

余敏

syu@acs-i.org

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如何使用SciFinder提高科研效率

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 - 结构式检索；分子式检索；物质属性检索
 - 如何获得物质的性质信息、谱图信息
 - 聚合物检索
- 反应检索
 - 结构编辑器的使用（绘图、限定反应的工具）
 - 如何进行锁环锁原子的结构反应检索
 - 如何进行亚结构反应检索，以及如何处理检索结果
 - 案例分享
 - 多氧簇金属的反应信息
 - MOF化合物反应信息



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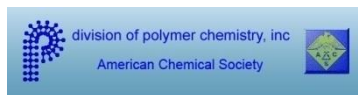
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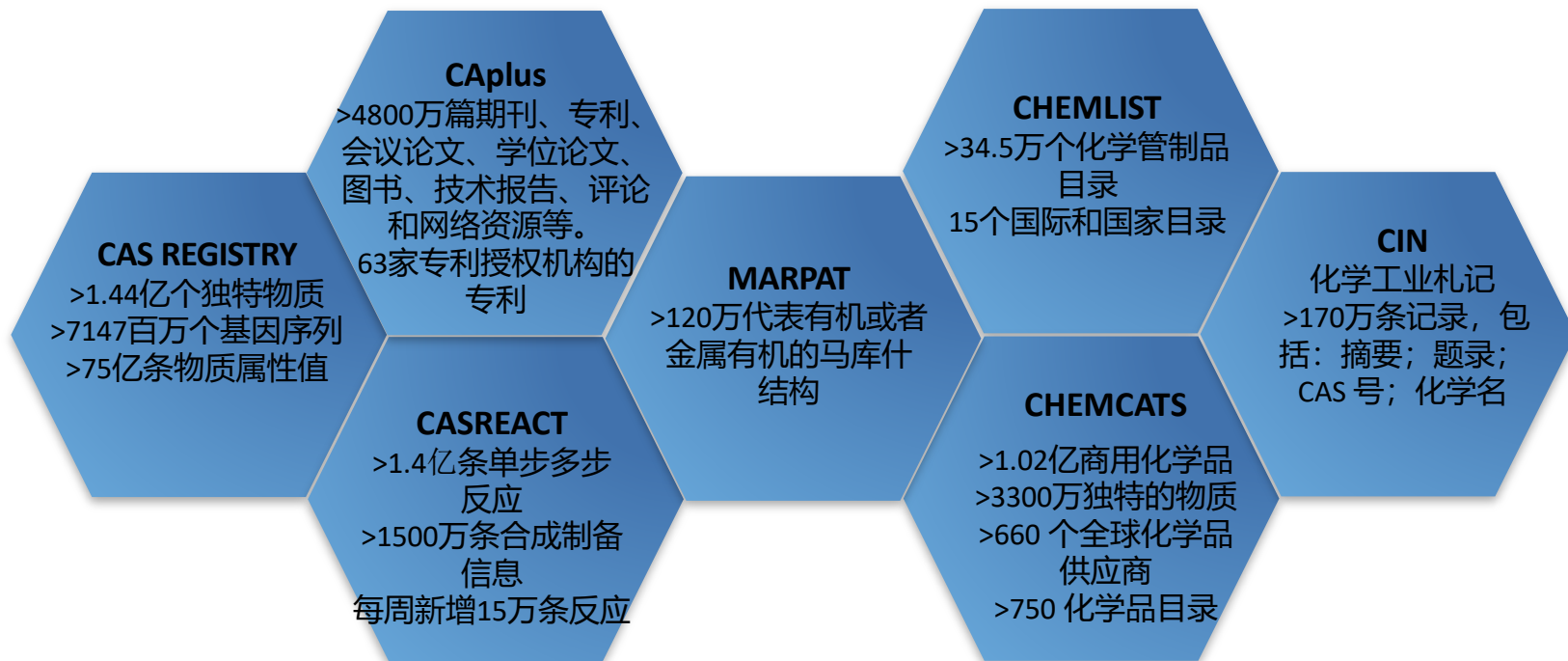


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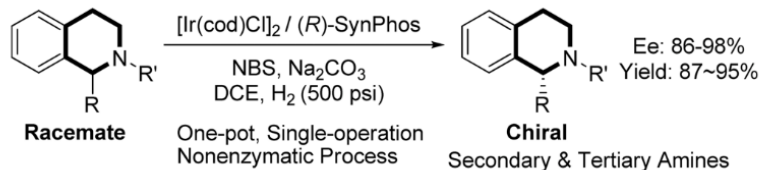
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CAS数据库最具价值的内容——人工标引

1. Concise Redox Deracemization of Secondary and Tertiary Amines with a Tetrahydroisoquinoline Core via a **Nonenzymatic Process**

By: Ji, Yue; Shi, Lei; Chen, Mu-Wang; Feng, Guang-Shou; Zhou, Yong-Gui

A concise deracemization of racemic secondary and tertiary amines with a tetrahydroisoquinoline core has been successfully realized by orchestrating a redox process consisted of N-bromosuccinimide oxidn. and iridium-catalyzed asym. hydrogenation. This compatible redox combination enables one-pot, single-operation deracemization to generate chiral 1-substituted 1,2,3,4-tetrahydroisoquinolines with up to 98% ee in 93% yield, offering a simple and scalable synthetic technique for chiral amines directly from racemic starting materials.



Indexing

Heterocyclic Compounds (One Hetero Atom) (Section27-17)

Concepts

Enantioselective synthesis Hydrogenation catalysts
Oxidation

stereoselective prepn. of tetrahydroisoquinoline derivs. via iridium-catalyzed deracemization in presence of chiral phosphine ligands

Chiral ligands

stereoselective prepn. of tetrahydroisoquinoline derivs. via iridium-catalyzed deracemization in presence of chiral phosphine ligands

Catalyst use; Uses

Substances

12112-67-3 Dichlorobis(cyclooctadiene)diiridium
76189-55-4
133545-16-1
445467-61-8
503538-68-9 (S)-SynPhos
503538-60-0

stereoselective prepn. of tetrahydroisoquinoline derivs. via iridium-catalyzed deracemization in presence of chiral phosphine ligands

Catalyst use; Uses

QUICK LINKS

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SOURCE

Journal of the American Chemical Society
Volume137
Issue33
Pages10496-10499
Journal; Online Computer File
2015
CODEN:JACSAT
ISSN:0002-7863
DOI:10.1021/jacs.5b06659

COMPANY/ORGANIZATION

State Key Laboratory of Catalysis, Dalian Institute of Chemical Physics
Chinese Academy of Sciences
Dalian, Peop. Rep. China
116023

ACCESSION NUMBER

2015:1340032
CAN163:231216

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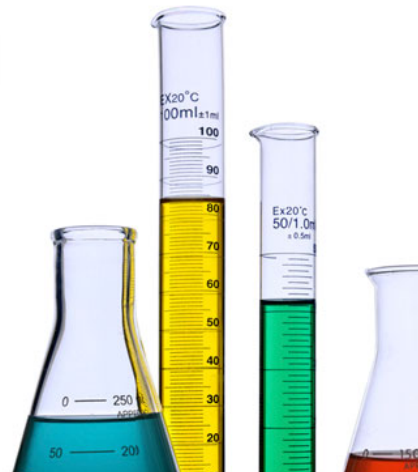
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- Reaction Structure

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

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- Mar 12, 2016(1)
- Mar 05, 2016(2)
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10

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- 检索式: water splitting with solar

REFERENCES: RESEARCH TOPIC ?

water splitting with solar

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The effect of antibiotic residues on dairy products
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1. Enhanced solar absorption of water splitting composite

Quick View Other Sources

By Abed, J.; AlMheiri, M.; Alexander, F.; Ra...
From Solar Energy Materials & Solar Cells (2017), Ahead of Print. | Language: English, Database: CAPLUS

We report on the effect of thermal annealing on the microstructure, optical properties and wettability of TiO₂-based water-splitting (WS) composite using full solar spectrum as source of energy. The WS material used in this study is composed of three layers (SiO₂, Al₂O₃ and TiO₂) on top of which a distribution of Localized Surface Plasmon Resonance structures such as gold are formed to obtain a multilayer composite material. The fabricated samples are then annealed at 450-1100 °C temps. range under atm. conditions. The crystal structure and chem. compn. are detd. using X-ray Diffractometer,...

2. Photocatalytic water splitting solar-to-hydrogen energy conversion: Perovskite-type hydride XBeH₃ (X = Li or Na) as active photocatalysts

Quick View Other Sources

By Reshak, A. H.
From Journal of Catalysis (2017), Ahead of Print. | Language: English, Database: CAPLUS

A highly enhanced photocatalytic hydrogen prodn. system has been achieved, by substitution of Na by Li and moving from cubic to orthorhombic phase in XBeH₃ system. Ab-initio calcns. from first- to second-principles methods were performed to investigate the suitability of the perovskite-type hydride namely; NaBeH₃ and LiBeH₃ in cubic phase and LiBeH₃ in orthorhombic phase to be used as active photocatalysts. We found significant increases in the fundamental energy band gap when we move from NaBeH₃-cubic (0.94 eV) → LiBeH₃-cubic (1.34 eV) → LiBeH₃-orthorhombic (2.44 eV). The obtained energy b...

3. Highly efficient synthesis of hydrogen storage material of formate from bicarbonate and water with general Zn powder

Quick View Other Sources

By Song, Jingwen; Yang, Yang; Yao, Guodong; Zhong, Heng; He, Runtian; Jin, Binbin; Jing, Zhenzi; Jin, Fangming
From Industrial & Engineering Chemistry Research (2017), Ahead of Print. | Language: English, Database: CAPLUS



Formate, as an excellent hydrogen-storage material, has recently become increasingly important, because formic acid is low toxic, easy to store and transport, and contains relatively high energy d. In this paper, we give an overview of the recent strategy in the conversion of bicarbonate into formate by water splitting with a general metallic Zn powder, which mainly includes: 1) hydrogen

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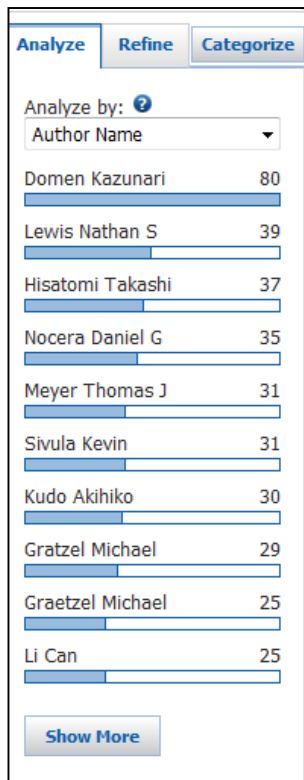
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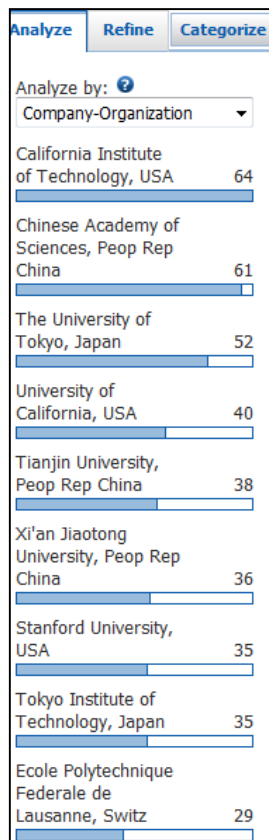
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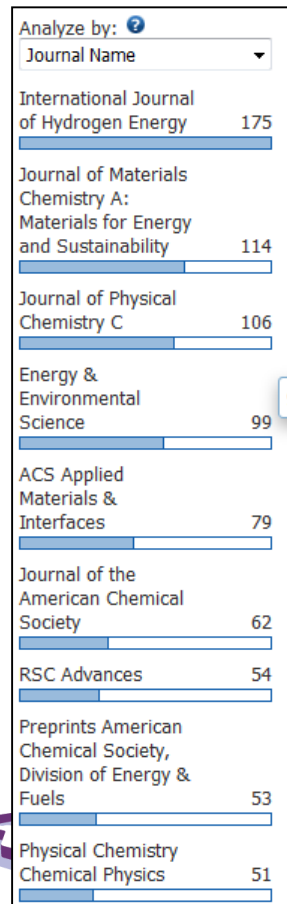
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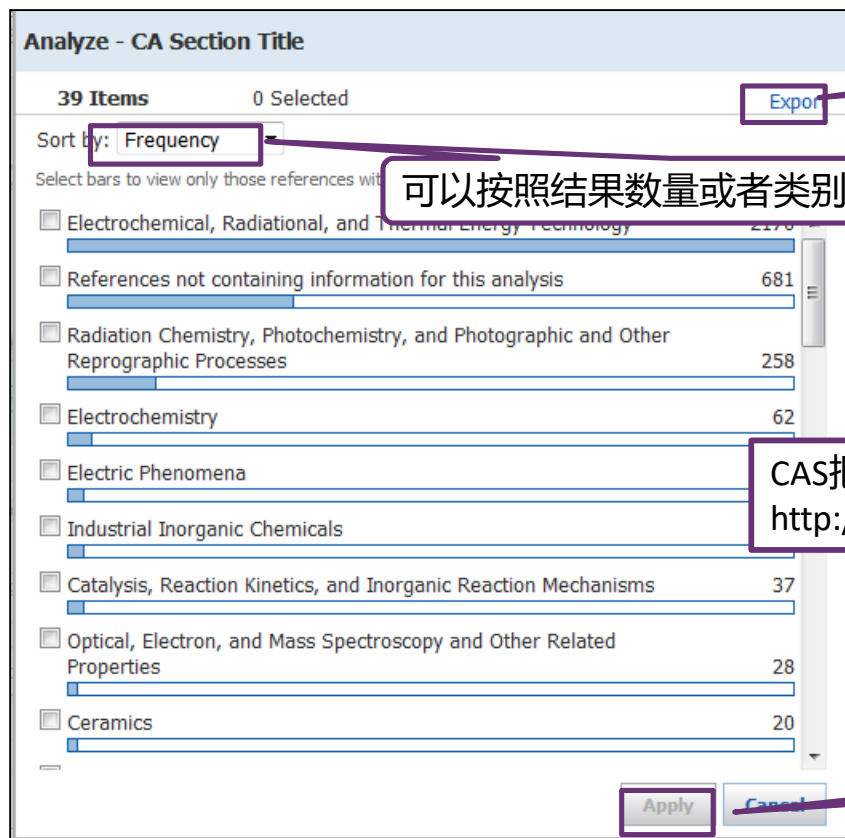
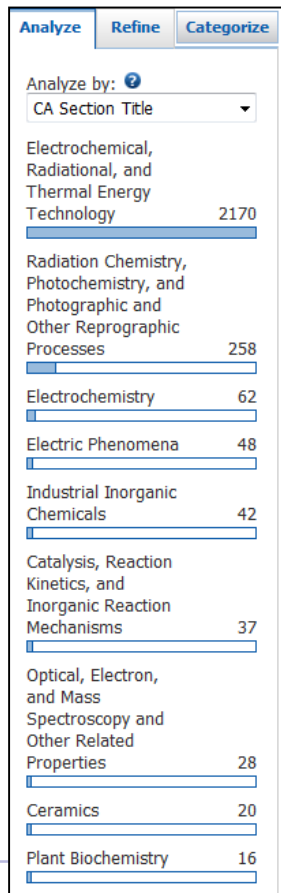
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| Photocurrent | 495 |
| Electric current-potential relationship | 429 |
| Photoelectrochemical cells | 421 |
| Photocatalysts | 396 |
| Photolysis | 332 |
| Solar cells | 330 |
| Photolysis catalysts | 321 |

