

钱欣博士

Application Specialist

cqian@acs-i.org

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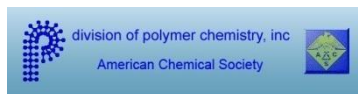
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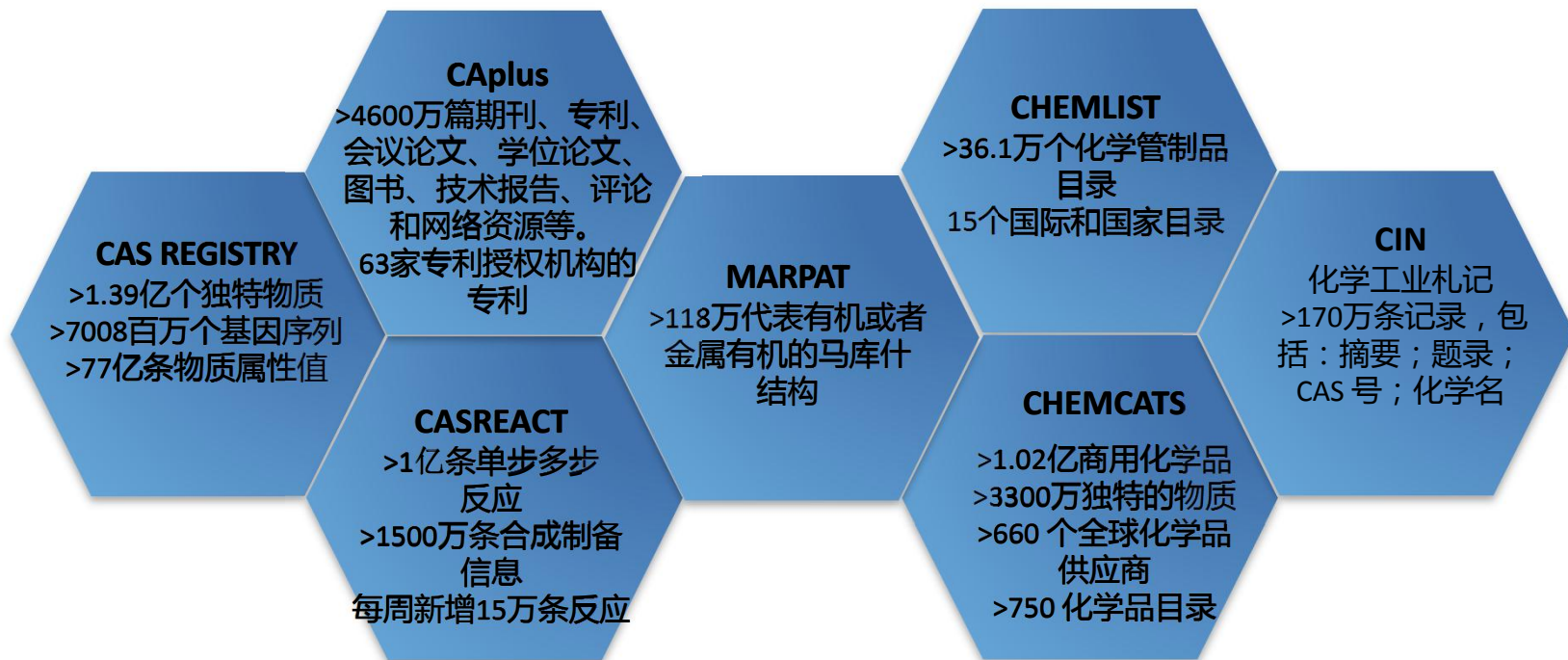


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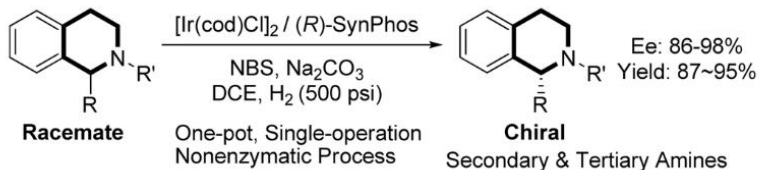
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CAS数据库最具价值的内容——人工标引

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
503538-68-9

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

Catalyst use; Uses

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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
CAN15:232316

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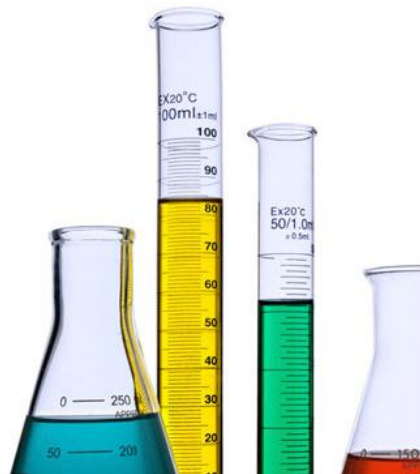
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- Chemical Structure
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- Reaction Structure

REFERENCES: RESEARCH TOPIC

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9

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- 检索式 : water splitting with solar

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1. **Enhanced solar absorption of water splitting composite**
Quick View Other Sources
By Abed, J.; AlMheiri, M.; Alexander, F.; Ray...
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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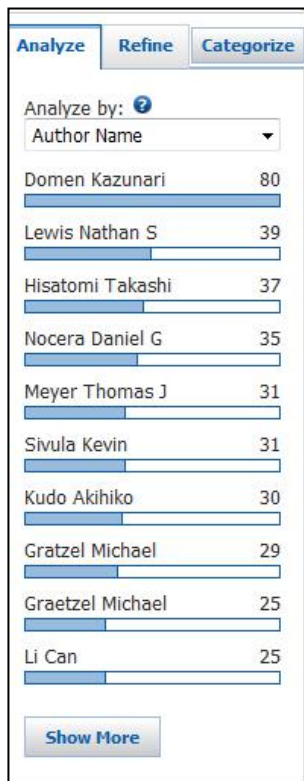
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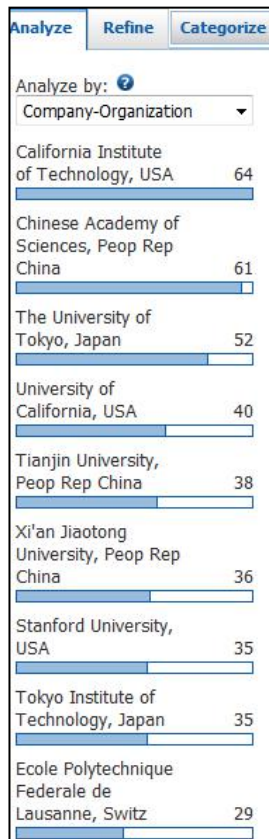
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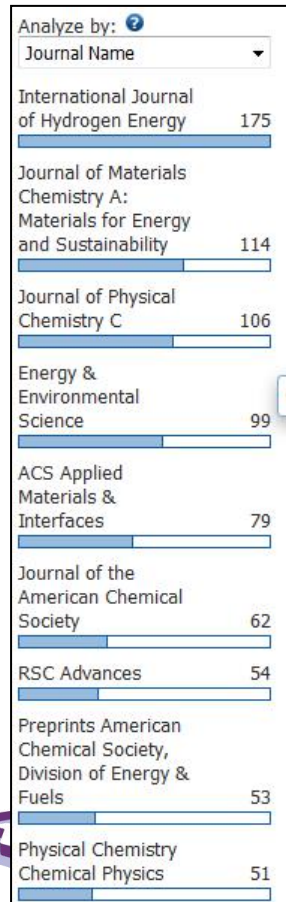
主要研究人员



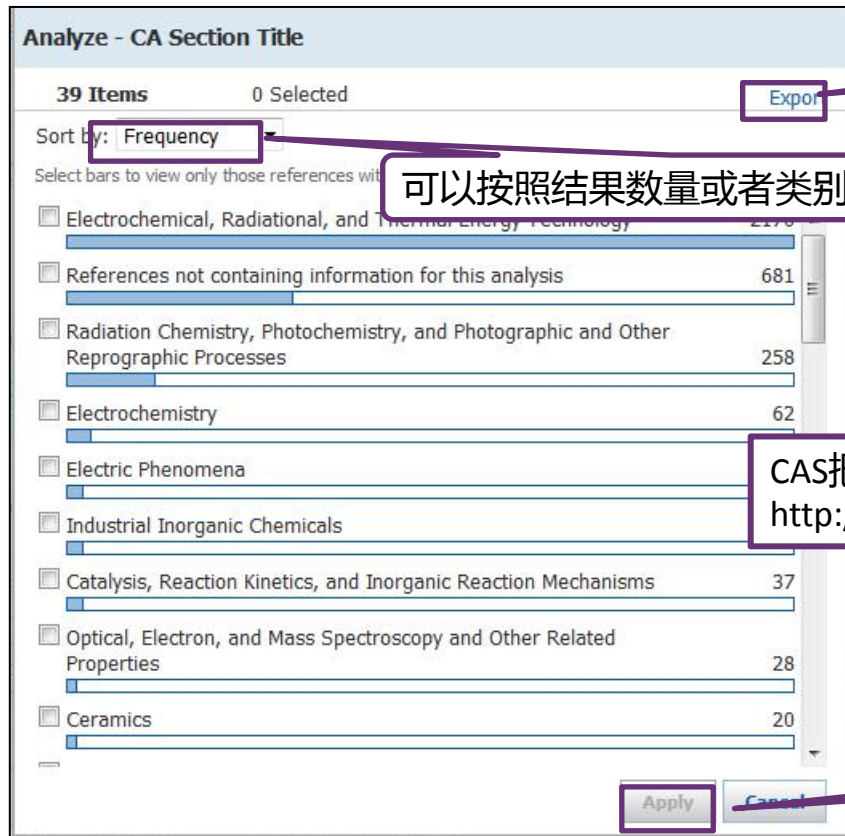
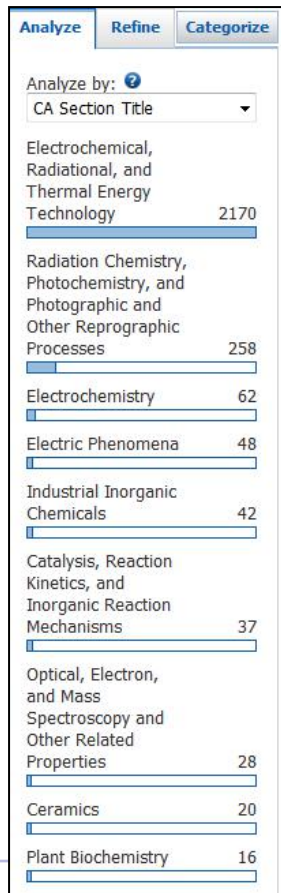
主要研究机构， 合作伙伴，竞争对手



