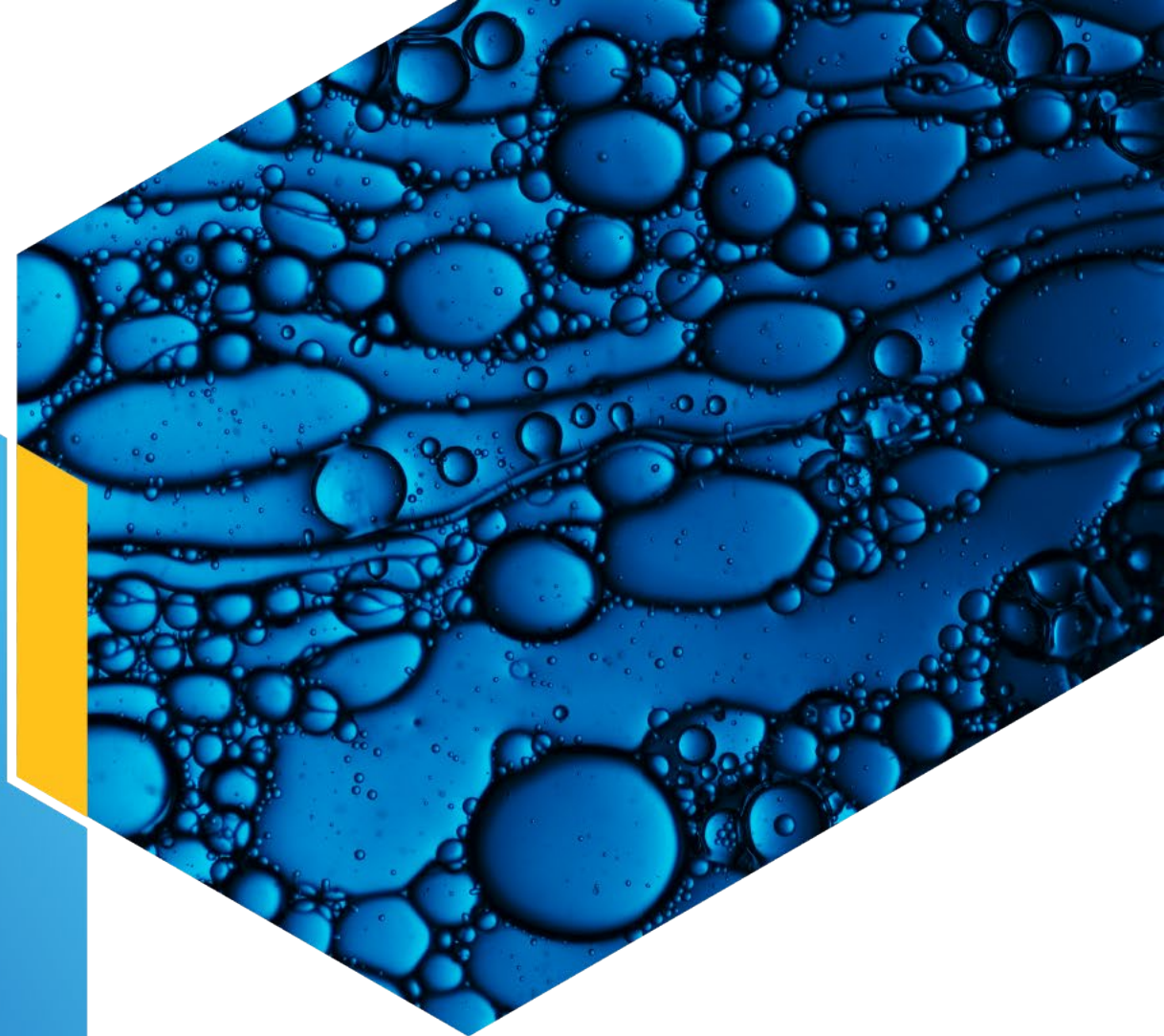


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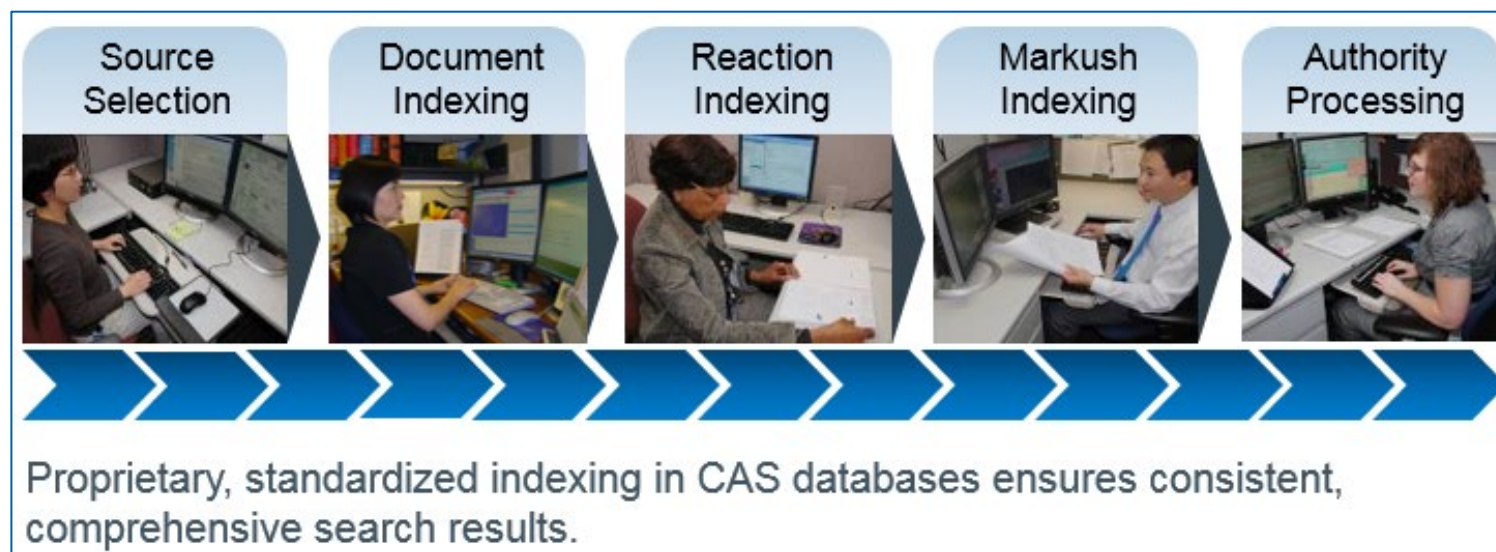
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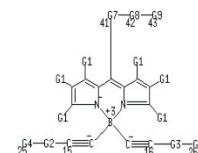
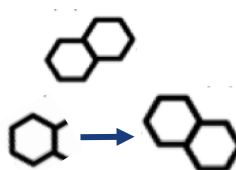
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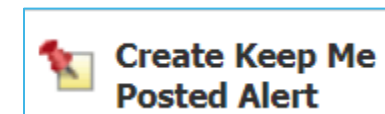
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Zhang Qiang	13

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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 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...

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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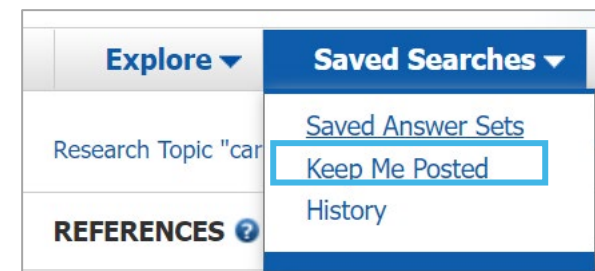
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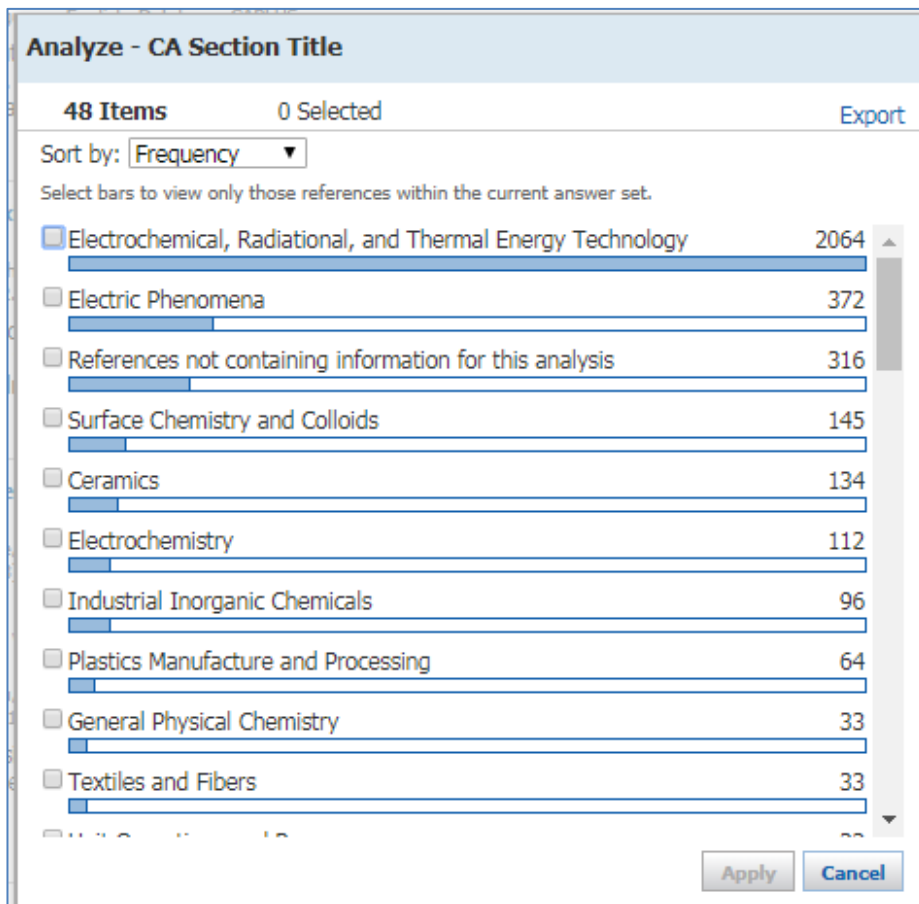
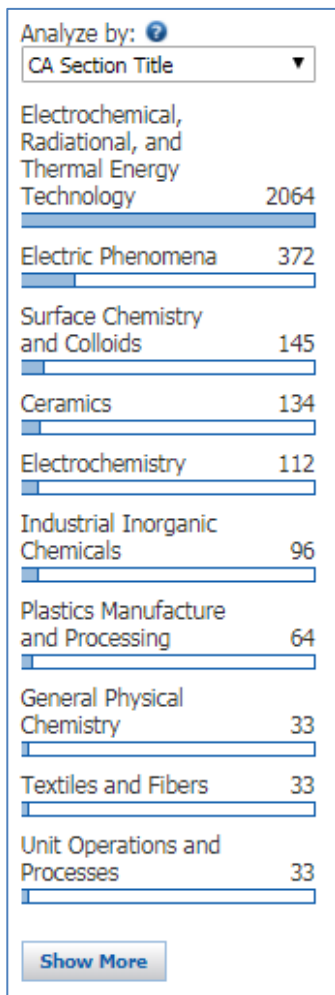
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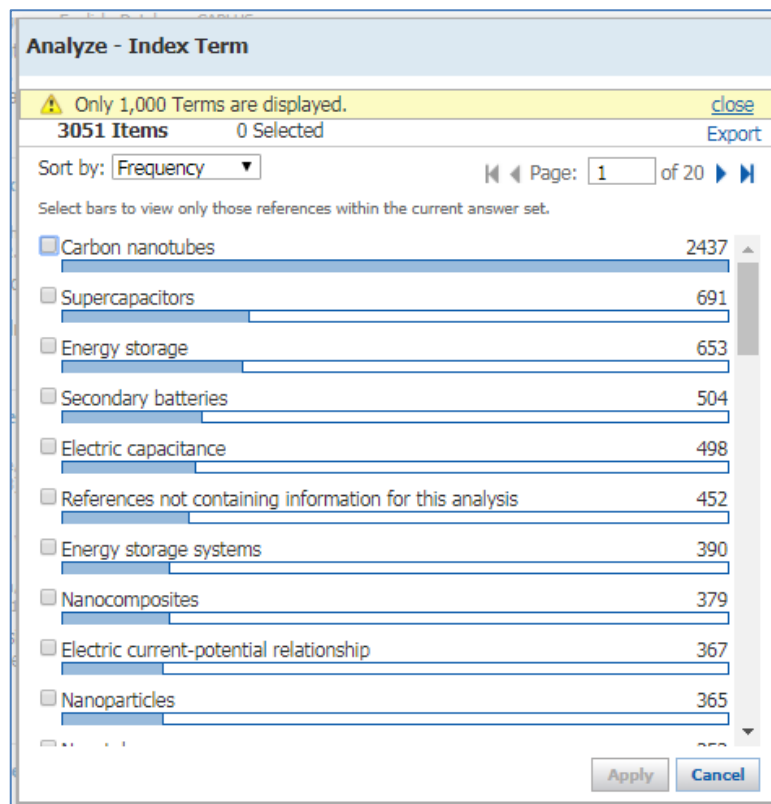
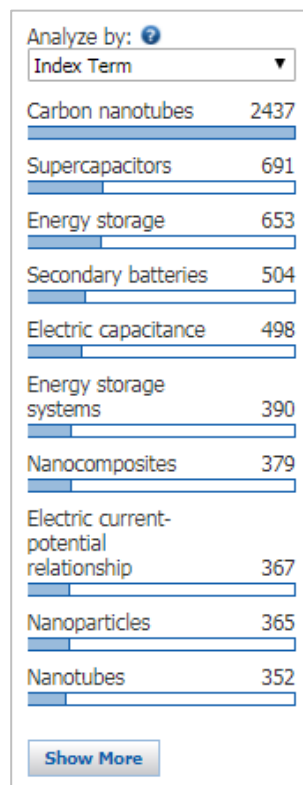
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Research Topic

secondary battery

Examples:

The effect of antibiotic residues on dairy products

Photocyanation of aromatic compounds

Refine

1. **Attempts to improve the energy capacity of capacitive electrochemical energy storage devices**

Quick View Other 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 View Other 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 (MnO_x) nanosheets composed of MnO₂ and Mn₃O₄ 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 View Other 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 View Other 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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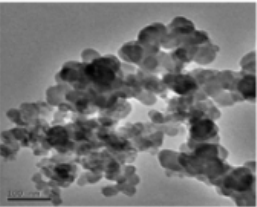
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- 1. Composite electrode material, preparation method and application thereof**
Quick View PATENTPAK
By Wang, Yue; Liang, Minghui; Jiang, Peng; Zhang, Xianfeng; Wei, Hang; Li, Xin; Liu, Yongguang
From Faming Zhuanli Shenqing (2017), CN 107359054 A 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**
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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. 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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Analytical chemistry		<input type="checkbox"/> Solar cells 34	
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General chemistry	Materials & products (369)	<input type="checkbox"/> Graphene 277	<input checked="" type="checkbox"/> Physical chemistry > Surface phenomena (3 Terms)
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Polymer chemistry	Metallurgy (153)	<input type="checkbox"/> Graphite 193	
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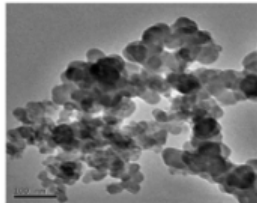
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- Composite electrode material, preparation method and application thereof**
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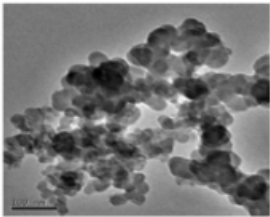
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From Faming Zhuanli Shenqing (2017), CN 107359054 A 20171117. | Language: Chinese, Database: CAPLUS

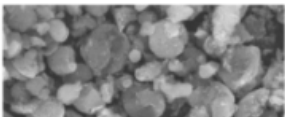


The title method comprises mixing coordination dissolved metal oxide and/or hydroxide soln. with **carbon** material, through evapn. of ligand soln., in situ growing metal oxide and/or metal hydroxide on **carbon** material surface, and obtaining the composite electrode material. The method is simple 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 ...

2. **Lithium ion battery cathode material and preparation method thereof**
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. **Micro-nano structuralized carbon silicon composite microsphere and preparation method and application thereof**
PATENTPAK
By Li, Xianglong; Zhang, Xinghao; Zhi, Linjie
From Faming Zhuanli Shenqing (2017), CN 107240677 A 20171010. | Language: Chinese, Database: CAPLUS



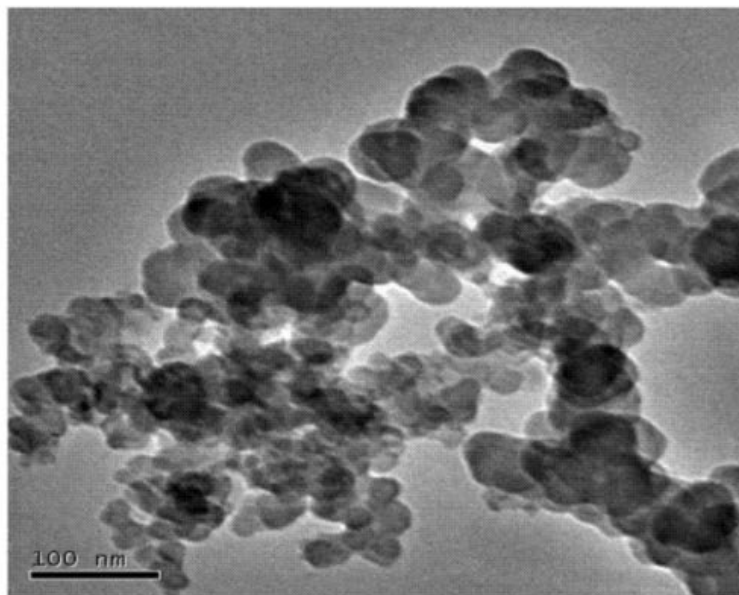
The method comprises using spray drying method for compounding and micro-nano structuralization of silica nanoparticle, protective agent and **carbon** nanomaterial, carrying out heat treatment under non-oxidn. atm. to prep. **carbon**/silica composite microsphere, and using metal thermal redn. method 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
<p>Batteries Electrodes Energy storage systems Lithium-ion secondary batteries Supercapacitors</p> <p>Carbon nanotubes Energy storage Evaporation Nanostructured materials</p>		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		<p>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</p>
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		

物质功能描述

定位信息

标准概念词列表

物质CAS RN,
物质名称



ACS
International



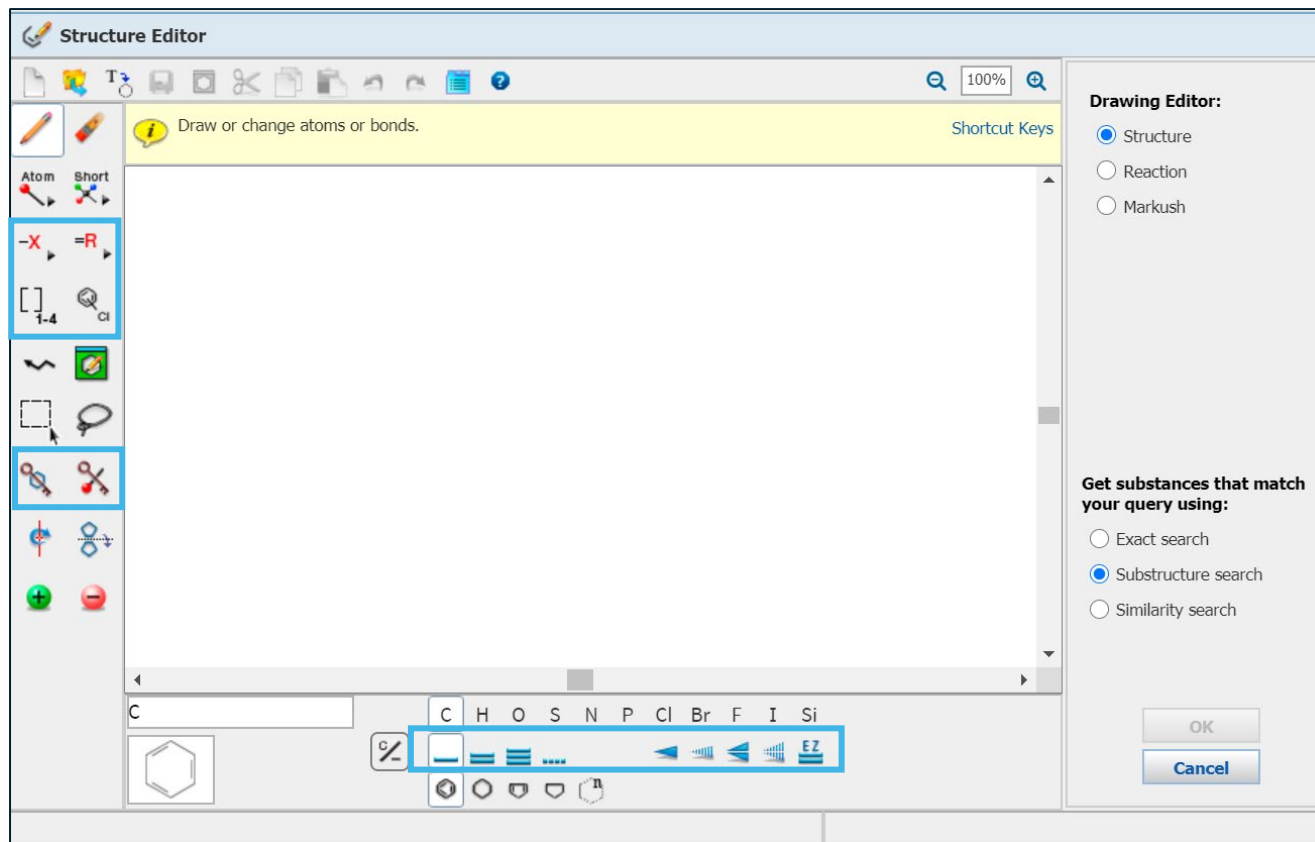
A division of the
American Chemical Society

大纲

- CAS SciFinder数据介绍
- 纳米储能材料的研究调研与追踪
- **生物、催化和医药研究的物质根基**
- 结构视角下的专利风险规避
- 制备反应研究的技术支撑



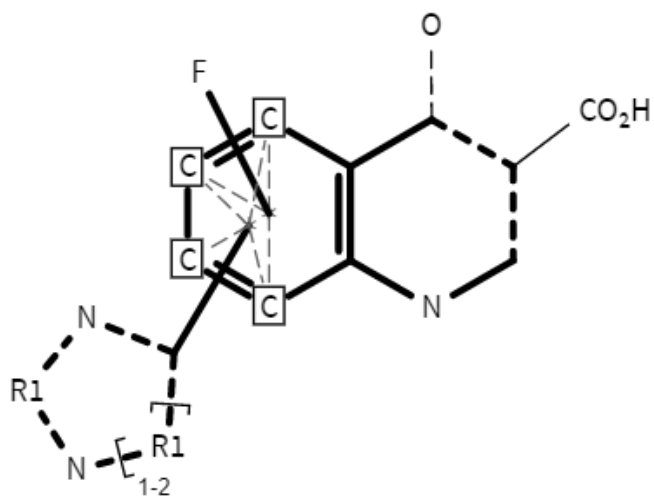
结构编辑器的使用



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

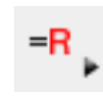
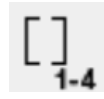
有机化合物: 通式结构的绘制



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)