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1. **Enhanced solar absorption of gold plasmon assisted TiO₂-based water splitting composite**
Quick View Other Sources
By Abed, J.; AlMheiri, M.; Alexander, F.; Rajput, N. S.; Viegas, J.; Jouiad, M.
From Solar Energy Materials & Solar Cells (2017), Ahead of Print. | Language: English, Database: CAPLUS

We report on the effect of thermal annealing on the microstructure, optical properties and wettability of TiO₂-based water splitting composite. The WS material used in this study is composed of three layers (SiO₂, Al₂O₃ and TiO₂) on top of structures such as gold are formed to obtain a multilayer composite material. The fabricated samples are then analyzed. The crystal structure and chem. compn. are detd. using X-ray Diffractometer,...

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Quick View Other Sources
By Reshak, A. H.
From Journal of Catalysis (2017), Ahead of Print. | Language: English, Database: CAPLUS

A highly enhanced photocatalytic hydrogen prodn. system has been achieved, by substitution of Na by Li and moving calcns. from first- to second-principles methods were performed to investigate the suitability of the perovskite-type hydride in orthorhombic phase to be used as active photocatalysts. We found significant increases in the fundamental energy band gap of LiBeH₃-cubic (1.34 eV) → LiBeH₃-orthorhombic (2.44 eV). The obtained energy band structure shows that the perovskite-type hydride is an excellent hydrogen-storage material, has recently been reported to be a good hydrogen storage material, contains relatively high energy density. In this study, we investigate the photocatalytic prodn. from water with Zn; 2) formate syntheses from bicarbonate with Zn/ZnO interface and reducing role of active intermediate of Zn hydride species.

3. **Highly efficient synthesis of hydrogen storage material of formate from bicarbonate and water with general photocatalytic water splitting**
Quick View Other Sources
By Song, Jingwen; Yang, Yang; Yao, Guodong; Zhong, Heng; He, Runtian; Jin, Binbin; Jing, Zhenzi; Jin, Fangming
From Solar Energy Materials & Solar Cells (2017), Ahead of Print. | Language: English, Database: CAPLUS

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$Zn + H_2O \rightarrow ZnO$

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307. Efficient water reduction with gallium phosphide nanowires

By: Standing, Anthony; Assali, Simone; Gao, Lu; Verheijen, Marcel A.; van Dam, Dick; Cui, Yingchao; Notten, Peter H. L.; Haverkort, Jos E. M.; Bakkers, Erik P. A. M.

Photoelectrochem. hydrogen prodn. from solar energy and water offers a clean and sustainable fuel option for the future. Planar III/V material systems have shown the highest efficiencies, but are expensive. By moving to the nanowire regime the demand on material quantity is reduced, and new materials can be uncovered, such as wurtzite gallium phosphide, featuring a direct bandgap. This is one of the few materials combining large solar light absorption and (close to) ideal band-edge positions for full water splitting. Here we report the photoelectrochem. redn. of water, on a p-type wurtzite gallium phosphide nanowire photocathode. By modifying geometry to reduce elec. resistance and enhance optical absorption, and modifying the surface with a multistep platinum deposition, high current densities and open circuit potentials were achieved. Our results demonstrate the capabilities of this material, even when used in such low quantities as in nanowires.

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SOURCE
Nature Communications
Volume6
Pages7824

Indexing

Electrochemical, Faradaic efficiency (Section52)

Concepts

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|--------------------------------|---|
| Annealing | Band gap |
| Catalysts | Electric current-potential relationship |
| Electric resistance | Electrolytes |
| Evaporation | Fuels |
| Nanowires | Open circuit potential |
| Optical absorption | Particle size distribution |
| Photoelectrochemical reduction | Semiconductor materials |
| Sol-gel processing | Solar energy |
| Solutions | pH |

efficient water redn. with gallium phosphide nanowires

重要技术术语

Substances

| |
|------------------------------------|
| 557-20-0 Di-ethyl zinc |
| 1333-74-0 Hydrogen |
| 1445-79-0 Tri-methyl gallium |
| 7440-06-4 Platinum |
| 7601-90-3 Perchloric acid |
| 7803-51-2 Phosphine |
| 9011-14-7 Poly-methyl-methacrylate |
| 12024-21-4 Gallium oxide |
| 12063-98-8 Gallium phosphide |
| 16941-12-1 |

efficient water redn. with gallium phosphide nanowires

Properties; Technical or engineered material use; Uses

重要物质

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LANGUAGE



PatentPak——专利工作流程解决方案：检索案例：金属储氢材料

- 检索式：hydrogen storage material with metal

23. **A hydrogen storage pellet**

Quick View PATENTPAK

By Bennington, St
From PCT Int. App

Figure 1

Arthur; Mooring, Lyndsey; Headen, Tom
Language: English, Database: CAPLUS

and **hydrogen storage** pellet is composed of a core
($< 50 \mu\text{m}$) to impart structural integrity and protection
the **material** is selected from boron-**hydrogen** comp
hydride, etc. **Hydrogen** is released, esp. by heating of

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| Patent No. | Kind | Language |
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PatentPak浏览器

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The screenshot displays the PatentPak Viewer interface. On the left, there is a sidebar with three entries for chemical substances: Li, Li-NH₂, and Cl-Mg-NH₃-Cl. The main area shows patent text with blue location markers. A callout box labeled '下载PDF文件' (Download PDF file) points to a 'DOWNLOAD PDF' button in the top toolbar. Another callout box labeled '专利PDF文件' (Patent PDF file) points to a specific location marker in the text. A third callout box labeled '在PatentPak Viewer中点击物质下面的灯泡，快速定位到PDF文件中的物质信息' (Click the lightbulb under the substance in PatentPak Viewer to quickly locate the substance information in the PDF file) points to a lightbulb icon below the text.

Key Substances in Patent

- Li -
Search in SciFinder | View Detail
Analyst Markup Location
page 32
- CAS RN 7782-89-0
Li — NH₂
Search in SciFinder | View Detail
Analyst Markup Location
page 32
- CAS RN 133598-88-6
NH₃
· Cl —²⁺ Mg — Cl ·
Search in SciFinder | View Detail

PAGE 33 / 40 ZOOM

DOWNLOAD PDF

下载PDF文件

专利PDF文件

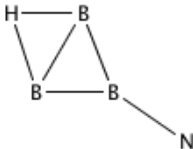
在PatentPak Viewer中点击物质下面的灯泡，快速定位到PDF文件中的物质信息

PatentPak——专利工作流程解决方案

SUBSTANCES: CHEMICAL STRUCTURE ?

Structure Editor:

Java Non-Java



Click image to change structure or view detail.

Import CXF

Search

Advanced Search

Search Type:

- Exact Structure
- Substructure
- Similarity

Show precision analysis

CD ChemDraw[®]
Launch a SciFinder[®] Search
More

从PatentPak Viewer直接跳转到结构检索界面，同时无需绘制，系统会自动将相应的结构直接导入到绘图面板，点击Search即开始SciFinder检索，拓展新的研究方向

如何使用SciFinder提高科研效率

- 以“光解水”为例，如何利用SciFinder：
 - 获取研究全景
 - 对文献结果进行分析、筛选、及精准定位所需信息
- 物质检索
 - 如何从大量物质结果集中快速定位目标物质
 - 结构式检索；分子式检索；物质属性检索
 - 如何获得物质的性质信息、谱图信息
 - 聚合物检索
- 反应检索
 - 结构编辑器的使用（绘图、限定反应的工具）
 - 如何进行锁环锁原子的结构反应检索
 - 如何进行亚结构反应检索，以及如何处理检索结果
 - 案例分享
 - 多氧簇金属的反应信息
 - MOF化合物反应信息



通过文献获得不同研究领域的物质

The screenshot displays the SciFinder interface with a search history: Research Topic "water splitting with solar" > references (3442) > refine "Journal" (2690) > refine "English" (2570) > refine "CAPLUS" (2458) > refine "2010-" (2148). The main area shows a list of references, with the first one selected: "1. Emerging energy applicat...". A dialog box titled "Get Substances" is open, allowing the user to retrieve substances from the selected references. The dialog box has two radio buttons: "All references" (selected) and "Selected references". Under "Limit results to:", there are several checkboxes: "Adverse Effect, including toxicity", "Analytical Study", "Biological Study", "Combinatorial Study", "Formation, nonpreparative", "Miscellaneous", "Occurrence", "Preparation", "Process", "Properties", "Prophetics in Patents", "Reactant or Reagent", and "Uses" (checked). The "Get" and "Cancel" buttons are at the bottom right of the dialog box.

REFERENCES ?

Get Substances Get Reactions

Analyze Refine Categorize

Sort by: Accession Number

0 of 936 References Selected

Analyze by: Index Term

| | |
|---|-----|
| Water splitting | 234 |
| Photoanodes | 211 |
| Photocurrent | 167 |
| Photocatalysts | 158 |
| Photoelectrochemical cells | 153 |
| Solar energy | 152 |
| Electric current-potential relationship | 150 |
| Photolysis | 131 |

1. Emerging energy applicat...
By Late, Dattatray J.; Rout, Chandr
From Canadian Chemical Transactio
Atomically thin semiconduct
easy synthesis using various
more suitable for nanoelectr
WS₂, MoSe₂, WSe₂, InSe,
2. Understanding photovolt...
By Scheuermann, Andrew G.; Chidse
From ECS Transactions (2015), 69(

In the pursuit of a photosynthetic and efficient **water splitting** device, efforts have focused on optimizing specific aspects of anode stability, and kinetics among other aspects. Improvement in one aspect can, however, often require fundamental trade-offs. To achieve a c.d. of interest for a **water splitting** device is an esp. important metric. High **solar** to-hydrogen efficiency is a reporting efficiency in a half cell can be misleading. This report invest...

3. Ultrathin planar hematite film for solar photoelectrochemical water splitting
Quick View Other Sources

Get Cancel

光解水中有关用途的物质

[SUBSTANCES](#)
[Get References](#)
[Get Reactions](#)
[Get Commercial Sources](#)
[Tools](#)
[Create Keep Me Posted Alert](#)
[Send to SciPlanner](#)

Analyze [Refine](#)
 Sort by: CAS Registry Number [↑](#)
[Display Options](#)

0 of 881 Substances Selected

[◀](#) Page: 10 of 18 [▶](#)

Analyze by:

Substance Role

Uses 877

Properties 867

Process 784

Preparation 778

Reactant or Reagent 695

Formation, Nonpreparative 654

Analytical Study 638

Biological Study 605

Occurrence 589

Miscellaneous 499

[Show More](#)

451. [13494-90-1](#)

(Component: 7697-37-2)

~2448 ~21

• 1/3 Ga

Ga . 3 H N O₃
Nitric acid, gallium salt (3:1)

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

452. [13530-65-9](#)

(Component: 7738-94-5)

~1428 ~10

• Zn

Cr H₂ O₄ . Zn
Chromic acid (H₂CrO₄), zinc salt (1:1)

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

453. [13587-35-4](#)

~320 ~12

| Component | Component Ratio |
|-----------|-----------------|
| O | 4 |
| Cu | 1 |
| W | 1 |

Cu . O . W
Copper tungsten oxide (CuWO₄)

[Regulatory Information](#)

454. [13595-86-3](#)

~993 ~3

455. [13595-87-4](#)

~135 ~10

456. [13597-19-8](#)

~274 ~7

ACS / Proprietary and Confidential / Do Not Distribute

SCIFINDER
 A CAS SOLUTION

24

物质检索结果——Analyze

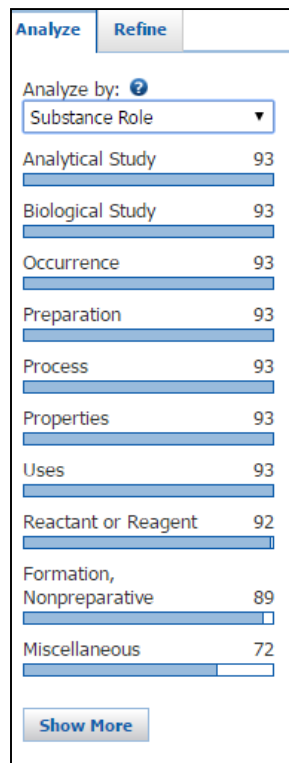
六种分析选项

Analyze by: ?

