier

REACTIONS

- Reaction Structure

SUBSTANCES: CHEMICAL STRUCTURE

Structure Editor:

Java **Non-Java**

CC1=CN=C1C(=O)C

Search Type:

- Exact Structure
- Substructure
- Similarity

Show precision analysis

Click image to change structure or view detail.

Import CXF

Search

SciFinder会依据相似度给出相似度表格，选择高分值的看

SciFinder

Preferences | SciFinder Help ▾ Sign Out

Welcome Sam Yu

Chemical Structure similarity

SUBSTANCES

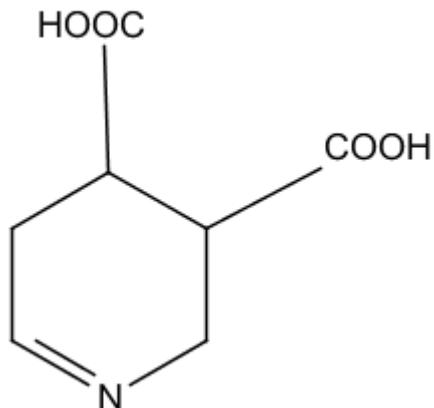
Select All Deselect All

5 of 6 Similarity Candidates Selected

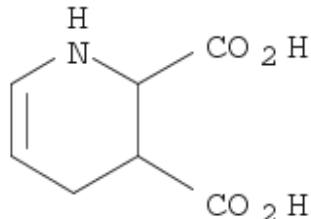
	Substances	
<input type="checkbox"/>	≥ 99 (most similar)	0
<input type="checkbox"/>	95-98	0
<input type="checkbox"/>	90-94	0
<input checked="" type="checkbox"/>	85-89	6
<input checked="" type="checkbox"/>	80-84	1
<input checked="" type="checkbox"/>	75-79	16
<input checked="" type="checkbox"/>	70-74	32
<input checked="" type="checkbox"/>	65-69	1689
<input type="checkbox"/>	0-64 (least similar)	2093

