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- 反应相关信息的获取策略
 - 反应的获取方法
 - 反应结果分析、精炼及详情
 - 如何高效获取反应详情 (Synthetic Methods)
- 如何高效获取分析方法详情 (CAS Analytical Methods)

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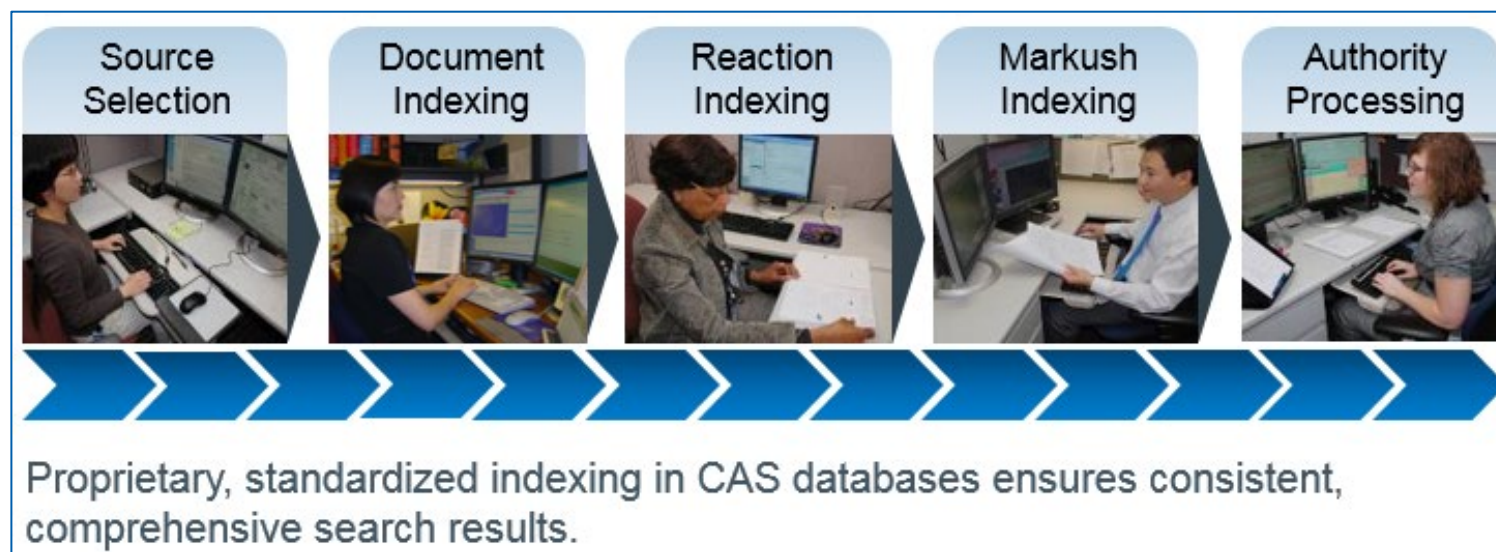
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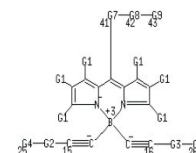
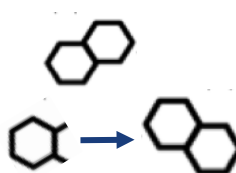
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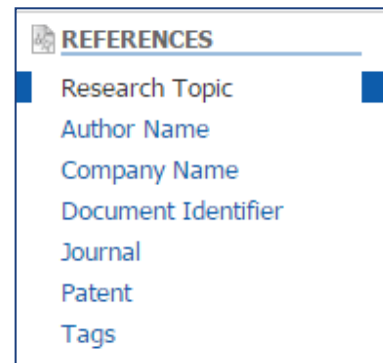
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☐ 1. Carbon nanotube and preparation method and application thereof [Machine Translation].
Quick View Other Sources
By Ding, Bing; Chen, Shuang; Zhang, Xiaogang; Lin, Qingyang; Hu, Ben
From Faming Zhuanli Shenqing (2021), CN 112750627 A 20210504. | Language: Chinese, Database: CAPLUS
[Machine Translation of Descriptors]. The invention provides a carbon nano tube and a prepn. method and application thereof, and belongs to the tech. field of carbon nano materials.The prepn. method of the carbon nano tube provided by the invention comprises the following steps:Carrying out ball milling on the transition metal salt, the phenolic compd. and the nonionic block copolymer to obtain a gel precursor material;Carbonizing the gel-like precursor material in a protective atm., and then washing to obtain the carbon nanotube.The prepn. method of the carbon nanotube based on the solid-pha...

☐ 2. Simultaneous improvements in conversion and properties of molecularly controlled CNT fibres
Quick View Other Sources
By Mikhailchian, Anastasiia; Vila, Maria; Arevalo, Luis; Vilatela, Juan J.
From Carbon (2021), 179, 417-424. | Language: English, Database: CAPLUS
Fibers of ultralong and aligned carbon nanotubes (CNT) have axial properties above ref. engineering materials, proving to be exceptional materials for application in structural composites, energy storage and other devices. For CNT fibers produced by direct spinning from floating catalyst chem. vapor deposition (FCCVD), a scaled-up method, the challenge is to simultaneously achieve high process conversion and high-performance properties. This work presents a parametric study of the CNT fiber spinning process by establishing the relation between synthesis conditions, mol. compn. (i.e. CNT type...

☐ 3. Energy storage battery for new energy vehicle [Machine Translation].
Quick View Other Sources
By Gong, Geling; Tang, Bing
From Faming Zhuanli Shenqing (2021), CN 112713276 A 20210427. | Language: Chinese, Database: CAPLUS
[Machine Translation of Descriptors]. The invention relates to an energy storage battery for a new energy vehicle, which comprises a pos. electrode, a neg. electrode and a solid electrolyte positioned between the pos. electrode and the neg. electrode, wherein the pos. electrode comprises a pos. electrode active material with a core-shell structure, the core is a pos. electrode active particle, and the shell comprises a first coating coated on the surface of the pos. electrode active particle and a second coating coated on the surface of the first coating;The first coating is a mixed layer of ...

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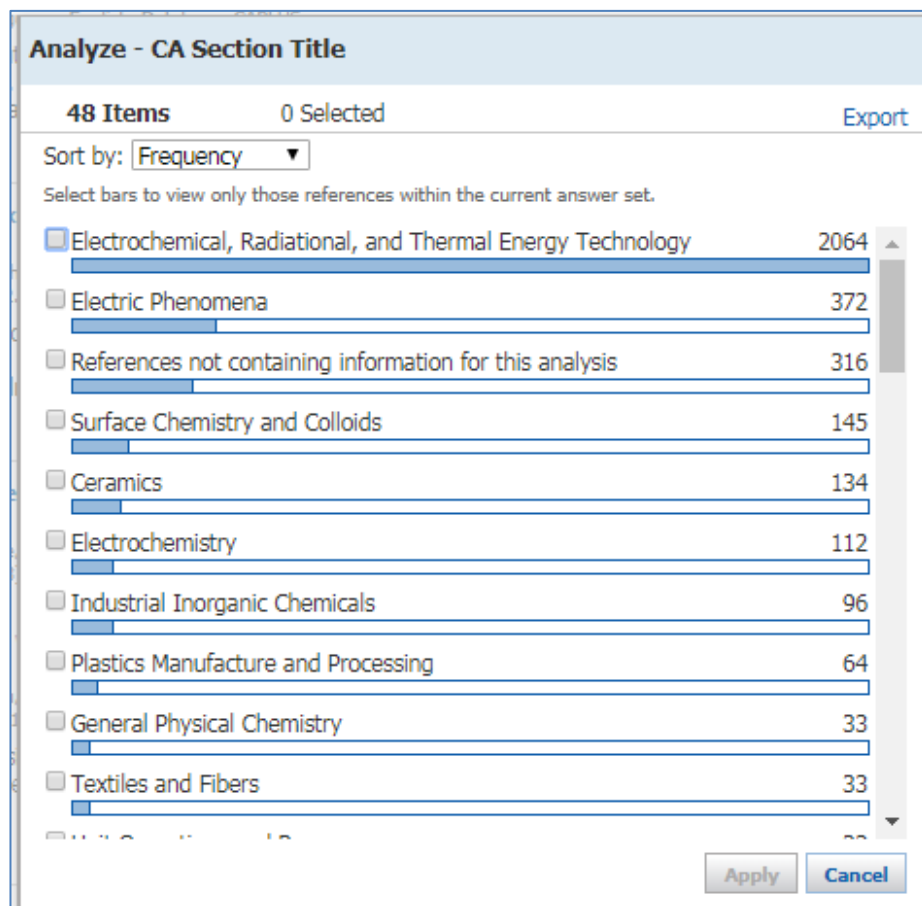
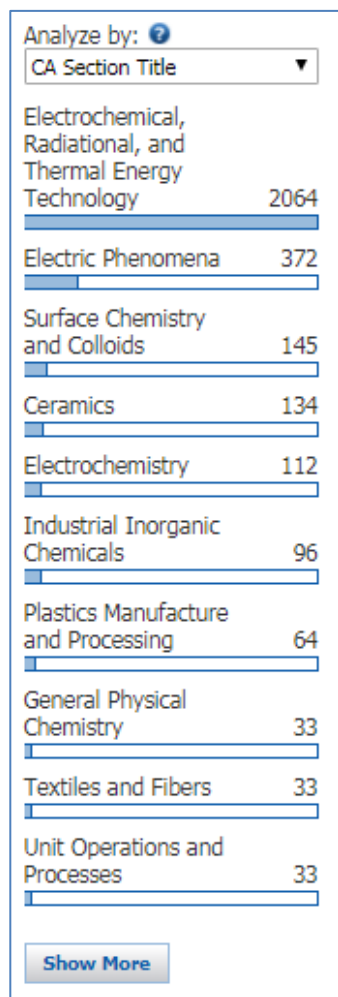
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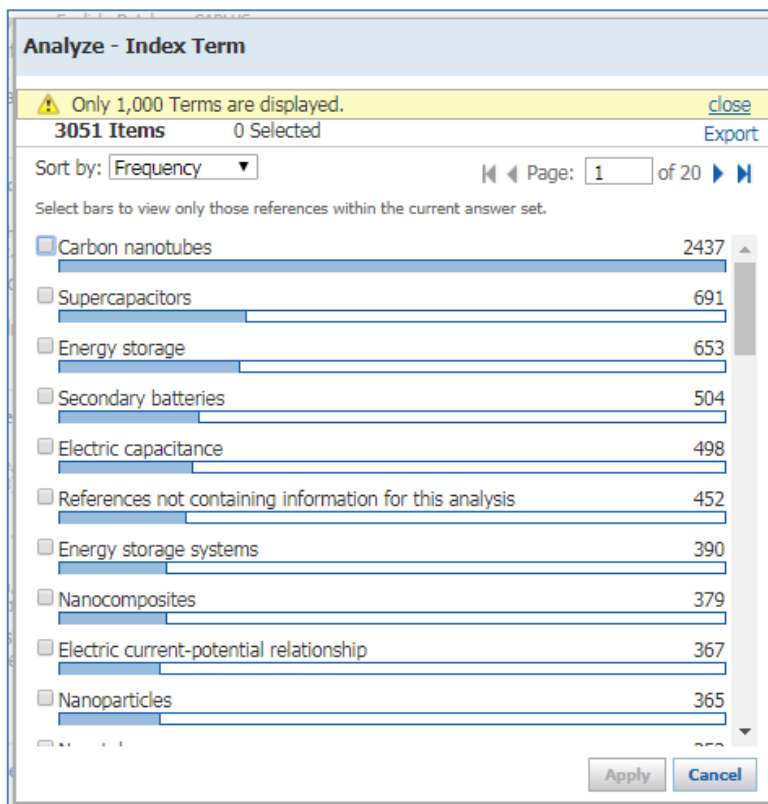
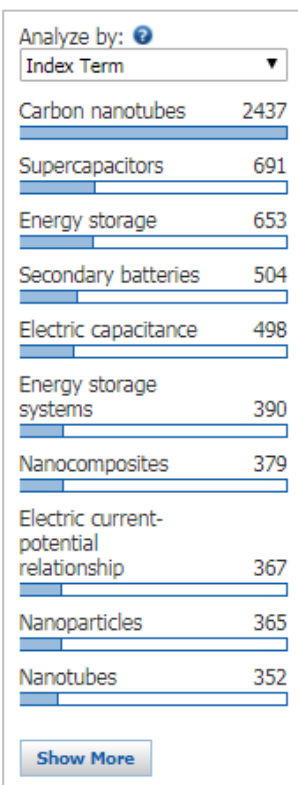
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secondary battery

Examples:
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1. Attempts to improve the energy capacity of capacitive electrochemical energy storage devices
Quick ViewOther Sources
By Yu, Lin-po; Chen, George Z.
From Dianhuaxue (2017), 23(5), 533-547. | Language: English, Database: CAPLUS
A review selected literatures from the authors' research group on the development of capacitive electrochem. energy storage (EES) devices, focusing on supercapacitors and supercapatteries at both the electrode material level and device level. Electronically conducting polymers (ECPs) and transition metal oxides (TMOs) composited with carbon nanotubes (CNTs) were found to be able to improve the capacitance performance as capacitive faradaic storage electrode. Carbon materials, like activated carbon (Act-C) and carbon black, were used to fabricate non-faradaic capacitive storage electrode. It...

2. 3D Porous Mixed-Valent Manganese Oxide Nanosheets Electrodeposited onto Flexible Ag-CNT Textiles for Highly Improved Capacitive Performances
Quick ViewOther Sources
By Ko, Wen-Yin; Chung, Chia-Ching; Lin, Kuan-Jiuh
From ChemistrySelect (2017), 2(35), 11503-11512. | Language: English, Database: CAPLUS
A simple yet efficient one-pot ultrasonication process for the green prepn. of a silver-carbon nanotube (Ag-CNT) ink, which was then used to fabricate conductive flexible thin films by a simple immersion process, is reported. A novel three-dimensional (3D) porous, hierarchical Ag-MnO_x-CNT nanocomposite was synthesized by electrodeposition of manganese oxide (MnO₂) nanosheets composed of MnO₂ and Mn₂O₄ onto the Ag-CNT films. The unique Ag-MnO_x-CNT electrode showed a specific capacitance of 842 F/g at 1 A/g and excellent charge-discharge cycling stability, with a capacitance retention of 148% ...

3. Stretchable Electronics: Stretchable Electrode Based on Laterally Combed Carbon Nanotubes for Wearable Energy Harvesting and Storage Devices (Adv. Funct. Mater. 48/2017)
Quick ViewOther Sources
By Hong, Seungki; Lee, Jongsu; Do, Kyungsik; Lee, Minbaek; Kim, Ji Hoon; Lee, Sangkyu; Kim, Dae-Hyeon
From Advanced Functional Materials (2017), 27(48), n/a. | Language: English, Database: CAPLUS

4. Composite "LiCl/MWCNT" as advanced water sorbent for thermal energy storage: Sorption dynamics
Quick ViewOther Sources
By Grekova, Alexandra D.; Gordeeva, Larisa G.; Lu, Zisheng; Wang, Ruzhu; Aristov, Yuri I.
From Solar Energy Materials & Solar Cells (2018), 176, 273-279. | Language: English, Database: CAPLUS
Sorption heat storage (SHS) is a promising technol. towards efficient use of renewable energy sources. Composite materials based on hygroscopic salts have a high potential for SHS in term of the heat storage capacity. Recently, a new sorbent "LiCl confined to Multi-Wall Carbon NanoTubes (MWCNT)" with enhanced storage capacity (1.7 kJ/g) has been suggested for SHS. This work addresses the dynamic study of water sorption on this material under operating conditions of a daily heat storage cycle. The study consists of three parts: (1) shaping the LiCl/MWCNT composite as grains (GP) and pellets...

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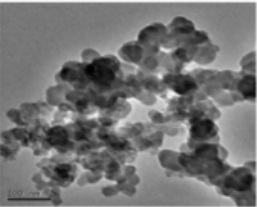
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1. Composite electrode material, preparation method and application thereof

Quick View PATENTPAK

By Wang, Yue; Liang, Minghui; Jiang, Peng; Zhang, Xianfeng; Wei, Hang; Li, Xin; Liu, Yongguang
From Faming Zhuanli Shenqing (2017), CN 107359054 A 20171117. | Language: Chinese, Database: CAPLUS



The title method comprises mixing coordination dissolved metal oxide and/or hydroxide soln. with **carbon** material, through evapn. of ligand soln., in situ growing metal oxide and/or metal hydroxide on **carbon** material surface, and obtaining the composite electrode material. The method is simple to operate, has low cost, is green and environmental protection, without aftertreatment, and provides possibility for the industrialized scale operation of electrode materials. The composite electrode material prepd. by the method of the invention has excellent property in terms of power **storage**. Such ...

2. Lithium ion battery cathode material and preparation method thereof

Quick View PATENTPAK

By Mao, Fanghui; Yang, Yujie
From Faming Zhuanli Shenqing (2017), CN 107275597 A 20171020. | Language: Chinese, Database: CAPLUS

The invention belongs to the field of **energy storage**. The title lithium ion **battery** cathode material has a particle of D1 of 1 μm -200 μm . The lithium ion **battery** cathode material has **secondary** particle structure. The **secondary** particle comprises primary particles and **secondary** particles from the electron conduction components. The primary particle diam. has $D2 \leq 0.5D1$. The primary particle diam. and the graphene sheet layer are uniformly distributed. Graphene is porous. The porous graphene layer has thickness of $h1 \leq 100 \text{ nm}$. The pore diam. is D3. The continuous portion between two hol...

3. A lithium-carbon nanotube composite for stable lithium anodes

Quick View Other Sources

By Wang, Yalong; Shen, Yanbin; Du, Zhaolong; Zhang, Xiaofeng; Wang, Ke; Zhang, Haiyang; Kang, Tuo; Guo, Feng; Liu, Chenghao; Wu, Xiaodong; et al
From Journal of Materials Chemistry A: Materials for Energy and Sustainability (2017), 5(45), 23434-23439. | Language: English, Database: CAPLUS

Li metal has been considered as the ultimate anode material for high-d. electrochem. **energy storage** technol. because of its extremely high specific capacity (3860 mAh/g), lowest redox potential, and ability to enable **battery** chemistries with Li free cathode materials. However, the practical application of Li metal anodes is still prohibited by its low Coulombic efficiency (CE) and growth of Li dendrites during Li dissoln./deposition. We report the prepn. of a Li **C nanotube** (Li-CNT) composite via a facile and scalable molten impregnation method. When used as an anode material, the Li-CNT com...

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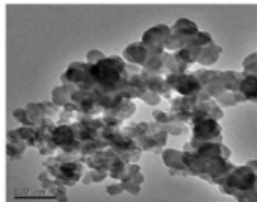
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1. Composite electrode material, preparation method and application thereof

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By Wang, Yue; Liang, Minghui; Jiang, Peng; Zhang, Xianfeng; Wei, Hang; Li, Xin; Liu, Yongguang
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By Mao, Fanghui; Yang, Yujie
From Faming Zhuanli Shenqing (2017), CN 107275597 A 20171020. | Language: Chinese, Database: CAPLUS

The invention belongs to the field of **energy storage**. The title lithium ion **battery** cathode material has a particle of D1 of 1 μm-200 μm. The lithium ion **battery** cathode material has **secondary** particle structure. The **secondary** particle comprises primary particles and **secondary** particles from the electron conduction components. The primary particle diam. has $D2 \leq 0.5D1$. The primary particle diam. and the graphene sheet layer are uniformly distributed. Graphene is porous. The porous graphene layer has thickness of $h1 \leq 100$ nm. The pore diam. is D3. The continuous portion between two hol...

3. A lithium-carbon nanotube composite for stable lithium anodes

Quick View Other Sources

By Wang, Yalong; Shen, Yanbin; Du, Zhaolong; Zhang, Xiaofeng; Wang, Ke; Zhang, Haiyang; Kang, Tuor; Guo, Feng; Liu, Chenghao; Wu, Xiaodong; et al
From Journal of Materials Chemistry A: Materials for Energy and Sustainability (2017), 5(45), 23434-23439. | Language: English, Database: CAPLUS

Li metal has been considered as the ultimate anode material for high-d. electrochem. **energy storage** technol. because of its extremely high specific capacity (3860 mAh/g), lowest redox potential, and ability to enable **battery** chemistries with Li free cathode materials. However, the practical application of Li metal anodes is still prohibited by its low Coulombic efficiency (CE) and growth of Li dendrites during Li dissoln./deposition. We report the prepn. of a Li **C nanotube** (Li-CNT) composite via a facile and scalable molten impregnation method. When used as an anode material, the Li-CNT com...

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REFERENCES ⓘ

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Carbon black 159

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Energy storage systems 108

Battery cathodes 102

Lithium-ion secondary batteries 91

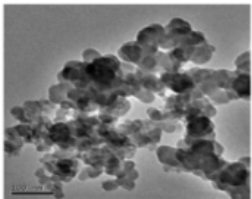
Battery electrodes 81

Show More

☐ 1. Composite electrode material, preparation method and application thereof

Quick View PATENTPAK ▾

By Wang, Yue; Liang, Minghui; Jiang, Peng; Zhang, Xianfeng; Wei, Hang; Li, Xin; Liu, Yongguang
From Faming Zhuanli Shenqing (2017), CN 107359054 A 20171117. | Language: Chinese, Database: CAPLUS



The title method comprises mixing coordination dissolved metal oxide and/or hydroxide soln. with **carbon** material, through evapn. of ligand soln., in situ growing metal oxide and/or metal hydroxide on **carbon** material surface, and obtaining the composite electrode material. The method is simple to operate, has low cost, is green and environmental protection, without aftertreatment, and provides possibility for the industrialized scale operation of electrode materials. The composite electrode material prep'd. by the method of the invention has excellent property in terms of power **storage**. Such ...