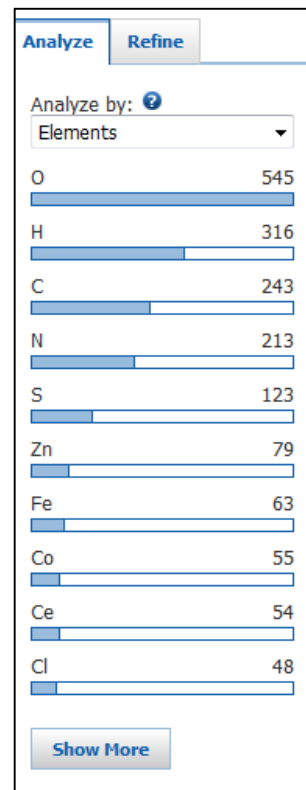
- Bioactivity Indicators
- Commercial Availability
- Elements**
- Reaction Availability
- Substance Role
- Target Indicators

可以按照生物活性，
商业可获得性，元素，
反应可获得性，
物质角色和靶点进行分析

物质角色



元素



物质检索结果——Refine

Analyze Refine

Refine by: ?

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

可以按照化学结构，
包含同位素化合物/金属化合物，
商业可获得性，
性质可获得性，
性质数值，文献可获得性
对结果进行限定

Analyze Refine

Refine by: ?

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

Retrieve substances with:

- Any property
- Any predicted property
- Any experimental property
- Any selected experimental property

Refine

SUBSTANCES ?

Analyze Refine

Sort by: Re

Get Refer

1. 50

~21151

C₁₇H₂₁N
8-Azabicy
8-methyl-

Key PI
Regulatory
Spectra
Experiment

Properties - 0 selected

Experimental

- Boiling Point
- Melting Point

Predicted

- H Acceptors
- H Donors
- Molecular Weight
- logP
- Freely Rotatable Bonds
- Bioconcentration Factor
- Boiling Point
- Density
- Enthalpy of Vaporization
- Flash Point
- H Acceptor/Donor Sum
- Koc
- logD
- Mass Intrinsic Solubility
- Mass Solubility
- Molar Intrinsic Solubility
- Molar Solubility



SCIFINDER®
A CAS SOLUTION

如何使用SciFinder提高科研效率

- 以“光解水”为例，如何利用SciFinder：
 - 获取研究全景
 - 对文献结果进行分析、筛选、及精准定位所需信息
- 物质检索
 - 如何从大量物质结果集中快速定位目标物质
 - 结构式检索；分子式检索；物质属性检索
 - 如何获得物质的性质信息、谱图信息
 - 聚合物检索
- 反应检索
 - 结构编辑器的使用（绘图、限定反应的工具）
 - 如何进行锁环锁原子的结构反应检索
 - 如何进行亚结构反应检索，以及如何处理检索结果
 - 案例分享
 - 多氧簇金属的反应信息
 - MOF化合物反应信息



化学结构检索：结构编辑器

直接导入已保存的.cxf或者.mol文件
direct import saved .cxf or .mol files

画笔pencil
原子atom
可变基团variables
重复单元 repeating group
碳链 chain
旋转/翻转 Rotate, flip fragment

橡皮eraser
常用官能团shortcut
自定义取代基defined
取代位点不确定variable attachment point
模板structure template
环/原子锁定rock ring, rock atom
阴阳离子 positive, negative charge

碳/单键恢复
Reset to carbon or single bond

常用原子,化学键,各种环
Common used atoms, bonds, and rings

结构反应马库什
精确检索
亚结构检索
相似检索

Structure Editor

Click and drag to select objects. Ctrl-click to select or

Add to Editor

Enter CAS Registry Number, SMILES, or InChI:

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

OK Cancel

Drawing Editor:

Structure
 Reaction
 Markush

Get substances that match your query using:

Exact search
 Substructure search
 Similarity search

Cancel

举例：不固定位置取代

The image displays two side-by-side screenshots of a chemical structure editor interface, illustrating the process of adding a chlorine atom to a benzene ring at a non-fixed position.

Left Screenshot: The editor shows a benzene ring with a single bond extending from the top vertex. The text "Draw or change atoms or bonds." is visible in the top yellow bar. The left sidebar contains various drawing tools, with the "Cl" atom tool highlighted by a purple box. The bottom toolbar shows the chemical formula input field containing "Cl".

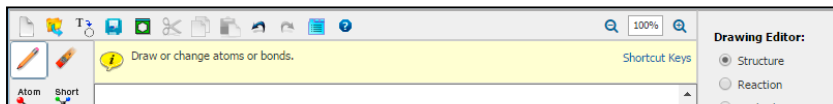
Right Screenshot: The editor shows the same benzene ring with a red "Cl" atom being added to the ring. The text "Click and drag from the substituent position to each ring position where attachment may occur." is visible in the top yellow bar. The "Cl" atom tool in the left sidebar is still highlighted. The bottom toolbar shows the chemical formula input field containing "Cl".

Right Panel: The "Drawing Editor" panel is visible on the right side of the interface. It contains three radio buttons: "Structure" (selected), "Reaction", and "Markush". Below this, the "Get substances that match your query using:" section contains three radio buttons: "Exact search", "Substructure search" (selected), and "Similarity search". At the bottom of the panel are "OK" and "Cancel" buttons.

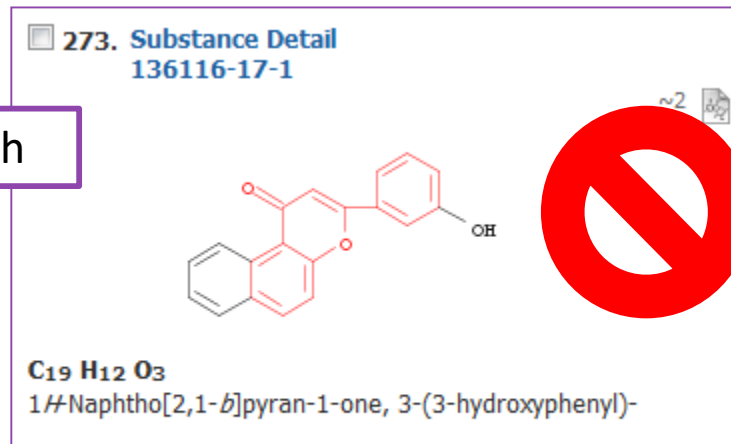
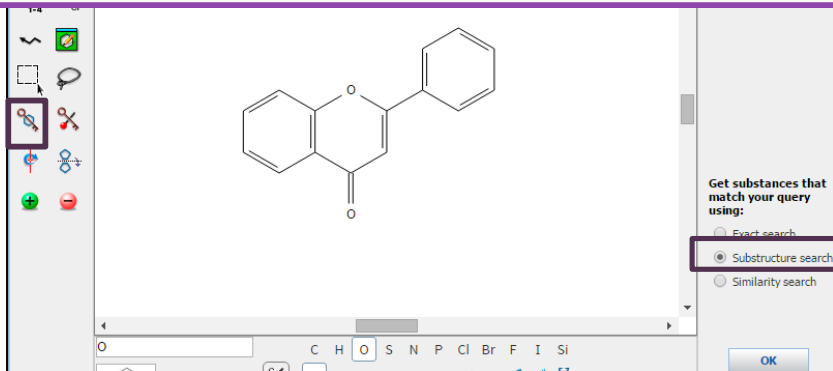
举例：环锁定



环锁定，被锁定的结构上不会出现新的环结构



If we use “ring lock” button in substructure search



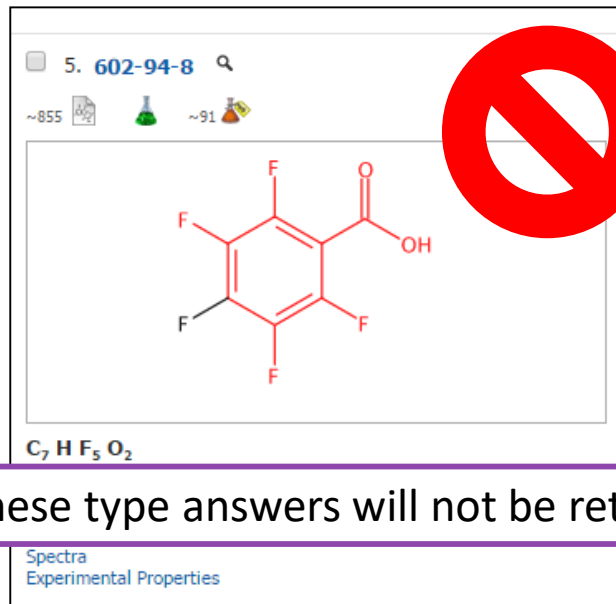
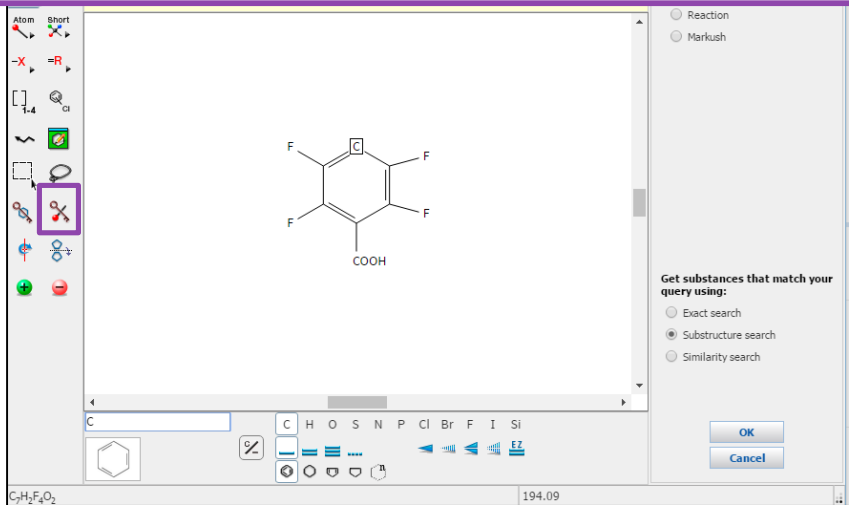
These type answers will not be retrieved.

举例：原子锁定



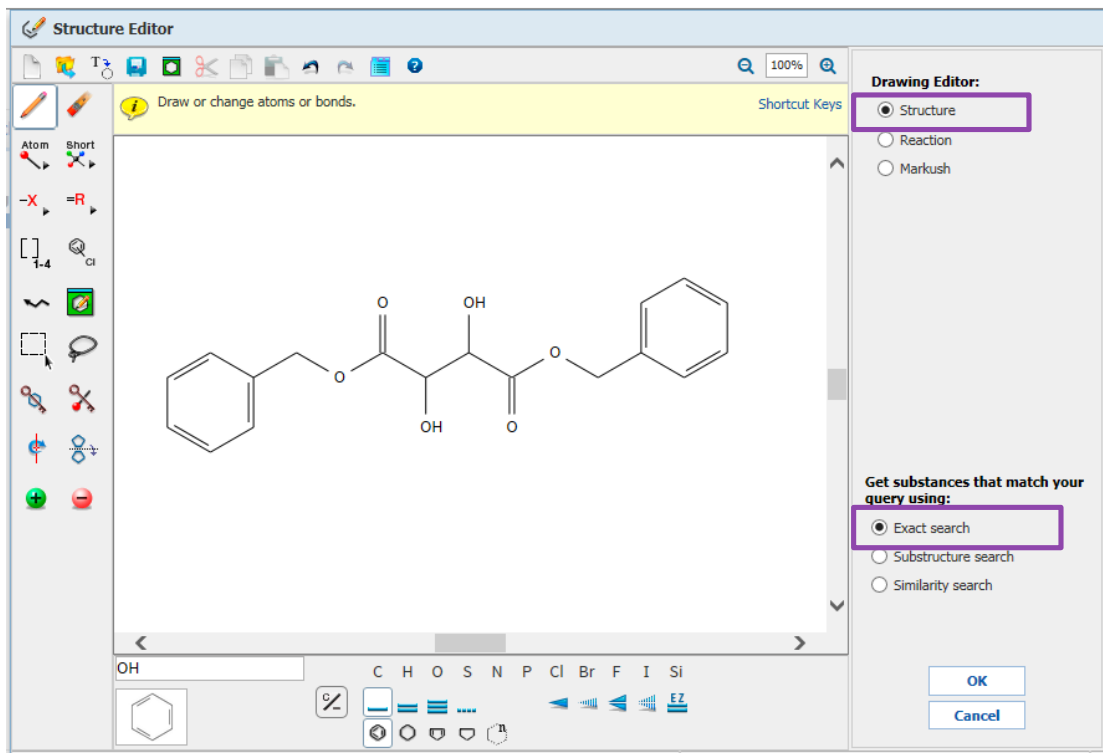
被锁定的原子上不会出现非氢取代

If we use “ring atom” button in substructure search



These type answers will not be retrieved.

化学结构检索: 精确结构检索



结构式中的原子和环
全部被锁定,不可被取代
All atom and ring are locked,
No substituents

物质结构结果集

0 of 20 Subst

1. 622-00-4 **手性化合物**
Chiral compound

Absolute stereochemistry.,Rotation (+).

$C_{18}H_{18}O_6$
Butanedioic acid, 2,3-dihydroxy-, 1,4-bis(phenylmethyl) ester
▶ **Key Physical Properties**
Experimental Properties

2. 4136-22-5

Absolute stereochemistry.,Rotation (-).

$C_{18}H_{18}O_6$
Butanedioic acid, 2,3-dihydroxy-, 1,4-bis(phenylmethyl) ester, (2S,3S)-
▶ **Key Physical Properties**

3. 93993-87-4 **非手性化合物**
Non-chiral compound

$C_{18}H_{18}O_6$
Butanedioic acid, 2,3-dihydroxy-, 1,4-bis(phenylmethyl) ester
▶ **Key Physical Properties**

4. 4079-56-5

Relative stereochemistry.