Get Substances

和原本结构相似的结构



Score: 81
 4. Substance Detail
 41819-46-9

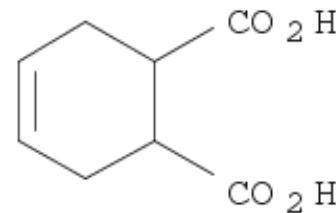


C₇H₉N₀4
 2,3-Pyridinedicarboxylic acid, 1,2,3,4-tetrahydro-

~1 

结构存在相似，但又不一样，可依据这些化合物的制备方法，制备目标化合物

Score: 68
 43. Substance Detail
 88-98-2



C₈H₁₀O₄
 4-Cyclohexene-1,2-dicarboxylic acid

~471 



Spectra
 Experimental Properties

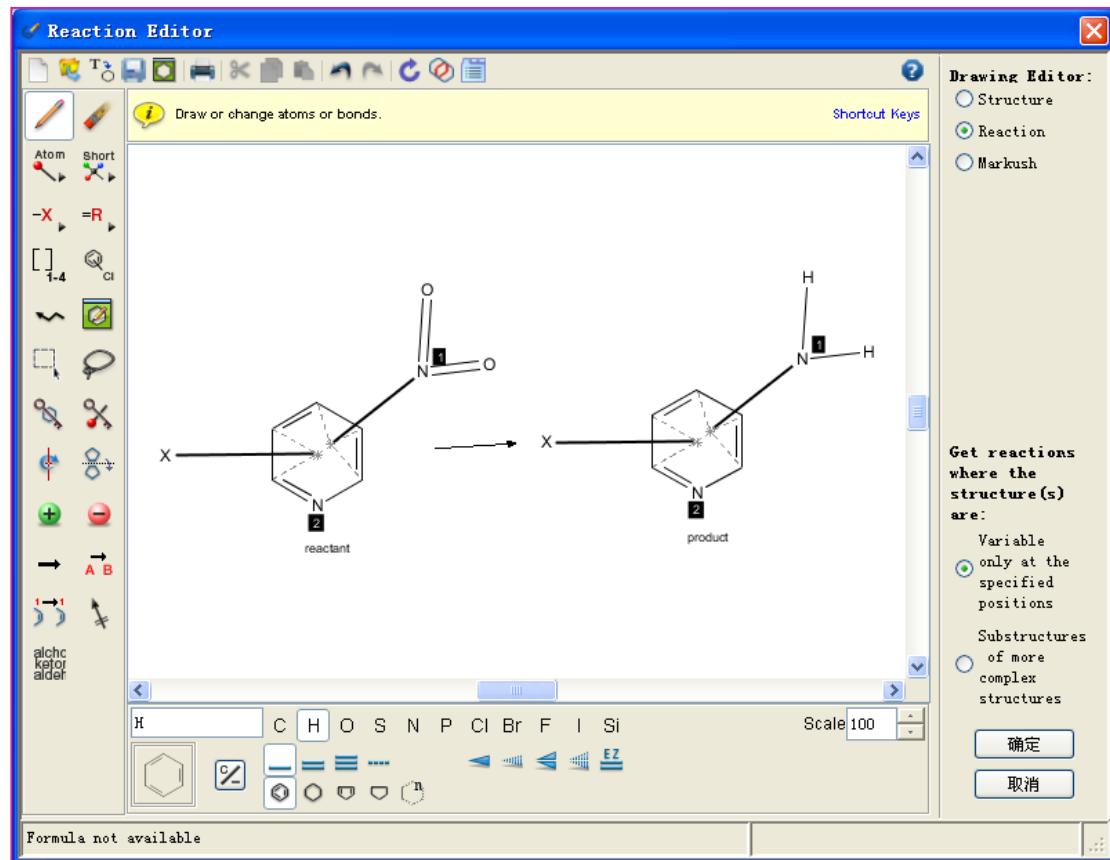
精确结构， 亚结构， 相似结构检索区别

- 精确结构
 - 检索到结构的盐，混合物，配合物，聚合物等
 - 母体结构不能改变，不能修饰
- 亚结构
 - 检索到结构的本身，衍生物结构
 - 母体结构不能改变，但可以修饰
- 相似结构
 - 检索到和结构本身相似度在**60分以上**的物质
 - 母体结构可以改变，可以修饰，用相似度控制结果范围

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反应检索



检索要求:

1: 吡啶环2, 3, 4位上存在一个硝基还原成氨基

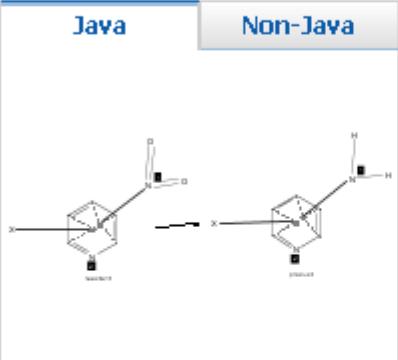
2: 吡啶环5, 6位上存在一个卤素

SciFinder Web中的检索

REACTIONS: REACTION STRUCTURE

Structure Editor:

Java Non-Java



Click image to change structure or view detail.

[Import CXF](#)

[Search](#)

[Advanced Search](#)

Search Type:

Allow variability only as specified
 Substructure

如果之前选择检索模式，可以在
此处进行修改

SciFinder中的检索结果

SciFinder® Welcome Sam Yu

Explore ▾ Saved Searches ▾ SciPlanner Save Print Export

Reaction Structure structure variable only at spe... > reactions (56)

REACTIONS Get References Tools ▾ Send to SciPlanner

Analyze Refine Group by: No Grouping Sort by: Accession Number NEW! Display Options

Analyze by: Reagent (New) 0 of 56 Reactions Selected Page: 1 of 3

Reagent (New) 26
H₂
Fe 9
KF 6
Mg 5
NH₃ 5
TiCl₄ 5
HCl 4

1. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.



