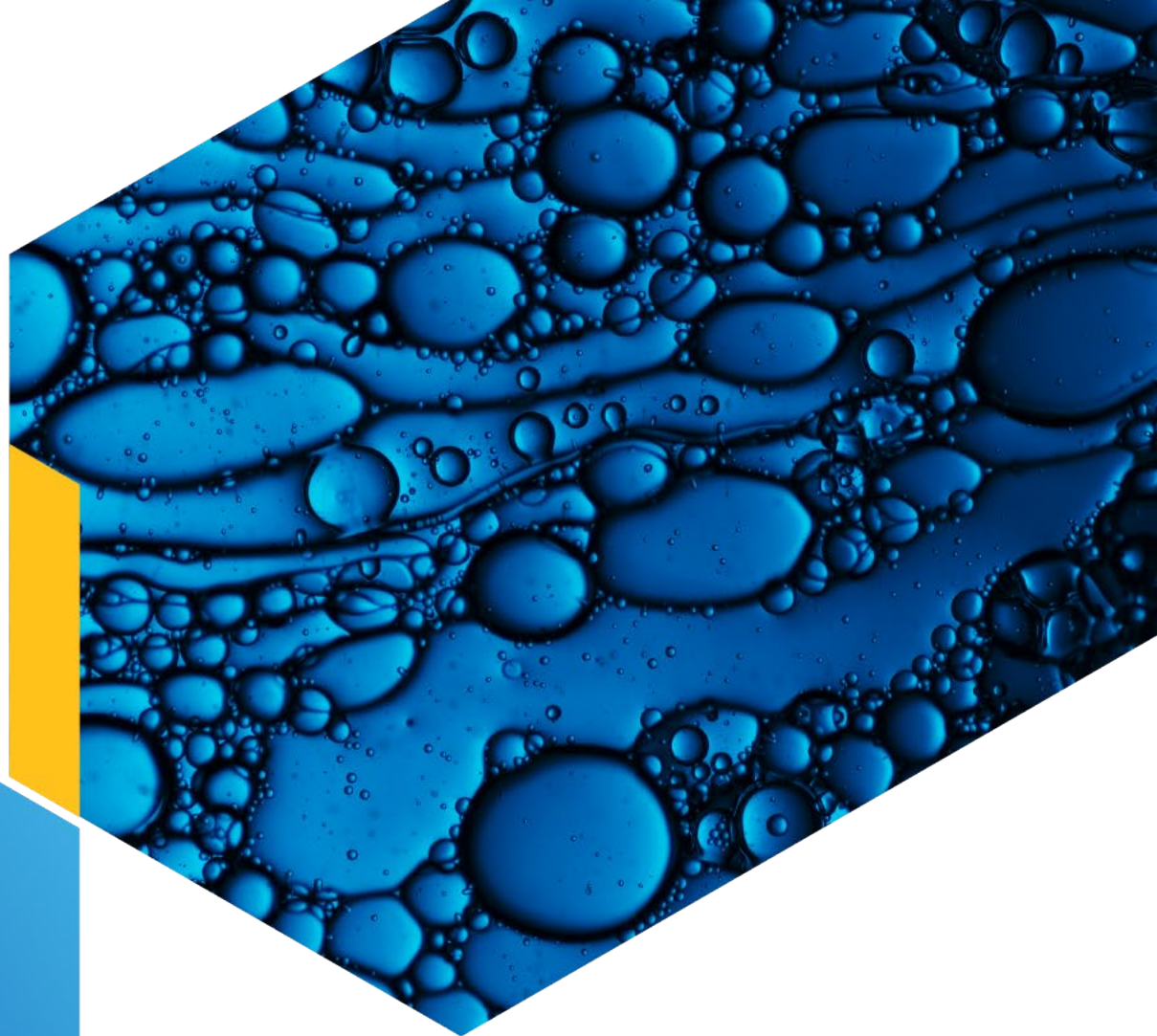


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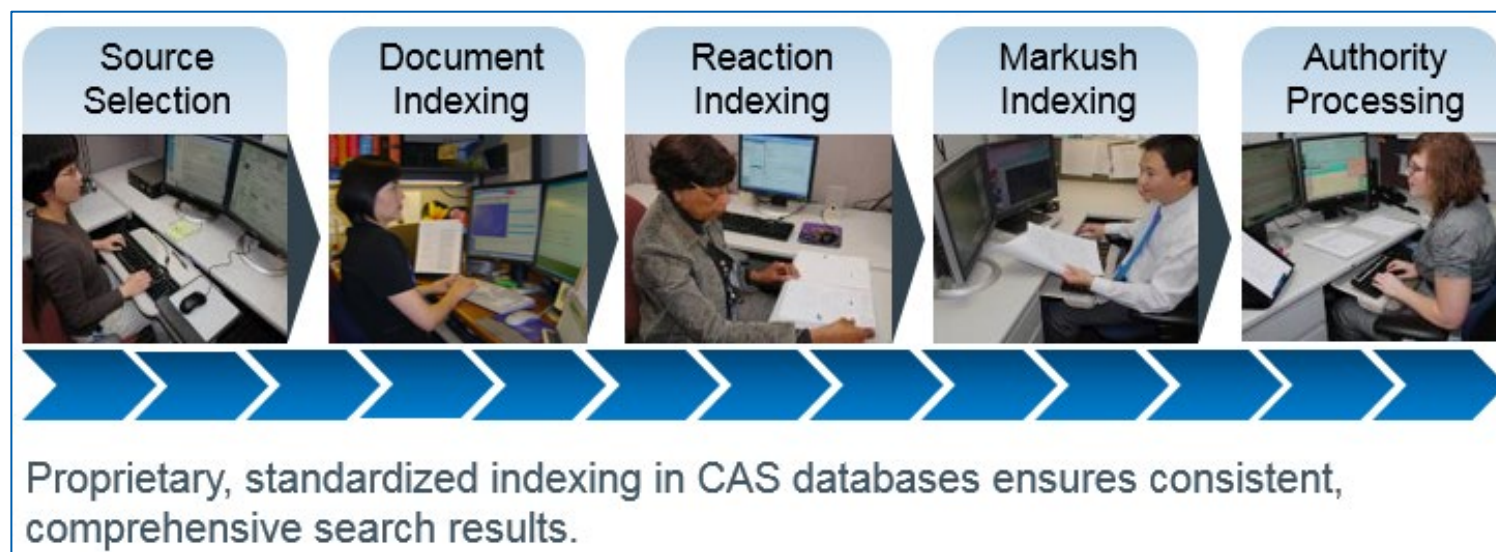
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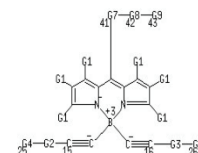
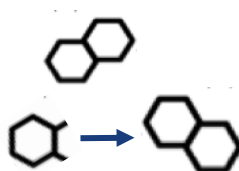
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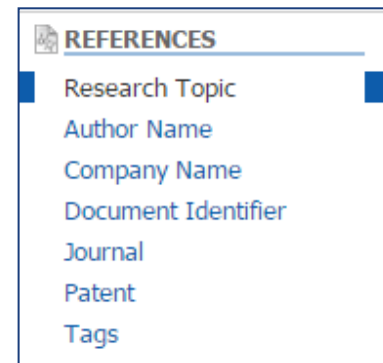
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Page: 1 of 24

Analyze by: Author Name

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Peng Huisheng	21
Wei Fei	20
Iyakutti K	14
Sakaida Yasushi	14
Dai Liming	13
Gogotsi Yury	13
Kim Seon Jeong	13
Lu Yunfeng	13
Zhang Qiang	13

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- Carbon nanotube and preparation method and application thereof [Machine Translation].**
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By Ding, Bing; Chen, Shuang; Zhang, Xiaogang; Lin, Qingyang; Hu, Ben
From Faming Zhuanyi 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...
- Simultaneous improvements in conversion and properties of molecularly controlled CNT fibres**
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By Mikhailchan, 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...
- Energy storage battery for new energy vehicle [Machine Translation].**
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By Gong, Geling; Tang, Bing
From Faming Zhuanyi 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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Document Type	
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Author Name ▼

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Zhang Qiang	30
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Liu Chang	21
Li Feng	19
Zhang Xiaogang	19
Chen Jun	18

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Tsinghua university, Peop Rep China	69
Fudan University, Peop Rep China	64
Massachusetts Institute of Technology, USA	40
Nanyang Technological University, Singapore	35
University of California, USA	33
USA	26
Zhejiang University, Peop Rep China	24
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Journal	2413
Online Computer File	1748
Patent	890
General Review	337
Conference	292
Meeting Abstract	211
Article	79
JOURNAL ARTICLE	79
Computer Optical Disk	71
RESEARCH SUPPORT NONUS GOVT	32

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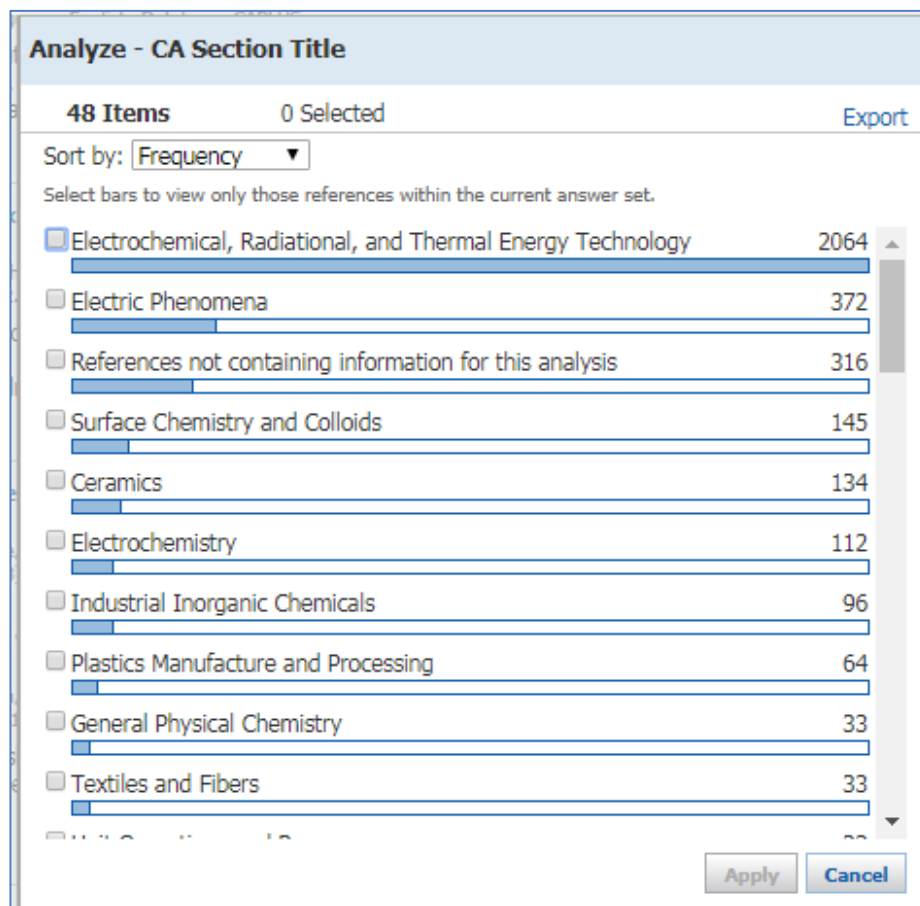
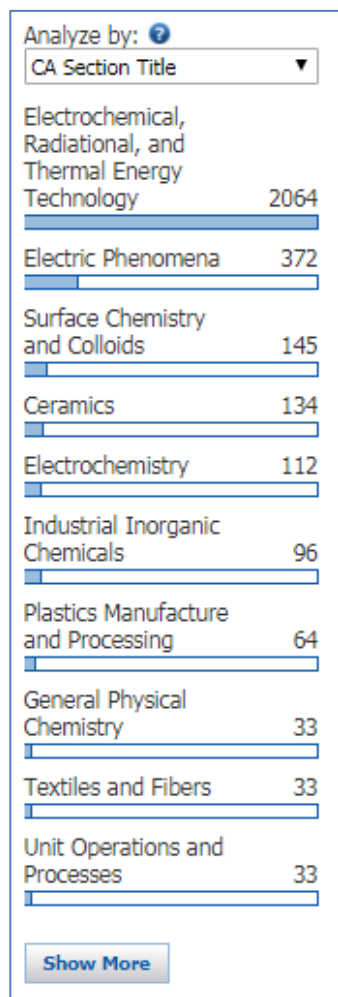
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Journal Name ▼