$C_{18}H_{18}O_6$
Butanedioic acid, 2,3-dihydroxy-, 1,4-bis(phenylmethyl) ester, (2R,3R)-rel

5. 4079-57-6

Relative stereochemistry.

$C_{18}H_{18}O_6$
Butanedioic acid, 2,3-dihydroxy-, 1,4-bis(phenylmethyl) ester, (2R,3S)-rel
▶ **Key Physical Properties**

6. 89960-73-6 **聚合物单体的组合物**
Monomer of polymer

622-00-4
 $C_{18}H_{18}O_6$

Absolute stereochemistry.,Rotation (+).

101-68-8
 $C_{15}H_{10}N_2O_2$

精确结构检索获得被检索结构的盐，混合物，配合物，聚合物等，被检结构不能被取代

高级检索——提前限定

Search

[Advanced Search](#) Always Show

Characteristics

- Single component
- Commercially available
- Included in references

Classes

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

Studies

- Analytical
- Biological
- Preparation
- Reactant or reagent



0 of 7 Substances Selected

1. **622-00-4** 🔍

~105 ~57

Absolute stereochemistry., Rotation (+).

C₁₈ H₁₈ O₆
Butanedioic acid, 2,3-dihydroxy-, 1,4-bis(phenylmethyl) ester
(phenylmethyl) ester

▶ **Key Physical Properties**
Experimental Properties

3. **93993-87-4** 🔍

~9 ~7

Absolute stereochemistry.

C₁₈ H₁₈ O₆
Butanedioic acid, 2,3-dihydroxy-, 1,4-bis(phenylmethyl) ester

▶ **Key Physical Properties**

6. **896448-46-7** 🔍

~2 ~3

Relative stereochemistry.

C₁₈ H₁₈ O₆
Butanedioic acid, 2,3-dihydroxy-, 1,4-bis(phenylmethyl) ester,
(2*R*,3*R*)-*rel*

▶ **Key Physical Properties**

去除混合物, 组合物, 配合物, 盐
Exclude mixture, polymer, complex, salts

化学结构检索：亚结构检索

母体骨架结构不变,
母体中的开放位点可以被取代

Search

Advanced Search Always Show

Characteristics Single component
 Commercially available
 Included in references

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

Studies Analytical
 Biological
 Preparation
 Reactant or reagent

将两个结构片段限定在
同一物质中

物质结果集

Chemical Structure substructure with limiters > substances (49240)

SUBSTANCES

Get References

Get Reactions

Get Commercial Sources

Tools

Create Keep Me Posted Alert

Send to SciPlanner

Analyze Refine

Sample Analysis:

Substance Role

Preparation ≥ 6761

Biological Study ≥ 5629

Uses ≥ 4822

Prophetic in Patents ≥ 1649

Reactant or Reagent ≥ 1241

Properties ≥ 369

Process ≥ 49

Combinatorial Study ≥ 25

Analytical Study ≥ 17

Occurrence ≥ 7

Show More

Sort by: CAS Registry Number

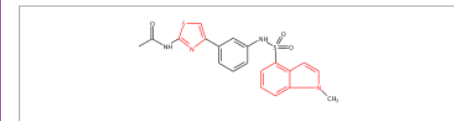
0 of 49240 Substances Selected

Page: 1 of 3283

Display Options

1. 1997357-70-6

~1

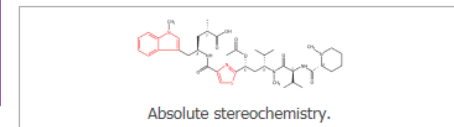


C₂₀ H₁₈ N₄ O₃ S₂
Acetamide, *N*-[4-[3-[[[1-methyl-1*H*-indol-4-yl]sulfonyl]amino]phenyl]-2-thiazolyl]-

[Key Physical Properties](#)

4. 1995847-80-7

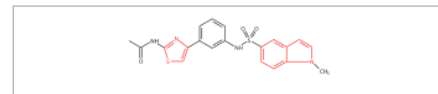
~1



C₄₀ H₅₈ N₆ O₇ S
1*H*-Indole-3-pentanoic acid, γ -[[[2-[(1*R*,3*R*)-1-(acetyloxy)-4-

2. 1997357-68-2

~1

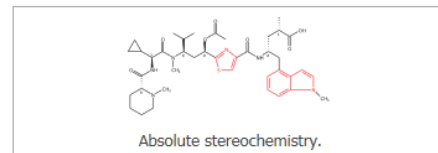


C₂₀ H₁₈ N₄ O₃ S₂
Acetamide, *N*-[4-[3-[[[1-methyl-1*H*-indol-5-yl]sulfonyl]amino]phenyl]-2-thiazolyl]-

[Key Physical Properties](#)

5. 1995846-52-0

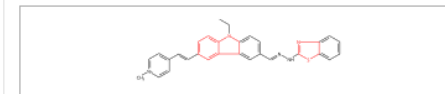
~1



C₂₀ H₁₈ N₄ O₃ S

3. 1995871-38-9

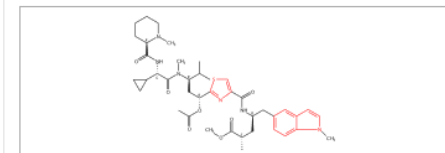
~0



C₃₀ H₃₈ N₅ S
Pyridinium, 4-[2-[6-[[[2-(2-benzothiazolyl)hydrazinylidene]methyl]-9-ethyl-9*H*-carbazol-3-yl]ethenyl]-1-methyl-

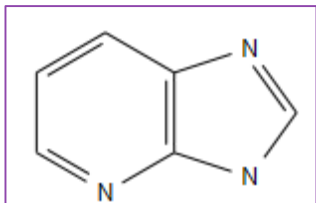
6. 1995844-98-8

~1



Absolute stereochemistry.

化学结构检索: 相似结构检索



Purin

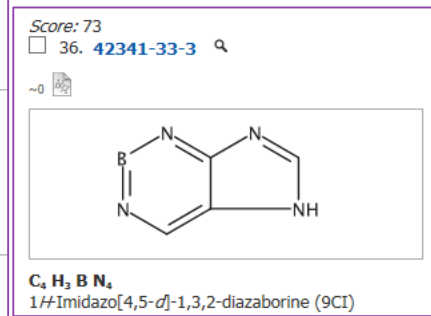
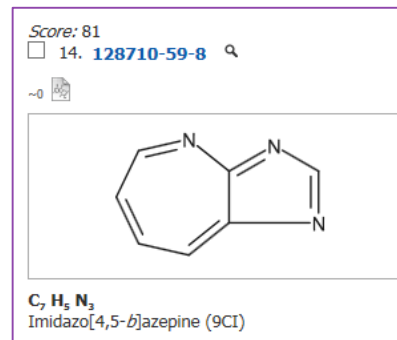
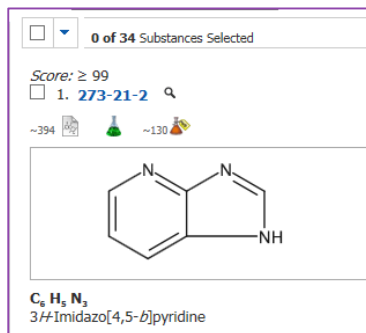
母体结构被拆分成分子片段



| 0 of 7 Similarity Candidates Selected | | Substances |
|---------------------------------------|----------------------|------------|
| <input type="checkbox"/> | ≥ 99 (most similar) | 26 |
| <input type="checkbox"/> | 95-98 | 0 |
| <input type="checkbox"/> | 90-94 | 0 |
| <input type="checkbox"/> | 85-89 | 8 |
| <input type="checkbox"/> | 80-84 | 23 |
| <input type="checkbox"/> | 75-79 | 179 |
| <input type="checkbox"/> | 70-74 | 199 |
| <input type="checkbox"/> | 65-69 | 997 |
| <input type="checkbox"/> | 0-64 (least similar) | 2321 |

Get Substances

相似度越高, 结构越相似



物质检索——理化性质检索

The screenshot displays the SciFinder web interface. On the left, there is a navigation menu with sections for REFERENCES, SUBSTANCES, and REACTIONS. The SUBSTANCES section is active, with 'Property' selected. The main content area features a 'SUBSTANCE' search box with a dropdown menu for 'Select Property...'. The dropdown list includes various physical and chemical properties, with 'Molecular Weight' highlighted. Below the dropdown is a 'Search' button. To the right of the search box, there are two input fields, each with the text 'Examples: 44, 25-35, >125' below it. The top of the page shows the SciFinder logo and navigation tabs like 'Explore' and 'Saved Searches'.

提纲

- SciFinder物质检索
 - 通过文献获得物质
 - 物质检索结果的处理：分析和限定
 - 物质信息详情
 - 理化性质检索
 - 分子式检索
 - 物质标识符检索

物质检索——分子式检索

REFERENCES

Research Topic
Author Name
Company Name
Document Identifier
Journal
Patent
Tags

SUBSTANCES

Chemical Structure
Markush
Molecular Formula
Property
Substance Identifier

REACTIONS

SUBSTANCES: MOLECULAR FORMULA ?

C₁₂ H₂₆ O₄ S . Na

Examples:

H₄SiO₄

(C₃H₆O.C₂H₄O)_x

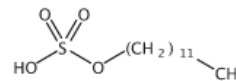
Search

无机金属盐：金属离子和阴离子间用点 (.) 分开

40. 151-21-3

(Component: 151-41-7)

~79363 ~283



• Na

C₁₂ H₂₆ O₄ S . Na

Sulfuric acid monododecyl ester sodium salt (1:1)

Key Physical Properties

Regulatory Information
Spectra
Experimental Properties

分子式输入需要遵守Hill排序规则:不含碳化合物,按元素符号的字母顺序排列;分子式为含碳化合物时,则“C”在前;如有氢则紧随其后,其它元素符号按字母顺序排在氢的后面



SCIFINDER®

A CAS SOLUTION

合金的检索：钴铁锰合金

Molecular Formula "Co . Fe . Mn" > substances (249)

REFERENCES

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

SUBSTANCES

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

REACTIONS

- Reaction Structure

SUBSTANCES: MOLECULAR FORMULA

Co.Fe.Mn
Examples:
H4SiO4
(C3H6O C2H4O)x

用 "." 将不同组分隔开
使用排序功能 (可按照第一个组分的成分排序提高检索效率)

SUBSTANCES

Get References Get Reactions Get Commercial Sources Tools

Sort by: CAS Registry Number
CAS Registry Number
Number of References
Number of Commercial Sources
Molecular Weight
Molecular Formula

Analyze by: Substance Role

Uses 149
Properties 134
Process 111
Preparation 27
Analytical Study 3
Reactant or Reagent 3
Biological Study 2
Formation, Nonpreparative 2
Miscellaneous 1

1. 1632299-35-4
Component Component Percent
Mn 69
Fe 26
Co 4.3
Co . Fe . Mn
Manganese alloy, base, Mn 69,Fe 26,Co 4.3

2. 1632299-35-4
Component Component Percent
Mn 70
Fe 28
Co 2.1
Co . Fe . Mn
Manganese alloy, base, Mn 70,Fe 28,Co 2.1

3. 1612139-04-4
Component Component Percent
Co 35
Fe 33
Mn 32
Co . Fe . Mn
Cobalt alloy, base, Co 35,Fe 33,Mn 32

4. 1585186-25-9
Component Component Percent
Co 34
Fe 34
Mn 32

5. 1446711-14-3
Component Component Percent
Fe 62 - 79
Mn 20 - 32
Co 1.1 - 9.5

6. 1383688-58-1
Component Component Ratio
Co 30
Mn 3
Fe 70

物质检索案例：

如何查找MOF化合物，以Cu-BTC为例

方法1：若已知物质的CAS号码，物质名称，使用Substance Identifier

方法2：若已知MOF化合物单元分子式，可以使用分子式检索

方法3：若已知配合物配体，可以先用结构检索配体，然后获得相关配合物

方法4：若已知MOF化合物单元结构式，可以绘制完整结构进行检索

方法1：若已知物质的CAS号码，物质名称，使用Substance Identifier

Explore ▾ Saved Searches ▾ SciPlanner

Substance Identifier "222404-02-6" > substances (1) > 222404-02-6

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 ?

222404-02-6

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

Search

Explore ▾ Saved Searches ▾ SciPlanner

Substance Identifier "Cu-BTC" > substances (1)

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 ?