▶ Overview

Group By Document

Get References Tools ▾

Group by: **Document** Sort

No Grouping

Document Selected

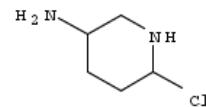
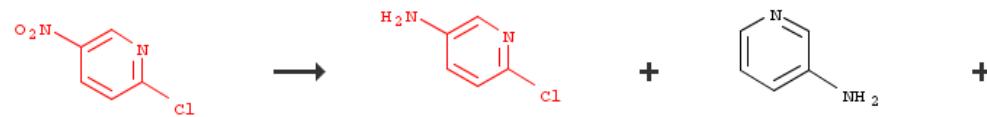
Transformation

1. **View Reaction Detail**

Group By Document 将来自同篇文献的反应合并

6. Selective catalytic hydrogenation of nitro groups in the presence of activated heteroaryl halides Quick View Full Text
 4 Reactions Similar Reactions

Single Step Hover over any structure for more options.

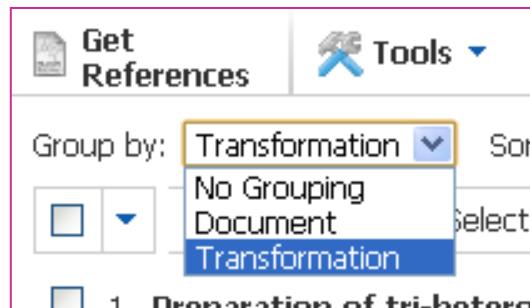


▶ Overview

▶ Experimental Procedure

10. N-Pyridyl and Pyrimidine Benzamides as KCNQ2/Q3 Potassium Channel Openers for the Treatment of Epilepsy Quick View
 Full Text
 3 Reactions

Group By Transformation



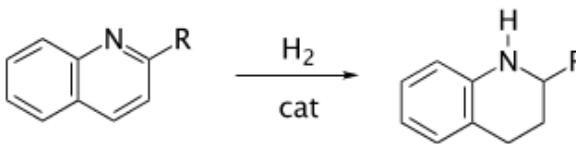
将所有同类型变化的反
应合并

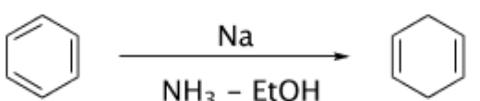
0 of 56 Reactions Selected

- 1. Reduction of Nitro Compounds to Amines
49 Reactions

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

$$\text{R}-\text{X} \longrightarrow \text{R}-\text{H}$$
- 4. Reduction of Aromatic Rings/ Birch or Benkeser Reduction
1 Reaction




Similary Reaction

1. Preparation of tri-heterocyclic derivatives as Flt3 kinase inhibitors
[1 Reaction](#) [Similar Reactions](#)

[Quick View](#) [Full Text](#)

Single Step Hover over any structure for more options.



[▶ Overview](#)

对单步反应提供相似反应检索，
Broad: 仅反应中心相同
Medium: 反应中心和附属原子相同
Narrow: 反应中心及扩展原子和键相同

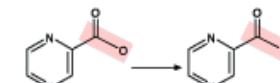
Get Similar Reactions

Retrieve similar reactions from:

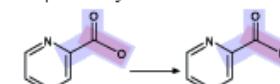
- All reactions
- Current answer set

Include this level of similarity:

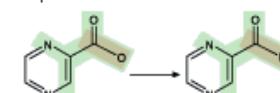
- Broad - Reaction centers only (96991)



- Medium - Reaction centers plus adjacent atoms and bonds (92590)



- Narrow - Reaction centers plus extended atoms and bonds (88722)



[Get Reactions](#)

[Cancel](#)

相似反应结果

1. Preparation of tri-heterocyclic derivatives as Flt3 kinase inhibitors [Quick View](#) [Full Text](#)

[1 Reaction](#) [Similar Reactions](#)

Single Step Hover over any structure for more options.