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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, F... gy (Section52)

重要技术术语

重要物质

Concepts

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

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

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- 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

Patent No.	Kind	Language
WO 2014096865	A1	English
Patent Family		
US 20140178291	A1	English
KR 2015097788	A	Korean
CN 104884382	A	Chinese
JP 2016502968	T	Japanese

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

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

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Key Substances in Patent

CAS RN 57808-44-3

CN(B)B

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Analyst Marking Location
page 32

CAS RN 12447-26-6

[NH4+].[B-]

• NH₄⁺

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5 methylamine borane, tri-methylamine borane, hydrazine borane, hydrazine bisborane, ethane 1,2-di-amineborane, ammonia triborane, ammonium octahydrotriborane or a mixture of two or more thereof.

6. The pellet according to any one of claims 3 to 5 wherein the borane comprises ammonia borane, methylamine borane, dimethylamine borane, phenylamine borane, hydrazine borane, hydrazine bisborane, ethane 1,2-di-amineborane, ammonia triborane, ammonium octahydrotriborane or a mixture of two or more thereof.

10

15 7. The pellet according to any of the preceding claims wherein the hydrogen storage material comprises or consists of ammonia borane.

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Chemical structures are shown for the key substances in the patent, including a complex borane-amine adduct and a triborane-amine structure. The triborane-amine structure is highlighted with a callout box containing the text: "CAS Registry Number 57808-44-3", "B₃H₁₀N", "Triborane(7), 3-ammine-", "Melting Point (Experimental) Value: 73 °C", and "Other Names: Triborane(7), ammoniate (6Cl); Triborane(7), monoammoniate; Ammonia triborane; Ammonia-triborane(7)".

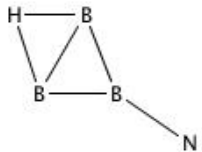
Annotations in Chinese provide instructions: "点击view detail, 直接查看物质信息详情" (Click view detail, directly view substance information details) points to the "View Detail" button. "可在PatentPak Viewer中直接返回SciFinder进行结构、马库什和反应检索" (Can directly return to SciFinder in PatentPak Viewer for structure, Markush, and reaction search) points to the "Search in SciFinder" button.

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（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：手性反应检索专题**
 - 手性化合物合成方法检索
 - 手性反转反应
 - 手性拆分反应
- 聚合物检索专题
 - 聚合物物质检索
 - 聚合物反应检索



通过文献获得不同研究领域的物质

The screenshot shows the SciFinder interface with a search for "water splitting with solar". The search results are filtered to 2148 references. A dialog box titled "Get Substances" is open, allowing the user to retrieve substances from the selected references. The dialog box has two main sections: "Retrieve substances for:" and "Limit results to:".

Retrieve substances for:

- All references
- Selected references

Limit results to:

- Adverse Effect, including toxicity
- Analytical Study
- Biological Study
- Combinatorial Study
- Formation, nonpreparative
- Miscellaneous
- Occurrence
- Preparation
- Process
- Properties
- Prophetics in Patents
- Reactant or Reagent
- Uses

The background interface shows a list of references under the heading "REFERENCES". The first reference is titled "1. Emerging energy applicat..." and the second is "2. Understanding photovolt...".

光解水中有关用途的物质

Substances interface showing search results for various compounds. The interface includes a navigation bar with options like "Get References", "Get Reactions", and "Get Commercial Sources". A sidebar on the left provides filters for "Analyze by" (Substance Role, Uses, Properties, Process, Preparation, Reactant or Reagent, Formation, Analytical Study, Biological Study, Occurrence, Miscellaneous) and a "Show More" button. The main area displays a grid of search results, each with a CAS number, a chemical structure, and a component list.

Sort by: CAS Registry Number

0 of 881 Substances Selected

Page: 10 of 18

451. 13494-90-1
(Component: 7697-37-2)
~2448
O=[N+]([O-])O
• 1/3 Ga

452. 13530-65-9
(Component: 7738-94-5)
~1428
[O-][Cr](O)(=O)O
• Zn

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

物质检索结果——Analyze

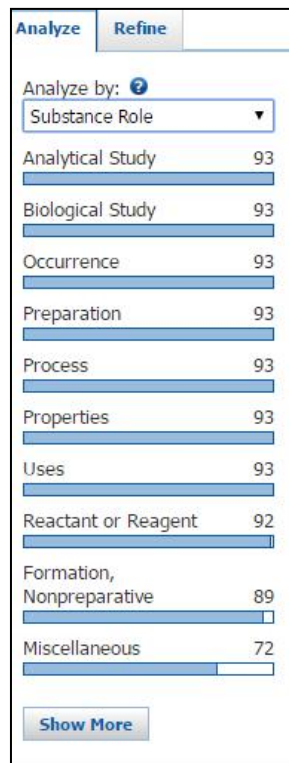
六种分析选项

Analyze by: ?

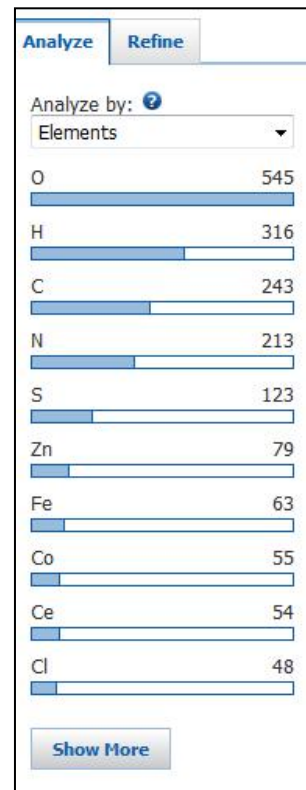
- Bioactivity Indicators
- Commercial Availability
- Elements**
- Reaction Availability
- Substance Role
- Target Indicators

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



SCIFINDER[®]
A CAS SOLUTION

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

1. 50

~21151

C₁₇H₂₁N
8-Azabicy
8-methyl-

Key PI
Regulatory
Spectra
Experiment

Get Refer

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

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 substituent group
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

精确检索
亚结构检索
相似检索

结构
反应
马库什

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A CAS SOLUTION

28

举例：不固定位置取代

The image displays two sequential screenshots of the Structure Editor software interface, illustrating the process of adding a chlorine atom to a benzene ring at a non-fixed position.

Left Screenshot: The main workspace shows a benzene ring with a single bond extending from the top vertex. To the right of the ring, a chlorine atom (Cl) is present. The left-hand toolbar has a purple box around the chlorine atom icon. The top status bar reads "Draw or change atoms or bonds."

Right Screenshot: The same workspace is shown, but now a dashed line indicates the attachment point on the ring. A red circle with the number "1" is positioned at the end of the bond, indicating the specific attachment site. The top status bar reads "Click and drag from the substituent position to each ring position where attachment may occur."

Right Panel (Drawing Editor): This panel contains the following options:

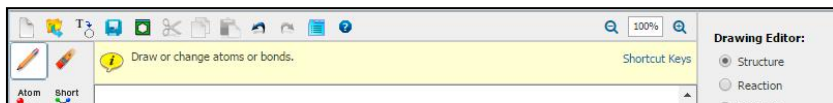
- Drawing Editor:**
 - Structure
 - Reaction
 - Markush
- Get substances that match your query using:**
 - Exact search
 - Substructure search
 - Similarity search

Buttons for "OK" and "Cancel" are located at the bottom of the right panel.