Faming Zhuanli Shenqing	391
PCT Int. Appl.	192
U.S. Pat. Appl. Publ.	152
Journal of Materials Chemistry A: Materials for Energy and Sustainability	146
ACS Applied Materials & Interfaces	87
RSC Advances	84
Electrochimica Acta	74
Journal of Power Sources	70
Advanced Materials (Weinheim, Germany)	62
Carbon	59

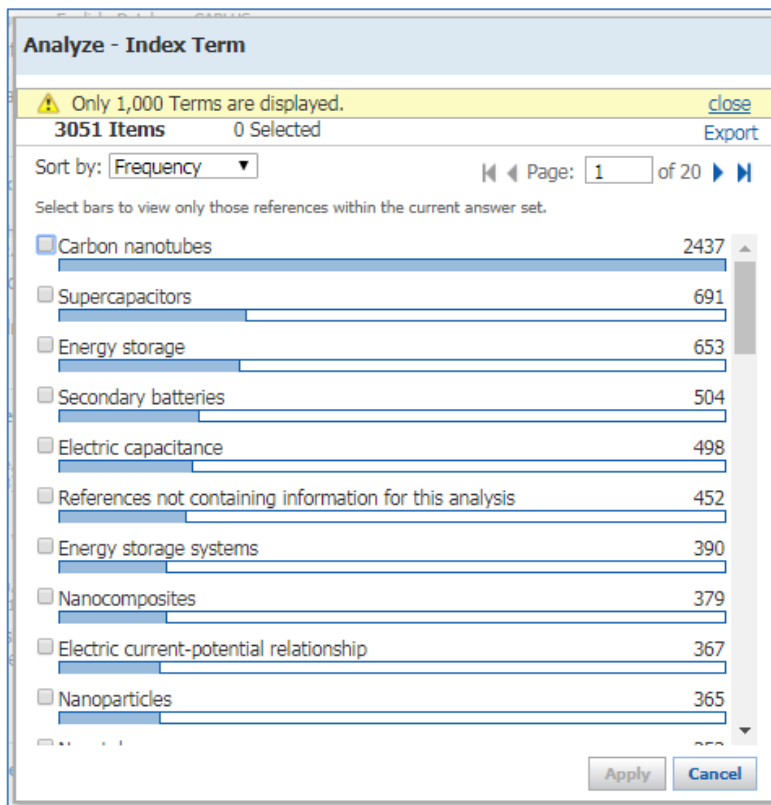
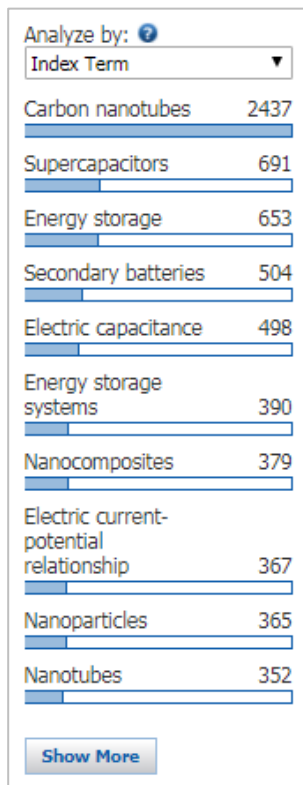
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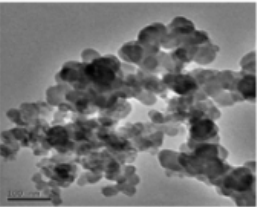
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Carbon nanotubes	663
Secondary batteries	504
Lithium-ion secondary batteries	262
Battery anodes	253
Carbon black	196
Battery cathodes	186
Fluoropolymers	176
Battery electrodes	171
Energy storage systems	145
Nanoparticles	127

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

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From Journal of Materials Chemistry A: Materials for Energy and Sustainability (2017), 5(45), 23434-23439. | Language: English, Database: CAPLUS

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Genetics & protein chemistry	Ceramics (12)	<input type="checkbox"/> Energy storage 124	
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Environmental chemistry	Imaging & recording (25)	<input type="checkbox"/> Secondary battery separators 50	
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Biology		<input type="checkbox"/> Sodium-ion secondary batteries 29	
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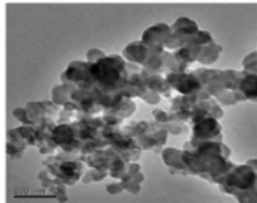
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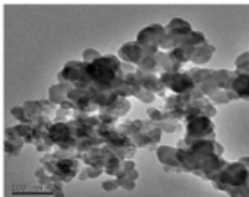
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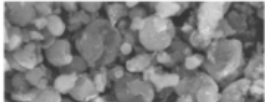
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Carbon nanotubes	321
Secondary batteries	256
Carbon black	159
Fluoropolymers	129
Battery anodes	114
Carbon fibers	113
Energy storage systems	108
Battery cathodes	102
Lithium-ion secondary batteries	91
Battery electrodes	81

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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 $h1 \leq 100 \text{ nm}$. 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


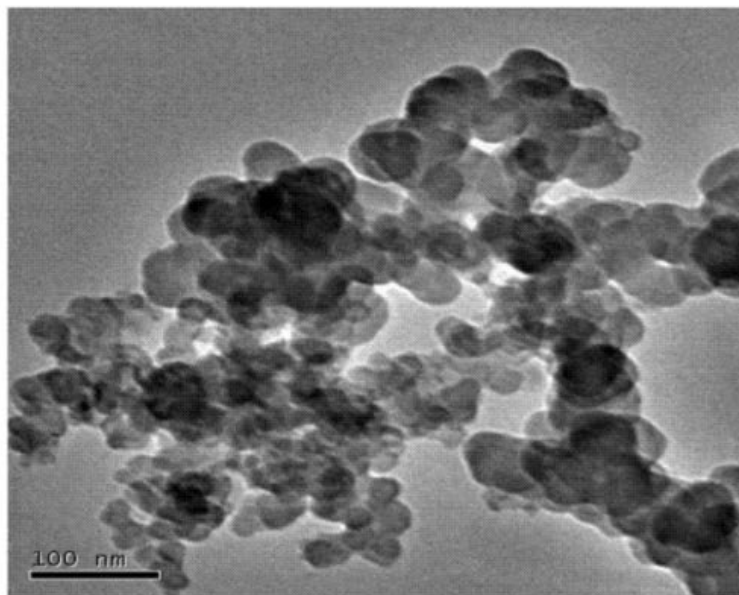
The method comprises using spray drying method for compounding and micro-nano structuralization of silica nanoparticle, protective agent and **carbon** nanomaterial, carrying out heat treatment under non-oxidn. atm. to prep. **carbon**/silica composite microsphere, and using metal thermal redn. method 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 prepd. 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. prepd. 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	PATENTPAK 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		Substances
Batteries Electrodes Energy storage systems Lithium-ion secondary batteries Supercapacitors Carbon nanotubes Energy storage Evaporation Nanostructured materials		7440-44-0 Activated carbon, uses  Page 2 in PATENTPAK
composite electrode material, prepn. method and application thereof		activated; composite electrode material, prepn. method and application thereof Physical, engineering or chemical process; Properties; Technical or engineered material use; Process; Uses
Carbon fibers		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  Page 2 in PATENTPAK 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		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		

标准概念词列表

物质CAS RN,
物质名称

物质功能描述

定位信息

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

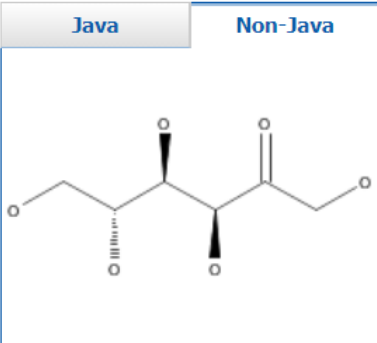
REACTIONS

- Reaction Structure

SUBSTANCES: CHEMICAL STRUCTURE

Structure Editor:

Java Non-Java



Click image to change structure or view detail.

Search Type:

- Exact Structure
- Substructure
- Similarity

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Search

[Advanced Search](#)

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

大纲

- CAS SciFinder介绍
- 文献相关信息的获取策略
 - 文献检索方法
 - 文献结果分析、精炼和详情
- 物质相关信息的获取策略
 - 物质检索方法
 - 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

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

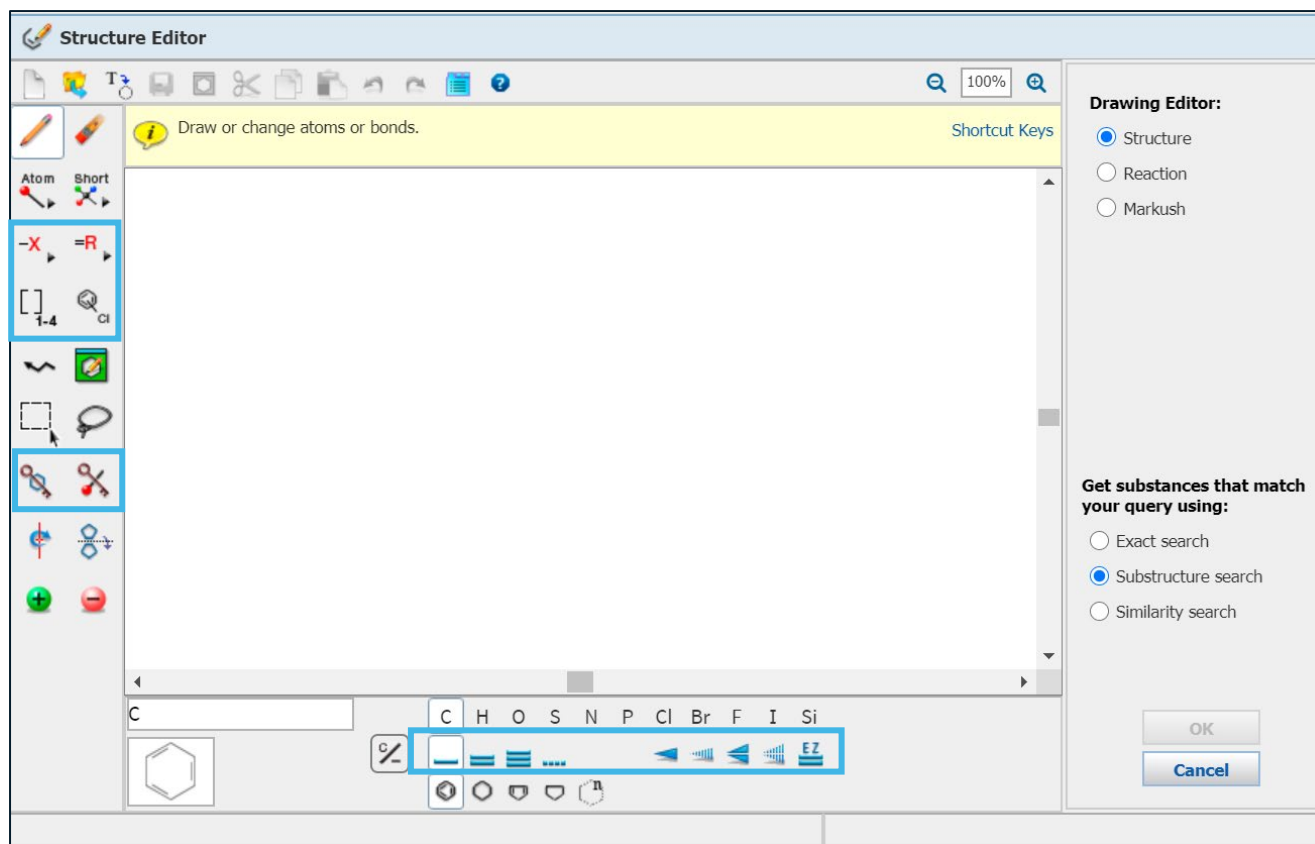
Molecular Formula

Property

Substance Identifier



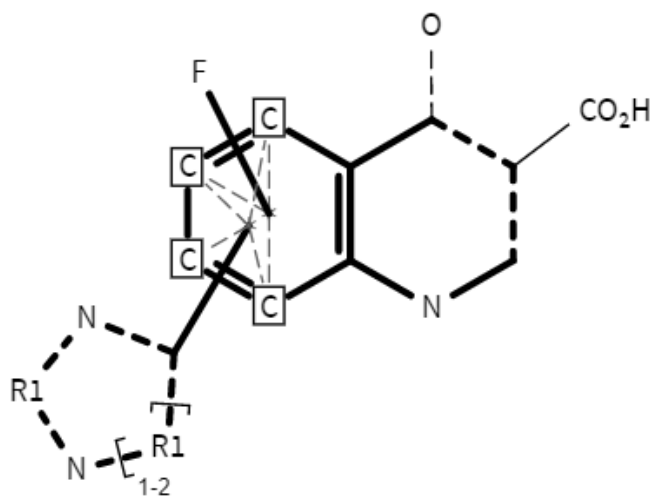
结构编辑器的使用



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

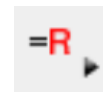
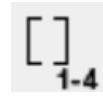
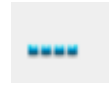
有机化合物: 通式结构的绘制



