

CAS SciFinder Discovery Platform

全面高效获取科技信息



陈开乾 博士

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

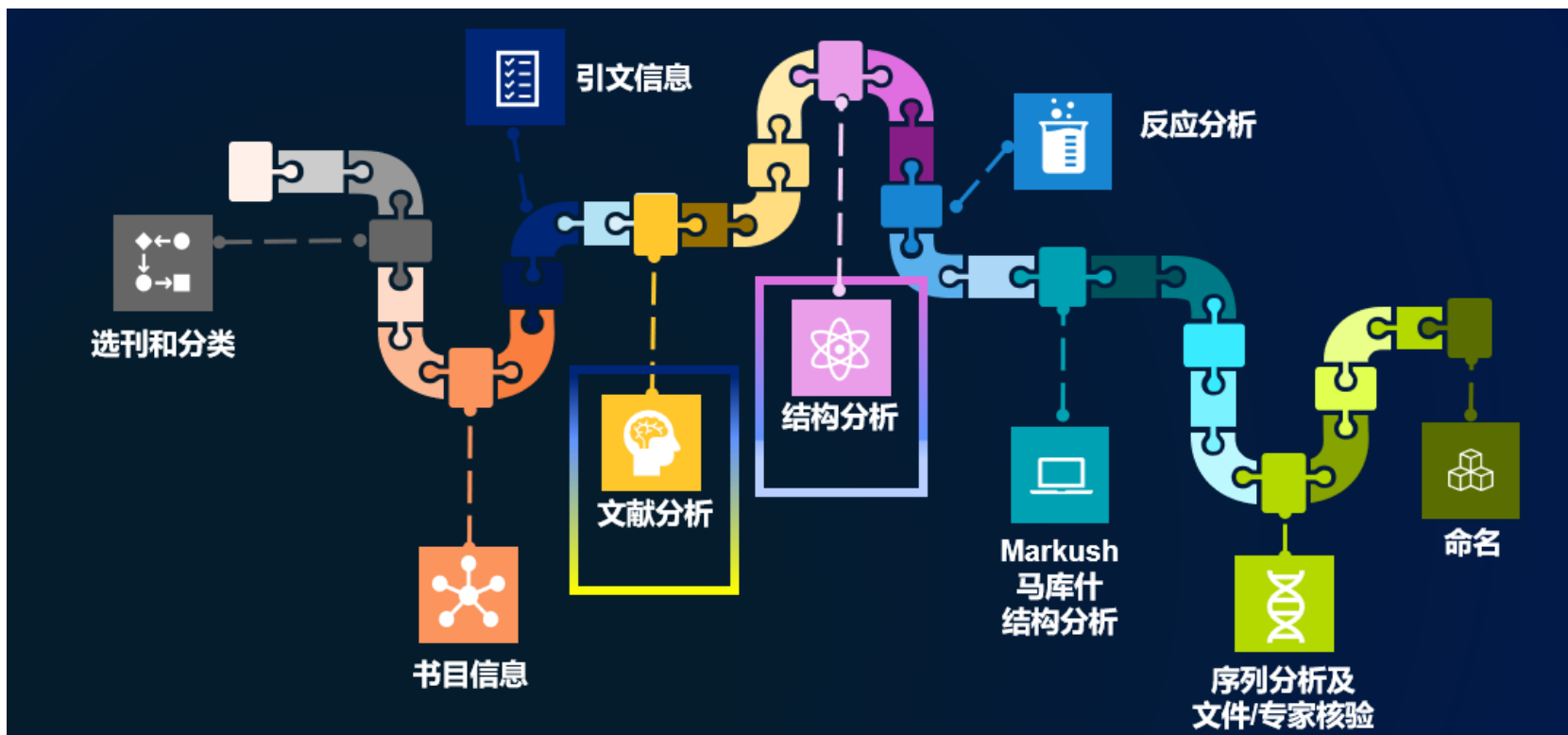


来源：

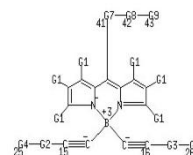
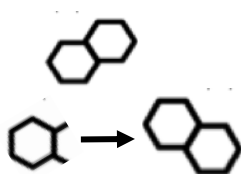
<https://www.cas.org/cas-data>

