

# CAS SciFinder Discovery Platform

## 全面高效获取科技信息



陈开乾 博士

[kchen@acs-i.org](mailto:kchen@acs-i.org)

美国化学文摘社(CAS)北京代表处

# 大纲

## CAS及CAS SciFinder Discovery Platform 简介

### 科研信息的高效查阅

- 全面的文献调研与拓展助力开题
- 多角度出发检索物质结构及相关属性
- 探索实验方案以获取反应与合成相关策略
- 高效获取分析方法及配方制剂信息

### 常见问题Q&A



# CAS SciFinder Discovery Platform 涵盖的工作流程解决方案



新一代的权威科学研究工具，是化学及相关学科智能研究平台，提供全球全面、可靠的化学及相关学科研究信息和分析工具



独特的分析方法详情数据库，有助于分析科学家快速获取详尽的分析方法信息、直接用于实验，并启发新方法的建立



专业的制剂/配方数据库，助力配方研究科学家快速评估配方、寻找可替代供应商和探索监管信息

# CAS 内容合集来源于化学、超越化学

5大类80小类

- 有机化学各领域：
  - 脂肪/环族化合物、杂环化合物、有机金属化合物、生物分子、碳水化合物
- 物理、无机、分析化学各领域：
  - 电化学、表面化学、催化剂、相平衡、核现象
- 大分子化学各领域：
  - 合成高聚物化学；塑料的制造、加工、成型与应用；涂料、墨水
  - 染料、有机颜料；合成橡胶；纺织品、纤维
- 应用化学各领域：
  - 大气污染、陶瓷、精油、化妆品、化石燃料、黑色金属、合金
- 生物化学：
  - 药理学、农化产品管控信息、生化遗传学、发酵、免疫化学

来源：<https://www.cas.org/support/documentation/references/ca-sections>

# CAS独特的内容合集

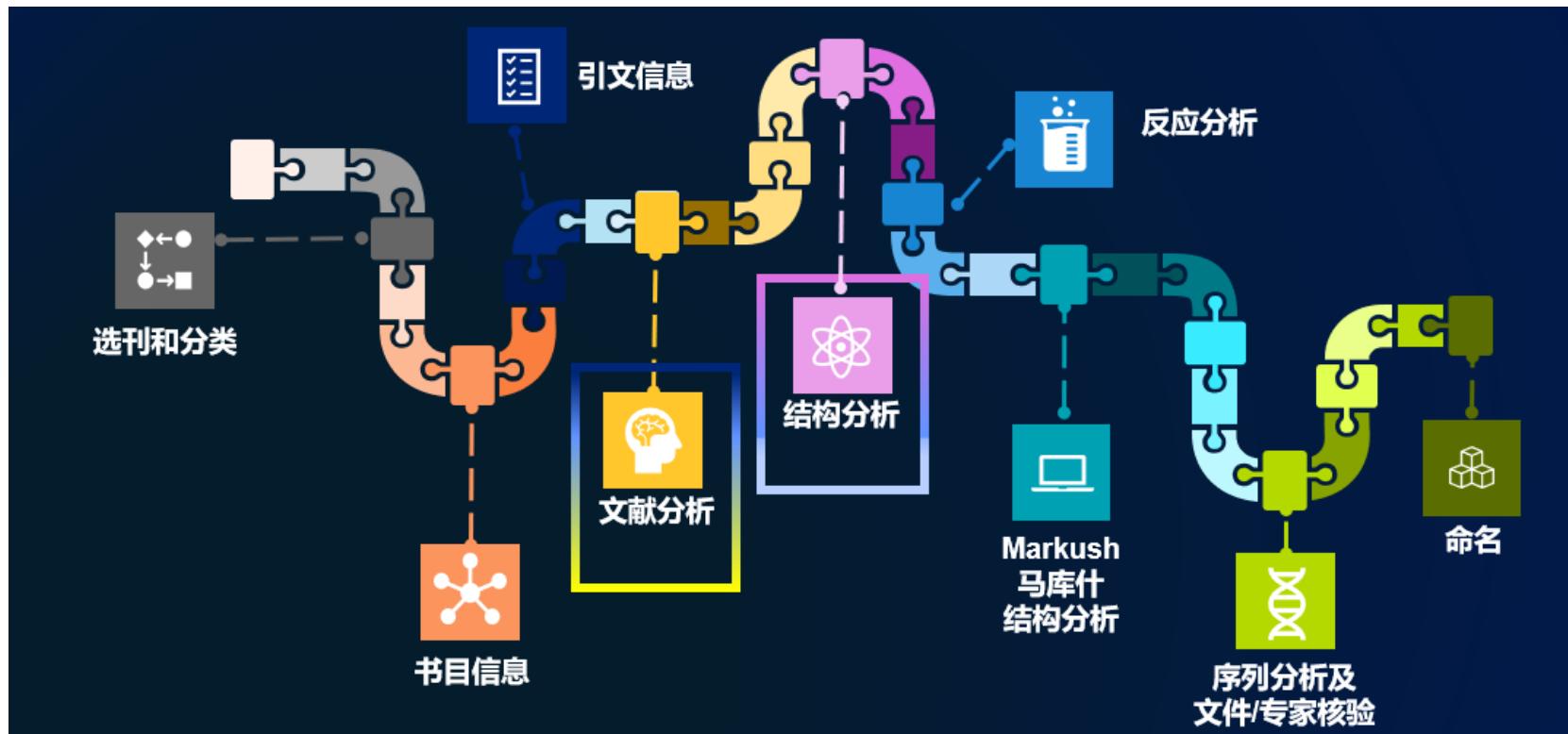


来源：

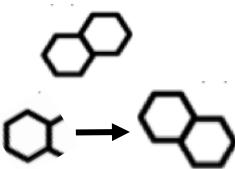
<https://www.cas.org/cas-data>

<https://www.cas.org/about/cas-content>

# CAS科学家的智力标引



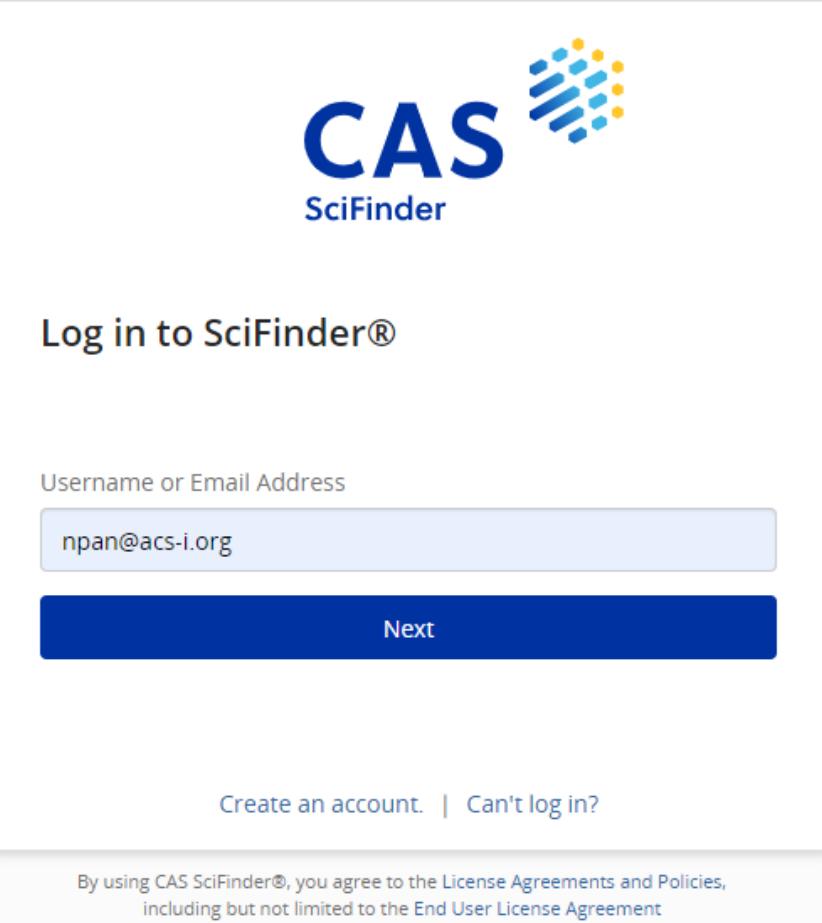
A small icon of a document or file, represented by a rectangle with horizontal lines inside.



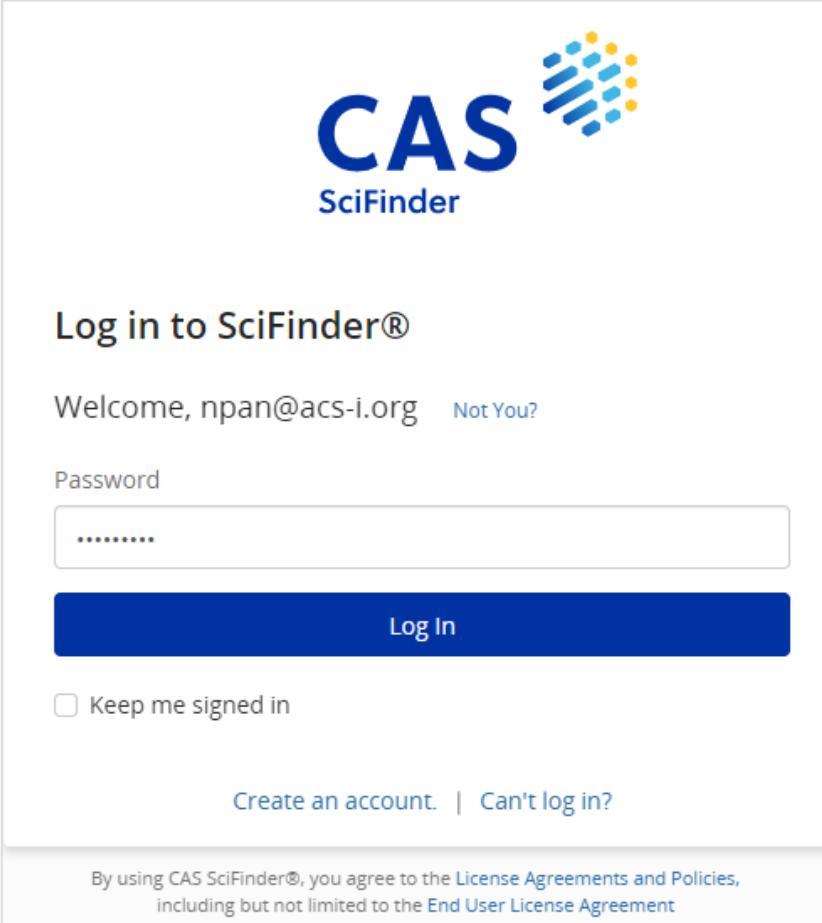
## Androst-4-en-3-one, 17-hydroxy-17-methyl-, (17 $\beta$ )-

**CAS科学家利用人类智慧对公开内容进行揭示，使相关信息更容易被挖掘**

# CAS SciFinder 登录网址: <https://scifinder-n.cas.org/>



The screenshot shows the first step of the CAS SciFinder login process. At the top, the CAS SciFinder logo is displayed. Below it, the text "Log in to SciFinder®" is centered. A light gray input field is labeled "Username or Email Address" and contains the text "npan@acs-i.org". Below this field is a large blue rectangular button with the word "Next" in white. At the bottom of the screen, there are two links: "Create an account." and "Can't log in?". A small note at the very bottom states: "By using CAS SciFinder®, you agree to the License Agreements and Policies, including but not limited to the End User License Agreement".



The screenshot shows the second step of the CAS SciFinder login process. At the top, the CAS SciFinder logo is displayed. Below it, the text "Log in to SciFinder®" is centered. Above the input field, the text "Welcome, npan@acs-i.org" is shown, followed by a link "Not You?". A light gray input field is labeled "Password" and contains several dots, indicating a password has been entered. Below this field is a large blue rectangular button with the word "Log In" in white. To the left of the "Log In" button is a small checkbox labeled "Keep me signed in". At the bottom of the screen, there are two links: "Create an account." and "Can't log in?". A small note at the very bottom states: "By using CAS SciFinder®, you agree to the License Agreements and Policies, including but not limited to the End User License Agreement".

## 使用CAS SciFinder账号登录

# 如何获取CAS SciFinder账号

登录本校图书馆网站，查看注册相关的链接和说明

<https://lib.jiangnan.edu.cn/info/1131/1637.htm>

## | 使用说明：

### 1、CAS SciFinder-n 账号注册须知

读者在使用CAS SciFindern之前**须用江南大学的学校域名邮箱地址注册账号**（如果已经注册了CAS SciFinder账号，请用该账号直接登录CAS SciFinder-n），根据提示输入相应信息，提交注册申请后系统将自动发送一个链接到您所填写的邮箱中，进入邮箱激活此链接即可完成注册。

### 2、SciFinder账号注册链接

<https://scifinder.cas.org/registration/index.html?corpKey=F1455EF5X86F35055X2E756CE85D18B16693>

### 3、CAS SciFinder-n检索网址

<https://scifinder-n.cas.org/>

### 4、CAS SciFinder-n培训材料及视频：

<https://www.cas.org/support/training/scifinder-n>

# 清晰简洁的检索界面



# 大纲

## CAS及CAS SciFinder Discovery Platform 简介

### 科研信息的高效查阅

- 全面的文献调研与拓展助力开题
- 多角度出发检索物质结构及相关属性
- 探索实验方案以获取反应与合成相关策略
- 高效获取分析方法及配方制剂信息

### 常见问题Q&A



# 通过文献标识符快速获取文献

支持使用：主题词、DOI、文献号、专利号、物质名词、CAS登记号等

The screenshot displays two side-by-side search results from the SciFinder database.

**Left Panel (DOI Search):**

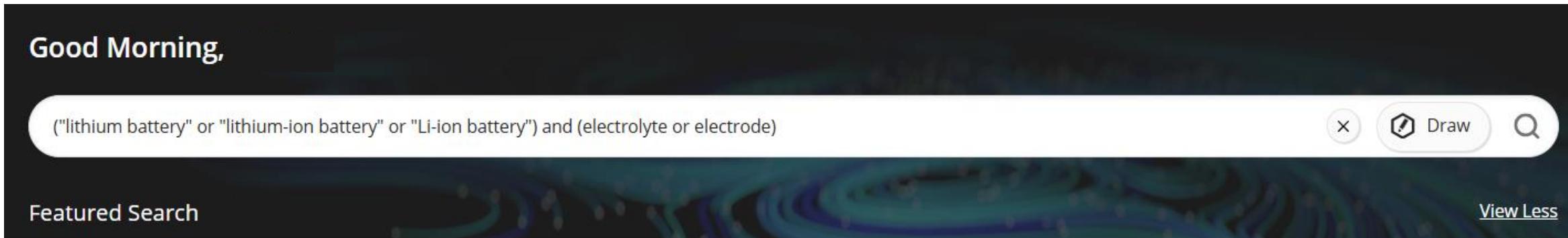
- Search bar: 10.1021/acssuschemeng.5b00981
- Filter Results sidebar:
  - Behavior: Filter by (selected), Exclude
  - Search Within Results
  - Document Type: Journal (1)
  - Flags
  - Language
- Result list:
  - Pyrrolinium-based Ionic Liquid as a Flame Retardant (ACS Sustainable Chemistry & Engineering, 2016, 4(2), 497-505)
- View More button
- Bottom navigation: Full Text, 11, 3, 43, 0

**Right Panel (Reference Search):**

- Search bar: An In Situ Polymeric Electrolyte with Low Interfacial Resistance on Electrodes for Lithium-Ion Batteries
- Filter Results sidebar:
  - Behavior: Filter by (selected), Exclude
  - Search Within Results
  - Document Type: Journal (1)
  - Flags
  - Language
- Result list:
  - An In Situ Polymeric Electrolyte with Low Interfacial Resistance on Electrodes for Lithium-Ion Batteries (Advanced Materials Interfaces, 2022, 9(3), 2101958)
- View More button
- Bottom navigation: View: Partial Abstract, Full Text, 5, 3, 3, 0

# 如何精准构建检索主题？

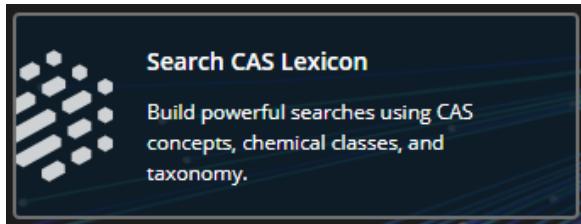
- 支持布尔逻辑运算符(and, or, not)
- 默认运算顺序or > and > not, ( )优先运算
- “”不允许词形变化，但可出现单数或复数
- 通配符\*代表0或多个字符；?代表0或1个字符



示例：("lithium battery" or "lithium-ion battery" or "Li-ion battery")  
and (electrolyte or electrode)

# CAS Lexicon 快速开启检索

对新的研究方向了解不深，不知道从何入手？



- CAS科学家标引的概念词(Concepts) 和重要物质
- 选择感兴趣的技术词来建立检索式(最多可用1000个词)

Search CAS Lexicon      Learn more about CAS Lexicon searching.

Search a concept to start (ex. Biomass)...      Search Concept

Preferred Concept

Primary batteries ⓘ  
This will search synonyms: Nonrechargeable batteries; Primary battery

Broader Concepts (1)      Select All  
 Batteries ⓘ

Narrower Concepts (10)      Select All  
 Button-type primary batteries  
 Dry cell primary batteries  
 Lithium primary batteries ⓘ  
 Nuclear batteries  
 Primary batteries, reserve  
[View All](#)

Related Concepts (4)      Select All  
 Battery electrodes ⓘ  
 Battery electrolytes  
 Electrolytic capacitors

AND      OR      NOT      Add to Query      Clear Query      Search

Primary batteries - Preferred Concept ⓘ      Remove All

OR

Primary batteries - Narrower Concept (1)  
Lithium primary batteries ⓘ

Primary batteries - Related Concept (1)  
Battery electrolytes

主题词示例：  
primary batteries (干电池)

- 干电池的上位词
- 干电池的下位词
- 干电池相关词汇

# 自定义组合检索

## Advanced Search

Select a search type, and then add multiple search fields to build a query. [?](#)

[Learn more about Advanced Search.](#)

Substance:  References  Clear All

Search by Keyword, Substance/Functional Group Name, CAS RN, Concept, Patent Number, PubMed ID, AN, CAN, and/or DOI.

Publication Name: Journal of the American Chemical Society

Volume (Optional)

Issue (Optional)

Starting Page (Optional)

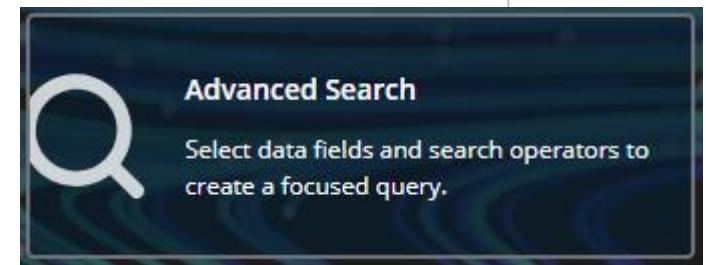
AND Publication Year: 2020 to 2025

+ Add Advanced Search Field

AND  
OR  
NOT

Authors/Inventors  
Publication Name  
Organization  
Title  
Abstract/Keywords  
Concept  
Substances  
Life Science Data   
Publication Year  
Document Identifier  
Patent Identifier  
Publisher

Search



检索方法可单独使用，也可联用：

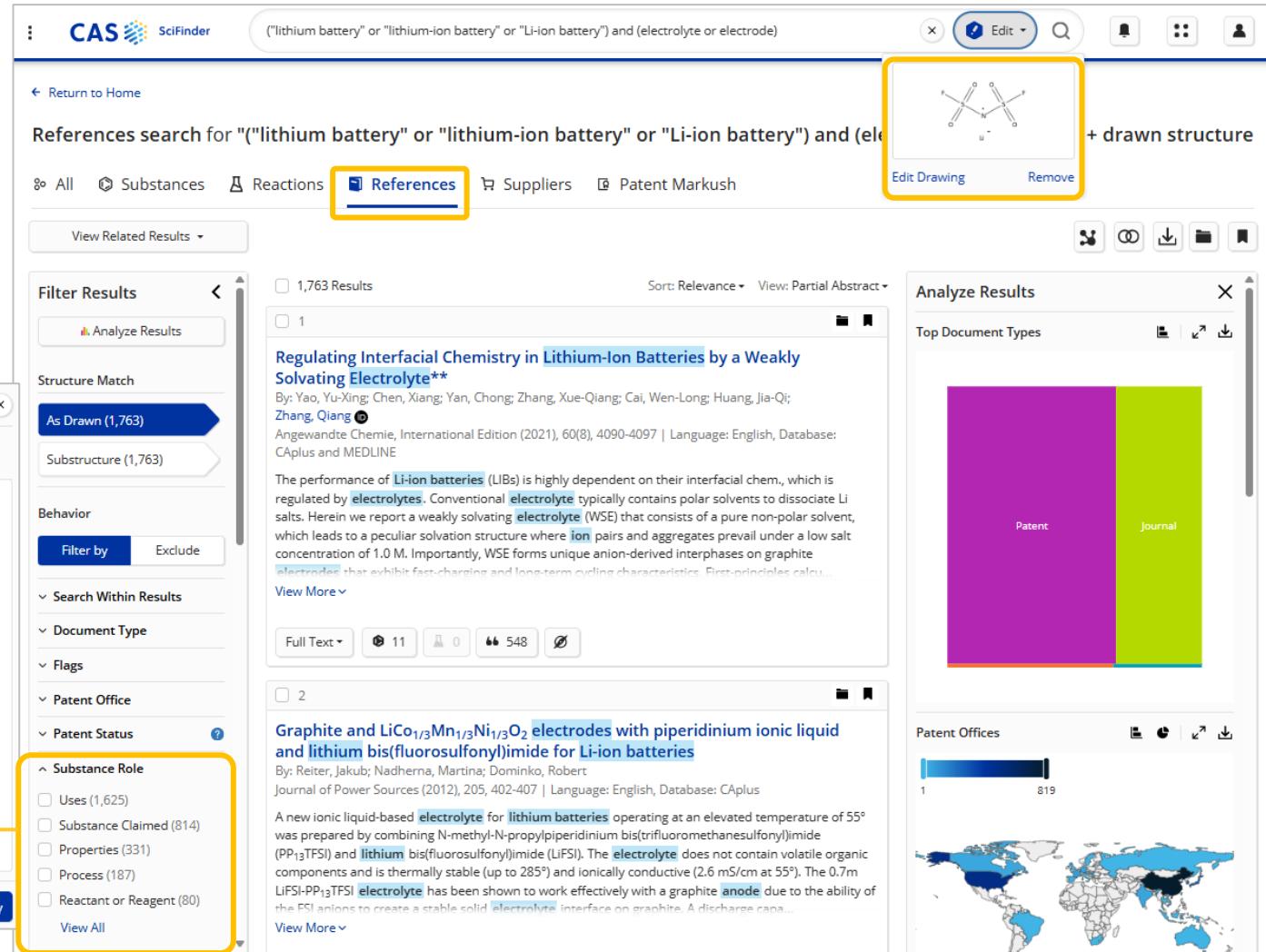
- 关键词、物质名称、CAS RN、文献号
- 高级检索（刊物名、机构名、Concepts、标题等）