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

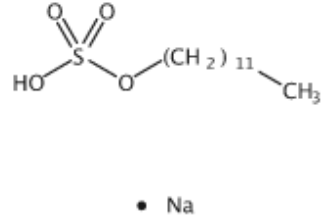
分子式输入需要遵守Hill排序规则:不含碳化合物,按元素符号的字母顺序排列;分子式为含碳化合物时,则“C”在前;如有氢则紧随其后,其它元素符号按字母顺序排在氢的后面

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 🧪

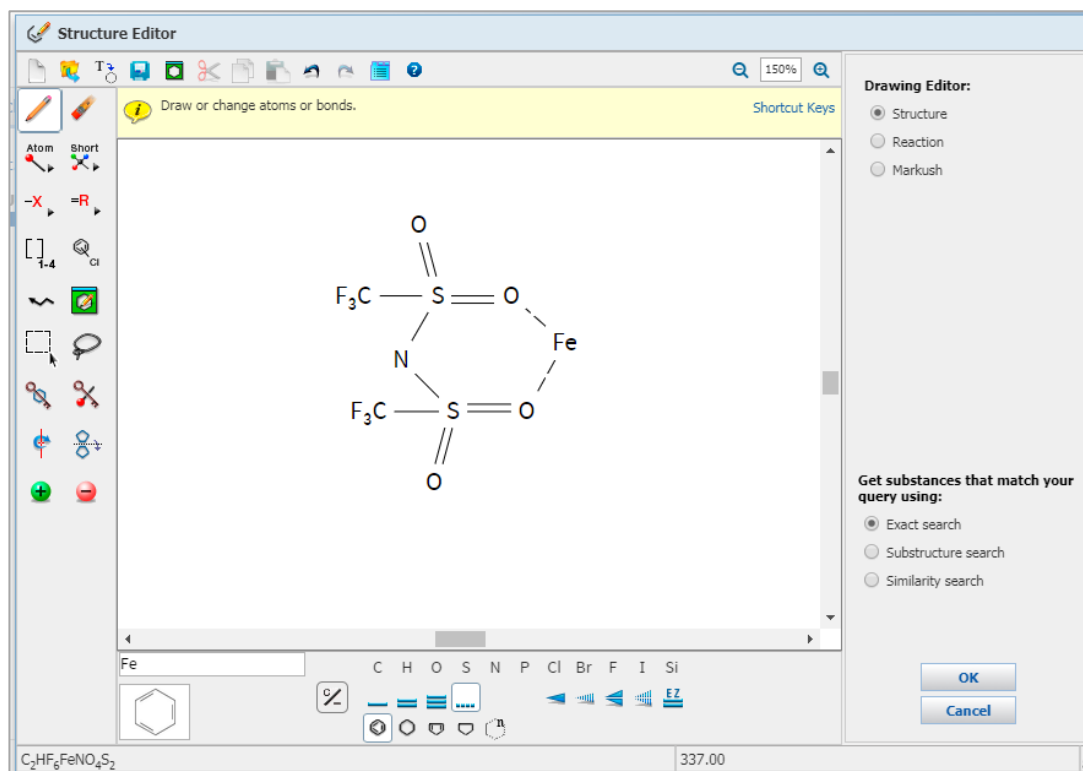


C₁₂ H₂₆ O₄ S . Na
Sulfuric acid monododecyl ester sodium salt (1:1)

▶ **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)

$C_2H_6N_4S_2 \cdot \frac{1}{2} Fe$
Methanesulfonamide, 1,1,1-trifluoro-*N*[(trifluoromethyl)sulfonyl]-, iron(2+) salt (2:1)

5. 1912405-54-9

1933513-70-2 (Component: 82113-65-3)
 $C_2H_6N_4S_2 \cdot \frac{1}{2} Fe$
Methanesulfonamide, 1,1,1-trifluoro-*N*[(trifluoromethyl)sulfonyl]-, iron(2+) salt (2:1)

6. 1706814-99-4

1706814-96-1
 $C_2F_6N_4S_2 \cdot \frac{1}{2} Fe H_{12}O_6$
98837-98-0
 $C_2F_6N_4S_2$

15365-81-8
 $Fe H_{12}O_6$

$C_2F_6N_4S_2 \cdot \frac{1}{2} Fe H_{12}O_6 \cdot 2 H_2O$
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

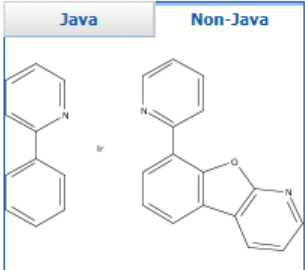
REACTIONS

- Reaction Structure

SUBSTANCES: CHEMICAL STRUCTURE

Structure Editor:

Java Non-Java



Search Type:

- Exact Structure
- Substructure
- Similarity

Show precision analysis

ChemDraw
Launch a SciFinder substance or reaction
More

Click image to change structure or view detail.

Import CXF

Search

Advanced Search Always Show

Characteristics

- Single component
- Commercially available
- Included in references

Classes

- Alloys
- Coordination compounds
- Incompletely defined
- Mixtures

Chemical Structure exact with limiters > substances (1)

SUBSTANCES

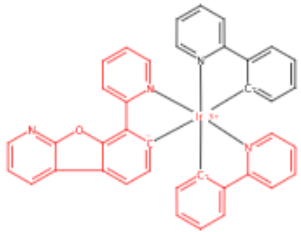
Get References Get Reactions Get Commercial Sources

Analyze Refine

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]-

Preparation 1
Process 1
Properties 1
Uses 1

Show More

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)

REFERENCES

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

SUBSTANCES

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

REACTIONS

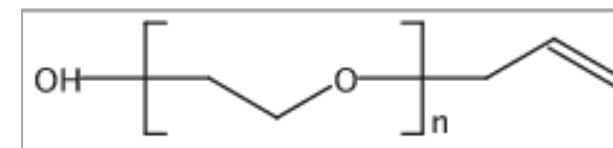
- Reaction Structure

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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Create Keep Me Posted Alert Send to SciPlanner

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

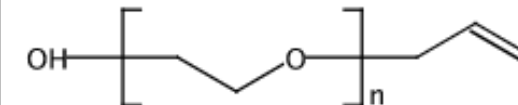
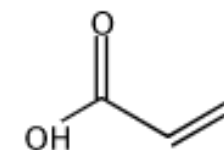
REACTIONS

- Reaction Structure

SUBSTANCES: MOLECULAR FORMULA

Examples:
H4SiO4
(C3H6O.C2H4O)x

Search



通过聚合物的重复结构单元来检索聚合物

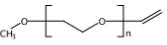
Get References | Get Reactions | Get Commercial Sources | Tools

Sort by: CAS Registry Number

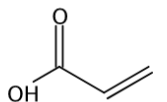
0 of 6 Substances Selected

1. 1580002-57-8

50856-25-2
(C₂H₄O)_n C₃H₆O



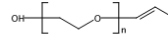
79-10-7
C₃H₄O₂



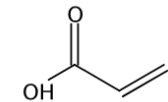
(C₃H₄O₂ · (C₂H₄O)_n C₃H₆O)_x
2-Propenoic acid, polymer with α-ethenyl-ω-methoxypoly(oxy-1,2-ethanediyl), graft

2. 1314225-78-9

191403-44-8
(C₂H₄O)_n C₃H₆O



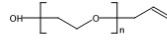
79-10-7
C₃H₄O₂



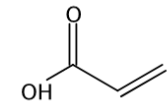
(C₃H₄O₂ · (C₂H₄O)_n C₃H₆O)_x
2-Propenoic acid, polymer with α-1-propen-1-yl-ω-hydroxypoly(oxy-1,2-ethanediyl), graft

3. 1010818-79-7

27274-31-3
(C₂H₄O)_n C₃H₆O



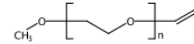
79-10-7
C₃H₄O₂



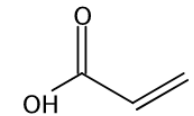
(C₃H₄O₂ · (C₂H₄O)_n C₃H₆O)_x
2-Propenoic acid, polymer with α-2-propen-1-yl-ω-hydroxypoly(oxy-1,2-ethanediyl), block

4. 250591-73-2

50856-25-2
(C₂H₄O)_n C₃H₆O



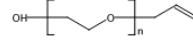
79-10-7
C₃H₄O₂



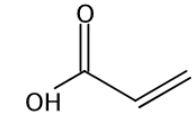
(C₃H₄O₂ · (C₂H₄O)_n C₃H₆O)_x
2-Propenoic acid, polymer with α-ethenyl-ω-methoxypoly(oxy-1,2-ethanediyl) (9CI)

5. 185506-87-0

27274-31-3
(C₂H₄O)_n C₃H₆O



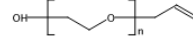
79-10-7
C₃H₄O₂



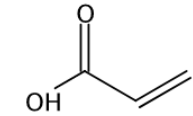
(C₃H₄O₂ · (C₂H₄O)_n C₃H₆O)_x
2-Propenoic acid, polymer with α-2-propen-1-yl-ω-hydroxypoly(oxy-1,2-ethanediyl), graft
Regulatory Information

6. 82850-00-8

27274-31-3
(C₂H₄O)_n C₃H₆O



79-10-7
C₃H₄O₂



(C₃H₄O₂ · (C₂H₄O)_n C₃H₆O)_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

Draw or change atoms or bonds. Shortcut Keys

Drawing Editor:

- Structure
- Reaction
- Markush

Get substances that match your query using:

- Exact search
- Substructure search
- Similarity search

Search Criteria:

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

Advanced Search Always Show

Characteristics

- Single component
- Commercially available
- Included in references

Classes

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

Studies

- Analytical
- Biological
- Preparation
- Reactant or reagent

通过聚合物的重复结构单元来检索聚合物

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

Analyze Refine Sort by: CAS Registry Number Display Options

0 of 134 Substances Selected Page: 1 of 9

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 Q
~1
 $(C_{56}H_{76}O_6S_2)_n$
INDEX NAME NOT YET ASSIGNED

2. 2089459-95-8 Q
~1
 $(C_{59}H_{79}F_2N_3S_4)_n$
INDEX NAME NOT YET ASSIGNED

3. 2056259-78-8 Q
~1
 $(C_{74}H_{122}N_2S_4)_n$
INDEX NAME NOT YET ASSIGNED

4. 1974335-87-9 Q
~1
 $(C_{62}H_{80}N_2O_2S_2)_n$
INDEX NAME NOT YET ASSIGNED

5. 1974335-85-7 Q
~1
 $(C_{70}H_{96}N_2O_2S_2)_n$
INDEX NAME NOT YET ASSIGNED

6. 1909267-21-5 Q
~1
 $(C_{32}H_{10}N_6S_5)_n$
INDEX NAME NOT YET ASSIGNED

通过聚合物的重复结构单元来检索聚合物

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Analyze Refine

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- Metal-Containing
- Commercial Availability
- Property Availability
- Property Value
- Reference Availability
- Atom Attachment