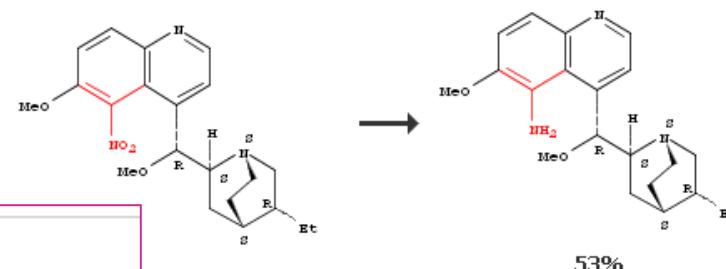


[▶ Overview](#)

0 of 88722 Reactions Selected

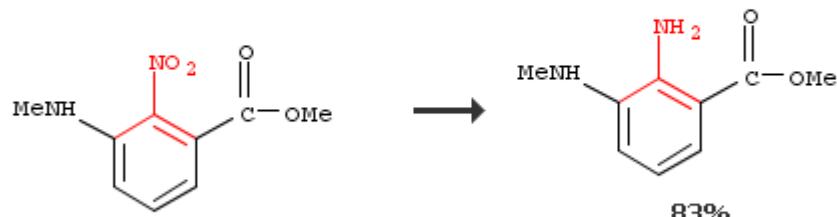
1. [View Reaction Detail](#) [Link](#) [Similar Reactions](#)

Single Step Hover over any structure for more options.



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

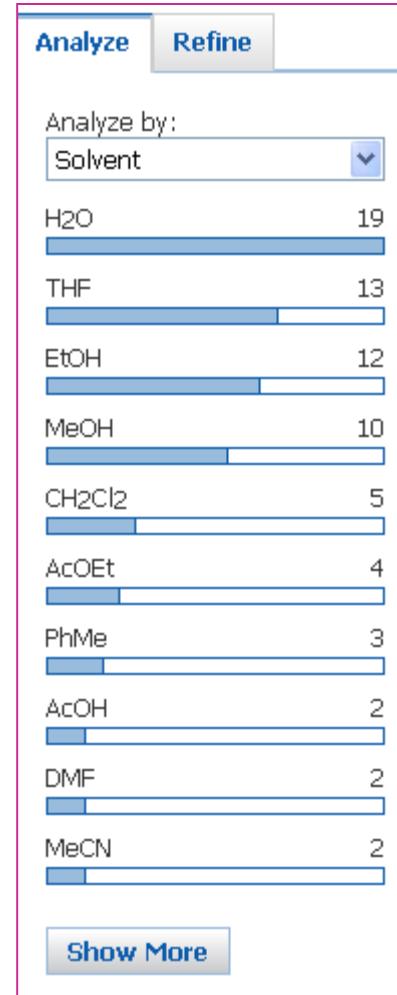
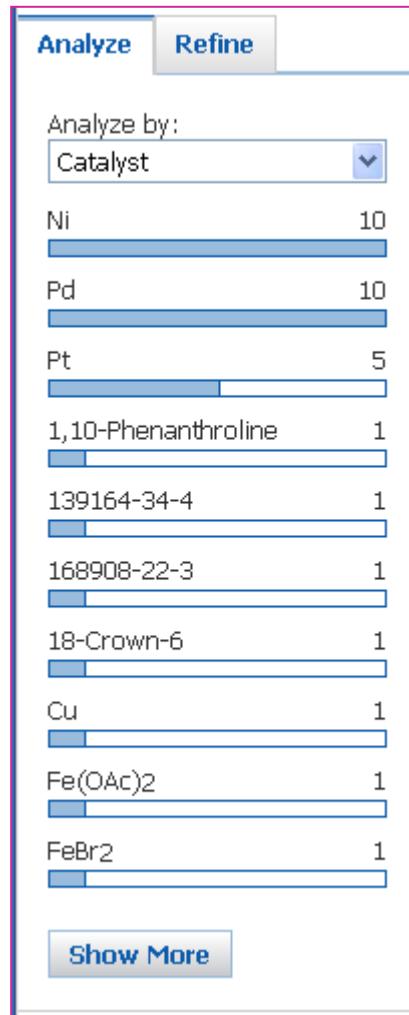
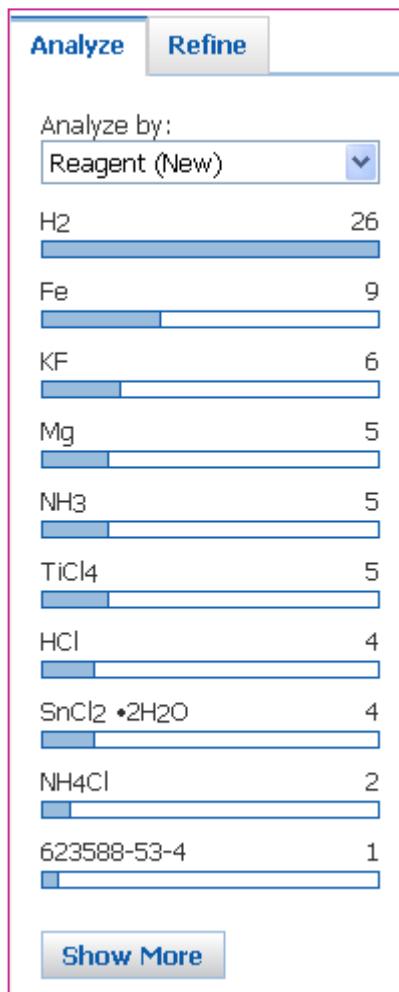
Single Step Hover over any structure for more options.