☐ 2. Lithium ion battery cathode material and preparation method thereof

Quick View PATENTPAK ▾

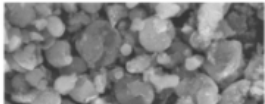
By Mao, Fanghui; Yang, Yujie
From Faming Zhuanli Shenqing (2017), CN 107275597 A 20171020. | Language: Chinese, Database: CAPLUS

The invention belongs to the field of **energy storage**. The title lithium ion **battery** cathode material has a particle of D1 of 1 μm-200 μm. The lithium ion **battery** cathode material has **secondary** particle structure. The **secondary** particle comprises primary particles and **secondary** particles from the electron conduction components. The primary particle diam. has $D2 \leq 0.5D1$. The primary particle diam. and the graphene sheet layer are uniformly distributed. Graphene is porous. The porous graphene layer has thickness of $h1 \leq 100$ nm. The pore diam. is D3. The continuous portion between two hol...

☐ 3. Micro-nano structuralized carbon silicon composite microsphere and preparation method and application thereof

Quick View PATENTPAK ▾

By Li, Xianglong; Zhang, Xinghao; Zhi, Linjie
From Faming Zhuanli Shenqing (2017), CN 107240677 A 20171010. | Language: Chinese, Database: CAPLUS



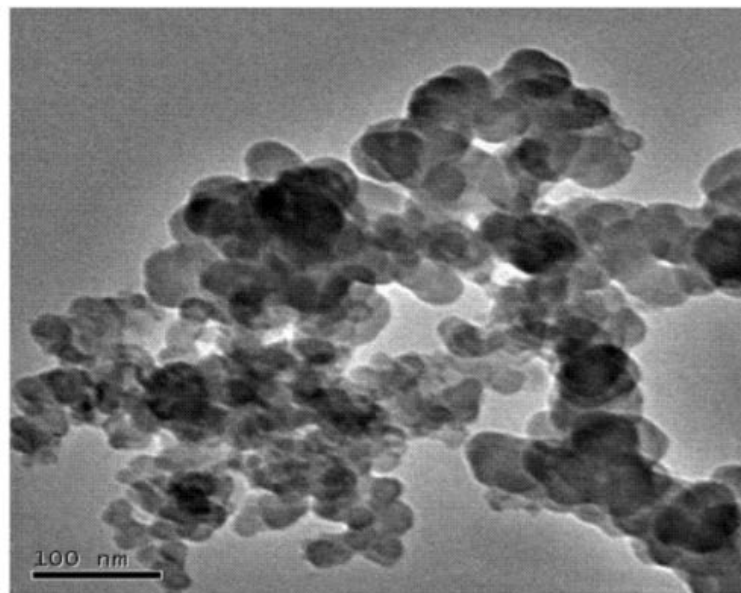
The method comprises using spray drying method for compounding and micro-nano structuralization of silica nanoparticle, protective agent and **carbon** nanomaterial, carrying out heat treatment under non-oxidn. atm. to prep. **carbon**/silica composite microsphere, and using metal thermal redn. method to obtain micro-nano structuralized **carbon** silicon composite microsphere. The prepn. method of the present invention has low cost, simple technique, and low **energy** consumption. The **carbon** silicon nanoparticle of the obtained micro-nano structuralized **carbon** silicon composite microsphere has core-hollow...

文献详情

1. Composite electrode material, preparation method and application thereof

By: Wang, Yue; Liang, Minghui; Jiang, Peng; Zhang, Xianfeng; Wei, Hang; Li, Xin; Liu, Yongguang
Assignee: National Center for Nanoscience and Technology, Peop. Rep. China

The title method comprises mixing coordination dissolved metal oxide and/or hydroxide soln. with carbon material, through evapn. of ligand soln., in situ growing metal oxide and/or metal hydroxide on carbon material surface, and obtaining the composite electrode material. The method is simple to operate, has low cost, is green and environmental protection, without aftertreatment, and provides possibility for the industrialized scale operation of electrode materials. The composite electrode material prep. by the method of the invention has excellent property in terms of power storage. Such as the nickel hydroxide-activated carbon composite electrode material with 5% of loading amt. prep. by the method of the invention under sweep speed of 5 mV/s, the complete electrode specific discharge capacity reaches 294 F/g, and the active substance specific capacity is up to 4917 F/g.



QUICK LINKS

0 Tags, 0 Comments

PATENT INFORMATION

Nov 17, 2017
CN 107359054
A

APPLICATION

May 9, 2016
CN 2016-10301475

PRIORITY

May 9, 2016
CN 2016-10301475

SOURCE

Faming Zhuanli Shenqing
13pp.
Patent
2017
CODEN:CNXXEV

ACCESSION NUMBER

2017:1811624
CAN168:7562
CAPLUS

LANGUAGE

Chinese

Patent Information

Patent No.	Kind	Language	Date	Application No.	Date
CN 107359054	A		Nov 17, 2017	CN 2016-10301475	May 9, 2016
Priority Application					
CN 2016-10301475			May 9, 2016		

文献详情

Indexing

学科领域

重要的物质列表

Electrochemical, Radiational, and Thermal Energy Technology (Section52-2)

Concepts

Batteries

Electrodes

Energy storage systems

Lithium-ion secondary batteries

Supercapacitors

Carbon nanotubes

Energy storage

Evaporation

Nanostructured materials

composite electrode material, prepn. method and application thereof

Carbon fibers

composite electrode material, prepn. method and application thereof

Physical, engineering or chemical process; Properties; Technical or engineered material use; Process; Uses

标准概念词列表

物质CAS RN,
物质名称

Substances

7440-44-0 Activated carbon, uses

Page 2 in PATENTPAK

activated; composite electrode material, prepn. method and application thereof

Physical, engineering or chemical process; Properties; Technical or engineered material use; Process; Uses

1313-99-1 Nickel oxide, uses

Page 2 in PATENTPAK

1314-13-2 Zinc oxide, uses

Page 2 in PATENTPAK

1335-25-7 Lead oxide

Page 2 in PATENTPAK

1344-69-0 Copper hydroxide

Page 2 in PATENTPAK

1344-70-3 Copper oxide

Page 2 in PATENTPAK

11104-61-3 Cobalt oxide

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11113-84-1 Ruthenium oxide

Page 2 in PATENTPAK

11129-60-5 Manganese oxide

Page 2 in PATENTPAK

12054-48-7 Nickel hydroxide

Page 2 in PATENTPAK

12626-88-9 Manganese hydroxide

Page 2 in PATENTPAK

12645-46-4 Iridium oxide

Page 2 in PATENTPAK

12672-51-4 Cobalt hydroxide

Page 2 in PATENTPAK

12673-77-7 Silver hydroxide

Page 2 in PATENTPAK

19783-14-3 Lead hydroxide

Page 2 in PATENTPAK

20427-58-1 Zinc hydroxide

Page 2 in PATENTPAK

20667-12-3 Silver oxide

Page 2 in PATENTPAK

56321-86-9 Ruthenium hydroxide

Page 2 in PATENTPAK

57425-17-9 Iridium hydroxide

Page 2 in PATENTPAK

composite electrode material, prepn. method and application thereof

Physical, engineering or chemical process; Properties; Technical or engineered material use; Process; Uses

74-89-5 Methylamine, uses

Page 2 in PATENTPAK

物质功能描述

定位信息

CAS PatentPak: 高效的专利工作流程解决方案

CAS Solutions

SciFinder

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A CAS SOLUTION

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ZOOM

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Key Substances in Patent

CAS RN 57-48-7

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Analyst Markup Locations (1)

page 2

CAS RN 69-79-4

Search in SciFinder | View Detail

Analyst Markup Locations (1)

page 2

CN 107240677 A

权 利 要 求 书

1/2 页

1. 一种微纳结构化碳硅复合微球的制备方法, 其特征在于, 所述方法包括如下步骤:
以二氧化硅颗粒与保护剂的混合溶液作为喷雾干燥的前驱体溶液, 进行喷雾干燥并热处理, 制备得到微纳结构化碳/二氧化硅复合微球, 然后, 通过金属热还原法制备微纳结构化碳硅复合微球。

2. 如权利要求1所述的方法, 其特征在于, 所述保护剂为葡萄糖、蔗糖、果糖、麦芽糖、壳聚糖、柠檬酸、尿素、抗坏血酸、淀粉、蛋白质、明胶、阿拉伯胶、海藻酸盐、纤维素、酚醛树脂、聚偏二氟乙烯、聚氨基酸、聚乙烯吡咯烷酮、聚碳酸酯、聚乙烯醇、聚乙二醇、聚甲基丙烯酸甲酯、聚甲基丙烯酸乙酯、聚丙烯酸树脂、聚氯乙烯、聚丙烯腈、聚乳酸或聚苯乙烯中的任意一种或至少两种的混合物。

3. 如权利要求1或2所述的方法, 其特征在于, 所述二氧化硅颗粒为气相二氧化硅颗粒;
优选地, 所述二氧化硅颗粒的粒径为5nm-300nm;
优选地, 所述喷雾干燥的前驱体溶液中, 溶剂为水和/或有机溶剂;
优选地, 所述喷雾干燥的前驱体溶液中, 溶质的质量浓度为0.1%-60%, 优选为15%;
优选地, 所述二氧化硅和保护剂的质量比为1:(0.1-50);

无缝连接进行新的检索

Explore ▼ Saved Searches ▼ SciPlanner

Patent "CN107240677" > references (1)

REFERENCES

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

SUBSTANCES

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

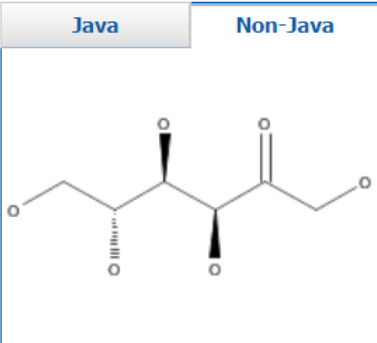
REACTIONS

- Reaction Structure

SUBSTANCES: CHEMICAL STRUCTURE ?

Structure Editor:

Java Non-Java



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Advanced Search

Search Type:

- ☐ Exact Structure
- ☒ Substructure
- ☐ Similarity

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文献检索小结：

- 主题检索时，使用介词 **in, with, of** 等作为连接词
- 根据检索要求选择合适的候选项
- 通过 **SciFinder** 的 **Analyze/Refine** 功能来缩小检索的范围
- 使用 **Categorize** 可以让系统来实现自动分类
- 充分利用文献详情中增值标引信息
- **CAS PatentPak** 高效获取专利中重要的化学信息

大纲

- CAS SciFinder介绍
- 文献相关信息的获取策略
 - 储能材料文献检索方法
 - 文献结果分析、精炼和详情
 - 如何高效阅读专利文献详情(CAS PatentPak)
- 物质相关信息的获取策略
 - 如何检索无机化合物、配位化合物和聚合物
 - 物质结果分析、精炼和详情
- 反应相关信息的获取策略
 - 反应的获取方法
 - 反应结果分析、精炼及详情
 - 如何高效获取反应详情 (Synthetic Methods)
- 如何高效获取分析方法详情 (CAS Analytical Methods)

物质检索的方法

- 物质检索方法
 - 结构式检索
 - 分子式检索
 - 理化性质检索
 - 物质标识符检索：化学名称，CAS RN
- 物质检索策略推荐
 - 有机化合物，天然产物：结构检索
 - 无机物，合金：分子式检索
 - 高分子化合物：分子式检索和结构检索



SUBSTANCES

Chemical Structure

Markush

Molecular Formula

Property

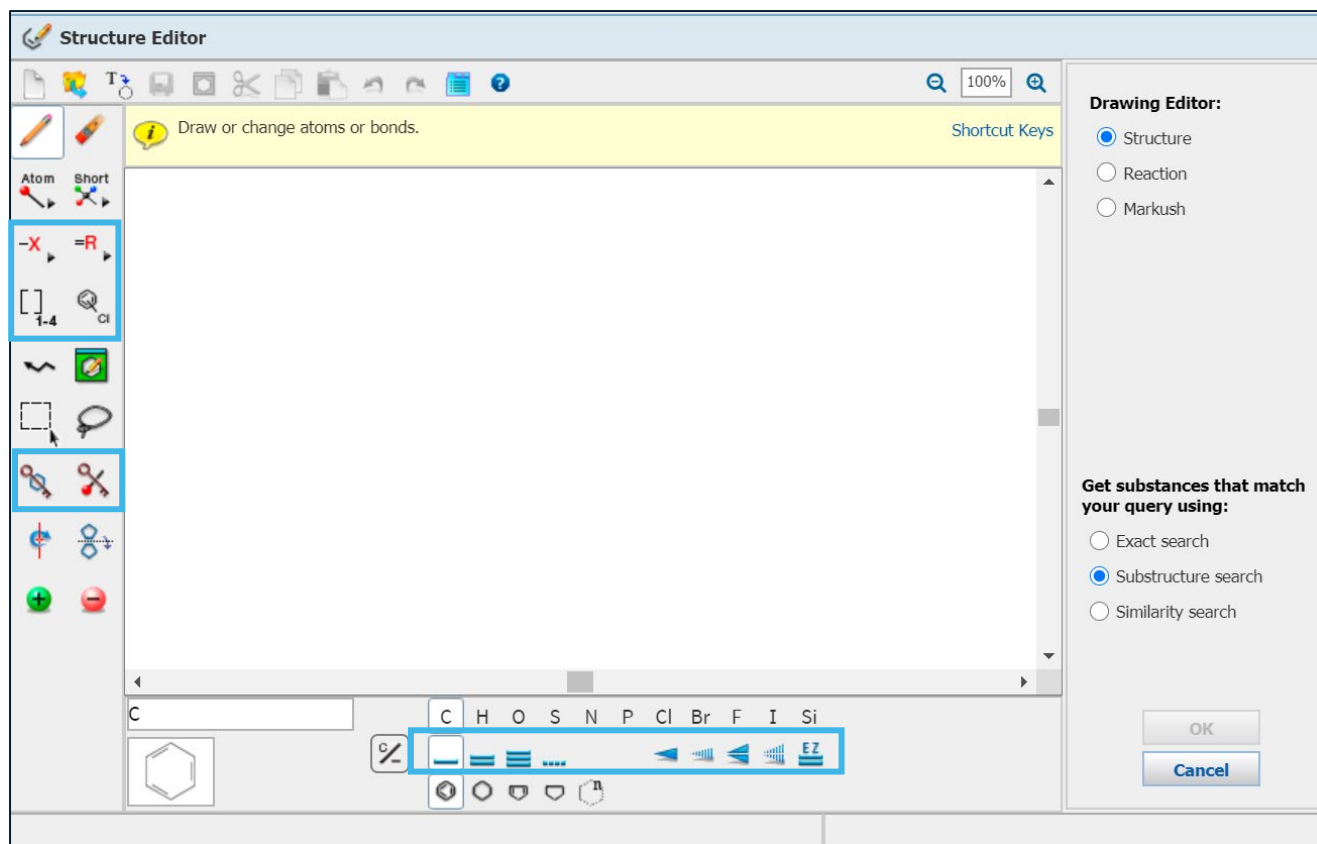
Substance Identifier



ACS
International



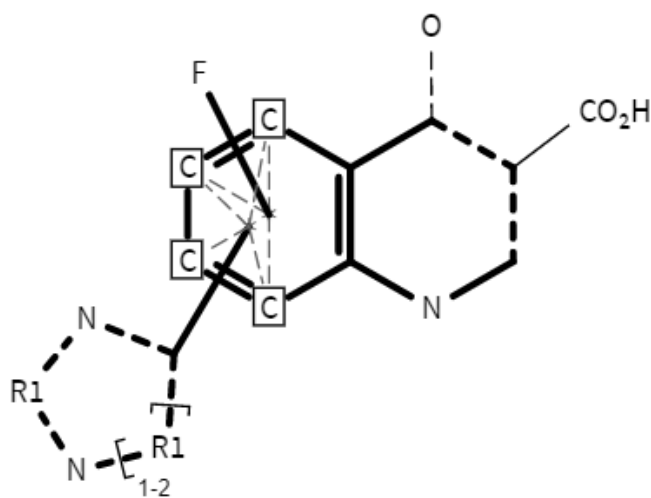
结构编辑器的使用



重要绘制工具注释

-  选择可变基团
-  自定义R基团
-  重复工具
-  取代位置可变
-  锁环工具
-  锁原子工具

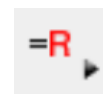
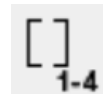
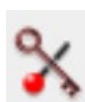
有机化合物: 通式结构的绘制



R1 = C, O

要求:

1. 两个环系不能与其他环 (系) 形成新的稠环 (系) 或桥环 (系) ;
2. 六元含氮环上可出现互变异构, 比如烯酮;
3. 六元碳环上有一个F取代和一个五至六元的饱和或非饱和杂环取代。
杂环的1,3位为N原子, R1为C或O;
4. 六元碳环上有且只有杂环和F取代, 且连接位点不确定。



根据分子式检索无机化合物

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

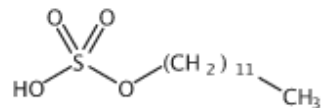
分子式输入需要遵守Hill排序规则:不含碳化合物,按元素符号的字母顺序排列;分子式为含碳化合物时,则“C”在前;如有氢则紧随其后,其它元素符号按字母顺序排在氢的后面

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)

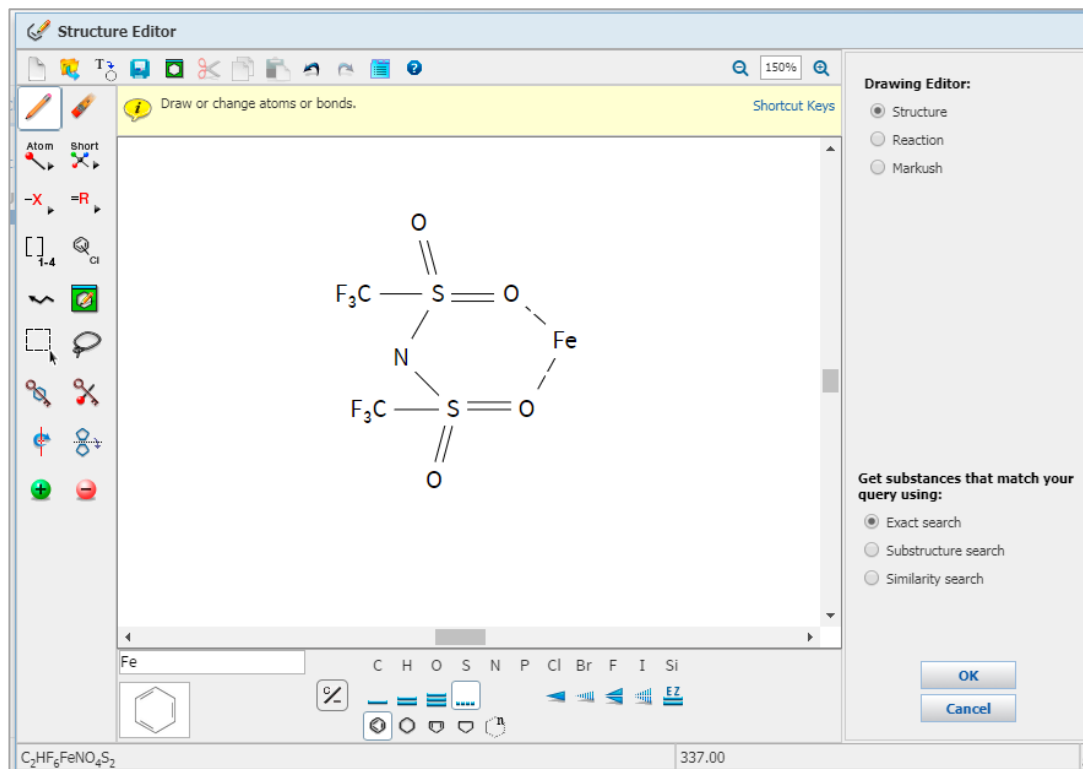
► **Key Physical Properties**

Regulatory Information

Spectra

Experimental Properties

根据络合物的结构来检索配位化合物



4. 1933513-70-2 (Component: 82113-65-3)

~3

$\bullet 1/2 \text{ Fe(II)}$

C₂H₆FeNO₄S₂ · 1/2 Fe
Methanesulfonamide, 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]-, iron(2+) salt (2:1)

5. 1912405-54-9

~0

1933513-70-2 (Component: 82113-65-3)
C₂H₆FeNO₄S₂ · 1/2 Fe

$\bullet 1/2 \text{ Fe(II)}$

C₂H₆FeNO₄S₂ · 1/2 Fe
Methanesulfonamide, 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]-, iron(2+) salt (2:1)

6. 1706814-99-4

~1

1706814-96-1
C₂H₆FeNO₄S₂ · 1/2 Fe H₁₂O₆
98837-98-0
C₂H₆FeNO₄S₂

15365-81-8
Fe H₁₂O₆

C₂H₆FeNO₄S₂ · 1/2 Fe H₁₂O₆ · 2 H₂O
INDEX NAME NOT YET ASSIGNED

根据配体结构和中心金属原子来检索配位化合物

REFERENCES

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

SUBSTANCES

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

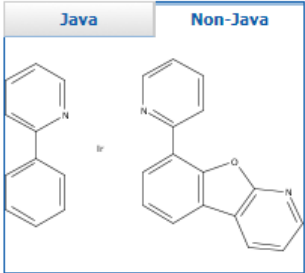
REACTIONS

- Reaction Structure

SUBSTANCES: CHEMICAL STRUCTURE

Structure Editor:

Java **Non-Java**



Search Type:

- ☒ Exact Structure
- ☐ Substructure
- ☐ Similarity

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ChemDraw
Launch a SciFinder substance or reactant
[More](#)

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Import CFX

Search

[Advanced Search](#) ☐ Always Show

Characteristics

- ☐ Single component
- ☐ Commercially available
- ☐ Included in references

Classes

- ☐ Alloys
- ☒ Coordination compounds
- ☐ Incompletely defined
- ☐ Mixtures

Chemical Structure exact with limiters > **substances (1)**

SUBSTANCES [Get References](#) [Get Reactions](#) [Get Commercial Sources](#) [Tools](#)

Analyze **Refine**

Analyze by: [?](#)
Substance Role

Preparation 1

Process 1

Properties 1

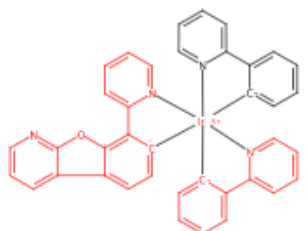
Uses 1

[Show More](#)

Sort by: CAS Registry Number

0 of 1 Substance Selected

1. **1609368-28-6**



C₃₈ H₂₅ Ir N₄ O
Iridium, [8-(2-pyridinyl-κN)benzofuro[2,3-b]pyridin-7-yl-κC]
bis[2-(2-pyridinyl-κN)phenyl-κC]-

通过聚合物的重复结构单元来检索聚合物

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Molecular Formula "(C2 H4 O)n C3 H6 O" > substances (4)

REFERENCES

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

SUBSTANCES

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

REACTIONS

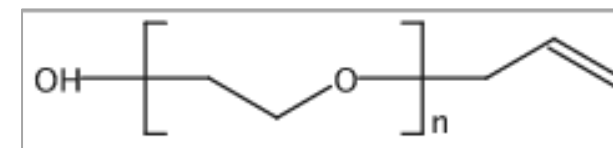
- Reaction Structure

SUBSTANCES: MOLECULAR FORMULA ?