# 如何获得结构相关的文献？

文本与结构是“and”关系

示例：关注锂电池技术中特定的热点材料

策略：从References出发，主题词+结构联用检索



# 文献结果的筛选与定题追踪

排序方式

Relevance  
Times Cited  
Accession Number: Ascending  
Accession Number: Descending  
Publication Date: Newest  
Publication Date: Oldest

Save and Alert  
Share Results  
Copy Search to Clipboard

Save Results  
Name: Project XXX  
Search Options: All Answers (Up to 20,000)  
Add Existing Tags (Optional): Agriculture, Chinese Medicine, Cigarette, Diabetes, Food  
New Tag (Optional): Add tag name, Tag Color: Light Blue  
Alerts  
Frequency: As Available  
Add Email(s): Add Recipient(s)

设置定题追踪

1,763 Results

Sort: Relevance ▾ View: Partial Abstract ▾

1 Regulating Interfacial Chemistry in Lithium-Ion Batteries by a Weakly Solvating Electrolyte\*\*  
By: Yao, Yu-Xing; Chen, Xiang; Yan, Chong; Zhang, Xue-Qiang; Cai, Wen-Long; Huang, Jia-Qi; Zhang, Qiang  
Angewandte Chemie, International Edition (2021), 60(8), 4090-4097 | Language: English, Database: Cplus and MEDLINE  
The performance of Li-ion batteries (LIBs) is highly dependent on their interfacial chem., which is regulated by electrolytes. Conventional electrolyte typically contains polar solvents to dissociate Li salts. Herein we report a weakly solvating electrolyte (WSE) that consists of a pure non-polar solvent, which leads to a peculiar solvation structure where ion pairs and aggregates prevail under a low salt concentration of 1.0 M. Importantly, WSE forms unique anion-derived interphases on graphite electrodes that exhibit fast-charging and long-term cycling characteristics. First-principles calcu...  
View More

2 e and LiCo<sub>1/3</sub>Mn<sub>1/3</sub>Ni<sub>1/3</sub>O<sub>2</sub> electrodes with piperidinium ionic liquid lithium bis(fluorosulfonyl)imide for Li-ion batteries  
Jakub, Nadherna, Martina; Dominko, Robert  
Power Sources (2012), 205, 402-407 | Language: English, Database: Cplus  
A new ionic liquid-based electrolyte for lithium batteries operating at an elevated temperature of 55° was prepared by combining N-methyl-N-propylpiperidinium bis(trifluoromethanesulfonyl)imide (PP<sub>13</sub>TFSI) and lithium bis(fluorosulfonyl)imide (LiFSI). The electrolyte does not contain volatile organic components and is thermally stable (up to 285°) and ionically conductive (2.6 mS/cm at 55°). The 0.7m LiFSI-PP<sub>13</sub>TFSI electrolyte has been shown to work effectively with a graphite anode due to the ability of the FS<sub>I</sub> anions to create a stable solid electrolyte interface on graphite. A discharge capa...  
View More

数据关联

View Related Results ▾  
How are these results different? Learn more.  
Substances  
Reactions  
Citing  
As Drawn (1,763)  
Substructure (1,763)  
Behavior  
Filter by  
Exclude  
Search Within Results  
Search for up to 3 text strings within the result set.  
Enter a query...  
Search  
Document Type  
Flags  
Patent Office  
Patent Status  
Substance Role  
Uses (1,625)

Analyze Results

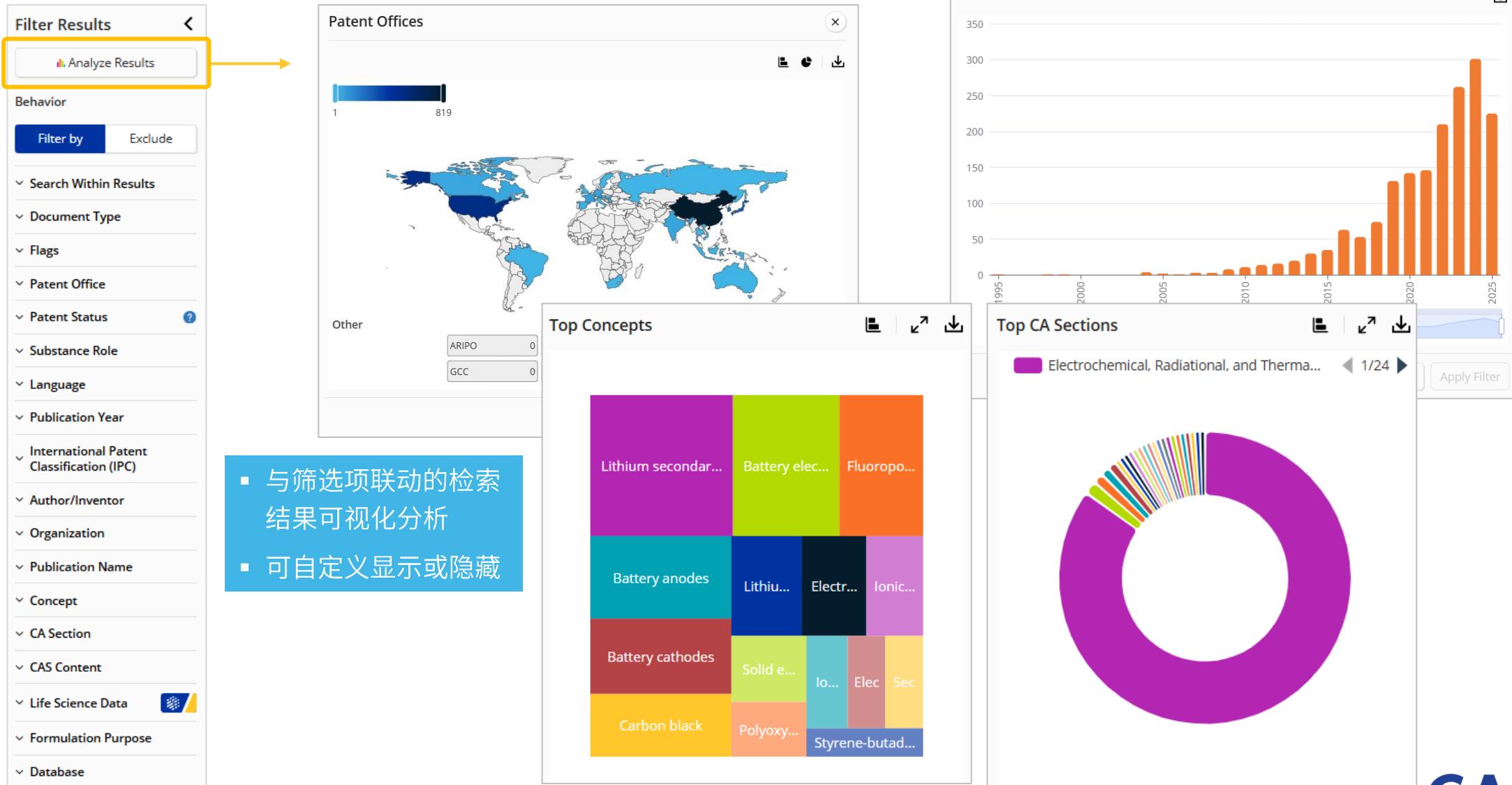
Top Document Types

Patent journal

Patent Offices

1 819

# 文献结果的筛选与可视化分析



# 筛选工具 CA Section & Concept

**CAS标引的学科研究方向**

**CA Section**

By Count Alphanumeric

3 Selected

- Electrochemical, Radiational, and Thermal Energy Technology (1,618)
- Chemistry of Synthetic High Polymers (28)
- Industrial Inorganic Chemicals (22)
- Electrochemistry (19)
- Plastics Fabrication and Uses (18)
- Plastics Manufacture and Processing (10)
- Organometallic and Organometalloidal Compounds (9)
- Aliphatic Compounds (8)
- Heterocyclic Compounds (More Than One Hetero Atom) (5)
- Inorganic Chemicals and Reactions (5)
- Electric Phenomena (3)
- Benzene, Its Derivatives, and Condensed Benzenoid Compounds (2)
- Ceramics (2)
- Heterocyclic Compounds (One Hetero Atom) (2)
- Phase Equilibria, Chemical Equilibria, and Solutions (2)
- Unit Operations and Processes (2)

**CAS标引的核心研究点**

**Concept**

Top Count Alphanumeric Search

6 Selected

- Lithium secondary batteries (1,110)
- Battery electrolytes (828)
- Fluoropolymers (652)
- Battery anodes (642)
- Battery cathodes (588)
- Carbon black (488)
- Lithium-ion secondary batteries (389)
- Electrolytes (356)
- Ionic conductivity (312)
- Solid electrolytes (274)
- Polyoxyalkylenes (227)
- Ionic liquids (210)
- Electric current collectors (193)
- Secondary battery separators (192)
- Styrene-butadiene rubber (183)
- Cellulose products (5)
- Gene expression (5)
- Physical polymers (5)
- Surface chemistry (5)
- Synthetic polymers (5)
- Textiles (5)
- Water treatment (5)

**精准定位感兴趣的  
核心研究点**

**支持使用通配符**

Concept Name: nano\*

6 Selected

- Carbon nanofibers (30)
- Carbon nanostructured materials (1)
- Carbon nanotube fibers (5)
- Carbon nanotubes (160)
- Core-shell nanoparticles (2)
- Graphite nanofibers (5)
- Ion beam nanolithography (1)
- Multi-walled carbon nanotubes (9)
- Nanoconfinement (1)
- Nanocrystals (3)
- Nanodisks (11)
- Nanofabrication (2)
- Nanofibers (22)
- Nanofilms (2)
- Nanohorns (2)
- Nanoparticles (66)
- Nanoparticle size distribution (45)
- Polyarnides (45)
- Separators (43)
- Electric resistance (42)

Cancel Apply

**CAS**  
A division of the American Chemical Society

# 文献详情：通过CAS科学家的增值标引，快速概览重要信息

An In Situ Polymeric Electrolyte with Low Interfacial Resistance on Electrodes for Lithium-Ion Batteries

By: Jin, Lei; Jang, Giseok; Lim, Hyunmin; Zhang, Wei; Kim, Whangi; Jang, Hohyun  
DOI: 10.1002/admi.202101958

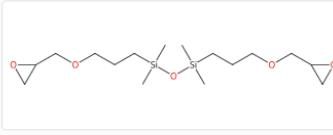
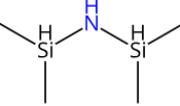
Due to their high energy d. and safety, polymer electrolytes are considered a promising alternative to the com. liquid electrolytes used in lithium-ion batteries (LIBs). However, in practical application, polymer electrolytes are limited by the high interface resistance between electrodes and electrolyte, leading to low ionic conductivity at room temperature (RT). In the present work, an in situ cationic ring-opening technique is introduced using LiFSI as an initiator to address the issue of interfacial contact between electrolyte and electrodes in LIBs. Herein, a series of in situ poly(siloxane-epoxy)-based polymer electrolytes (PSEPEs) are synthesized, which present good thermal stability (158°C), low glass transition temperature ( $T_g$ ) (-42°C), high ionic conductivity of  $1.16 \times 10^{-4} \text{ S cm}^{-1}$ , and good  $t_{50}$  of 0.61 at RT. The PSEPEs also show a wide electrochem. window (>4.7 V vs Li/Li<sup>+</sup>), and excellent compatibility with the lithium anode with an assembled LiFePO<sub>4</sub>/PSEPEs/Li cell. This work contributes to developing a new polymer electrolyte fabricated by in situ cationic polymerization, and its effects on the reduction of the interfacial resistance of electrodes-electrolyte.

Keywords: polysiloxane epoxy electrolyte lithium ion battery electrode thermal stability

View Source Full Text ▾

Substances

原文中重点研究的物质信息

171611-11-3  • Li F <sub>2</sub> HNO <sub>4</sub> S <sub>2</sub> .Li Lithium bis(fluorosulfonyl)imide Role: Technical or Engineered Material Use, Uses	31305-85-8  (C <sub>16</sub> H <sub>34</sub> O <sub>5</sub> Si <sub>2</sub> ) <sub>x</sub> Disiloxane, 1,1,3,3-tetramethyl-1,3-bis[3-(2-oxiranylmethoxy)propyl]-, homopolymer... Role: Physical, Engineering or Chemical Process, Properties, Synthetic Preparation, Technical or Engineered Material Use, Process, Preparation, Uses	15933-59-2  C <sub>4</sub> H <sub>15</sub> NSi <sub>2</sub> Tetramethyldisilazane Role: Reactant, Reactant or Reagent
--	---	---

物质研究角色

核心研究点

Amorphous structure

Battery anodes

Battery cathodes

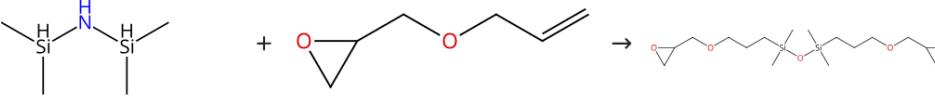
Battery electrolytes

Reactions

31-614-CAS-31042382

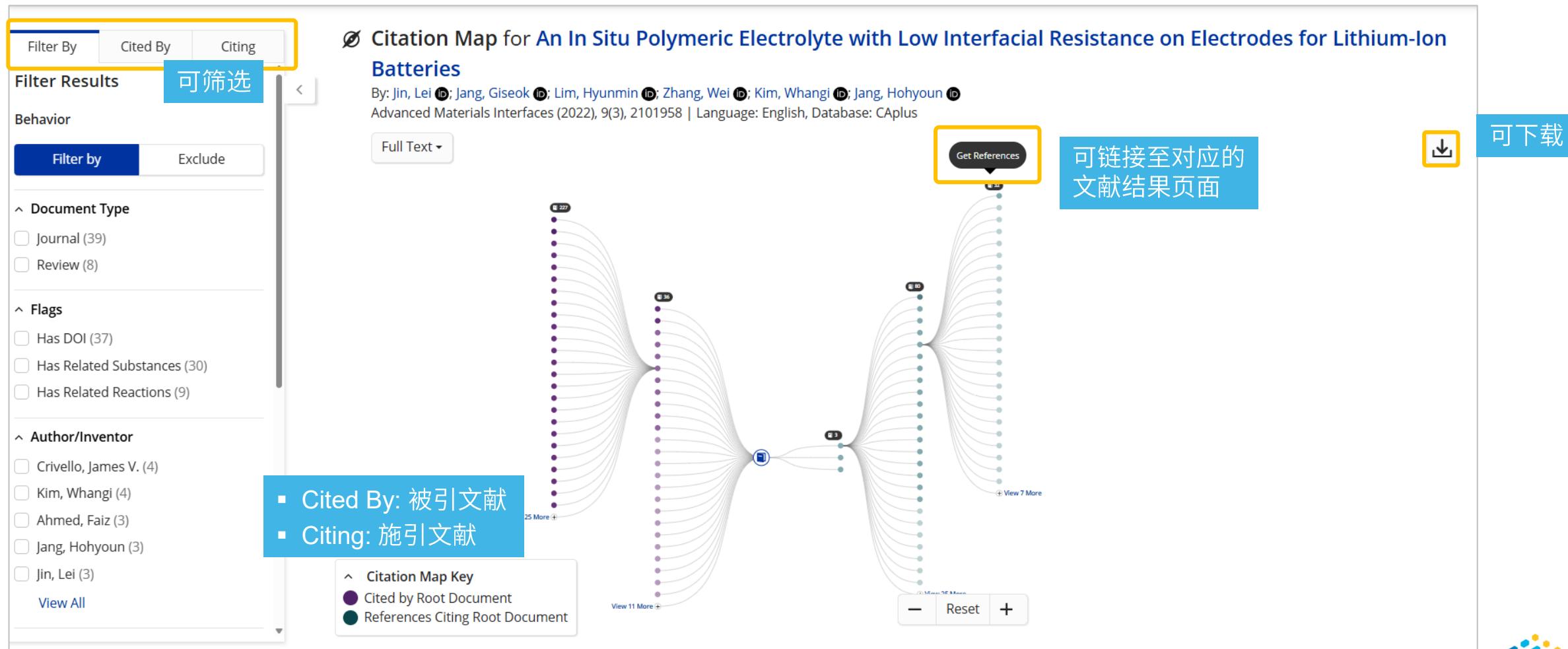
31-614-CAS-31042381

涉及的反应



# 如何快速获取引文信息？——可视化的引文地图

Citation Map



# 深入专利文献详情

## Claims

Claims text may be based on automatic Optical Character Recognition processes.

- 1 What is claimed is:  
A rechargeable lithium battery cell comprising an anode, a cathode, and a hybrid quasi-solid or solid-state electrolyte in ionic communication with the anode and the cathode, wherein: the hybrid electrolyte, having a lithium ion conductivity from  $10^{-5}$  S/cm to  $5 \times 10^{-2}$  S/cm, comprises a mixture of a polymer and an inorganic solid electrolyte; the polymer is a polymerization or crosslinking product of a reactive additive, wherein the reactive additive comprises (i) a first liquid solvent that is polymerizable, (ii) an initiator or curing agent, and (iii) a lithium salt; wherein the first liquid solvent occupies from 1% to 99% by weight based on the total weight of the reactive additive; the polymer is present in the anode, the cathode, the separator, an interface between the anode and the separator, and/or an interface between the cathode and the separator; and the hybrid electrolyte forms a contiguous phase in the cathode or in the anode, and occupies from 3% to 40% by volume of the cathode or from 3% to 40% by volume of the anode.
- 2 The rechargeable lithium cell of claim 1 , wherein the inorganic solid electrolyte material is selected from an oxide type, sulfide type, hydride type, halide type, borate type, phosphate type, lithium phosphorus oxynitride (LiPON), garnet-type, lithium superionic conductor (LISICON) type, sodium superionic conductor (NASICON) type, or a combination thereof.
- 3 The rechargeable lithium cell of claim 1 , wherein the first liquid solvent is selected from the group consisting of vinylene carbonate, ethylene carbonate, fluoroethylene carbonate, ethylene glycol phenyl ether acrylate) (PEGPEA), ethoxylated trimethyl propyl triacrylate (ETPTA), tetrahydrofuran (THF), vinyl sulfite, vinyl ethylene sulfite, vinyl ethylene carbonate, 1,3-propyl sultone, 1,3,5-trioxane (TXE), 1,3-acrylic-sultones, methyl ethylene sulfone, methyl vinyl sulfone, ethyl vinyl sulfone, methyl methacrylate, vinyl acetate, acrylamide, 1,3-dioxolane (DOL), fluorinated ethers, fluorinated esters, sulfones, sulfides, dinitriles, acrylonitrile (AN), sulfates, siloxanes, silanes, N-methylacetamide, acrylates, ethylene glycols, phosphates, phosphonates, phosphinates, phosphines, phosphine oxides, phosphonic acids, phosphorous acid, phosphites, phosphoric acids, phosphazene compounds, derivatives thereof, and combinations thereof.

## 权利要求

## Patent Family

## 专利家族

Patent	Language	Full Text	Publication Date	Application Number	Application Date	Patent Status ?	Status Date
US20230096724 A1	English	PatentPak PDF	2023-03-30	US2021-17410282	2021-08-24	Alive	2023-04-06
US12272791 B2	English	PatentPak PDF	2025-04-08	US2021-17410282	2021-08-24	Alive	2023-04-06
WO2023028514 A1	English	PatentPak PDF	2023-03-02	WO2022-US75385	2022-08-23	Alive	2023-03-09

## 专利状态

Keywords: flame resistant solid state composite electrolyte lithium ion battery

PatentPak

Get Prior Art Analysis

Full Text ▾

## Classifications

## 分类信息

Patent	Classification	Codes
US20230096724 A1	IPCI	H01M 10/0569; H01M 10/0525
	CPCI	H01M 10/0569; H01M 10/0525; H01M 2300/0028
US12272791 B2	IPCI	H01M 4/62; H01M 10/0525; H01M 10/0569
	CPCI	H01M 10/0569; H01M 10/0525; H01M 2300/0028
WO2023028514 A1	IPCI	H01M 10/056; H01M 10/42; H01M 4/62; H01M 10/052; H01M 12/08

# CAS PatentPak: 高效浏览专利

一键定位专利原文中的核心研究物质

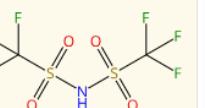
**PAGE** 26 /32 **ZOOM** **DOWNLOAD**  
PDF | PDF+

**Key Substances in Patent**

**Analyst Markup Locations (2)**

- Page 26
- Page 29

**CAS RN 90076-65-6**

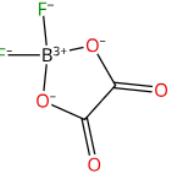


• Li

**Analyst Markup Locations (3)**

- Page 26
- Page 31
- Page 31

**CAS RN 409071-16-5**



• Li<sup>+</sup>

**Analyst Markup Locations (2)**

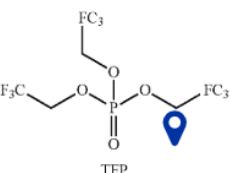
and a solid-state electrolyte-based separator composed of particles of  $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$  embedded in a poly(vinylidene fluoride)-hexafluoropropylene (PVDF-HFP) matrix (inorganic solid electrolyte/PVDF-HFP ratio=4/6). This cell was then injected with the reactive solution mixture (10% by weight based on the total cell weight). The cell was then irradiated with electron beam at room temperature until a total dosage of 40 Gy was reached. In-situ polymerization of the polymerizable first liquid solvent in the battery cell was accomplished, resulting in a quasi-solid electrolyte that permeates into the cathode to wet the surfaces of  $\text{LiCoO}_2$  particles, impregnates the porous separator, and comes in contact with the lithium metal in the anode.