Structure Editor:

Java Non-Java

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Search type: **Substructure**

Only retrieve substances that:

- Have references
- Are commercially available
- Are a single component
- Are in specific substance

<input type="checkbox"/> 1. 2096989-39-6 ~1 (C ₅₆ H ₇₆ O ₆ S ₂) _n INDEX NAME NOT YET ASSIGNED	<input type="checkbox"/> 2. 2089459-95-8 ~1 (C ₅₉ H ₇₉ F ₂ N ₃ S ₄) _n INDEX NAME NOT YET ASSIGNED	<input type="checkbox"/> 3. 2056259-78-8 ~1 (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 	<input type="checkbox"/> 8. 1909267-19-1 ~1 	<input type="checkbox"/> 9. 1909267-18-0 ~1

Structure Editor

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Atom Report

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
C₇₄H₁₂₂N₂S₄

85.13

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

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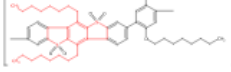
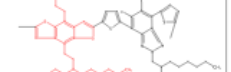
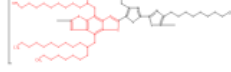
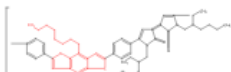
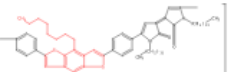
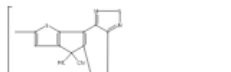





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 Are in specific substance classes
 Are in specific types of studies

 $(C_{56} H_{76} O_6 S_2)_n$ 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-d]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
 $C_{48}H_{70}Br_2N_2S_4$
 $(C_{48}H_{70}Br_2N_2S_4)_x$
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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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

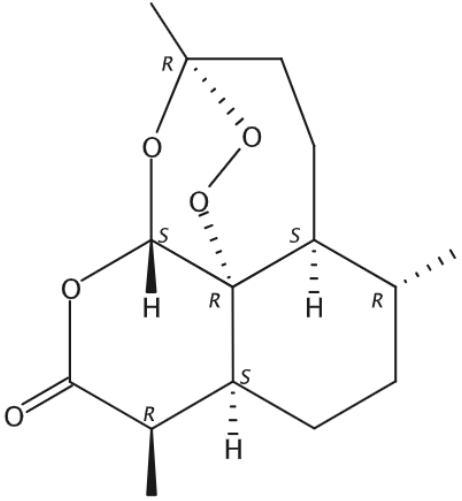
提示：
• 一次最多可输入25个物质。
• 每行一个物质标识符。

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

1. 63968-64-9

~6028 ~132



Absolute stereochemistry.

C₁₅H₂₂O₅
3,12-Epoxy-12H-pyrano[4,3-j]-1,2-benzodioxepin-10(3H)-one, octahydro-3,6,9-trimethyl-, (3R,5aS,6R,8aS,9R,12S,12aR)-

▶ **Key Physical Properties**
Regulatory Information
Spectra
Experimental Properties

CAS Registry Number: 63968-64-9

- » View Substance Detail
- 🔍 Explore by Structure ▶
- Synthesize this...
- Get Reactions where Substance is a ▶
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SUBSTANCE DETAIL [Get References](#) [Get Reactions](#) [Get Commercial Sources](#)

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CAS Registry Number 63968-64-9

~6,028 ~132

C₁₅H₂₂O₅
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*)-

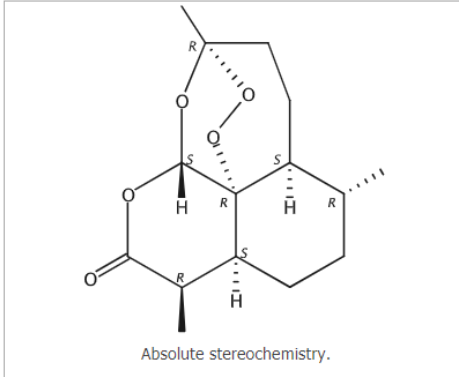
Molecular Weight
282.33

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
(+)-Arteannuin
(+)-Artemisinin
(+)-Qinghaosu
[View more...](#)



Absolute stereochemistry.

EXPERIMENTAL PROPERTIES

EXPERIMENTAL SPECTRA

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

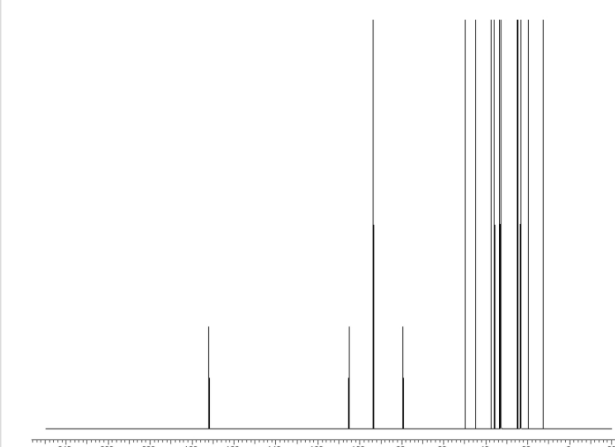
BIOACTIVITY INDICATORS

TARGET INDICATORS

CAS REFERENCE ROLES

ADDITIONAL DETAILS

Carbon-13 NMR Spectrum



SPECTRUM ID
7MED36_38.C

CAS REGISTRY NUMBER
63968-64-9

FORMULA
C₁₅H₂₂O₅

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

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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

(71) Applicant (for all designated States except US): ASTRAZENECA AB [SE/SE]; S-151 85 Södertälje (SE).

(71) Applicant (for MG only): ASTRAZENECA UK LIMITED (GB/GB); 15 Starhope 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, 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 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;

R₁ is aryl, heteroaryl, (C₁-C₆)alkyl, aralkyl, heterocycloalkyl, or heteroaralkyl;

R₂ and R₂' 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_c is H or (C₁-C₆)alkyl;

R_d 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, R₂', R₃, R₄, R_c, R_d 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

PATENTPAK
A CAS SOLUTION

PAGE 28 / 72 ZOOM DOWNLOAD PDF PDF+

Key Substances in Patent

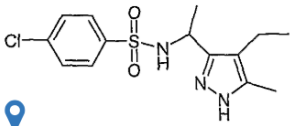
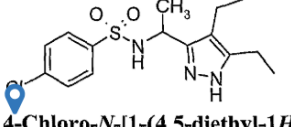
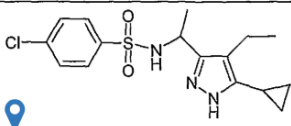
CAS RN 957128-74-4
Analyst Markup Locations (1)
Page 28

CAS RN 957128-75-5
Analyst Markup Locations (1)
Page 28

CAS RN 957128-76-6
Analyst Markup Locations (1)
Page 28

CAS RN 957128-77-7
Analyst Markup Locations (1)
Page 29

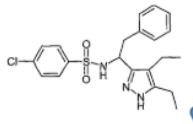
Table 1

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-D6) 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-D6) 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	 N-[1-(5-amino-1-[(4-chlorophenyl)sulfonyl]-4-ethyl-1H-pyrazol-3-yl)-2-phenylethyl]-4-chlorobenzamide	(400 MHz, DMSO-D6) 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

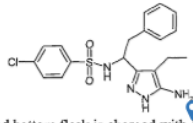
0.81 mmol) is then added in one portion, and the mixture is allowed to stir at 0 °C for 2 min and is allowed to warm to room temperature over 3 min. Glacial HOAc (0.50 mL) is added to quench the reaction, followed by absolute EtOH (2 mL). Hydrazine monohydrate (150 μL, 3.1 mmol) is added, and the mixture 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-chlorobenzesulfonamide (**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-chlorobenzamide (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

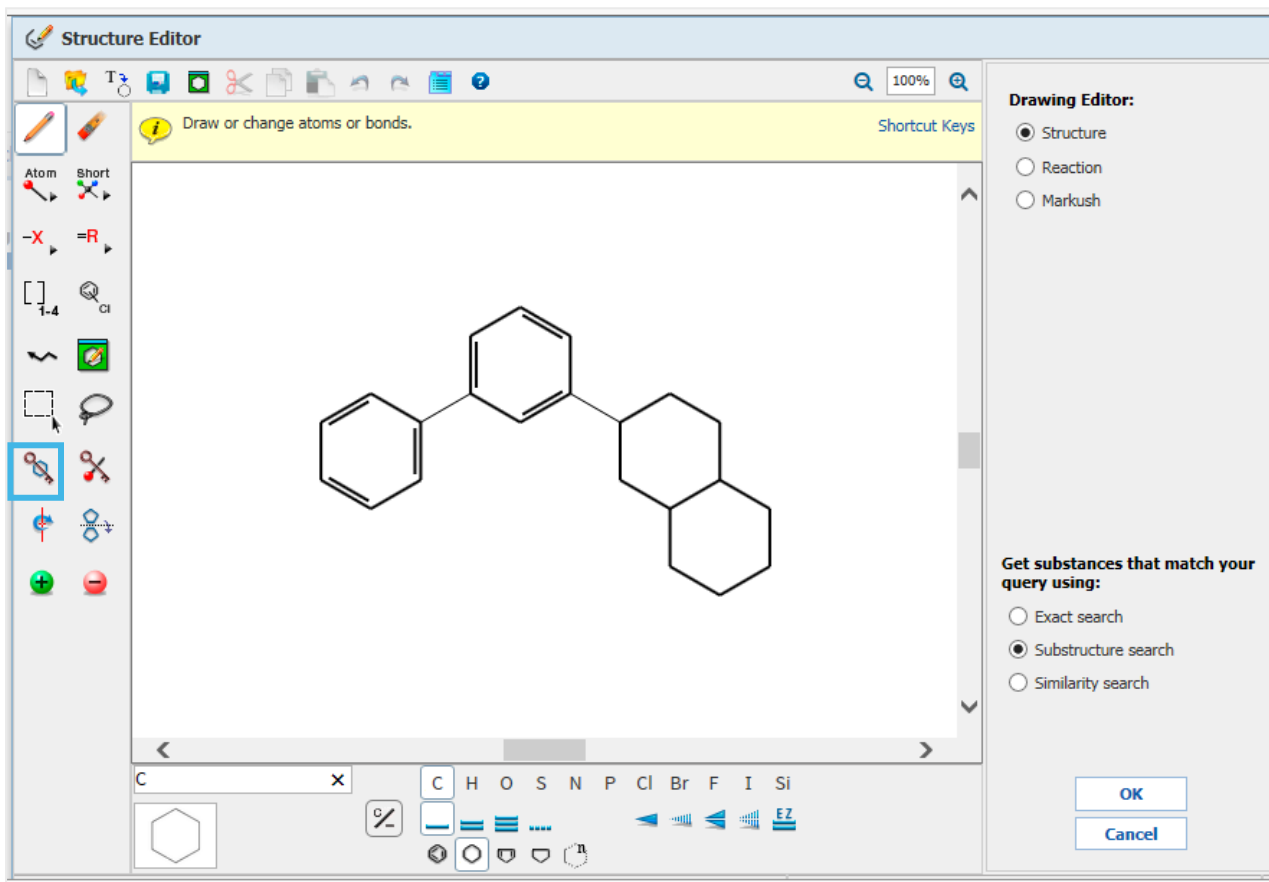
■ 确定物质[Specific Substance]:

- 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

The screenshot displays the SciFinder web interface. At the top, the SciFinder logo is visible, along with navigation links for 'CAS Solutions', 'Preferences', 'SciFinder Help', and 'Sign Out'. The user is logged in as 'Sunny Yu'. Below the navigation bar, there are tabs for 'Explore', 'Saved Searches', and 'SciPlanner'. A yellow warning banner indicates that the search for 'Explore Substances' resulted in 0 substances, with a 'Return' link. The main content area shows the search path 'Chemical Structure substructure > substances (0)'. There is a 'SUBSTANCES' section with 'Analyze' and 'Refine' buttons. The 'Analyze by:' section shows 'No substances available'. At the bottom, there are links for 'Contact Us' and 'Legal', and a copyright notice for the American Chemical Society.