Cu-BTC

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

Search

方法2: 已知MOF化合物单元分子式, 可以使用分子式检索

Explore ▾ Saved Searches ▾ SciPlanner

Chemical Structure exact with limiters > substances (7)

REFERENCES

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

SUBSTANCES

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

REACTIONS

- Reaction Structure

SUBSTANCES: MOLECULAR FORMULA

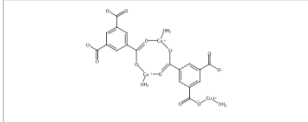
C18 H12 Cu3 O15

Examples:
H4SiO4
(C3H6O.C2H4O)x

Search

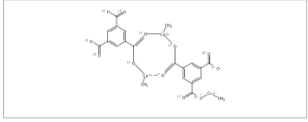
0 of 4 Substances Selected

1. 2019181-18-9



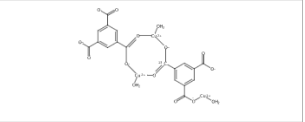
C₁₈ H₁₂ Cu₃ O₁₅
INDEX NAME NOT YET ASSIGNED

2. 1685249-53-9



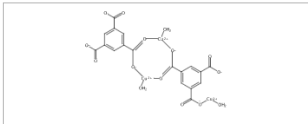
C₁₈ H₁₂ Cu₃ O₁₅
INDEX NAME NOT YET ASSIGNED

3. 1416961-85-7



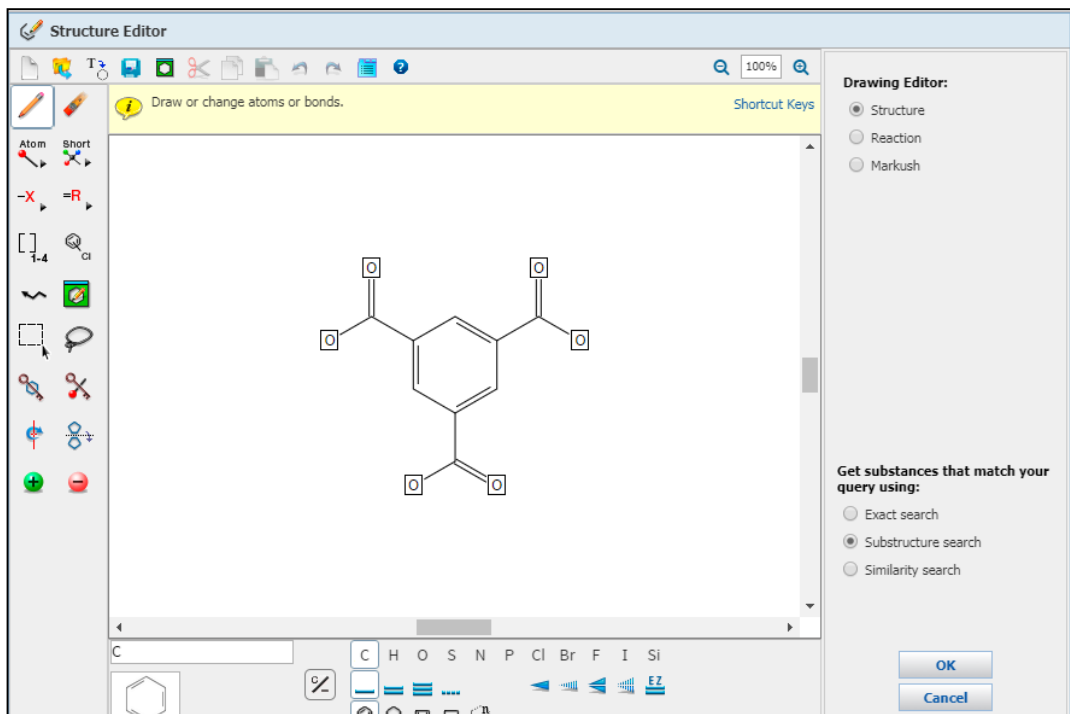
C₁₈ H₁₂ Cu₃ O₁₅
Copper, triaqu[μ-[1,3,5-benzenetricarboxylato(3-)-κO²:κO²]]
[[μ₂-[1,3,5-benzenetricarboxyl-1-κO(3-)-κO²:κO²]]
tri-

4. 222404-02-6



C₁₈ H₁₂ Cu₃ O₁₅

方法3: 已知配合物配体, 可以先用结构检索配体, 然后获得相关配合物



Search

Advanced Search Always Show

Characteristics

- Single component
- Commercially available
- Included in references

Classes

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

Studies

- Analytical
- Biological
- Preparation
- Reactant or reagent

在结果集中通过Analyze by Elements, 选择Cu

Chemical Structure substructure with limiters > substances (2434)

SUBSTANCES

Get References Get Reactions Get Commercial Sources Tools

Analyze Refine

Sort by: Relevance

0 of 2434 Substances Selected

Analyze by:

Elements

| | |
|----|------|
| C | 2434 |
| O | 2434 |
| H | 2427 |
| N | 1685 |
| Zn | 540 |
| Cu | 350 |
| Co | 340 |
| Cd | 313 |
| Ni | 223 |
| Mn | 109 |

Show More

1. 1001196-71-9

$C_9 H_3 O_6 Zn$
Zincate(1-), [1,3,5-benzenetricarboxylato(3-)-κO²]-

2. 1805003-23-9

$C_9 H_3 Cd O_6$
INDEX NAME NOT

4. 1804937-55-0

(Component: 1805003-23-9)

5. 951026-11-9

MOL_10_16_2017_....mol

如果结果中有不相关的信息，可以通过结构等进一步进行筛选

Explore ▾ Saved Searches ▾ SciPlanner

Chemical Structure substructure with limiters > substances (2434) > keep analysis "Elements" (350)

SUBSTANCES ⓘ

Get References Get Reactions Get Commercial Sources Tools ▾

Analyze Refine

Analyze by: ⓘ
Elements ▾

| | |
|----|-----|
| C | 350 |
| Cu | 350 |
| H | 350 |
| O | 350 |
| N | 288 |
| Cl | 16 |
| S | 15 |
| Mn | 6 |

Sort by: Number of References ▾

- Relevance
- CAS Registry Number
- Number of References
- Number of Commercial Sources
- Molecular Weight
- Molecular Formula

1. ~1274

C₁₈ H₁₂ Cu₃ O₁₅
Copper, triaqua[μ-[1,3,5-benzenetricarboxylato(3-)-κO²:κO²]]
[[μ₂-[1,3,5-benzenetricarboxylato(3-)-κO²:κO²]]tri-
▶ **Key Physical Properties**
Experimental Properties

2. 222403-98-7 🔍
(Component: 222404-02-6)

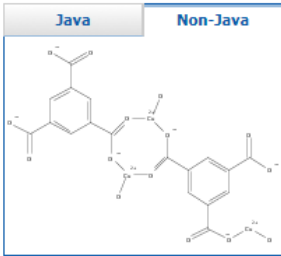
~38

C₁₈ H₁₂ Cu₃ O₁₅ · x H₂O
Copper, triaqua[μ-[1,3,5-benzenetricarboxylato(3-)-κO²:κO²]]
[[μ₂-[1,3,5-benzenetricarboxylato(3-)-κO²:κO²]]tri-
hydrate (1:?)

方法4: 已知MOF化合物单元结构式, 可以绘制完整结构进行检索

Structure Editor:

Java Non-Java



Click image to change structure or view detail.

Import CXF


Search

Advanced Search Always Show

Search Type:

- Exact Structure
- Substructure
- Similarity

Show precision analysis

 ChemDraw
Launch a SciFinder substance
[More](#)

Characteristics



- Single component
- Commercially available
- Included in references

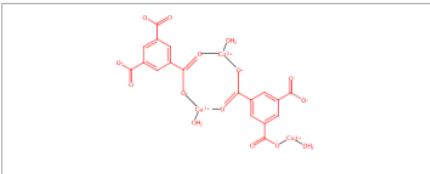
Classes

- Alloys
- Coordination compounds

0 of 7 Substances Selected

1. **222404-02-6** 🔍

~1274  





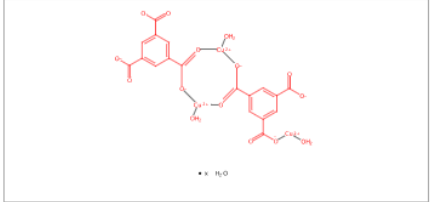
C₁₈ H₁₂ Cu₃ O₁₅
Copper, triaqua[μ-[1,3,5-benzenetricarboxylato(3-)-κO⁻:κO¹]]
[[μ₂-[1,3,5-benzenetricarboxylato(3-)-κO⁻:κO²:κO³]]tri-

Key Physical Properties
[Experimental Properties](#)

2. **222403-98-7** 🔍



(Component: 222404-02-6)

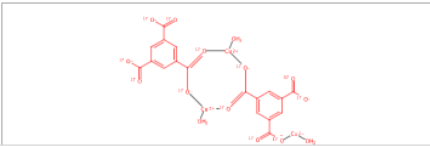
~38  





C₁₈ H₁₂ Cu₃ O₁₅ · x H₂O
Copper, triaqua[μ-[1,3,5-benzenetricarboxylato(3-)-κO⁻:κO¹]]
[[μ₂-[1,3,5-benzenetricarboxylato(3-)-κO⁻:κO²:κO³]]tri-,
hydrate (1:?)

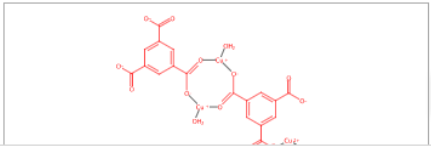
4. **1685249-53-9** 🔍

~1  



5. **2019181-18-9** 🔍

~1  



SciFinder中的物质记录

Substance Identifier "222404-02-6" > substances (1) > 222404-02-6 > get reactions (222)

Get References **Get Reactions** **Get Commercial Sources** **Tools**

Analyze Refine

Analyze by: Substance Role

Analytical Study 1

Biological Study 1

Formation, Nonpreparative 1

Occurrence 1

Preparation 1

Process 1

Properties 1

Reactant or Reagent 1

Uses 1

Show More

Sort by: CAS Registry Number

0 of 1 Substance Selected

1. **222404-02-6**

~1274

C₁₈ H₁₂ Cu₃ O₁₅
Copper, triaqua[μ-[1,3,5-benzenetricarboxylato(3-)-κO²:κO¹]]₃[μ₃-[1,3,5-benzenetricarboxylato(3-)-κO²:κO¹]]tri-

Key Physical Properties
Experimental Properties

CAS Registry Number: 222404-02-6

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

获得其文献、反应和供应商信息

点击CAS号, 获得物质信息详情

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

SciFinder中的物质记录

Substance Identifier "222404-02-6" > substances (1) > 222404-02-6

SUBSTANCE DETAIL ⓘ

Get References

Get Reactions

Return

CAS Registry Number 222404-02-6

~1,274  

C₁₈ H₁₂ Cu₃ O₁₅

Copper, triqua[μ-[1,3,5-benzenetricarboxylato(3-)-κO⁻:κO²⁻]][μ₃-[1,3,5-benzenetricarboxylato(3-)-κO⁻:κO²⁻:κO²⁻]]tri-

Coordination Compound

Density (Experimental)

Value: 0.879 g/cm³

Other Names

Copper, triqua[μ-[1,3,5-benzenetricarboxylato(3-)-κO⁻:κO²⁻]][μ₃-

[1,3,5-benzenetricarboxylato(3-)-κO⁻:κO²⁻:κO²⁻]]tri- (9CI)

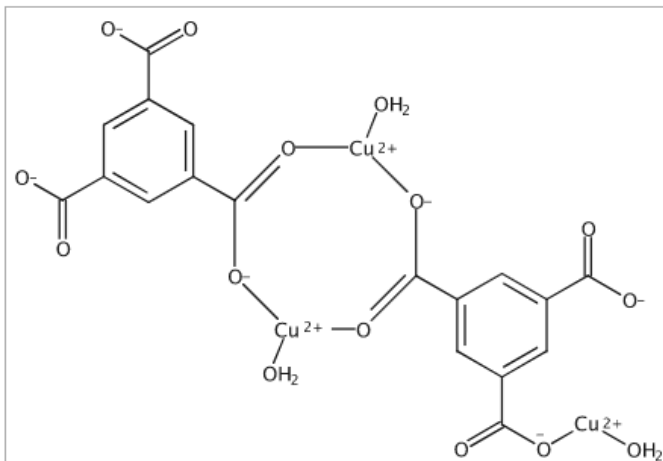
Triaqua[μ-[1,3,5-benzenetricarboxylato(3-)-κO⁻:κO²⁻]][μ₃-[1,3,5-benzenetricarboxylato(3-)-κO⁻:κO²⁻:κO²⁻]]tricopper

Basolite C 300

Cu-BTC

Cu₃BTC₂

[View more...](#)



实验数据与实验谱图

▼ EXPERIMENTAL PROPERTIES

Density Electrical Mechanical Nuclear Optical and Scattering Structure Related Thermal

| Density Properties | Value | Condition | Note |
|--------------------|-------------------------|-----------|--------|
| Density | 0.879 g/cm ³ | | (5)CAS |
| Density | See full text | 1 of 3 | (6)CAS |

Notes

(5) Chen, Banglin; US 20110269984 A1 2011 CAPLUS 🔍

(6) Liu, Ying Dan; Chemical Communications (Cambridge, United Kingdom) 2012, V48(45), P5635-5637 CAPLUS 🔍

▼ EXPERIMENTAL SPECTRA

¹H NMR ¹³C NMR IR Raman UV and Visible X-Ray Additional Spectra

| ¹ H NMR Properties | Value | Condition | Note |
|-------------------------------|---------------|-----------|---------|
| Proton NMR Spectrum | See full text | | (15)CAS |

Notes

(15) Chen, Joseph J.; Angewandte Chemie, International Edition 2013, V52(46), P12043-12046 CAPLUS 🔍

SciFinder中的物质记录

▼ CAS REFERENCE ROLES

| Roles | Patents | Nonpatents | Nonspecific Derivatives from Patents | Nonspecific Derivatives from Nonpatents |
|---------------------------|---------|------------|--------------------------------------|---|
| Analytical Study | ✓ | ✓ | ✓ | ✓ |
| Biological Study | ✓ | ✓ | ✓ | ✓ |
| Combinatorial Study | ✓ | ✓ | ✓ | |
| Formation, Nonpreparative | ✓ | ✓ | ✓ | ✓ |
| Miscellaneous | ✓ | ✓ | ✓ | ✓ |
| Occurrence | ✓ | ✓ | ✓ | ✓ |
| Preparation | ✓ | ✓ | ✓ | ✓ |
| Process | ✓ | ✓ | ✓ | ✓ |
| Properties | | ✓ | ✓ | |
| Prophetic in Patents | | | ✓ | |
| Reactant or Reagent | | | ✓ | ✓ |
| Uses | ✓ | ✓ | ✓ | ✓ |