Example 6: 1,3-Dioxolane (DOL) as the Polymerizable First Solvent and an Unsaturated Phosphazene, Alone or in Combination with EC, as a Second Solvent

[0187] In this study, all of the electrolytes were prepared in an Ar-filled glovebox. The polymerizable liquid electrolyte composition comprises anhydrous DOL (99.8%, containing approximately 75 ppm butylated hydroxytoluene (BHT) as inhibitor; Sigma-Aldrich). A total of 0.6 M LiTFSI (TCI America) and 0.4 M LiDFOB (Sigma-Aldrich) were added to the above solvent to prepare the electrolytes. One electrolyte was prepared by dissolving the salts in pure DOL. In several electrolytes, a ternary salt composition (0.6 M LiTFSI+0.2 M LiDFOB and 0.2 M LiBOB [Sigma-Aldrich]) was used to prepare the electrolytes using the same process. Aluminum triflate ( $\text{Al}(\text{OTf})_3$ , 99%; Alfa Aesar) with a concentration of 2 mM was also added to accelerate the polymerization reaction. Electrolyte compositions used in the study were created by diluting the homogeneous solutions of DOL- $\text{Al}(\text{OTf})_3$  with appropriate amounts of DOL-LiTFSI to create initially liquid DOL electrolytes containing variable fractions of  $\text{Al}(\text{OTf})_3$ . All of the electrolytes were respectively injected into dry cells to facilitate

and Trifluoro-Phosphate (TFP) as the Second Liquid Solvent

[0189] In this study, VC or FEC was used as the first liquid solvent, azodiisobutyronitrile (AIBN) as the initiator, lithium difluoro(oxalate) borate (LiDFOB) as the lithium salt, and TFP as the second flame-retardant liquid solvent. TFP has the following chemical structure:



[0190] Solutions containing 1.5 M LiDFOB in VC and FEC, respectively, and 0.2 wt % AIBN (vs VC or FEC) were prepared. Then, TFP (TFPNC or TFP/FEC ratios being from 10/90 to 50/50) was added into the solution to form mixed electrolyte solutions. The electrolyte solutions were separately injected into different dry battery cells, allowing the electrolyte solution to permeate into the anode (wetting out particles of the ISE obtained in Example 3 and the anode active material; e.g., graphite particles), into the cathode (wetting out the ISE and the cathode active material; e.g., NCM-532 particles), and into the porous separator layer (porous PE/PP film or nonwoven of electro-spun PAN nano-fibers). The battery cells were stored at 60° C. for 24 h and then 80° C. for another 2 h to obtain polymerized VC or polymerized FEC that contained TFP in their matrix of polymer chains. The polymerization scheme of VC is shown below (Reaction scheme 1):

## CAS PatentPak:

- 快速理解专利
- 一键下载原文
- 快速定位专利中的物质
- 阅读其他语言撰写的等同专利

# AI+科学家训练的模型，提升现有技术分析效率和精度



基于指定信息的现有技术探索

❖ Prior Art Discovery

Prior Art Discovery uses CAS AI tools to find similar patents and non-patent literature results. [Learn more about Prior Art Discovery.](#)

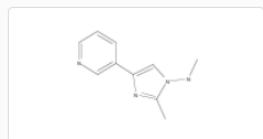
This disclosure is related to the field of processes to produce molecules that are useful as pesticides (e.g., acari-cides, insecticides, molluscicides, and nematicides), such molecules, and processes of using such molecules to control pests. In general, the molecules of Formula One may be used to control pests e.g. beetles, earwigs, cockroaches, flies, aphids, scales, whiteflies, leafhoppers, ants, wasps, termites, moths, butterflies, lice, grasshoppers, locusts, crickets, fleas, thrips, bristletails, mites, ticks, nematodes, and symphylans. Generally, when the molecules disclosed in Formula One are used in a formulation, such formulation can also contain other components. These components include, but are not limited to, (this is a non-exhaustive and non-mutually exclusive list) wetters, spreaders, stickers, penetrants, buffers, sequestering agents, drift reduction agents, compatibility agents, anti-foam agents, cleaning agents, and emulsifiers.

输入不少于200个英文字符的自然语言，进行现有技术探索

Priority Date: 08-12-2025 [Edit](#) [自定义日期](#) 962 / 10,000 characters [Clear Text](#)

Add Structure (Optional)

[Edit](#)



[Edit Drawing](#) [Remove](#)

[Search](#)

支持文本+结构检索，使结果更精准

# AI赋能自然语言便捷获取文献检索结果总结，快速掌握关键发现

References search for "Polyols from depolymerization of polyurethanes"

Query Interpretation ?

All Substances Reactions References Suppliers Patent Markush

[View Related Results](#)

Filter Results

Analyze Results

Behavior

[Filter by](#)

[Exclude](#)

Search Within Results

Search for up to 3 text strings within the result set.

Enter a query...

[Search](#)

Document Type

Journal (167)

Patent (174)

Review (16)

Conference (10)

Flags

[347 Results](#)

[+ AI Summary](#)

Sort: Relevance View: Partial Abstract

[View All](#)

Based on the search results, here's a summary of key findings related to polyols and depolymerization and polyurethanes:

The search results highlight various methods for the depolymerization of polyurethanes to produce polyols, which can be used in the production of new polyurethane materials. Hydrolysis, glycolysis, and acidolysis are among the techniques used for the depolymerization of polyurethanes, with the aim of creating bio-based polyols from waste materials. These methods can be applied to different types of polyurethanes, including rigid and flexible foams, and can achieve high recovery rates of polyols. Additionally, the use of lignin as a source of bio-based polyols is explored, with depolymerization methods such as hydrolysis and acidolysis being used to produce bio-based polyols. The resulting polyols can be used in the production of new polyurethane materials, such as rigid polyurethane foams. The analysis also highlights the potential of lignin as a source of bio-based polyols for rigid polyurethane foam production. The use of lignin as a source of bio-based polyols has been explored, with depolymerization methods such as hydrolysis and acidolysis being used to produce bio-based polyols. The resulting polyols can be used in the production of new polyurethane materials, such as rigid polyurethane foams. The analysis also highlights the potential of lignin as a source of bio-based polyols for rigid polyurethane foam production.

Analyze Results

Top Document Types

Patent

Review

Patent Offices

+ AI Summary

Based on the search results, here's a summary of key findings related to polyols and depolymerization and polyurethanes:

The search results highlight various methods for the depolymerization of polyurethanes to produce polyols, which can be used in the production of new polyurethane materials. Hydrolysis, glycolysis, and acidolysis are among the techniques used for the depolymerization of polyurethanes, with the aim of creating bio-based polyols from waste materials. These methods can be applied to different types of polyurethanes, including rigid and flexible foams, and can achieve high recovery rates of polyols. Additionally, the use of lignin as a source of bio-based polyols is explored, with depolymerization methods such as hydrolysis and acidolysis being used to produce bio-based polyols. The resulting polyols can be used in the production of new polyurethane materials, such as rigid polyurethane foams. The analysis also highlights the potential of lignin as a source of bio-based polyols for rigid polyurethane foam production. The use of lignin as a source of bio-based polyols has been explored, with depolymerization methods such as hydrolysis and acidolysis being used to produce bio-based polyols. The resulting polyols can be used in the production of new polyurethane materials, such as rigid polyurethane foams. The analysis also highlights the potential of lignin as a source of bio-based polyols for rigid polyurethane foam production.

基于由科学家训练的AI模型生成的总结，确保科学准确性并提供可追溯的引用来源

Key Findings:

#### 1. Depolymerization Techniques:

- Hydrolysis, glycolysis, and acidolysis are effective methods for depolymerizing polyurethanes to produce polyols. (2) (7)
- Multi-stage degradation (MSD) method can efficiently degrade polyurethane materials to recover polymerizable polyols. (8)

#### 2. Bio-Based Polyols:

- Lignin can be depolymerized to produce bio-based polyols for rigid polyurethane foam production. (1) (12)
- Corn cob lignin can be depolymerized into bio-polyols with low molecular weight and suitable hydroxyl number for rigid polyurethane foam synthesis. (12)

#### 3. Waste Utilization:

- Waste polyurethane foams can be depolymerized to produce polyols for the formulation of new polyurethane materials. (13) (14)
- Continuous production equipment and method for regeneration of polyol via depolymerization of waste polyurethane can produce polyether polyols with good performance. (15)

#### 4. Industrial Applications:

- Recovered polyols can be used in the production of phenol formaldehyde resoles and lignin-based epoxy resins with high bio-content. (16)
- Solvent-free synthesis of acetal-containing polyols for use in recyclable polyurethanes is possible under mild and industrially applicable conditions. (19)

# 小结

1. 检索主题的构建：利用CAS Lexicon精准选词，使用布尔逻辑算符及通配符等工具灵活构建检索主题，利用高级检索选项进行自定义组合检索。
2. 主题词+结构联合检索，快速获得文献。
3. 利用多维的筛选工具，如Concept、CA Section等快速缩小范围，锁定目标文献。
4. 检索结果趋势分析、引文地图。
5. 文献详情中可快速获取关键信息，CAS PatentPak浏览专利详情。

# 大纲

## CAS及CAS SciFinder Discovery Platform 简介

### 科研信息的高效查阅

- 全面的文献调研与拓展助力开题
- 多角度出发检索物质结构及相关属性
- 探索实验方案以获取反应与合成相关策略
- 高效获取分析方法及配方制剂信息

### 常见问题Q&A



# 灵活的检索方式，满足各种物质类别的检索

The screenshot shows the CAS Advanced Search interface. On the left, there's a sidebar with 'Advanced Search' and 'Select a search type, and then add multiple search fields to bu...'. Below it are buttons for 'Substances' (highlighted in blue), 'References', and 'Clear All'. A search bar says 'Search by Substance Name, Functional Group, CAS RN...'. To the right is a dropdown menu with 'Molecular Formula' selected (highlighted with a yellow box). Other options include 'CAS Registry Number', 'Chemical Identifier', 'Document Identifier', and 'Patent Identifier'. On the right, a main search area has a title 'Advanced Search' and instructions 'Select data fields and search operators to create a focused query.' It features a magnifying glass icon, a 'Draw' button (highlighted with a yellow box), and a standard search button. A yellow arrow points from the 'Molecular Formula' dropdown towards the main search area.

Advanced Search  
Select a search type, and then add multiple search fields to bu...

Substances References Clear All

Search by Substance Name, Functional Group, CAS RN...

Molecular Formula Enter a mole...

+ Add

Molecular Formula  
CAS Registry Number  
Chemical Identifier  
Document Identifier  
Patent Identifier

Experimental Spectra  
Life Science Data  
Biological  
Chemical Properties  
Density  
Electrical  
Lipinski  
Magnetic  
Mechanical  
Optical and Scattering  
Structure Related  
Thermal

/or DOI.  
Exam...

Advanced Search  
Select data fields and search operators to create a focused query.

Draw

检索策略推荐

- 有机化合物，金属配合物，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

# 物质检索—物质标识符

PEG

Results for "PEG"

All Substances Reactions References Suppliers Patent Markush

Substances Showing 1 of 619 Results

View All Substances →

25322-68-3 PEG

OC(O)Cn(CCO)C(=O)c1ccccc1 + O=C1CC1

1.1 Catalysts: Triethylborane, N-[P,P-Bis(dimethylamino)-N-(1,1-dimethylethyl)phosphoryl]benzylamine  
1.2 Reagents: Acetic acid; rt

References Showing 20 of 650,680 Results

PEG-modified biopharmaceuticals By: Ballon, Pascal; Won, Chee-Youb Expert Opinion on Drug Delivery (2009), 6(1), 1-16 | Database: CPlus, MEDLINE

Full Text 1 0 293

PEG-Peptide Conjugates By: Hamley, Ian W. Biomacromolecules (2014), 15(5), 1543-1559 | Database: CPlus, MEDLINE

Properties Boiling Point: 227 °C Density: 1.2 g/cm³ Temp: 20 °C; Press: 758.54 Torr

Substances search for "PEG"

All Substances Reactions References Suppliers Patent Markush

View Related Results

Filter Results

Behavior

Filter by Exclude

Search Within Results

Reaction Role

Reference Role

Life Science Data

Commercial Availability

Number of Components

Molecular Weight

Element

Functional Group

Aromatic Rings

Substance Class

Polymer Class

Isotopes

Metals

Experimental Property

Experimental Spectrum

GHS Hazard Statements

619 Results

1 25322-68-3 OC(O)Cn(CCO)C(=O)c1ccccc1 (C<sub>2</sub>H<sub>4</sub>O)<sub>n</sub>H<sub>2</sub>O PEG 499K 69K 714

2 1370345-22-4 O=C1CC1 (C<sub>2</sub>H<sub>4</sub>O)<sub>x</sub> Oxirane, homopolymer Preferred RN: 25322-68-3 0 0 0

3 934660-23-8 OC(O)Cn(CCO)C(=O)c1ccccc1 (C<sub>2</sub>H<sub>4</sub>O)<sub>n</sub>(C<sub>2</sub>H<sub>4</sub>O)<sub>n</sub>C<sub>2</sub>H<sub>6</sub>O<sub>2</sub> Poly(oxy-1,2-ethanediyl),  $\alpha,\alpha'$ -1,2-ethanediylbis[ $\omega$ -hydroxy-] 0 0 0

4 166024-40-4 Image Not Available Notes: A PEG-modified polyacrylamide (Poland) Unspecified Instar G 5 2 0 0

5 121449-01-2 Image Not Available Notes: An arylphenyl ether of PEG Unspecified Syn Fac 334-10 1 0 0

6 1630005-99-0 Image Not Available Notes: A PEG-based adhesive Unspecified SurPhys 078 2 2 0

7 76050-61-8 Image Not Available Notes: A PEG acid deriv. (Russia) Unspecified Laurex 9 0 0 0

8 58339-86-9 Image Not Available Notes: PEG monoalkyl ether (Russia). Indexed also at Surfactants and PEG Unspecified 0 0 0

9 854918-94-8 Image Not Available Notes: A blend of PEG castor oil and PEG oleate (Rhodia) Unspecified 0 0 0

- 可同时检索多个物质识别符（物质名称或CAS RN）
- 不同物质使用空格隔开 (<2000个字符)

# 分子式检索：高效检索聚合物或无机化合物

- 含碳化合物，C排第一位，H排第二位，其他元素符号按照首字母顺序进行排列
- 不含碳化合物，按照元素符号的首字母顺序进行排列
- 不同组分之间用“.”隔开，如：高熵碳化物 C.Hf.Nb.Ta.Ti.Zr
- 无机含氧盐：阳离子和阴离子用点（.）分开；阴离子以氢补齐至电中性 Na<sub>2</sub>SO<sub>4</sub>：H<sub>2</sub>O<sub>4</sub>S.2Na

The screenshot shows a search interface for substances. In the search bar at the top left, the query "C.Hf.Nb.Ta.Ti.Zr" is entered. A yellow arrow points from this input field to the search results area. The results are displayed in three columns, each showing a substance entry with its CAS number, component ratio table, and a detailed description.

Component	Ratio
C	1
Zr	0.20
Hf	0.20
Ti	0.20
Ta	0.20
Nb	0.20

**Substances search for "C.Hf.Nb.Ta.Ti.Zr"**

All Substances Reactions References Suppliers Patent Markush

View Related Results

Filter Results

Behavior

Filter by Exclude

Search Within Results

Reaction Role

Reference Role

Commercial Availability

Number of Components

Element

Aromatic Rings

Substance Class

Isotopes

Sort: Relevance | View: Partial |

1 2304767-82-4 Component Ratio ...

2 1427190-21-3 Component Ratio ...

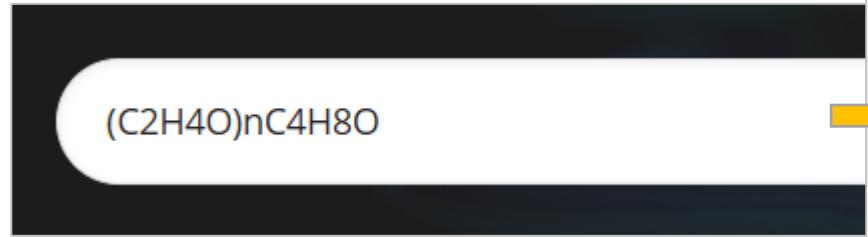
3 2649374-42-3 Component Ratio ...

?

适用于分子式检索的物质类型包括：

- 无机化合物：合金，无机表格化合物，多氧簇金属化合物等
- 聚合物

# 分子式检索：高效检索聚合物或无机化合物



- (C<sub>2</sub>H<sub>4</sub>O)<sub>n</sub>C<sub>4</sub>H<sub>8</sub>O: 括号中是重复结构单元，括号外为n

- (C<sub>5</sub>H<sub>6</sub>O<sub>4</sub>.C<sub>4</sub>H<sub>6</sub>O<sub>2</sub>.C<sub>3</sub>H<sub>4</sub>O<sub>2</sub>)<sub>x</sub> : 括号中是单体，括号外为x

Substances search for "(C<sub>2</sub>H<sub>4</sub>O)<sub>n</sub>C<sub>4</sub>H<sub>8</sub>O"

All Substances Reactions References Suppliers Patent Markush

View Related Results

Filter Results

Behavior

Filter by Exclude

13 Results

1 31497-33-3 ...  
2 27252-80-8 ...  
3 85600-94-8 ...

Sort: Relevance View: Partial

1,905 1,728 13  
1,055 588 12  
45 21 0

Substances search for "(C<sub>5</sub>H<sub>6</sub>O<sub>4</sub>.C<sub>4</sub>H<sub>6</sub>O<sub>2</sub>.C<sub>3</sub>H<sub>4</sub>O<sub>2</sub>)<sub>x</sub>"

All Substances Reactions References Suppliers Patent Markush

View Related Results

Filter Results

Behavior

Filter by Exclude

6 Results

1 97384-95-7 ...  
2 63899-49-0 ...  
3 56280-96-7 ...

Sort: Relevance View: Partial

30 5 0  
7 2 0  
3 0 1

(C<sub>5</sub>H<sub>6</sub>O<sub>4</sub>.C<sub>4</sub>H<sub>6</sub>O<sub>2</sub>.C<sub>3</sub>H<sub>4</sub>O<sub>2</sub>)<sub>x</sub>  
Components: 3  
Butanedioic acid, 2-methylene-, polymer with 2-methyl-2-propenoic acid and 2-pro...  
(C<sub>5</sub>H<sub>6</sub>O<sub>4</sub>.C<sub>4</sub>H<sub>6</sub>O<sub>2</sub>.C<sub>3</sub>H<sub>4</sub>O<sub>2</sub>)<sub>x</sub>  
Components: 3  
Butanedioic acid, 2-methylene-, polymer with ethenyl acetate and 2-propenoic aci...  
(C<sub>5</sub>H<sub>6</sub>O<sub>4</sub>.C<sub>4</sub>H<sub>6</sub>O<sub>2</sub>.C<sub>3</sub>H<sub>4</sub>O<sub>2</sub>)<sub>x</sub>  
Components: 3  
2-Butenedioic acid (2Z)-, 1-methyl ester, polymer with ethenyl acetate and 2-pro...

# 属性值联用检索物质

The screenshot shows the CAS Advanced Search interface. At the top, there are tabs for 'Substances' (highlighted with a yellow border), 'References', and 'Clear All'. Below the tabs is a search bar with placeholder text: 'Search by Substance Name, Functional Group, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI.' To the right of the search bar is a large magnifying glass icon and the text 'Advanced Search' followed by 'Select data fields and search operators to create a focused query.' Further down, there's a 'Draw' button and a standard search button.

On the left side, there's a sidebar with a list of search fields:

- Molecular Formula (selected)
- CAS Registry Number
- Chemical Identifier
- Document Identifier
- Patent Identifier
- Experimental Spectra (selected)
- Life Science Data
- Biological
- Chemical Properties
- Density
- Electrical
- Lipinski
- Magnetic
- Mechanical
- Optical and Scattering
- Structure Related
- Thermal

Under 'Experimental Spectra', a dropdown menu lists: Proton NMR, Carbon-13 NMR, Nitrogen-15 NMR, Fluorine-19 NMR, and Phosphorus-31 NMR. The text 'Enter a molecular formula.' is displayed above the search bar, and examples of search terms are shown below it: C6H6 | (C8H8)x | C22H26CuN2O5.C2H3N.

**高级检索字段：**

- CAS RN (物质、组份)、物质标识符、分子式、文献号、专利号
- 实验谱图:  $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{15}\text{N}$ ,  $^{19}\text{F}$ ,  $^{31}\text{P}$  NMR
- 化学标识符: 化学名称、InChI key
- 生物: 生物富集因子、LD50
- 化学: Koc, LogD, LogP、溶解度、分子量、pKa、蒸汽压
- 密度属性: 密度、摩尔体积
- 电学: 电导/电导率、电阻/电阻率
- Lipinski: 自由旋转键、H受体/供体
- 磁: 磁力矩
- 机械属性: 拉伸强度
- 光散射: 旋光性、折射率
- 结构: 极性表面积
- 热学: 熔点、沸点、闪电、玻璃转化温度、蒸发焓

# 属性值、谱图数据联用检索物质

## Advanced Search

Select a search type, and then add multiple search fields to build a query. [?](#)

Substances Advanced search for 3 fields

View Related Results [?](#)

Filter Results [?](#)

Filtering: Life Science Data: 3 Selected [X](#)

Clear All Filters

Sort: Relevance [?](#) View: Partial [?](#)

Molecular Weight: 220 to 280  
Predicted values only.

pKa: 1.3 to 1.8  
Predicted values only.