(C2 H4 O)n C3 H6 O

Examples:
H4SiO4
(C3H6O.C2H4O)x

Search



通过聚合物的重复结构单元来检索聚合物

Molecular Formula "(C₂ H₄ O)_n C₃ H₆ O" > substances (4)

SUBSTANCES

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Analyze **Refine** Sort by: CAS Registry Number

0 of 4 Substances Selected

Analyze by: Substance Role

Preparation 4

Reactant or Reagent 3

Uses 3

Biological Study 2

Process 2

Properties 2

Analytical Study 1

Formation, Nonpreparative 1

Occurrence 1

Show More

1. 1500029-22-0

~2

(C₂ H₄ O)_n C₃ H₆ O
Poly(oxy-1,2-ethanediyl), α-(1-methylethenyl)-ω-hydroxy-

2. 191403-44-8

~5

(C₂ H₄ O)_n C₃ H₆ O
Poly(oxy-1,2-ethanediyl), α-1-propen-1-yl-ω-hydroxy-

3. 50856-25-2

~64 ~1

(C₂ H₄ O)_n C₃ H₆ O
Poly(oxy-1,2-ethanediyl), α-ethenyl-ω-methoxy-

4. 27274-31-3

~1386 ~14

(C₂ H₄ O)_n C₃ H₆ O
Poly(oxy-1,2-ethanediyl), α-2-propen-1-yl-ω-hydroxy-
[Regulatory Information](#)

通过聚合物的重复结构单元来检索聚合物

Explore ▾ Saved Searches ▾ SciPlanner

Molecular Formula "(C2 H4 O)n C3 H6 O" > substances (4) > 27274-31-3

REFERENCES

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

SUBSTANCES

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

REACTIONS

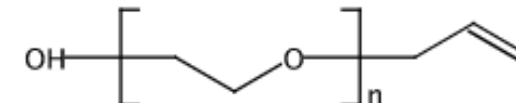
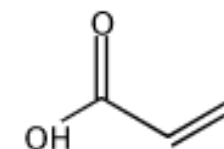
- Reaction Structure

SUBSTANCES: MOLECULAR FORMULA ?

(C3 H4 O2 . (C2 H4 O)n C3 H6 O)x

Examples:
H4SiO4
(C3H6O.C2H4O)x

Search



通过聚合物的重复结构单元来检索聚合物

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Sort by: CAS Registry Number

0 of 6 Substances Selected

1. 1580002-57-8

50856-25-2
(C₂ H₄ O)_n C₃ H₆ O

79-10-7
C₃ H₄ O₂

(C₃ H₄ O₂ · (C₂ H₄ O)_n C₃ H₆ O)_x
2-Propenoic acid, polymer with α-ethenyl-ω-methoxypoly(oxy-1,2-ethanediyl), graft

2. 1314225-78-9

191403-44-8
(C₂ H₄ O)_n C₃ H₆ O

79-10-7
C₃ H₄ O₂

(C₃ H₄ O₂ · (C₂ H₄ O)_n C₃ H₆ O)_x
2-Propenoic acid, polymer with α-1-propen-1-yl-ω-hydroxypoly(oxy-1,2-ethanediyl), graft

3. 1010818-79-7

27274-31-3
(C₂ H₄ O)_n C₃ H₆ O

79-10-7
C₃ H₄ O₂

(C₃ H₄ O₂ · (C₂ H₄ O)_n C₃ H₆ O)_x
2-Propenoic acid, polymer with α-2-propen-1-yl-ω-hydroxypoly(oxy-1,2-ethanediyl), block

4. 250591-73-2

50856-25-2
(C₂ H₄ O)_n C₃ H₆ O

79-10-7
C₃ H₄ O₂

(C₃ H₄ O₂ · (C₂ H₄ O)_n C₃ H₆ O)_x
2-Propenoic acid, polymer with α-ethenyl-ω-methoxypoly(oxy-1,2-ethanediyl) (9CI)

Regulatory Information

5. 185506-87-0

27274-31-3
(C₂ H₄ O)_n C₃ H₆ O

79-10-7
C₃ H₄ O₂

(C₃ H₄ O₂ · (C₂ H₄ O)_n C₃ H₆ O)_x
2-Propenoic acid, polymer with α-2-propen-1-yl-ω-hydroxypoly(oxy-1,2-ethanediyl), graft

Regulatory Information

6. 82850-00-8

27274-31-3
(C₂ H₄ O)_n C₃ H₆ O

79-10-7
C₃ H₄ O₂

(C₃ H₄ O₂ · (C₂ H₄ O)_n C₃ H₆ O)_x
2-Propenoic acid, polymer with α-2-propen-1-yl-ω-hydroxypoly(oxy-1,2-ethanediyl)

Regulatory Information

通过聚合物的重复结构单元来检索聚合物

The screenshot displays the ChemDraw software interface. The central workspace shows a chemical structure of a polymer repeat unit, which is a benzene ring fused to two thiophene rings, with two 'Ak' labels indicating the points of polymer chain extension. The left sidebar contains various drawing tools. The top status bar indicates 'Draw or change atoms or bonds.' and 'Shortcut Keys'. The right sidebar is divided into several sections:

- Drawing Editor:** Includes radio buttons for 'Structure' (selected), 'Reaction', and 'Markush'.
- Get substances that match your query using:** Includes radio buttons for 'Exact search', 'Substructure search' (selected), and 'Similarity search'.
- Advanced Search:** A list of search criteria with checkboxes:
 - X Any halogen
 - M Any metal
 - A Any atom except H
 - Q Any atom except C or H
 - Ak Any alkyl chain (highlighted)
 - Cy Any cycle
 - Cb Any carbocycle
 - Hy Any heterocycle
- Advanced Search (Always Show):** A section with checkboxes for various characteristics, classes, and studies:
 - Characteristics:** Single component (checked), Commercially available, Included in references.
 - Classes:** Alloys, Coordination compounds, Incompletely defined, Mixtures, Polymers (checked), Organics, and others not listed.
 - Studies:** Analytical, Biological, Preparation, Reactant or reagent.

The bottom status bar shows the chemical formula 'Ak' and a list of elements: C, H, O, S, N, P, Cl, Br, F, I, Si.

通过聚合物的重复结构单元来检索聚合物

SUBSTANCES ?

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Analyze Refine

Sort by: CAS Registry Number

0 of 134 Substances Selected

Analyze by: Substance Role

Uses 101

Preparation 84

Properties 75

Process 29

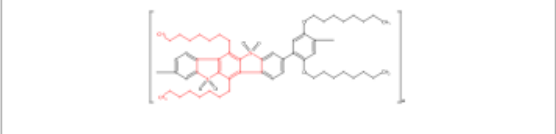
Prophetic in Patents 3

Reactant or Reagent 3

Occurrence 1

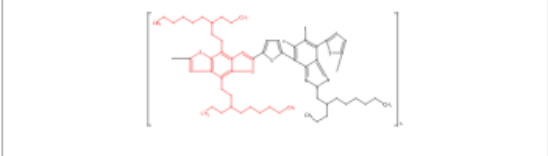
Show More

1. 2096989-39-6



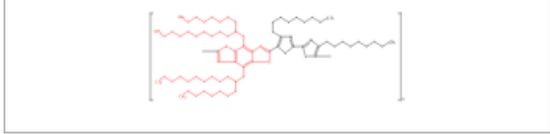
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INDEX NAME NOT YET ASSIGNED

2. 2089459-95-8



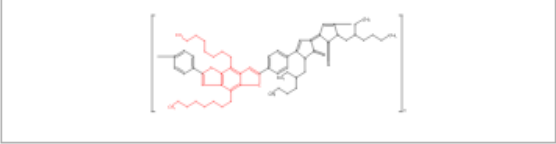
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INDEX NAME NOT YET ASSIGNED

3. 2056259-78-8



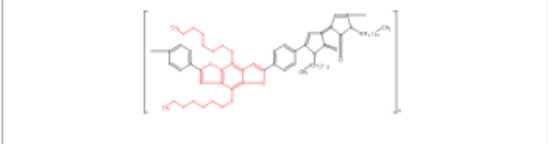
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INDEX NAME NOT YET ASSIGNED

4. 1974335-87-9



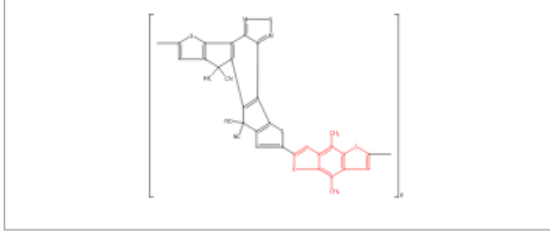
$(C_{62}H_{80}N_2O_2S_2)_n$
INDEX NAME NOT YET ASSIGNED

5. 1974335-85-7



$(C_{70}H_{96}N_2O_2S_2)_n$
INDEX NAME NOT YET ASSIGNED

6. 1909267-21-5



$(C_{32}H_{10}N_6S_5)_n$
INDEX NAME NOT YET ASSIGNED

通过聚合物的重复结构单元来检索聚合物

SUBSTANCES

Analyze Refine

Sort by: CAS Registry Number

0 of 134 Substances Selected

Refine by:

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

Structure Editor:

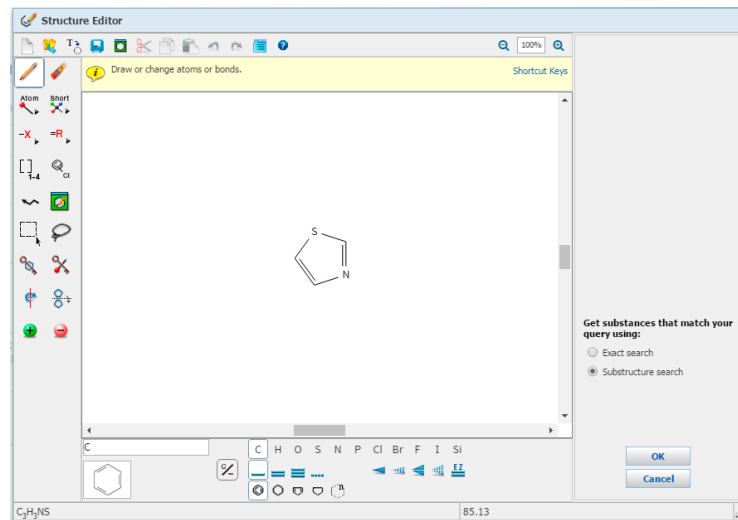
Java Non-Java

Click image to change structure or view detail.
Search type: **Substructure**

Only retrieve substances that:

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- ☐ Are a single component
- ☐ Are in specific substance


<p>1. 2096989-39-6 </p> <p>~1 </p> <p>(C₅₆ H₇₆ O₆ S₂)_n INDEX NAME NOT YET ASSIGNED</p>	<p>2. 2089459-95-8 </p> <p>~1 </p> <p>(C₅₉ H₇₉ F₂ N₃ S₄)_n INDEX NAME NOT YET ASSIGNED</p>	<p>3. 2056259-78-8 </p> <p>~1 </p> <p>(C₇₄ H₁₂₂ N₂ S₄)_n INDEX NAME NOT YET ASSIGNED</p>
<p>4. 1974335-87-9 </p> <p>~1 </p> <p>(C₆₂ H₈₀ N₂ O₂ S₂)_n INDEX NAME NOT YET ASSIGNED</p>	<p>5. 1974335-85-7 </p> <p>~1 </p> <p>(C₇₀ H₉₆ N₂ O₂ S₂)_n INDEX NAME NOT YET ASSIGNED</p>	<p>6. 1909267-21-5 </p> <p>~1 </p> <p>(C₃₂ H₁₀ N₆ S₅)_n INDEX NAME NOT YET ASSIGNED</p>
<p>7. 1909267-20-4 </p> <p>~1 </p>	<p>8. 1909267-19-1 </p> <p>~1 </p>	<p>9. 1909267-18-0 </p> <p>~1 </p>



通过聚合物的重复结构单元来检索聚合物

☐ Property Availability
☐ Property Value
☐ Reference Availability
☐ Atom Attachment

Structure Editor:

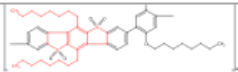
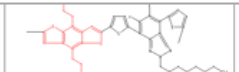
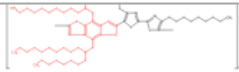

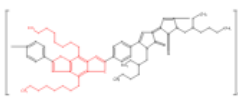

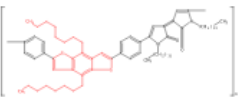

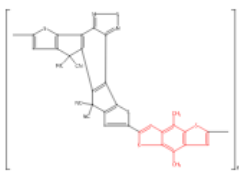

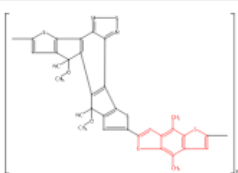

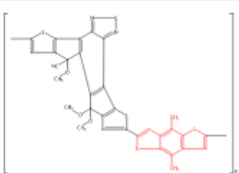

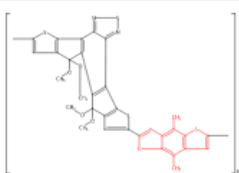


Click image to change structure or view detail.

Search type: **Substructure**

Only retrieve substances that:

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

 $(C_{66} H_{76} O_6 S_2)_n$ INDEX NAME NOT YET ASSIGNED	 $(C_{59} H_{79} F_2 N_3 S_4)_n$ INDEX NAME NOT YET ASSIGNED	 $(C_{74} H_{122} N_2 S_4)_n$ INDEX NAME NOT YET ASSIGNED
<input type="checkbox"/> 4. 1974335-87-9 🔍 ~1   $(C_{62} H_{80} N_2 O_2 S_2)_n$ INDEX NAME NOT YET ASSIGNED	<input type="checkbox"/> 5. 1974335-85-7 🔍 ~1   $(C_{70} H_{96} N_2 O_2 S_2)_n$ INDEX NAME NOT YET ASSIGNED	<input type="checkbox"/> 6. 1909267-21-5 🔍 ~1   $(C_{32} H_{10} N_6 S_5)_n$ INDEX NAME NOT YET ASSIGNED
<input type="checkbox"/> 7. 1909267-20-4 🔍 ~1   $(C_{32} H_{16} N_4 O_2 S_5)_n$ INDEX NAME NOT YET ASSIGNED	<input type="checkbox"/> 8. 1909267-19-1 🔍 ~1   $(C_{32} H_{19} N_3 O_3 S_5)_n$ INDEX NAME NOT YET ASSIGNED	<input type="checkbox"/> 9. 1909267-18-0 🔍 ~1   $(C_{32} H_{22} N_2 O_4 S_5)_n$ INDEX NAME NOT YET ASSIGNED

通过聚合物的重复结构单元来检索聚合物

Chemical Structure substructure with limiters > substances (134) > refine "substructure" (5)

SUBSTANCES

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Analyze Refine

Sort by: Relevance

0 of 5 Substances Selected

Analyze by:

Substance Role

Uses 5

Preparation 4

Properties 4

Show More

1. 1306688-43-6

~1

$(C_{54}H_{72}N_2S_6)_n$
Poly[thiazolo[5,4-c]thiazole-2,5-diyl-2,5-thiophenediyl[4,8-bis(2-hexyldecyl)benzo[1,2-b:4,5-b']dithiophene-2,6-diyl]-2,5-thiophenediyl]

2. 1437802-52-2

~1

$(C_{48}H_{70}N_2S_4)_n$
Poly[(4,4'-dioctyl[5,5'-bithiazole]-2,2'-diyl)(4,8-dioctylbenzo[1,2-b:4,5-b']dithiophene-2,6-diyl)]

3. 1437802-51-1

~2

1437802-50-0
 $C_{48}H_{70}Br_2N_2S_4$
Thiazole, 2,2'-(4,8-dioctylbenzo[1,2-b:4,5-b']dithiophene-2,6-diyl)bis[5-bromo-4-octyl-, homopolymer]

4. 2056259-78-8

~1

$(C_{74}H_{122}N_2S_4)_n$
INDEX NAME NOT YET ASSIGNED

5. 1246920-83-1

~1

$(C_{58}H_{78}N_2S_6)_n$
Poly[(4,4'-dinonyl[2,2'-bithiazole]-5,5'-diyl)-2,5-thiophenediyl[4,8-bis(2-ethylhexyl)benzo[1,2-b:4,5-b']dithiophene-2,6-diyl]-2,5-thiophenediyl]

物质标识符检索

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SciPlanner

Research Topic "nano with Immunotherapy of can..." > references (1547) > refine by categories > Gold nanospheres and nanorods ...

REFERENCES

Research Topic

Author Name

Company Name

Document Identifier

Journal

Patent

Tags

SUBSTANCES

Chemical Structure

Markush

Molecular Formula

Property

Substance Identifier

REACTIONS

Reaction Structure

SUBSTANCES: SUBSTANCE IDENTIFIER ?

qinghaosu

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

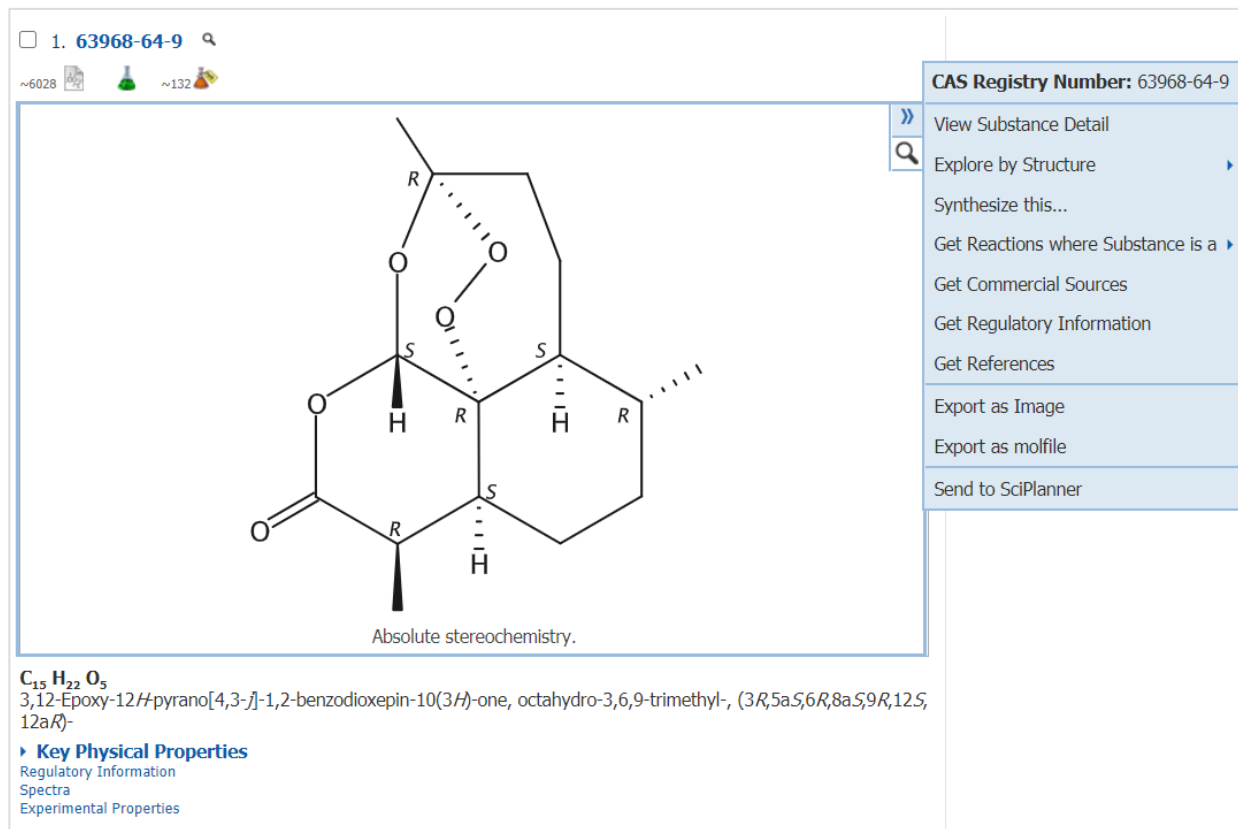
Search

提示：

- 一次最多可输入25个物质。
- 每行一个物质标识符。

物质标识符包括CAS RN和化学名称，化学名称可以是通用名称、商品名、俗名。

物质结果



点击CAS RN获取物质详情

SUBSTANCE DETAIL

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[Return](#)

CAS Registry Number 63968-64-9

~6,028

~132

C₁₅ H₂₂ O₅
3,12-Epoxy-12*H*-pyrano[4,3-*f*]-1,2-benzodioxepin-10(3*H*)-one, octahydro-3,6,9-trimethyl-, (3*R*,5*aS*,6*R*,8*aS*,9*R*,12*S*,12*aR*)-

Molecular Weight
282.33

Melting Point (Experimental)
Value: 156-157 °C

Boiling Point (Predicted)
Value: 389.9±42.0 °C | Condition: Press: 760 Torr

Density (Experimental)
Value: 1.300 g/cm³

Other Names
3,12-Epoxy-12*H*-pyrano[4,3-*f*]-1,2-benzodioxepin-10(3*H*)-one, octahydro-3,6,9-trimethyl-, [3*R*-(3*a*,5*a*β,6β,8*a*β,9*a*,12β,12*aR**)]-(3*R*,5*aS*,6*R*,8*aS*,9*R*,12*S*,12*aR*)-Octahydro-3,6,9-trimethyl-3,12-epoxy-12*H*-pyrano[4,3-*f*]-1,2-benzodioxepin-10(3*H*)-one
(+)-Artemannuin
(+)-Artemisinin
(+)-Qinghaosu
[View more...](#)

Absolute stereochemistry.