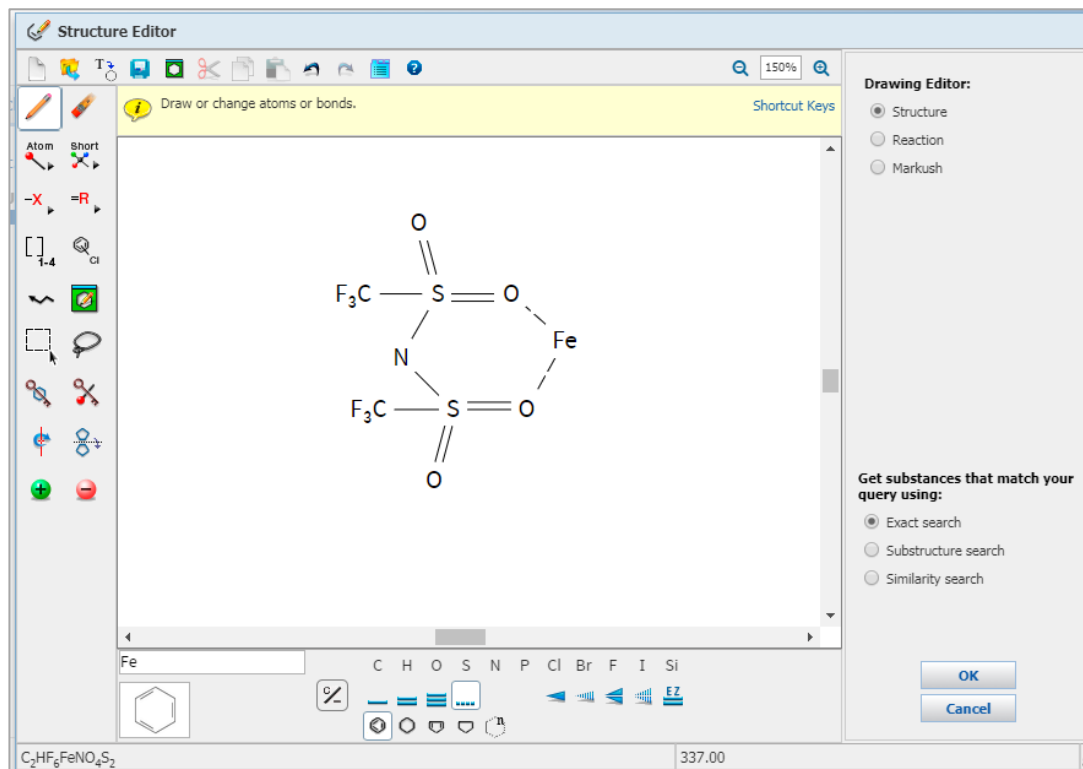
~79363 ~283

• 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 $\text{C}_2\text{H F}_6\text{N O}_4\text{S}_2 \cdot \frac{1}{2}\text{Fe}$
(Component: 82113-65-3)
~3
C2HF6FeNO4S2
 $\bullet \frac{1}{2} \text{Fe(II)}$
 $\text{C}_2\text{H F}_6\text{N O}_4\text{S}_2 \cdot \frac{1}{2}\text{Fe}$
Methanesulfonamide, 1,1,1-trifluoro-*N*[(trifluoromethyl)sulfonyl]-, iron(2+) salt (2:1)

5. 1912405-54-9 $\text{C}_2\text{H F}_6\text{N O}_4\text{S}_2 \cdot \frac{1}{2}\text{Fe}$
~0
C2HF6FeNO4S2
 $\bullet \frac{1}{2} \text{Fe(II)}$
 $\text{C}_2\text{H F}_6\text{N O}_4\text{S}_2 \cdot \frac{1}{2}\text{Fe}$
Methanesulfonamide, 1,1,1-trifluoro-*N*[(trifluoromethyl)sulfonyl]-, iron(2+) salt (2:1)

6. 1706814-99-4 $\text{C}_2\text{F}_6\text{N O}_4\text{S}_2 \cdot \frac{1}{2}\text{Fe H}_{12}\text{O}_6$
~1
1706814-96-1
 $\text{C}_2\text{F}_6\text{N O}_4\text{S}_2 \cdot \frac{1}{2}\text{Fe H}_{12}\text{O}_6$
98837-98-0
C2F6FeNO4S2
 $\text{C}_2\text{F}_6\text{N O}_4\text{S}_2$
 $\text{Fe H}_{12}\text{O}_6$
 $\text{C}_2\text{F}_6\text{N O}_4\text{S}_2 \cdot \frac{1}{2}\text{Fe H}_{12}\text{O}_6 \cdot 2\text{H}_2\text{O}$
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

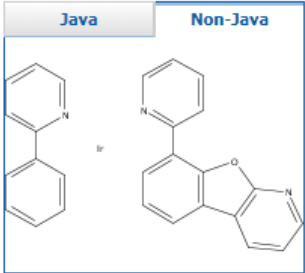
REACTIONS

- 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

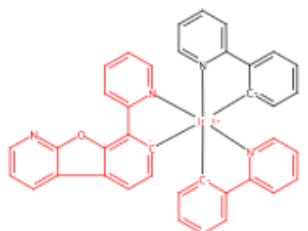
Get References Get Reactions Get Commercial Sources

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

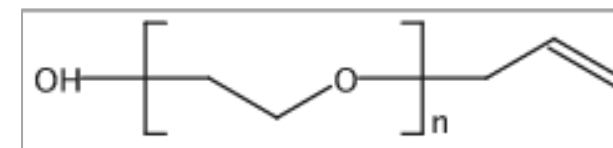
- Reaction Structure

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 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 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

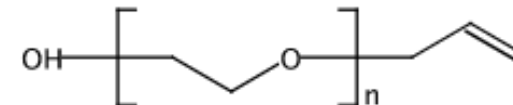
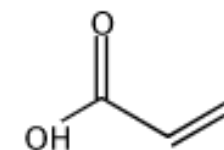
REACTIONS

- 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

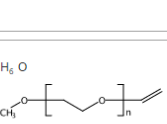
Get References Get Reactions Get Commercial Sources Tools

Sort by: CAS Registry Number

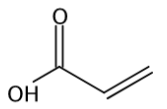
0 of 6 Substances Selected

1. 1580002-57-8

50856-25-2
(C₂H₄O)_n C₃H₆O



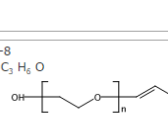
79-10-7
C₃H₄O₂



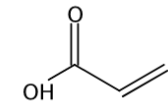
(C₃H₄O₂ · (C₂H₄O)_n C₃H₆O)_x
2-Propenoic acid, polymer with α-ethenyl-ω-methoxypoly(oxy-1,2-ethanediyl), graft

2. 1314225-78-9

191403-44-8
(C₂H₄O)_n C₃H₆O



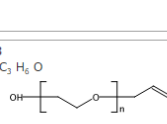
79-10-7
C₃H₄O₂



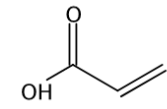
(C₃H₄O₂ · (C₂H₄O)_n C₃H₆O)_x
2-Propenoic acid, polymer with α-1-propen-1-yl-ω-hydroxypoly(oxy-1,2-ethanediyl), graft

3. 1010818-79-7

27274-31-3
(C₂H₄O)_n C₃H₆O



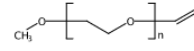
79-10-7
C₃H₄O₂



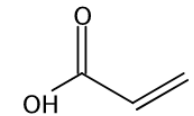
(C₃H₄O₂ · (C₂H₄O)_n C₃H₆O)_x
2-Propenoic acid, polymer with α-2-propen-1-yl-ω-hydroxypoly(oxy-1,2-ethanediyl), block

4. 250591-73-2

50856-25-2
(C₂H₄O)_n C₃H₆O



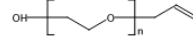
79-10-7
C₃H₄O₂



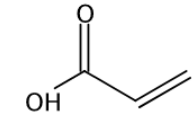
(C₃H₄O₂ · (C₂H₄O)_n C₃H₆O)_x
2-Propenoic acid, polymer with α-ethenyl-ω-methoxypoly(oxy-1,2-ethanediyl) (9CI)

5. 185506-87-0

27274-31-3
(C₂H₄O)_n C₃H₆O



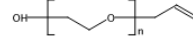
79-10-7
C₃H₄O₂



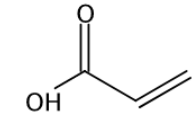
(C₃H₄O₂ · (C₂H₄O)_n C₃H₆O)_x
2-Propenoic acid, polymer with α-2-propen-1-yl-ω-hydroxypoly(oxy-1,2-ethanediyl), graft
Regulatory Information

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

The screenshot displays a chemical drawing editor with a central workspace containing a benzothiazole-like structure with two 'Ak' labels indicating the repeat unit. The interface includes a toolbar on the left, a 'Drawing Editor' panel on the right with search options (Structure, Reaction, Markush), and a search results panel on the far right. The search results panel shows a list of filters under 'Advanced Search' and 'Always Show', with 'Polymers' checked under 'Characteristics'. Below the filters, there is a 'KEEP ME POSTED' section with a list of recent search results.

Drawing Editor:

- Structure
- Reaction
- Markush

Get substances that match your query using:

- Exact search
- Substructure search
- Similarity search

Search Results Panel:

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

KEEP ME POSTED

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

View All

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

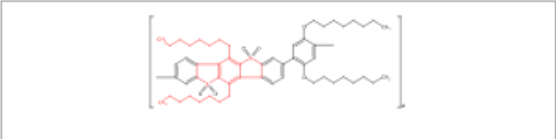
Analyze Refine Sort by: CAS Registry Number Display Options

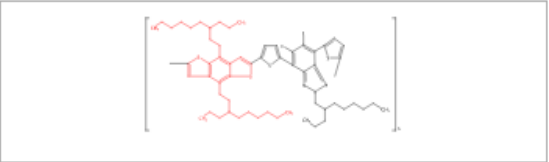
0 of 134 Substances Selected Page: 1 of 9

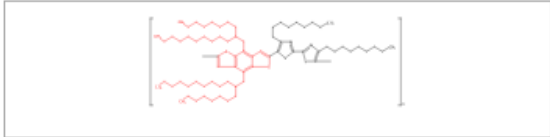
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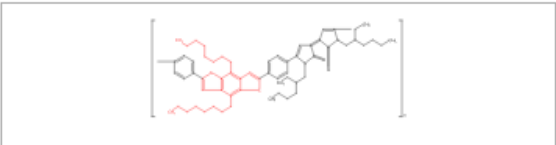
Uses 101
Preparation 84
Properties 75
Process 29
Prophetic in Patents 3
Reactant or Reagent 3
Occurrence 1

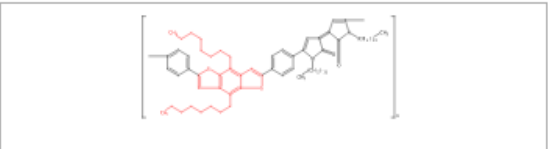
Show More

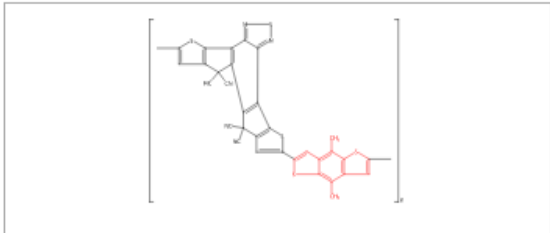
1. 2096989-39-6 Q
~1 
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INDEX NAME NOT YET ASSIGNED

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

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

Analyze Refine

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- Property Value
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Structure Editor:

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

Only retrieve substances that:

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- 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

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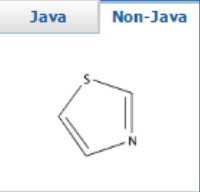
C₆H₆N₂S

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

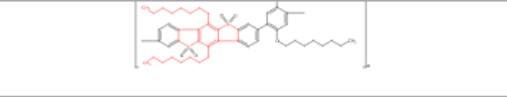
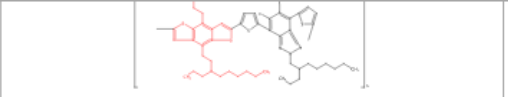
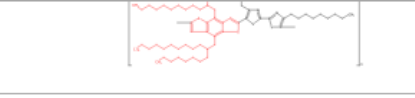


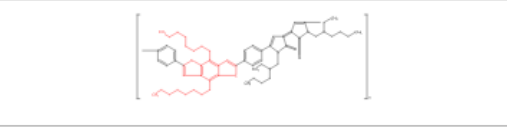


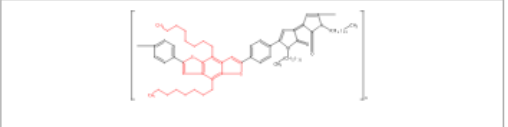

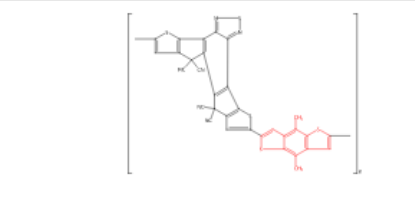

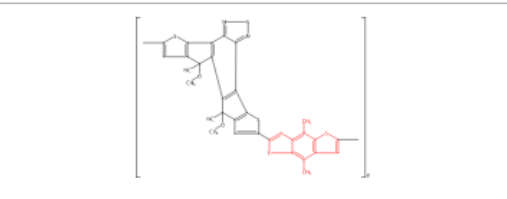

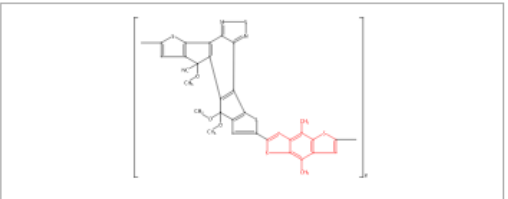

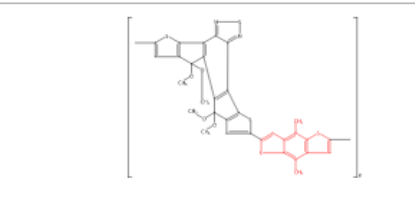
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 Are in specific substance classes
 Are in specific types of studies