Carbon-13 NMR: 114 to 171, 96, 11.5  
Allowance of  $\pm 2$  ppm.

+ Add Advanced Search Field

Filter Results [?](#)

Behavior

Filter by [Exclude](#)

Search Within Results

Reaction Role

Reference Role

Life Science Data

Pharmacological Data (13)

ADME (2)

Toxicity (1)

Commercial Availability

Number of Components

Molecular Weight

LogP

Stereochemistry

Element

Functional Group

13 Results

1 57498-78-9

C<sub>13</sub>H<sub>12</sub>N<sub>2</sub>O<sub>2</sub>  
9H-Pyrido[3,4-b]indole, 7-methoxy-1-methyl-, 2-oxide

16 11 2

31K 1,090 116

2 723-46-6

C<sub>10</sub>H<sub>11</sub>N<sub>3</sub>O<sub>3</sub>S  
Sulfamethoxazole

3 442571-27-9

C<sub>11</sub>H<sub>12</sub>N<sub>2</sub>O<sub>2</sub>S<sub>2</sub>  
2-[(5,6-Dimethylthieno[2,3-d]pyrimidin-4-yl)propionic acid

2 4 31

4 50995-74-9

C<sub>14</sub>H<sub>15</sub>NO<sub>4</sub>  
7-Diethylaminocoumarin-3-carboxylic acid

5 1628224-40-7

Absolute stereochemistry shown, Rotation (-)

C<sub>9</sub>H<sub>13</sub>N<sub>3</sub>O<sub>5</sub>  
(dS)-a-Amino-3-(carboxymethoxy)-5-methyl-1H-pyrazole-4-propanoic acid

6 1631737-39-7

Absolute stereochemistry shown, Rotation (-)

C<sub>10</sub>H<sub>15</sub>N<sub>3</sub>O<sub>5</sub>  
(2R,3R,4S,5R)-4,5-Dihydro-5-(hydroxymethyl)-3'-methylSpiro[furan-2(3H),7'(6'H)-...

16 4 31

Yellow arrow pointing from the 'Add Advanced Search Field' button to the 'Filter Results' sidebar.

- 分子量: 220至280之间
- pKa: 1.3至1.8之间
- C谱特征峰: 114至171之间, 96, 11.5

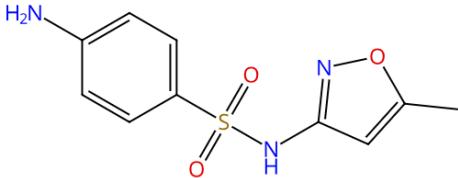
# 物质的详情页

CAS Registry Number: 723-46-6

31K 1,079 123 View in CAS BioFinder

该物质被专利Claims保护的系列专利信息

Patents Claimed In



C<sub>10</sub>H<sub>11</sub>N<sub>3</sub>O<sub>3</sub>S

Benzenesulfonamide, 4-amino-N-(5-methyl-3-isoxazolyl)-

Properties

Molecular Weight

Melting Point (Experimental)

Boiling Point (Predicted)

Density (Experimental)

pKa (Experimental)

Experimental Properties | Spectra

Other Names and Identifiers

Experimental Properties

实验属性

Experimental Spectra

实验谱图

Pharmacological Data

ADME

Toxicity

Predicted Properties

Predicted Spectra

Bioactivity Indicators

Target Indicators

Regulatory Information

GHS Hazard Statements

GHS危害信息

Triazine desulfurizer containing triazine methoxazole and tetracarboxylic acid oxazolidine used for desulfurization of crude oil

Role: Reactant

Patent Number: CN120349810

Publication Date: 2025-07-22

Method for co-treating organic wastewater using peroxymonosulfate and peroxydisulfate

Role: Pollutant

Patent Number: CN120349021

Publication Date: 2025-07-22

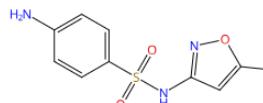
External antibacterial liquid containing sulfamethoxazole, alcohol and water

Role: Therapeutic Use

Patent Number: CN120305271

Publication Date: 2025-07-15

723-46-6



C<sub>10</sub>H<sub>11</sub>N<sub>3</sub>O<sub>3</sub>S

CAS Name  
Sulfamethoxazole

Conditions

Working Frequency  
400 MHz

Solvent

Dimethyl sulfoxide (67-68-5)

Carbon tetrachloride (56-23-5)

Temperature

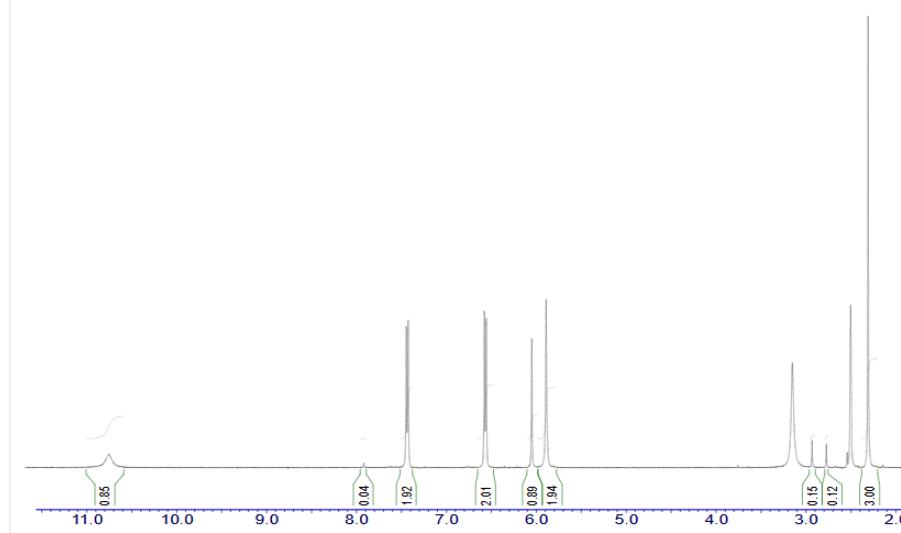
20 °C

Spectrum Summary

Spectrum ID  
F0175-0013

Source

Spectral data were obtained from  
Life Chemicals



Solvent	Source
Dimethyl sulfoxide; Carbon tetrachloride	(1) LC
-	(2) ENAMINE
-	(2) ENAMINE
-	(3) BIORAD
Chloroform-d; DMSO-d <sub>6</sub> (1:1)	(3) BIORAD

# 扩展问答类型，快速聚焦物质谱图和安全信息

Results for "the Raman spectra of luminol"

All Substances Reactions References Suppliers Patent Markush

Spectrum 自然语言查阅拉曼光谱

Showing 1 of 1 Result

521-31-3  
Luminol  
Viewing 1 of 1

- Reset +

View All Spectra →

Results for "the proton spectra of ibuprofen"

All Substances Reactions References Suppliers Patent Markush

Spectra 自然语言查阅核磁共振谱图

Showing 5 of 28 Results

15687-27-1  
Ibuprofen  
Viewing 1 of 5

Experimental View Spectra Details

Proton NMR Spectrum

Conditions  
Working Frequency 300 MHz  
Solvent Chloroform-d (865-49-6)

View All Spectra →

Results for "What are the hazards of bisphenol A"

All Substances Reactions References Suppliers Patent Markush

GHS Hazard Table 自然语言查阅物质安全信息

Showing 5 of 62 Results

Code	Hazard Statement
H272	May intensify fire; oxidizer
H302	Harmful if swallowed
H304	May be fatal if swallowed and enters airways
H313	May be harmful in contact with skin
H317	May cause allergic skin reaction

Regulatory List

View in Detail Page →

AII, AREC, CANL, DSL, EECI, EINECS, ENCS, FDA, HAP, HHAZ, HTU, IECSC, INSQ, ITC, IUR, JDATA, NZIoC, PICCS, PII, PROP, REACH, RSTR, S313, SIDS, State\_CA\_PROP65, State\_MA, State\_NJ, State\_OR, State\_PA, State\_VT, State\_WA, STOR, STY, TCSI, TDCA, TSCA, VNECI, VOC, WGK

Confidential Business Information: Public

Regulatory Synonyms (35)

Details by Country/International & Other Lists

# 支持自然语言直接检索物质理化性质，直观高效

Results for "what is the boiling point of DMF"

All Sub Suppliers Patent Markush

自然语言查询物质沸点

68-12-2  
**DMF**

Boiling Point  
**153 °C**  
Condition Press: 760 Torr  
Source "Hazardous Substances Data Bank" data were obtained from the National Library of Medicine (US)

Boiling Point Properties  
Showing 5 of 210 Results

Value	Condition	Source
153 °C	Press: 760 Torr	"Hazardous Substances Data Bank" data were obtained from the ...

View in Detail Page →

Results for "the logP of olaparib"

All Sub Suppliers Patent Markush

自然语言查询物质logP

763113-22-0  
**Olaparib**

logP  
**1.037±0.00**  
Condition Temp: 25 °C  
Source Calculated using Advanced Chemistry Development (ACD/Labs) Software (© 1994-2025 ACD/Labs)

logP Properties  
Showing 1 of 1 Result

Value	Condition	Source
1.037±0.00	Temp: 25 °C	Calculated using Advanced Chemistry Development (ACD/Labs) S...

View in Detail Page →

Results for "pKb of alanine"

All Sub Suppliers Patent Markush

自然语言查询物质pKb

56-41-7  
**Alanine**

pKb  
**9.62**  
Source Harutyunyan, Lusine R.; Tenside, Surfactants, Detergents, (2017), 54(2), 141-159, CPlus

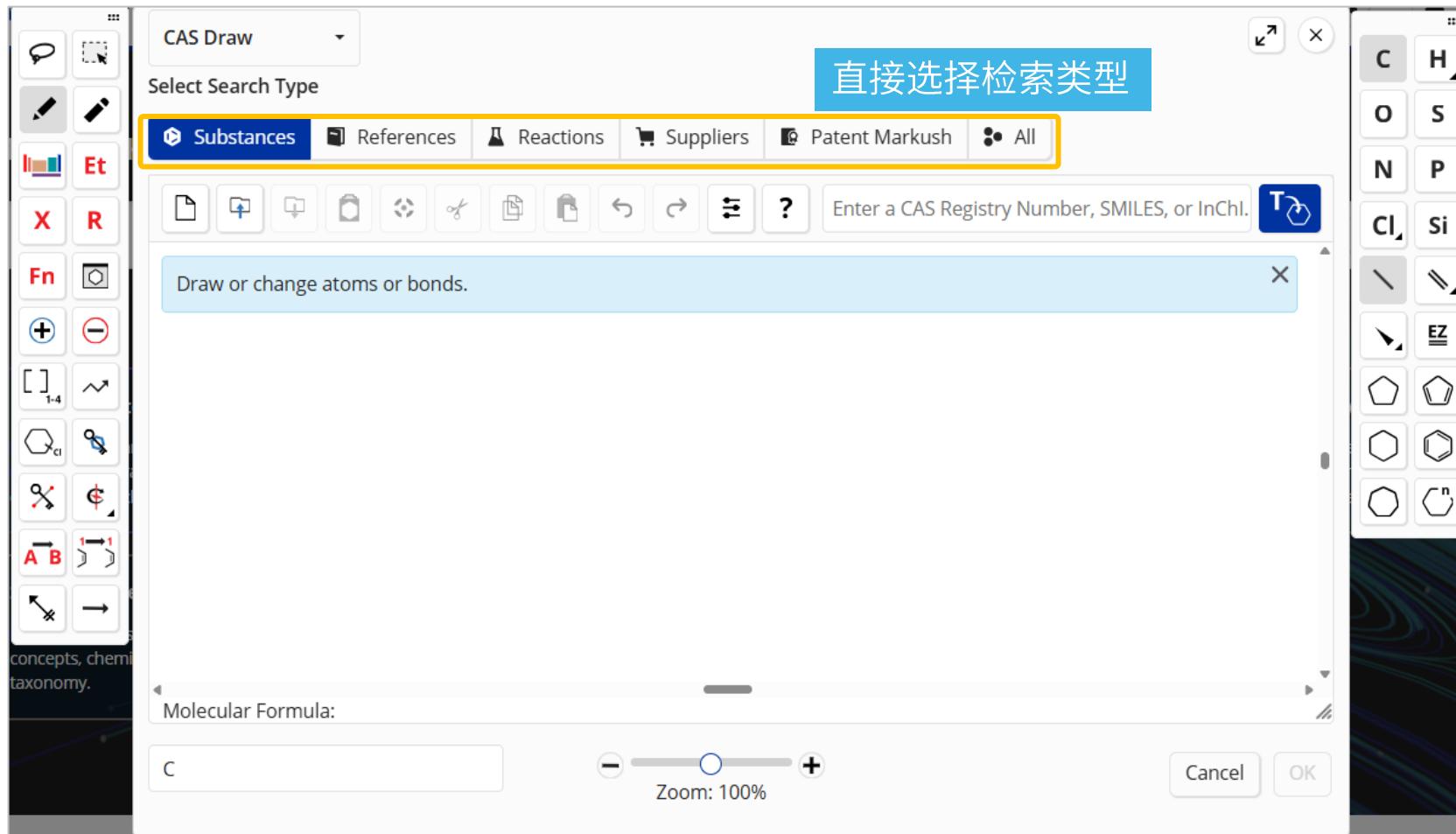
pKb Properties  
Showing 1 of 1 Result

Value	Condition	Source
9.62	-	Harutyunyan, Lusine R.; Tenside, Surfactants, Detergents, (2017), ...

View in Detail Page →

# 物质检索—CAS Draw：结构绘制面板

- X 选择可变基团
- R 自定义R基团
- Fn 片段结构
- [ ]<sub>1-4</sub> 重复工具
- C<sub>l</sub> 取代位置可变
- 环锁定工具
- 原子锁定工具



线上学习短视频：

CAS 美国化学文摘社



# 结构检索结果

结构检索类别：

- As Drawn: 可变结构可变，其他位点锁环锁原子。
- Substructure 亚结构：包含 As Drawn结果，有取代基。
- Similarity 相似结构：母体结构可以被取代，也可以被改变的相似结果。

Substances search for drawn structure

All **Substances** Reactions References Suppliers Patent Markush

View Related Results

Filter Results **Structure Match** 1,095 Results

As Drawn (0) **Substructure (1,095)** Similarity (2)

Analyze Structure Precision

Behavior Filter by Exclude

Search Within Results

Reaction Role Product (398) Reactant (115) Reagent (3) Catalyst (81)

Reference Role

Life Science Data

Commercial Availability

Number of Components

Molecular Weight

结构匹配度

Sort: Number of References: Descending View: Parti 多样的排序方式

R1: Cr, Fe, Co, Ni, Cu, Zn, Mn

Chemical structures and details for results 1-6:

- 1. 1929551-26-7: C<sub>30</sub>H<sub>29</sub>BrMnNO<sub>2</sub>P<sub>2</sub>. (OC-6-42)-Bromodicarbonyl[2-(diphenylphosphino- $\kappa P$ )-N-[2-(diphenylphosphino- $\kappa P$ )...]
- 2. 1929551-26-7: C<sub>30</sub>H<sub>53</sub>BrMnNO<sub>2</sub>P<sub>2</sub>. Stereoisomer of bromodicarbonyl[2-(dicyclohexylphosphino- $\kappa P$ )-N-[2-(dicyclohexylphosphino- $\kappa P$ )...]
- 3. 53687-39-1: C<sub>42</sub>H<sub>43</sub>CoNP<sub>3</sub>. Cobalt, [2-(diphenylphosphino)-N,N-bis[2-(diphenylphosphino)ethyl]ethanamine-N,P...
- 4. 1418299-84-9: C<sub>32</sub>H<sub>63</sub>CoNP<sub>2</sub>Si. (SP-4-1)-[2-(Dicyclohexylphosphino- $\kappa P$ )-N-[2-(dicyclohexylphosphino- $\kappa P$ )ethyl]etha...
- 5. 1428439-31-9: C<sub>32</sub>H<sub>64</sub>CoNP<sub>2</sub>Si.C<sub>32</sub>H<sub>12</sub>BF<sub>24</sub>. Components: 2

Relevance

CAS RN: Ascending  
CAS RN: Descending  
Molecular Formula: Ascending  
Molecular Formula: Descending  
Molecular Weight: Ascending  
Molecular Weight: Descending  
Number of References: Ascending  
Number of References: Descending  
Number of Suppliers

# 自定义关键物理性质的优先展示

支持自定义感兴趣的物理性质，优先展示在物质结果集上

Substances search for drawn structure

View Related Results ▾

Filter Results  36,710 Results Sort: Number of References: Descending ▾ View: Partial ▾

Structure Match As Drawn (1) Substructure (36K) **Similarity (594K)** Analyze Structure Precision Behavior Filter by Exclude

1415607-60-1 1241891-64-4 1980037-96-4

C<sub>33</sub>H<sub>19</sub>N<sub>3</sub> 10-Phenylspiro[acridine-9(10H),9'-[9H]fluorene]-2',7'-dicarbonitrile C<sub>31</sub>H<sub>20</sub>BrN 2'-Bromo-10-phenylspiro[acridine-9(10H),9'-[9H]fluorene]-2',7'-dicarbonitrile C<sub>46</sub>H<sub>30</sub>N<sub>4</sub> 10-[4-(4,6-diaminophenoxy)-2-phenyl-1,3-dihydro-2H-pyrazolo[4,3-f]quinoline-7,9-dione]

Substance Properties Display Boiling Point X Density X Molecular Weight X pKa X 4 of 6 properties selected **Reset to**

Acoustic  Sound Velocity  Density  Molar Volume  Optical and Scattering  Optical Rotatory Power  Refractive Index  Polar Surface Area  Thermal  Autoignition Temperature  Boiling Point  Combustion Enthalpy  Critical Point  Enthalpy of Vaporization  Entropy  Electrical  Dielectric Constant  Electric Conductance  Electric Resistance  Electric Resistivity  Viscosity  IUPAC  **View All Settings** Cancel Save

Reaction Role  Search Within Results  Reaction Role  **Search Within Results**  Reaction Role  **Reaction Role**

可以选取最多六个性质在物质结果上显示

Substances search for drawn structure

View Related Results ▾

Filter Results  36,710 Results Sort: Number of References: Descending ▾ **View: Full** ▾

Structure Match As Drawn (1) Substructure (36K) **Similarity (594K)** Analyze Structure Precision Behavior Filter by Exclude

1415607-60-1

C<sub>33</sub>H<sub>19</sub>N<sub>3</sub> 10-Phenylspiro[acridine-9(10H),9'-[9H]fluorene]-2',7'-dicarbonitrile

Properties	Value	Condition
Molecular Weight	457.53	-
Boiling Point (Predicted)	638.074±55.00 °C	Press: 760.00 Torr
Density (Predicted)	1.385±0.10 g/cm <sup>3</sup>	Temp: 25 °C; Press: 760 Torr
pKa (Predicted)	-3.680±0.20	Most Basic Temp: 25 °C

Spectra

# 快速筛选物质结果集，助力聚焦领域核心技术

Reference Role **物质研究角色**

By Count Alphanumeric

0 Selected

- Biological Study (2.2M)
- Uses (2.1M)
- Preparation (2M)
- Synthetic Preparation (1.9M)
- Prophetic Synthesis or Use (1.5M)
- Agricultural Use (1.5M)
- Biological Study, Unclassified (1.2M)
- Therapeutic Use (1.2M)
- Pharmacological Activity (1M)
- Properties (452K)
- Analytical Study (200K)
- Analyte (182K)
- Diagnostic Use (178K)
- Process (55K)
- Technical or Engineered Material Use (53K)
- Industrial Manufacture (51K)
- Physical, Engineering, or Chemical Process (51K)
- Biological Use, Unclassified (45K)
- Modifier or Additive Use (37K)
- Adverse Effect (32K)
- Purification or Recovery (28K)
- Other Use, Unclassified (28K)
- Catalyst Use (27K)
- Formation, Non-preparative (26K)
- Occurrence (26K)
- Analytical Role, Unclassified (26K)
- Pharmacokinetics (19K)
- Combinatorial Study (19K)
- Food or Feed Use (19K)
- Removal or Disposal (18K)
- Biochemical Process (17K)
- Polymer in Formulation (15K)
- Occurrence, Unclassified (15K)
- Nanoscale (15K)
- Byproduct (13K)
- Miscellaneous (12K)
- Natural Product Occurrence (9,062)
- Analytical Matrix (8,759)
- Bioindustrial Manufacture (8,177)

Cancel Apply

## 物质类别

### Substance Class

- Organic/Inorganic Small Molecule (2M)
- Protein/Peptide Sequence (470K)
- Mixture (83K)
- Salt and Compound With (30K)
- Manual Registration (18K)
- Coordination Compound (9,189)
- Polymer (8,017)

### Aromatic Rings

- No aromaticity (208K)
- 1 (294K)
- 2 (994K)
- 3 (799K)
- 4 (165K)

芳环数量

### Functional Group

- Halide (1.6M)
- Amide (1.3M)
- Imine (1.2M)
- Alkene (1.1M)
- Alkyl halide (1M)

官能团

## 聚合物类别

### Polymer Class

- Polyacrylic (2,224)
- Polyether (1,563)
- Polyether (1,531)
- Polyamide (1,116)
- Manual registration (1,080)