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

CAS科学家的智力标引




1990
Smith, M.
anthracene



Androst-4-en-3-one, 17-hydroxy-17-methyl-, (17β)-

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/>




Log in to SciFinder®

Username or Email Address

[Next](#)

[Create an account.](#) | [Can't log in?](#)

By using CAS SciFinder®, you agree to the [License Agreements and Policies](#), including but not limited to the [End User License Agreement](#)



Log in to SciFinder®

Welcome, npan@acs-i.org [Not You?](#)

Password

[Log In](#)

☐ Keep me signed in

[Create an account.](#) | [Can't log in?](#)

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>

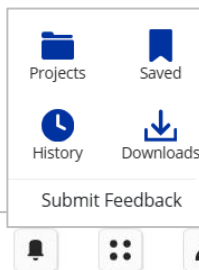
3、CAS SciFinder-n检索网址

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

4、CAS SciFinder-n培训材料及视频:

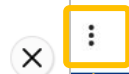
<https://www.cas.org/support/training/scifinder-n>

清晰简洁的检索界面



检索结果管理
和账号设置

更新结果提醒



CAS SciFinder

Good Morning,

Proton nmr spectral data for C13H13Br

Draw

结构绘制面板

Featured Search

View Less

Prior Art Discovery
Discover prior art in patents and non-patent literature using AI-enhanced search technology.

现有技术探索

Patent Markush
Search Patent Markush by structure and view associated references.

专利Markush检索

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

高级检索选项

Retrosynthetic Analysis
Make reaction plans with conditions, yields, catalysts, and experimental

逆合成路线设计

Search CAS Lexicon
Build powerful searches using CAS concepts, chemical classes, and taxonomy.

CAS词库

Search CAS Sequences
Query BLAST, CDR, and Motif algorithms for nucleotide and protein based sequences.

CAS序列检索

History For You

近期检索历史

Recent Search History

View All Search History

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 image displays two screenshots of the CAS SciFinder interface, illustrating the process of searching for literature using different identifiers.

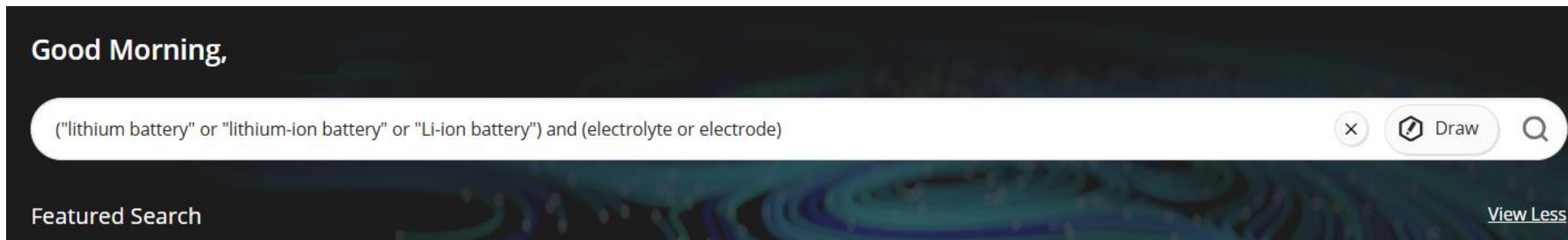
Left Screenshot: The search query is "10.1021/acssuschemeng.5b00981". The results show a paper titled "Pyrrolinium-based Ionic Liquid as a Flame Retardant" by Kim, Hyung-Tae; Kang, Jaesik; Mun, Junyoung; Oh, Seung M.; Yoon, J. H. The paper is published in ACS Sustainable Chemistry & Engineering (2016), 4(2), 497-505. The interface includes a "Filter Results" sidebar with options for "Behavior", "Search Within Results", "Document Type", and "Flags".

Right Screenshot: The search query is "An In Situ Polymeric Electrolyte with Low Interfacial Resistance on Electrodes for Lithium-Ion Batteries". The results show a paper titled "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, Whangl; Jang, Hohyouon. The paper is published in Advanced Materials Interfaces (2022), 9(3), 2101958. The interface includes a "Filter Results" sidebar with options for "Behavior", "Search Within Results", "Document Type", and "Flags".

Both screenshots feature a "智能识别检索意图" (Smart Identification of Search Intent) overlay, indicating that the system has interpreted the query as a reference title and suggests rerunning the query as a general search.