Refine

 <p>(C₅₆ H₇₆ O₆ S₂)_n INDEX NAME NOT YET ASSIGNED</p>	 <p>(C₅₉ H₇₉ F₂ N₃ S₄)_n INDEX NAME NOT YET ASSIGNED</p>	 <p>(C₇₄ H₁₂₂ N₂ S₄)_n INDEX NAME NOT YET ASSIGNED</p>
<p><input type="checkbox"/> 4. 1974335-87-9 🔍</p> <p>~1  </p>  <p>(C₆₂ H₈₀ N₂ O₂ S₂)_n INDEX NAME NOT YET ASSIGNED</p>	<p><input type="checkbox"/> 5. 1974335-85-7 🔍</p> <p>~1  </p>  <p>(C₇₀ H₉₆ N₂ O₂ S₂)_n INDEX NAME NOT YET ASSIGNED</p>	<p><input type="checkbox"/> 6. 1909267-21-5 🔍</p> <p>~1 </p>  <p>(C₃₂ H₁₀ N₆ S₅)_n INDEX NAME NOT YET ASSIGNED</p>
<p><input type="checkbox"/> 7. 1909267-20-4 🔍</p> <p>~1 </p>  <p>(C₃₂ H₁₆ N₄ O₂ S₅)_n INDEX NAME NOT YET ASSIGNED</p>	<p><input type="checkbox"/> 8. 1909267-19-1 🔍</p> <p>~1 </p>  <p>(C₃₂ H₁₉ N₃ O₃ S₅)_n INDEX NAME NOT YET ASSIGNED</p>	<p><input type="checkbox"/> 9. 1909267-18-0 🔍</p> <p>~1 </p>  <p>(C₃₂ H₂₂ N₂ O₄ S₅)_n INDEX NAME NOT YET ASSIGNED</p>

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

Explore ▾ Saved Searches ▾ SciPlanner

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

REFERENCES

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

SUBSTANCES

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

REACTIONS

- Reaction Structure

SUBSTANCES: SUBSTANCE IDENTIFIER ?

qinghaosu

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

Search

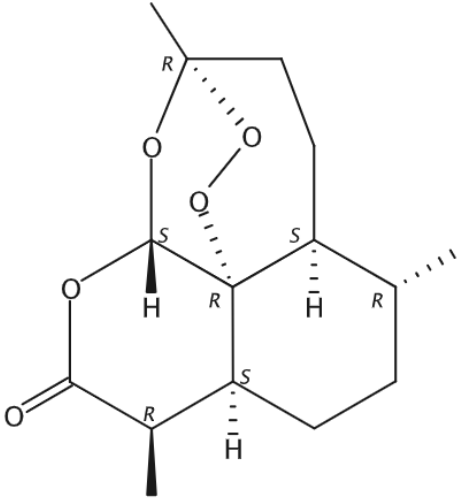
提示：
• 一次最多可输入25个物质。
• 每行一个物质标识符。

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 ▶
- Get Commercial Sources
- Get Regulatory Information
- Get References
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- Export as molfile
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SUBSTANCE DETAIL [Get References](#) [Get Reactions](#) [Get Commercial Sources](#)

[Return](#)

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*)-

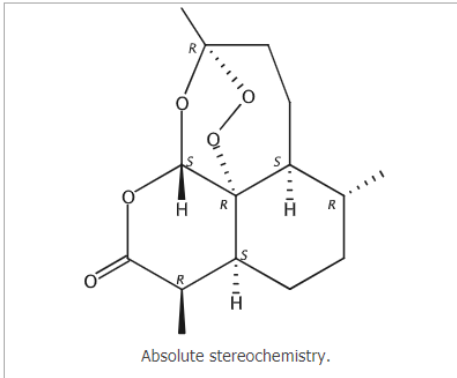
Molecular Weight
282.33

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

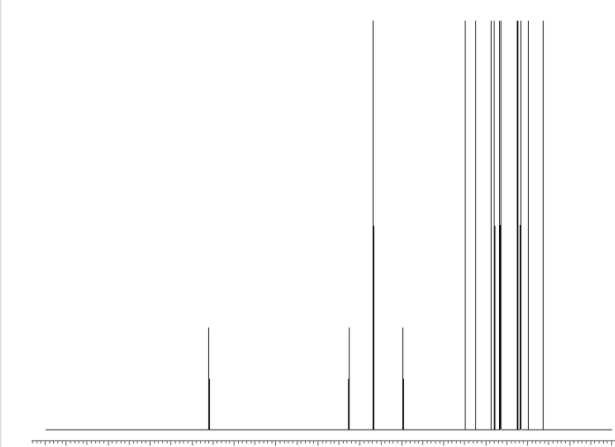
BIOACTIVITY INDICATORS

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.

大纲

- CAS SciFinder数据介绍
- 纳米储能材料的研究调研与追踪
- 生物、催化和医药研究的物质根基
- **结构视角下的专利风险规避**
- 制备反应研究的技术支撑



结构检索的原理与示例

US005480883A

5,480,883

1 BIS MONO- AND BICYCLIC ARYL AND HETEROARYL COMPOUNDS WHICH INHIBIT EGF AND/OR PDGF RECEPTOR TYROSINE KINASE

BACKGROUND OF THE INVENTION

This application is a continuation-in-part application of U.S. Ser. No. 07/988,515, filed Dec. 10, 1992, now abandoned which is a continuation-in-part application of U.S. Ser. No. 07/698,420, filed May 10, 1991 now abandoned and a continuation-in-part application of PCT International Application Ser. No. PCT/US92/03736 filed May 6, 1992.

FIELD OF THE INVENTION

This invention relates to the modulation and/or inhibition of cell signaling, cell proliferation, cell inflammatory response, the control of abnormal cell growth and cell reproduction. More specifically, this invention relates to the use of bis mono- and/or bicyclic aryl and/or heteroaryl compounds in inhibiting cell proliferation, including compounds which are useful protein tyrosine kinase (PTK) inhibitors.

Normal cellular reproduction is believed to be triggered by the exposure of the cellular substrate to one or more growth factors, examples of which are insulin, epidermal growth factor (EGF) and platelet-derived growth factor (PDGF). Such growth factor receptors are imbedded in and penetrate through the cellular membrane. The initiation of cellular reproduction is believed to occur when a growth factor binds to the corresponding receptor on the external surface of the cellular membrane. This growth factor-receptor binding alters the chemical characteristics of that portion of the receptor which exists within the cell and which functions as an enzyme to catalyze phosphorylation of either an intracellular substrate or the receptor itself, the latter being referred to as autophosphorylation. Examples of such phosphorylation enzymes include tyrosine kinases, which catalyze phosphorylation of tyrosine amino acid residues of substrate proteins.

Many disease states are characterized by the uncontrolled reproduction of cells. These disease states involve a variety of cell types and include disorders such as leukemia, cancer, psoriasis, inflammatory diseases, bone diseases, atherosclerosis and restenosis occurring subsequent to angioplastic procedures. The inhibition of tyrosine kinase is believed to have utility in the control of uncontrolled cellular reproduction, i.e., cellular proliferative disorders.

Initiation of autophosphorylation, i.e., phosphorylation of the growth factor receptor itself, and of the phosphorylation of a host of intracellular substrates are some of the biochemical events which are involved in mediator release mitogenesis and cell proliferation. Autophosphorylation of the insulin receptor and phosphorylation of substrate proteins by other receptors are the earliest identifiable biochemical hormonal responses.

Elimination of the protein tyrosine kinase (PTK) activity of the insulin receptor and of the epidermal growth factor (EGF) receptor by site-directed mutagenesis of the cellular genetic material which is responsible for generation of insulin and EGF results in the complete elimination of the receptor's biological activity. This is not particularly desirable because insulin is needed by the body to perform other biological functions which are not related to cell proliferation. Accordingly, compounds which inhibit the PTK portion of the EGF and/or PDGF receptor at concentrations less than

2

the concentrations needed to inhibit the PTK portion of the insulin receptor could provide valuable agents for selective treatment of cell proliferation disorders.

REPORTED DEVELOPMENTS

It has been reported that the most potent inhibitors of EGF receptors inhibit EGF-induced proliferation of A431/clon 15 cells with little or no effect on the proliferation of such cells when induced by other growth factors. It has been reported also that erbstatin inhibits the autophosphorylation of the EGF receptor in membranes of A431 cells. Higher concentrations of erbstatin are required to inhibit cyclic adenosine 3',5'-monophosphate (cAMP)-dependent protein kinase.

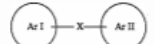
SUMMARY OF THE INVENTION

In accordance with the present invention, there is provided a method of inhibiting abnormal cell proliferation in a patient suffering from a disorder characterized by such proliferation comprising the administration to a patient of an EGF and/or PDGF receptor inhibiting effective amount of a bis mono- and/or bicyclic aryl compound exhibiting protein tyrosine kinase inhibition activity wherein each aryl group is a ring system containing 0-4 hetero atoms, said compound being optionally substituted or polysubstituted.

Another aspect of the present invention relates to pharmaceutical compositions comprising, in admixture with a pharmaceutically acceptable carrier, a pharmaceutically effective amount of a compound of the aforementioned type. Another aspect of this invention comprises compounds useful in the practice of the present method.

With respect to the method aspects of this invention, the compounds described by Formula I below constitute a class of the aforementioned bis mono- and/or bicyclic aryl, heteroaryl, carbocyclic or heterocarbocyclic compounds for use in the practice of the present invention:

Formula 1



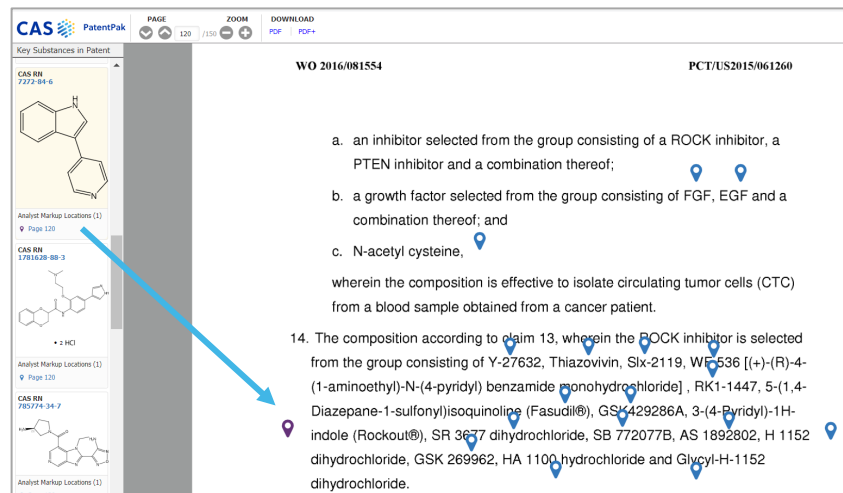
where:

Ar I and Ar II are independently a substituted or unsubstituted mono- or bicyclic ring, said rings optionally substituted with 0 to about 3 R groups; and

X is (CHR₁)_m or (CHR₁)_n-Z-(CHR₂)_n, where Z is O, NR, S, SO or SO₂, m and n are 0-3 and m+n=0-3 and R₁ and R₂ are independently hydrogen or alkyl; or a pharmaceutically acceptable salt thereof.

Preferably, Ar I is a substituted or unsubstituted mono- or bicyclic aryl or heteroaryl ring system of about 5 to about 12 atoms and where each monocyclic ring may contain 0 to about 3 hetero atoms, and each bicyclic ring may contain 0 to about 4 hetero atoms selected from N, O and S provided said hetero atoms are not vicinal oxygen and/or sulfur atoms and where the substituents may be located at any appropriate position of the ring system and are described by R₁.