### LogP

No Min to No Max Apply

Available Range: -25.829 to 87.223

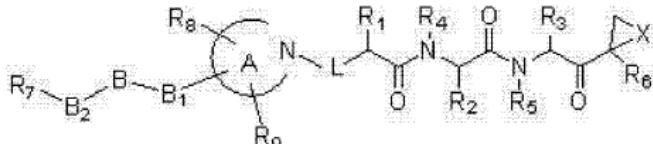
# CAS Markush检索，助力结构查新

CN 104945470 A

## 权利要求书

1/3 页

1. 一种杂环构建的三肽环氧酮类化合物，具有下述结构通式 I：



I

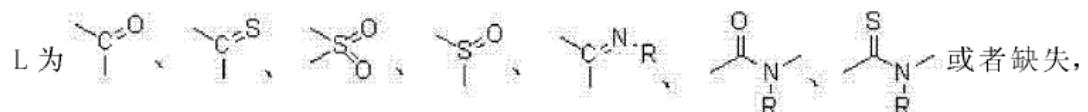
其中：

R<sub>1</sub>, R<sub>2</sub>, R<sub>3</sub> 各自独立选自 H、C<sub>1-6</sub> 烷基 -D、卤代的 C<sub>1-6</sub> 烷基 -D、C<sub>1-6</sub> 羟基烷基、C<sub>1-6</sub> 硫基烷基、C<sub>1-6</sub> 烷氧基烷基、芳基、芳烷基、杂芳基或杂芳烷基；其中 :D 为 N(R<sub>a</sub>) (R<sub>b</sub>) 或缺失, R<sub>a</sub>, R<sub>b</sub> 各自独立选自 H、OH、C<sub>1-6</sub> 烷基、卤代的 C<sub>1-6</sub> 烷基或 N 末端保护基；

R<sub>4</sub>, R<sub>5</sub> 各自独立选自 H、OH、C<sub>1-6</sub> 烷基、卤代的 C<sub>1-6</sub> 烷基或芳烷基；

R<sub>6</sub> 选自 H, C<sub>1-6</sub> 烷基, 卤代的 C<sub>1-6</sub> 烷基, C<sub>1-6</sub> 羟基烷基, C<sub>1-6</sub> 烷氧基, 卤代的 C<sub>1-6</sub> 烷氧基, C(O)O-C<sub>1-6</sub> 烷基, C(O)NH-C<sub>1-6</sub> 烷基, 芳烷基；

X 为 O、S、NH、N-C<sub>1-6</sub> 烷基或 N- 卤代的 C<sub>1-6</sub> 烷基；



其中 R 选自 H、C<sub>1-6</sub> 烷基或卤代的 C<sub>1-6</sub> 烷基；

环 A 选自 5 ~ 7 元的饱和脂肪杂环、不饱和杂环、或者有取代的 5 ~ 7 元的饱和脂肪杂环、不饱和杂环，所述的杂环包含 0 ~ 3 个选自 O、N 和 S 的杂原子并任选地被 R<sub>8</sub>、R<sub>9</sub> 和 B<sub>1</sub> 基团取代；

R<sub>8</sub>, R<sub>9</sub> 分别独立选自 H、OH, C<sub>1-6</sub> 烷基, C<sub>1-6</sub> 烷氧基, C<sub>1-6</sub> 羟基烷基, C<sub>1-6</sub> 硫基烷基, C<sub>1-6</sub> 烷

## 具体物质[Specific Substance]

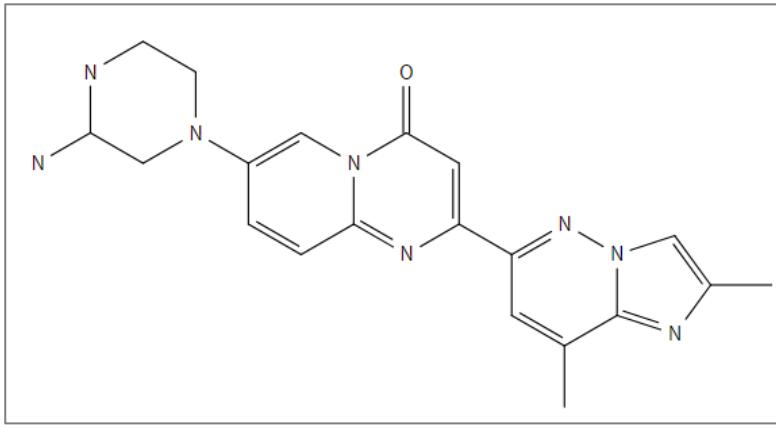
- 以具体化学结构陈述的特定物质，会被分配CAS 登记号

## 预测性物质[Prophetic Substance]

- 使用Markush结构陈述的预测物质，一个Markush可以陈述上千甚至更多的结构
- 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登记号
- Markush 检索，能检索到通过 Substance 可能检索不到的结构

# CAS Markush检索

该结构进行精准结构，亚结构均无结果，能够确定它没有被公开吗？



此时您检索的是CAS REGISTRY数据库，它是专利审查员的重要参考依据之一。

Substances search for drawn structure

View Related Results ▾

Filtering: Similarity: 3 Selected X Number of Components: 1 X Clear All Filters

Sort: Relevance ▾ View: Partial ▾

Filter Results

Structure Match

As Drawn (0)  Substructure (0)  Similarity (116K)

Behavior

Filter by Exclude

Search Within Results

Similarity

95-98 (2)  
 90-94 (54)  
 85-89 (232)  
 80-84 (265)  
 75-79 (310)

View All

Reaction Role

Product (255)  
 Reactant (21)

Reference Role

Biological Study (285)

Filtering: Similarity: 3 Selected X Number of Components: 1 X

288 Results

Rank	Similarity	Count
1	95 ***	1825352-54-2
2	95 ***	1825352-53-1
3	95 ***	1825352-79-1
4	95 ***	1825352-78-0
5	95 ***	1825352-52-0
6	95 ***	2097817-67-7

1825352-54-2: C<sub>21</sub>H<sub>23</sub>N<sub>7</sub>O, 2-(2,8-Dimethylimidazo[1,2-b]pyridazin-6-yl)-7-[(3R)-3-methyl-1-piperazinyl]-4H-...  
1825352-53-1: C<sub>21</sub>H<sub>23</sub>N<sub>7</sub>O, 2-(2,8-Dimethylimidazo[1,2-b]pyridazin-6-yl)-7-[(3S)-3-methyl-1-piperazinyl]-4H-...  
1825352-79-1: C<sub>21</sub>H<sub>23</sub>N<sub>7</sub>O, 9-Methyl-2-(2-methylimidazo[1,2-b]pyridazin-6-yl)-7-[(3R)-3-methyl-1-piperazinyl]...  
1825352-78-0: C<sub>21</sub>H<sub>23</sub>N<sub>7</sub>O, 9-Methyl-2-(2-methylimidazo[1,2-b]pyridazin-6-yl)-7-[(3S)-3-methyl-1-piperazinyl]...  
1825352-52-0: C<sub>22</sub>H<sub>25</sub>N<sub>7</sub>O, rel-2-(2,8-Dimethylimidazo[1,2-b]pyridazin-6-yl)-7-[(3R,5S)-3,5-dimethyl-1-piper...  
2097817-67-7: C<sub>22</sub>H<sub>25</sub>N<sub>7</sub>O, 2-(2,8-Dimethylimidazo[1,2-b]pyridazin-6-yl)-7-[(3S,5S)-3,5-dimethyl-1-piperazinyl]...

# CAS Markush检索



- CAS专利马库什数据集，是专利审查员进行可专利性检索的重要参考依据。
- 马库什检索可以使用具体结构、骨架结构和通式结构来进行迭代检索，确保获得完整的公开结构信息
- 用户可以根据必要性使用 CAS 文献数据集 CAplus 进行文本检索补充

Patent Markush search for drawn structure

View Related Results

Filter Results

Patent Markush Match

As Drawn (1)

Substructure (1)

Behavior

Filter by Exclude

1 Result

WO2017081111 Markush Details

Preparation of substituted 2-(imidazo[1,2-b]pyridazin-6-yl)-pyrido[1,2-a]pyrimidin-4-ones for treating amyotrophic lateral sclerosis

Assignees: F. Hoffmann-La Roche AG; Hoffmann-La Roche Inc.

World Intellectual Property Organization, WO2017081111 A1 2017-05-18 | Language: English, Database: CAplus

Patent Status: Dead

Patent claim 1

PatentPak Full Text

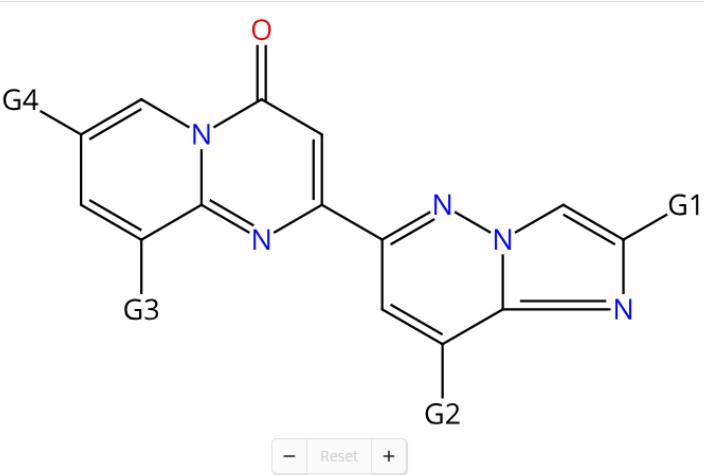
453,454,455,456,457: opt. substd. by G22

629: opt. substd.

# 直观的 Markush 详情页

Patent Markush 1

PatentPak Full Text ▾



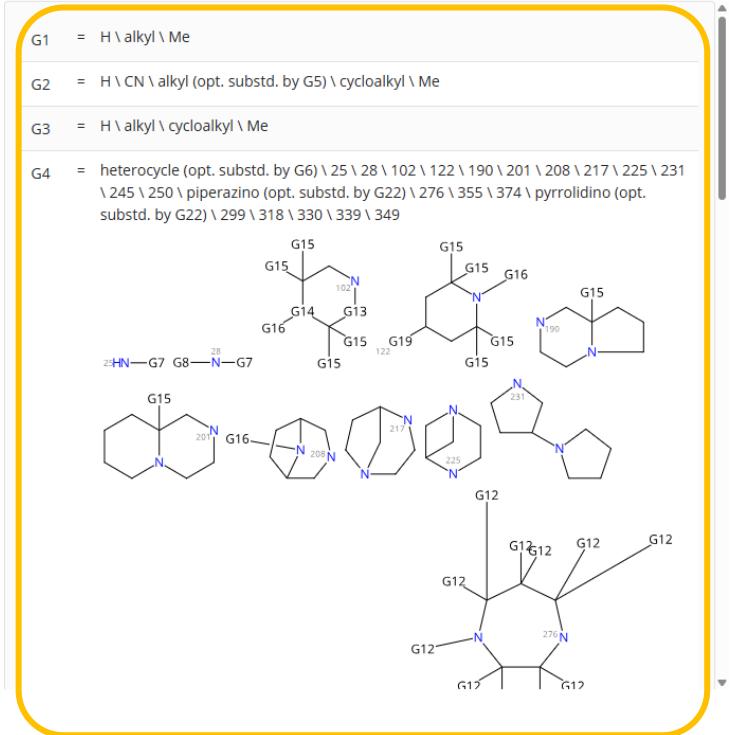
Publication Information

Assignees: F. Hoffmann-La Roche AG; Hoffmann-La Roche Inc.  
World Intellectual Property Organization, WO2017081111 A1 2017-05-18 | Language: English, Database: Cplus

Notes

Patent claim 1  
or pharmaceutically acceptable salts  
substitution is restricted  
additional ring formation also claimed

G1 = H \ alkyl \ Me  
G2 = H \ CN \ alkyl (opt. substd. by G5) \ cycloalkyl \ Me  
G3 = H \ alkyl \ cycloalkyl \ Me  
G4 = heterocycle (opt. substd. by G6) \ 25 \ 28 \ 102 \ 122 \ 190 \ 201 \ 208 \ 217 \ 225 \ 231 \ 245 \ 250 \ piperazino (opt. substd. by G22) \ 276 \ 355 \ 374 \ pyrrolidino (opt. substd. by G22) \ 299 \ 318 \ 330 \ 339 \ 349

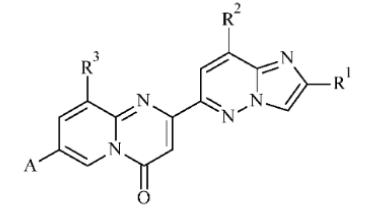


清晰直观展示原文中复杂Markush结构的拆解与解读，  
助力发现专利文件中隐藏的结构保护信息

## 原文中Markush结构

### Claims

#### 1. The compound of formula (I)

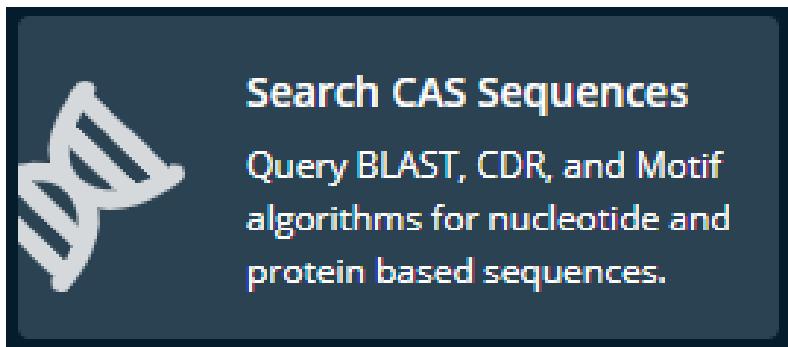


wherein

- 5       $R^1$  is hydrogen or  $C_{1-7}$ -alkyl;  
R<sup>2</sup> is hydrogen, cyano,  $C_{1-7}$ -alkyl,  $C_{1-7}$ -haloalkyl or  $C_{3-8}$ -cycloalkyl;  
R<sup>3</sup> is hydrogen,  $C_{1-7}$ -alkyl, or  $C_{3-8}$ -cycloalkyl;  
10     A is N-heterocycloalkyl or  $NR^{12}R^{13}$ , wherein N-heterocycloalkyl comprises 1 or 2 nitrogen ring atoms and is optionally substituted with 1, 2, 3 or 4 substituents selected from  $R^{14}$ ;  
 $R^{12}$  is heterocycloalkyl comprising 1 nitrogen ring atom, wherein heterocycloalkyl is optionally substituted with 1, 2, 3 or 4 substituents selected from  $R^{14}$ ;  
 $R^{13}$  is hydrogen,  $C_{1-7}$ -alkyl or  $C_{3-8}$ -cycloalkyl;  
15      $R^{14}$  is independently selected from hydrogen,  $C_{1-7}$ -alkyl, amino, amino- $C_{1-7}$ -alkyl,  $C_{3-8}$ -cycloalkyl and heterocycloalkyl or two  $R^{14}$  together form  $C_{1-7}$ -alkylene;

# CAS SciFinder 中的序列检索

- BLAST
- CDR
- Motif



# 小结

1. 物质检索方法：物质、文献标识符检索；分子式、物性参数、谱图数据检索；及结构式检索，充分利用结构绘制工具，合理扩大或限定结构检索范围
2. 使用自然语言检索，快速获取物质的理化性质、谱图数据等信息
3. 正确理解As Drawn、Substructure、Similarity检索结果集的意义和范围
4. 充分利用物质筛选选项准确定位目标物质：Reaction Role、Reference Role等
5. 利用CAS Markush检索尽可能全面的获得结构的公开信息
6. 利用CAS Sequences高效获取生物序列检索结果。

# 大纲

## CAS及CAS SciFinder Discovery Platform 简介

### 科研信息的高效查阅

- 全面的文献调研与拓展助力开题
- 多角度出发检索物质结构及相关属性
- 探索实验方案以获取反应与合成相关策略
- 高效获取分析方法及配方制剂信息

### 常见问题Q&A



# 使用标识符直接检索

支持使用：CAS反应登记号、物质名称、CAS登记号、文献号等

示例：丙烯酸异丁酯的相关反应

CAS SciFinder reaction of 106-63-8

All Substances Reactions References Suppliers Patent Markush

View Related Results

Filter Results

Behavior

Filter by Exclude

Search Within Results

Substance Role

Yield

Number of Steps

Non-Participating Functional Groups

Reaction Mapping

Reaction Scale

Experimental Protocols

Reaction Type

Stereochemistry

Reagent

Catalyst

Tetraphenylphosphine palladium (649K)

[1,1'-Bis(diphenylphosphino)ferrocene]dichloropalladium (215K)

Palladium diacetate (129K)

Dichloro[1,1'-bis(diphenylphosphino)ferrocene] palladium(II) dichloro methane adduct (119K)

Dichlorobis(triphenylphosphine)palladium (89K)

View All

Full Text

1.470 Results

Scheme 1 (5 Reactions)

1.1 Reagents: Potassium carbonate  
Catalysts: Dichloro[1,1'-bis(diphenylphosphino)ferrocene]pall...  
Solvents: 1,4-Dioxane, Water; 60 - 90 min, 120 - 140 °C

1.1 Reagents: Ethylene gly..., Potassium acetate  
Catalysts: Palladium  
Solvents: Dimethyl sulf...; 2 h, 120 °C

1.1 Reagents: Palladate(6-), dichlorobis[3,3',3"-phosphini...  
Catalysts: Glycerol; 4 h, 80 °C

Supplier (96)

Supplier (51)

Supplier (1)

Supplier (4)

Supplier (101)

Supplier (3)

点击进入反应详情页

CAS SciFinder Suzuki coupling reaction 人名反应智能识别

Reactions search for "Suzuki coupling reaction"

All Substances Reactions References Suppliers Patent Markush

View Related Results

Yield

Number of Steps

Non-Participating Functional Groups

Reaction Mapping

Reaction Scale

Experimental Protocols

Reaction Type

Stereochemistry

Reagent

Catalyst

1,478,164 Results

Scheme 1 (1 Reaction)

31-179-CAS-11123183

Preparation of pyrazolo[3,4-d]pyrimidine derivatives useful as inhibitors of Bruton's tyrosine kinase

Assignee: Redx Pharma Limited  
World Intellectual Property Organization, WO2014188173 A1 2014-11-27

PatentPak Full Text

Scheme 2 (1 Reaction)

Supplier (1)

Supplier (51)

Absolute stereochemistry shown

Absolute stereochemistry shown

Supplier (1)

Supplier (51)

Supplier (1)

Supplier (4)

Supplier (101)

Supplier (3)

Steps: 1 Yield: 100% \*\*\*

# 利用自然语言检索反应，降低检索难度

使用CAS数据训练的AI，智能识别检索意向，提供最相关反应检索结果

Reactions search for "Dehalogenation in isopropanol catalyzed by palladium"

All Substances Reactions References Suppliers Patent Markush

View Related Results

Filter Results

Behavior Filter by Exclude

Search Within Results Yield Number of Steps Non-Participating Functional Groups Reaction Mapping Reaction Scale Experimental Protocols Reaction Type Stereochemistry Reagent Catalyst Solvent Commercial Availability Reaction Notes

155,676 Results Scheme 1 (1 Reaction)

Absolute stereochemistry shown, Rotation (-) → Absolute stereochemistry shown, Rotation (+)

Supplier (1)

31-113-CAS-5796848 Steps: 1 Yield: 100% \*\*\* Cobalt-Catalyzed Asymmetric Hydrogenation of 1,1-Diarylethenes By: Chen, Jianhui; et al Organic Letters (2016), 18(7), 1594-1597

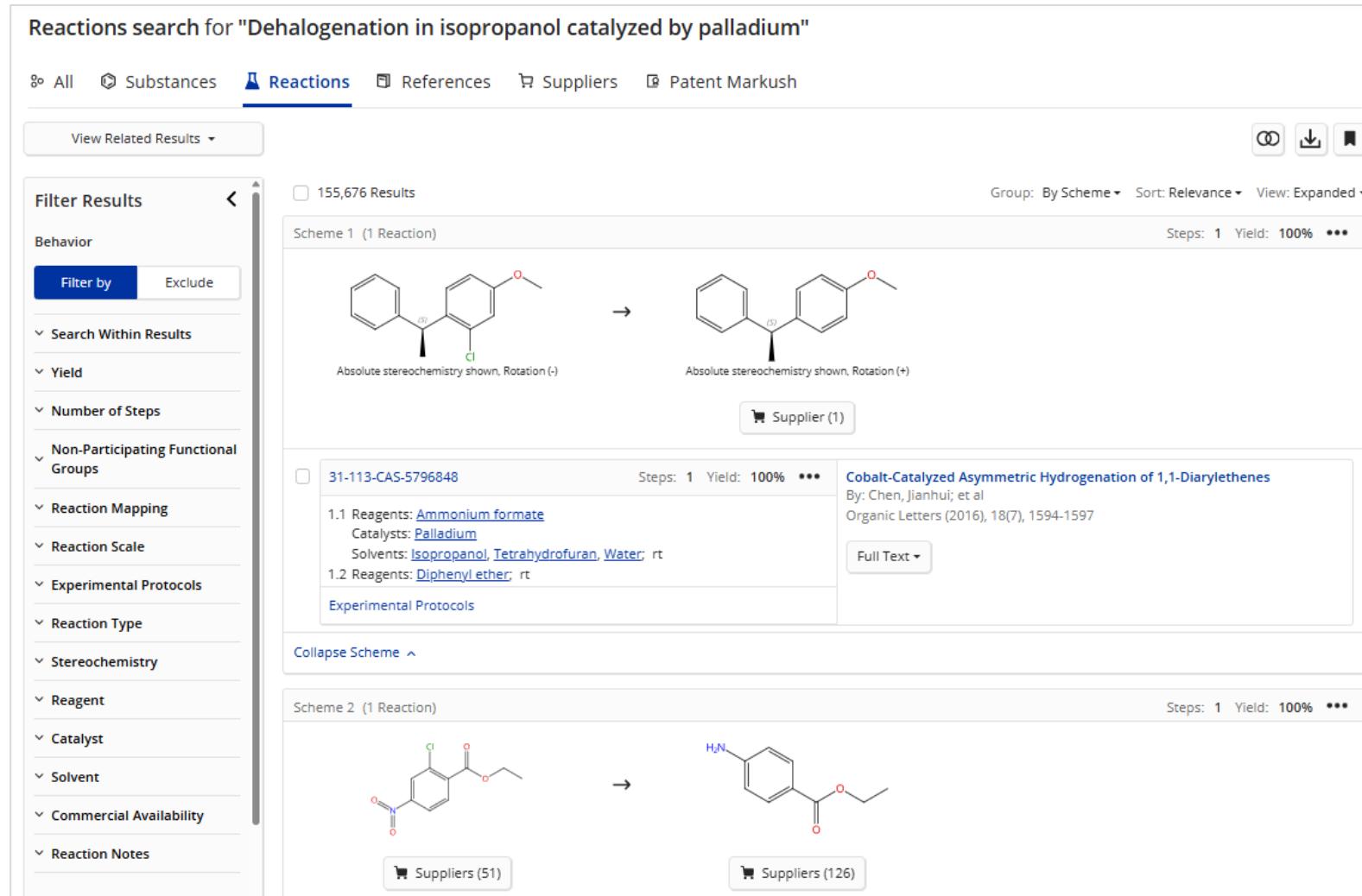
1.1 Reagents: Ammonium formate Catalysts: Palladium Solvents: Isopropanol, Tetrahydrofuran, Water, rt  
1.2 Reagents: Diphenyl ether, rt

Experimental Protocols

Collapse Scheme

Scheme 2 (1 Reaction)

Supplier (51) → Supplier (126)



支持检索：

- 反应转化类型
- 物质类别和官能团
- 物质名称、CAS RN、分子式

支持指定反应参与角色：

- 产物 synthesis/preparation /manufacture of
- 反应物 from
- 溶剂 in
- 催化剂 catalyzed by
- 试剂 mediated by

# 不止具体反应，还可便捷检索某一类反应

Reactions search for "Synthesis of aldehyde catalyzed by Palladium diacetate" 乙酸钯催化合成醛类化合物

All Substances Reactions References Suppliers Patent Markush

View Related Results

Filter Results

Behavior

Filter by Exclude

Search Within Results

Yield

Number of Steps

Non-Participating Functional Groups

Reaction Mapping

Reaction Scale

Milligram (78K)

Gram (74K)

Kilogram (48)

No Scale Provided (33K)

Experimental Protocols

Collapse Scheme ▾

Scheme 1 (1 Reaction)

114,093 Results

31-614-CAS-27980971 Steps: 1 Yield: 100%

1.1 Reagents: Sodium carbonate, Triethyls...  
Catalysts: Palladium dia..., 1,1-Bis(diphenylphosphino)...  
Solvents: Acetonitrile; 16 h, 80 °C

Experimental Protocols

Scheme 2 (1 Reaction)

Suppliers (58) Suppl...