如何精准构建检索主题？

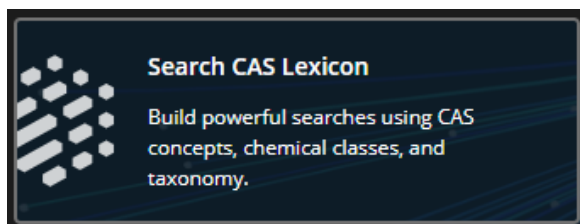
- 支持布尔逻辑运算符(and, or, not)
- 默认运算顺序or > and > not, ()优先运算
- “”不允许词形变化，但可出现单数或复数
- 通配符*代表0或多个字符；?代表0或1个字符



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

Primary batteries - Preferred Concept ⓘ [×](#)

OR [Remove All](#)

^ 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

AND OR NOT [Add to Query](#) [Clear Query](#) [Search](#)

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.](#)

Substances **References** Clear All

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

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

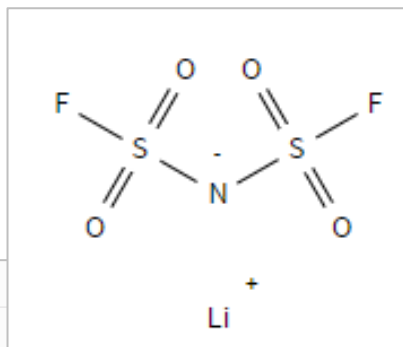
Advanced Search
Select data fields and search operators to create a focused query.

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?

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



文本与结构是“and”关系

定位物质在文献中的研究角色

文献结果的筛选与定题追踪

References search for "lithium battery" or "lithium-ion battery" or "Li-ion battery" and (electrolyte or electro... + drawn structure

All Substances Reactions **References** Suppliers Patent Markush

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

Sort: Relevance ▾ View: Partial Abstract ▾

1,763 Results

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: CAlplus 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 ▾

Full Text ▾ 11 0 548

2

Li-ion battery and LiCo_{1/3}Mn_{1/3}Ni_{1/3}O₂ electrodes with piperidinium ionic liquid lithium bis(fluorosulfonyl)imide for Li-ion batteries
Jakub; Nadherná, Martina; Dominko, Robert
Power Sources (2012), 205, 402-407 | Language: English, Database: CAlplus

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 (PP₁₃TFSI) 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-PP₁₃TFSI **electrolyte** has been shown to work effectively with a graphite **anode** due to the ability of the FSI anions to create a stable solid **electrolyte** interface on graphite. A discharge capa...

View More ▾

Document Type
Flags
Patent Office
Patent Status
Substance Role
Uses (1,625)

Analyze Results
Top Document Types

Patent Journal

Patent Offices
1 819

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
☐ Query Only ☐ Selected Answers ☒ 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)

Cancel Save

设置定题追踪

文献结果的筛选与可视化分析

Filter Results <

Analyze Results

Behavior

Filter by Exclude

Search Within Results

Document Type

Flags

Patent Office

Patent Status ?

Substance Role

Language

Publication Year

International Patent Classification (IPC)