Ar II may be as described for Ar I or at least one ring is a substituted or unsubstituted saturated carbocyclic of about 3 to about 7 atoms where each monocyclic ring may contain 0 to about 2 hetero atoms, and each bicyclic ring may contain 0 to about 4 hetero atoms selected from N, O and S provided said hetero atoms are not vicinal oxygen and/or sulfur atoms and where the substituents may be located at



Key Substances in Patent

WO 2016/081554 PCT/US2015/061260

CAS RN 7272-84-6

CAS RN 1781628-88-3

CAS RN 782774-34-7

Analyst Markup Locations (1) Page 120

Analyst Markup Locations (1) Page 120

Analyst Markup Locations (1) Page 120

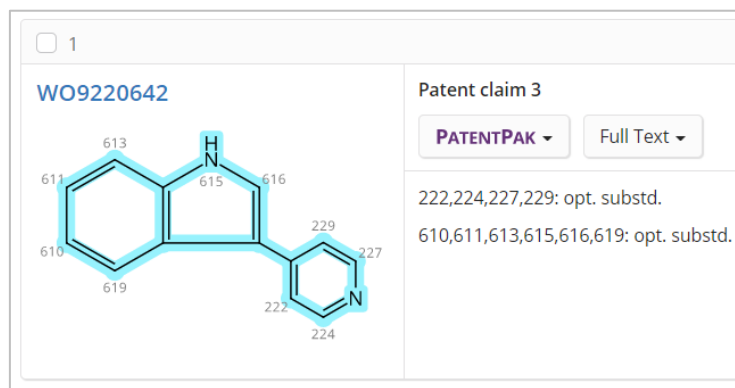
- an inhibitor selected from the group consisting of a ROCK inhibitor, a PTEN inhibitor and a combination thereof;
- a growth factor selected from the group consisting of FGF, EGF and a combination thereof; and
- N-acetyl cysteine,

wherein the composition is effective to isolate circulating tumor cells (CTC) from a blood sample obtained from a cancer patient.

14. The composition according to claim 13, wherein the ROCK inhibitor is selected from the group consisting of Y-27632, Thiazovivin, Six-2119, WF-536 [(+)-(R)-4-(1-aminoethyl)-N-(4-pyridyl) benzamide monohydrochloride], RK1-1447, 5-(1,4-Diazepan-1-sulfonyl)isoquinoline (Fasudil®), GSK429286A, 3-(4-Pyridyl)-1H-indole (Rockout®), SR 3677 dihydrochloride, SB 772077B, AS 1892802, H 1152 dihydrochloride, GSK 269962, HA 1100 hydrochloride and Glycyl-H-1152 dihydrochloride.

CAS REGISTRY

CAS REGISTRY



1

WO9220642

Patent claim 3

PATENTPAK Full Text

222,224,227,229: opt. substd.

610,611,613,615,616,619: opt. substd.

CAS Markush

Chemistry & Biology, Vol. 12, 385-395, 2005

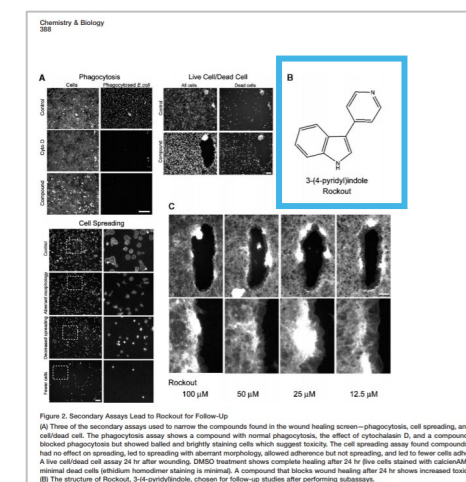


Figure 2. Secondary Assays Lead to Rockout for Follow-Up

(A) Three of the secondary assays used to narrow the compounds found in the wound healing screen—phagocytosis, cell spreading, and live cell/dead cell. The phagocytosis assay shows a compound with normal phagocytosis, the effect of cytochalasin D, and a compound that blocked phagocytosis but showed barrel and long-pyramidal cells which suggest toxicity. The cell spreading assay found compounds that had no effect on spreading, led to spreading with aberrant morphology, allowed adherence but not spreading, and led to fewer cells adhering. A live cell/dead cell assay 24 hr after wounding. DMSO treatment shows complete healing after 24 hr for live cells stained with calcein-AM and minimal dead cells (barrel homodimer staining is minimal). A compound that blocks wound healing after 24 hr shows increased toxicity. (B) The structure of Rockout, 3-(4-pyridyl)indole, chosen for follow-up studies after performing subscreens.



ACS
International

CAS
A division of the
American Chemical Society

结构检索的原理与示例

专利中物质的标引方式：

- 具体物质[Specific Substance]：

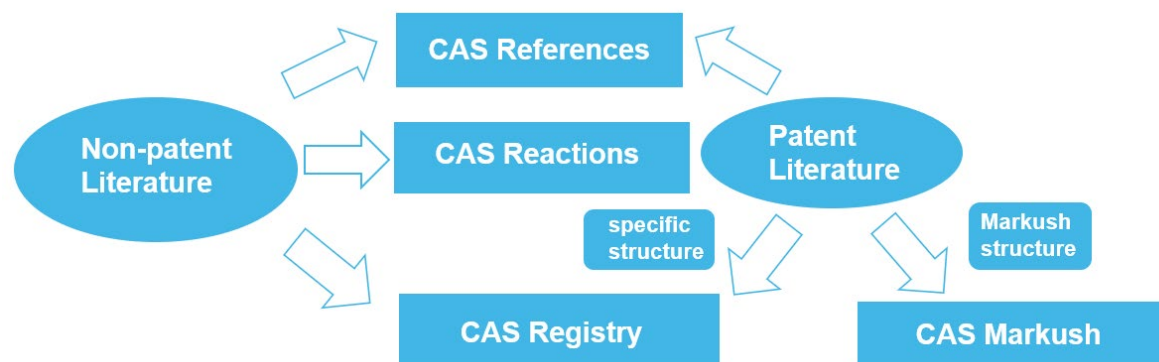
- 以具体化学结构陈述的特定物质，会被分配CAS RN

- 预测性物质[Prophetic Substance]：

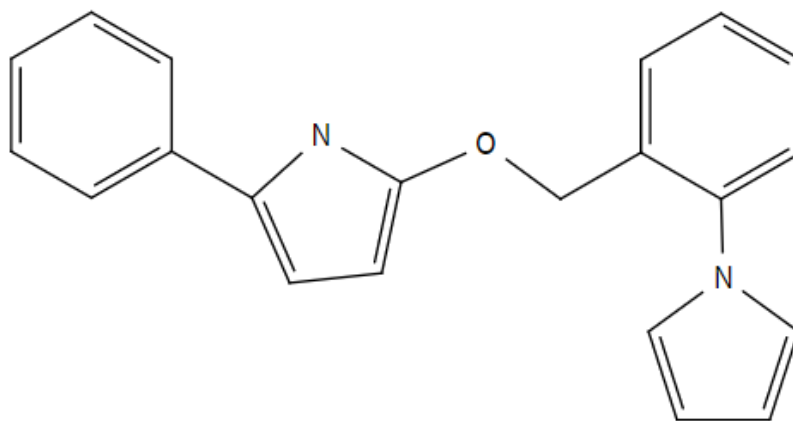
- 使用Markush结构陈述的预测物质，一个Markush可以陈述上百或上千个化学物质

- 被Markush结构包含，但未被实施或呈现在表格、权利要求书或说明书中的结构，不会被CAS分配CAS Registry Number

- Markush检索，能检索到通过结构检索检不到的专利

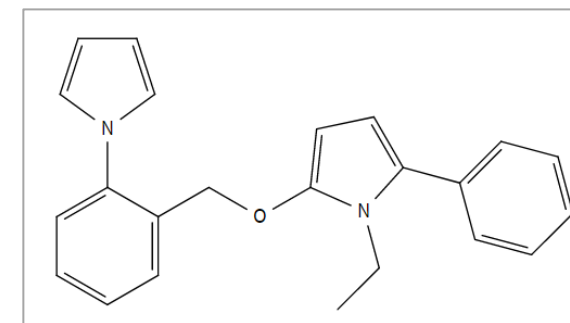


例：此结构是否已被相关文献披露？是否被包含在已公开专利文献的通式结构中？



先在CAS Registry中进行物质结构检索

The screenshot shows the CAS Registry search interface. At the top, there are navigation tabs: "Explore", "Saved Searches", and "SciPlanner". Below these, a breadcrumb trail reads "Chemical Structure substructure > substances (0)". The left sidebar contains three main sections: "REFERENCES" with options like "Research Topic", "Author Name", "Company Name", "Document Identifier", "Journal", "Patent", and "Tags"; "SUBSTANCES" with options like "Chemical Structure", "Markush", "Molecular Formula", "Property", and "Substance Identifier"; and "REACTIONS" with "Reaction Structure". The main content area is titled "SUBSTANCES: CHEMICAL STRUCTURE" and features a "Structure Editor" with a chemical structure of a query molecule. To the right of the editor are search options: "Search Type:" with radio buttons for "Exact Structure", "Substructure" (which is selected), and "Similarity"; and a checkbox for "Show precision analysis". Below the search options is a "ChemDraw" logo and a button to "Launch a SciFinder/SciFinder ChemDraw. Learn More". At the bottom of the main area is a large blue "Search" button and a link for "Advanced Search".



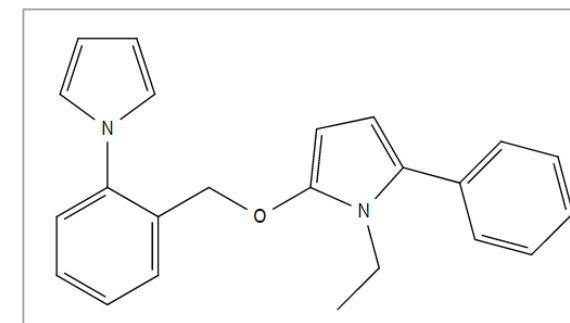
Query

Exact Structure, Substructure结果为0

先在CAS Registry中进行物质结构检索

1 of 3 Similarity Candidates Selected		Substances
<input type="checkbox"/>	≥ 99 (most similar)	0
<input type="checkbox"/>	95-98	0
<input type="checkbox"/>	90-94	0
<input type="checkbox"/>	85-89	0
<input type="checkbox"/>	80-84	0
<input type="checkbox"/>	75-79	0
<input checked="" type="checkbox"/>	70-74	13
<input type="checkbox"/>	65-69	113
<input type="checkbox"/>	0-64 (least similar)	2741

[Get Substances](#)



Query

Chemical Structure similarity > substances (13)

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

Analyze Refine Sort by: Similarity Score [Display Options](#)

Analyze by: Substance Role Preparation 9 Reactant or Reagent 6 [Show More](#)

0 of 13 Substances Selected

<p>Score: 73</p> <p>1. 2546026-51-7</p> <p>C₁₈H₁₈N₂O₂ 1H-Pyrrol-2-ol, 1-(5-amino-2-methylphenyl)-5-(phenylmethoxy)- Key Physical Properties</p>	<p>Score: 73</p> <p>2. 2588894-62-4</p> <p>C₁₆H₁₈N₂O₂ 1H-Pyrrol-2-ol, 1-(3-amino-4-methylphenyl)-5-(phenylmethoxy)- Key Physical Properties</p>	<p>Score: 72</p> <p>3. 183614-37-1</p> <p>C₂₄H₂₁N O 1H-Pyrrole, 5-ethoxy-1,2,3-triphenyl- Key Physical Properties</p>	<p>Score: 72</p> <p>4. 824935-40-2</p> <p>C₁₈H₁₇N O₂ 1H-Pyrrol-2-ol, 5-(4-methylphenyl)-1-phenyl-, 2-acetate Key Physical Properties Experimental Properties</p>
<p>Score: 72</p> <p>5. 1170700-44-3</p> <p>C₁₈H₁₇N O₂</p>	<p>Score: 72</p> <p>6. 1191052-68-2</p> <p>C₂₆H₁₇N O₄ Benzoic acid, 4-[2-(acetoxyl)-5-phenyl-1H-pyrrol-1-yl]-</p>	<p>Score: 72</p> <p>7. 2437287-69-7</p> <p>C₁₈H₁₇N O₃ 1H-Pyrrol-2-ol, 1-(3-hydroxy-4-methylphenyl)-5-(phenylmethoxy)-</p>	<p>Score: 71</p> <p>8. 2563403-40-5</p> <p>C₁₈H₁₇N O₃ 1H-Pyrrol-2-ol, 1-(2-hydroxy-5-methylphenyl)-5-(phenylmethoxy)-</p>

Similarity结果中物质最大相似度
仅为73%

再在CAS Markush中进行物质Markush结构检索

Markush substructure > references (1)

REFERENCES ?