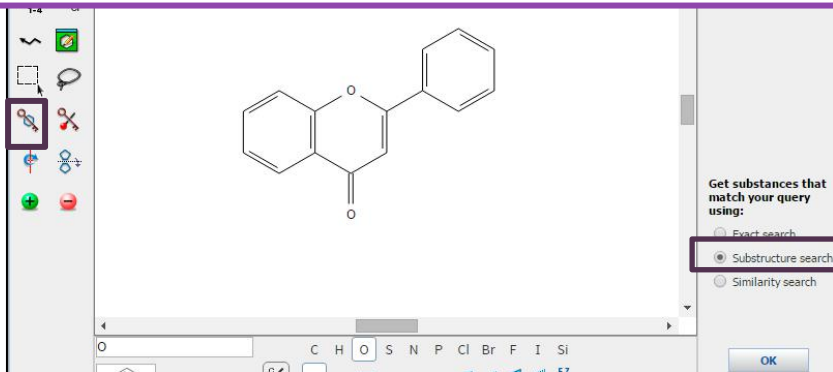
举例：环锁定



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

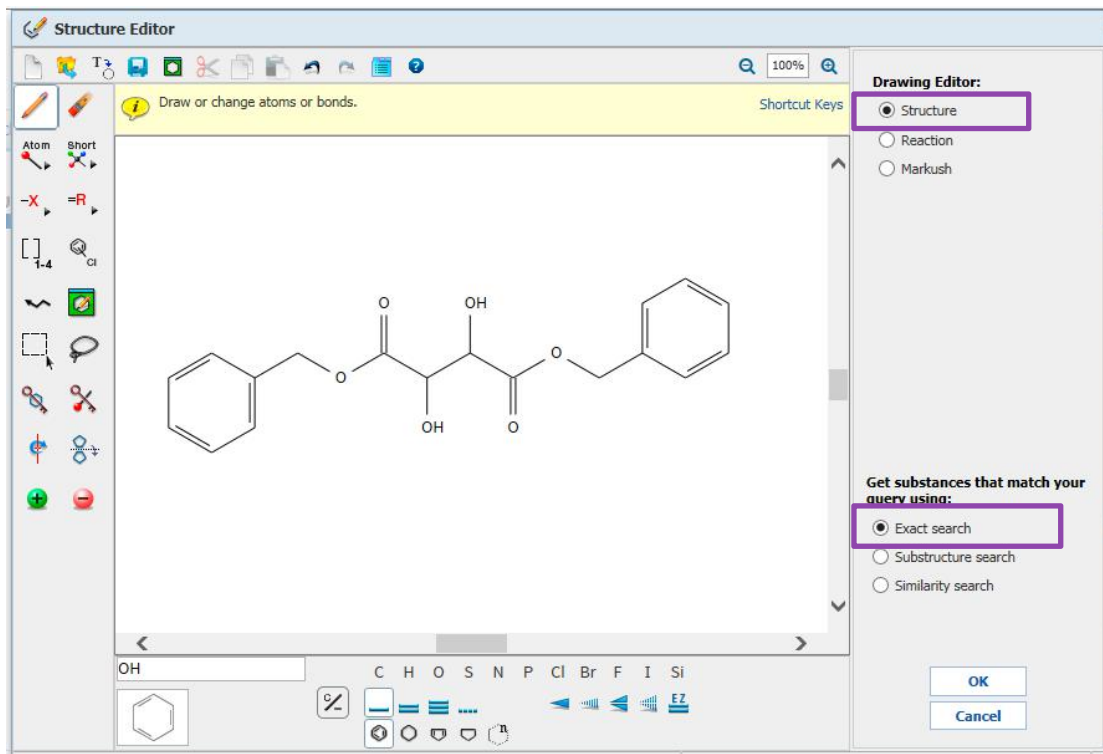


273. Substance Detail
136116-17-1

$C_{19}H_{12}O_3$
1#Naphtho[2,1-*b*]pyran-1-one, 3-(3-hydroxyphenyl)-

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

<p>0 of 20 Subst</p> <p>1. 622-00-4 </p> <p>~105 ~57 </p> <p>手性化合物 Chiral compound</p> <p>Absolute stereochemistry.,Rotation (+).</p> <p>C₁₈ H₁₈ O₆ Butanedioic acid, 2,3-dihydroxy-, 1,4-bis(phenylmethyl) ester</p> <p>▶ Key Physical Properties Experimental Properties</p>	<p>2. 4136-22-5 </p> <p>~46 </p> <p>Absolute stereochemistry.,Rotation (-).</p> <p>C₁₈ H₁₈ O₆ Butanedioic acid, 2,3-dihydroxy-, 1,4-bis(phenylmethyl) ester, (2S,3S)-</p> <p>▶ Key Physical Properties</p>	<p>3. 93993-87-4 </p> <p>~9 ~7 </p> <p>C₁₈ H₁₈ O₆ Butanedioic acid, 2,3-dihydroxy-, 1,4-bis(phenylmethyl) ester</p> <p>▶ Key Physical Properties</p>
<p>4. 4079-56-5 </p> <p>~5 </p> <p>Relative stereochemistry.</p> <p>C₁₈ H₁₈ O₆ Butanedioic acid, 2,3-dihydroxy-, 1,4-bis(phenylmethyl) ester, (2R,3R)-rel</p>	<p>5. 4079-57-6 </p> <p>~5 ~1 </p> <p>Relative stereochemistry.</p> <p>C₁₈ H₁₈ O₆ Butanedioic acid, 2,3-dihydroxy-, 1,4-bis(phenylmethyl) ester, (2R,3S)-rel</p> <p>▶ Key Physical Properties</p>	<p>6. 89960-73-6 </p> <p>~2 </p> <p>Absolute stereochemistry.,Rotation (+).</p> <p>622-00-4 C₁₈ H₁₈ O₆</p> <p>101-68-8 C₁₅ H₁₀ N₂ O₂</p>

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- (2*R*,3*R*)-, 1,4-bis(phenylmethyl) ester

▶ **Key Physical Properties**
Experimental Properties

4. **4079-56-5** 🔍

~5

Relative stereochemistry.

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

▶ **Key Physical Properties**

3. **93993-87-4** 🔍

~9 ~7

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

▶ **Key Physical Properties**

6. **896448-46-7** 🔍

~2 ~3

Absolute stereochemistry.

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

▶ **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

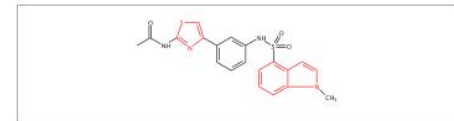
Show More

Sort by: CAS Registry Number

0 of 49240 Substances Selected

Page: 1 of 3283

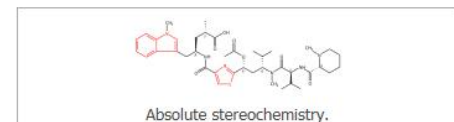
1. 1997357-70-6



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

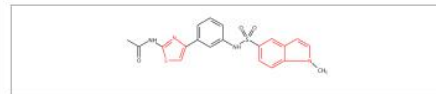
[Key Physical Properties](#)

4. 1995847-80-7



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

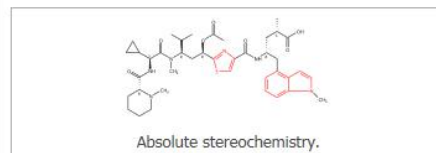
2. 1997357-68-2



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

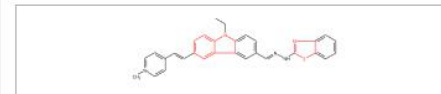
[Key Physical Properties](#)

5. 1995846-52-0



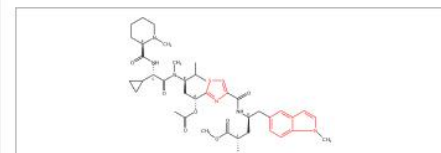
C₂₀ H₁₈ N₄ O₃ S₂

3. 1995871-38-9



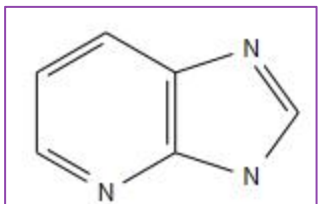
C₃₀ H₂₆ N₅ S
Pyridinium, 4-[2-[6-[[[2-(2-benzothiazolyl)hydrazinylidene]methyl]-9-ethyl-9*H*-carbazol-3-yl]ethenyl]-1-methyl-

6. 1995844-98-8



C₃₀ H₂₆ N₅ S
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

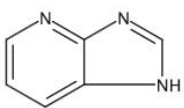
相似度越高, 结构越相似



0 of 34 Substances Selected


Score: ≥ 99
 1. [273-21-2](#)

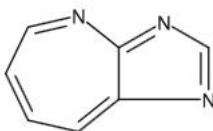
~394   ~130 



C₆ H₅ N₃
3H-Imidazo[4,5-b]pyridine


Score: 81
 14. [128710-59-8](#)

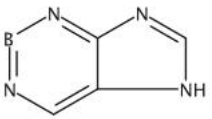
~0 



C₇ H₅ N₃
Imidazo[4,5-b]azepine (9CI)

Score: 73
 36. [42341-33-3](#)

~0 



C₄ H₃ B N₄
1H-Imidazo[4,5-d]-1,3,2-diazaborine (9CI)

物质检索——理化性质检索：寻找电阻率大于125ohm的含铁物质

CAS Solutions

SCIFINDER
A CAS SOLUTION

Explore Saved Searches SciPlanner

REFERENCES

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

SUBSTANCES

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

REACTIONS

- Reaction Structure

SUBSTANCES: PROPERTY ?

Experimental

Select Property...
Select Property...
Boiling Point (°C)
Density (g/cm³)
Electric Conductance (S)
Electric Conductivity (S/cm)
Electric Resistance (ohm)
Electric Resistivity (ohm*cm)
Glass Transition Temp. (°C)
Magnetic Moment (μB)
Median Lethal Dose (LD50) (mg/kg)
Melting Point (°C)
Optical Rotatory Power (degrees)
Refractive Index
Tensile Strength (MPa)

Examples: 44, 25-35, >125

Examples: 44, 25-35, >125

物质检索——理化性质性质检索

The screenshot displays the SciFinder web interface. The top navigation bar includes 'Apps', 'SciFinder - Sign In', and 'CAS(美国化学)'. The main header features the SciFinder logo and 'A CAS SOLUTION'. Below the header, there are 'Explore' and 'Saved Searches' buttons. The left sidebar contains three main sections: 'REFERENCES' (with sub-items: Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, Tags), 'SUBSTANCES' (with sub-items: Chemical Structure, Markush, Molecular Formula, Property, Substance Identifier), and 'REACTIONS' (with sub-item: Reaction Structure). The 'SUBSTANCES' section is currently active, showing a 'SUBSTANCE' search area. A dropdown menu is open, listing various physical and chemical properties: Bioconcentration Factor, Boiling Point (°C), Density (g/cm³), Enthalpy of Vaporization (kJ/mol), Flash Point (°C), Freely Rotatable Bonds, H Donor/Acceptor sum, H Acceptors, H Donors, Koc, logD, logP, Mass Intrinsic Solubility (g/L), Mass Solubility (g/L), Molar Intrinsic Solubility (mol/L), Molar Solubility (mol/L), Molar Volume (cm³/mol), **Molecular Weight** (highlighted), pKa, and 'Select Property...'. Below the dropdown, there are two input fields with the text 'Examples: 44, 25-35, >125'. A blue 'Search' button is positioned below the input fields.