Author/Inventor

Organization

Publication Name

Concept

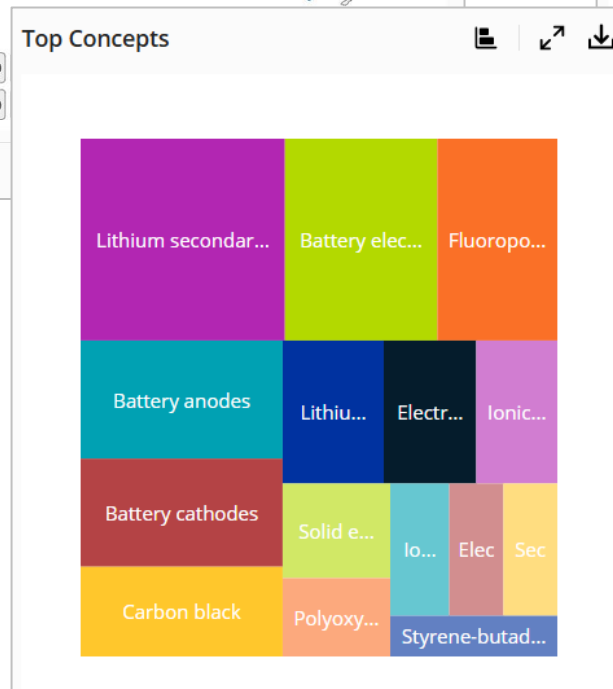
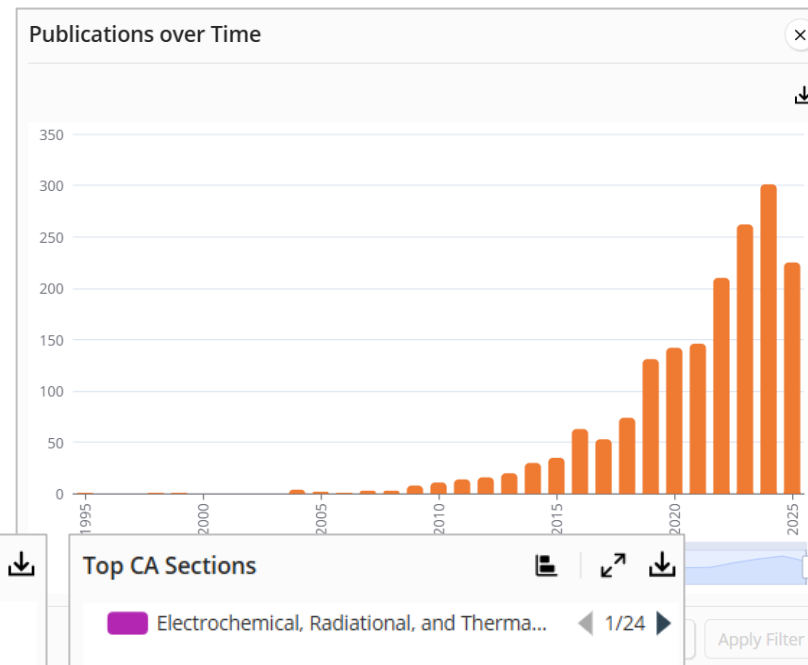
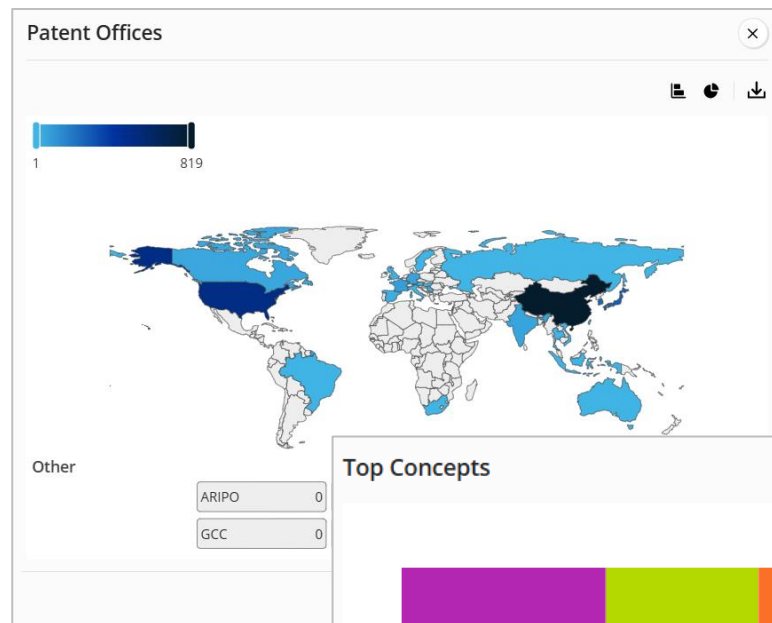
CA Section

CAS Content

Life Science Data

Formulation Purpose

Database



- 与筛选项联动的检索结果可视化分析
- 可自定义显示或隐藏

筛选工具 CA Section & Concept

CA Section

CAS标引的学科研究方向

By CountAlphanumeric

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)

☐ Heterocyclic Compounds (One Hetero Atom) (2)

☐ Phase Equilibria, Chemical Equilibria, and Solutions (2)

☐ Unit Operations and Processes (2)

☐ Cellulose Products (5)

☐ Gene Products (5)

☐ Gene Products (5)

☐ Physicochemical Properties (5)

☐ Surface Properties (5)

☐ Synthetic Polymers (5)

☐ Textiles (5)

☐ Water (5)