EXPERIMENTAL PROPERTIES

EXPERIMENTAL SPECTRA

¹H NMR

¹³C NMR

Hetero NMR

IR

Mass

Raman

UV and Visible

Additional Spectra

¹³ C NMR Properties	Value	Condition	Note
Carbon-13 NMR Spectrum	See spectrum		(3)ACD
Carbon-13 NMR Spectrum	See spectrum		(4)ACD
Carbon-13 NMR Spectrum	See full text	1 of 8	(5)CAS

Notes
(3) ACD: Spectral data were obtained from Advanced Chemistry Development, Inc.
(4) Han, Jaehong; Journal of Natural Products 2001, V64(9), P1201-1205 CAPLUS
(5) Yadav, J. S.; Tetrahedron 2010, V66(11), P2005-2009 CAPLUS

PREDICTED PROPERTIES

PREDICTED SPECTRA

REGULATORY INFORMATION

BIOACTIVITY INDICATORS

TARGET INDICATORS

CAS REFERENCE ROLES

ADDITIONAL DETAILS

Carbon-13 NMR Spectrum

Print

SPECTRUM ID
7MED36_38.C

CAS REGISTRY NUMBER
63968-64-9

FORMULA
C₁₅ H₂₂ O₅

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

NUCLEUS
13C

SOURCE
Spectral data were obtained from Advanced Chemistry Development, Inc.

专利Markush检索的意义

(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(19) World Intellectual Property Organization
International Bureau

(43) International Publication Date
15 November 2007 (15.11.2007)

(10) International Publication Number
WO 2007/129019 A1

(51) International Patent Classification:
C07D 231/12 (2006.01) A61P 9/10 (2006.01)
C07D 231/20 (2006.01) A61P 19/02 (2006.01)
C07D 231/38 (2006.01) A61P 31/00 (2006.01)
C07D 261/08 (2006.01) A61P 35/00 (2006.01)
C07D 261/10 (2006.01) A61K 31/415 (2006.01)
C07D 261/12 (2006.01) A61K 31/42 (2006.01)
C07D 275/02 (2006.01) A61P 7/02 (2006.01)

(21) International Application Number:
PCT/GB2007/001427

(22) International Filing Date: 20 April 2007 (20.04.2007)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data:
60/745,295 21 April 2006 (21.04.2006) US

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(71) Applicant (for MG only): ASTRAZENECA UK LIMITED [GB/GB]; 15 Stanhope Gate, London Greater London W1K 1LN (GB).

(72) Inventors; and
(75) Inventors/Applicants (for US only): GREWAL, Gurnit [US/US]; AstraZeneca R & D Boston, 35 Gatehouse Drive, Waltham, Massachusetts 02451 (US). HENNESSY, Edward [US/US]; AstraZeneca R & D Boston, 35 Gatehouse Drive, Waltham, Massachusetts 02451 (US). KAMHI, Victor [US/US]; AstraZeneca R & D Boston, 35 Gatehouse Drive, Waltham, Massachusetts 02451 (US). LI, Danyang [CN/US]; AstraZeneca R & D Boston, 35 Gatehouse Drive, Waltham, Massachusetts 02451 (US).

(74) Agent: GLOBAL INTELLECTUAL PROPERTY; AstraZeneca AB, S-SE-151 85 Södertälje (SE).

(81) Designated States (unless otherwise indicated, for every kind of national protection available): AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW.

(84) Designated States (unless otherwise indicated, for every kind of regional protection available): ARIPO (BW, GH, GM, KE, LS, MW, MZ, NA, SD, SE, SZ, TZ, UG, ZM, ZW), Eurasian (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European (AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR), OAPI (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG).

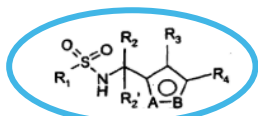
Published:
— with international search report

For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.

(54) Title: SULFONAMIDE COMPOUNDS USEFUL AS ADG RECEPTOR MODULATORS

(57) Abstract: The present invention relates to compounds of formula (I) that mediate Edg, including Edg-1, processes for their preparation, pharmaceutical compositions containing them as the active ingredient, to their use as medicaments and to their use in the manufacture of medicaments for use in the treatment in warm-blooded animals such as humans of diseases that have a significant vascularization or inflammatory component such as in tumor-related diseases. The present invention also relates to compounds that inhibit α5β1, and also that exhibit appropriate selectivity profile(s) against other integrins.

WO 2007/129019 A1



WO 2007/129019 1 PCT/GB2007/001427

SULFONAMIDE COMPOUNDS USEFUL AS ADG RECEPTOR MODULATORS

BACKGROUND OF THE INVENTION

EDG (endothelial differentiation gene) receptors belong to a family of closely related, lipid activated G-protein coupled receptors. EDG-1, EDG-3, EDG-5, EDG-6, and EDG-8 (also known as SIP1, SIP3, SIP2, SIP4, and SIP5) are identified as receptors specific for sphingosine-1-phosphate (SIP). EDG2, EDG4, and EDG7 (known also as LPA1, LPA2, and LPA3, respectively) are receptors specific for lysophosphatidic (LPA). Among the SIP receptor isotypes, EDG-1, EDG-3 and EDG-5 are widely expressed in various tissues, whereas the expression of EDG-6 is confined largely to lymphoid tissues and platelets, and that of EDG-8 to the central nervous system.

EDG receptors are responsible for signal transduction and are thought to play an important role in cell processes involving cell development, proliferation, maintenance, migration, differentiation, plasticity and apoptosis. Certain EDG receptors are associated with diseases mediated by the *de novo* or deregulated formation of vessels—for example, for diseases caused by ocular neovascularisation, especially retinopathies (diabetic retinopathy, age-related macular degeneration); psoriasis; hemangiomas such as “strawberry-marks”; various inflammatory diseases, such as arthritis, especially rheumatoid arthritis, arterial atherosclerosis and atherosclerosis occurring after transplants, endometriosis or chronic asthma; and tumor diseases; or by lymphocyte interactions, for example, in transplantation rejection, autoimmune diseases, inflammatory diseases, infectious diseases and cancer. An alteration in EDG receptor activity contributes to the pathology and/or symptomatology of these diseases. Accordingly, molecules that themselves alter the activity of EDG receptors are useful as therapeutic agents in the treatment of such diseases.

SUMMARY OF THE INVENTION

These and other needs are met by the present invention which is directed to a compound of formula I

in free or pharmaceutically acceptable salt form, wherein:

WO 2007/129019 2 PCT/GB2007/001427

A and B are each independently N, NR_a, O, S, or CR_b;

R_a is H, (C₁-C₆)alkyl, C(O)-(C₁-C₆)alkyl, C(O)-NR'R'', CO₂(C₁-C₆)alkyl;

R_b is H, halo, (C₁-C₆)alkyl, cyano, -C(O)-(C₁-C₆)alkyl, -CO₂(C₁-C₆)alkyl, C(O)-NR'R'', wherein R' and R'' are each independently at each occurrence H or (C₁-C₆)alkyl or X-R_c; -CO₂H, -SO₂NHR;

R_c is aryl, heteroaryl, (C₁-C₆)alkyl, aralkyl, heterocycloalkyl, or heteroaralkyl;

R₂ and R₃ are each independently H, (C₁-C₆)alkyl, aryl, heteroaryl, aralkyl, or heteroaralkyl, or taken together with the carbon to which they are attached form C=O;

R₃ and R₄ are each independently H, halo, (C₁-C₆)alkyl, (C₃-C₆)cycloalkyl, (C₃-C₆)cycloalkyl(C₁-C₆)alkyl, heterocycloalkyl, aralkyl, aryl, (C₂-C₆)alkenyl, (C₂-C₆)alkynyl, or heteroaralkyl, or X-R_c;

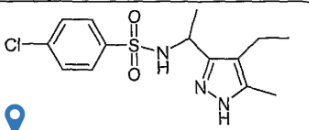
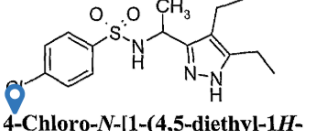
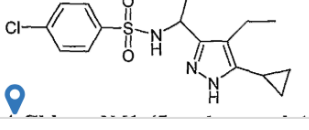
X is S, O, or NR_d;

R_d is H or (C₁-C₆)alkyl;

R₄ is H, (C₁-C₆)alkyl, aryl, heteroaryl, heterocyclo, (C₂-C₆)alkenyl, (C₂-C₆)alkynyl, aralkyl, heteroaralkyl, (C₃-C₆)cycloalkyl(C₁-C₆)alkyl, heterocycloalkyl(C₁-C₆)alkyl, acyl, acyloxy, acylamino, or (C₁-C₆)alkoxycarbonyl(C₁-C₆)alkyl, or cyano; and

each R₁, R₂, R₃, R₄, R₅, R₆, R₇, and R₈ may be optionally substituted on carbon by azido, halo, nitro, cyano, hydroxy, trifluoromethoxy, NR'R'', -CO₂H, C(O)-(C₁-C₆)alkyl, -CO₂(C₁-C₆)alkyl, -C(O)-NR'R'', S(C₁-C₆), SO₂(C₁-C₆)alkyl, SO₂NH(C₁-C₆)alkyl, SO₂NR'R'' (C₂-C₆)alkenyl, (C₂-C₆)alkynyl, or (C₁-C₆)alkoxy, wherein R' and R'' are each independently hydrogen, (C₁-C₆)alkyl, (C₃-C₆)cycloalkyl, (C₃-C₆)cycloalkyl(C₁-C₆)alkyl, or aryl.

专利中的物质表达

Table 1				
Ex	Compound	¹ H NMR	M/Z	Int
1	 4-Chloro-N-[1-(4-ethyl-5-methyl-1H-pyrazol-3-yl)ethyl]benzenesulfonamide	(400 MHz, DMSO-D ₆) δ ppm 0.82 - 0.92 (m, 3 H) 1.23 (d, 3 H) 1.99 (s, 3 H) 2.10 - 2.21 (m, 2 H) 4.30 - 4.39 (m, 1 H) 7.53 (m, 2 H) 7.61 - 7.70 (m, 2 H) 7.99 (d, 1 H) 11.99 (s, 1 H)		1
2	 4-Chloro-N-[1-(4,5-diethyl-1H-pyrazol-3-yl)ethyl]benzenesulfonamide	(400 MHz, DMSO-D ₆) δ ppm 0.89 (t, <i>J</i> =7.58 Hz, 3 H) 1.06 (t, <i>J</i> =7.58 Hz, 3 H) 1.24 (d, <i>J</i> =7.07 Hz, 3 H) 2.11 - 2.22 (m, 2 H) 2.38 (q, <i>J</i> =7.58 Hz, 2 H) 4.33 - 4.44 (m, 1 H) 7.49 - 7.59 (m, 2 H) 7.63 - 7.65 (m, 2 H) 8.02 (m, 1 H), 12.01 (broad s, 1 H).	341	1
3	 4-Chloro-N-[1-(4-ethyl-5-methyl-1H-pyrazol-3-yl)ethyl]benzenesulfonamide	(400 MHz, DMSO-D ₆) δ ppm 0.54 - 0.65 (m, 2 H) 0.75 - 0.85 (m, 2 H) 0.93 (t, 3 H) 1.24 (d, 3 H)		1

WO 2007/129019

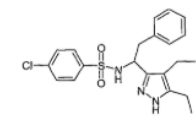
34

PCT/GB2007/001427

0.81 mmol) is then added in one portion, and the mixture is allowed to stir at 0 °C for 2 min and is allowed to warm to room temperature over 3 min. Glacial HOAc (0.50 mL) is added to quench the reaction, followed by absolute EtOH (2 mL). Hydrazine monohydrate (150 μL, 3.1 mmol) is added, and the mixture is allowed to stir at room temperature. After 45 min, the reaction is partitioned between EtOAc and H₂O. The aqueous layer is extracted with EtOAc, and the combined organics are washed with brine, dried (MgSO₄), filtered, and concentrated. The crude material is purified by silica gel chromatography (gradient elution; R_f in 50:50 hexanes:EtOAc = 0.23) to give a viscous oil that is lyophilized to give a colorless solid (54 mg, 28%).

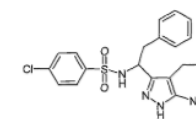
Example 5 may be prepared in two steps from intermediate 2a as outlined below:

4-Chloro-N-[1-(4,5-diethyl-1H-pyrazol-3-yl)-2-phenylethyl]benzenesulfonamide; (Example 5):



A 25 mL round bottom flask is charged with *N*-(1-benzyl-3-ethyl-2,4-dioxohexyl)-4-chlorobenzenesulfonamide (**Intermediate 2a**, 104 mg, 0.25 mmol) and MeOH (4.0 mL). Hydrazine monohydrate (50 μL, 1.03 mmol) is added, and the solution is allowed to stir at room temperature for 1 h. The volatile components are removed under reduced pressure, and the crude material is purified by silica gel chromatography (EtOAc as eluent) to give a colorless oil. Lyophilization affords a solid material (16 mg, 15%).

***N*-[1-(5-Amino-4-ethyl-1H-pyrazol-3-yl)-2-phenylethyl]-4-chlorobenzenesulfonamide (Example 6):**



A 50 mL round bottom flask is charged with *N*-(1-[5-amino-1-[(4-chlorophenyl)sulfonyl]-4-ethyl-1H-pyrazol-3-yl]-2-phenylethyl)-4-

专利中的物质表达方式

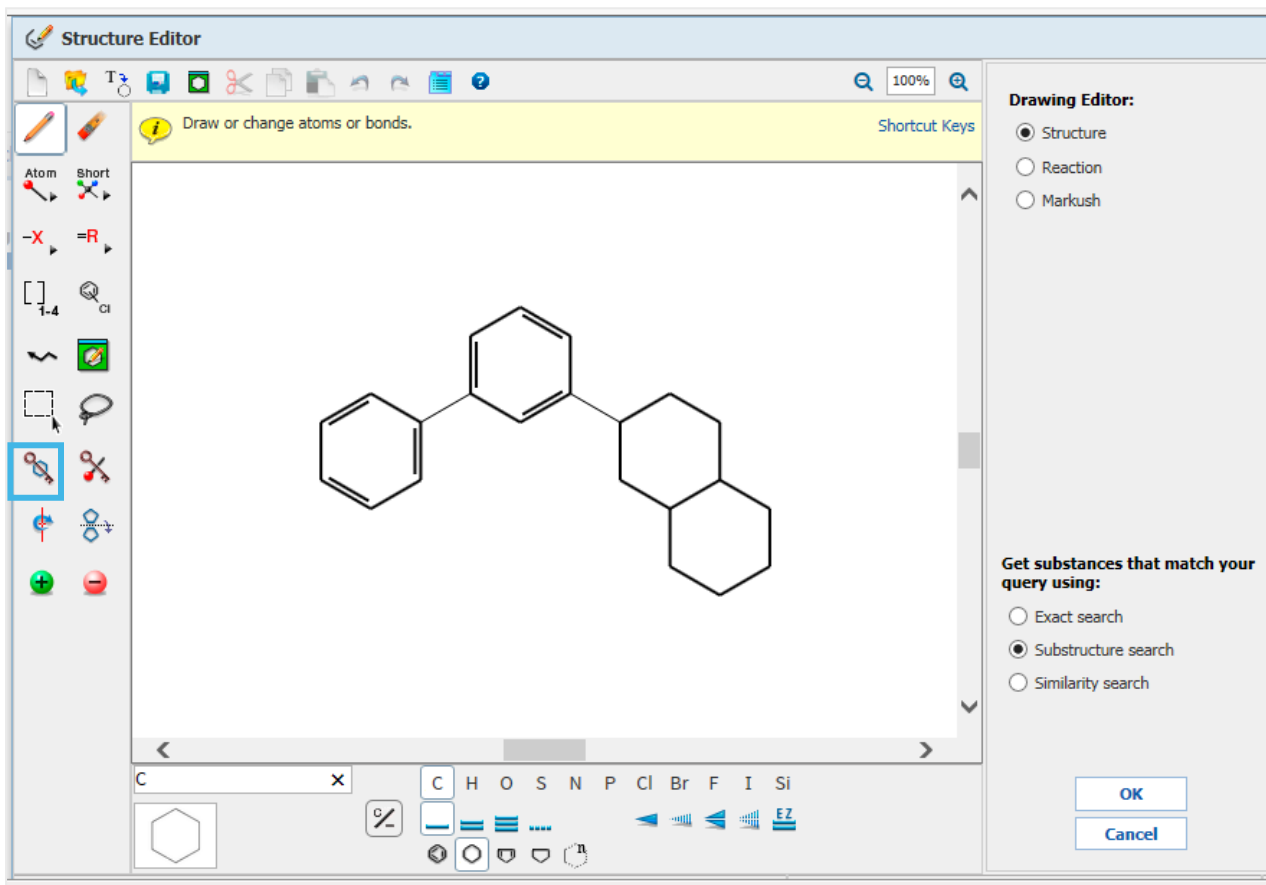
■ 确定物质[Specific Substance]:

- 具有表征数据的物质（一般为实施例中的物质，会被CAS Registry收录）
- 专利中其他确定物质（只有有充分的证据证明此物质存在，才会被CAS Registry收录）

■ 预测性物质[Prophetic Substance]:

- 使用通式结构（CAS Markush）表示的预测物质，一个通式结构可以表示上百或上千个化学物质（会被CAS Markush数据库收录）
- 通常，实施例中只表征Markush结构中的部分物质，更大量的结构则被隐藏在Markush结构中，受到保护

绘制结构，并检索文献中报道的确定结构的物质



物质亚结构检索结果为零

CAS Solutions

SciFINDER[®]
A CAS SOLUTION

Preferences | SciFinder Help | Sign Out

Welcome Sunny Yu

Explore | Saved Searches | SciPlanner

⚠ Explore Substances resulted in 0 substances [Return](#)

Chemical Structure substructure > substances (0)