Group: By Scheme Sort: Relevance View: Expanded

Reactions search for "Reduction of Ketones to Alcohols catalyzed by Carbonyl reductase" 羰基还原酶催化还原酮为醇类化合物

All Substances Reactions References

View Related Results

Filter Results

Behavior

Filter by Exclude

Search Within Results

Yield

Number of Steps

Non-Participating Functional Groups

Reaction Mapping

Reaction Scale

Experimental Protocols

Reaction Type

Stereochemistry

Br-CH<sub>2</sub>-C(=O)-C<sub>6</sub>H<sub>4</sub>-Br → Br-CH<sub>2</sub>-CH(OH)(R)-C<sub>6</sub>H<sub>4</sub>-Br

Absolute stereochemistry shown, Rotation (-)

Suppliers (86) Suppl...

Group: By Scheme Sort: Relevance View: Expanded

335,050 Results

31-614-CAS-23937123 Steps: 1 Yield: 100% \*\*\*

1.1 Reagents: 1,3-Dibromo-5,5-dimethylhy...  
Catalysts: p-Toluenesulfoni..., Carbonyl reductase  
Solvents: Methanol, Water; 180 min, pH 7, 30 °C; 3 h, 30 °C

One-pot chemo-enzymatic synthesis of chiral α-halogenated aryl alcohols  
By: Yang, Jingwen; et al  
Youji Huaxue (2018), 38(7), 1811-1816

Full Text ▾

31-513-CAS-10291418 Steps: 1 Yield: 99% \*\*\*

1.1 Solvents: Ethanol; 18 h, 30 °C

Chiral pharmaceutical intermediaries obtained by reduction of 2-Halo-1-(4-substituted phenyl)-ethanones mediated by Geotrichum candidum CCT 1205 and Rhodotorula glutinis CCT 2182  
By: Fardelone, Lucidio C.; et al  
Enzyme Research (2011), 976368, 8 pp.

Full Text ▾

# 直接绘制反应进行检索

Reactions search for drawn structure

All Substances Reactions References Suppliers Patent Markush

[View Related Results](#)

Filter Results

Structure Match

As Drawn (34)

Substructure (8,161)

Similarity (0)

结构匹配度

Behavior

Filter by

Exclude

Search Within Results

Yield

Number of Steps

Non-Participating Functional Groups

Reaction Mapping

Reaction Scale

Experimental Protocols

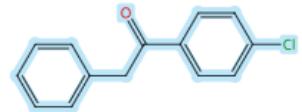
Reaction Type

Stereochemistry

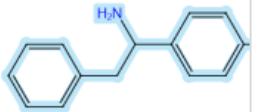
Reagent

34 Results

Scheme 1 (5 Reactions)



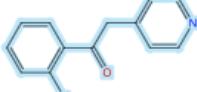
→



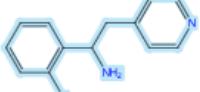
[Suppliers \(79\)](#)

Expand Scheme

Scheme 2 (1 Reaction)



→



[Suppliers \(43\)](#)

31-614-CAS-28968228

Steps: 1 Yield: 76% \*\*\*

1.1 Reagents: O-Methylhydroxylamine hydro...

Solvents: Pyridine; rt; 1 h, 50 °C

1.2 Reagents: (7,4)-Trihydro[*tetra*hydro...

Solvents: Tetrahydrofuran; rt; 3 h, reflux; reflux → 0 °C

1.3 Reagents: Sodium hydroxide

Solvents: Water; overnight, reflux; reflux → rt

[Experimental Protocols](#)

By Scheme

By Document

By Transformation

Group: By Scheme

Sort: Relevance View: Expanded

Steps: 1 Yield: 85% \*\*\*



Relevance

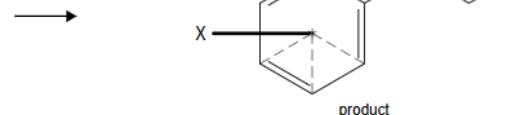
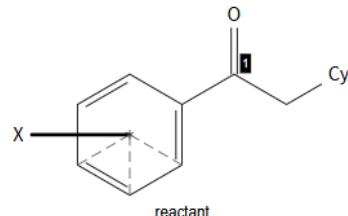
Publication Date: Newest

Publication Date: Oldest

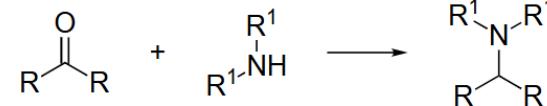
Yield

Number of Steps: Ascending

Number of Steps: Descending



聚焦反应类型



Filter Results

Structure Match

As Drawn (34)

Substructure (8,161)

Similarity (0)

Behavior

Filter by

Exclude

Search Within Results

Yield

Number of Steps

Non-Participating Functional Groups

Reaction Mapping

Reaction Scale

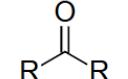
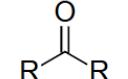
PatentPak

Full

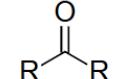
8,161 Results

1 Reductive Alkylation of Ammonia or Amines

[View 121 Related Reactions](#)



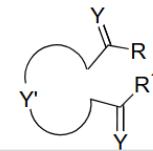
聚  
焦  
反  
应  
类  
型



2

Formation of N/O/S Heterocycles

[View 54 Related Reactions](#)



# 反应结果的筛选

## 筛选/排除，二次检索

Filter Behavior

**Filter by**      Exclude

^ Search Within Results  
Search for up to 3 structures within the result set.

 Draw

## 试剂

^ Reagent

Sodium hydride (17K)  
 Sodium hydroxide (9,054)  
 Water (7,867)  
 Hydrochloric acid (6,933)  
 Triethylamine (6,070)

[View All](#)

## 反应规模

### Reaction Scale

- Milligram (5,818)
- Gram (4,525)
- Kilogram (12)
- No Scale Provided (26K)

## 催化剂

### Catalyst

- Tetrabutylammonium hydrogen sulfate (3,656)
- 4-(Dimethylamino)pyridine (2,697)
- Tetrakis(triphenylphosphine) palladium (2,381)
- Palladium diacetate (1,455)
- Palladium (1,426)

[View All](#)

## 不参与反应官能团

### Non-Participating Functional Groups

- Alkene (8,230)
- Cyclic alkene (8,230)
- Halide (4,370)
- Ether (2,466)
- Amine (2,197)

[View All](#)

## 溶剂

### Solvent

- Water (21K)
- Tetrahydrofuran (19K)
- Dichloromethane (15K)
- Dimethylformamide (13K)
- Methanol (5,501)

[View All](#)

## 反应注释

### Reaction Notes

- Stereoselective (53) 立体选择性
- Chemoselective (25) 化学选择性
- Regioselective (10) 区域选择性
- Thermal (8)
- Photochemical (7) 光化学
- Prophetic Reaction (5)
- Combinatorial (4)
- Green Chemistry (3) 绿色化学
- Electrochemical (2) 电化学
- Green Chemistry-Process Simplification (1) 绿色化学-工艺简化

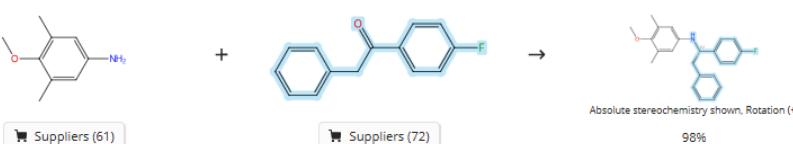
[View Fewer](#)

# 高效获取CAS科学家增值的合成路线详情

## Synthetic Methods——CAS科学家增值标引的合成制备详情

CAS Reaction Number: 31-614-CAS-41195127

Get Similar Reactions



Suppliers (61)      Suppliers (72)

Absolute stereochemistry shown. Rotation (+) 98%

Reaction Overview  
Steps: 1 Yield: 98%

JOURNAL  
Nickel-catalyzed enantioselective reductive amination of benzylic ketones in alcohols  
By: Wang, XiuHua; et al  
View All ▾  
Science China: Chemistry (2024), 67(8), 2566-2570

View Source Full Text ▾

Company/Organization  
State Key Laboratory of Chemical Oncogenomics, School of Chemical Biology and Biotechnology  
Peking University Shenzhen Graduate School  
Shenzhen 518055  
China

Step 1

Stage	Reagents	Catalysts	Solvent
1	Isopropanol Titanium isopropoxide	-	-
2	-	Bis[1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]-κO]methanesulfonamido-κO[nickel] (R,R)-Ph-BPE	-

Experimental Protocols

Synthetic Methods

Products Benzeneethanamine, α-(4-fluorophenyl)-N-(4-methoxy-3,5-dimethylphenyl)-(αS), Yield: 98%

Reactants 1-(4-Fluorophenyl)-2-phenylethanone  
3,5-Dimethyl-4-methoxyaniline

Reagents Isopropanol  
Titanium isopropoxide

Catalysts Bis[1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]-κO]methanesulfonamido-κO[nickel]  
(R,R)-Ph-BPE

Procedure

1. Add aniline (0.2 mmol), ketone (0.1 mmol), Ti(O*i*Pr)<sub>4</sub> (34.1 mg, 0.12 mmol) and dry isopropanol (0.2 mL) to a dry 10-mL Schlenk tube.
2. Heat the mixture with stirring at 100°C for 24 hours.
3. Monitor the partial formation of ketimine by GC.
4. Cool the reaction to room temperature.
5. Add Ni(*i*NTf)<sub>2</sub> (3.1 mg, 0.005 mmol, 5 mol%), (R)-Ph-BPE (3.1 mg, 0.006 mmol, 6 mol%) and GC standard n-C<sub>12</sub>H<sub>26</sub> (10 μL) in an argon-filled glove box.
6. Stir the reaction mixture in an oil bath maintained at 70°C for 48 hours.
7. Cool the reaction mixture to room temperature.
8. Purify the crude product by flash chromatography (ethyl acetate/petroleum ether 1:15) to obtain (S)-N-(3,5-dimethyl-4-methoxyphenyl)-1-(4-fluorophenyl)-2-phenylethan-1-amine.

Transformation Reductive Alkylation of Ammonia or Amines

Characterization Data

^ Benzeneethanamine, α-(4-fluorophenyl)-N-(4-methoxy-3,5-dimethylphenyl)-(αS)-

Proton NMR Spectrum	(400 MHz, CDCl <sub>3</sub> ): δ 7.31 - 7.27 (m, 4H), 7.25 - 7.22 (m, 1H), 7.12 - 7.10 (m, 2H), 7.02 - 6.98 (m, 2H), 6.12 (s, 2H), 4.50 (dd, <i>J</i> = 7.9, 6.0 Hz, 1H), 3.90 (br s, 1H), 3.61 (s, 3H), 3.07 (dd, <i>J</i> = 13.8, 6.0 Hz, 1H), 2.99 (dd, <i>J</i> = 13.8, 7.9 Hz, 1H), 2.13 (s, 6H)
Carbon-13 NMR	(100 MHz, CDCl <sub>3</sub> ): δ 162.0 (d, <i>J</i> <sub>C,F</sub> = 243.0 Hz), 149.2, 143.3, 139.5 (d, <i>J</i> <sub>C,F</sub> = 3.0 Hz), 137.7, 131.3, 129.4, 128.7, 128.1 (d, <i>J</i> <sub>C,F</sub> = 8.0 Hz), 126.9, 115.5 (d, <i>J</i> <sub>C,F</sub> = 21.0 Hz), 113.8, 60.0, 59.2, 45.5, 16.4
Fluorine-19 NMR	(376.6 MHz, CDCl <sub>3</sub> ): δ -116.0
Optical Rotatory Power	[α] <sup>25</sup> <sub>D</sub> = +5.6° (c = 1.0, CHCl <sub>3</sub> )
Enantiomeric Excess	90%
HRMS	(ESI <sup>+</sup> ): Calcd for C <sub>23</sub> H <sub>25</sub> FNO [M+H] <sup>+</sup> : 350.1915; found: 350.1916
State	yellow oil

Reaction Notes stereoselective (ee = 90%)

清晰的实验操作

产物表征

反应用注释

^ Experimental Protocols

 Synthetic Methods (449) Experimental Procedure (5,678)

# 获取相似反应，拓展实验设计思路

Scheme 4 (15 Reactions)

Absolute stereochemistry shown

Absolute stereochemistry shown, Rotation (-)

Suppliers (120) Suppliers (75)

31-614-CAS-42267257 Steps: 1 Method and system for the Get Similar Reactions

1.1 Solvents: Methanol, Water; 2.4 MPa, 179 °C; 183.8 °C

Get Similar Reactions

Set Reaction Similarity

Broad (34,980) Reaction centers only

Medium (4,709) Reaction centers plus adjacent atoms and bonds

Narrow (596) Reaction centers plus extended atoms and bonds

Cancel Get Reactions

Steps: 1 Yield: 60% \*\*\*

Reactions similar to 31-614-CAS-42267257

References Save

Filter Behavior

Filter by Exclude

4,709 Results Group: By Scheme Sort: Publication Date: Newest View: Expanded

Scheme 1 (3 Reactions) Steps: 1 Yield: 78% \*\*\*

Suppliers (83) Suppliers (63)

31-614-CAS-42231899 Steps: 1 Yield: 78% \*\*\* Pyrrolidinone urea fpr2 agonists treating atherosclerosis

1.1 Reagents: Hexamethyldisilazane Assignee: Bristol-Myers Squibb Company  
Solvents: Acetonitrile; 40 h, rt → reflux World Intellectual Property Organization, WO2024220482 A1  
1.2 Solvents: Methanol; 0 °C; 30 min, rt 2024-10-24

PatentPak Full Text

31-367-CAS-21603883 Steps: 1 Yield: 78% \*\*\* Preparation of phenylpyrrolidinone formyl peptide 2 receptor agonists

1.1 Reagents: Hexamethyldisilazane Assignee: Bristol-Myers Squibb Company  
Solvents: Acetonitrile; 40 h, rt → reflux United States, US20190270704 A1 2019-09-05  
1.2 Solvents: Methanol; 0 °C; 30 min, rt

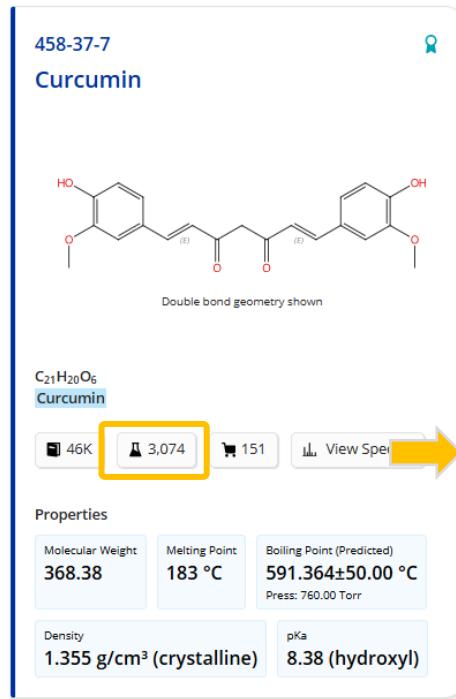
PatentPak Full Text

31-367-CAS-19142997 Steps: 1 \*\*\* Preparation of sulfonamides compound as cccDNA inhibitor for treating hepatitis B

1.1 Reagents: Hexamethyldisilazane Assignees: Chia Tai Tianqing Pharmaceutical Group Co., Ltd.;  
Solvents: Acetonitrile; rt → reflux; 48 h, reflux Medshine Discovery Inc.

根据反应中心与相邻原子的相似性获取相似反应

# 如何检索重要化合物的相关反应与合成工艺?



Reactions for 458-37-7

View Related Results ▾

Filter Results

Substance Role: Product X

341 Results

Scheme 1 (1 Reaction)

Suppliers (84) Suppliers (146) Suppliers (151)

31-614-CAS-43010367 Steps: 1 Yield: 94% \*\*\*

Preparation of curcumin and its symmetrical derivatives  
Assignee: Zhaoqing Juyuan Biochemical Co., Ltd.  
China, CN118084637 A 2024-05-28

1.1 Reagents: Trimethyl borate  
Catalysts: Butylamine  
Solvents: Dimethylformamide: 50 min, 60 - 70 °C; 1.5 h, 60 - 70 °C  
1.2 Reagents: Sulfuric...  
Solvents: Methanol; neutralized  
1.3 Reagents: Hydrochloric...  
Solvents: Methanol, Water: 2 h, 60 - 70 °C

PatentPak ▾ Full Text ▾

Collapse Scheme ▾

Scheme 2 (2 Reactions)

Steps: 1 Yield: 94% \*\*\*

Double bond geometry shown

- 通过物质结构、名称或其他物质标识符检索物质
- 一键链接到相关反应
- 限定物质角色为产物，通过产率筛选较优的反应条件
- 可进一步筛选反应规模、实验详情等

# 使用联用检索——结构与关键词检索反应

Friedel-crafts acylation

Featured Search

- Prior Art Discovery
- Patent Markush
- Advanced Search

Edit Drawing Remove experimental procedures.

References search for "Friedel-crafts acylation" + drawn structure

All Substances Reactions References Suppliers Patent Markush

View Related Results

Filter Results

Analyze Results

Structure Match

As Drawn (1,364)

Substructure (2,999)

Behavior

Filter by Exclude

Search Within Results

Document Type

1,364 Results

1 ZrCl<sub>4</sub>-Mediated Regio- and Chemoselective Friedel-Crafts Acylation of Indole

By: Guchhait, Sankar K.; Kashyap, Maneesh; Kamble, Harshad  
Journal of Organic Chemistry (2011), 76(11), 4753-4758 | Language: English, Database: CPlus and MEDLINE

An efficient method for regio- and chemoselective Friedel-Crafts acylation of indoles using acyl chlorides has been discovered. It minimizes/eliminates common competing reactions that occur due to high and m character of indole. In this method, a wide range of aryl, heteroaryl, alkenyl, and alkanoyl chlorides undergo acylation with various indoles without NH protection and afford 3-acylindoles in good to high yields.