选中任何一项即可获得相关文献

物质检索案例——聚合物检索

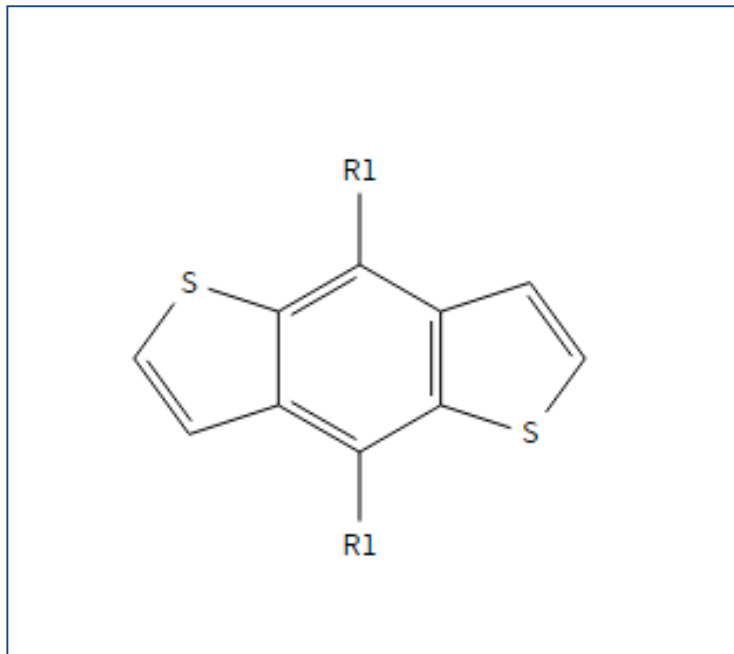
- 结构检索
- 分子式检索

REGISTRY中有两种方法表示聚合物

- **Starting materials** – 被描述成组分单体（这个单体将会联合起来形成聚合物）
- **Final product** – 被表示为结构重复单元 (SRU)

聚合物检索——结构式检索

- 案例：检索以下结构作为聚合单体的均聚物信息并对检索结果进行筛选



R1 = alkyl chains

Draw or change atoms or bonds. Shortcut Keys

100%

Drawing Editor:

- Structure
- Reaction
- Markush

Get substances that match your query using:

- Exact search
- Substructure search
- Similarity search

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

Close

Create Saved Answer
View All | Import

KEEP ME POSTED

C-N bond activation
Dec 05, 2015(1)
Nov 28, 2015(1)
Nov 21, 2015(1)

View All

OK
Cancel

Ak

C H O S N P Cl Br F I Si

 Advanced Search Always Show

Characteristics Single component
 Commercially available
 Included in references

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

Studies Analytical
 Biological
 Preparation
 Reactant or reagent

物质检索案例——聚合物检索

- 结构检索
- 分子式检索

聚合物检索——分子式检索

- 聚合物的分子式表现形式

分子式中带有括号

括号外为n，嵌段聚合物（有首尾端或无首尾段都可）

有端基嵌段聚合物分子式： $(C_6H_{10}O_2)_n C_3H_4O_2$

无端基嵌段聚合物分子式： $(C_{12} H_{12} O_4)_n$

括号外为x，对于均聚物和共聚物，将以单体进行标引，聚合度不影响标引

共聚物： $(C_2 H_4 . C_2 F_4)_x$

均聚物： $(C_2H_4)_x$

如何使用SciFinder提高科研效率

- 以“光解水”为例，如何利用SciFinder：
 - 获取研究全景
 - 对文献结果进行分析、筛选、及精准定位所需信息
- 物质检索
 - 如何从大量物质结果集中快速定位目标物质
 - 结构式检索；分子式检索（合金，多氧簇金属，MOF化合物）；物质属性检索
 - 如何获得物质的属性信息、谱图信息
- 反应检索
 - 结构编辑器的使用（绘图、限定反应的工具）
 - 如何进行精确结构反应检索，并获得实验详情
 - 如何进行亚结构反应检索，以及如何处理检索结果
 - 案例分享
 - 多氧簇金属的反应信息
 - MOF化合物反应信息

结构编辑器：绘制反应工具

The screenshot shows the Structure Editor software interface. On the left, a 'Functional Groups' panel is open, listing various chemical groups such as Alcohols (13), Alkenes (11), Alkynes (4), Amines (11), Carbonate Derivatives (7), Carboxy Derivatives (17), Halides (16), Heterocycles (54), Ketones (6), Organometallics (19), Non-Rings (136), and Rings (71). The main workspace contains a toolbar with icons for drawing atoms, bonds, and rings. A yellow banner at the top of the workspace reads 'Draw or change atoms or bonds.' On the right, a 'Drawing Editor' panel is visible, with radio buttons for 'Structure', 'Reaction', and 'Markush', and a section for 'Get reactions where the structure(s) are:' with options for 'Variable only at the specified positions' and 'Substructures of more complex structures'. The bottom status bar shows 'CH₄' and '16.04'. Four purple callout boxes with white text and arrows point to specific features: '角色定义' (Role Definition) points to the 'C' atom in the workspace; '反应箭头' (Reaction Arrow) points to the arrow icon in the toolbar; '化学键变化' (Chemical Bond Change) points to the bond change icon in the toolbar; and '官能团列表' (Functional Group List) points to the 'Functional Groups' panel.

Functional Groups

Enter 3 or more characters...

- Alcohols (13)
- Alkenes (11)
- Alkynes (4)
- Amines (11)
- Carbonate Derivatives (7)
- Carboxy Derivatives (17)
- Halides (16)
- Heterocycles (54)
- Ketones (6)
- Organometallics (19)
- Non-Rings (136)
- Rings (71)

Close

Structure Editor

Draw or change atoms or bonds.

Shortcut Keys

Drawing Editor:

- Structure
- Reaction
- Markush

Get reactions where the structure(s) are:

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

OK

Cancel

角色定义

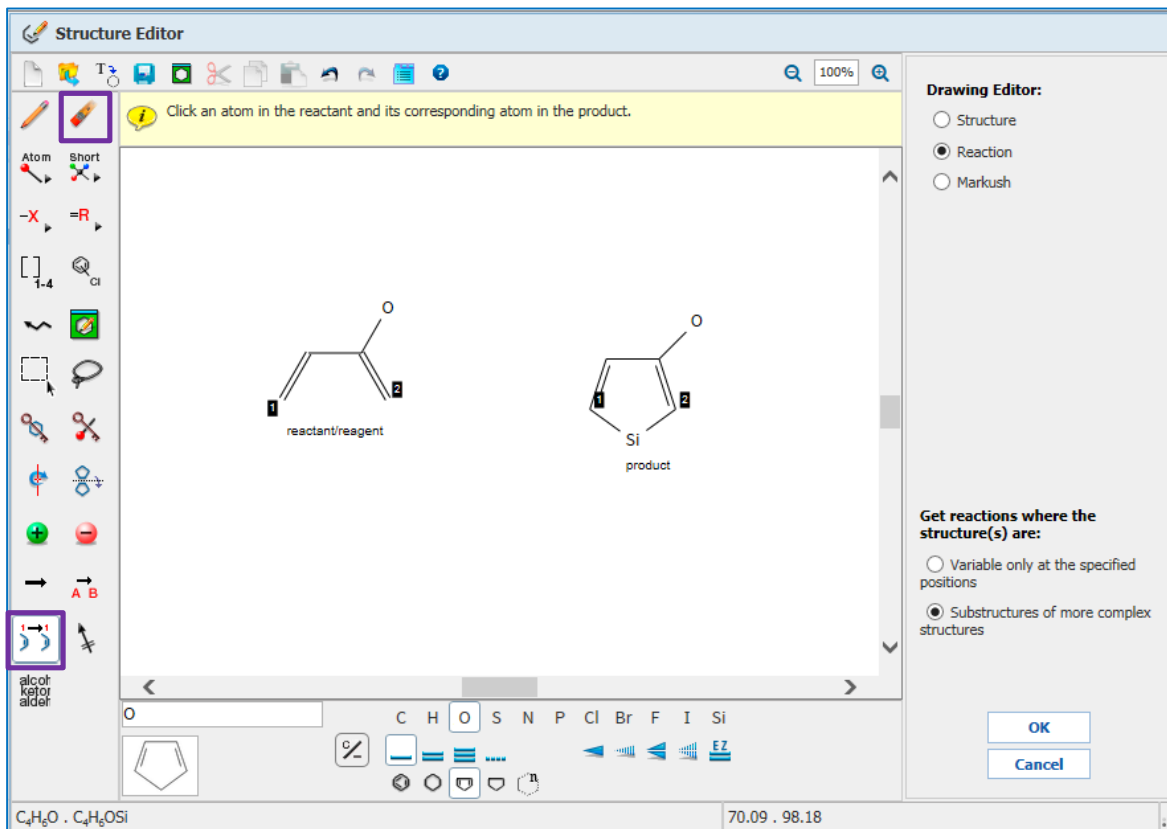
反应箭头

化学键变化

原子标记

官能团列表

例1：反应前后物质中的原子标记



例2：发生变化的化学键标记

Structure Editor

Click bonds to be formed or broken during the reaction.

reactant/reagent

product

化学键的变化：键的断裂，生成，迁移等。

Drawing Editor:

- Structure
- Reaction
- Markush

Get reactions where the structure(s) are:

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

OK

Cancel

C_4H_8O · C_4H_8OSi 70.09 . 98.18

锁环、锁结构的反应检索：绘制反应式

The screenshot displays the 'Structure Editor' software interface. The main workspace shows a chemical reaction: a benzothiazole ring (labeled 'reactant') reacts to form a benzothiazole ring with an acetyl group (labeled 'product'). The interface includes a toolbar on the left with various drawing tools, a top menu bar with icons for file operations, and a right-hand 'Drawing Editor' panel. In the 'Drawing Editor' panel, the 'Reaction' radio button is selected and highlighted with a purple box, with the Chinese characters '反应' (Reaction) written next to it. Below this, the 'Get reactions where the structure(s) are:' section has the 'Variable only at the specified positions' radio button selected and highlighted with a purple box. A callout bubble points to this selection with the text '执行的是锁环锁原子的检索' (Executing the search for locked ring and locked atoms). At the bottom of the interface, there is a search bar containing the letter 'C' and a list of chemical elements: C, H, O, S, N, P, Cl, Br, F, I, Si. Below the element list are icons for aromaticity and stereochemistry.

执行的是锁环
锁原子的检索

NDER®

锁环、锁结构的反应检索：查看反应结果集

Explore Saved Searches SciPlanner Save Print **Export**

Reaction Structure structure variable only at spe... > reactions (8)

REACTIONS **分组, 排序**

Get References Tools

Analyze Refine

Group by: No Grouping Sort by: Number of Steps

0 of 8 Reactions Selected

1. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.

C1=CC=C2C(=C1)S=N2 + CC(C)C(=O)N

~85 ~102

Overview

Steps/Stages

1.1 R:BuLi, S:THF, S:Me(CH₂)₂, -78°C; 1 h, -78°C

Export

Export: All Selected Range Example: 2-20

For: Offline review Portable Document Format (*.pdf) Rich Text Format (*.rtf)

Saving locally Answer Key eXchange (*.akx)

Details: File Name: * Reaction_05_05_2017_171255 X

Format: Summary Detail

Include: Experimental Procedure (if available) MethodsNow™ Protocols (if available) Overview Task History

Export Cancel

点击Export导出结果

锁环、锁结构的反应检索：查看反应结果集

点击Document，合并来自同一篇文章的反应；
点击Transformation，获得反应类型的分类。

Reaction Structure structure variable only at spe... > reactions (8)

REACTIIONS ?

Get References Tools

Analyze Refine

Analyze by: Reagent

| | |
|--------------------------------|---|
| BuLi | 4 |
| t-BuOOH | 3 |
| HCl | 2 |
| 19468-88-3 | 1 |
| H ₂ O | 1 |
| H ₂ SO ₄ | 1 |

Show More

Group by: No Grouping Document Transformation
Sort by: Relevance

0 of 8 Reactions Selected

1. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.

~101 ~93 90% ~83

1. Decarboxylative Alkylation, Acylation and Carbalkoxylation of Nitrogen Heterocycle
5 Reactions

R⁴ = R, COR¹, OCOR³

2. Uncategorized Single-Step Reactions
2 Reactions

3. Multi-Step Reactions
1 Reaction

Overview

Steps/Stages

1.1 R: t-BuOOH, S: Me(CH₂)₃Me, 24 h, 80°C
1.2 R: H₂O

Notes

optimized on amount of TBHP, amount of phosphate, temperature and solvent, using hydrogen peroxide in MeCN resulted in lower yield, optimization study, Reactants: 2, Reagents: 2, Solvents: 1, Steps: 1, Stages: 2, Most stages in any one step: 2

References

Peroxides as "Switches" of Dialkyl H-Phosphonate: Two Mild and Metal-Free Methods for

锁环、锁结构的反应检索：查看反应结果集

Explore ▾ Saved Searches ▾ SciPlanner Save Print Export

Reaction Structure structure variable only at spe... > reactions (8)

REACTIONS **?** Get References Tools

Analyze Refine

Analyze by: Reagent

| | |
|--------------------------------|---|
| BuLi | 4 |
| <i>t</i> -BuOOH | 3 |
| HCl | 2 |
| 19468-88-3 | 1 |
| H ₂ O | 1 |
| H ₂ SO ₄ | 1 |

Show More

Group by: No Grouping Sort by: **Number of Steps**

0 of 8 Reactions Selected

1. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.

CN1C=NC2=CC=CC=C1S2 + CC(=O)Cl → CC(=O)C1=NC2=CC=CC=C1S2

~85 ~102 58% ~79

Overview

Steps/Stages

1.1 R:BuLi, S:THF, S:Me(CH₂)₂Me, -78°C; 1 h, -78°C

Notes

ice-bath removed after stirring at -78°C for 1 hour (stage 2), Reactants: 2, Reagents: 2, Catalysts: 2, Steps: 1, Stage: 2, Most stages is any one step?