[▶ Overview](#)

这些都和原有的反应，在反应中心，及扩展的原子和键上是一致的

SciFinder Web中的反应后处理



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）

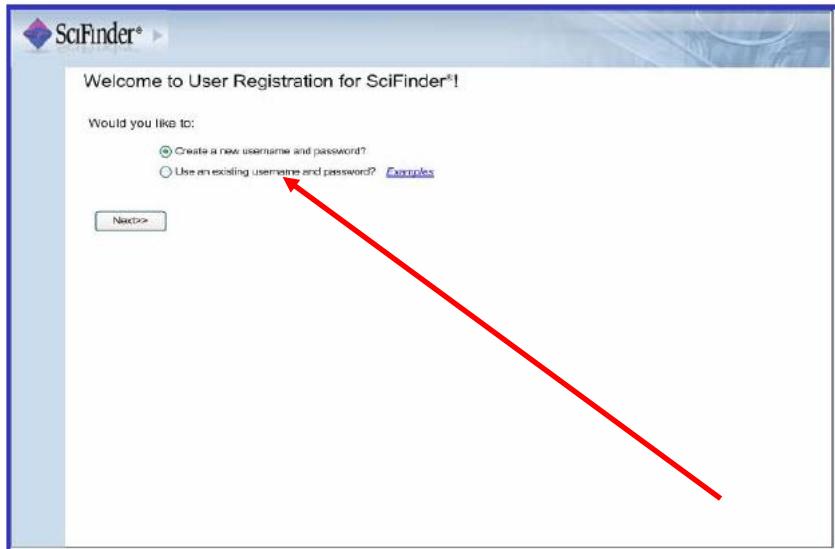
在图书馆相关页面上找到SciFinder Web注册用的网址

千万别用360浏览器，用其他浏览器的时候，也请关闭360安全卫士



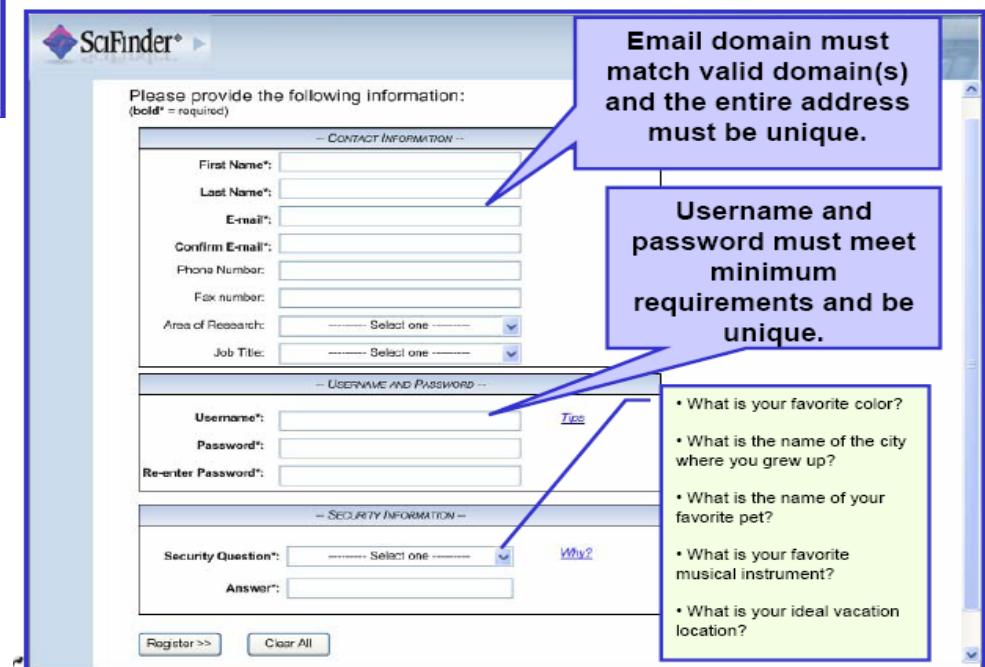
The screenshot shows the homepage of the East China University of Science and Technology Library. At the top, there is a banner featuring the university's logo and name in Chinese and English, along with a modern building image. Below the banner, a navigation bar includes links for 首页 (Home), 资源导航 (Resource Navigation), 读者服务 (Reader Services), 关于本馆 (About the Library), 帮助指南 (Help Guide), and a date/time stamp (2014年3月17日 星期一). A search bar with the placeholder "站内搜索" (Search within site) is also present. The main content area features a heading "美国化学文摘[WEB版]使用指南" (Guide to ACS Web Edition) and a sub-section titled "如果您已经注册请直接访问《美国化学文摘WEB版》" (If you have registered, please directly visit the ACS Web Edition). It also includes a warning message "请不要重复注册!" (Please do not register again!). Below this, there is explanatory text about the registration process using SciFinder Web, mentioning the URL <https://scifinder.cas.org/registration/index.html>, a corpKey value, and instructions for completing the registration form. At the bottom, there are links for "详细的注册方法请看: 使用帮助" (For detailed registration methods, see: Help) and "常见问题请看: 常见问题" (For common questions, see: Frequently Asked Questions). To the right of the main content, there are two small images of library buildings.

点击URL创建SciFinder Web账号



开始创建SciFinder Web帐号

创建ID所用的IP不能是代理服务器的IP



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

CONTACT INFORMATION

- First Name*: [Input Field]
- Last Name*: [Input Field]
- E-mail*: [Input Field]
- Confirm E-mail*: [Input Field]
- Phone Number*: [Input Field]
- Fax number*: [Input Field]
- Area of Research*: [Select one]
- Job Title*: [Select one]

USERNAME AND PASSWORD

- Username*: [Input Field] *Type*
- Password*: [Input Field]
- Re-enter Password*: [Input Field]

SECURITY INFORMATION

- Security Question*: [Select one] *Why?*
- Answer*: [Input Field]