Concept

CAS标引的核心研究点

Top CountAlphanumericSearch

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)

☐ Organic solvents (83)

☐ Carbon fibers (83)

☐ Electrodes (83)

☐ Electric capacitor relationships (83)

☐ Molecular simulation (83)

☐ Current efficiency (83)

☐ Solid-state batteries (7)

☐ Cyclic voltammetry (7)

☐ Binding energy (7)

☐ Polymers (7)

☐ Density functional theory (7)

☐ Electric conductivity (7)

☐ Polyesters (7)

☐ Anodes (67)

☐ Fire-resistant materials (67)

☐ Lithium primary batteries (66)

☐ Diffusion (51)

☐ Carbon nanotubes (51)

☐ Nanoparticles (51)

Concept

精准定位感兴趣的核心研究点

Top CountAlphanumericSearch

Concept Name

nano*

支持使用通配符

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

☐ Nanoribbons (6)

☐ Nanorods (3)

☐ Nanoscale analysis (1)

☐ Nanoscale particle size (1)

☐ Nanosheets (21)

☐ Nanospheres (3)

☐ Nanostructured materials (4)

☐ Nanostructures (6)

☐ Nanotubes (8)

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

5 3 3 Citation Map

By: Jin, Lei ; Jang, Giseok ; Lim, Hyunmin ; Zhang, Wei ; Kim, Whangi ; Jang, Hohyoun

DOI: 10.1002/admi.202101958

Due to their high energy density and safety, polymer electrolytes are considered a promising alternative to the common 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_{Li^+} of 0.61 at RT. The PSEPEs also show a wide electrochem. window (>4.7 V vs Li/Li^+), and excellent compatibility with the lithium anode with an assembled $\text{LiFePO}_4/\text{PSEPEs}/\text{Li}$ 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](#)

CAS Concepts

核心研究点

- Amorphous structure
- Battery anodes
- Battery cathodes
- Battery electrolytes

In this Reference

- [CAS Concepts](#)
- [Substances](#)
- [Reactions](#)
- [Cited Documents](#)

导航速览

Substances

原文中重点研究的物质信息

171611-11-3

$\text{F}_2\text{HNO}_4\text{S}_2\text{Li}$
Lithium bis(fluorosulfonyl)imide

Role: Technical or Engineered Material Use, Uses

物质研究角色

31305-85-8

$(\text{C}_{16}\text{H}_{34}\text{O}_5\text{Si}_2)_x$
Disiloxane, 1,1,3,3-tetramethyl-1,3-bis[3-(2-oxiranylmethoxy)propyl]-, homopolym...

Role: Physical, Engineering or Chemical Process, Properties, Synthetic Preparation, Technical or Engineered Material Use, Process, Preparation, Uses