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

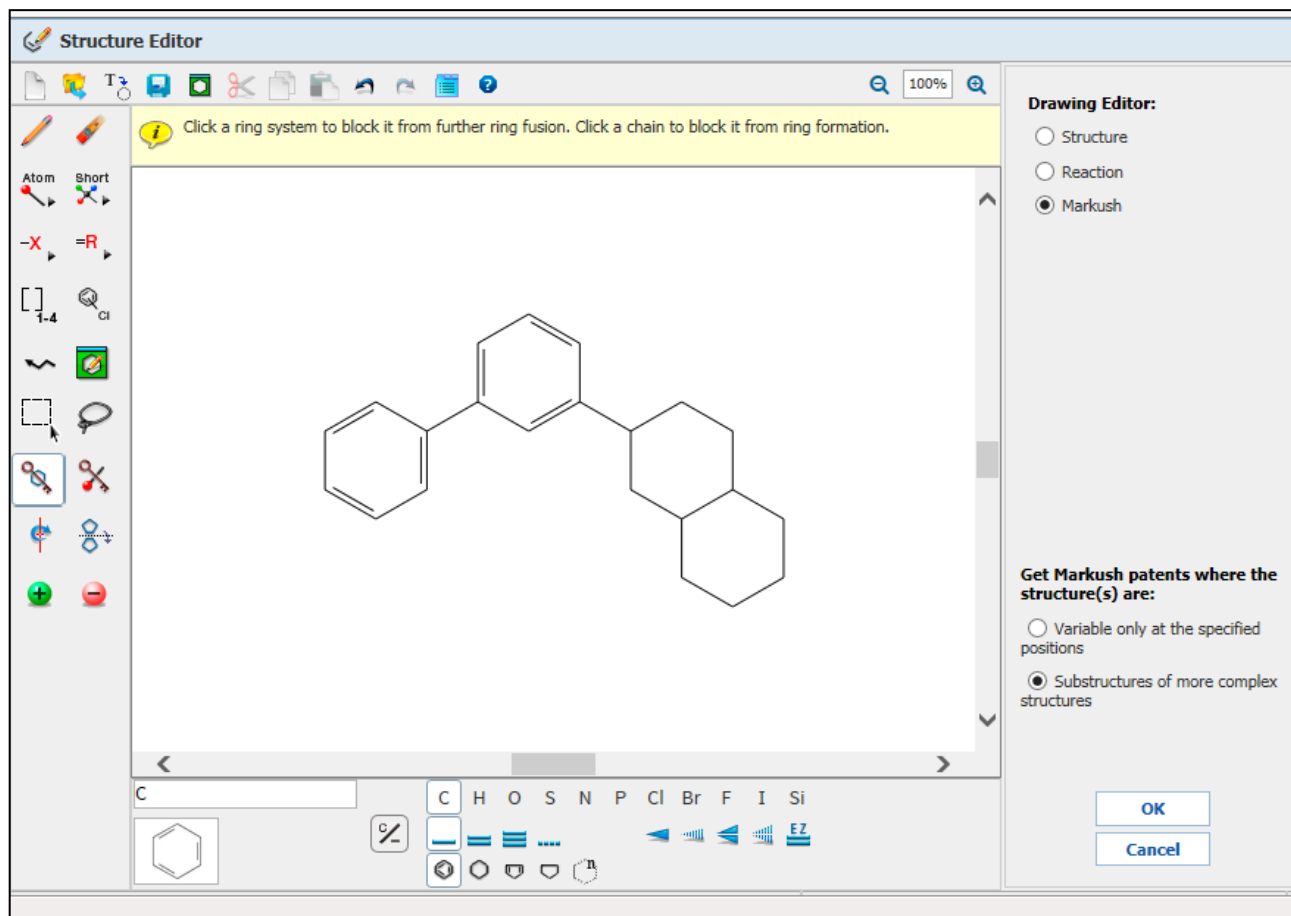
Analyze | Refine

Analyze by:
No substances available

[Contact Us](#) | [Legal](#)

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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 Save Print Export

Markush substructure > references (24)

REFERENCES ⓘ Get Substances Get Reactions Get Related Citations Tools ▾ Create Keep Me Posted Alert Send to SciPlanner

Analyze Refine Categorize Sort by: Accession Number ▾ ↓ 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

0 of 24 References Selected

- 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 prepg. 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；
- 充分使用结构编辑器中的绘图工具，灵活绘制结构；
- 有机物、无机物、配位化合物和聚合物等物质的检索方法；
- 物质Markush结构检索，规避专利风险

大纲

- CAS SciFinder介绍
- 文献相关信息的获取策略
 - 文献检索方法
 - 文献结果分析、精炼和详情
- 物质相关信息的获取策略
 - 物质检索方法
 - 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

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

The screenshot displays a search results page from a chemical database. At the top, there are navigation buttons: 'REFERENCES', 'Get Substances', 'Get Reactions', 'Get Related Citations', and 'Tools'. On the right, there are options to 'Create Keep Me Posted Alert' and 'Send to SciPlan'. Below the navigation bar, there are tabs for 'Analyze', 'Refine', and 'Categorize'. The 'Analyze' tab is active, showing a list of authors and their corresponding number of results. The main content area shows two search results. The first result is titled '1. A kind of method for catalyzed synthesis of aspirin by using choline eutectic solvent [Machine Translation]'. It includes a 'Quick View' button, a 'PATENTPAK' icon, and the authors 'Wang, Yinglei; Li, Wenhuan; Liu, Xueguo; Du, Chaojun; Li, Jin'. The second result is titled '2. Synthesis of novel aspirin analogs for medicinal testing'. It includes a 'Quick View' button, an 'Other Sources' icon, and the authors 'Albasrawi, Hadeel K.; Timmons, Shannon C.'. The interface also shows a 'Sort by: Accession Number' dropdown, a 'Display Options' link, and a pagination bar indicating 'Page: 1 of 3'.

REFERENCES ?

Get Substances Get Reactions Get Related Citations Tools

Create Keep Me Posted Alert Send to SciPlan

Analyze Refine Categorize

Sort by: Accession Number

0 of 227 References Selected

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

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 'Get References' dialog box overlaid on a substance detail page. The dialog box has a title bar 'Get References' and a 'Limit results to:' section with two columns of checkboxes. The 'Preparation' checkbox is checked. Below this is a 'For each sequence, retrieve:' section with one checkbox for 'Additional related references, e.g., activity studies, disease studies.' There are 'Get' and 'Cancel' buttons at the bottom right of the dialog box.

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 'Get Reactions' dialog box overlaid on a substance detail page. The dialog box has a title bar 'Get Reactions' and a 'Retrieve reactions for:' section with two radio buttons. The 'All substances' radio button is selected. Below this is a 'Limit results by reaction role:' section with a list of radio buttons. The 'Product' radio button is selected. There are 'Get' and 'Cancel' buttons at the bottom right of the dialog box.

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

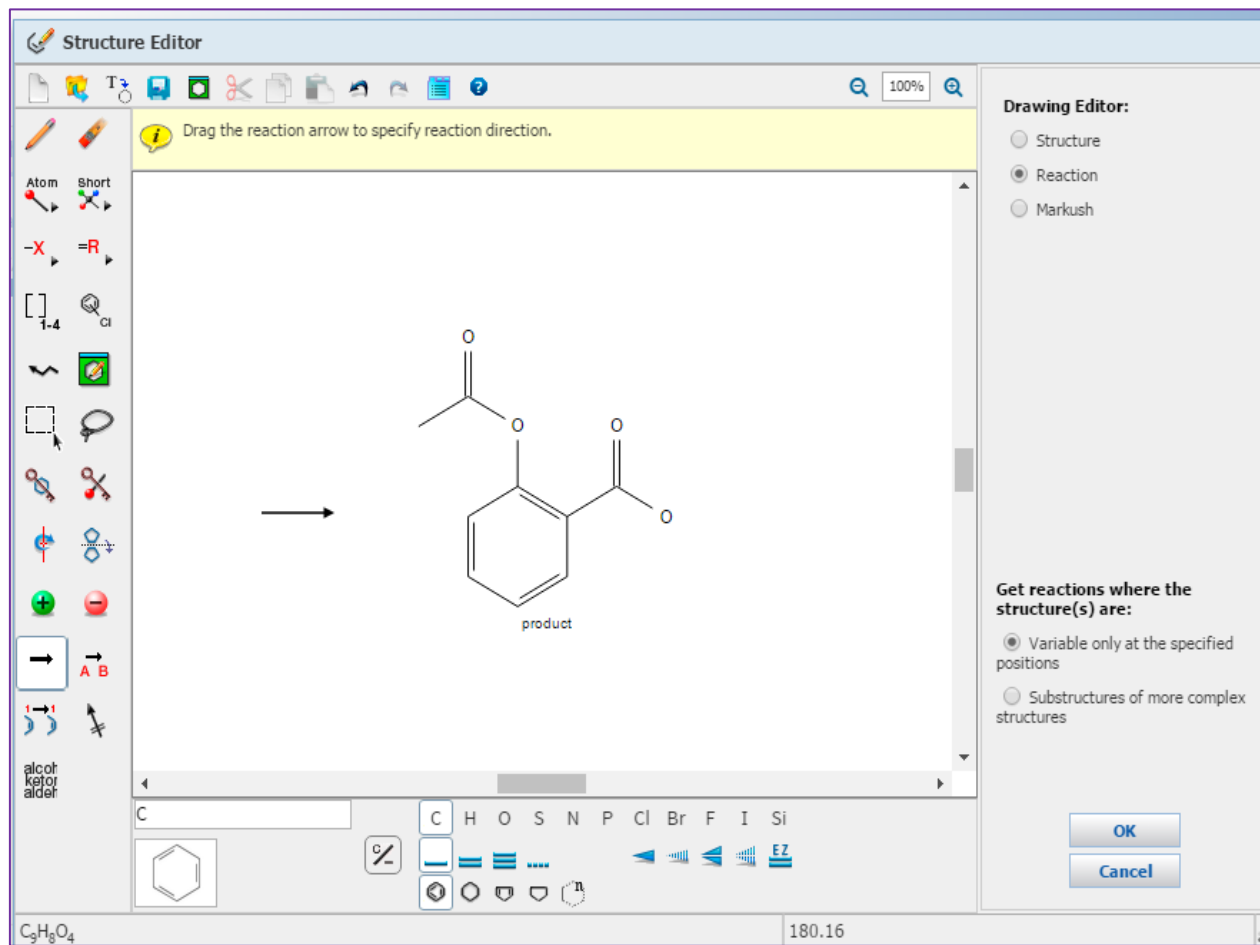
Other Names
Rhodine (7CI)
Salicylic acid acetate (8CI)
2-(Acetyloxy)benzoic acid
2-Acetoxybenzoic acid

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

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

The screenshot displays the Structure Editor software interface. On the left, a 'Functional Groups' panel lists various chemical categories such as Alcohols (13), Alkenes (11), Alkynes (4), Amines (11), Carbonate Derivatives (7), Carboxy Derivatives (17), Halides (16), Heterocycles (54), Ketones (6), Organometallics (19), Non-Rings (136), and Rings (71). The main workspace is titled 'Structure Editor' and contains a toolbar with icons for drawing atoms, bonds, and reactions. A yellow banner at the top of the workspace reads 'Draw or change atoms or bonds.' and 'Shortcut Keys'. On the right, a 'Drawing Editor' panel allows switching between 'Structure', 'Reaction', and 'Markush' modes. Below this, there are options to 'Get reactions where the structure(s) are:' with radio buttons for 'Variable only at the specified positions' and 'Substructures of more complex structures'. At the bottom, there are 'OK' and 'Cancel' buttons. The status bar at the bottom shows 'CH₄' and '16.04'. Four blue callout boxes with white text and arrows point to specific features: '反应箭头' (Reaction Arrow) points to the reaction arrow icon; '原子标记' (Atom Label) points to the atom label icon; '官能团列表' (Functional Group List) points to the Functional Groups panel; and '化学键变化' (Chemical Bond Change) points to the bond change icon.