SUBSTANCES

Create Keep Me Posted Alert

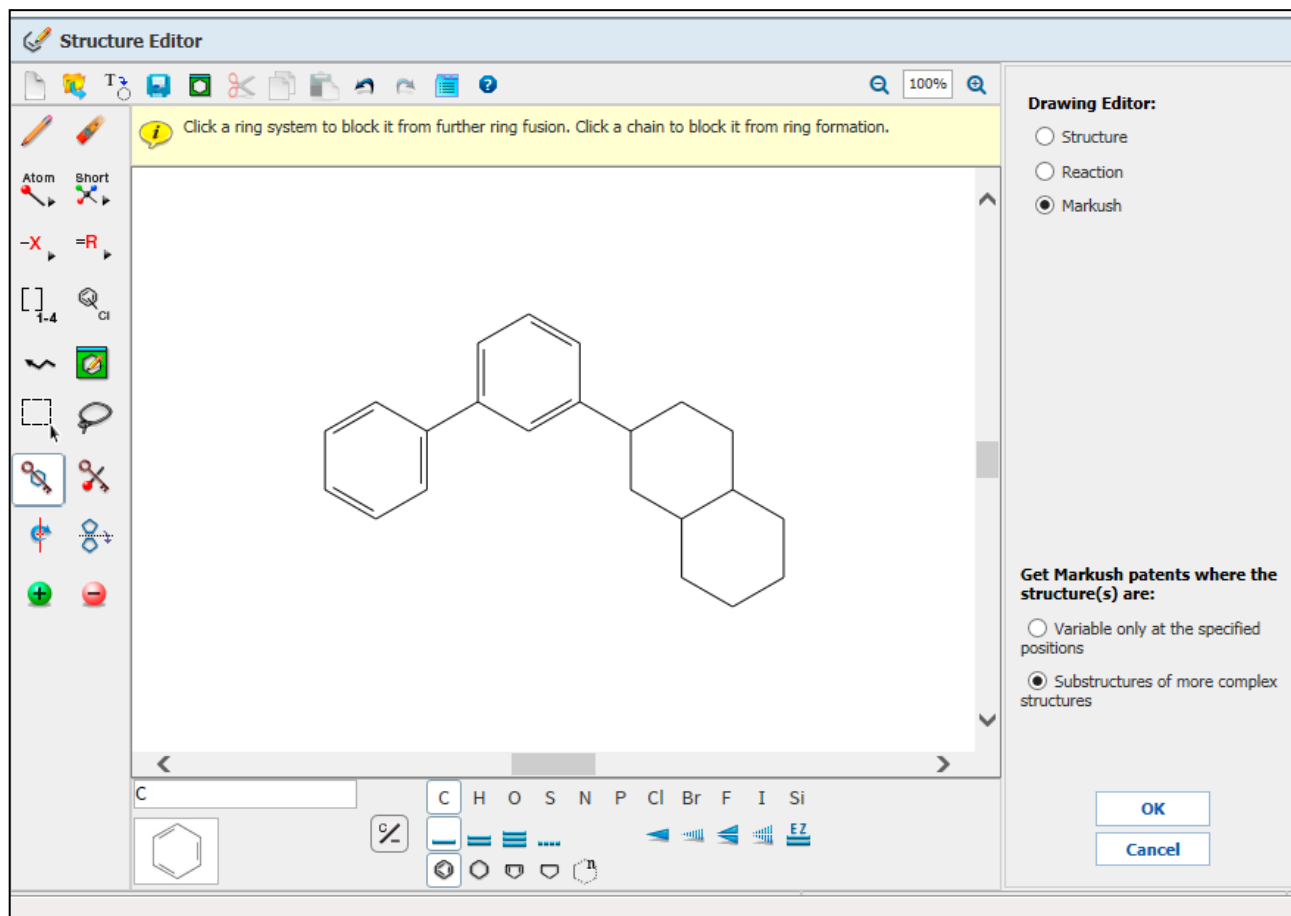
Analyze Refine

Analyze by:
No substances available

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物质Markush结构检索



在SciFinder中进行Markush检索
(系统在进行Markush检索时,
将自动进行环锁定)

第一种是指除了所设置的可变基团外,
其他位点默认锁定。
第二种是开放位点允许有取代

Markush检索结果集：24项专利文献

Explore
Saved Searches
SciPlanner

SavePrintExport

Markush substructure > references (24)

REFERENCES
Get Substances
Get Reactions
Get Related Citations
Tools

Create Keep Me Posted AlertSend to SciPlanner

Analyze
Refine
Categorize

Sort by: Accession Number
0 of 24 References Selected
Display Options

Analyze by:
Author Name

Hirata Shinichi 3
Brown Richard James 2
Castro Peter Paul 2
Frasier Deborah Ann 2
Happersett Constance 2
Hsieh Yu Ying 2
Krause Joachim 2
Sternberg Charlene Gross 2

☐ 1. Compounds for the modulation of proprotein convertase subtilisin/kexin type 9 (PCSK9)
Quick View PATENTPAK
By Bowers, Simeon; Karbarz, Mark; Zhu, Jiang; Barta, Thomas E.; Bourne, Jonathan William; Pandey, Anjali
From PCT Int. Appl. (2020), WO 2020252383 A2 20201217. | Language: English, Database: CAPLUS
The present disclosure relates to novel compds. capable of binding to PCSK9, thereby modulating PCSK9 biol. activity. Also provided are compns. comprising these compds., methods of prep. the compds., and methods for use of the compds. in the treatment of PCSK9-related conditions and diseases.

☐ 2. Preparation of hole transport material for OLED
Quick View PATENTPAK
By Wang, Yalong; Li, Hongyan; Xue, Zhen; Wang, Jinping; Chen, Zhiwei; Li, Lingang; Yan, Shan; Wang, Weijun; Ren, Zenggang
From Faming Zhuanli Shenqing (2019), CN 110156746 A 20190823. | Language: Chinese, Database: CAPLUS
The title hole transport material with general formula of $R^1Ar^1-N(Ar^2R^3)-Ar^3R^2$, wherein, Ar^1-Ar^3 are independently selected from substituted or unsubstituted C6-30 arylene, including phenylene, bis-phenylene, heteroarylene, etc.; R^1-R^3 are independently selected from H, substituted or unsubstituted C8-30 alkyl, substituted or unsubstituted C8-30 alkenyl, substituted or unsubstituted C8-30 alkynyl, etc. The inventive hole transport material is not only suitable for solar cells, but also suitable for org. semiconductor and other photoelec. fields.

☐ 3. Process for the reduction of the NOx emissions with combustion engines by fuel additives.
Quick View PATENTPAK
By Kantlehner, Willi
From Ger. Offen. (2019), DE 102018001260 A1 20190822. | Language: German, Database: CAPLUS

物质检索小结：

- 物质的检索方法汇总和适用性；
- 结构编辑器的使用方法；
- 无机物、配位化合物和聚合物等物质的检索方法；
- 物质识别符检索；
- 物质Markush结构检索

大纲

- CAS SciFinder介绍
- 文献相关信息的获取策略
 - 储能材料文献检索方法
 - 文献结果分析、精炼和详情
 - 如何高效阅读专利文献详情(CAS PatentPak)
- 物质相关信息的获取策略
 - 如何检索无机化合物、配位化合物和聚合物
 - 物质结果分析、精炼和详情
- 反应相关信息的获取策略
 - 反应的获取方法
 - 反应结果分析、精炼及详情
 - 如何高效获取反应详情 (Synthetic Methods)
- 如何高效获取分析方法详情 (CAS Analytical Methods)



化合物制备信息的获取方法

方法1： 基于物质名称和主题词获取到合成制备信息；

方法2： 基于物质的CAS号检索合成制备信息；

方法3： 在CAS REACT中获取到该结构的精确合成信息；

方法4： 在CAS REACT中获取到该结构的精确反应信息、该结构的盐、同位素、立体构型等合成信息。

反应的检索方法

方法1：在文献检索Research Topic中输入preparation of 50-78-2或者synthesis of aspirin进行检索

REFERENCES ?

Get Substances

Get Reactions

Get Related Citations

Tools

Create Keep Me Posted Alert

Send to SciPlann

Analyze Refine Categorize

Sort by: Accession Number

Display Options

Analyze by: ?

Author Name

Patrono C 4

Valles Juana 4

Dineen Annie E 3

Fahey Jodie T 3

Moscardo Antonio 3

Nizankowska E 3

Pulliam Curtis R 3

Wennmalm A 3

0 of 227 References Selected

1. A kind of method for catalyzed synthesis of aspirin by using choline eutectic solvent [Machine Translation].
Quick View PATENTPAK
By Wang, Yinglei; Li, Wenhuan; Liu, Xueguo; Du, Chaojun; Li, Jin
From Faming Zhuanli Shenqing (2017), CN 106928055 A 20170707. | Language: Chinese, Database: CAPLUS
[Machine Translation of Descriptors]. The present invention belongs to environment-friendly org. **synthesis** chem. tech. field, particularly relates to a kind of method for catalyzed **synthesis** of **aspirin** by using choline eutectic solvent. The method comprises: adding choline eutectic solvent, salicylic acid, acetic anhydride into reaction vessel, after heating reaction 15 ~ 40min at 70 ~ 80 DEG C; purifying the crude products obtained by reaction, obtaining the **aspirin**. The method catalyzed **synthesis** of **aspirin** by using choline eutectic solvent of the present invention has simple operation, gent...

2. Synthesis of novel aspirin analogs for medicinal testing
Quick View Other Sources
By Albasrawi, Hadeel K.; Timmons, Shannon C.
From Abstracts, 48th Central Regional Meeting of the American Chemical Society, Dearborn, MI, United States, June 6-9 (2017), CERM-66. | Language: English, Database: CAPLUS
Aspirin is a common nonsteroidal anti-inflammatory drug used to treat pain, fever, and inflammation. It is one of the most widely used medications in the world with an estd. 40,000 tons produced and consumed annually. Recent research has shown that this inexpensive age-old drug holds promise as an anticancer agent. Studies have shown that **aspirin** has a remarkable ability to inhibit the proliferation of colorectal cancer cells in vitro, for example. Although the mechanism of action has not yet been established, it is clear that the **synthesis** of **aspirin** analogs to further probe this finding ...

反应的检索方法

方法2：检索物质后，在物质信息详情页面，可以由此物质获得制备 (preparation) 相关文献或者产物为此物质的反应。

The screenshot shows the 'SUBSTANCE DETAIL' page for CAS Registry Number 50-36-2. The substance is 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(benzoyloxy)-8-methyl ester, (1R,2R,3S,5S)-. The 'Get References' dialog box is open, showing options to limit results to various categories. The 'Preparation' checkbox is selected. The 'For each sequence, retrieve:' section has the option 'Additional related references, e.g., activity studies, disease studies.' checked.

Get References

Limit results to:

- ☐ Adverse Effect, including toxicity
- ☐ Analytical Study
- ☐ Biological Study
- ☐ Combinatorial Study
- ☐ Crystal Structure
- ☐ Formation, nonpreparative
- ☐ Miscellaneous
- ☐ Occurrence
- ☒ Preparation
- ☐ Process
- ☐ Properties
- ☐ Prophetic in Patents
- ☐ Reactant or Reagent
- ☐ Spectral Properties
- ☐ Uses

For each sequence, retrieve:

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

Get Cancel

The screenshot shows the 'Searches' page in SciFinder for substance 50-78-2. The 'Get Reactions' dialog box is open, showing options to retrieve reactions for all substances or selected substances. The 'Limit results by reaction role:' section has the 'Product' role selected.

Get Reactions

Retrieve reactions for:

- ☒ All substances
- ☐ Selected substances

Limit results by reaction role:

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

Get Cancel

反应的检索方法

方法3：也可以点击物质结构右上角的蓝色双箭头，点击 Synthesis this，获得相关反应

SUBSTANCE DETAIL ?

Get References

Get Reactions

Get Commercial Sources

[Return](#)

CAS Registry Number 50-78-2

~39,113

~106

C₉H₈O₄
Benzoic acid, 2-(acetyloxy)-

Molecular Weight
180.16

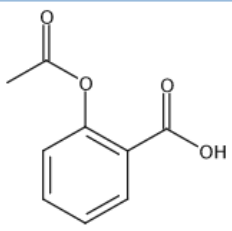
Melting Point (Experimental)
Value: 135 °C

Boiling Point (Experimental)
Value: 197-200 °C | Condition: Press: 7 Torr

Density (Experimental)
Value: 1.40 g/cm3

pKa (Predicted)
Value: 3.48±0.10 | Condition: Most Acidic Temp: 25 °C

Other Names
Rhodine (7CI)
Salicylic acid acetate (8CI)
2-(Acetyloxy)benzoic acid
2-Acetoxybenzoic acid



CAS Registry Number: 50-78-2

[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](#)

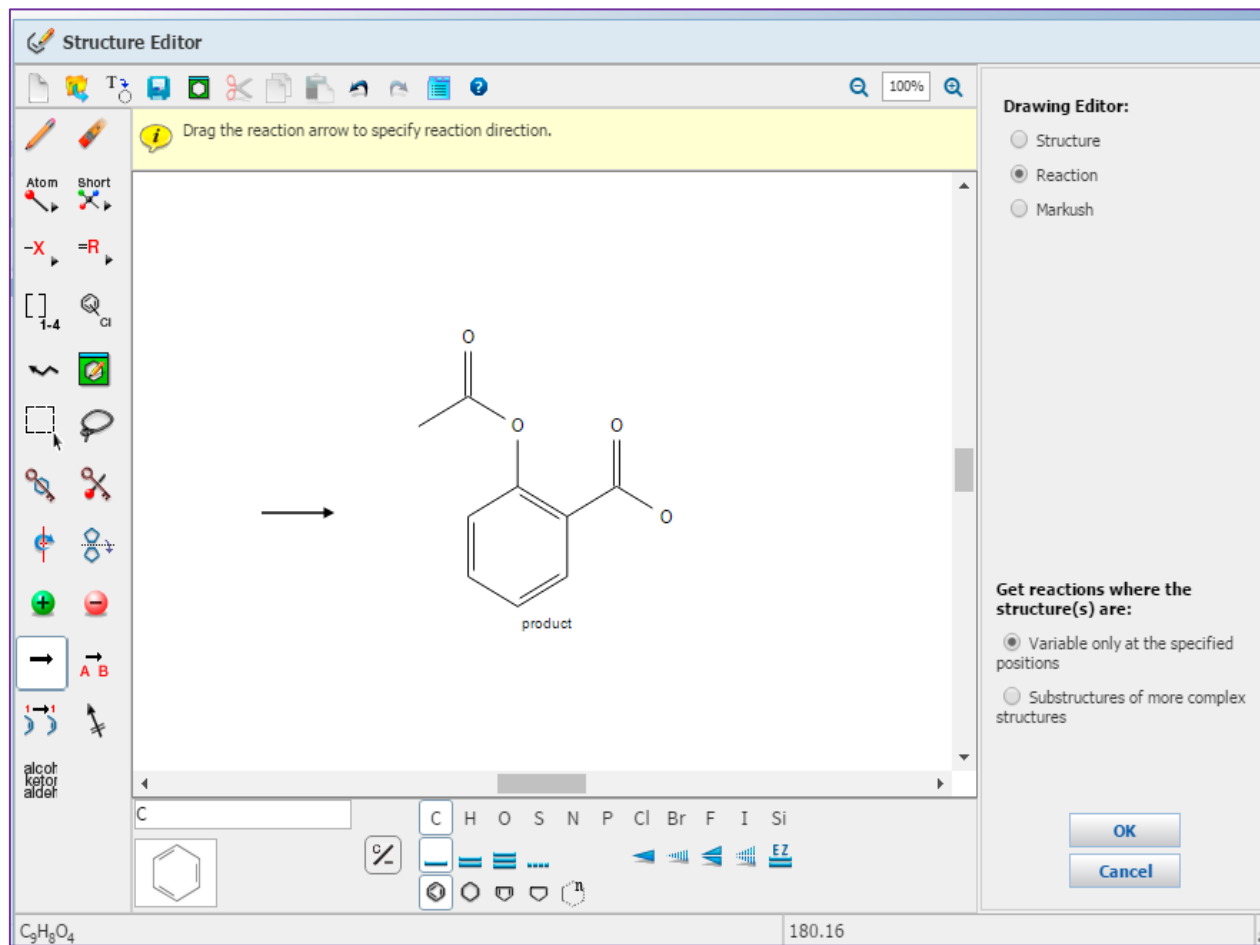
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**ACS**
International

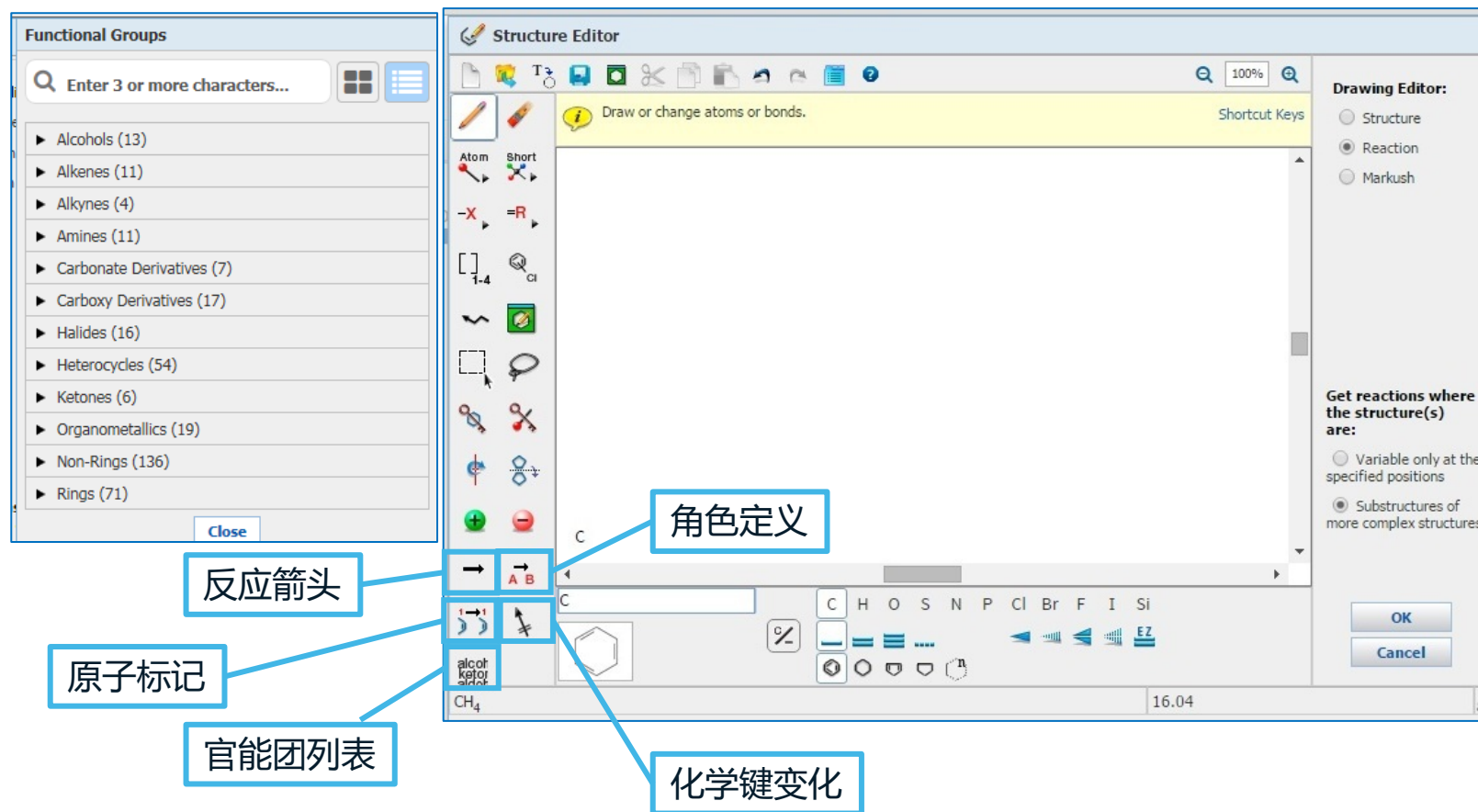
CAS
A division of the
American Chemical Society