Full Text ▾ 40 21 108

2 Hexafluoro-2-propanol-Promoted Intermolecular Friedel-Crafts Acylation Reaction

By: Vekariya, Rakesh H.; Aube, Jeffrey  
Organic Letters (2016), 18(15), 3534-3537 | Language: English, Database: CPlus and MEDLINE

联用检索提高检索效率

21 Results

Scheme 1 (1 Reaction)

Suppliers (82) Suppliers (114) Suppliers (15)

31-091-CAS-326053 Steps: 1 Yield: 82% \*\*\* ZrCl<sub>4</sub>-Mediated Regio- and Chemoselective Friedel-Crafts Acylation of Indole By: Guchhait, Sankar K.; et al Journal of Organic Chemistry (2011), 76(11), 4753-4758 Full Text ▾

Collapse Scheme ▾

Scheme 2 (1 Reaction)

Suppliers (102) Suppliers (81) Suppliers (9)

31-091-CAS-6828122 Steps: 1 Yield: 78% \*\*\* ZrCl<sub>4</sub>-Mediated Regio- and Chemoselective Friedel-Crafts Acylation of Indole By: Guchhait, Sankar K.; et al Journal of Organic Chemistry (2011), 76(11), 4753-4758 Full Text ▾

Collapse Scheme ▾

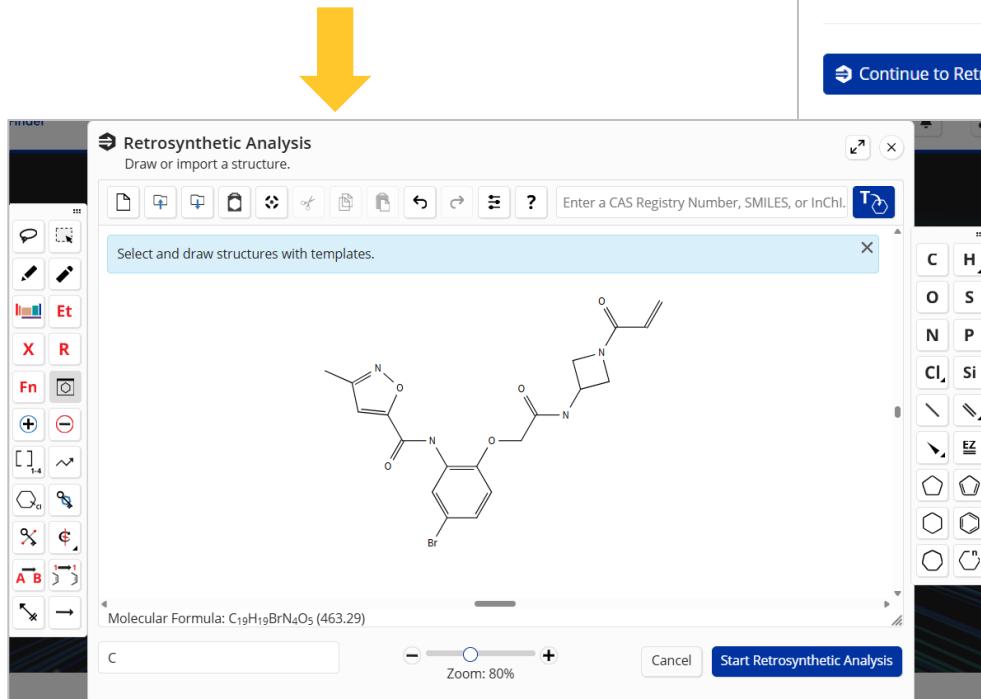
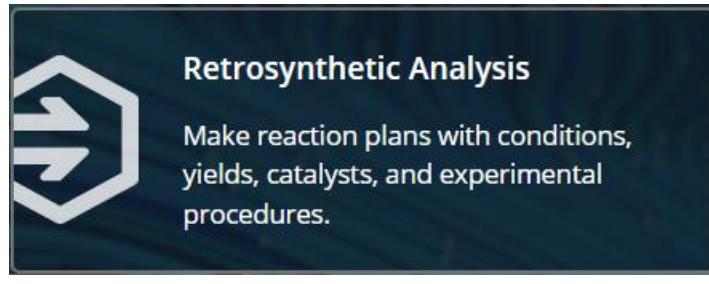
Scheme 3 (1 Reaction)

Suppliers (43) Suppliers (102) Suppliers (32)

31-091-CAS-12409550 Steps: 1 Yield: 77% \*\*\* ZrCl<sub>4</sub>-Mediated Regio- and Chemoselective Friedel-Crafts Acylation of Indole By: Guchhait, Sankar K.; et al

# Retrosynthetic Analysis——拓展反应路线设计思路

结合先进的AI技术和CAS科学家标引的高质量反应数据，为已知或未知分子设计合成路线



## Retrosynthesis Plan Options for drawn structure

Set Rules Supporting Predicted Reactions [Learn more](#)

- Common
- Uncommon (includes common rules)
- Rare (includes common and uncommon rules)

反应规则的常见性

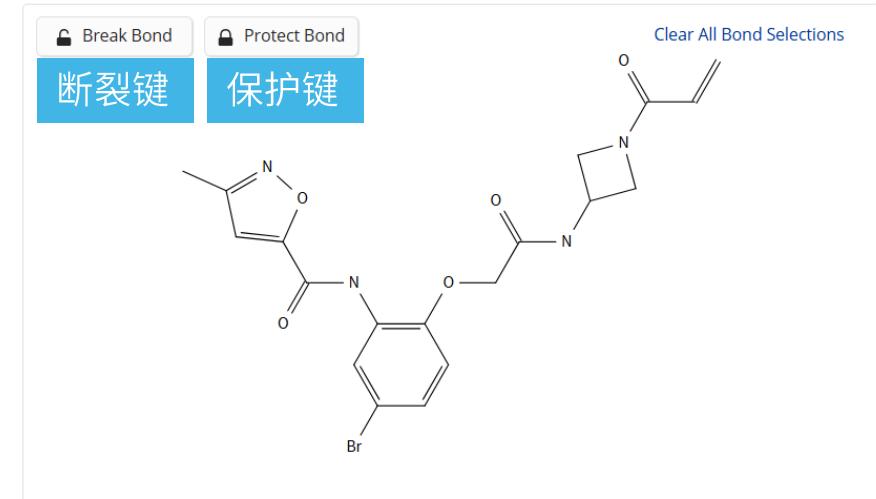
[Continue to Retrosynthesis Plan](#)

[Edit Structure](#)

## Break and Protect Bonds (Optional)

Select a bond within the box to break or protect. You may break a single bond or protect multiple bonds in the target molecule. [Learn more](#)

Break Bond  
 Protect Bond  
断裂键  
保护键



# 逆合成路线详情

Retrosynthesis Plan for drawn structure

Build Status: Complete Estimated Yield: 1% Overall Price: \$7926.40

Customize Plan

Selected Options  Edit

Predicted Rules: Common

Break and Protect Bonds: None

Filters

View Excluded Options

Step Type

Experimental Steps

Predicted Steps

At least one step type must be turned on to display a plan.

Starting Material Cost Limit

300 USD/mol

Reset filter

起始原料价格

已知反应

预测反应

Copyright © 2025 American Chemical Society. All Rights Reserved.

可自由拖动、缩放的路线图

步骤纵览

查看关注步骤的设计依据、可替换路线

Viewing All Steps

A  $\Rightarrow$  B + C Avg Yield: 70%

1.1 Reagents : 1-Ethyl-3-(3'-dimethylaminopropyl)carbodiimide, 1-Hydroxybenzotriazole, Diisopropylethylamine  
Solvents : Dichloromethane; 16 h, rt  
[Experimental Protocols](#)

Evidence Alternative Steps  Exclude

B  $\Rightarrow$  D + E Avg Yield: 63%

1.1 Reagents : Ethyl acetate, Diisopropylethylamine  
Solvents : Dichloromethane; rt

Evidence Alternative Steps  Exclude

C  $\Rightarrow$  O Max Yield: 50%

No Evidence Summary

Alternative Steps  Exclude

D  $\Rightarrow$  F Max Yield: 50%

?

# 了解其他反应路线，拓宽实验设计思路

查看可替代反应

筛选可替代反应路线

直观查看替代反应

路线依据

The screenshot displays a chemical synthesis planning interface. On the left, a main panel shows four reaction steps (B, C, D, E) with their respective reagents, yields, and costs. Step B: Reagent B reacts with reagent D to produce product D (Avg Yield: 63%). Step C: Reagent C reacts with reagent D to produce product D (Max Yield: 50%). Step D: Reagent D reacts with reagent E to produce product E. Step E: Reagent E reacts with reagent D to produce product D (Avg Yield: 63%). A central panel titled "B → D + E" lists "Alternative Steps (34)" with a "Filters" section. A yellow box highlights the "Evidence" dropdown menu. Below, two examples of alternative steps are shown: step 4 of 34 (Predicted Step, Average Yield: 63%) and step 5 of 34 (Predicted Step). A yellow box highlights the "Evidence" dropdown menu for step 5. A detailed view of step 5 evidence is shown in a separate window, titled "Viewing Evidence", which includes chemical structures, reagents, solvents, and experimental protocols. A yellow box highlights the "Evidence" dropdown menu in this window.

58

© 2025 American Chemical Society. All rights reserved.

**CAS**  
A division of the  
American Chemical Society

# 设计该步反应的依据从何而来？

The screenshot displays a chemical synthesis planning interface with several key components:

- Left Panel:** Shows a reaction scheme starting from compound B (a benzyl amine derivative) and leading through steps B → D + E, D → Product, and E → Product. It includes yield calculations (Avg Yield: 63%), cost information (\$73639.59), and a reaction tool for drawing structures.
- Middle Panel:** A detailed view of step B → D + E. It shows the reaction scheme (Scheme 1), reagents (1-Ethyl-3-(3'-dimethylaminopropyl)carbodiimide, HOAc), solvents (Dimethylformamide), and conditions (0 °C; 0 °). It also lists alternative steps (34).
- Right Panel:** A search interface for reactions. It features a search bar ("Search Within Results: Drawn Structure"), a results table, and a "Get 500 Reactions" button highlighted with a yellow arrow. The results table includes entries for various schemes and their reagents, yields, and suppliers.
- Bottom Center:** A summary statement: "进一步明确底物/产物的结构特征 筛选最感兴趣的合成路线" (Further clarify the structure characteristics of substrates/products to select the most interesting synthesis route).

# 小结

1. 通过自然语言、标识符、结构式进行反应信息检索
2. 反应结果集的浏览与筛选
3. 关键词与反应式的联合检索
4. 获取已知化合物或新化合物的逆合成路线，查看文献支持，自定义选择替代路线

# 大纲

## CAS及CAS SciFinder Discovery Platform 简介

### 科研信息的高效查阅

- 全面的文献调研与拓展助力开题
- 多角度出发检索物质结构及相关属性
- 探索实验方案以获取反应与合成相关策略
- 高效获取分析方法及配方制剂信息

### 常见问题Q&A



# 关注文献关联的分析方法？

在CAS SciFinder的文献结果集页面，点击CAS Content中的 Analytical Methods获得有具体分析实验方法的文献，从文献详情页中链接至分析实验方法

The screenshot illustrates the CAS SciFinder interface for searching the literature. On the left, the search bar shows "ciprofloxacin". Below it, the "References" tab is selected. A sidebar on the left lists various filtering options under "Filter Results", with "CAS Content: Analytical Methods" checked. A yellow arrow points from this checked box to the "Method Title" section of the main content area.

**References Tab:**

- All
- Substances
- Reactions
- References**
- Suppliers
- Patent Markush

**Filter Results:**

- Analyze Results
- Behavior
- Filter by (selected)
- Exclude
- Search Within Results
- Document Type
- Flags
- Substance Role
- Language
- Publication Year
- Author/Inventor
- Organization
- Publication Name
- Concept
- CA Section
- CAS Content** (highlighted)
- Analytical Methods (3,595)** (highlighted)
- Formulations (2,495)

**Method Title:** Analysis of Ciprofloxacin in Blood plasma by Solid phase extraction

**Details of the Analytical Method:**

**High-performance liquid chromatographic determination of ciprofloxacin in plasma samples**  
By: Vybiralova, Z.; Nobilis, M.; Zoulova, J.; Kvetina, J.; Petr, P.  
DOI: 10.1016/j.jpba.2004.09.034

A new bioanal. high-performance liquid chromatog. (HPLC) method for the determination of **ciprofloxacin** with norfloxacin as an internal standard was developed and validated for blood plasma samples. Norfloxacin is structural homolog of **ciprofloxacin** and exhibits similar retention properties. The quality of resp. peak separation is strongly influenced by amphoteric character of **ciprofloxacin** and norfloxacin as well. In previously published HPLC methods on conventional C18 reversed-phase, ion pair reagents were added into the mobile phase to suppress peak tailing. In comparison with end-capped and high purity silica reversed-phase sorbent (Purospher RP-18e, Merck), which yielded sym. peaks, separation efficiency was further enhanced in the authors' method. Gradient elution mode using acetonitrile and phosphate buffer pH 3 on the pentafluorophenylpropyl stationary phase (250-4.6 mm Discovery HS F5, 5 µm, Supelco) was carried out. The resolution of 4.1 for **ciprofloxacin**-norfloxacin peaks was achieved. Sample preparation by SPE C18 (Supelclean) with recovery 72% was performed. Fluorescence detection with  $\lambda_{\text{excit}} = 280 \text{ nm}$ ,  $\lambda_{\text{emis}} = 446 \text{ nm}$  was used. After the validation, the bioanal. HPLC method was applied to pharmacokinetic studies.

**Keywords:** **ciprofloxacin** determination blood HPLC pharm

**Substances:**

85721-33-1  
CN1CC[C@H]2[C@@H]1Cc3cc(F)c4cc(O)c(=O)c4[n+]32  
**C17H18FN3O3**  
**Ciprofloxacin**  
Role: Analyte, Pharmacokinetics, Therapeutic Use, Analytical Study, Biological Study, Uses

# CAS科学家增值标引的分析方法详情

## Analysis of Ciprofloxacin in Blood plasma by HPLC

CAS Method Number	Method Category	Technique
1-101-CAS-44938	Active Pharmaceutical Ingredient and Metabolite Analysis	UV-visible spectroscopy; HPLC
Analyte	Matrix	Material
Ciprofloxacin	Blood plasma	Silanized glass tube Eppendorf tube Glass syringe ACE 5 C18 column (250 mm × 4.6 mm, 5 µm) <a href="#">View All</a>
Reagent	Biological Reagent	-
Acetonitrile Methanol Phosphate-buffered saline solutions	-	-

Source	文献来源
JOURNAL	A simple HPLC-UV method for the determination of ciprofloxacin in human plasma
Vella, Janis; Busuttil, Francesca; Bartolo, Nicolette Sammut; Sammut, Carmel; Ferrito, Victor; Serracino-Ingott, Anthony; Azzopardi, Lilian M.; LaFerla, Godfrey	<a href="#">View Abstract</a> <a href="#">Full Text</a>
Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences (2015), 989, 80 - 85. Elsevier B.V.	
CODEN : JCBAAI   ISSN : 15700232   DOI : 10.1016/j.jchromb.2015.01.006	

Equipment Used	所用仪器
HPLC unit, Pro Star, Varian	
Online degasser	
Column oven	
UV-vis detector	
Analytical balance, XS104, Mettler Toledo	
Automated evaporation system, LV, TurboVap	
Concentrator, Turbovap	
Centrifuge	

Validation	数据验证
Linearity Range	0.05 - 8 µg/mL
Limit of Detection	0.01 µg/mL
Limit of Quantitation	0.05 µg/mL
Recovery	97.50, 96.75, 95.50, 93.25, 100.00% in 3.90, 3.87, 3.82, 3.73, 4.00 µg/mL calculated quantity
Accuracy	96.1117, 99.0000, 90.0000% in 6, 2, 0.5 µg/mL spiked
Precision	1.1268, 2.3273, 1.688, 3.8570, 8.8059, 0.0455, 13.0820% (RSD, intraday); 0.9989, 4.7934, 2.0837, 4.1180, 4.4613, 6.0831, 12.0374% (RSD, interday) in 8, 6, 4, 2, 0.5, 0.1, 0.05 µg/mL added
Retention Time	3.26 min

## Instructions

### Preparation of the mobile phase

## 操作步骤

1. Prepare 0.02 M phosphate buffer at pH 2.7 using disodium hydrogen phosphate and orthophosphoric acid.
2. Elute together with acetonitrile to dilute mobile phase of buffer and acetonitrile 77:23 (v/v).
3. Keep reagents in amber glass bottles.

### Plasma sample preparation using silanized tubes

1. Transfer spiked 400 mL of plasma with ciprofloxacin to 1.5 mL Eppendorf tubes.
2. Add 30 mL of internal standard (IS, sulfadimidine sodium) working solution in water (100 g/mL) to each tube.
3. Add 1 drop of 10 M phosphate buffer (pH 2.7).
4. Vortex mix for 3 min.
5. Add 500 mL of ice cold acetonitrile using a glass syringe.
6. Vortex mix the tubes for 5 min.
7. Centrifuge the samples at 3500 × g for 5 min.
8. Pour the supernatant into 8 mL silanized glass tubes.
9. Place the silanized tubes in a Turbovap concentrator with the water bath set at 50 °C for 20 min.
10. Reconstitute the dried residue with 100 µL mobile phase.
11. Vortex mix for 3 min.
12. Re-centrifuge at 15000 rpm for 3 min.
13. Inject 50 mL of the clear supernatant into the HPLC unit.

### Standard solution preparation

1. Prepare 1 mg/mL ciprofloxacin stock solution in methanol.
2. Obtain working solutions from the stock solution by dilution with mobile phase.
3. Store at 4 °C.

### HPLC-UV analysis

1. Perform HPLC-UV analysis using Varian Pro Star HPLC unit consisting of an online degasser, column oven and UV-vis detector.
2. Carry out separation on a reversed phase ACE 5 C18 column (250 mm × 4.6 mm, 5 µm; Advances chromatography Technologies, Aberdeen, Scotland) protected by Agilent Pursuit 5 C18 Meta guard column (10 mm × 4.6 mm, 5 µm; Agilent Technologies, Amstelveen, Netherlands).
3. Maintain column and injection temperature at 25 °C.
4. Program the system isocratically.
5. Set the flow rate at 1.5 mL/min.
6. Inject fixed sample through a loop having a volume of 50 µL.
7. Perform detection at 277 nm.

- CAS科学家增值标引的分析实验详情  
- 无需购买、浏览全文，高效获取所需实验信息

# 通过CAS Analytical Methods获取分析方法详情

方法(2): 登录<https://methods.cas.org>, 主题检索或分类浏览

The screenshot illustrates the search process on the CAS Analytical Methods website. On the left, the homepage features a search bar and two main navigation buttons: 'Explore Methods' (highlighted with a yellow box and arrow) and 'Advanced Search'. The 'Explore Methods' section lists various analytical categories. A yellow arrow points from the 'Explore Methods' button to the 'Search Methods' button at the bottom of the page. On the right, the search results for 'Active Pharmaceutical Ingredient and Metabolite Analysis' are displayed. The results page includes a sidebar for filtering by analyte, matrix, method category, technique, validation, and year. Two specific results are shown: 'Analysis of Ketoconazole by Cyclic voltammetry' and 'Analysis of Rabeprazole in Blood serum by Ion mobility spectrometry'. Both results provide details on the analyte, matrix, reagents, and equipment used.

Good Morning,

Search for keywords, matrices or analyte.

Explore Methods  
Search methods using criteria like method categories and subcategories.

Advanced Search  
Search methods using criteria like keywords, analytes, matrices and more.

## Explore Methods

Category	Category Name	Include Keywords (Optional)
Agricultural Applications / Analysis	Active Pharmaceutical Ingredient	Enter a keyword... + Add Another Keyword
Bioassays	Addictive Drug Assay	
Biomolecule Isolation	Forensic Analysis	
Environmental Analysis	Genetic Analysis	
Food Analysis	Nanomaterial Analysis	
Fuels / Geology / Biofuels	Organic Compound Analysis	
Historical Analysis / Dating	Toxicity Assay	
Miscellaneous	Toxin Assay	
Organic Compound Analysis		
Organometallics / Inorganics		
<b>Pharmacology / Toxicology</b>		
Polymer Analysis		
Water Analysis		

Search Methods

Results for Active Pharmaceutical Ingredient and Metabolite Analysis

Filter By

Analyte

- Acetaminophen (2993)
- Flavonoids (2578)
- Phenols (2482)
- Ciprofloxacin (1704)
- Ibuprofen (1394)

[View All](#)

Matrix

- Pharmaceutical tablets (27081)
- Blood plasma (17543)
- Urine (9378)
- Blood serum (5721)
- Pharmaceutical capsules (4423)

[View All](#)

Method Category

Technique

Equipment Used

114,515 Results

Sort: Relevance Group: By Method

**Analysis of Ketoconazole by Cyclic voltammetry**

By: Alagumalai, Krishnapandi; Muthukutty, Balamurugan; Sivakumar, Mani; Lee, Daeho; Kim, Seong-Cheol  
Surface-grafted MoS<sub>2</sub> for ketoconazole sensing in biological and aqua samples  
Colloids and Surfaces, A: Physicochemical and Engineering Aspects (2025), 706, -. Elsevier B.V.