SciFinder物质检索结果

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

Refine by: ?

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

Structure Editor:

Java
Non-Java

Click to Edit

Search type: **Exact Structure**

0 of 137 Substances Selected

1. **1360099-47-3** 🔍

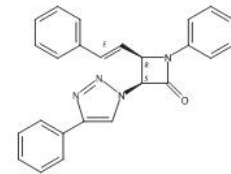
~189

Component	Component Ratio
Te	x
Cd	x
Hg	x

Cd . Hg . Te
Cadmium mercury telluride
[Experimental Properties](#)

2. **1262894-47-2** 🔍

~2



Double bond geometry as shown.,Relative stereochemistry.

C₂₅ H₂₆ N₄ O
2-Azetidinone, 1-phenyl-4-[(1E)-2-phenylethenyl]-3-(4-phenyl-1H-1,2,3-triazol-1-yl)-, (3R,4S)-rel
[Key Physical Properties](#)
[Experimental Properties](#)

3. **1160936-40-2** 🔍

~1

Component	Component Ratio
Te	1.8
Se	0.2
In	0.1
Cu	0.1
Cd	1.8

Cd . Cu . In . Se . Te
Cadmium copper indium selenide telluride
(Cd_{1.8}Cu_{0.1}In_{0.1}Se_{0.2}Te_{1.8})
[Experimental Properties](#)

4. **1160936-38-8** 🔍

~1

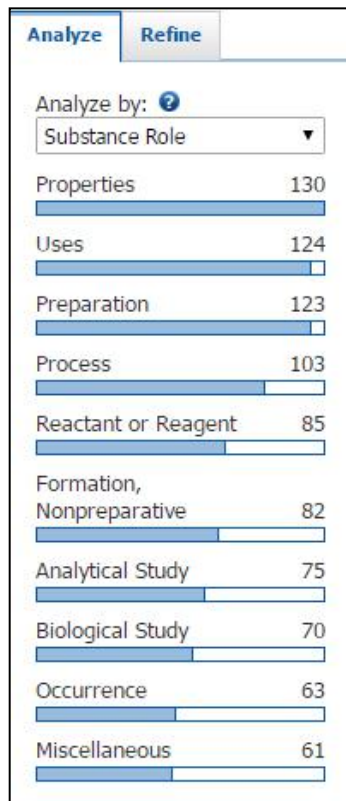
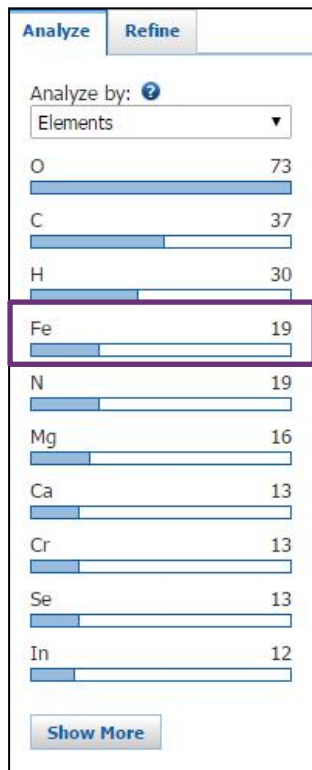
5. **1160936-37-7** 🔍

~1

6. **1034343-98-0** 🔍

~86194 ~48

通过分析/限定工具筛选结果



Analyze Refine

Refine by: ?

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

Structure Editor:

Java Non-Java

Click to Edit

Search type: **Exact Structure**

Only retrieve substances that:

Only retrieve substances that:

- Have references
- Are commercially available
- Are a single component
- Are in specific substance classes
 - Alloys
 - Coordination compounds
 - Incompletely defined
 - Mixtures
 - Polymers
 - Organics, and others not listed
- Are in specific types of studies

Refine

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

- Reaction

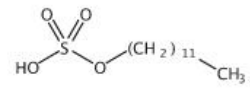
SUBSTANCES: MOLECULAR FORMULA ?

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

C₁₂H₂₆O₄S . 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

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

Analyze Refine

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

Occurrences 1

Component Component Percent

Component	Component Percent
Mn	69
Fe	26
Co	4.3

Co . Fe . Mn
Manganese alloy, base, Mn 69,Fe 26,Co 4.3

Component	Component Percent
Mn	70
Fe	28
Co	2.1

Co . Fe . Mn
Manganese alloy, base, Mn 70,Fe 28,Co 2.1

Component	Component Percent
Co	35
Fe	33
Mn	32

Co . Fe . Mn
Cobalt alloy, base, Co 35,Fe 33,Mn 32

Component	Component Percent
Co	34
Fe	34
Mn	32

Co . Fe . Mn

Component	Component Percent
Fe	62 - 79
Mn	20 - 32
Co	1.1 - 9.5

Co . Fe . Mn

Component	Component Ratio
Co	30
Mn	3
Fe	70

Page: 1 of 5

多氧簇金属：七钼酸铵

CAS Registry Number 12027-67-7

(Component: 12274-10-1)

~7,729   ~40 

$\text{H}_4 \text{N} \cdot \frac{1}{6} \text{Mo}_7 \text{O}_{24}$

Molybdate ($\text{Mo}_7\text{O}_{24}^{6-}$), ammonium (1:6)

Coordination Compound

Other Names

Ammonium molybdate(VI) ($(\text{NH}_4)_6\text{Mo}_7\text{O}_{24}$) (6CI)

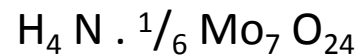
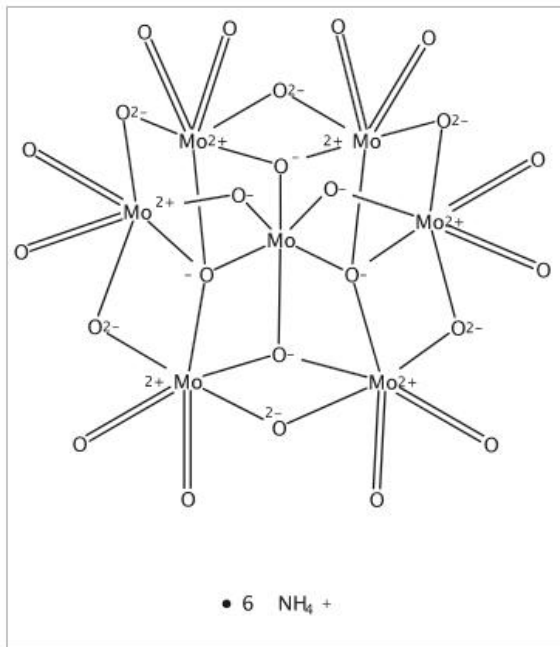
Molybdate ($\text{Mo}_7\text{O}_{24}^{6-}$), hexaammonium (9CI)

Molybdic acid ($\text{H}_2\text{Mo}_7\text{O}_{24}$), hexaammonium salt (8CI)

Ammonium heptamolybdate

Ammonium heptamolybdate ($(\text{NH}_4)_6\text{Mo}_7\text{O}_{24}$)

[View more...](#)



SCIFINDER®
A CAS SOLUTION

如何查找MOF化合物，以Cu-BTC为例

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-)-κ^O:κ^O]]₃[μ₃-[1,3,5-benzenetricarboxylato(3-)-κ^O:κ^O:κ^O]]tri-

Coordination Compound

Density (Experimental)

Value: 0.879 g/cm³

Other Names

Copper, triqua[μ-[1,3,5-benzenetricarboxylato(3-)-κ^O:κ^O]]₃[μ₃-[1,3,5-benzenetricarboxylato(3-)-κ^O:κ^O:κ^O]]tri- (9CI)

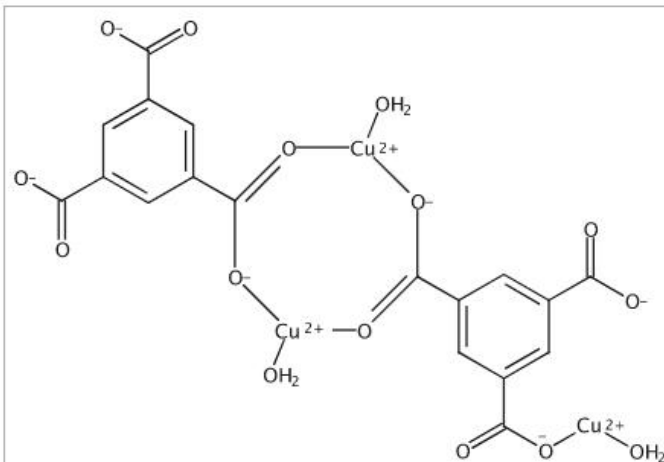
Triaqua[μ-[1,3,5-benzenetricarboxylato(3-)-κ^O:κ^O]]₃[μ₃-[1,3,5-benzenetricarboxylato(3-)-κ^O:κ^O:κ^O]]tricopper