反应的检索方法

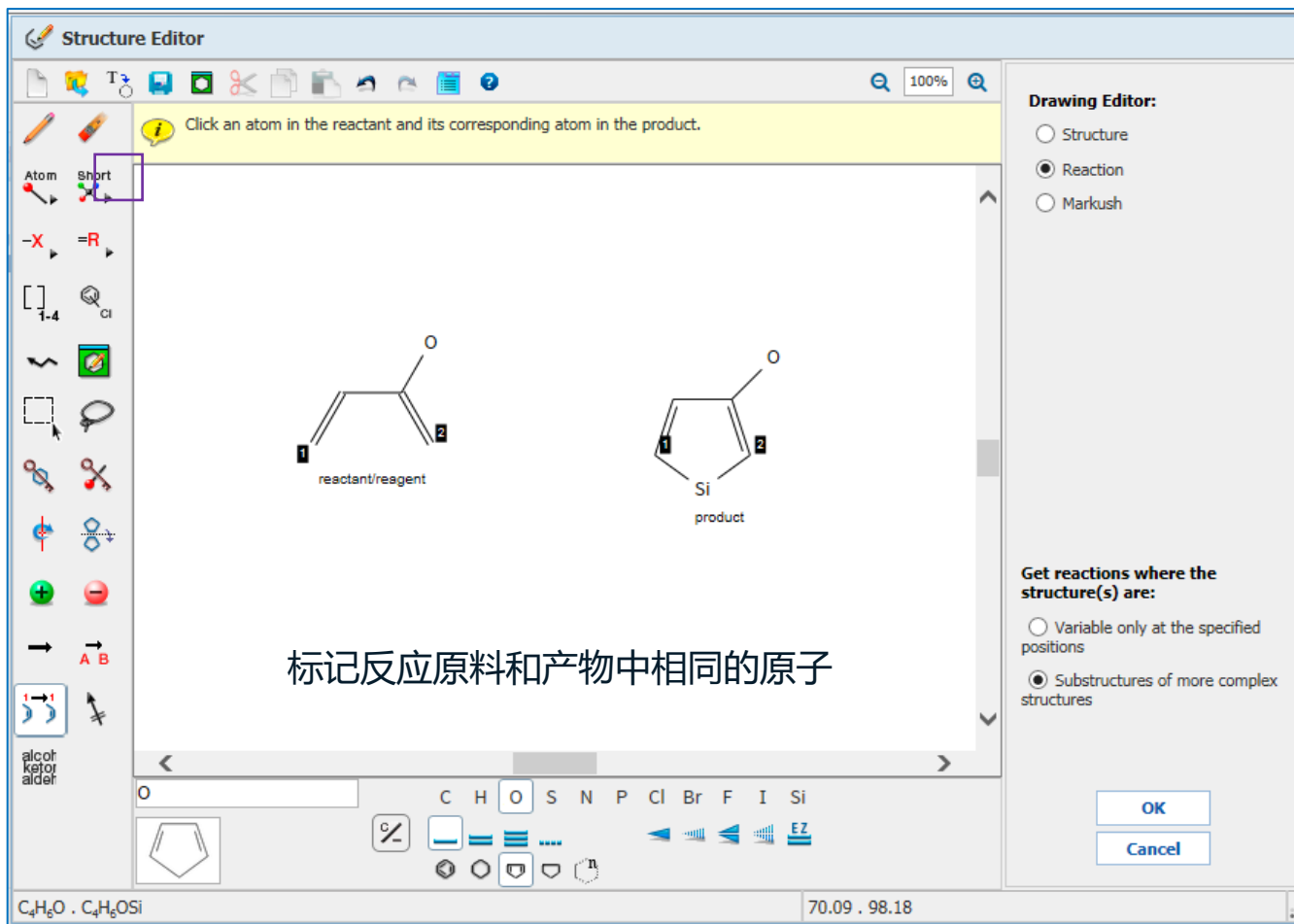
方法4：在SciFinder反应检索编辑器中绘制结构，获得反应。



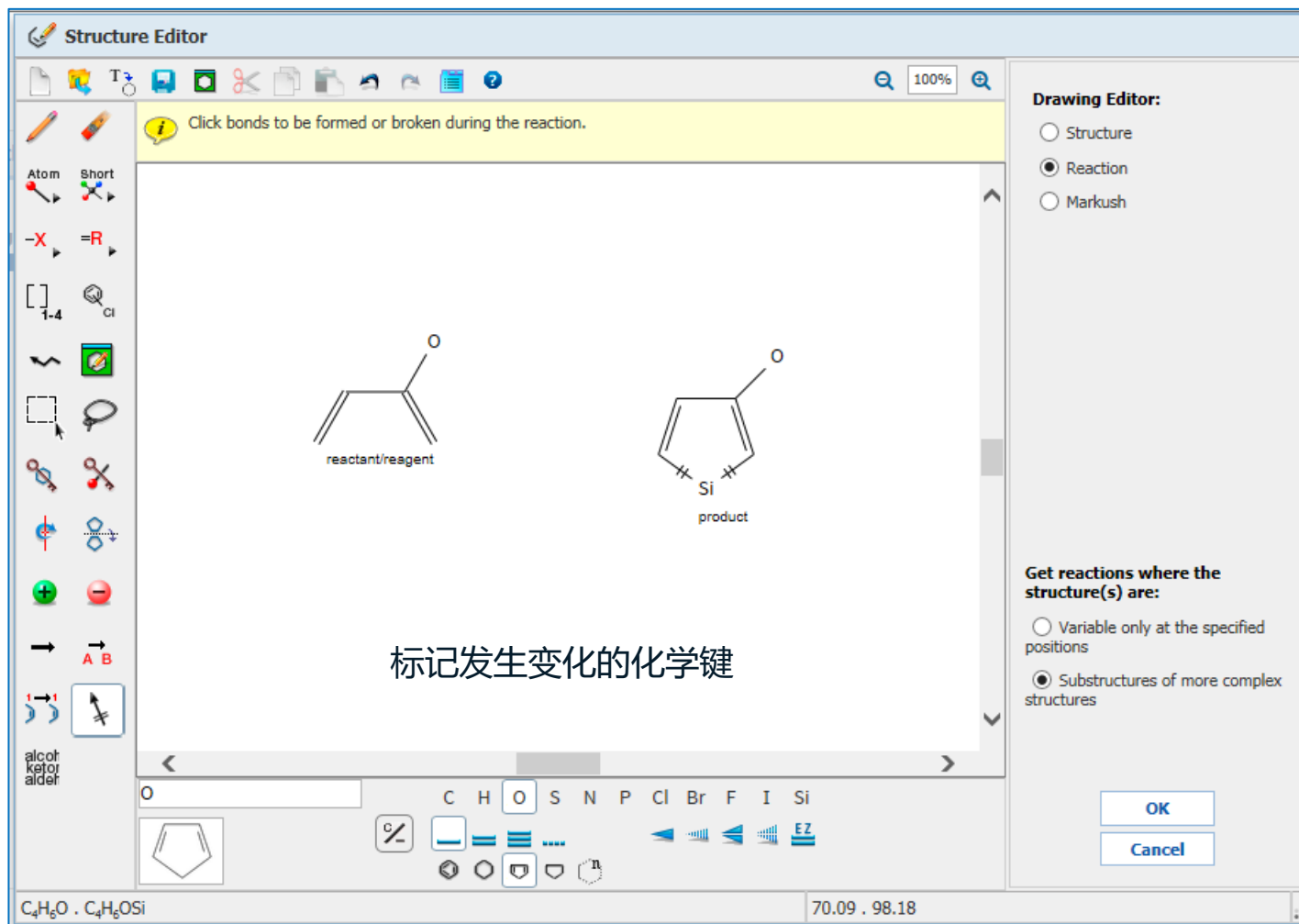
结构编辑器：绘制反应工具



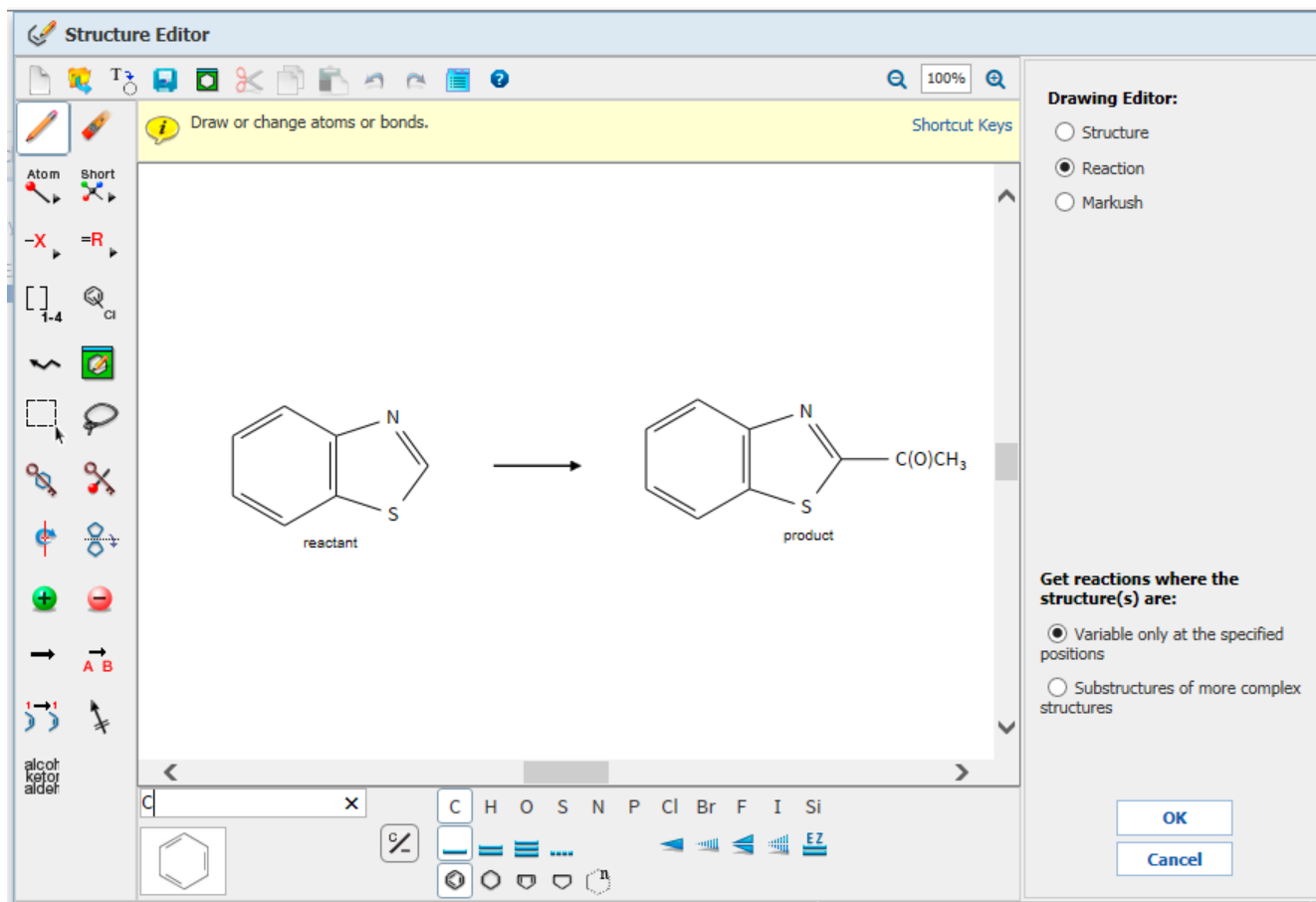
反应前后物质中的原子标记



发生变化的化学键标记



精确结构反应检索：绘制反应式



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) 分组, 排序

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

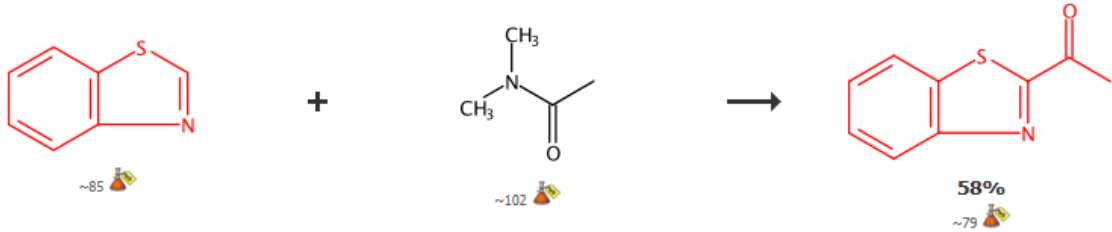
Show More

Group by: No Grouping ▾ 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 ⓘ 58% ~79 ⓘ

▼ Overview

Steps/Stages	Notes
1.1 R:BuLi, S:THF, S:Me(CH ₃) ₂ , -78°C; 1 h, -78°C	ice-bath removed after stirring at -78°C for 1 hour (stage 2), Reactants: 2, Reagents: 2, Solvents: 2, Steps: 1, Stages: 2. Most stages in new reaction set.

精确结构反应检索：查看反应结果集

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

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

REACTIONS ?

Get References Tools

Analyze Refine

Analyze by: Reagent

BuLi 4
t-BuOOH 3
HCl 2
19468-88-3 1
H₂O 1
H₂SO₄ 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)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

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 ▾

Relevance
Accession Number
Experimental Procedure
MethodsNow
Number of Steps
Product Yield
Publication Year

排序：相关度，入库号，实验步骤，MethodsNow, 步数，产率，发表年份

Analyze Refine

Analyze by: ⓘ
Reagent ▾

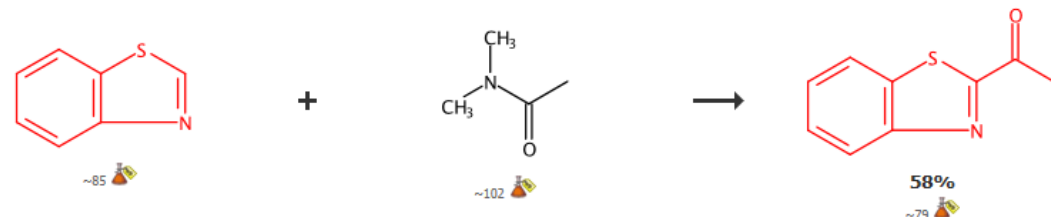
BuLi 4
t-BuOOH 3
HCl 2
19468-88-3 1
H₂O 1
H₂SO₄ 1

Show More

Group by: No Grouping ▾ Sort by: 0 of 8 Reactions Selected

1. 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)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, Solvents: 2, Stages: 1, Steps: 2, Most steps in previous stage?

精确结构反应检索：查看反应结果集

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

REACTIIONS ?

Get References Tools

Send to SciPlanner

Analyze Refine

Analyze by: Reagent

BuLi 4

t-BuOOH 3

HCl 2

19468-88-3 1

H₂O 1

H₂SO₄ 1

Show More

Group by: No Grouping Document Transformation

Sort by: Relevance

Display Options

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

~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

精确结构反应检索： 获取相似反应

相似度限制：

Broad： 仅反应中心相似

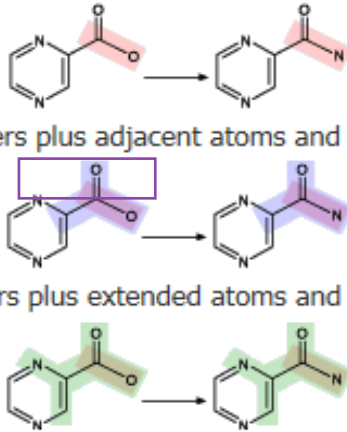
Medium： 反应中心及附属原子和键

Narrow： 反应中心及扩展的原子和键

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



精确结构反应检索：查看感兴趣的反应信息

REACTIONS ?

Analyze

Refine

Analyze by: ?

Reagent

Author Name

Catalyst

Company-Organization

Document Type

Experimental Procedure

Journal Name

Language

MethodsNow

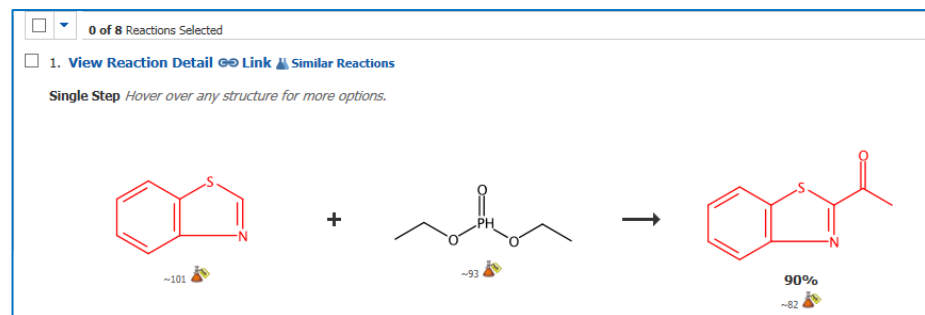
Number of Steps

Product Yield

Publication Year

Reagent

Solvent



Overview

Steps/Stages

1.1 R: t -BuOOH, S: $\text{Me}(\text{CH}_2)_4\text{Me}$, 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_3CN (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.

实验步骤

CAS Synthetic Methods实验详情

REACTIONS ?

Analyze Refine

Analyze by: ?

Reagent

Author Name

Catalyst

Company-Organization

Document Type

Experimental Procedure

Journal Name

Language

MethodsNow

Number of Steps

Product Yield

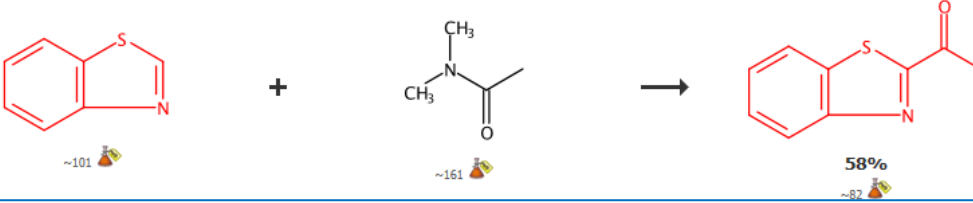
Publication Year

Reagent

Solvent

☐ 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...](#)

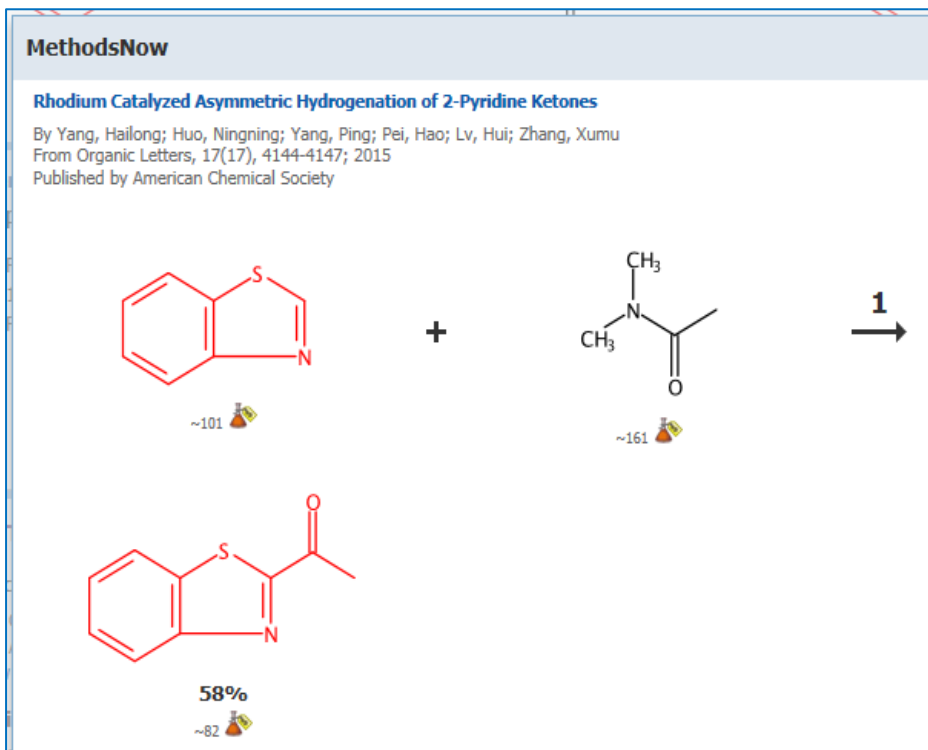
Available Experimental Data

¹H NMR, ¹³C NMR, State

[View with MethodsNow](#)

点击查看MethodsNow窗口

MethodsNow Synthesis: 实验详情展示

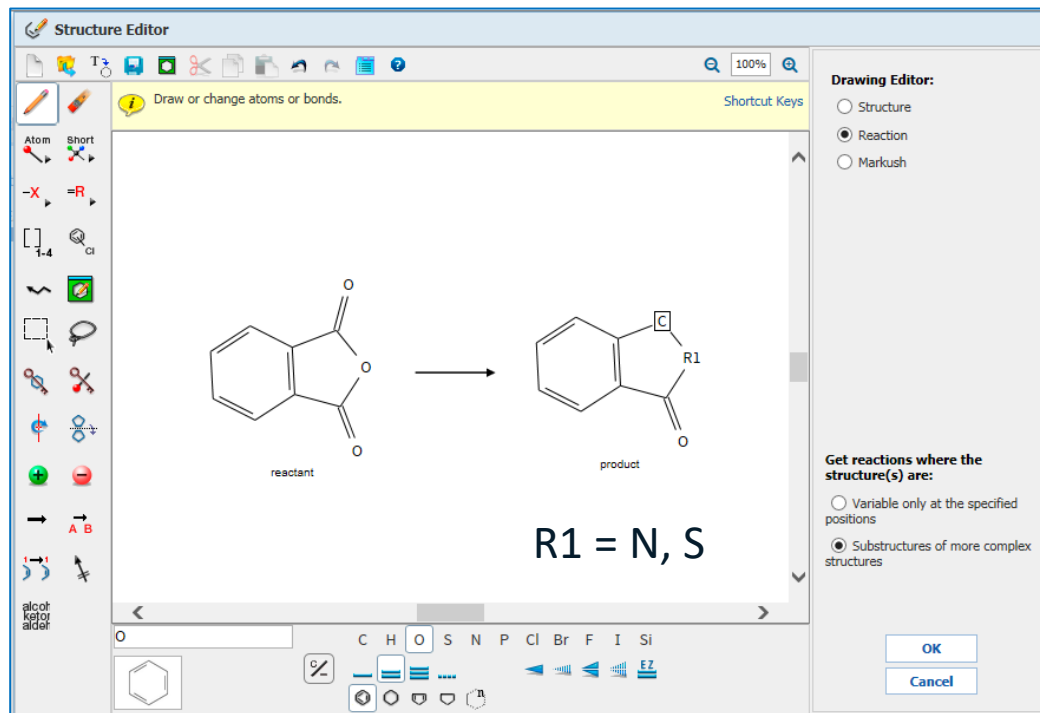


产物, 反应物, 试剂, 溶剂, 步骤,
反应类型, 规模, 核磁氢谱, 核磁碳谱,
产物状态, CAS方法号

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"> 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). 3. Keep the resulted mixture for 1 h under -78 °C. 4. Add N,N-dimethylacetamide (1 equiv, 5 mmol) to the stirred solution at -78 °C. 5. Stir the mixture was continuously for 1 h. 6. Remove the cold bath and stir the mixture for additional 10 min. 7. Hydrolyze with concd hydrochloric acid (1 mL). 8. Stir the acidic solution continuously until the temperature reach to room temperature. 9. Pour the mixture into same amount of water. 10. Extract the aqueous mixture with ethyl acetate 3 times. 11. Dry the combined organic solution with Na₂SO₄. 12. Purify by flash column chromatography to afford product.
Transformation	Decarboxylative Alkylation, Acylation and Carbalkoxylation of Nitrogen Heterocycle
¹ H 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);
¹³ C 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

Print/Export Close

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

Group by: No Grouping Sort by: Relevance

0 of 1208 Reactions Selected

Page: 1 of 81

Refine by: ?