Get Substances Get Reactions Get Related Citations Tools

Create Keep Me Posted Alert Send to SciPlanner

Analyze Refine Categorize

Sort by: Accession Number

0 of 1 Reference Selected

Analyze by: Author Name

Chang So Young 1

Choi Junghwan 1

Jo Su Yeon 1

Kang Sun Hee 1

Kim Young Mi 1

Kong Sun Ju 1

Lee Ji Hye 1

Min Ji Young 1

Park Kaapjoo 1

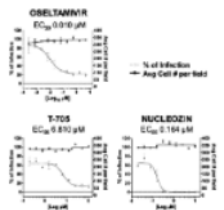
Show More

1. Preparation of heteroaryl compounds as antiviral agents

Quick View PATENTPAK

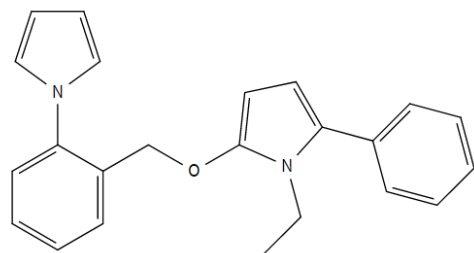
By Min, Ji Young; Chang, So Young; Lee, Ji Hye; Kang, Sun Hee; Kong, Sun Ju; Jo, Su Yeon; Park, Kaapjoo; Kim, Young Mi; Choi, Junghwan
From PCT Int. Appl. (2018), WO 2018062978 A1 20180405. | Language: Korean, Database: CAPLUS

Disclosed are compds. I or II [X¹ = O, S or -N(Et)-; X², X³ = independently N or CH; Y = absent, -CH₂-, -CH₂NH-, etc.; Z = absent, -CH₂S-, -CH₂NH-, etc.; R¹ = Q¹, Ph (optionally substituted with halo, alkyl, cycloalkyl, etc.), pyridin-2-yl, etc.; R^a = halo, alkyl, (un)substituted Ph, etc.; n = 0-3; R² = H, Q², naphthalen-1-yl, etc.; R^b = Ph (optionally substituted with alkyl or halo), alkyl, methoxy, etc.; m = 0-2; or enantiomers, diastereomers or pharmaceutically acceptable salts thereof]. Thus, compd. III was prepd. from 4-bromo-3,5-dimethyl-1H-pyrazole via conversion into 2-[(4-bromo-3,5-d...

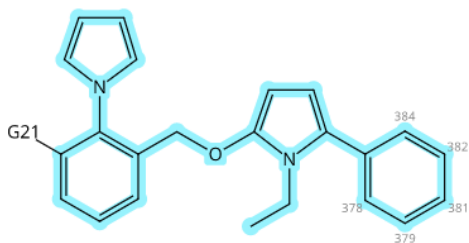


Patent No.	PatentPak Options	Kind	Language
WO 2018062978	PDF PDF+ Viewer	A1	Korean
Patent Family			
KR 2018036415	PDF PDF+ Viewer	A	Korean
US 20200031816	PDF	A1	English
US 11149033	PDF	B2	English

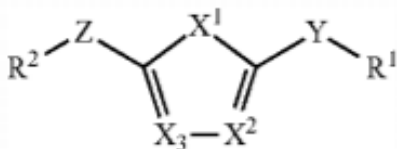
CAS科学家对专利原文中的Markush结构进行直观标引



Query structure



Indexed structure



Markush structure

What is claimed is:

1. Compound represented by the following Chemical formula 1 or Chemical formula 2, an enantiomer thereof, a diastereomer thereof, or a pharmaceutically acceptable salt thereof:

[Chemical formula 1]

or

[Chemical formula 2]

wherein

X¹ is O, S or —N(CH₂CH₃)—,
X² and X³ are each independently N or CH,
Y is absent, or, is —CH₂—; —CH₂NH—; —C(=O)—;
—CH₂CH₂—; —NH—; —NHC(=O)—; —C(=O)
NH—; —CH(CH₃)—; —CF₂—; —CH(OCH₃)—;
—CH₂O—; —N(CH₃)—; or —CH₂NHC(=O)—,
Z is absent, or, is —CH₂S—; —CH₂S(=O)—;
—CH₂NH—; —CH(R^c)S—; —CH₂CH₂S—; —CH₂N
(CH₃)—;

—CH=CH—; —S—; —CH₂—; —O—; —CH₂S(=O)
₂—; —C(=O)—; —SCH₂—; —CH₂CH₂—; —CH
(OH)—; —CH(CH₃)CH₂—; —OCH₂—; —C(=O)
CH₂S—; —C(=O)—NH—; —CH=C(CH₃)—; —CH₂-
cyclopropyl—; —NH—S(=O)₂—; —S(=O)₂—NH—; or
—NH—C(=O)—,
R^c is benzene,
R¹ is

benzene unsubstituted, or substituted with one or more selected from the group consisting of halogen, linear or branched C₁₋₄ alkyl, C₃₋₆ cycloalkyl, —OCF₃, —CF₃, —CHF₂, —OH, phenoxy, phenyl, C₁₋₄ alkoxy, —CN, —NH₂, and —N(CH₃)₂;

pyridine unsubstituted, or substituted with halogen; naphthalene unsubstituted, or substituted with C₁₋₄ alkoxy; benzotriazole; quinoline or isoquinoline unsubstituted, or substituted with C₁₋₄ alkyl, C₁₋₄ alkoxy or halogen; indazole unsubstituted, or substituted with C₁₋₄ alkyl; C₃₋₆ cycloalkyl; benzothiazophene; benzofuran; indole unsubstituted, or substituted with C₁₋₄ alkyl; or thiophene,

R^a is halogen; linear or branched C₁₋₄ alkyl; OCF₃; CF₃; or unsubstituted benzene,
R^c is benzene,
n is an integer in the range of 0 to 3,
R² is H;

C₁₋₄ alkyl; naphthalene unsubstituted, or substituted with halogen;

benzene unsubstituted, or substituted with one or more selected from the group consisting of halogen, linear or branched C₁₋₄ alkyl, C₃₋₆ cycloalkyl, —OCF₃, —CF₃, —CHF₂, —OH, phenoxy, phenyl, C₁₋₄ alkoxy, —CN, —NH₂, and —N(CH₃)₂;

benzofuran unsubstituted, or substituted with halogen; benzodioxole unsubstituted, or substituted with halogen; quinoline or isoquinoline unsubstituted, or substituted with halogen; pyrazole unsubstituted, or substituted with linear or branched C₁₋₄ alkyl or halogen; indole substituted with C₁₋₄ alkyl; or imidazopyridine,

R^b is benzene unsubstituted, or substituted with one or more selected from the group consisting of linear C₁₋₄ alkyl and halogen; linear C₁₋₄ alkyl; branched C₃₋₅ alkyl; —OCH₃; 5-membered or 6-membered heteroaryl comprising N, O or S; cycloalkyl of 5 to 7 carbon atoms; —C(=O)CH₃; —OR^c; —C(=O)OCH₃; —CH₂R^c; —CF₃; —OCF₃; —OH; —N(CH₃)₂; —C(=O)—OH; pyrrolidine; piperidine; pyrrole; furan; thiophene; morpholine; C₁₋₄ alkoxy substituted with morpholine; —NRdRe (wherein Rd is H or methyl, and Re is —CH₂CH₂OCH₃ or —CH₂CH₂Ph); or halogen,
R^c is benzene unsubstituted, or substituted with halogen; C₁₋₄ alkyl; or halogen, and
m is an integer in the range of 0 to 2.

R^a is C₁₋₄ alkyl; halogen; or unsubstituted benzene,
R^c is benzene,
n is an integer in the range of 0 to 3,
R² is

US 2020/0031816 A1

107

Jan. 30, 2020

CAS PatentPak: 查看专利中重要的物质信息

WO2018062978

PATENTPAK
A CAS SOLUTION

PAGE 62 / 181 ZOOM DOWNLOAD PDF

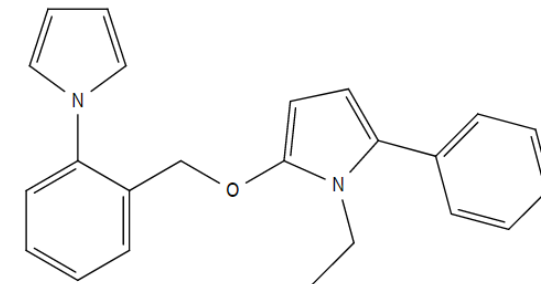
Key Substances in Patent

CAS RN 2215969-90-5
Search in SciFinder | View Detail
Analyst Markup Locations (1)
page 62

CAS RN 2215969-91-6
Search in SciFinder | View Detail
Analyst Markup Locations (1)
page 62

CAS RN 2215969-93-8

[852] C1 합성의 일반적인 방법
[853] 물질 A2 (405 mg, 1.55 mmol)를 무수 EtOH (6 mL)에 용해시켰다.



Query

大纲

- CAS SciFinder数据介绍
- 纳米储能材料的研究调研与追踪
- 生物、催化和医药研究的物质根基
- 结构视角下的专利风险规避
- 制备反应研究的技术支撑



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 rings. 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 has radio buttons for 'Structure', 'Reaction', and 'Markush', with 'Reaction' selected. Below this, there are options for 'Get reactions where the structure(s) are:' with radio buttons for 'Variable only at the specified positions' and 'Substructures of more complex structures'. The bottom of the interface features a periodic table and a search bar. Four blue callout boxes with white text 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

角色定义

反应箭头

原子标记

官能团列表

化学键变化

例1: 双膦配体钴催化剂可以催化哪些类型反应

Author Name
Company Name
Document Identifier
Journal
Patent
Tags

SUBSTANCES

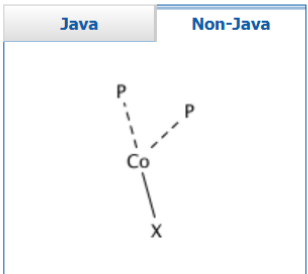
- Chemical Structure
- Markush
- Molecular Formula
- Property
- Substance Identifier

REACTIONS

- Reaction Structure

Structure Editor:

Java Non-Java



Search Type:

- Exact Structure
- Substructure
- Similarity

Show precision analysis

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

ChemDraw
Launch a SciFinder/SciFind latest version of ChemDraw

CAS Solutions
SCIFINDER
A CAS SOLUTION

Explore Saved Searches SciPlanner

Chemical Structure substructure with limiters > substances (9232) > get

SUBSTANCES

Get References Get Reactions

Analyze Refine

Sort by: CAS Registry Number

0 of 9232 Substances Selected

Analyze by: Substance Role

Preparation 6163

Properties 3978

Reactant or Reagent 1769

Process 1022

Uses 1014

Biological Study 250

Formation, Nonpreparative 208

1. 2471733-36-3

75-05-8
C₂ H₃ N

CH₃ — C≡

2471700-16-8
C₂₆ H₄₆ Co₂ N₂ S₂ · 2 F₆ P

2471700-15-7
C₂₆ H₄₆ Co₂ N₂ S₂

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

Group by Transformation: 锁定反应类型

Chemical Structure substructure with limiters > substances (9232) > **get reactions (8570)** > reactions with tra

REACTIONS ? Get References Tools

Analyze Refine

Analyze by: ?
Reagent ▼


H ₂ O	1479
H ₂	1341
Zn	1338
O ₂	1041
<i>t</i> -BuOK	1018
NH ₄ Cl	934
BuLi	825
HCl	701

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

▼ No Grouping
Document ns Selected
Transformation

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

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



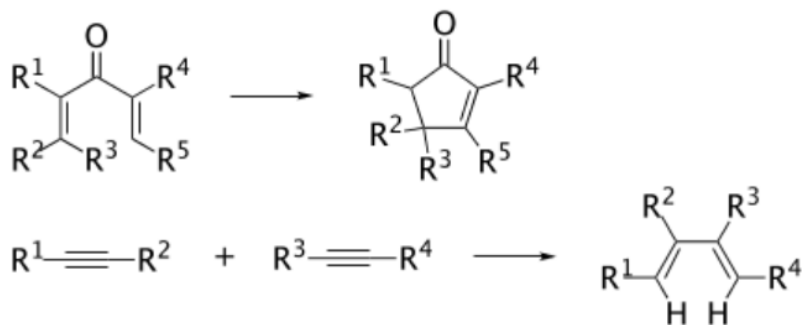
Overview

Steps/Stages

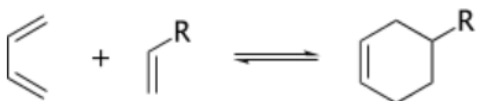
- 1.1 C:2430461-60-0, C:EtAlCl₂, S:PhMe, 30 min, 40°C, 5 atm
- 1.2 R:HCl, S:H₂O, neutralized