Basolite C 300

Cu-BTC

Cu₃BTC₂

[View more...](#)



SCIFINDER
A CAS SOLUTION

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

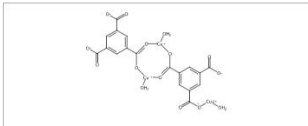
SUBSTANCES: MOLECULAR FORMULA

Examples:
H4SiO4
(C3H6O.C2H4O)x

Search

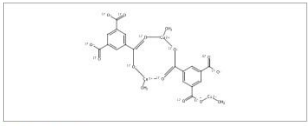
0 of 4 Substances Selected

1. 2019181-18-9



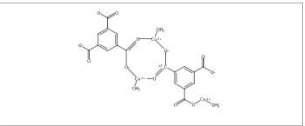
C₁₈ H₁₂ Cu₃ O₁₅
INDEX NAME NOT YET ASSIGNED

2. 1685249-53-9



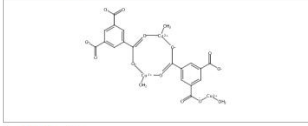
C₁₈ H₁₂ Cu₃ O₁₅
INDEX NAME NOT YET ASSIGNED

3. 1416961-85-7



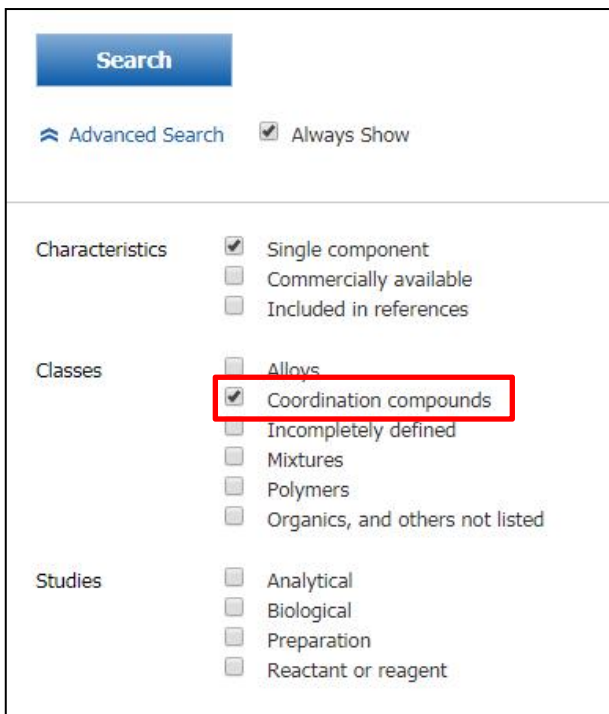
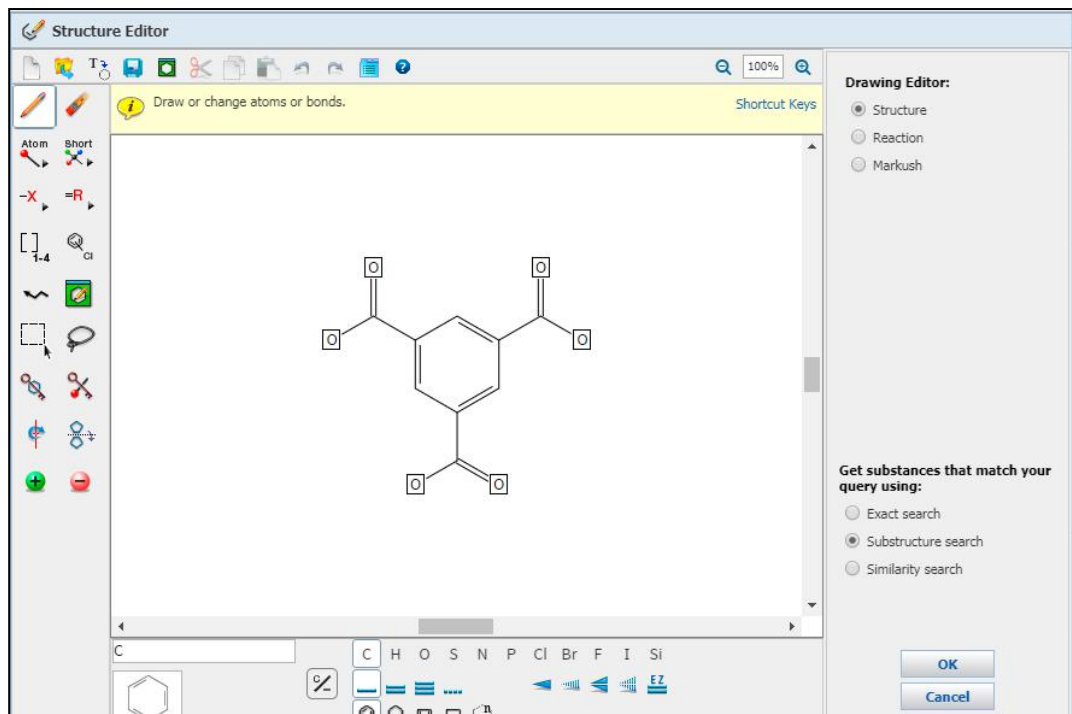
C₁₈ H₁₂ Cu₃ O₁₅
Copper, triaquo[μ-[1,3,5-benzenetricarboxylato(3-)-κO⁻:κO²⁻]]
[[μ₂-[1,3,5-benzenetricarboxyl-1⁻κO⁻:κO²⁻]]
tri-

4. 222404-02-6



C₁₈ H₁₂ Cu₃ O₁₅

方法3：已知配合物配体，可以先结构检索配体，然后获得相关配合物



注：此种方法可能结果噪音较多

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

MOL_10_16_2017_...mol ^

1. **1001196-71-9**

C₉ H₃ O₆ Zn
Zincate(1-), [1,3,5-benzenetricarboxylato(3-)-κO²]-

2. **1805003-23-9**

C₉ H₃ Cd O₆
INDEX NAME NOT

4. **1804937-55-0**

(Component: 1805003-23-9)

5. **951026-11-9**

结果会有噪音，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
- 1. Number of Commercial Sources
- Molecular Weight
- Molecular Formula

~1274

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

▶ **Key Physical Properties**
Experimental Properties

2. **222403-98-7**

(Component: 222404-02-6)

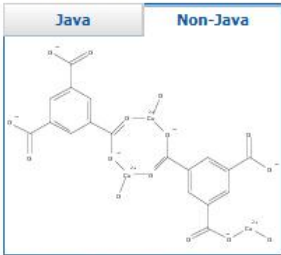
~38

C₁₈ H₁₂ Cu₃ O₁₅ · x H₂O
Copper, triaqua[μ-[1,3,5-benzenetricarboxylato(3-)-κO²:κO²]]
[μ₃-[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


Characteristics Single component
 Commercially available
 Included in references

Classes Alloys
 Coordination compounds



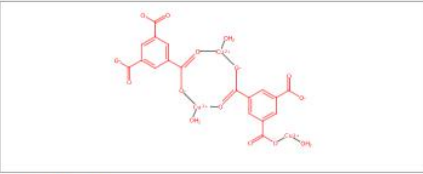
Search Type:



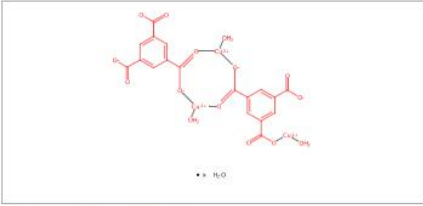
Exact Structure
 Substructure
 Similarity



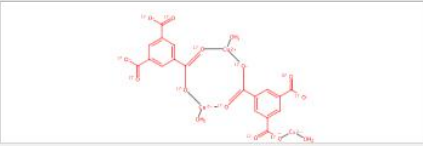
Show precision analysis



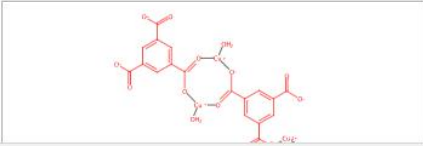
 ChemDraw
Launch a SciFinder substance
More

0 of 7 Substances Selected

1. **222404-02-6** 🔍
~1274  

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

2. **222403-98-7** 🔍
(Component: 222404-02-6)
~38  

C₁₈ H₁₂ Cu₃ O₁₅ · x H₂ O
Copper, triaqua[μ-[1,3,5-benzenetricarboxylato(3-)-κO¹]]
[μ₂-[1,3,5-benzenetricarboxylato(3-)-κO¹:κO²]]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

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

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

Key Physical Properties
Experimental Properties

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

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

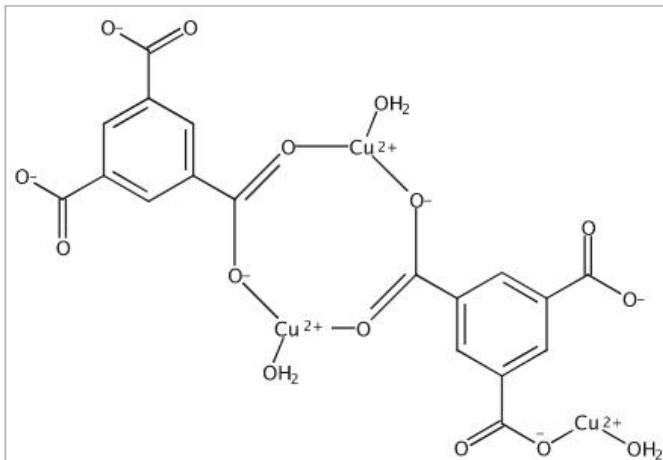
Triaqua[μ-[1,3,5-benzenetricarboxylato(3-)-κO⁻:κO²⁺]][μ₃-[1,3,5-benzenetricarboxylato(3-)-κO⁻:κO²⁺:κO²⁺]]tricopper