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

Structure Editor:

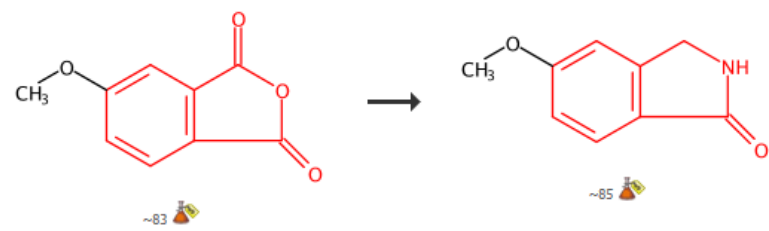
Java Non-Java

Click image to change structure or view detail.
Search type: Substructure

Refine

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

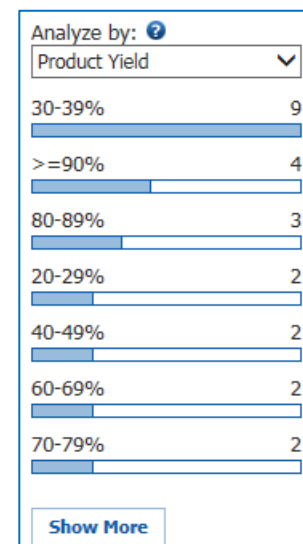
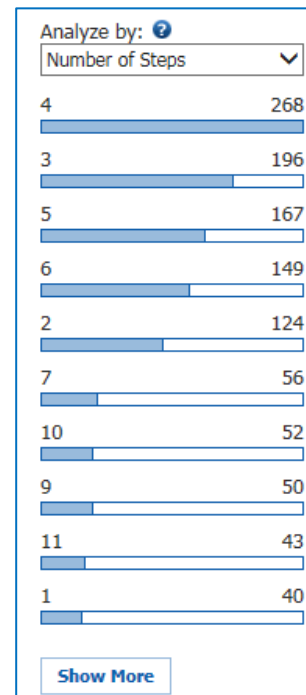
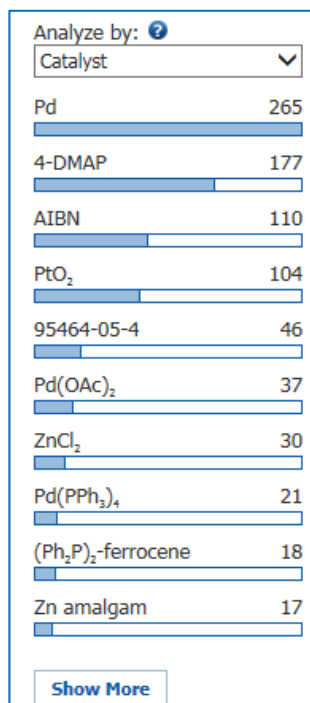
Studies on the chemistry of isoindoles and isoindolenines. XXVII. 3-Alkoxy-1H-isoindoles: syntheses and properties
Quick View Other Sources
By Hennige, Hans et al
From Chemische Berichte, 121(2), 243-52; 1988

亚结构反应检索：分析处理

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



亚结构反应检索：筛选处理

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

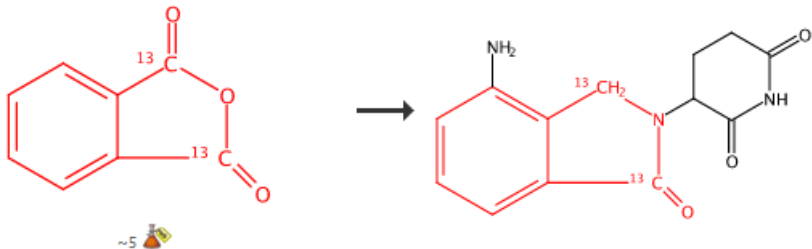
☐ Regioselective

☐ 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

0 of 1154 Reactions Selected

1. View Reaction Detail

2 Steps Hover over any structure for more options.

~83 ~85

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

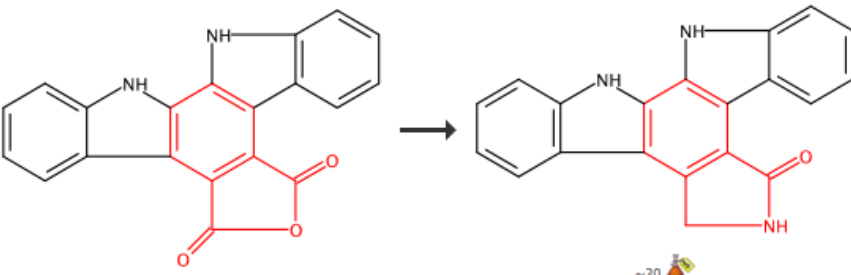
Analyze Refine

Group by: No Grouping Sort by: Relevance

0 of 435 Reactions Selected

1. View Reaction Detail [Link](#)

2 Steps Hover over any structure for more options.



~30

2 Selected Clear Selections

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

Non-participating Functional Group(s)

View: Classes 10

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

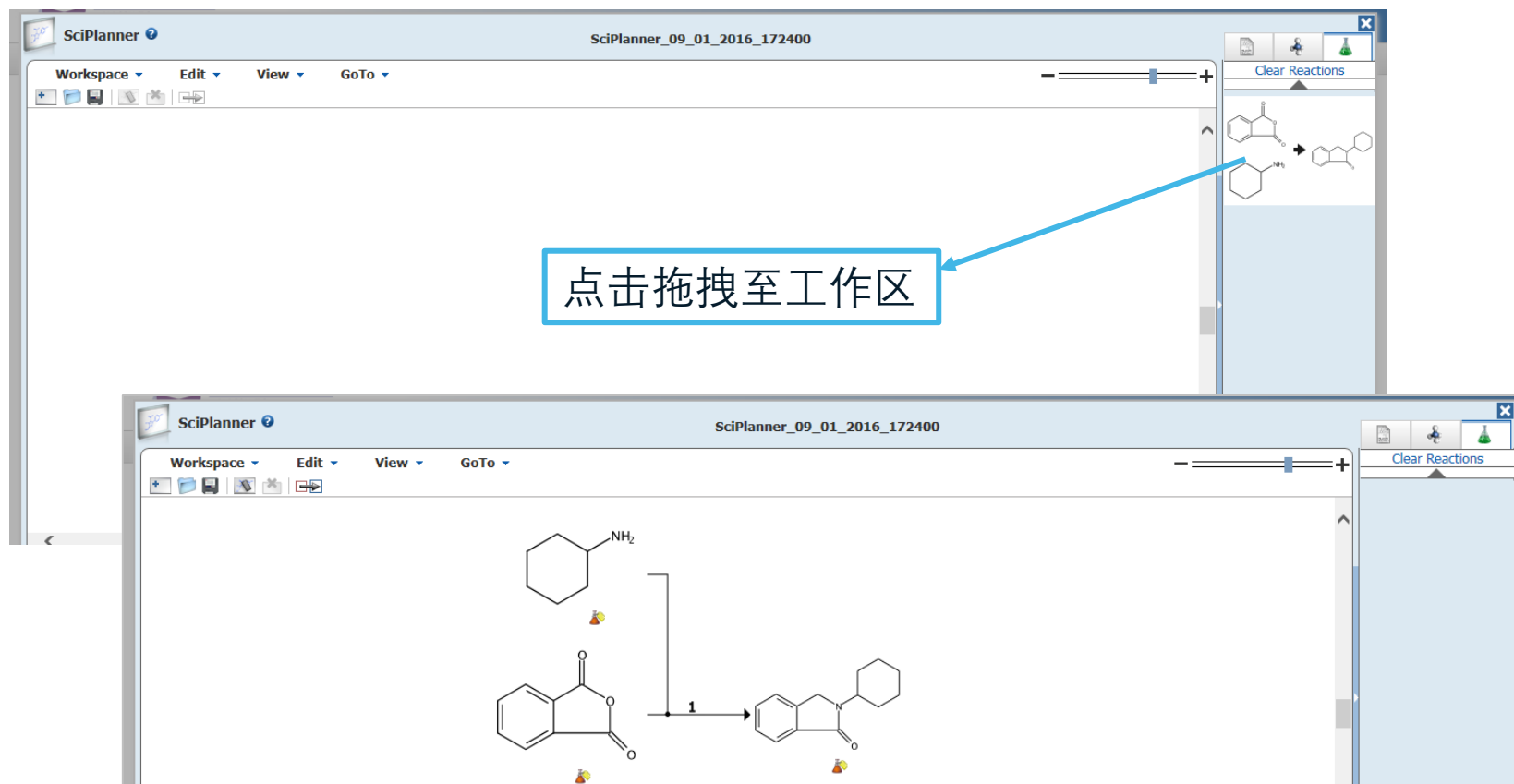
利用SciPlanner设计拟合成反应路线

点击打开SciPlanner工作界面

The screenshot shows the SciPlanner web interface. At the top, there are tabs for 'Explore', 'Saved Searches', and 'SciPlanner'. Below the tabs, the breadcrumb trail reads 'Reaction Structure substructure > reactions (1208) > refine "Catalyzed" (535)'. The main content area is divided into 'REACTANTS' and 'PRODUCTS' sections. Under 'REACTANTS', there is a list of reactions with columns for 'Group by' (No Grouping) and 'Sort by' (Number of Steps). A list of 535 reactions is shown, with the first reaction selected. The reaction details show a chemical reaction scheme: a benzene ring with a carboxylic acid group reacts with a cyclohexylamine to form a benzene ring with an amide group. The reaction is labeled '1. View Reaction Detail' and 'Link Similar Reactions'. The yield is 87%.

选择感兴趣的反应，点击send to SciPlanner

SciPlanner工作界面

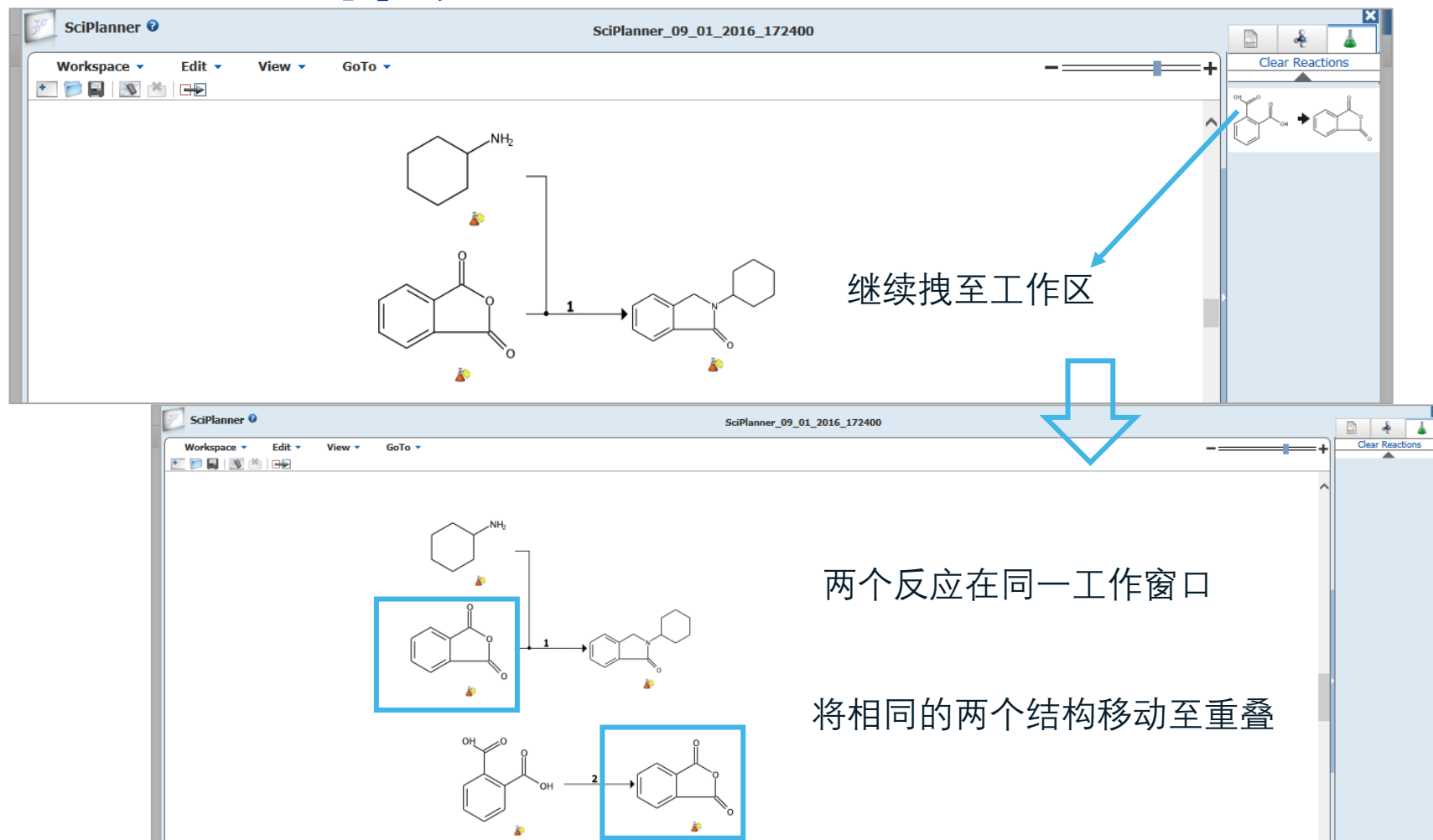


SciPlanner工作界面

The screenshot shows the SciPlanner web interface. At the top, the title bar reads "SciPlanner" and "SciPlanner_09_01_2016_172400". Below the title bar is a menu bar with "Workspace", "Edit", "View", and "GoTo". The main workspace displays a chemical structure of cyclohexylamine (N[C@H]1CCCCC1). A context menu is open over the structure, showing options: "View Substance Detail", "Explore by Structure", "Synthesize this...", "Get Reactions where Substance is a", "Get Commercial Sources", "Get Regulatory Information", and "Get References". A blue callout box points to the "Synthesize this..." option with the text: "点击物质右上角的双箭头, 检索其合成方法".

The screenshot shows the results page of the SciPlanner interface. The top section includes a "Get References" button and a "Tools" dropdown. Below this, there are filters for "Group by: No Grouping" and "Sort by: Accession Number". A summary bar indicates "1 of 382 Reactions Selected". The main content area shows a reaction scheme for the synthesis of cyclohexylamine from cyclohexanone (O=C1CCCCC1) and cyclohexylamine (N[C@H]1CCCCC1). The reaction is labeled "4. View Reaction Detail" and "Single Step". A blue callout box points to the "Send to SciPlanner" button in the top right corner of the results section with the text: "从结果中选择感兴趣的反应, 继续推送至SciPlanner".

SciPlanner工作界面



SciPlanner——设计拟合成的反应路线

SciPlanner 09_01_2016_172400

Workspace Edit View GoTo

导出设计的路线

合二为一的合成路线

Export

Export

Details

File Name: * SciPlanner_09_01_2016_172400

Title

Include:

SciPlanner Image

Reaction Details

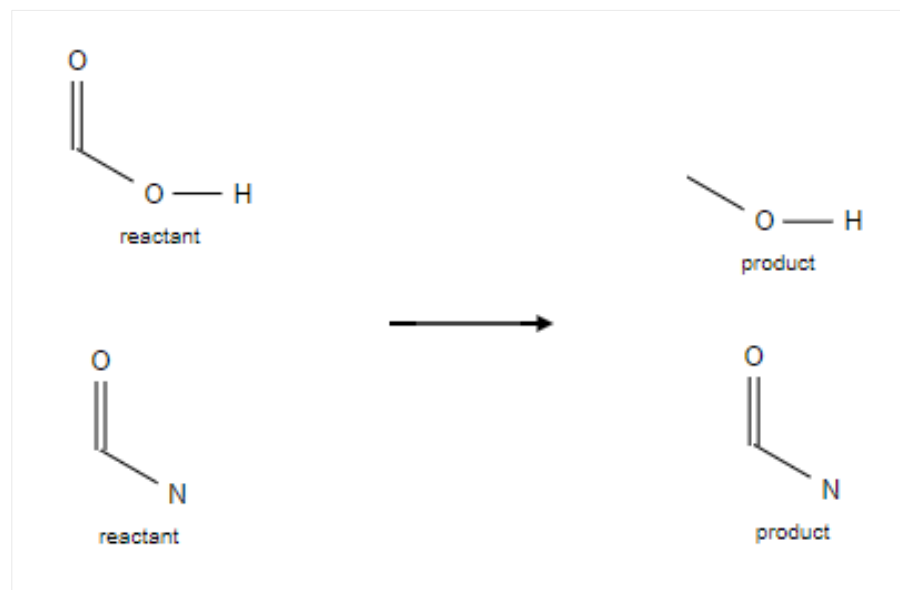
Substance Details

Reference Details

Export Cancel

The screenshot displays the SciPlanner software interface. The main workspace shows a chemical reaction scheme with three steps. Step 1 involves the reaction of a cyclohexylamine derivative with a benzene ring. Step 2 involves the reaction of a carboxylic acid derivative with a benzene ring. The final product is a complex molecule. An 'Export' dialog box is open on the right, showing options for 'Offline Review' (Portable Document Format, Citations, Image) and 'Saving Locally' (SciPlanner eXchange). The 'Details' section includes fields for 'File Name' and 'Title', and a list of items to include in the export (SciPlanner Image, Reaction Details, Substance Details, Reference Details). The 'Export' button is highlighted.

片段结构的化学选择性反应



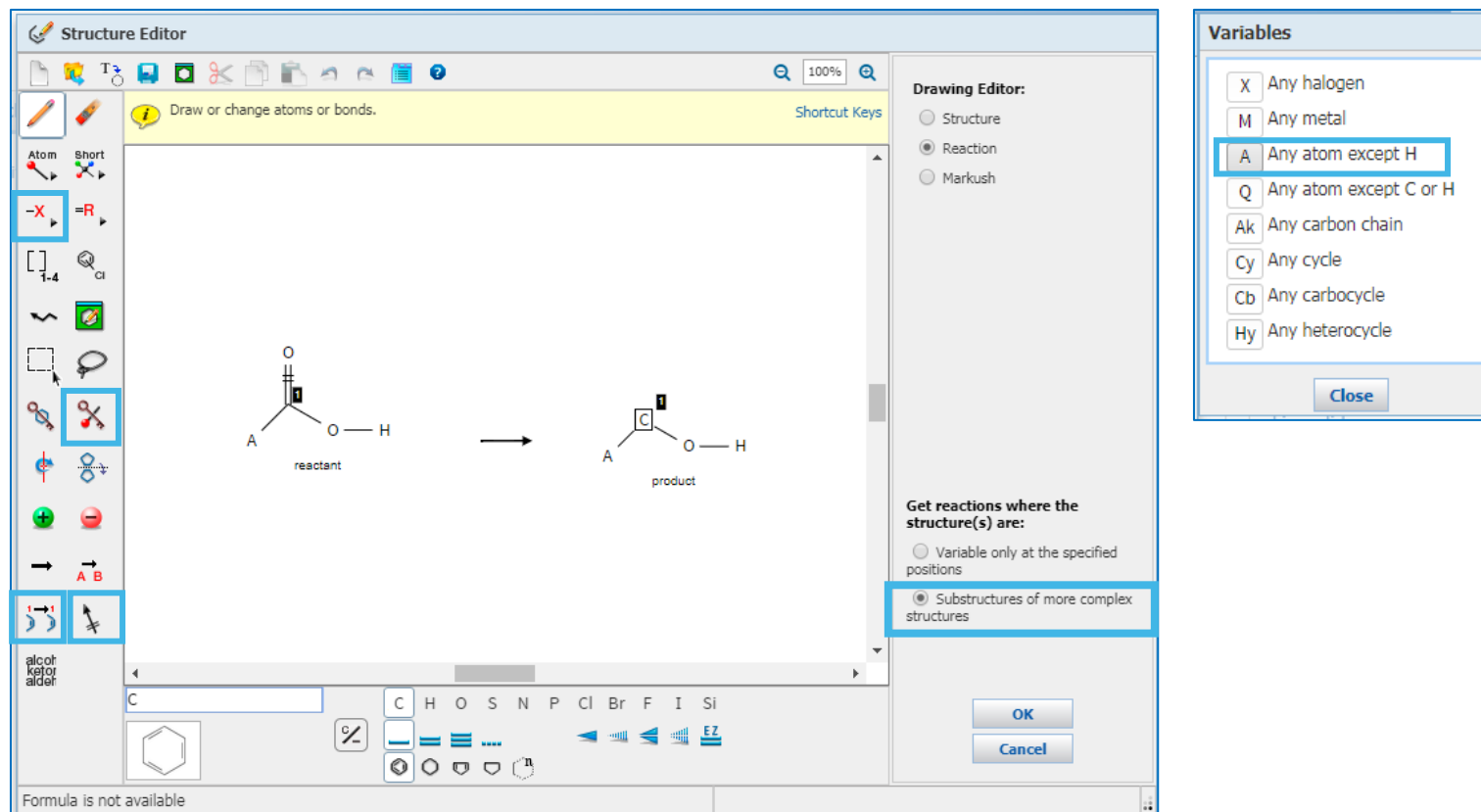
检索要求:

1. 反应物中含有羧基和酰胺基团;
2. 反应物种的羧基被还原为产物中的羟基;
3. 反应物中的酰胺基在反应后没有发生变化。

分析:

化学选择性反应可以使用non-participating functional groups来限定不参与反应的官能团。

绘制反应式



可提前选择不参与反应的官能团

The screenshot displays the ACS Reaxys search interface. On the left is a sidebar with navigation options: Author Name, Company Name, Document Identifier, Journal, Patent, Tags, SUBSTANCES (with sub-options: Chemical Structure, Markush, Molecular Formula, Property, Substance Identifier), and REACTIONS (with sub-option: Reaction Structure). The main area is titled 'Structure Editor' and includes tabs for 'Java' and 'Non-Java'. Below these is a chemical reaction scheme showing a reactant with a carbonyl group reacting to form a product. To the right of the reaction scheme are 'Search Type' options: 'Allow variability only as specified' and 'Substructure' (selected). Below the reaction scheme is a 'Click image to change structure or view detail.' instruction and an 'Import CXF' button. A 'Search' button is prominently displayed. Below the 'Search' button is a link to 'Advanced Search' and an 'Always Show' checkbox. At the bottom, there is a 'Solvents' section with a 'Select Solvents' button and a 'Non-participating Functional Groups' section with a 'Close' button. The 'Non-participating Functional Groups' list includes: 'All' (selected), '217' (dropdown), '1 Selected', 'Clear Selections', 'pi-Allyl', 'Allyl Alcohol', 'Allyl Halide', 'Amide' (checked), and 'Amidine'.