Functional Groups

Enter 3 or more characters...

Alcohols (13)

Alkenes (11)

Alkynes (4)

Amines (11)

Carbonate Derivatives (7)

Carboxy Derivatives (17)

Halides (16)

Heterocycles (54)

Ketones (6)

Organometallics (19)

Non-Rings (136)

Rings (71)

Close

Structure Editor

Draw or change atoms or bonds.

Shortcut Keys

Drawing Editor:

Structure

Reaction

Markush

Get reactions where the structure(s) are:

Variable only at the specified positions

Substructures of more complex structures

OK

Cancel

反应箭头

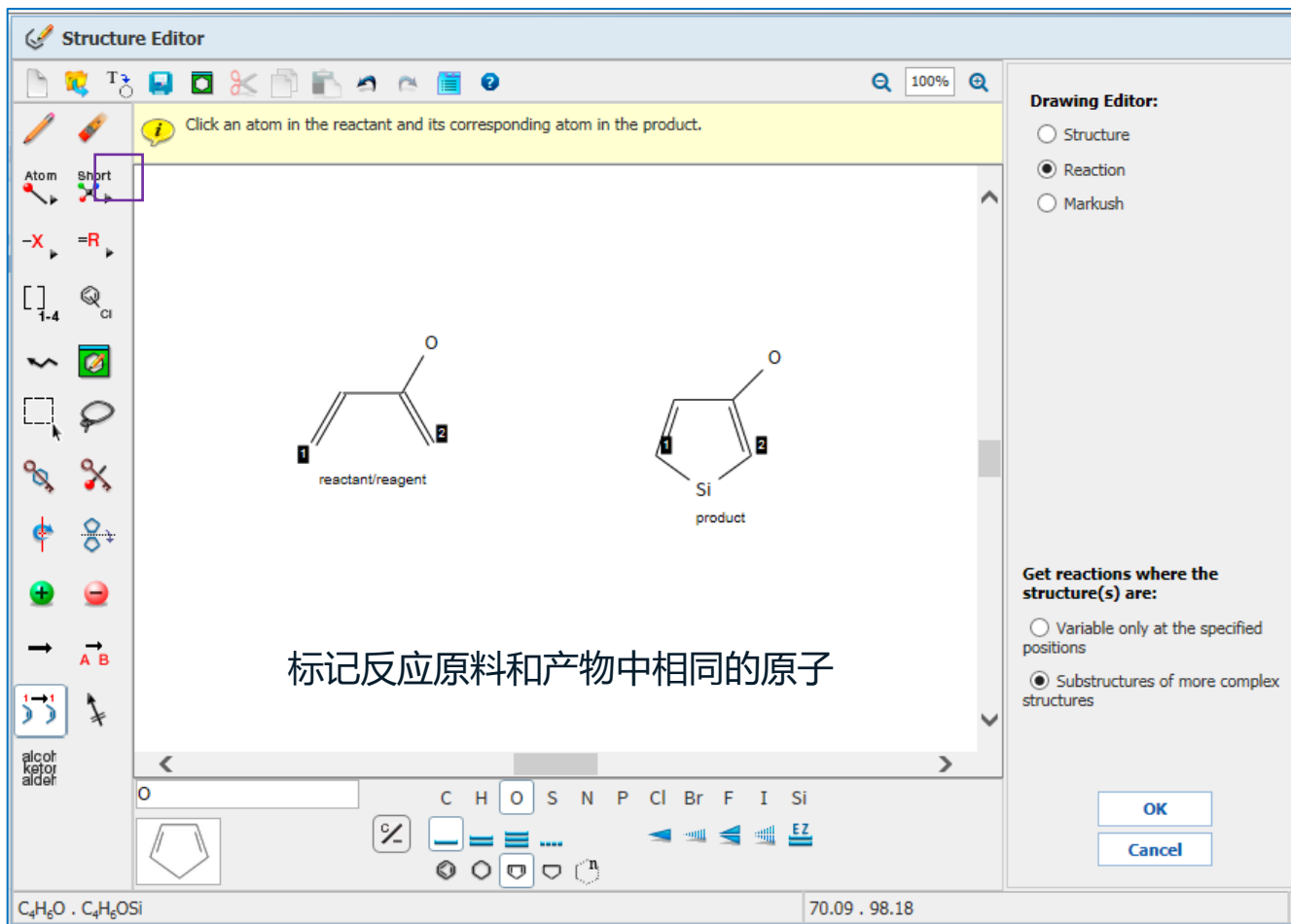
原子标记

官能团列表

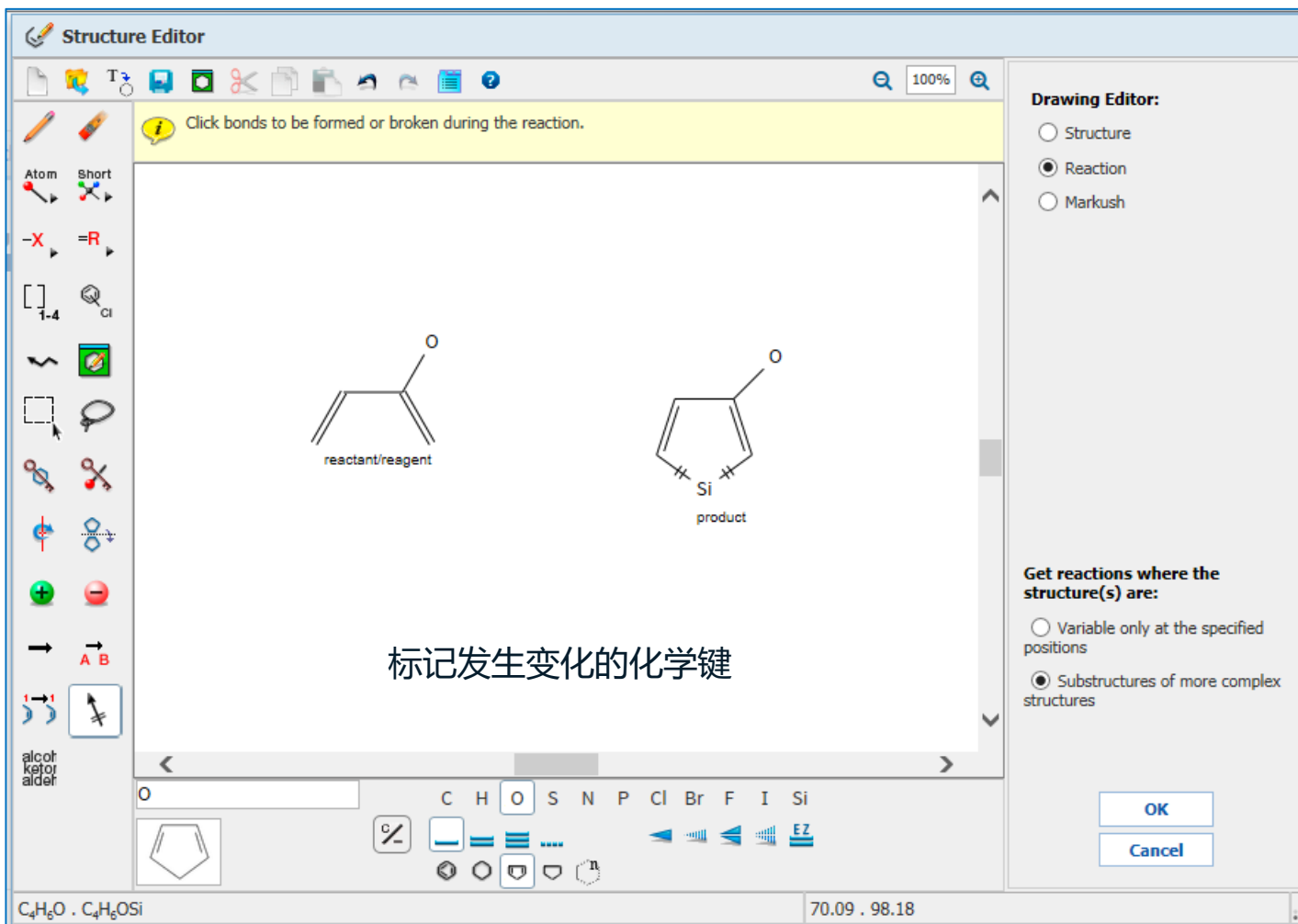
角色定义

化学键变化

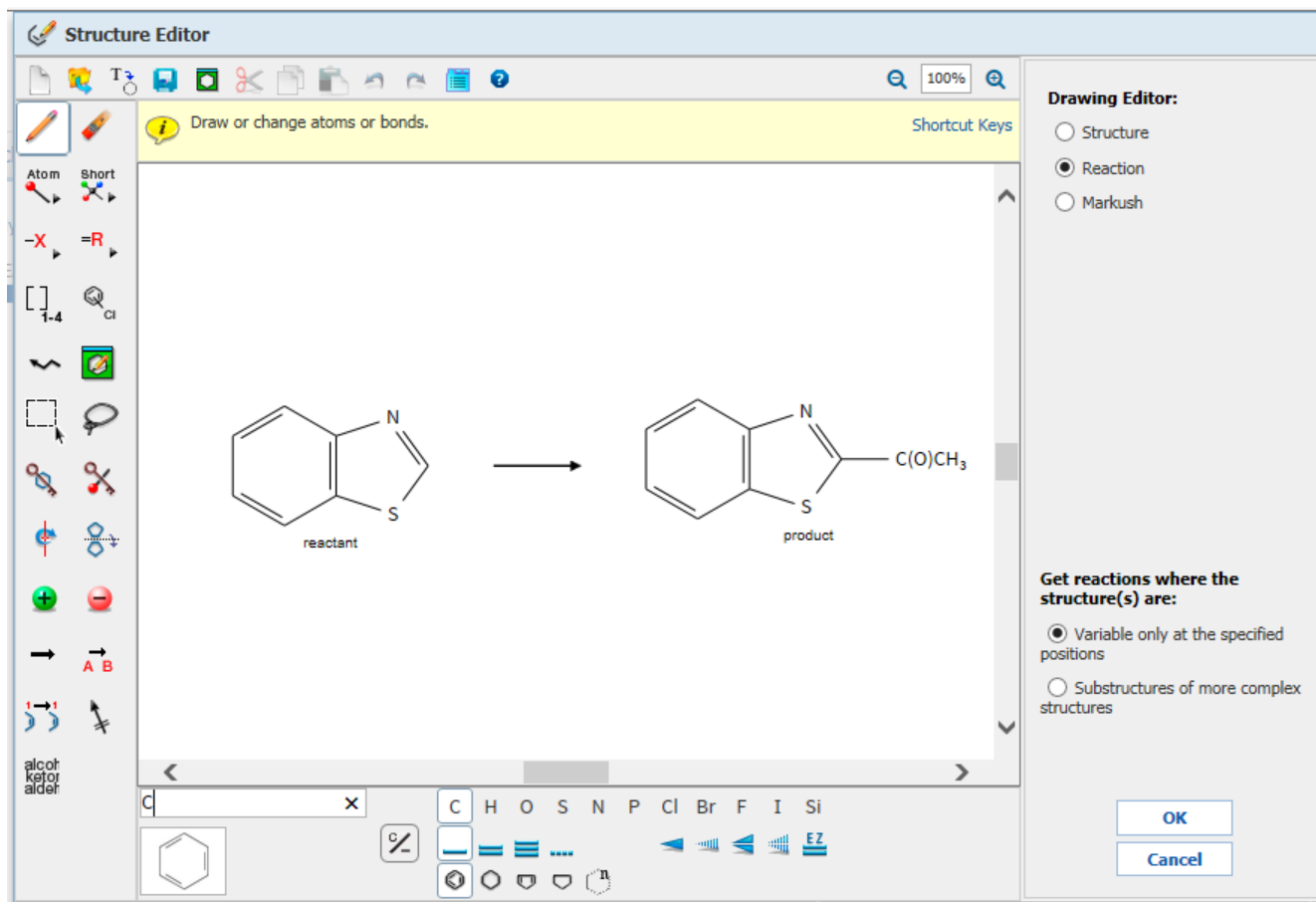
反应前后物质中的原子标记



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 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

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

Notes

ice-bath removed after stirring at -78C for 1 hour (stage 2), Reactants: 2, Reagents: 2, Solvents: 2, Steps: 1, Stage: 2, Most stages in new page step: 2

精确结构反应检索：查看反应结果集

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

REACTIONS ? Get References Tools Send to SciPlanner

Analyze ? Refine

Analyze by: Reagent

BuLi 4
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](#)

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

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**

RCO_2H
 R^1CHO
 $\text{R}^2\text{COCO}_2\text{R}^3$

$\text{R}^4 = \text{R}, \text{COR}^1, \text{OCOR}^3$

2. Uncategorized Single-Step Reactions **2 Reactions**

3. Multi-Step Reactions **1 Reaction**

精确结构反应检索：查看反应结果集

Explore Saved Searches SciPlanner Save Print Export

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

REACTIONS Get References Tools

Sort by: Relevance, Accession Number, Experimental Procedure, MethodsNow, **Number of Steps**, Product Yield, Publication Year

Group by: No Grouping

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

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

Notes

ice-bath removed after stirring at -78C for 1 hour (stage 2), Reactants: 2, Reagents: 2, Columns: 2, Steps: 1, Steps: 2, Most steps in sequence: 2

Analyze Refine

Analyze by: Reagent

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

Show More

Send to SciPlanner Display Options

精确结构反应检索：查看反应结果集

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

REACTIONS ? Get References Tools Send to SciPlanner

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

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

Document Transformation

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)₃Me, 24 h, 80°C
- 1.2 R: H₂O

Notes

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

References

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

精确结构反应检索：获取相似反应

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 ?