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：

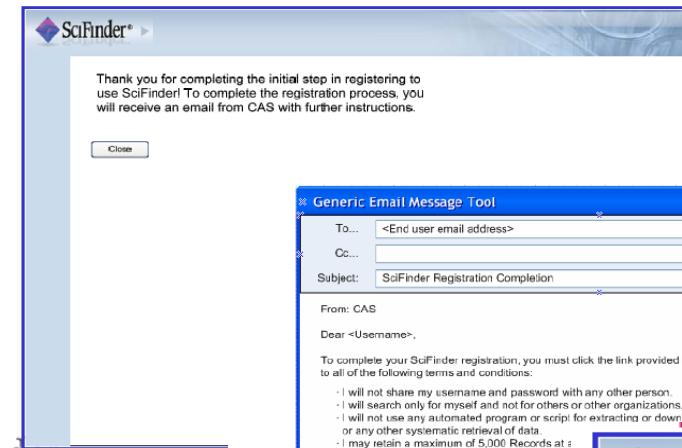
必须包含 7-15 个字符，并且至少包含三个以下字符：

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

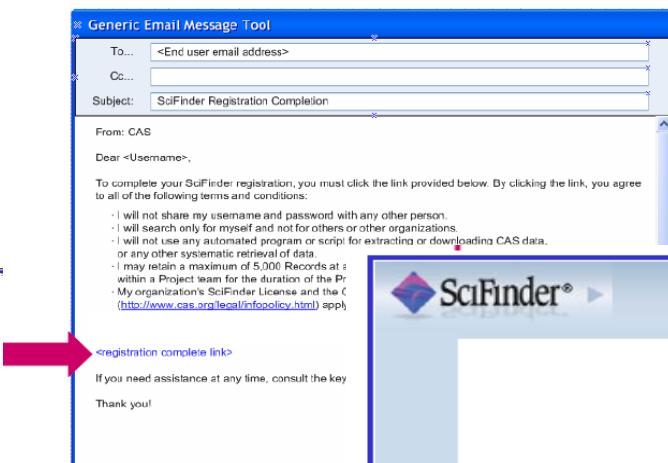
密码设置小技巧：

- 1：不要和账号中有重复的字符
- 2：密码格式最好是abc@123

对新ID的Email确认



需要点击邮件中的确认链接



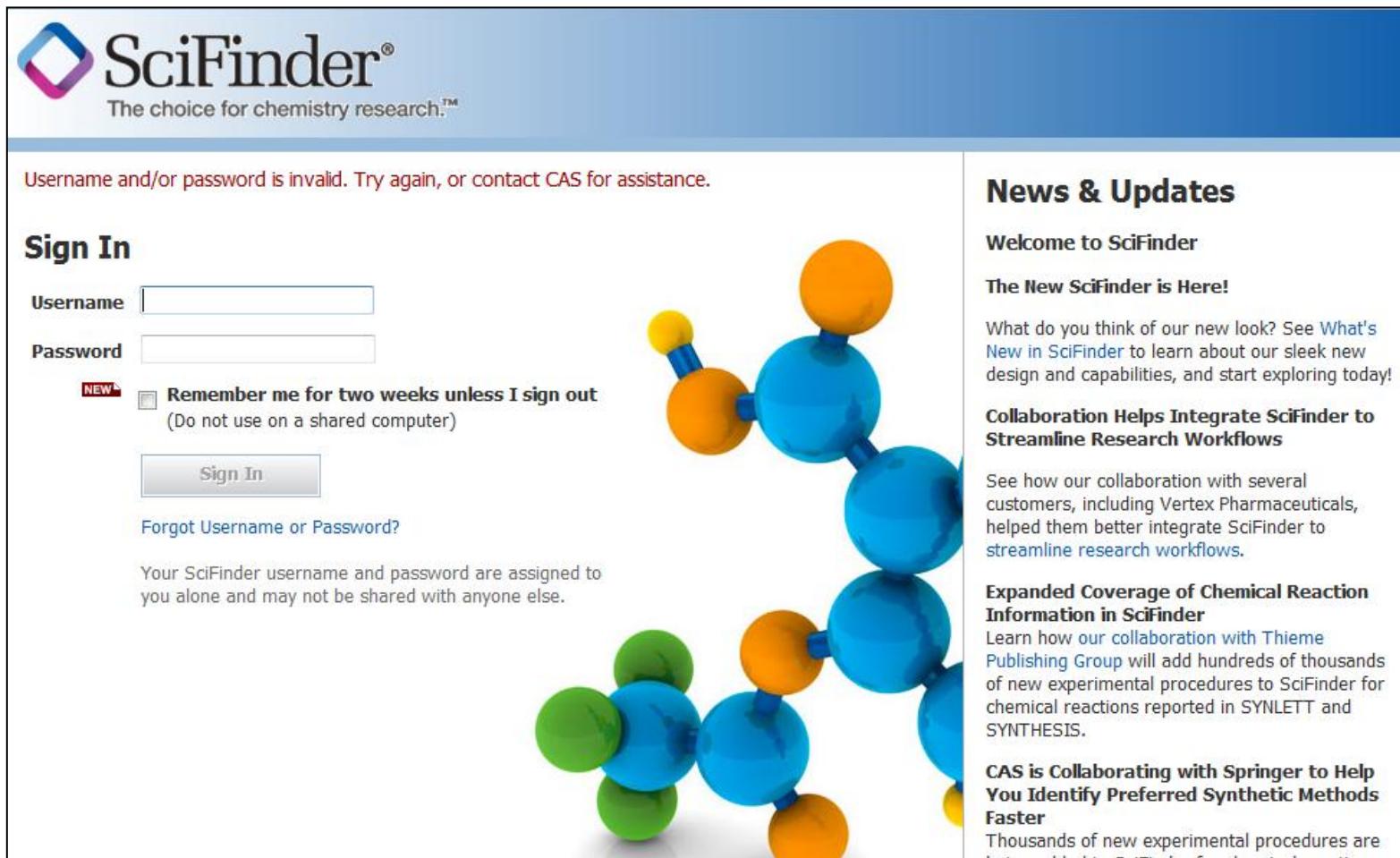
Welcome to SciFinder!

You have successfully registered.
To login, follow the link below.

<http://scifinder.cas.org>

Http://scifinder.cas.org

SciFinder Web 常见问题



The screenshot shows the SciFinder Web sign-in page. At the top, the SciFinder logo and tagline "The choice for chemistry research.™" are displayed. Below the logo, an error message in red text reads: "Username and/or password is invalid. Try again, or contact CAS for assistance." The sign-in form includes fields for "Username" and "Password", both with placeholder text "Enter Username" and "Enter Password". A "Remember me for two weeks unless I sign out" checkbox is present, with the note "(Do not use on a shared computer)". A "Sign In" button is located below the checkbox. To the right of the sign-in form is a large, stylized 3D molecular model composed of spheres in various colors (blue, orange, yellow, green). On the right side of the page, there is a "News & Updates" section with several articles:

- 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 from Springer.

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>



将页面截图下来，一并发给图书馆

SciFinder使用注意事项

1. 单次下载只能下载50条记录，严禁过量下载SciFinder中的记录，如遇大量记录，请使用Analyze/Refine工具缩小检索范围，或使用Save功能，保存在网上
2. 请合理使用SciFinder，检索完，点击Sign Out退出
3. SciFinder使用南方答疑群：207211509（群满），258225168（新群）
4. 不能使用360浏览器登录SciFinder，即使在使用其他浏览器的时候，也请关闭360有关的任何软件

Thank You

俞靓

SciFinder 培训专员

Mail: Sam@igroup.com.cn

Tel:021-64453167-8004