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

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
 - 化合物分析方法检索
- 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 categories like 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 various drawing tools, a central canvas with a benzene ring structure, and a 'Drawing Editor' panel on the right with options for Structure, Reaction, and Markush. A yellow status bar at the top of the canvas reads 'Draw or change atoms or bonds.' and 'Shortcut Keys'. Several callout boxes with Chinese text point to specific features: '角色定义' (Role Definition) points to the 'C' atom in the benzene ring; '反应箭头' (Reaction Arrow) points to the arrow tool in the toolbar; '原子标记' (Atom Labeling) points to the 'A B' tool; '化学键变化' (Chemical Bond Change) points to the bond change tool; 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

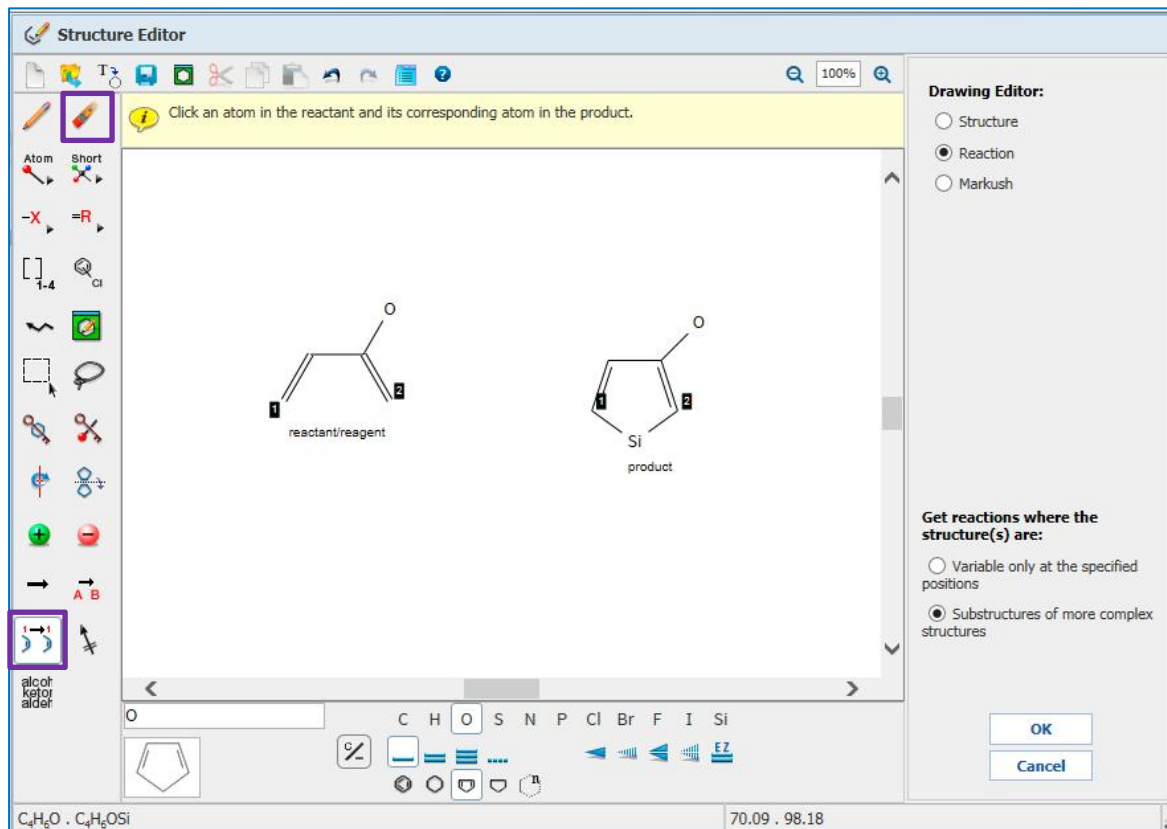
原子标记

官能团列表

化学键变化

CH₄ 16.04

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

精确结构反应检索：绘制反应式

The screenshot shows the 'Structure Editor' software interface. The main drawing area displays a chemical reaction: a benzothiazole derivative (reactant) reacts to form a benzothiazole derivative with an acetyl group (product). The reaction arrow is highlighted with a purple box. The 'Drawing Editor' panel on the right has the 'Reaction' radio button selected and highlighted with a purple box. Below it, 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. The 'OK' and 'Cancel' buttons are visible at the bottom of the panel.

Structure Editor

Draw or change atoms or bonds. Shortcut Keys

Atom Short

-X =R

1-4 Cl

reactant product

C H O S N P Cl Br F I Si

alcohol ketone aldehyde

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

反应

执行的是锁环
锁原子的检索

NDER®

精确结构反应检索：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

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.



~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 (*.alx)

Details:

File Name: *

Reaction_05_05_2017_171255 X

Format:

Summary
 Detail

Include:

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

* Required

Send to SciPlanner

Export Cancel

Click Export to export results

分组, 排序

精确结构反应检索：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

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

1. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.

~101 ~93 90% ~83

Overview

Steps/Stages

1.1 R: t-BuOOH, S: Me(CH₂)₂Me, 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

Get References Tools

Group by: Transformation Sort by: Frequency

0 of 8 Reactions Selected

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

精确结构反应检索：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

Sort by: **Number of Steps**

0 of 8 Reactions Selected

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

1. View Reaction Detail ⓘ Link Similar Reactions

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

C1CN2C(S1)C=CC=C2 + CC(=O)N(C)C → CC(=O)N1C=CC2C(S1)C=CC=C2

~85 ~102 58% ~79

Overview

Steps/Stages

Notes

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

ice-bath removed after stirring at -78°C for 1 hour (stage 2), Reactants: 2, Reagents: 2,

精确结构反应检索：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

精确结构反应检索：获取相似反应

Get Similar Reactions ?

Retrieve similar reactions from:

All reactions

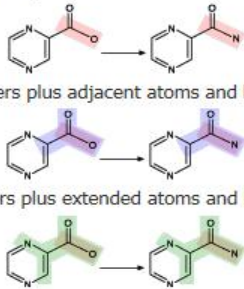
Current answer set

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



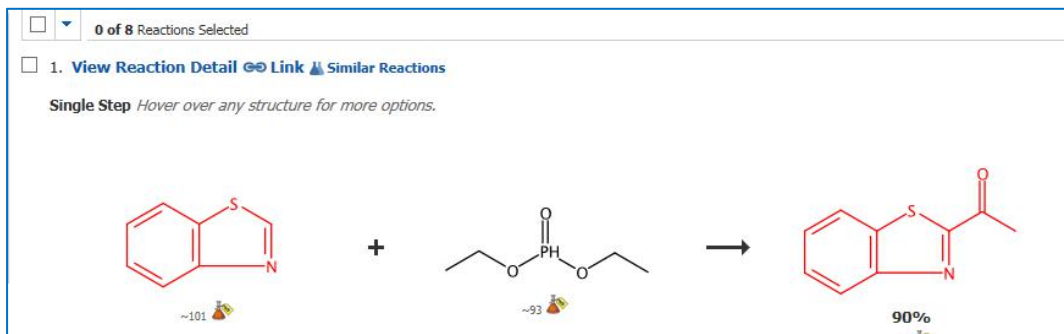
相似度限制：

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

精确结构反应检索：查看感兴趣的反应信息



Overview

Steps/Stages

- 1.1 R: tBuOOH, S: Me(CH₂)₂Me, 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 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 CH₂CN (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 MgSO₄. 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, CDCl₃) 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); ¹³C NMR (100 MHz, CDCl₃) δ 26.2, 122.5, 125.5, 127.0, 127.7, 137.5, 153.6, 166.5, 193.2; HRMS (ESI) calcd for C₉H₇NOS [M + H]⁺, 178.0321, found 178.0320.

实验步骤

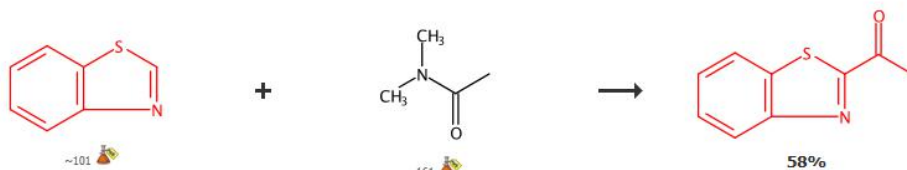
MethodsNow Synthesis——人工标引的反应信息，节省您宝贵的时间

- 详细、明确的物质信息
- 全面、有条理的实验过程信息
- 更好的阅读体验——表格形式
- 无需查看原文直接获取实验详情——反应物，反应条件，步骤，产物性质，谱图等

MethodsNow Synthesis: 通过Analyze, 选择有MethodsNow标引的反应, 点击MethodsNow查看实验详情

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

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



Overview

Steps/Stages

- 1.1 R: BuLi, S: THF, S: Me(CH₂)₄Me, -78°C; 1 h, -78°C
- 1.2 1 h, -78°C; 10 min
- 1.3 R: HCl, S: H₂O, rt, acidify

Notes

ice-bath removed after stirring at -78C for 1 hour (stage 2), Reactants: 2, Reagents: 2, Solvents: 3, Steps: 1, Stages: 3, Most stages in any one step: 3

References

Rhodium Catalyzed Asymmetric Hydrogenation of 2-Pyridine Ketones
[Quick View](#) [Other Sources](#)
By Yang, Hailong et al
From Organic Letters, 17(17), 4144-4147; 2015

METHODSNOW™

Procedure

1. Cool the solution (0.5 M) of benzothiazole in dry THF under nitrogen to -78 °C.
2. Add dropwise nBuLi (1.1 equiv, 5.5 mmol, 2.3M in hexane).