排序：相关度，入库号，实验步骤，MethodsNow，步数，产率，发表年份

锁环、锁结构的反应检索：查看反应结果集

Reaction Structure structure variable only at spe... > reactions (8)

REACTIONS ? Get References Tools Send to SciPlanner

Analyze Refine

Analyze by: ?
Reagent

| | |
|--------------------------------|---|
| BuLi | 4 |
| <i>t</i> -BuOOH | 3 |
| HCl | 2 |
| 19468-88-3 | 1 |
| H ₂ O | 1 |
| H ₂ SO ₄ | 1 |

Show More

Group by: No Grouping Document Transformation Sort by: Relevance

1. View Reaction Detail Link Similar Reactions

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

对于一步反应，可以点击 similar Reaction, 获取相似反应

Overview

Steps/Stages

1.1 R: *t*-BuOOH, S: Me(CH₂)₃Me, 24 h, 80°C
1.2 R: H₂O

Notes

optimized on amount of TBHP, amount of phosphate, temperature and solvent, using hydrogen peroxide in MeCN resulted in lower yield, optimization study, Reactants: 2, Reagents: 2, Solvents: 1, Steps: 1, Stages: 2, Most stages in any one step: 2

References

[Peroxides as "Switches" of Dialkyl H-Phosphonate: Two Mild and Metal-Free Methods for](#)

锁环、锁结构的反应检索：获取相似反应

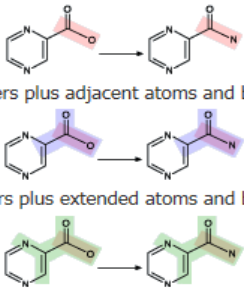
Get Similar Reactions ?

Retrieve similar reactions from:

- All reactions
- Current answer set

Include this level of similarity:

- Broad - Reaction centers only
- Medium - Reaction centers plus adjacent atoms and bonds
- Narrow - Reaction centers plus extended atoms and bonds



Get Reactions **Cancel**

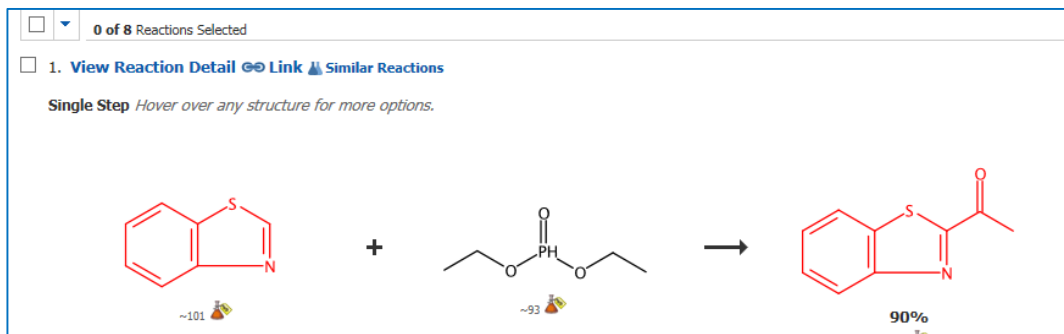
相似度限制：

Broad：仅反应中心相似

Medium：反应中心及附属原子和键

Narrow：反应中心及扩展的原子和键

锁环、锁结构的反应检索：查看感兴趣的反应信息



Overview

Steps/Stages

- 1.1 R: t -BuOOH, S: $\text{Me}(\text{CH}_2)_2\text{Me}$, 24 h, 80 °C
- 1.2 R: H_2O

Notes

optimized on amount of TBHP, amount of phosphate, temperature and solvent, using hydrogen peroxide in MeCN resulted in lower yield, optimization study, Reactants: 2, Reagents: 2, Solvents: 1, Steps: 1, Stages: 2, Most stages in any one step: 2

References

Peroxides as "Switches" of Dialkyl H-Phosphonate: Two Mild and Metal-Free Methods for Preparation of 2-Acylbenzothiazoles and Dialkyl Benzothiazol-2-ylphosphonates

[Quick View](#) [Other Sources](#)

By Chen, Xiao-Lan et al

From Journal of Organic Chemistry, 79(17), 8407-8416; 2014

Experimental Procedure

JOC
The Journal of Organic Chemistry

Experimental Procedures for the Synthesis of 2-Acylbenzothiazoles (3a-3ab). A mixture of benzothiazole (135.0 mg, 1.0 mmol), phosphonate (5.0 mmol), and TBHP (10.0 mmol) in CH_2CN (2.0 mL) was stirred at 80 °C for 24 h. The reaction mixture was quenched with water (5.0 mL) and extracted with ethyl acetate (3 x 5.0 mL). The combined organic layers were washed with brine (15.0 mL) and dried over anhydrous MgSO_4 . After filtration, the solvent was evaporated in vacuo. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 20/1) to give the desired product **1-(Benzo[d]thiazol-2-yl)ethanone (3a)**: yield 90%. mp 107–110 °C; ^1H NMR (400 MHz, CDCl_3) δ 2.83 (s, 3H), 7.53 (td, $J = 7.6, 1.3$ Hz, 1H), 7.58 (td, $J = 8.0, 1.3$ Hz, 1H), 7.98 (d, $J = 8.0$ Hz, 1H), 8.18 (d, $J = 7.8$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 26.2, 122.5, 125.5, 127.0, 127.7, 137.5, 153.6, 166.5, 193.2; HRMS (ESI) calcd for $\text{C}_8\text{H}_7\text{NOS}$ [$\text{M} + \text{H}$] $^+$, 178.0321, found 178.0320.

提纲

- SciFinder中获取化合物制备信息的方法
- 物质相关信息获取方法
 - 结构编辑器的使用（绘图工具，定义和限定化合物等）
 - 如何进行物质检索（结构，属性，识别号检索等）
 - 如何查看物质详情
- 反应相关信息获取方法
 - 结构编辑器的使用（绘图、限定反应的工具）
 - 如何进行精确结构反应检索，并获得实验详情
 - 如何进行亚结构反应检索，以及如何处理检索结果
 - 反应检索案例分享

亚结构反应检索: 绘制反应式

Structure Editor

Draw or change atoms or bonds. Shortcut Keys

Atom Short

-X -R

reactant

product

R1 = N, S

Drawing Editor:

- Structure
- Reaction
- Markush

Get reactions where the structure(s) are:

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

OK

Cancel

输入的反应物和产物结构可以被修饰，但母体结构不变

亚结构反应检索：获得反应结果集

REACTIONS

Get References Tools

Send to SciPlanner

Analyze Refine

Group by: No Grouping Sort by: Relevance

0 of 1208 Reactions Selected

1. View Reaction Detail Link

2 Steps *Hover over any structure for more options.*

Refine by:

- Reaction Structure
- Product Yield
- Number of Steps
- Reaction Classification
- Excluding Reaction Classification
- Non-participating functional groups

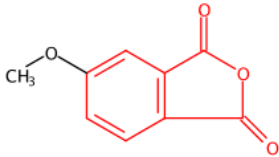
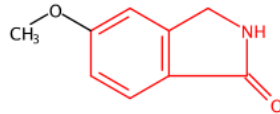
Structure Editor:

Java Non-Java

Click image to change structure or view detail.

Search type: **Substructure**

Refine

CH₃  \rightarrow  CH₃

~83 ~85

Overview

Steps/Stages

1.1 R:H₂NCHO
2.1 R:HCl, R:Sn, S:H₂O, S:EtOH

Notes

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

References

Studies on the chemistry of isoindoles and isoindolenines. XXVII. 3-Alkoxy-1H-isoindoles: syntheses and properties

Quick View Other Sources

By Hennige, Hans et al
From *Chemische Berichte*, 121(2), 243-52; 1988

亚结构反应检索：分析处理

13种分析选项

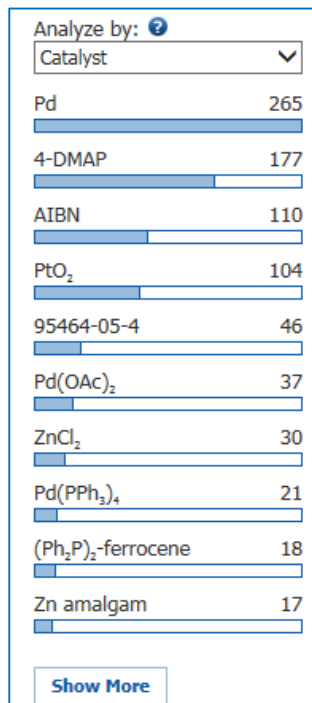
Analyze Refine

Analyze by: ?

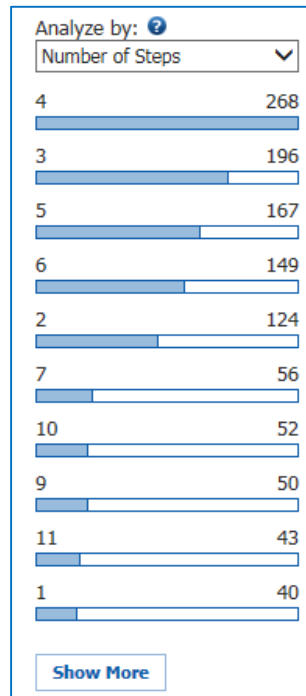
- Author Name
- Catalyst
- Company-Organization
- Document Type
- Experimental Procedure
- Journal Name
- Language
- MethodsNow
- Number of Steps
- Product Yield
- Publication Year
- Reagent
- Solvent



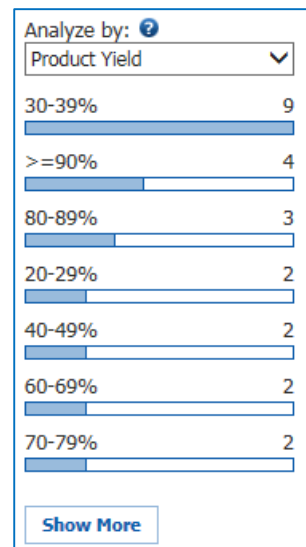
催化剂



反应步数



产率



亚结构反应检索：筛选处理

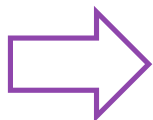
6种筛选选项：反应结构、产率、反应步数、包含/排除的反应类型(11种)、反应官能团(217种)

REACTIONS ?

Analyze Refine

Refine by: ?

- Reaction Structure
- Product Yield
- Number of Steps
- Reaction Classification
- Excluding Reaction Classification
- Non-participating functional groups



Reaction Classification(s):

- Biotransformation
- Catalyzed
- Chemoselective
- Combinatorial
- Electrochemical
- Gas-phase
- Non-catalyzed
- Photochemical
- Radiochemical
- Regioselective
- Stereoselective

Refine

- 生物转化
- 催化反应
- 化学选择性
- 组合化学
- 电子化学
- 气相反应
- 非催化反应
- 光化学
- 放射化学
- 区域选择反应
- 立体选择反应

亚结构反应检索：勾选反应类型

REACTIONS ? Get References Tools Send to SciPlanner

Analyze Refine

Group by: No Grouping Sort by: Relevance ↓

0 of 1217 Reactions Selected Page: 1 of 82

1. View Reaction Detail Link

2 Steps *Hover over any structure for more options.*

Reaction Classification(s):

- Biotransformation
- Catalyzed
- Chemoselective
- Combinatorial
- Electrochemical
- Gas-phase
- Non-catalyzed
- Photochemical
- Radiochemical
- Regioselective
- Stereoselective

Refine

Overview

Steps/Stages

- 1.1
- 2.1

Notes

1) no experimental details, prophetic reaction, 2) literature preparation, prophetic reaction, no experimental details, Reactants: 1, Steps: 2, Stages: 2, Most stages in any one step: 1

References

Lenalidomide isotopologues and their preparation and use for the treatment of diseases

Quick View PATENTPAK

By Muller, George W. and Man, Hon-Wah
From PCT Int. Appl., 2010093434, 19 Aug 2010

亚结构反应检索：排除反应类型

Reaction Structure substructure > reactions (1208) > refine "Electrochemical Gas-phase Phot..." (1154)

REACTIONS ? Get References Tools Send to SciPlanner

Analyze **Refine** Group by: No Grouping Sort by: Relevance Display Options

0 of 1154 Reactions Selected Page: 1 of 77

1. View Reaction Detail Link

2 Steps *Hover over any structure for more options.*

Refine by:

- Reaction Structure
- Product Yield
- Number of Steps
- Reaction Classification
- Excluding Reaction Classification
- Non-participating functional groups

Excluding Reaction Classification(s):

- Biotransformation
- Catalyzed
- Chemoselective
- Combinatorial
- Electrochemical
- Gas-phase
- Non-catalyzed
- Photochemical
- Radiochemical
- Regioselective
- Stereoselective

Overview

Steps/Stages

1.1 R:H₂NCHO
2.1 R:HCl, R:Sn, S:H₂O, S:EtOH

Notes

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

References

Studies on the chemistry of isoindoles and isoindolenines. XXVII. 3-Alkoxy-1H-isoindoles: syntheses and properties
[Quick View](#) [Other Sources](#)
By Hennig, Hans et al.