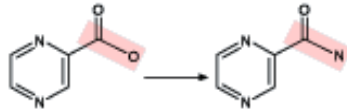
Retrieve similar reactions from:

All reactions

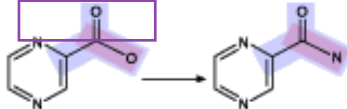
Current answer set

Include this level of similarity:

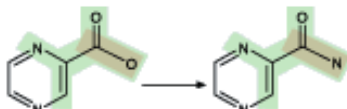
Broad - Reaction centers only



Medium - Reaction centers plus adjacent atoms and bonds



Narrow - Reaction centers plus extended atoms and bonds



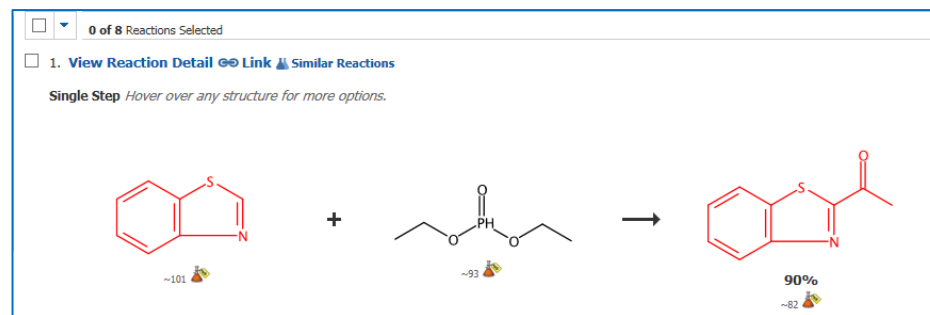
精确结构反应检索：查看感兴趣的反应信息

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

Notes

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

References

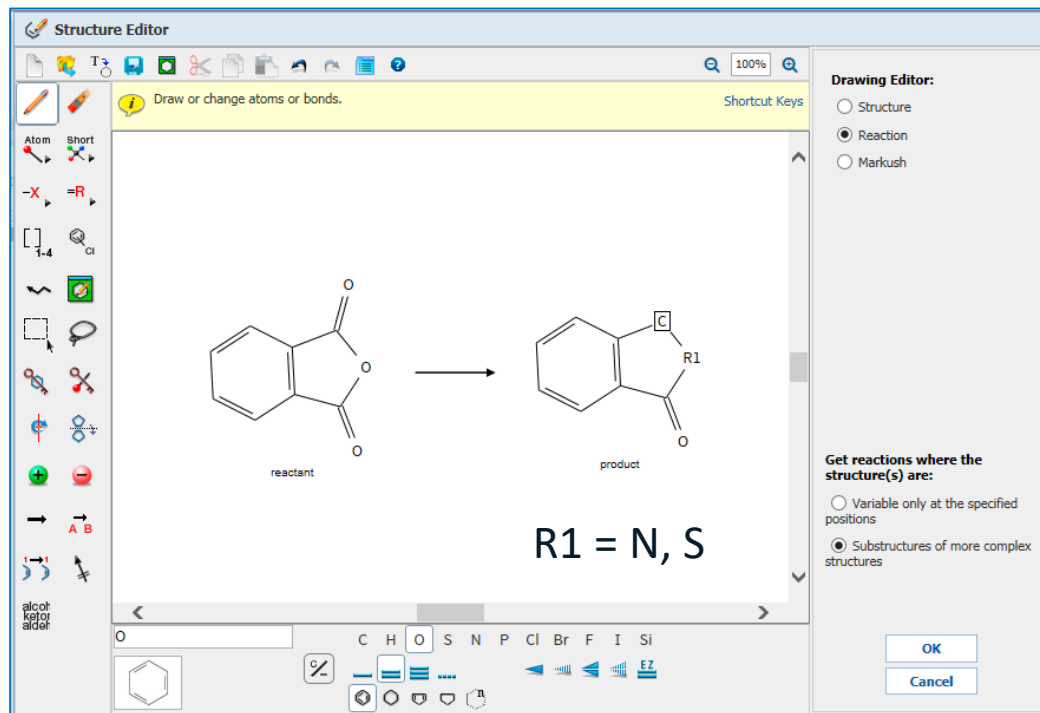
Peroxides as "Switches" of Dialkyl H-Phosphonate: Two Mild and Metal-Free Methods for Preparation of 2-Acylbenzothiazoles and Dialkyl Benzothiazol-2-ylphosphonates
Quick View Other Sources
By Chen, Xiao-Lan et al
From Journal of Organic Chemistry, 79(17), 8407-8416; 2014

Experimental Procedure

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

实验步骤

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

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

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

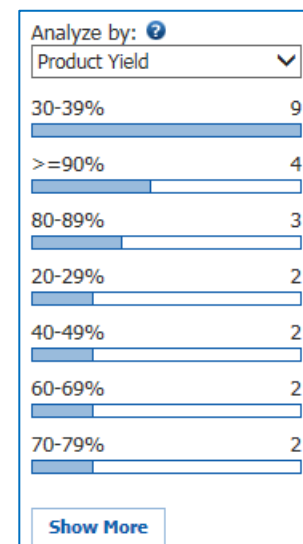
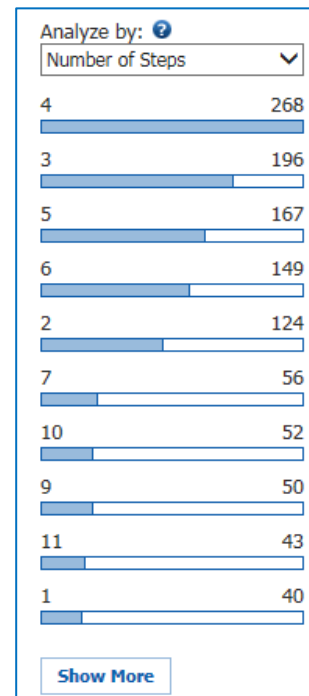
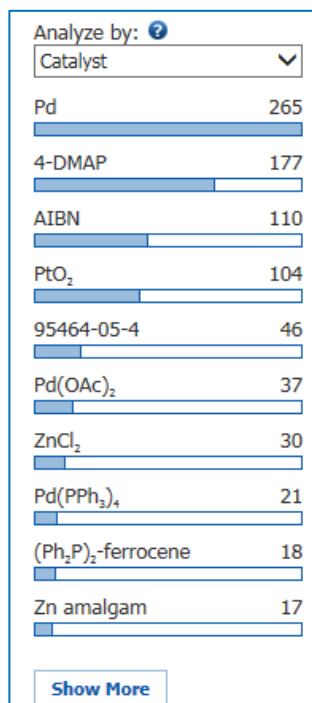
Studies on the chemistry of isoindoles and isoindolenines. XXVII. 3-Alkoxy-1H-isoindoles: syntheses and properties
Quick View Other Sources
By Hennige, Hans et al
From *Chemische Berichte*, 121(2), 243-52; 1988

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 Display Options

0 of 1217 Reactions Selected Page: 1 of 82

Refine by: ?

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

Reaction Classification(s):

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

Refine

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

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

Overview

Steps/Stages

- 1.1
- 2.1

Notes

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

References

Lenalidomide isotopologues and their preparation and use for the treatment of diseases
Quick View **PATENTPAK**
By Muller, George W. and Man, Hon-Wah
From PCT Int. Appl., 2010093434, 19 Aug 2010

亚结构反应检索：排除反应类型

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

REACTIONS Get References Tools Send to SciPlanner

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

0 of 1154 Reactions Selected Page: 1 of 77

Refine by:

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

Excluding Reaction Classification(s):

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

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

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

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

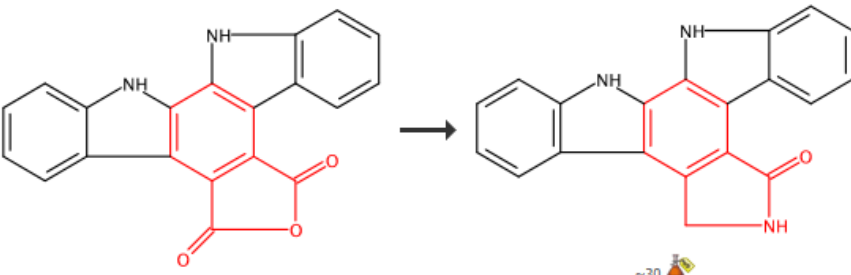
Analyze Refine

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

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

Refine by:

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

Non-participating Functional Group(s)