1. 点击高级检索;
2. 点击不参与反应官能团;
3. 选择酰胺amide。

反应结果分组

点击Group by中的Transformation, 显示反应类型

Reaction Structure substructure with limiters > reactions (4522)

REACTIONS ?

Get References Tools

Analyze Refine

Analyze by: ?
Reagent

NaBH ₄	1888
EtN(Pr-) ₂	1819
HCl	1745
Et ₃ N	1738
F ₃ CCO ₂ H	1345
NaOH	1345
AcOH	1261
H ₂	1238
NaHCO ₃	917
H ₂ O	766

Show More

Group by: No Grouping Sort by: Accession Number

1. View Reaction Detail Link

2 Steps Hover over any structure for more options.

Overview

2. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.

Group by Transformation 根据反应转化类型分组

Reaction Structure substructure with limiters > reactions (4522)

REACTIONS

Get References Tools

Analyze Refine

Analyze by:
 Reagent

NaBH ₄	1888
EtN(Pr- <i>i</i>) ₂	1819
HCl	1745
Et ₃ N	1738
F ₃ CCO ₂ H	1345
NaOH	1345
AcOH	1261
H ₂	1238
NaHCO ₃	917
H ₂ O	766

Show More

Group by: Transformation Sort by: Frequency

673 of 4522 Reactions Selected

☒ 1. Reduction of Carboxylic Acids to Alcohols
673 Reactions (673 Selected)

$$\text{R}-\text{C}(=\text{O})\text{OH} \longrightarrow \text{R}-\text{CH}_2\text{OH}$$

☐ 2. Acylation of Nitrogen Nucleophiles by Carboxylic Acids
102 Reactions (23 Selected)

$$\text{R}-\text{C}(=\text{O})\text{OH} + \text{R}^1-\text{NH}-\text{R}^1 \longrightarrow \text{R}-\text{C}(=\text{O})\text{N}(\text{R}^1)_2$$

☐ 3. Transamidation/ Zip Reaction
75 Reactions (16 Selected)

$$\text{R}^2-\text{C}(=\text{O})\text{N}(\text{R}^1)_2 + \text{R}-\text{NH}-\text{R}^1 \longrightarrow \text{R}^2-\text{C}(=\text{O})\text{N}(\text{R})_2 + \text{R}^1-\text{NH}-\text{R}^1$$

☐ 4. Formation of Alkyl Halides/ Alcohols from Ethers /Silyl Ethers
73 Reactions (5 Selected)

$$\text{R}-\text{O}-\text{R}^1 \xrightarrow{\text{HX}} \text{R}-\text{X} + \text{R}^1-\text{OH}$$

$\text{R}^1 = \text{CR}'_3, \text{SiR}'_3$

选择羧酸还原为醇的这类反应

获得反应结果

Reaction Structure substructure with limiters > reactions (4522) > reactions with transformation "Reduction of Carboxylic Acids ..." (673)

REACTIONS

Get References Tools

Analyze **Refine**

Analyze by:
 Reagent

NaBH ₄	401
Et ₃ N	151
N-Methylmorpholine	149
ClCO ₂ Bu- <i>i</i>	136
HCl	129
ClCO ₂ Et	110
BH ₃ -THF	74
H ₂ O	71
MeOH	54
LiAlH ₄	52

Show More

Group by: No Grouping Sort by: Accession Number

0 of 673 Reactions Selected

1. **View Reaction Detail** Similar Reactions

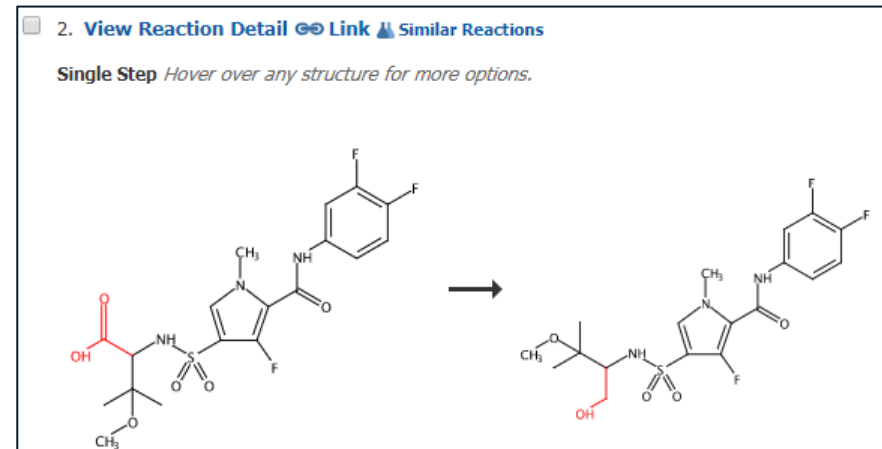
Single Step *Hover over any structure for more options.*

90%

Overview

2. **View Reaction Detail** Similar Reactions

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



反应检索小结：

- 反应检索方法汇总与区分；
- 反应绘制工具的灵活使用；
- 反应结果的快速纵览及筛选，例如non-participating functional group；
- 反应结果分组：Group by Transformation/Document
- 相似反应的获取获得更多启发
- CAS Synthetic Methods获取反应详情
- SciPlanner工具助于自定义设计拟合成反应路线

大纲

- CAS SciFinder介绍
- 文献相关信息的获取策略
 - 储能材料文献检索方法
 - 文献结果分析、精炼和详情
 - 如何高效阅读专利文献详情(CAS PatentPak)
- 物质相关信息的获取策略
 - 如何检索无机化合物、配位化合物和聚合物
 - 物质结果分析、精炼和详情
- 反应相关信息的获取策略
 - 反应的获取方法
 - 反应结果分析、精炼及详情
 - 如何高效获取反应详情 (Synthetic Methods)
- 如何高效获取分析方法详情 (CAS Analytical Methods)

高效获取分析方法详情

CAS Analytical Methods

- CAS Analytical Methods介绍
- 关键词检索
- 检索结果的分析、精炼与详情
- 多个分析方法的对照



CAS Analytical Methods分析方法类别

目前有13个大类，45个小类；某些子类属于多种方法分类：

Organic Compound Analysis: 天然产物分离分析，手性分离，活性药物成分及代谢产物分析…

Organometallics / Inorganics: 地质分析，无机物分析，金属有机化合物分析

Pharmacology / Toxicology: 成瘾药物检测，有毒物检测…

Bioassays: 生物探针，生物标定细胞实验，生物标定药物实验，生物医学材料分析，生物分子/生物组织分离测定…

Water Analysis: 阴阳离子分析，元素测定，痕量元素分析，废水分析，生物标记公共卫生分析…

Historical Analysis / Dating: 考古分析，同位素分析

Environmental Analysis: 土壤/空气/水分析，农药残留分析…

Agricultural Applications / Analysis: 除草剂分析…

Food Analysis: 脂肪酸分析，脂肪酸酯分析，蛋白质分析…

Fuels / Geology / Biofuels: 生物燃料分析，油气分析，石油产品分析，煤炭加工…

Miscellaneous: 化妆品分析，爆炸物分析，纳米材料分析…


Water: 阴阳离子分析、环境分析、废水分析、微量元素分析…


Polymer: 聚合物分析…




简洁易用的检索界面

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Search

Enter keyword, matrix, analyte, etc.


Advanced Search



Browse Method Categories

Agricultural Applications / Analysis	Fuels / Geology / Biofuels	Pharmacology / Toxicology
Bioassays	Historical Analysis / Dating	Polymer Analysis
Biomolecule Isolation	Miscellaneous	Water Analysis
Environmental Analysis	Organic Compound Analysis	
Food Analysis	Organometallics / Inorganics	

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- taxol d
- taxoleic acid

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AND ▾ Technique ▾ HPLC ×

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检索结果分析与精炼

分析物

基质

方法分类

技术&仪器

年份

Method Category

- ☐ Element Detection (47)
- ☐ Biomolecule Isolation Assay (30)
- ☐ Water / Wastewater / Sludge Analysis (30)
- ☐ Suboptimal Analysis (28)
- ☐ Toxin Assay (16)

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Technique

- ☐ Electrothermal atomic absorption spectroscopy (20)
- ☐ Solid phase extraction (18)
- ☐ Fluorescence spectroscopy (15)
- ☐ HPLC (14)
- ☐ Chemical vapor deposition (13)

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Year

- ☐ 2016 (36)
- ☐ 2007 (23)
- ☐ 2019 (23)
- ☐ 2009 (14)
- ☐ 2015 (14)

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CAS Analytical Methods

boron nitride

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Compare (0/3)

☐ Analysis of Atomic nitrogen in Boron nitride by Chemical digestion

CAS MN: 1-119-CAS-264573

[View Details & Instructions](#)

[Add to Compare](#)

Analyte	Atomic nitrogen
Matrix	Boron nitride
Other Materials	Reagent: Hydrofluoric acid; Methyl red; Sodium hydroxide; Ethanol; Methylene blue; Sulfuric acid Material: PTFE-container; Volumetric flask (100 mL); Erlenmeyer flask
Method Category	Element Detection
Technique	Acid-base titration; Chemical digestion
Equipment Used	High pressure decomposition device; Distillation device
Source	The precise determination of nitrogen in boron nitride Gruner, W.; Hassler, J.; Barth, P.; Behm, J.; Sunderkoetter, J. Journal of the European Ceramic Society (2009), 29 (10), 2029-2035. Elsevier Ltd.

[Full Text](#)

[Abstract](#)

分析方法详情

Method Detail

(1 of 192)

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↓

★

Analysis of Atomic nitrogen in Boron nitride by Chemical digestion

CAS MN: 1-119-CAS-264573

Method Category:

Element Detection

Technique:

Acid-base titration; Chemical digestion

Materials	Role	Image	CAS RN
Atomic nitrogen	analyte	View Structure	17778-88-0
Boron nitride	matrix	View Structure	10043-11-5
PTFE-container	material		
Volumetric flask (100 mL)	material		
Erlenmeyer flask	material		
Hydrofluoric acid	reagent	View Structure	7664-39-3
Methyl red	reagent	View Structure	493-52-7
Sodium hydroxide	reagent	View Structure	1310-73-2
Ethanol	reagent	View Structure	64-17-5
Methylene blue	reagent	View Structure	61-73-4
Sulfuric acid	reagent	View Structure	7664-93-9

所用材料、标题摘要、著录信息、仪器

Source

The precise determination of nitrogen in boron nitride

Gruner, W.; Hassler, J.; Barth, P.; Behm, J.; Sunderkoetter, J.

Journal of the European Ceramic Society (2009), 29 (10), 2029 - 2035. Elsevier Ltd.

CODEN: JECSER | ISSN: 09552219 | DOI: 10.1016/j.jeurceramsoc.2008.12.021

Full Text

Abstract

To further improve the high performance ceramic material BN it is necessary to advance its analytics. The quant. determination of the nitrogen content as main component is compared by three methods: the carrier gas hot extraction, the LiOH fusion, and the Kjeldahl method. Thereby specific methodical aspects are critically highlighted with respect to the trueness and precision of the nitrogen anal. The "chem." plays a fundamental role in all methods. In the case of the instrumental anal. by CGHE important critical aspects are the calibration of CGHE measurements and the improvement of reproducibility which needs a much better understanding of the chem. reactions in the crucible. In case of the Kjeldahl method it is of decisive importance to apply an adequate high temperature of 260° for decomposition, whereas the melt-decomposition with LiOH is affected by melt additions

Equipment Used

High pressure decomposition device, Berghof Products and Instruments GmbH, Germany

Distillation device, Vapodest 3, erhardt Laboratory Systems, Germany

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分析方法详情

操作步骤和数据有效性验证

Instructions

Boron nitride sample

1. Collect boron nitride sample containing 0.1% soluble boric oxide, 0.7% oxygen for analysis.

Digestion

1. Weigh 0.2 g of the BN sample in a PTFE-container with 10 mL of HF-acid (40%).
2. Decompose the sample for 20 h at a temperature of 260 °C in a high pressure decomposition device (Berghof Products and Instruments GmbH, Germany).
3. Cool the solution and transfer into a volumetric flask (100 mL).

Acid-base titration using Kjeldahl method

1. Measure 20 - 30 mL of the solution in a sample cup and transfer into the Kjeldahl container built into the distillation device (Vapodest 3, erhardt Laboratory Systems, Germany).
2. Titrate 30 mL sulfuric acid (0.05 mol/L) into an Erlenmeyer flask and dilute with approximately 120 mL of water.
3. Add 2 - 3 mL of indicator solution (0.2% methyl red + 0.1% methylene blue in ethanol p.a.).
4. Apply the solution of sodium hydroxide (40%) to the sample and distill with steam into the Erlenmeyer flask.
5. Titrate excessive sulfuric acid with sodium hydroxide solution (0.1 mol/L).
6. Calculate the nitrogen content as wt.% using the following equation: $N_{\text{total}}\% = (V_{\text{H}_2\text{SO}_4}f_{\text{H}_2\text{SO}_4} - V_{\text{NaOH}}f_{\text{NaOH}})F/m_S$; V_{acid} : consumption of 0.1 M H_2SO_4 [mL]; F : 70945 (titrimetric factor with 0.2 g solid sample); $f_{\text{H}_2\text{SO}_4}$: titration correction factor of H_2SO_4 solution; f_{NaOH} : titration correction factor of NaOH solution; m_S : sample mass of taken liquid [mg].

Validation

Precision	0.20% (RSD)
Concentration	55.76 ± 0.11% wt

浏览方法分类

Browse Method Categories

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Bioassays

Biomolecule Isolation

Environmental Analysis

Food Analysis

Fuels / Geology / Biofuels

Historical Analysis / Dating

Miscellaneous

Organic Compound Analysis

Organometallics / Inorganics

Pharmacology / Toxicology

Polymer Analysis

Water Analysis

[Browse Method Categories](#) > Organic Compound Analysis

Active Pharmaceutical Ingredient and Metabolite Analysis

Chiral Separation

Natural Product Isolation Analysis

Organic Compound Analysis

对照多个感兴趣的分析方法详情

CAS Solutions
Analytical Methods

Browse: Organic Compound Analysis

Return to Home

^ Analyte
☐ Naphthalene (1837)
☐ Toluene (1651)
☐ Anthracene (1543)
☐ Pyrene (1451)
☐ Phenanthrene (1411)
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^ Matrix
☐ Urine (941)
☐ Water (628)
☐ Drinking waters (555)
☐ Blood serum (515)
☐ River waters (498)
[View All](#)

^ Method Category

^ Technique

^ Year

Results (33850)

Sort Relevance

☐

☐ **Analysis of Sulfitecobalamin by Reversed-phase HPLC**
CAS MN: 1-132-CAS-468124

Analyte	Sulfitecobalamin
Other Materials	Reagent: Hypochlorous acid; Ethanol Material: Sep-Pak Vac (5 g) C ₁₈ cartridge; Reversed-phase HPLC column (Wakosil-II 5C18RS Φ 4.6 × 150 mm ² ; particle size 5 μm) View All
Method Category	Organic Compound Analysis
Technique	UV-visible spectroscopy; Reversed-phase HPLC; Solid phase extraction
Equipment Used	High-performance liquid chromatographic system; UV-Visible detector; System controller; Degasser; HPLC pumps; Column oven; Chromatodata processing system
Source	Food Additives (Hypochlorous Acid Water, Sodium Metabisulfite, and Sodium Sulfite) Strongly Affect the Chemical and Biological Properties of Vitamin B₁₂ in Aqueous Solution Okamoto, Naho; Bito, Tomohiro; Hiura, Nanami; Yamamoto, Ayaka; Iida, Mayu; Baba, Yasuhiro; Fujita, Tomoyuki; Ishihara, Atsushi; Yabuta, Yukinori; Watanabe, Fumio ACS Omega (2020), 5 (11), 6207-6214. American Chemical Society <input type="button" value="Full Text"/>

Results (33850) Sort Relevance ▾

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☐ **Analysis of Sulfitocobalamin by Reversed-phase HPLC**
 CAS MN: 1-132-CAS-468124
[View Details & Instructions](#) [Remove from Compare](#)

Analyte	Sulfitocobalamin
Other Materials	Reagent: Hypochlorous acid; Ethanol Material: Sep-Pak Vac (5 g) C ₁₈ cartridge; Reversed-phase HPLC column (Wakosil-II 5C18RS Φ 4.6 × 150 mm ² ; particle size 5 μm) View All ▾
Method Category	Organic Compound Analysis
Technique	UV-visible spectroscopy; Reversed-phase HPLC; Solid phase extraction
Equipment Used	High-performance liquid chromatographic system; UV-Visible detector; System controller; Degasser; HPLC pumps; Column oven; Chromatodata processing system
Source	Food Additives (Hypochlorous Acid Water, Sodium Metabisulfite, and Sodium Sulfite) Strongly Affect the Chemical and Biological Properties of Vitamin B₁₂ in Aqueous Solution

对照多个感兴趣的分析方法详情

Compare Methods			
<div>Expand All Collapse All</div>			
	1	2	3
Title	Analysis of Sulfitocobalamin by Reversed-phase HPLC	Analysis of Phenol by Spectrophotometry	Analysis of 2-Chlorophenol in Irrigation waters by Solid phase extraction
CAS Method Number	1-132-CAS-468124	1-132-CAS-467381	1-132-CAS-466437
Method Category	Organic Compound Analysis	Organic Compound Analysis	Organic Compound Analysis
Technique	UV-visible spectroscopy; Reversed-phase HPLC; Solid phase extraction	Spectrophotometry	Liquid chromatography diode array detectors; Reversed-phase HPLC; Solid phase extraction
Analyte	Sulfitocobalamin	Phenol	2-Chlorophenol; 2,4-Dichlorophenol; 3-Chlorophenol; 2,3-Dichlorophenol; Chlorophenols
Matrix			Irrigation waters
Other Materials	Hypochlorous acid; Ethanol; Sep-Pak Vac (5 g) C ₁₈ cartridge; Reversed-phase HPLC column (Wakosil-II 5C18RS Φ 4.6 × 150)	3-Methyl-2-benzothiazolinone hydrazone; Phosphate; Glutaraldehyde; Reed	Hydrochloric acid; Sodium hydroxide; 1,3,5-Triphenylbenzene; Dimethoxymethane; Iron chloride (FeCl ₃); Methanol; Dichloroethane;

Equipment Used	High-performance liquid chromatographic system, Shimadzu; UV-Visible detector, SPD-10AV, Shimadzu; System controller, SCL-10A	UV-Vis spectrophotometer, Lambda 2, PerkinElmer, Waltham, MA	HPLC-DAD instrument, LC-20AT, Shimadzu, Japan
Source	Food Additives (Hypochlorous Acid Water, Sodium Metabisulfite, and Sodium Sulfite) Strongly Affect the Chemical and Biological	Reed Membrane as a Novel Immobilization Matrix for the Development of an Optical Phenol Biosensor	Layered porous organic frameworks as a novel adsorbent for the solid phase extraction of chlorophenols prior to their
Preparation		Fabrication of the reed biosensor 1. Peel a reed membrane carefully from	Preparation of amorphous porous organic frameworks (A-POF) 1. Dissolve FeCl ₃ (4.87 g), 1,3,5-
Method	Treatment cyanocobalamin (CN-B ₁₂) 1. Treat cyanocobalamin (CN-B ₁₂) with hypochlorous acid water (an effective	Analysis of phenol by spectrophotometry 1. Perform the analysis on a UV-Vis spectrophotometer Lambda 2	Solid phase extraction 1. Prepare the SPE cartridge by packing an empty 3 mL SPE cartridge with 30
Retention Time	27.171 min		
Linearity Range		5 - 100 μM	
Limit of Detection		2.5 μM	
Recovery			30% in 80.0 ng/mL added concentration (read from figure), 2-chlorophenol, 39% in 80.0 ng/mL added concentration (read from

CAS Analytical Methods使用方法小结：

- CAS Analytical Methods目前有13个大类，45个小类；某些子类属于多种方法分类；
- 可通过关键词检索，或者浏览方法分类来获取分析方法结果；
- 检索结果可通过分析物、基质、方法分类、技术&仪器，以及年份来纵览或精炼；
- 所有的分析方法都可获取详情，包括所用材料、标题摘要、著录信息、仪器、实验条件、操作步骤和数据有效性验证等信息；
- 支持三种不同的分析方法之间的对照，以表格的形式清晰对比呈现所有的实验详情。

谢谢关注!



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