亚结构反应检索：筛选官能团

Reaction Structure substructure > reactions (1208) > refine "Electrochemical Gas-phase Phot..." (1154) > **refine "any HETEROCYCLES KETONES" (435)**

REACTIONS Get References Tools Send to SciPlanner

Analyze **Refine** Group by: No Grouping Sort by: Relevance Display Options

0 of 435 Reactions Selected Page: 1 of 29

Refine by:

- Reaction Structure
- Product Yield
- Number of Steps
- Reaction Classification
- Excluding Reaction Classification
- Non-participating functional groups

Non-participating Functional Group(s)
View: Classes 10

2 Selected Clear Selections

- AMINES
- CARBONATE DERIVAT
- CARBOXY DERIVATI
- HALIDES
- HETEROCYCLES
- KETONES
- ORGANOMETALLICS

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

2 Steps *Hover over any structure for more options.*

Overview

Steps/Stages

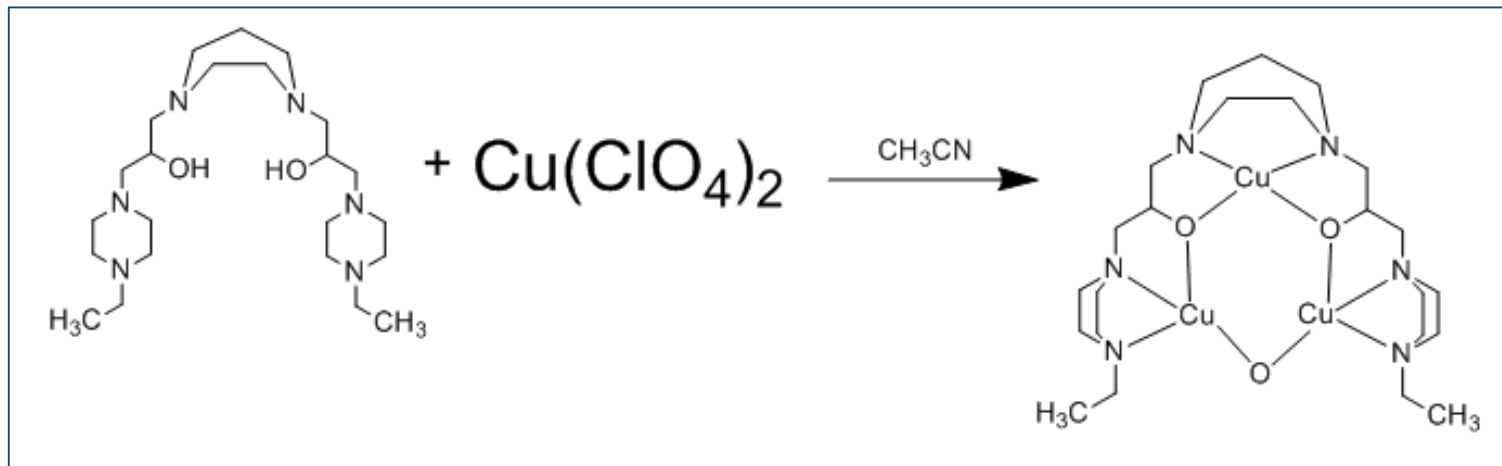
1.1 R:NH₂OAc, 3 h, 140°C
2.1

Notes

1) thermal, 2) literature preparation, no experimental detail, Reactants: 1, Reagents: 1, Steps: 2, Stages: 2, Most stages in any one step: 1

References

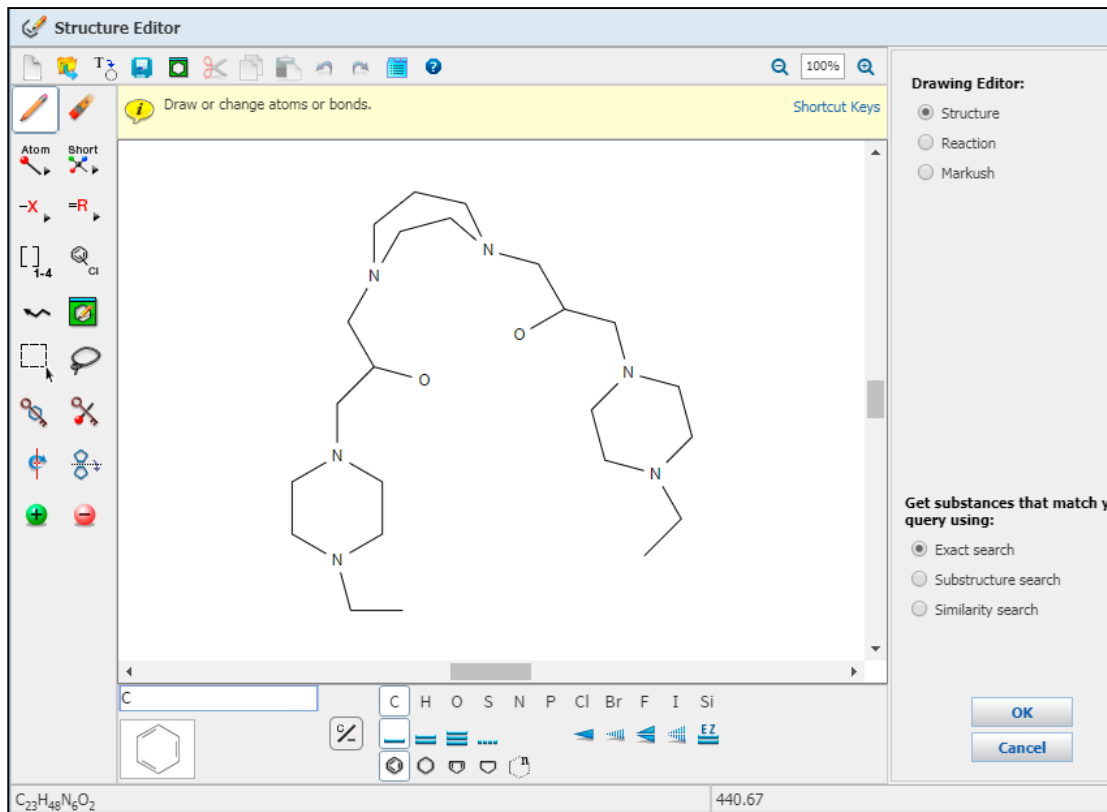
查找此反应



提纲

- SciFinder中获取化合物制备信息的方法
- 物质相关信息获取方法
 - 结构编辑器的使用（绘图工具，定义和限定化合物等）
 - 如何进行物质检索（结构，属性，识别号检索等）
 - 如何查看物质详情
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 - 结构编辑器的使用（绘图、限定反应的工具）
 - 如何进行精确结构反应检索，并获得实验详情
 - 如何进行亚结构反应检索，以及如何处理检索结果
 - 反应检索案例分享

在结构编辑器绘制配体



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获得此配体作为reagent 或者reactant的反应

The screenshot shows the SciFinder web interface. At the top, there are navigation tabs: 'Get References', 'Get Reactions', 'Get Commercial Sources', and 'Tools'. Below these, a search bar is set to 'Sort by: CAS Registry Number'. A dropdown menu indicates '0 of 1 Substance Selected'. The search results list item 1 with CAS number 1430236-09-1. Below the list is a chemical structure of 1#-1,4-Diazepine-1,4(5H)-diethanol, α^1, α^4 -bis[(4-ethyl-1-piperazinyl)methyl]tetrahydro-. The molecular formula is $C_{23}H_{48}N_6O_2$. Below the structure is a link for 'Key Physical Properties'. A 'Get Reactions' dialog box is overlaid on the right side of the screen. The dialog has a title bar 'Get Reactions' and contains the following options:

Retrieve reactions for:

- All substances
- Selected substances

Limit results by reaction role:

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

At the bottom right of the dialog are 'Get' and 'Cancel' buttons.

Explore ▾ Saved Searches ▾ SciPlanner

Chemical Structure exact > substances (1) > get reactions (2)

REACTIONS ⓘ

Get References Tools ▾

Analyze Refine

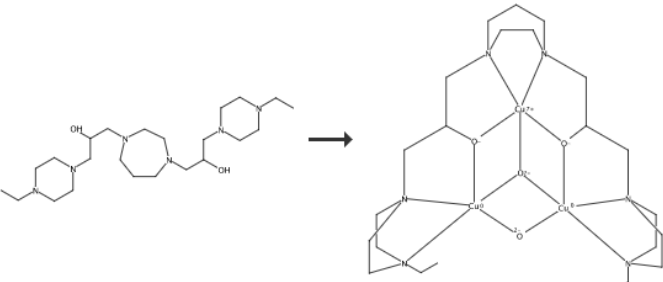
Analyze by: ⓘ
 Reagent ▾
 No reactions available

Group by: No Grouping ▾ Sort by: Accession Number ▾ ↓

0 of 2 Reactions Selected

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

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



▼ Overview
 Steps/Stages

1.1

Notes

literature preparation, no experimental detail, Reactants: 1, Steps: 1, S

References

[Efficient Oxidation of Methane to Methanol by Dioxygen Mediated by T](#)
Click View Other Sources
 By Chan, Sunney I. et al
 From *Angewandte Chemie, International Edition*, 52(13), 3731-3735; 2013

点此可查该文章的所有反应



[Return](#)**Efficient Oxidation of Methane to Methanol by Dioxygen Mediated by Tricopper Clusters**

By: Chan, Sunney I.; Lu, Yu-Jhang; Nagababu, Penumakki; Maji, Suman; Hung, Mu-Cheng; Lee, Marianne M.; Hsu, I.-Jui; Minh, Pham Dinh; Lai, Jeff C.-H.; Ng, Kok Yoah; Ramalingam, Sridevi; Yu, Steve S.-F.; Chan, Michael K.

Efficient oxidn. of methane to methanol by dioxygen mediated by tricopper clusters is discussed.

Indexing

Industrial Organic Chemicals, Leather, Fats, and Waxes (Section45-4)

Section cross-reference(s): 6, 22, 23, 34, 67, 78

Concepts**Alkanes**

C2-6; efficient oxidn. of methane to methanol by dioxygen mediated by tricopper clusters

Physical, engineering or chemical process; Properties; Reactant; Process; Reactant or reagent

Alcohols**Ketones**

C2-6; efficient oxidn. of methane to methanol by dioxygen mediated by tricopper clusters

Physical, engineering or chemical process; Properties; Synthetic preparation; Preparation; Process

Bioinorganic chemistry

Catalyst supports

ESR(electron spin resonance)

Emission spectra

Hydroxylation catalysts

Mass spectra

Oxidation

Oxidation kinetics

X-ray spectra

C-H bond cleavage

Coordination number

EXAFS spectra

Hydroxylation

Magnetic susceptibility

Molecular cloning

Oxidation catalysts

Singlet state

efficient oxidn. of methane to methanol by dioxygen mediated by tricopper clusters

Intermediates

efficient oxidn. of methane to methanol by dioxygen mediated by tricopper clusters

Catalyst use; Formation, unclassified; Physical, engineering or chemical process; Properties; Reactant; Formation, nonpreparative; Process; Uses; Reactant or reagent

Cluster compounds**Enzyme mimics****Substances**

1430342-15-6

efficient oxidn. of methane to methanol by dioxygen mediated by tricopper clusters

Catalyst use; Formation, unclassified; Physical, engineering or chemical process; Properties; Reactant; Formation, nonpreparative; Process; Uses; Reactant or reagent

7440-44-0 Carbon, processes

efficient oxidn. of methane to methanol by dioxygen mediated by tricopper clusters

Catalyst use; Physical, engineering or chemical process; Properties; Process; Uses

1430236-11-5

1430236-12-6

1430236-13-7

1430236-14-8

1430236-15-9

1430236-16-0

1430236-17-1

1430236-18-2

1430236-19-3

efficient oxidn. of methane to methanol by dioxygen mediated by tricopper clusters

Catalyst use; Physical, engineering or chemical process; Properties; Reactant; Process; Uses; Reactant or reagent

7440-50-8DP Copper, peptide complexes

1430236-09-1P

1430236-10-4P

1430342-17-8P

QUICK LINKS

0 Tags, 0 Comments

SOURCE

Angewandte Chemie, International Edition
Volume52
Issue13
Pages3731-3735
Journal
2013
CODEN:ACIEF5
ISSN:1433-7851
DOI:10.1002/anie.201209846

COMPANY/ORGANIZATION

Institute of Chemistry
Academia Sinica
Taipei, Taiwan 11529

ACCESSION NUMBER

2013:271245
CAN158:591813
CAPLUS

PUBLISHER

Wiley-VCH Verlag GmbH &
Co. KGaA

LANGUAGE

English

查看反应信息详情

Analyze Refine

Group by: No Grouping Sort by: Accession Number

0 of 12 Reactions Selected

1. View Reaction Detail [Link](#)

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

Analyze by: Reagent

KMnO₄ 6

TEA chloride 2

110743-42-5 1

Ce(NH₄)₂(NO₃)₆ 1

H₂O 1

Mn(OAc)₂ 1

Show More

complex with picoline

Overview

Steps/Stages

1.1 R:Ce(NH₄)₂(NO₃)₆, S:MeCN, rt; 15 min, rt

Notes

crystals formed after 3 days at room temperature, Reactants: 2, Reagents: 1, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Manganese/Cerium Clusters Spanning a Range of Oxidation Levels and CeMn8, Ce2Mn4, and Ce6Mn4 Nuclearities: Structural, Magnetic, and EPR Properties
By Lampropoulos, Christos et al
From Inorganic Chemistry, 53(13), 6805-6816; 2014

Experimental Procedure

Inorganic Chemistry General/Typical Procedure: **Method B.** To a stirred solution of [Mn₁₁O₁₂(O₂CMe)₂₅(H₂O)₄] (0.50 g, 0.25 mmol) in a solvent mixture comprising MeCN (15 mL) and pyridine (10 mL) was slowly added solid (NH₄)₂[Ce(NO₃)₆] (0.28 g, 0.50 mmol). The resulting solution was stirred for 15 min, during which time the color changed slightly from dark brown to red/brown. The solution was filtered and left undisturbed for a period of 3 d, during which time black needles of **1**·2py·6MeCN grew. They were isolated as for Method A; the yield was based on Ce. The identity of the product was confirmed by elemental analysis, IR spectral comparison, and unit cell determination to be identical to material from Method A. The picoline version [Ce₂Mn₄O₁₂(O₂CMe)₁₂(NO₃)₄(pic)₂] (**1'**) can be obtained in comparable yield by the same method using picoline instead of pyridine. Anal. Calcd (Found) for **1'**·2H₂O: C, 21.14 (21.25); H, 2.50 (2.75); N, 4.48 (4.26)%.

METHODS NOW™

Procedure

1. Slowly add solid (NH₄)₂[Ce(NO₃)₆] (0.28 g, 0.50 mmol) to a stirred solution of [Mn₁₁O₁₂(O₂CMe)₂₅(H₂O)₄] (0.50 g, 0.25 mmol) in a solvent mixture comprising MeCN (15 mL) and picoline (10 mL).
2. Stir the resulting solution for 15 min.

[View more...](#)

Available Experimental Data

Elemental Analysis

[View with MethodsNow](#)

谢谢关注!



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