[View more...](#)

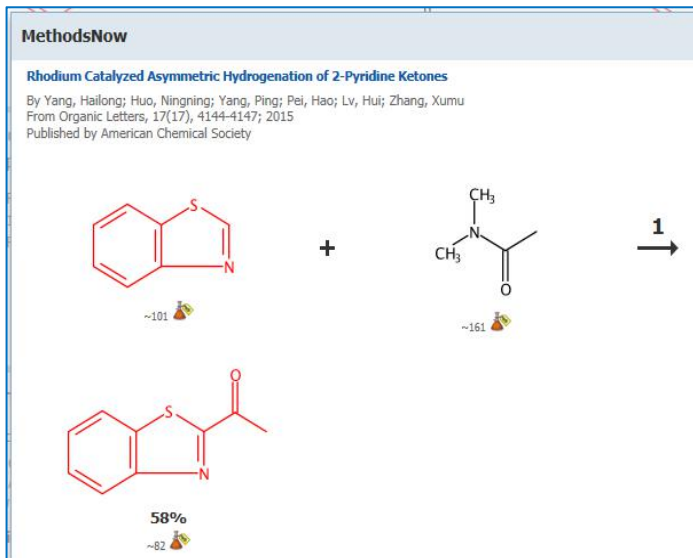
Available Experimental Data

¹H NMR, ¹³C NMR, State

[View with MethodsNow](#)

点击查看MethodsNow窗口

MethodsNow Synthesis: 实验详情展示窗口



产物，反应物，试剂，溶剂，步骤，
反应类型，规模，核磁氢谱，核磁碳谱，
产物状态，CAS方法号

Products	Ethanone, 1-(2-benzothiazolyl)-, 58%, CAS RN: 1629-78-3
Reactants	Benzothiazole, CAS RN: 95-16-9 Dimethylacetamide, CAS RN: 127-19-5
Reagents	Butyllithium, CAS RN: 109-72-8 Hydrochloric acid, CAS RN: 7647-01-0
Solvents	Tetrahydrofuran, CAS RN: 109-99-9 Hexane, CAS RN: 110-54-3 Water, CAS RN: 7732-18-5
Procedure	<ol style="list-style-type: none"> Cool the solution (0.5 M) of benzothiazole in dry THF under nitrogen to -78 °C. Add dropwise nBuLi (1.1 equiv, 5.5 mmol, 2.3M in hexane). Keep the resulted mixture for 1 h under -78 °C. Add N,N-dimethylacetamide (1 equiv, 5 mmol) to the stirred solution at -78 °C. Stir the mixture was continuously for 1 h. Remove the cold bath and stir the mixture for additional 10 min. Hydrolyze with concd hydrochloric acid (1 mL). Stir the acidic solution continuously until the temperature reach to room temperature. Pour the mixture into same amount of water. Extract the aqueous mixture with ethyl acetate 3 times. Dry the combined organic solution with Na₂SO₄. Purify by flash column chromatography to afford product.
Transformation	Decarboxylative Alkylation, Acylation and Carbalkoxylation of Nitrogen Heterocycle
¹H NMR	(400 MHz, CDCl ₃)δ8.22 (d, J = 8.0Hz, 1H), 8.01 (d, J = 7.6Hz, H), 7.55-7.63 (m, 2H), 2.87 (s, 3H);
¹³C NMR	(101MHz, CDCl ₃)δ193.2, 166.5, 153.6, 137.4, 127.7, 127.0, 125.5, 122.5, 26.2.
State	white solid
CAS Method Number	3-219-CAS-1662290

点击CAS RN, 即时查看物质

PDF or XLS格式

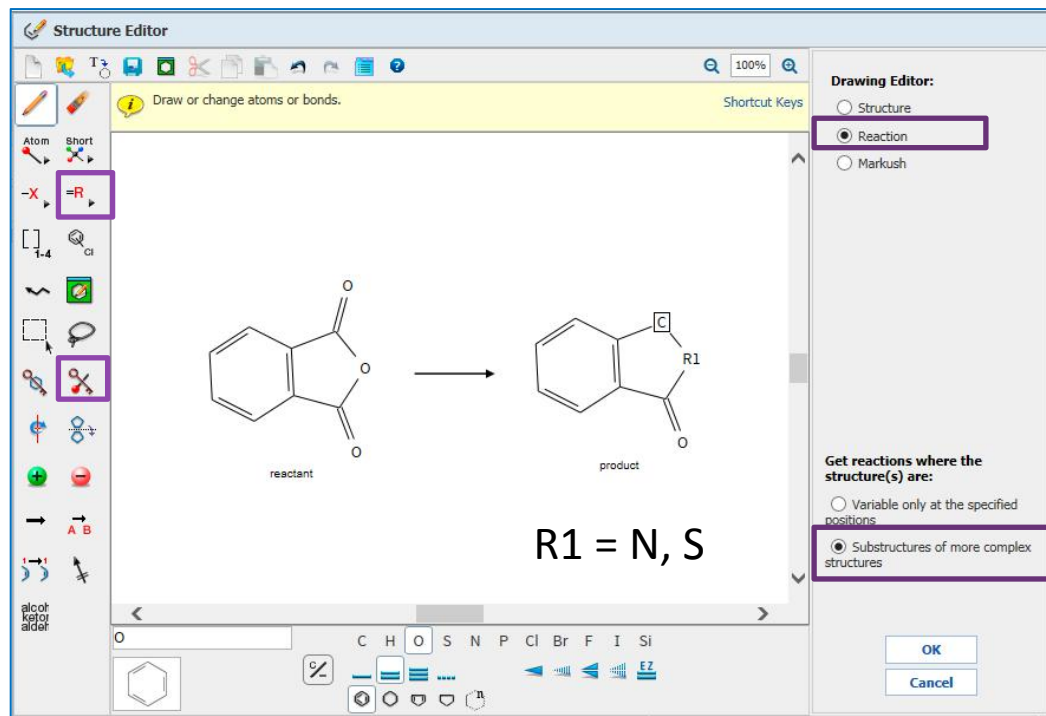
Print/Export Close



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



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

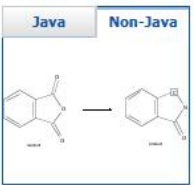
Analyze Refine

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**

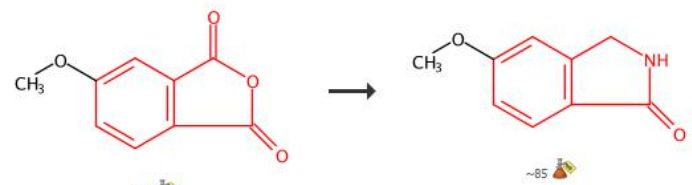
Refine

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.*



~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

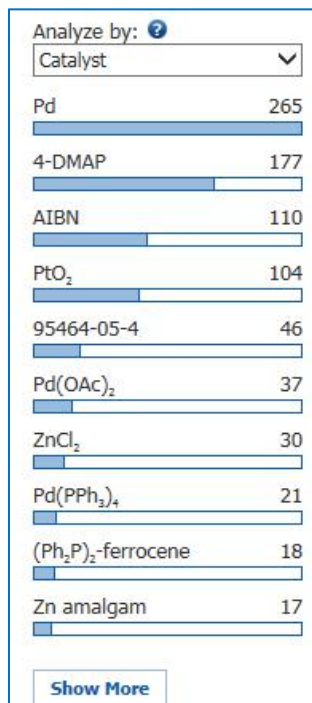
Analyze Refine

Analyze by: ?

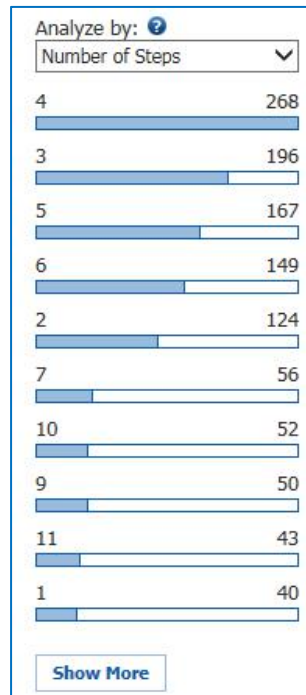
- Author Name
- Catalyst
- Company-Organization
- Document Type
- Experimental Procedure
- Journal Name
- Language
- MethodsNow
- Number of Steps
- Product Yield
- Publication Year
- Reagent
- Solvent



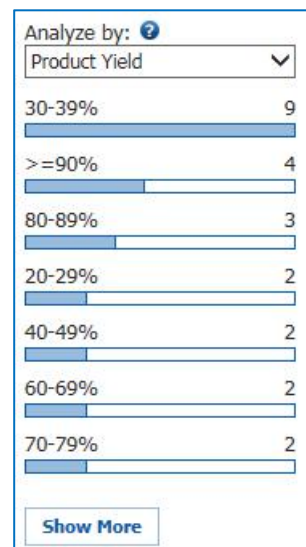
催化剂



反应步数



产率



亚结构反应检索：筛选处理

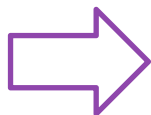
6种筛选选项：反应结构、产率、反应步数、包含/排除的反应类型(11种)、反应官能团(217种)

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

Refine by:

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

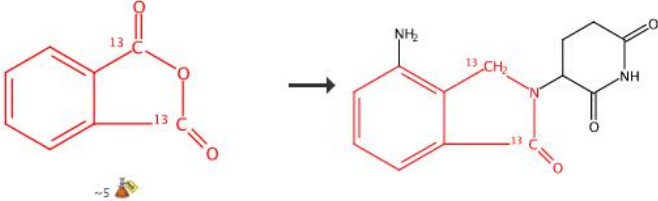
Reaction Classification(s):

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

Refine

1. View Reaction Detail [Link](#)

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



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.*

~83 ~85

Excluding Reaction Classification

- 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 DERIVATIV
- HALIDES
- HETEROCYCLES
- KETONES
- ORGANOMETALLICS

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

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

Overview

Steps/Stages

1.1 R: NH₄OAc, 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

查找多氧簇金属的反应信息：

CAS Registry Number 76210-25-8

$C_{32}H_{56}Mn_{12}O_{48}$

Manganese, hexadeca-
oxododeca-, compd. with acetic acid, hydrate (1:2:4)

Other Names

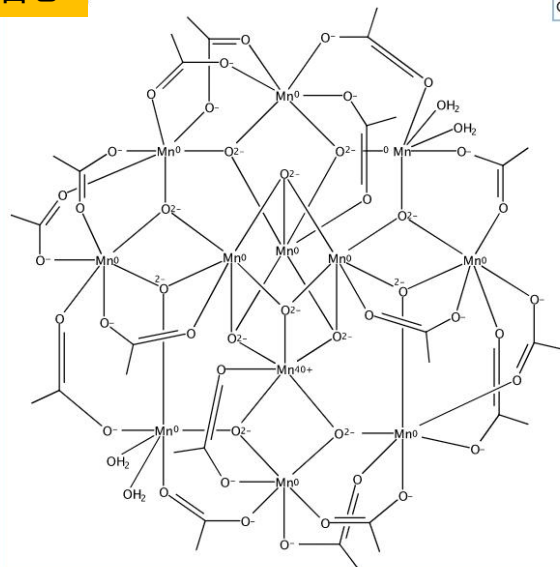
Manganese, hexadecakis[μ-(acetato-*O,O'*)]tetraaquadodeca-μ₃-
oxododeca-, compd. with acetic acid (1:2), tetrahydrate
Manganese, hexadecakis[μ-(acetato-*K,O,K'*)]tetraaquadodeca-μ₃-
oxododeca-, compd. with acetic acid (1:2), tetrahydrate (9CI)
Hexadecaacetatotetraaquadodecaoxododecamanganese-acetic acid
tetrahydrate (1:2)

Mn₁₂

Mn12 acetate

View more...

也可以获得反应信息



64-19-7
 $C_2H_4O_2$



CAS Registry Number: 76125-82-1

 View Substance Detail

Explore by Structure

Synthesize this...

Get Reactions where Substance is a

Product

Get Commercial Sources

Reactant

Get Regulatory Information

Reagent

Get References

Reactant/Reagent

Export as Image

Catalyst

Export as molfile

Solvent

Send to SciPlanner

Any Role

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

KMnO ₄	6
TEA chloride	2
110743-42-5	1
Ce(NH ₄) ₂ (NO ₃) ₆	1
H ₂ O	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)₁₂(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 reddrown. 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 [Ce₂Mn₁₀O₁₂(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)%.

METHODSNow™

Procedure

1. Slowly add solid (NH₄)₂[Ce(NO₃)₆] (0.28 g, 0.50 mmol) to a stirred solution of [Mn₁₁O₁₂(O₂CMe)₁₂(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

查找MOF的反应信息：

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⁻:κO⁻]][μ₃-[1,3,5-benzenetricarboxylato(3-)-κO⁻:κO⁻:κO⁻]]tri-

Coordination Compound

Density (Experimental)

Value: 0.879 g/cm³

Other Names

Copper, triqua[μ-[1,3,5-benzenetricarboxylato(3-)-κO⁻:κO⁻]][μ₃-[1,3,5-benzenetricarboxylato(3-)-κO⁻:κO⁻]]tri- (9CI)

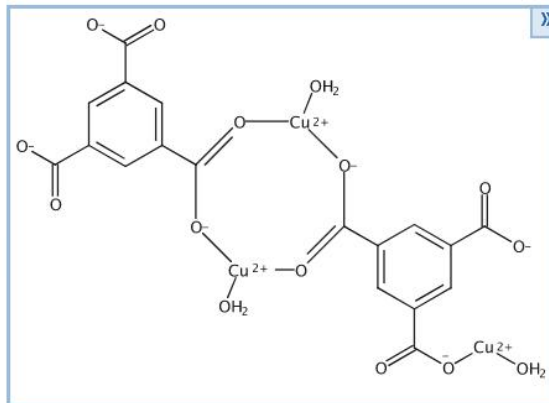
Triqua[μ-[1,3,5-benzenetricarboxylato(3-)-κO⁻:κO⁻]][μ₃-[1,3,5-benzenetricarboxylato(3-)-κO⁻:κO⁻:κO⁻]]tricopper

Basolite C 300

Cu-BTC

Cu₃BTC₂

View more...



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

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Send to SciPlanner

Product

Reactant

Reagent

Reactant/Reagent

Catalyst

Solvent

Any Role

EXPERIMENTAL PROPERTIES

EXPERIMENTAL SPECTRA

CAS REFERENCE ROLES

ADDITIONAL DETAILS

查看反应信息详情

Substance Identifier "222404-02-6" > substances (1) > 222404-02-6 > get reactions (222) > keep analysis "Experimental Procedure" (198)

REACTIONS Get References Tools Send to SciPlanner

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

0 of 198 Reactions Selected Page: 1 of 2

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

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

Overview

Steps/Stages

- 1.1 R:Cu(NO₃)₂, S:H₂O, S:MeOH, S:DMF, 10 min, 90°C

Notes

microwave irradiation, microwave synthesizer (500W) used, Reactants: 1, Reagents: 1, Solvents: 3, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Metal-Organic Frameworks with Incorporated Carbon Nanotubes: Improving Carbon Dioxide and Methane Storage Capacities by Lithium Doping
By Xiang, Zhonghua et al
From *Angewandte Chemie, International Edition*, 50(2), 491-494, S491/1-S491/17; 2011

METHODSNow™

Procedure

1. Sonicate the benzene-1,3,5-tricarboxylic acid (2.5 g) and copper nitrate hemihexahydrate (5 g) for 15 min in a 125 mL solvent consisting of equal parts of N,N-dimethylformamide (DMF), ethanol, and deionized water in a 300 mL wide mouth glass jar.
2. Place the jar inside laboratory microwave synthesizer (XH-MC-1, Xianghu Technology Co., Ltd.).

[View more...](#)
[View with MethodsNow](#)

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

Analyze by:

Solvent	
EtOH	143
H ₂ O	130
DMF	78
DMSO	7
MeOH	7
(CH ₂ OH) ₂	4
BuOH	3
174501-64-5	2
104371-26-8	1
111-30-8	1

[Show More](#)

已知配体查找MOF的合成信息

Structure Editor

Drag the reaction arrow to specify reaction direction.

首先可以只画出配体

reactant/reagent

OK

Cancel

Get reactions where the structure(s) are:

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

C H O S N P Cl Br F I Si

C₉H₆O₆ 210.14

在反应结果集中选择Analyze by Reagent, 找到相应金属盐

Reaction Structure structure variable only at spe... > reactions (7218)

REACTIONS **Analyze** Refine

Analyze by: Reagent

Et₃N 2942

F₃CCO₂H 2596

ETN(Pr-*i*)₂ 2542

132705-51-2 2111

Na ascorbate 2034

CuSO₄ 2024

K₂CO₃ 1941

NaHCO₃ 1910

NaN₃ 1902

H₂O 1694

Show More

Get References Tools

Group by: No Grouping Sort by: Relevance

0 of 7218 Reactions Selected

1. View Reaction Detail Link

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

100%

Overview
Steps/Stages
1.1 R:CuCl₂, R:Propylene oxide, R:

S:H₂O, 5 min

2. View Reaction Detail Link

Analyze - Reagent

682 Items 2 Selected Export

Sort by: Natural Order Page: 8 of 14

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

<input type="checkbox"/>	Cu	426
<input checked="" type="checkbox"/>	Cu acetylacetonate	1
<input checked="" type="checkbox"/>	Cu(BF ₄) ₂	1
<input type="checkbox"/>	Cu(CF ₃ SO ₂) ₂	1
<input type="checkbox"/>	Cu(ClO ₄) ₂	15
<input type="checkbox"/>	Cu(NO ₂) ₂	267
<input type="checkbox"/>	Cu(NO ₃) ₂ · 3H ₂ O	52
<input type="checkbox"/>	Cu(OAc) ₂	73
<input type="checkbox"/>	Cu(OAc) ₂ · H ₂ O	20
<input type="checkbox"/>	Cu(OH) ₂	17

Apply Cancel

获得相应反应信息

Analyze Refine

Group by: No Grouping Sort by: Relevance

0 of 7218 Reactions Selected

1. View Reaction Detail [Link](#)

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

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

100%

100%

Overview

Steps/Stages

1.1 R:CuCl₂, R:Propylene oxide, R:

Si:H₂O, 5 min

2. View Reaction Detail [Link](#)

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

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

100%

100%

Reagent

Et ₃ N	2942
F ₂ CCO ₂ H	2596
EtN(Pr-) ₂	2542
132705-51-2	2111
Na ascorbate	2034
CuSO ₄	2024
K ₂ CO ₃	1941
NaHCO ₃	1910
NaN ₃	1902
H ₂ O	1694

Show More

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