快速获取各类催化反应类型

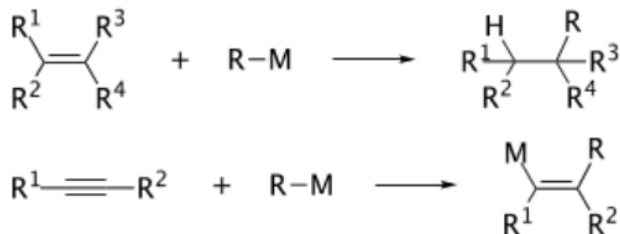
1. Addition of Alkenes/ Alkynes to Alkenes/ Alkynes/ Nazarov Cyclization
[552 Reactions](#)



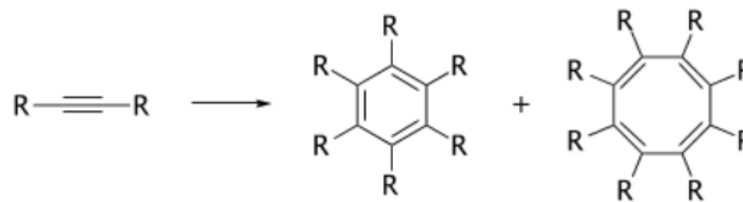
2. Diels-Alder Reaction and Retro-Diels-Alder Reaction
[352 Reactions](#)



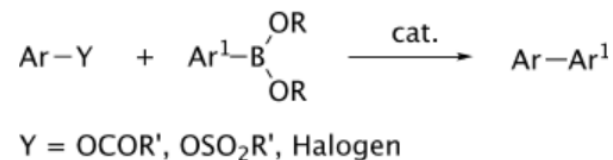
3. Addition of Organometallics to Unactivated Double or Triple Bonds
[196 Reactions](#)



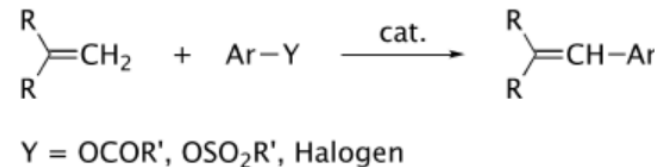
4. Cyclotrimerization and Cyclotetramerization of Alkynes
[190 Reactions](#)



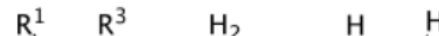
5. Coupling of Aryl Compounds with Arylboronic Acid Derivatives/ Suzuki Coupling
[140 Reactions](#)



6. Arylation and Alkylation of Alkenes/ Heck Reaction
[138 Reactions](#)



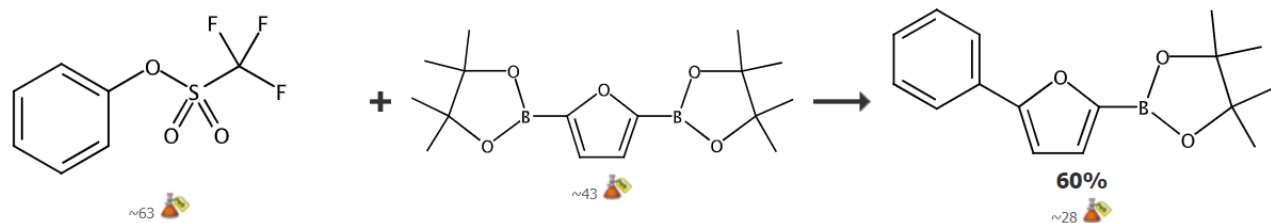
7. Reduction of Double or Triple Bonds/ Hydrogenation
[110 Reactions](#)



查看反应信息

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

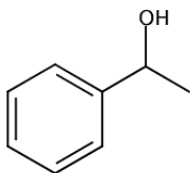
Single Step *Hover over any structure for more options.*



Overview

Steps/Stages

1.1 R:



• Na

C:1578190



Click for more options



Notes

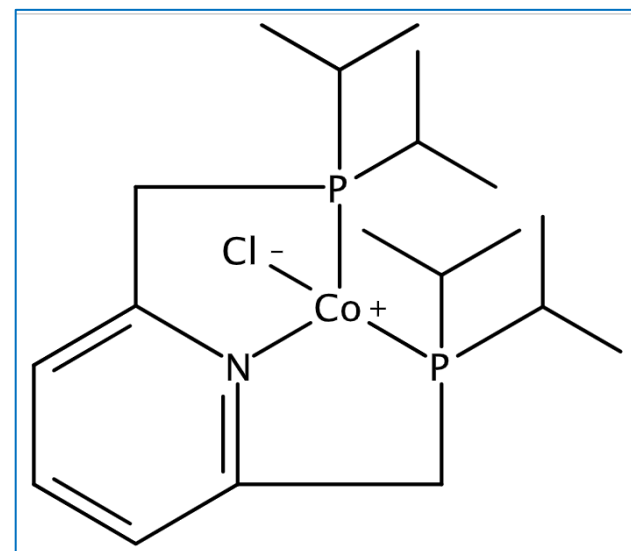
Suzuki-Miyaura cross coupling, scintillation sealed vial used, increment phenyl triflate, NaOCH(Ph)Me, (iPrPNP)CoCl, THF, catalyst prepared at Reactants: 2, Reagents: 1, Catalysts: 1, Solvents: 1, Steps: 1, Stages: stages in any one step: 1

References

Insight into Transmetalation Enables Cobalt-Catalyzed Suzuki-Miyaura Coupling

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

By Neely, Jamie M. et al
From ACS Central Science, 2(12), 935-942; 2016



例2：聚乙二醇单烯丙基醚的合成与修饰

The image displays a screenshot of the CAS database interface. The main window shows a search for the substance with CAS Registry Number 27274-31-3. The search results list the substance with its chemical structure and formula: $(C_2H_4O)_n C_3H_6O$, Poly(oxy-1,2-ethanediyl), α -2-propen-1-yl- ω -hydroxy-Regulatory Information. The interface includes navigation tabs for 'Analyze' and 'Refine', and buttons for 'Get References', 'Get Reactions', and 'Get Commercial Sources'. A 'Get Reactions' dialog box is open, showing the 'Limit results by reaction role:' section with the 'Product' role selected. The dialog box also includes 'Get' and 'Cancel' buttons.

Substance Identifier "27274-31-3" > substances (1)

Substances

Get References Get Reactions Get Commercial Sources Tools

Analyze Refine

Sort by: CAS Registry Number

0 of 1 Substance Selected

1. 27274-31-3

~2509 ~22

OC(CCO)nCC=C

$(C_2H_4O)_n C_3H_6O$
Poly(oxy-1,2-ethanediyl), α -2-propen-1-yl- ω -hydroxy-
Regulatory Information

Analyze by: Substance Role

Analytical Study 1
Biological Study 1
Formation, Nonpreparative 1
Occurrence 1
Preparation 1

Get Reactions

Limit results by reaction role:

Product
 Reactant
 Reagent
 Reactant or reagent
 Catalyst
 Solvent
 Any role

Get Cancel

获得聚乙二醇单烯丙基醚的合成制备反应

Substance Identifier "27274-31-3" > substances (1) > **get reactions (70)**

REACTIONS Get References Tools Send to SciPlanner

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

0 of 70 Reactions Selected Page: 1 of 2

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

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

C=CCO + C1CO1 >> OCC(OCCO)nCC=C

Overview

Steps/Stages

1.1 R:

S:THF, rt

Notes

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

References

Core-crosslinked worm-like micelles from polyether-based diblock terpolymers
[Quick View](#) [Other Sources](#)
By Elter, Johanna K. et al
From Polymer Chemistry, 10(40), 5425-5439; 2019

聚乙二醇单烯丙基醚的改性修饰

SUBSTANCES

Get References Get Reactions Get Commercial Sources Tools

Analyze **Refine**

Sort by: CAS Registry Number

0 of 1 Substance Selected

1. **27274-31-3**

~2509 ~22

(C₂H₄O)_nC₃H₆O
Poly(oxy-1,2-ethanediyl), α-2-propen-1-yl-ω-hydroxy-

Regulatory Information

Get Reactions

Limit results by reaction role:

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

Get Cancel

Refine: 精炼烯烃接枝后的结构变化

Substance Identifier "27274-31-3" > substances (1) > get reactions (1812)

REACTIONS **Get References** **Tools** removes for selected reactions **Send to SciPlanner**

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

0 of 1812 Reactions Selected Page: 1 of 37

1. View Reaction Detail [Link](#)

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

~22 ~80

Structure Editor:

Java Non-Java

Click to Edit

Search type: **Substructure**

Overview

Steps/Stages

- 1.1 S:H₂O, 58°C
- 1.2 3 h
- 1.3 R:HSCH₂CH₂CO₂H, S , 2 h, 63-65°C
- 1.4 R:NaOH, pH 5-7

Notes

initiator added at stage 2, Reactants: 2, Reagents: 4, Most stages in any one step: 4

References

Star-shaped poly(carboxylic acid) water-reducing admixtures using tannic acid azo compound as initiator **PATENTPAK**

REACTIONS **Get References** **Tools** removes for selected reactions **Send to SciPlanner**

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

0 of 214 Reactions Selected Page: 1 of 5

1. View Reaction Detail [Link](#)

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

~22 ~16

Overview

Steps/Stages

- 1.1 C:SiO₂, C:919-30-2, C:32267-20-2, C:Pt, 225 min, 100°C

Notes

catalyst prepared and used, Reactants: 2, Catalysts: 4, Steps: 1, Stages: 1, Most stages in any one step: 1

REACTIONS **Get References** **Tools** removes for selected reactions **Send to SciPlanner**

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

0 of 214 Reactions Selected Page: 1 of 5

1. View Reaction Detail [Link](#)

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

~22 ~16

Overview

Steps/Stages

- 1.1 C:SiO₂, C:919-30-2, C:32267-20-2, C:Pt, 225 min, 100°C

Notes

catalyst prepared and used, Reactants: 2, Catalysts: 4, Steps: 1, Stages: 1, Most stages in any one step: 1

聚乙二醇单烯丙基醚的羟基修饰

The screenshot displays a chemical reaction software interface. On the left, a drawing tool shows the reaction of a chlorosilane (reactant) to a trialkoxysilane (product). The main window shows a list of reactions with filters for 'Reaction Structure', 'Product Yield', 'Number of Steps', 'Reaction Classification', 'Excluding Reaction Classification', and 'Non-participating functional groups'. A selected reaction is shown in detail, including the chemical structures of the reactants and products, and a list of steps/stages. The reaction is: $\text{CH}_3\text{Si}(\text{Cl})(\text{CH}_3)_2 + \text{HO}[\text{CH}_2\text{CH}_2\text{O}]_n\text{CH}_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3\text{Si}(\text{OCH}_2\text{CH}_2\text{O})_n\text{CH}_2\text{CH}=\text{CH}_2$. The reaction conditions are: 1.1 R:Et₃N, S:Cyclohexane, rt; 0.5 h, 30°C. The interface also includes a 'Structure Editor' with 'Java' and 'Non-Java' tabs, and a 'References' section with a link to 'Preparation method of polyether-based trialkoxysilane'.

REACTIONS [?](#) [Get References](#) [Tools](#) ▼

Group by: No Grouping ▼ Sort by: Relevance ▼ ↓

0 of 142 Reactions Selected

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

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

$\text{CH}_3\text{—Si}(\text{Cl})(\text{CH}_3)_2 + \text{OH}[\text{—CH}_2\text{CH}_2\text{O}]_n\text{—CH}_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3\text{—Si}(\text{OCH}_2\text{CH}_2\text{O})_n\text{—CH}_2\text{CH}=\text{CH}_2$

~108 🔍 ~22 🔍

Overview

Steps/Stages

1.1 R:Et₃N, S:Cyclohexane, rt; 0.5 h, 30°C

Notes

green chemistry-process simplification, Reactants: 2, Reagent Steps: 1, Stages: 1, Most stages in any one step: 1

References

Preparation method of polyether-based trialkoxysilane [Quick View](#) [PATENTPAK](#) ▼

Structure Editor: Java Non-Java

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

例3：生物转化反应

The screenshot shows the SciFinder Structure Editor interface. On the left, there are navigation tabs for 'Explore' and 'Saved', and a list of 'REFERENCES' and 'SUBSTANCES'. The main area is the 'Structure Editor' with a toolbar and a central workspace. The workspace shows a chemical reaction: a benzene ring with a methyl group (labeled 'reactant') is converted to a benzene ring with an isopropyl alcohol group (labeled 'product'). The 'Drawing Editor' on the right has 'Reaction' selected. Below the workspace, there is a 'Get reactions where the structure(s) are:' section with two options: 'Variable only at the specified positions' and 'Substructures of more complex structures', with the latter selected. At the bottom, there is a 'Drawing Editor' section with 'Structure', 'Reaction', and 'Markush' options, and 'Reaction' is selected. There are also 'OK' and 'Cancel' buttons.