**Ketoconazole**  
Reagent: Hydrochloric acid; Phosphate;  $\beta$ -Cyclodextrin; Molybdenum sodium oxide; Thiourea; Sodium hydroxide; Acetic acid  
Material: Glassy carbon electrodes; Saturated KCl-based silver/silver chloride (Ag/AgCl) electrode; Platinum

[View Abstract](#) [Full Text](#) [View in CAS SciFinder](#)

**Analysis of Rabeprazole in Blood serum by Ion mobility spectrometry**

By: Mazidi, Fatemeh; Sheibani, Ali; Shishehbori, M. Reza  
Au NPs-CdS QDs nano-composite as a new adsorbent for quantitative determination of rabeprazole in biological and pharmaceutical samples using ion mobility spectrometry  
Analytical and Bioanalytical Chemistry Research (2025), 12 (1), 57-64. Iranian Chemical Society

**Rabeprazole**  
Matrix

Other Materials

Method Category

Technique

Equipment Used

[View Abstract](#) [Full Text](#) [View in CAS SciFinder](#)

# 分析方法检索结果的分析与精炼

分析物

基质

方法分类

技术&仪器

实验验证

年份

Results for Custom query

Filter By

28 Results

Sort: Relevance ▾ Group: By Method ▾

1 Analysis of Lapatinib in Blood plasma by HPLC-tandem mass spectrometry JOURNAL Compare

Analyte: Lapatinib  
Matrix: Blood plasma  
Other Materials: Reagent: Formic acid; Ethyl acetate; Methanol  
Material: XBridge C18 column (3.5 μm, 50 mm × 2.1 mm i.d.)  
Method Category: Active Pharmaceutical Ingredient and Metabolite Analysis  
Technique: HPLC-tandem mass spectrometry  
Equipment Used: LC system; Triple quadrupole mass spectrometer

View Abstract ▾ Full Text ▾ View in CAS SciFinder

2 Analysis of Lapatinib in Blood plasma by Solvent extraction JOURNAL Compare

Analyte: Lapatinib  
Matrix: Blood plasma  
Other Materials: Reagent: Dimethyl sulfoxide; Methanol  
Material: Poroshell 120 EC C18 column (70 × 3.0 mm, 2.7 μm)

点击标题，可进入分析方法详情。  
可同时对比3种分析方法  
可链接至SciFinder，查看文献详情页

Validation: Precision (28), Accuracy (25), Linearity Range (25), Limit of Quantitation (24), Recovery (18)  
Year: 2006 to 2024

No Min to No Max Apply

# 对照多个感兴趣的分析方法详情

Download   Cancel

Format

PDF
  XLS

Method 1		Method 2	
Analysis of Lapatinib in Blood plasma by HPLC-tandem mass spectrometry		Analysis of Lapatinib in Blood plasma by Atmospheric precipitation	
CAS Method Number	1-101-CAS-187473	1-101-CAS-43	Linearity Range 5 - 5000 ng/ml
Method Category	Active Pharmaceutical Ingredient and Metabolite Analysis	Active Pharm	Limit of Quantitation 5 ng/mL
Technique	HPLC-tandem mass spectrometry	HPLC-tandem spectrometry	Recovery $43\% \pm 14\%$ , $42\% \pm 10\%$ and $48\% \pm 12\%$ (recovery), for 5, 15, 800 and 4000 ng/mL spiked sample, repectively.
Analyte	Lapatinib	Lapatinib	Accuracy 102.1%, 98.6%, 102.5% and 98.3% (recovery), for 5, 15, 800 and 4000 ng/mL QC sample, repectively.
Matrix	Blood plasma	Blood plasma	Precision 4.6%, 3.4%, 2.3% and 2.4% (RSD, intra-day); 4.0%, 2.9% and 3.1% (RSD, inter-day), for 5, 15, 800 and 4000 ng/mL QC sample, repectively.
Other Materials	Formic acid; Methanol; Ethyl acetate; XBridge C18 column (3.5 $\mu$ m,50 mm $\times$ 2.1 mm i.d.)	Acetonitrile; A precipitation Security guar	Source JOURNAL A stable isotope-labeled internal standard is essential for correcting for the interindividual variability in the recovery of lapatinib from cancer patient plasma in quantitative LC-MS/MS analysis
Equipment Used	LC system., Alliance2695, Waters, Milford, MA, USA; Triple quadrupole mass spectrometer, Quattro Micromass, Waters	HPLC system, Shimadzu, Ky Kyoto, Japan; Sciex, Ontario	By: Wu, Jianmei; Wiegand, Richard; LoRusso, Patricia; Li, Jing Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences (2013), 941, 100 - 108. Full Text ▾
Conditions	Instrument: ionization mode-Positive; heated nebulized probe- 350 °C; pressure of collision gas (Argon) (mbar)- 5.92E-003, 5.92E-003 and 5.92E-003 for lapatinib, lapatinib-d3 and zileuton; dwell time (s)- 0.5, 0.5 and 0.5, for lapatinib, lapatinib-d3 and zileuton; cone voltage (V)- 60, 60 and 22 for lapatinib, lapatinib-d3 and zileuton; collision energy (eV)- 34, 34 and 12, for lapatinib, lapatinib-d3 and zileuton; transition- 581.4>364.96, 584.1>366 and 237.43>161.09, for lapatinib, lapatinib-d3 and zileuton.Chromatographic: XBridge C18 column (3.5 $\mu$ m,50 mm $\times$ 2.1 mm i.d.); internal standard- lapatinib-d3; temperature- 30 °C; mobile phase- methanol and 0.45% formic acid in water (50:50, v/v); isocratically; flow rate- 0.2 ml/min.	Instrument: C and security g 10 mM ammonium acetone ntrile; C supply 2: 80 a V; source gas declustering potential: 102 V and collision energy: 50 V for both lapatinib and internal standard	JOURNAL A sensitive LC-MS-MS assay for the determination of lapatinib in human plasma in subjects with end-stage renal disease receiving hemodialysis By: Kocan, Geralyn P.; Huang, Mike; Li, Fumin; Pai, Sudhakar Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences (2018), 1097-1098, 74 - 82. Full Text ▾

# 研究课题在产品中的应用？配方制剂的检索与设计

- 访问网址：<https://formulus.cas.org/>

The screenshot shows the CAS Formulus website interface. At the top, there is a navigation bar with the CAS logo, a menu icon, 'Help & Support', 'Alerts', 'Saved', and a user profile icon. Below the header, a banner says 'Good Evening,' followed by 'Formulations' and 'Ingredients' tabs, with 'Ingredients' being the active tab. A search bar at the top right contains the placeholder 'Search by Ingredient Name, CAS Registry Number, or Function' and a magnifying glass icon. To the left, there are two cards: 'Formulation Designer' (with a coffee cup icon) and 'Advanced Search' (with a magnifying glass icon). The 'Advanced Search' card has the text: 'Search Formulations using criteria like ingredients, targets, and more.' A yellow arrow points from this text to the 'Advanced Formulations Search' section on the right. The 'Advanced Formulations Search' section has a title 'Advanced Formulations Search ?' and a subtitle 'Searches the following content fields: Ingredient, Function, Purpose, Physical Form, Delivery Route, and Target.' It includes fields for 'Search For' (set to 'Ingredient'), 'Operator' (set to 'Required'), and a text input 'Enter one term' with the placeholder 'Ex: caffeine, sodium, 50-00-0'. Below these are buttons for 'Add Another Term' and a 'Search' button. To the right of the search form is a vertical list of search fields: All Fields, Form, Function, Ingredient, Purpose, Route, and Target. A dropdown menu next to 'Required' allows selecting 'Optional' or 'Excluded'. A large yellow arrow points from the 'Advanced Search' card to the 'Advanced Formulations Search' section. To the right of the search form, the text '针对形式、功能、成分、用途、途径或目标进行精确检索' is displayed. At the bottom left, there is a 'Recent Search History' section. The bottom right corner features the CAS logo with the text 'A division of the American Chemical Society'.

Good Evening,

Formulations Ingredients

Search by Ingredient Name, CAS Registry Number, or Function

Formulation Designer

Design custom formulation templates based on selections and ingredients

Advanced Search

Search Formulations using criteria like ingredients, targets, and more.

Advanced Formulations Search ?

Searches the following content fields: Ingredient, Function, Purpose, Physical Form, Delivery Route, and Target.

Search For: Ingredient Operator: Required Enter one term: Ex: caffeine, sodium, 50-00-0

Add Another Term

All Fields

Form

Function

Ingredient

Purpose

Route

Target

Required  
Optional  
Excluded

Recent Search History

针对形式、功能、成分、用途、途径或目标进行精确检索

CAS

A division of the American Chemical Society

# 多角度筛选精炼配方检索结果

领域  
用途  
物理形态  
物质状态  
递送途径  
所含信息  
文献类型  
机构/组织  
语言  
发表年份

Formulations search for "photoresists"

Get Additional References

Filter by

188 Results

Sort: Relevance ▾ Group: By Family ▾

1 点击标题，可进入制剂/配方详情。

Photoresist Composition

Location: Claim 22, 23, 27, 30, 37

Purpose: Photoresists

Compare

可同时对比3种制剂/配方

PATENT

Fluorinated monomers, fluorinated polymers having polycyclic groups with fused 4-membered heterocyclic rings, useful as photoresists, and processes for microlithography

Assignee: E. I. Du Pont De Nemours and Company  
WO2004014960  
Language: English

Patent PDF View in CAS SciFinder

可链接至SciFinder，查看文献详情页

Component	Function	Amount Reported
Group: fluorine-containing copolymer	Photoresists	-
fluorinated monomers, fluorinated polymers: Markush 2, claim 23		
3-Oxatricyclo[4.2.1.0 <sup>2,5</sup> ]non-7-ene, 4,4-bis(trifluoromethyl)-		
3-Oxatricyclo[4.2.1.0 <sup>2,5</sup> ]non-7-ene, 4-[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]-		
3-oxatricyclo[4.2.1.0(2,5)]non-7-ene		

# 制剂/配方详情页

 Positive Photosensitive Anionic Electrodeposition Coating Composition: Electrodeposition Coating Agents

## 配方用途

Purpose	Target	Delivery Route	Physical Form	Source
electrodeposition coating agents	Printed circuit boards	-	Solutions	<a href="#">View</a>

## Formulation Ingredients

## 配方成分

Component	Function	Amount Reported
Group: vinyl copolymer	-	122 wt. parts
4,4'-[1-[4-[1-(4-Hydroxyphenyl)-1-methylethyl]phenyl]ethylidene]bis[phenol]	-	15 wt. parts
1,2-Naphthoquinonediazide-5-sulfonic acid	-	-
Water	-	418.5 wt. parts
Water	-	111.1 wt. parts

## Source Patent

## 文献来源

Photosensitive anionic electro-deposition coating compositions for positive-working photoresists with good storage stability and high sensitivity

Assignee : Honey Kasei Co., Ltd.  
JP4302178  
Language: Japanese  
Location: Example 1, Table 1

[Patent PDF](#)[View in CAS SciFinder](#)

无需阅读原文  
即可获取配方详情

## Process

preparation of positive photosensitive anionic electrodeposition coating composition: mix vinyl copolymer (place 10.0 parts of isopropanol and 10.0 parts of butyl cellosolve in a 3-liter four-necked flask equipped with a stirrer, a reflux condenser and a nitrogen inlet tube, and heat to 90 °C. separately, 16.0 parts of isopropanol, 6 parts of acrylic acid, 1 part of 2-hydroxyethyl acrylate, 14 parts of 2-ethylhexyl acrylate, 10 parts of ethyl acrylate, 34 parts of n-butyl acrylate, 35 parts of methyl methacrylate, 1 part of mercaptoacetic acid, charge 2 parts of azobisisobutyronitrile into the dropping funnel and drop into the flask over 120 minutes, add 2 parts of isopropanol and 0.2 parts of azobisisobutyronitrile three times every 30 minutes, and the continue reaction at 90 °C. for 90 minutes at temperature was below 50 °C and add 2.3 parts of dimethylaminoethanol, stir) and 4,4'-[1-[4-[1-(4-hydroxyphenyl)-1-methylethyl]phenyl]ethylidene]bis[phenol] with 6-diazo-5,6-dihydro-5-oxonaphthalene-1-sulfonic acid, and add deionized water while stirring, continue to effect phase inversion emulsification and electrolysis (stock solution), add water and stock solution was added while stirring to obtain an electrodeposition solution.

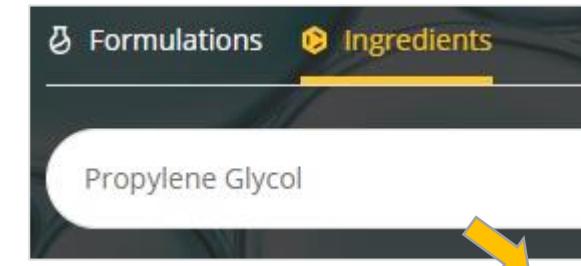
## Experimental Activity

Descriptor	Notes	
developability	the exposed printed circuit board was immersed in a 0.5% sodium metasilicate aqueous solution at 32 °C for 2 minutes to confirm whether development was possible.	Yes
etching solution resistance	after the developed printed circuit board was immersed in an etching solution of ferric chloride at 40 °C for 5 minutes, the electrodeposition coating film was checked for cracks and creases.	good
	the composition was allowed to stand for 24 hours, and the presence or absence of sediments deposited on the bottom of the container was confirmed.	No sedimentation
	-	10 µM

详细、直观的工艺步骤  
与实验数据



# 制剂、配方主要成分检索



- 使用该原料的制剂或配方
- 原料供应商信息
- 可将原料添加至设计工具

Formulation Designer

• 制剂或配方中，与该原料同时使用的其它配伍成分  
• 管控信息及清单  
• 实验属性

CAS RN: 57-55-6  
[View Details](#)

OCC(O)C  
 $C_3H_8O_2$

(±)-Propylene glycol Propylene glycol  
Key Physical Properties Value Condition

Molecular Weight	76.09	-
Melting Point (Experimental)	-59 °C	-
Boiling Point (Experimental)	188.2 °C	-
Density (Experimental)	1.036 g/cm <sup>3</sup>	Temp: 25 °C

Commonly Used As: Solvents; Humectants; Plasticizers; Preservatives; Carriers...

Similar Ingredients with Regulatory Information

37321-62-3	Lauroglycol
27194-74-7	Propylene glycol monolaurate
29387-86-8	Propylene glycol butyl ether

[View 14 More](#)

[Commonly Formulated With](#) | [Regulatory Information](#) | [Experimental Properties](#)

[Get Formulations](#) [Get Suppliers](#) [Add to Formulation Designer](#)

# Formulation Designer辅助设计制剂、配方

启发制剂配方设计

The screenshot shows the 'Formulation Designer' interface. At the top, there's a search bar with placeholder text 'Search for a product or ingredient'. Below it, a section titled 'Design custom formulation templates based on selections and ingredients' features a large yellow arrow pointing downwards. The main area displays a table with columns for Industry, Purpose, Physical Form, and a button to 'Add up to 5 Ingredients'. The 'Industry' column lists categories like Pharmaceutical, Cosmetics & Personal Care, Agrochemical, Cleaning & Surfactant Products, Inks, Paints, & Coatings (which is highlighted with a blue box), and Food & Related. The 'Purpose' column lists various coating materials. The 'Physical Form' column shows options like Liquids, Varnishes, Fluids, Solutions, and Paints (also highlighted with a blue box). A button labeled '+ Add Another Ingredient' is visible. At the bottom right of the main area is a 'Create Template' button.

The screenshot shows the 'Formulation Designer' interface with a template creation screen. At the top, there's a header with a back arrow and the text 'Formulation Designer'. On the right, there are buttons for 'Clear All Selections', 'Save', and 'Download'. Below the header, there's a section titled 'Your Template' with a table. The table has columns for Function, Ingredient, Regulatory Lists, Top Alternatives, and Amounts. The first row shows 'Active or Featured Ingredient' as 'Ethenol, homopolymer, 3-phenyl-2-propenoate' with a note 'Amount not available'. The second row shows 'Solvents' as 'Methyl ethyl ketone' with regulatory lists 'EPA Safer Chemical Ingredients; FDA Inactive Ingredients Database' and alternatives 'Isopropanol; N-Methyl-2-pyrrolidone' with a note 'Approximate Range: 20 - 25%'. The third row shows 'Photopolymerization catalysts' as '1H-Imidazole, 2-(2-chlorophenyl)-4,5-diphenyl-, dimer' with a note 'View More Alternatives'. The fourth row shows 'Bis(diethylamino)benzophenone; 2-(Dimethylamino)-2-(4-methylbenzyl)-1-[(4-morpholin-4-yl)phenyl]-1-butane; Bis(2,4,6-trimethylbenzoyl)phenylphosphine oxide; Poly(oxy-1,2-ethanediyl),  $\alpha,\alpha',\alpha''$ -1,2,3-propanetriyltris[ $\omega$ -[[phenyl(2,4,6-trimethylbenzoyl)phosphinyl]oxy]-Acrylic acid-butyl acrylate-styrene copolymer' with a note 'Approximately 1%'. There are also 'Edit Selections' and 'Clear' buttons at the bottom of the template table.

基于期刊、专利和产品说明书中标引的制剂、配方数据，获得见解。

# 文献关联的配方/制剂

在CAS SciFinder的文献结果集页面，点击CAS Content中的 Formulation 获得有具体配方或制剂信息的文献，从文献详情页中链接获取

References search for ""chronic heart failure" and "traditional Chinese medicine""

All Substances Reactions References Suppliers Patent Markush

View Related Results ▾

Publication Year International Patent Classification (IPC) Author/Inventor Organization Publication Name Concept CA Section

CAS Content Analytical Methods (9) Formulations (3)

Life Science Data Formulation Purpose Cardiovascular agents (3)

Databases 制剂用途/目的

583 Results 1

**Application of a traditional Chinese medicine composition for preparing medicines for preventing and/or treating myocardial hypertrophy**

In this Patent Inventors: Zhang, Minyu; Guo, Fefei; Wu, Hongwei; Yang, Hongjun; Wei, Junying; Wu, Sha

Claims Classifications CAS Concepts Formulations

The invention relates to the field of medicines, in particular to an application of a traditional Chinese medicine composition to preparation of a medicine for preventing and/or treating myocardial hypertrophy and an application to preparation of a medicine for preventing pressure-loaded chronic heart failure, and expands new indications of Yixinshu capsules. Curative effect and action mechanism for myocardial hypertrophy resistance are studied. A new thought and a new choice are provided for treating myocardial hypertrophy and malignant heart diseases caused by further development of myocardial hypertrophy.

Keywords: myocardial hypertrophy prevention traditional Chinese medicine composition

PatentPak Get Prior Art Analysis Full Text View in CAS Formulus

Formulations Formulation Title Traditional Chinese Medicine for Preventing and/or Treating Myocardial Hypertrophy: Cardiovascular Agents

2

**The traditional Chinese medicines treat chronic heart failure and their main bioactive constituents and mechanisms**

By: Chen, Jie; Wei, Xiaohong; Zhang, Qian; Wu, Yuzhuo; Xia, Guiyang; Xia, Huan; Wang, Lingyan; Shang, Hongcai; Lin, Sheng  
Acta Pharmaceutica Sinica B (2023), 13(5), 1919-1955 | Language: English, Database: CPlus and MEDLINE

A review. Chronic heart failure (CHF) is a severe public health problem with increasing morbidity and mortality, any treatment targeting a single session is insufficient to tackle this. CHF is characterized by reduced cardiac output resulting from neurohumoral dysregulation and cardiac remodeling, which might be related to oxidative stress, inflammation, endoplasmic reticulum stress, apoptosis, autophagy, mitochondrial function, and angiogenesis. These mol. mechanisms interact with each other through crosstalk. Historically, Chinese medicinal herbs have been widely applied in the treatment of...

# 小结

1. 利用**CAS Analytical Methods**进行主题检索或分类浏览获得分析方法，或通过文献查看关联的分析实验及数据详情
2. 利用**CAS Formulus**检索原料、配方/制剂，或通过文献结果集获得关联的配方/制剂信息；利用配方设计工具启发产品配方的开发

# 总结

- CAS 内容合集来源于化学并超越于化学，支持多学科、跨学科研创新
- 全面覆盖的内容确保不遗漏任何重要的信息
- CAS 科学家人工智慧与先进专有技术结合标引的数据，能够揭示隐藏在数据间的隐秘关联
- 强大的功能确保降低文献检索和分析的时间，将更多宝贵的时间应用于创新工作中，提升科研创新效率

# CAS SciFinder 检索浏览器推荐

浏览器推荐：

- Windows (7, 8.1, 10): Chrome 60及更高版本, Firefox 55及更高版本, Firefox 52 (ESR)、Edge 15及更高版本
- Mac OS X (10.11, 10.12, 10.13): Safari 9.3及更高版本, Chrome 60及更高版本, Firefox 55及更高版本, Firefox 52 (ESR)
- 不建议使用360浏览器，相关功能或插件会被自动拦截

# 常见问题

## Unauthorized IP Address

User registration is available only from IP addresses specified by the key contact at your organization. Please try to register again from an authorized location.

- 检查注册链接是否正确
- 确认连入校园网，且不是通过VPN连接
- 如果链接正确，且在校园内，请联系图书馆或china@acs-i.org



A division of the  
American Chemical Society

There was a problem verifying your account.

[Try Again](#)

[Contact Us](#)

Or [Log Out](#) and try again.

Reference Id: GU75LMF9iZnhTq8mymUog

- 确认账号密码是否正确
- 如果账号密码正确，请填写问题报告后联系图书馆或china@acs-i.org

A division of the  
American Chemical Society

# 使用注意事项

- 一人注册一个帐号
- 实名注册, 请提供真实姓名信息 (中文名用汉语拼音全拼)
- 不得过量下载 (<https://www.cas.org/legal/infopolicy>)
- 不得账号分享
- 不得将账号用于非学术研究

# CAS SCIFINDER DISCOVERY PLATFORM

## 2025 秋季专题论坛直播时间表



9月 25 日 | 在能源材料研发与产业化中的应用

演讲人：杜德鑫 博士



10月 23 日 | 最新进展及在知识产权工作流程中的应用

演讲人：钱欣 博士



11月 13 日 | 助力生物医药研发创新与可持续发展

演讲人：陈开乾 博士



12月 18 日 | 独特数据与AI技术结合赋能研发突破

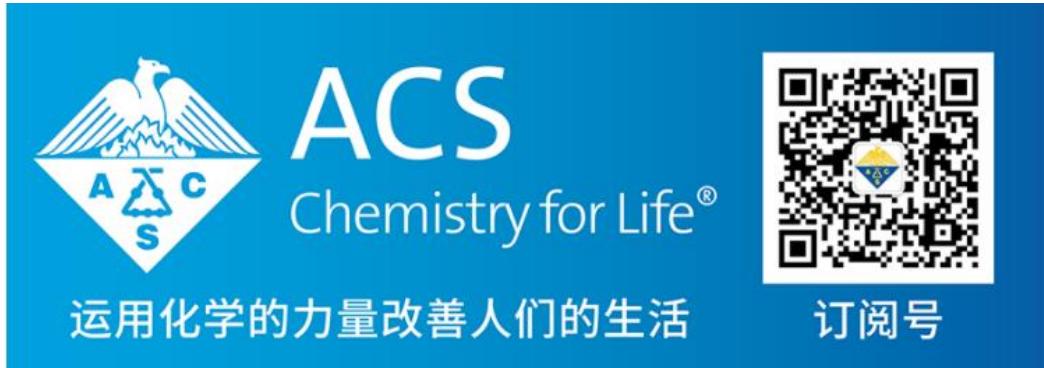
演讲人：钱欣 博士

“

扫描二维码，一键获取  
四场直播回放！



# 学习资源



1. 扫码关注 ACS 美国化学会官方公众号查看视频和课件
2. Bilibili 官方账号查看视频：  
<https://space.bilibili.com/630784162>

Three screenshots of mobile interfaces for ACS resources. The first screenshot shows the ACS WeChat official account with posts about ACS SciFinder tips and precision chemistry. The second screenshot shows the ACS website for the International Conference on Smart Materials and Chemical Engineering. The third screenshot shows the SciFinder learning center with sections for registration, short videos, specialized forums, and usage tips.



**Between problems  
and progress are  
connections that  
matter**



谢谢！

美国化学文摘社(CAS)北京代表处

China@acs-i.org  
+86-10-6250 8026/7