View: Classes 10

2 Selected Clear Selections

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

利用SciPlanner设计拟合成反应路线

点击打开SciPlanner工作界面

REACTIONS

Get References Tools

Analyze Refine

Analyze by: Catalyst

No reactions available

Group by: No Grouping Sort by: Number of Steps

1 of 535 Reactions Selected

1. View Reaction Detail Link Similar Reactions

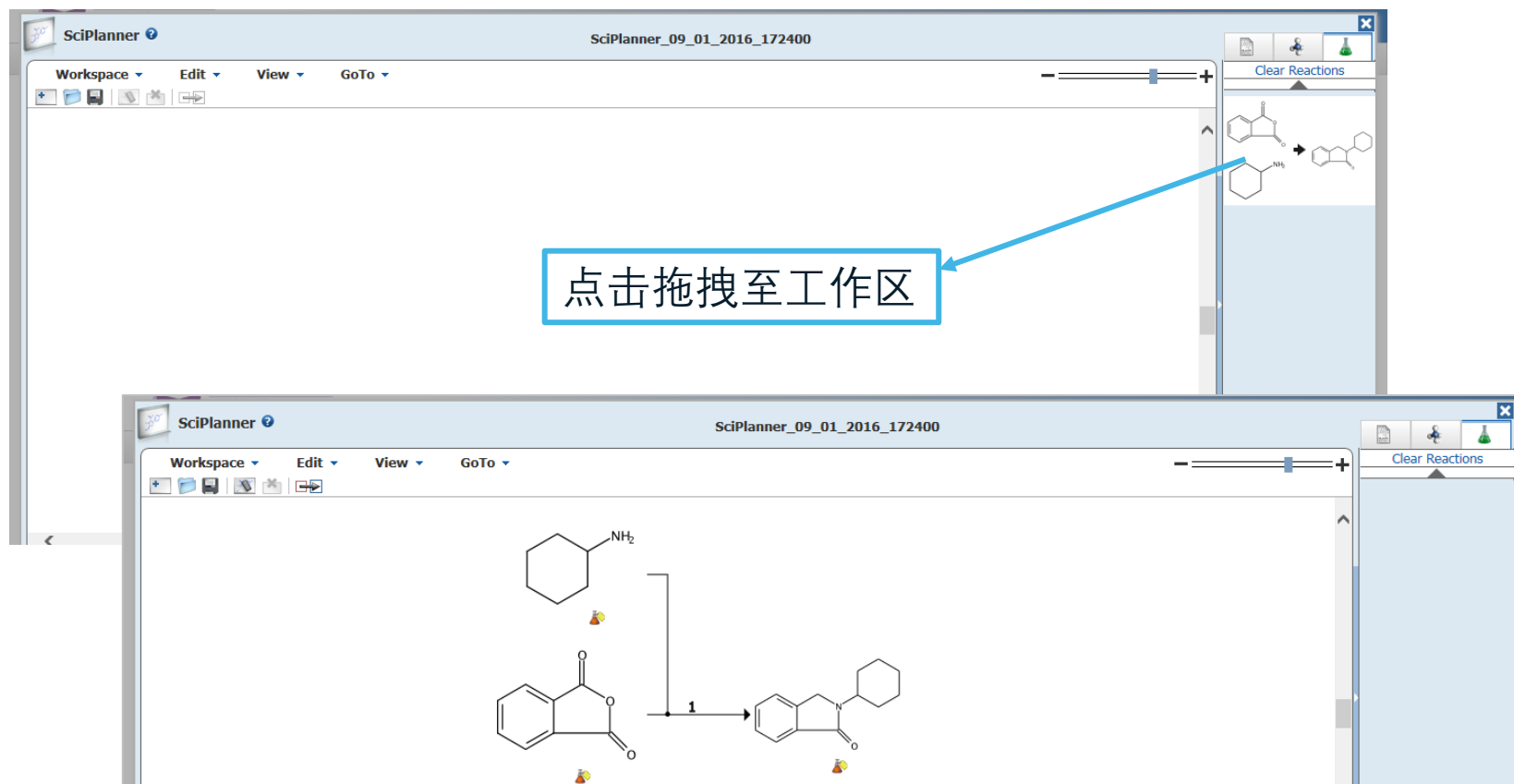
Single Step Hover over any structure for more options.

选择感兴趣的反应，点击send to SciPlanner

~136 ~95 87% ~1

The screenshot shows the SciPlanner interface with a search for "Catalyzed" reactions. A reaction is selected, and a callout box points to the "Send to SciPlanner" button. The reaction shown is the synthesis of a cyclic amide from a cyclic imide and a cyclic amine.

SciPlanner工作界面



SciPlanner工作界面

The screenshot shows the SciPlanner workspace with a chemical structure of cyclohexylamine. A context menu is open over the structure, listing options such as 'View Substance Detail', 'Explore by Structure', and 'Synthesize this...'. 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 for the search. It displays a reaction scheme where two molecules of salicylic acid react to form a cyclic product. The reaction is labeled '4. View Reaction Detail' and includes a 'Send to SciPlanner' button. A blue callout box points to this button 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

The image displays two screenshots of the SciPlanner software interface, illustrating how to manage multiple reactions in a single workspace.

The top screenshot shows a workspace with two reactions. Reaction 1 involves the synthesis of a cyclic amide from a cyclohexylamine derivative and a cyclic imide. Reaction 2 involves the synthesis of a cyclic imide from a diacid and a cyclic amine. A blue arrow points from the reaction scheme in the top right to the workspace, with the text "继续拽至工作区" (Continue to drag to workspace).

The bottom screenshot shows the same workspace with the two reactions overlaid. The reaction schemes are highlighted with blue boxes, and the text "两个反应在同一工作窗口" (Two reactions in the same workspace) and "将相同的两个结构移动至重叠" (Move the same two structures to overlap) is displayed.

SciPlanner——设计拟合成的反应路线

The screenshot displays the SciPlanner software interface. The main workspace shows a chemical reaction pathway starting from 2-oxo-3-phenylpropanoic acid, proceeding through an intermediate to a final product. The reaction is labeled with '2' and '1'. A menu is open on the left with 'Export' selected. An 'Export' dialog box is open on the right, showing options for file format (PDF, Citations, Image) and saving locally (SciPlanner eXchange). The dialog also includes fields for file name and title, and checkboxes for including image, reaction details, substance details, and reference details.

导出设计的路线

合二为一的合成路线

Export

Offline Review

- Portable Document Format (*.pdf)
- Citations (*.ris)
- Image (*.png)

Saving Locally

- SciPlanner eXchange (*.plx)

Details: * Required

File Name: *
SciPlanner_09_01_2016_172400

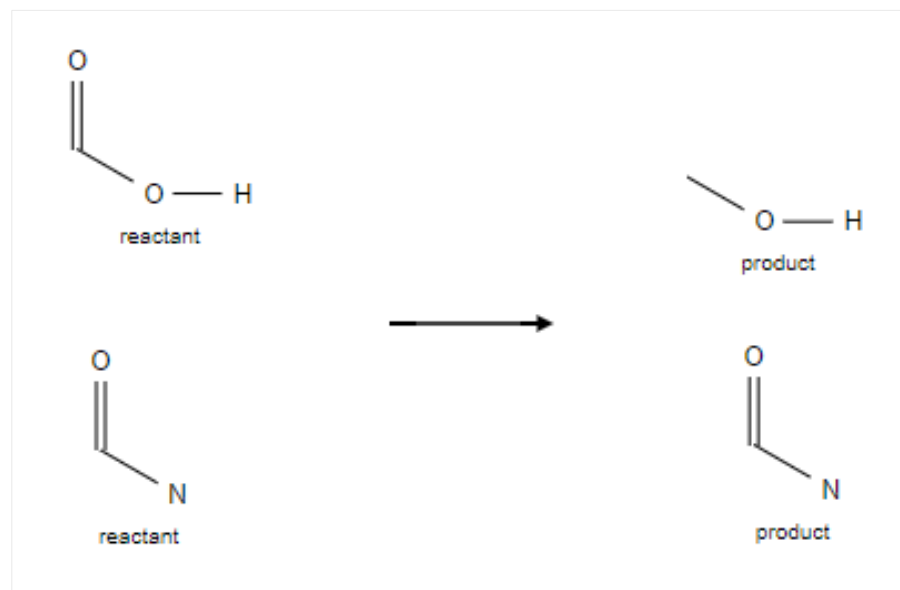
Title

Include:

- SciPlanner Image
- Reaction Details
- Substance Details
- Reference Details

Export Cancel

片段结构的化学选择性反应



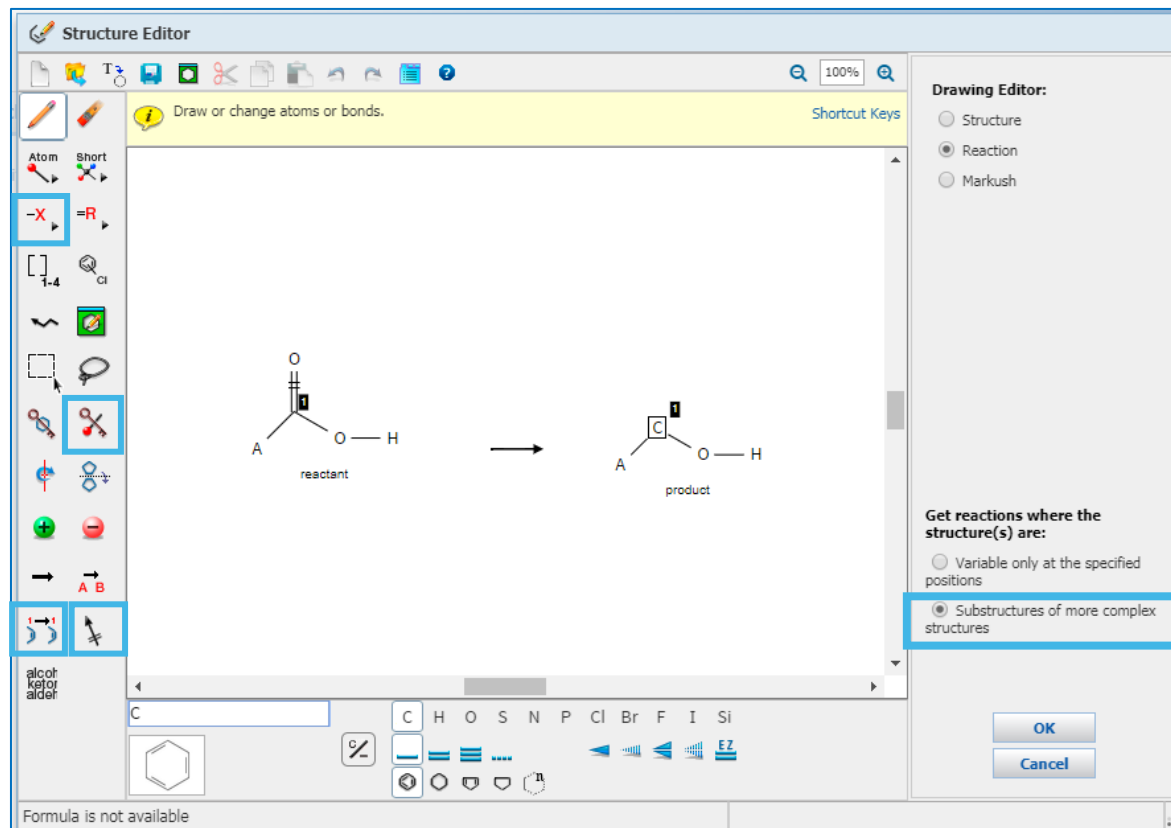
检索要求:

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



The 'Variables' dialog box lists several variables for defining reaction patterns:

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

A 'Close' button is located at the bottom of the dialog.

可提前选择不参与反应的官能团

The screenshot displays the ChemDraw software 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 contains a chemical reaction scheme with 'A' labels on the reactant and product. To the right of the editor are 'Search Type' options: 'Allow variability only as specified' (unselected) and 'Substructure' (selected). Below the editor is a 'Search' button and an 'Advanced Search' link. At the bottom, a 'Non-participating Functional Groups' dialog box is open, showing a list of functional groups with 'Amide' selected. A 'ChemDraw' logo and a 'Launch a SciFinder substance or reagent' button are also visible.

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- <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: No Grouping ▼ Sort by: Accession Number ▼ ↓

No Grouping Document None Selected

[Transformation](#)

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)

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

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

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

R¹ = CR'₃, 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](#) [Link](#) [Similar Reactions](#)

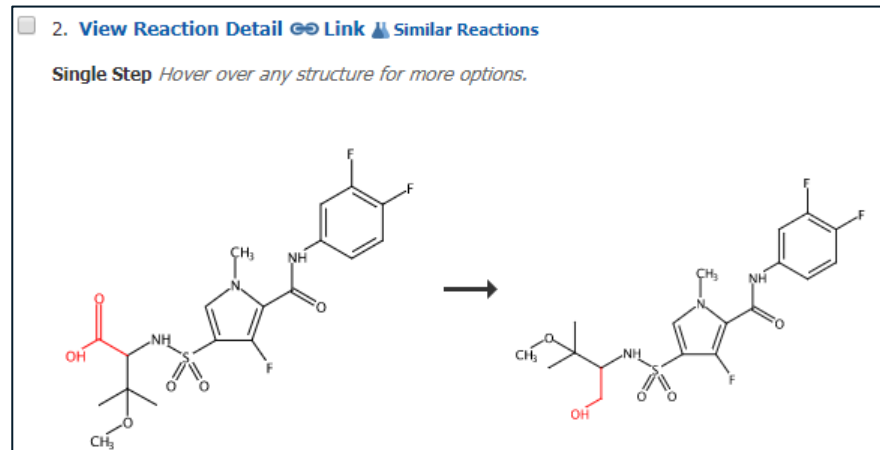
Single Step *Hover over any structure for more options.*

90%

[Overview](#)

2. [View Reaction Detail](#) [Link](#) [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
- SciPlanner工具助于自定义设计拟合成反应路线

谢谢关注!



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Unit 1010, Tower B, Raycom InfoTech Park
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