The screenshot shows the 'REACTIONS: REACTION STRUCTURE' search interface. It features a 'Structure Editor' section with 'Java' and 'Non-Java' tabs, and a 'Search Type:' section with 'Allow variability only as specified' and 'Substructure' options. The 'Substructure' option is selected. Below this, there is a 'Click image to change structure or view detail.' section with a 'Search' button. The 'Import CXF' section is also visible. The 'Solvents' section has a 'Select Solvents' button. The 'Non-participating Functional Groups' section has a 'Select Groups' button. The 'Number of Steps' section has a text input field with '1' and examples: '1, 1-3, 1-, -3'. The 'Classifications' section has 'Biotransformation' selected, and 'Catalyzed', 'Non-catalyzed', and 'Photochemical' options are also present. There are 'Advanced Search' and 'Always Show' options. At the bottom, there is a 'ChemDraw' logo and a 'Launch a SciFinder/SciFinder® subst...' button.

查看生物催化酶

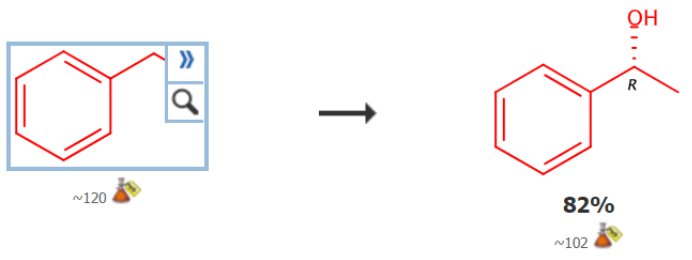
REACTIONS 🔍 Get References Tools Send to SciPlanner

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

0 of 4901 Reactions Selected Page: 1 of 99

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

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



~120

82%
~102

Overview

Steps/Stages

1.1 R:H₂O₂, C:Peroxidase, S:H₂O, 0.5 h, 24°C, pH 7

Notes

stereoselective, biotransformation, enzymic, phosphate buffered solution, Agrocybe aegerita peroxidase used, Reactants: 1, Reagents: 1, Catalysts: 1, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Stereoselective hydroxylation of alkyl aromatics using Agrocybe aegerita peroxidase

细胞色素P450酶可以催化哪些反应

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

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

Search

Substance Identifier "Cytochrome P 450" > substances (1)

Get References | Get Reactions | Get Commercial Sources | Tools

Sort by: CAS Registry Number

Analyze | Refine

0 of 1 Substance Selected

<input type="checkbox"/>	1. 9035-51-2	~51214	~10
	Substance Image		
	Cannot Be Displayed		
	9035-51-2		

Unspecified
Cytochrome P450

Get Reactions

Limit results by reaction role:

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

Get Cancel

Group by Transformation: 一键浏览反应类型

Substance Identifier "Cytochrome P 450" > substances (1) > get reactions (4762)

REACTIONS Get References Tools

Analyze Refine

Analyze by: Reagent

Coenzyme II	2815
NaHCO ₃	2058
NH ₄ Cl	1897
HCl	1667
Martin's reagent	1632
NaOH	1568
3671-99-6	1319
Me ₂ CO	1305
H ₂	1297
HF	1284

Group by: No Grouping Sort by: Accession Number

No Grouping 0 of 4762 Reactions Selected

Document

Transformation

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

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

[Overview](#) [Steps/Stages](#) [Notes](#)

Group by: Transformation Sort by: Frequency

0 of 4762 Reactions Selected

1. **Nitration of Aromatic Compounds**
567 Reactions

$$\text{Ar-H} \xrightarrow{\text{HNO}_3} \text{Ar-NO}_2$$

2. **Hydroxylation at an Aliphatic Carbon**
379 Reactions

$$\text{R-CH}_2\text{-R}^1 \longrightarrow \text{R-CH(OH)-R}^1$$

3. **Hydroxylation at an Aromatic Carbon**
73 Reactions

$$\text{Ar-H} \xrightarrow{\text{H}_2\text{O}_2} \text{Ar-OH}$$

4. **Hydroxylation of Aromatic Compounds**
72 Reactions

$$\text{Ar-H} + \text{R}^1\text{C(=O)OOH} \longrightarrow \text{Ar-OH}$$

5. **Epoxidation of Alkenes**
55 Reactions

$$\text{R}^1\text{-CH=CH-R}^3 \longrightarrow \text{R}^1\text{-CH(O)}\text{-CH(R}^3\text{)}$$

6. **Formation of Alkyl Halides/ Alcohols from Ethers /Silyl Ethers**
47 Reactions

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

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

7. **Oxidation of Aldehydes to Carboxylic Acids**
38 Reactions

$$\text{R-CHO} \longrightarrow \text{R-COOH}$$

8. **Oxidation of Methyl/Methylene to Carbonyl**
28 Reactions

$$\text{R-CO-CH}_2\text{-R}^1 \longrightarrow \text{R-CO-CO-R}^1$$

9. **Oxidation of Thioethers to Sulfoxides and Sulfones**
23 Reactions

$$\text{R-S-R}^1 \longrightarrow \begin{cases} \text{R-S(=O)-R}^1 \\ \text{R-S(=O)}_2\text{-R}^1 \end{cases}$$

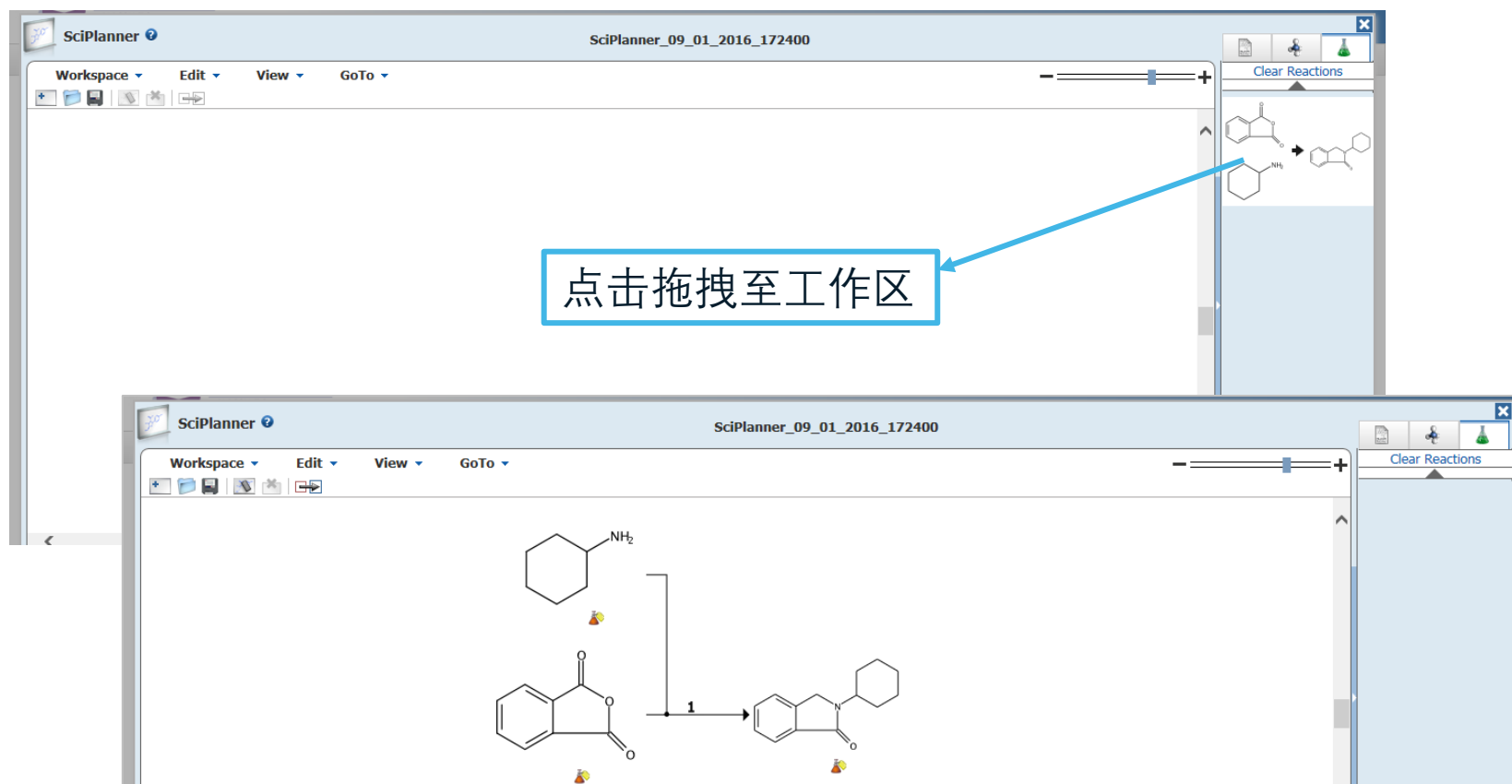
利用SciPlanner设计拟合成反应路线

点击打开SciPlanner工作界面

The screenshot displays the SciPlanner web interface. At the top, there are navigation tabs: 'Explore', 'Saved Searches', and 'SciPlanner'. Below the tabs, the breadcrumb path reads 'Reaction Structure substructure > reactions (1208) > refine "Catalyzed" (535)'. The main content area is titled 'REACTIONS' and includes options for 'Get References' and 'Tools'. A list of reactions is shown, with '1. View Reaction Detail' selected. A callout box points to a 'Send to SciPlanner' button. Below the list, a chemical reaction scheme is displayed, showing the synthesis of a bicyclic amide from a phthalimide derivative and cyclohexylamine. The reaction is labeled with a yield of 87% and a reaction number of ~1.

选择感兴趣的反应，点击send to SciPlanner

SciPlanner工作界面



SciPlanner工作界面

SciPlanner
SciPlanner_09_01_2016_172400

Workspace Edit View GoTo

CAS Registry Number: 85-44-9

- View Substance Detail
- Explore by Structure
- Synthesize this...
- Get Reactions where Substance is a
- Get Commercial Sources
- Get Regulatory Information
- Get References

点击物质右上角的双箭头，检索其合成方法

Get References Tools

Group by: No Grouping Sort by: Accession Number

1 of 382 Reactions Selected

4. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.

97%
~132 ~136

Send to SciPlanner

Display Options

Page: 1 of 26

从结果中选择感兴趣的反应，继续推送至SciPlanner

SciPlanner工作界面

The top screenshot shows a workspace with a chemical reaction (1) where cyclohexylamine reacts with a cyclic imide to form a substituted imide. A second reaction is partially visible on the right. A blue arrow points from the text '继续拽至工作区' to the reaction scheme.

The bottom screenshot shows the same workspace with two reactions (1 and 2) overlaid. Reaction 1 is the same as in the top screenshot. Reaction 2 shows the synthesis of the imide from a diacid and a cyclic amine. Blue boxes highlight the overlapping structures. A blue arrow points from the text '两个反应在同一工作窗口' to the overlapping structures.

继续拽至工作区

两个反应在同一工作窗口

将相同的两个结构移动至重叠

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 a starting material (a benzene ring with two carboxylic acid groups) and proceeding through two steps (labeled 1 and 2) to a final product (a benzene ring with a fused ring system and a cyclohexyl group). The text "导出设计的路线" (Export the designed route) is overlaid on the reaction scheme. Below the reaction scheme, the text "合二为一的合成路线" (Synthesis route combined into one) is visible. An "Export" dialog box is open on the right side of the screen, showing options for "Offline Review" (Portable Document Format, Citations, Image) and "Saving Locally" (SciPlanner eXchange). The "Details" section includes fields for "File Name" (SciPlanner_09_01_2016_172400) and "Title". The "Include" section has checkboxes for "SciPlanner Image", "Reaction Details", "Substance Details", and "Reference Details".

导出设计的路线

合二为一的合成路线

总结：

- CAS全面的数据内容、化学相关的广泛交叉学科覆盖和科学家的增值标引；
- 主题词构建及候选项的选择；设置提醒，及时跟踪最新研究进展；
- Analyze: CA Section Title锁定学科主题, Index Term精炼核心研究点；Categorize: 高效、精准锁定核心研究点；
- 各类物质的检索方法；结构编辑器的灵活应用；结构检索和Markush检索的数据基础，对规避专利风险的帮助；
- 基于物质和反应的关联，灵活获取反应信息；Substance Role, Reaction Role一键锁定物质在文献中和反应中的角色；Group by Transformation高效获取反应类型；SciPlanner根据感兴趣的反应自主设计拟合出反应路线。

谢谢关注!



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