15933-59-2

$\text{C}_4\text{H}_{15}\text{NSi}_2$
Tetramethyldisilazane

Role: Reactant, Reactant or Reagent

Reactions

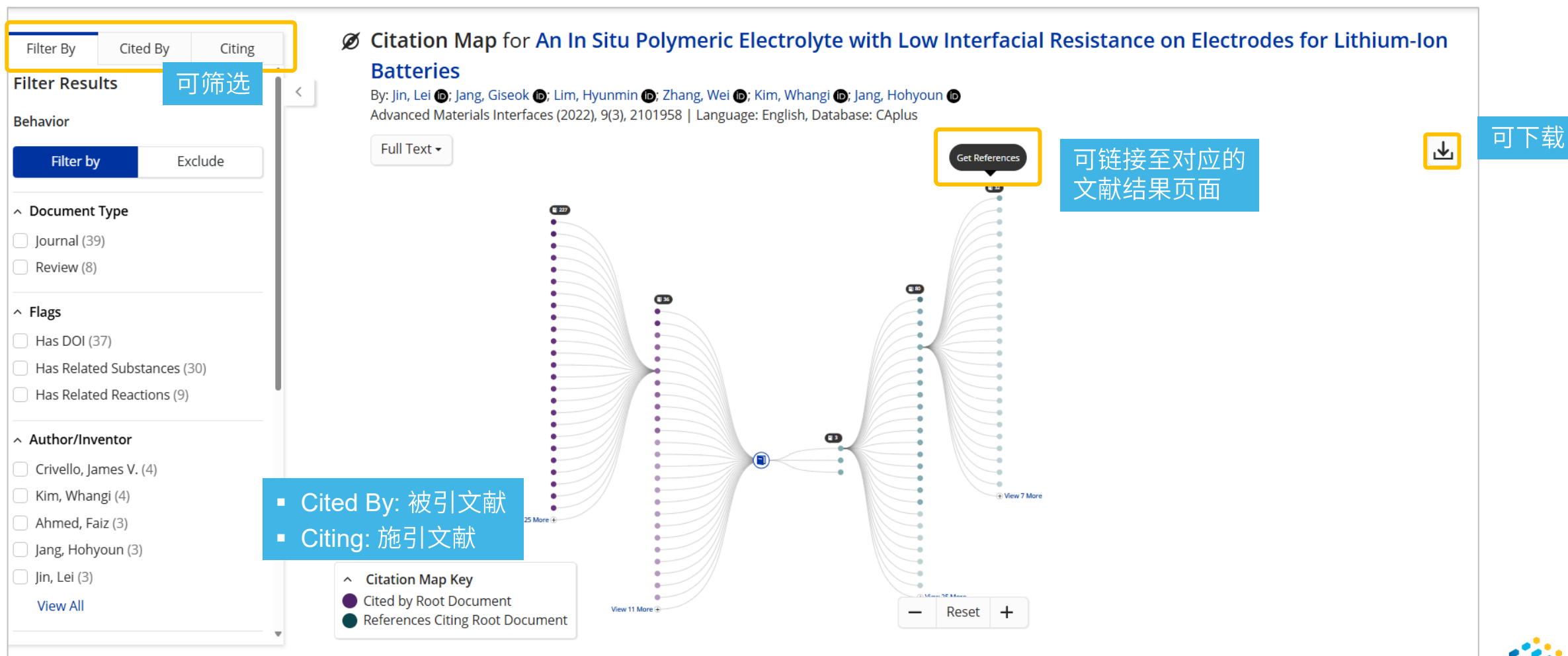
涉及的反应

31-614-CAS-31042382

31-614-CAS-31042381

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

权利要求

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 5×10^{-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.

Patent Family

专利家族

专利状态

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

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	IPC1	H01M 10/0569; H01M 10/0525
	CPCI	H01M 10/0569; H01M 10/0525; H01M 2300/0028
US12272791 B2	IPC1	H01M 4/62; H01M 10/0525; H01M 10/0569
	CPCI	H01M 10/0569; H01M 10/0525; H01M 2300/0028
WO2023028514 A1	IPC1	H01M 10/056; H01M 10/42; H01M 4/62; H01M 10/052; H01M 12/08

CAS PatentPak: 高效浏览专利

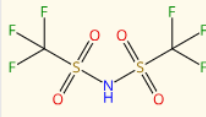
一键定位专利原文中的核心研究物质

CAS PatentPak

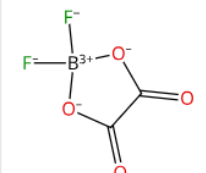
PAGE 26 / 32 ZOOM DOWNLOAD PDF PDF+

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⁺

Analyst Markup Locations (2)

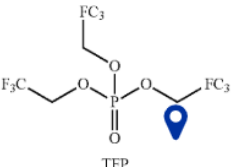
and a solid-state electrolyte-based separator composed of particles of $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ embedded in a poly(vinylidene fluoride)-hexafluoropropylene (PVDF-HFP) matrix (inorganic solid electrolyte/PVDF-HFP ratio=4/6). This cell was then injected with the reactive solution 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 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:

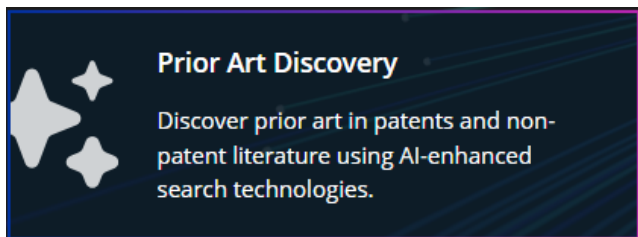


[0190] Solutions containing 1.5 M LiDFOB in VC and FEC, respectively, and 0.2 wt % AIBN (vs VC or FEC) were prepared. Then, TFP (TFPNC or TFP/FEC ratios being from 10/90 to 50/50) was added into the solution to form mixed electrolyte solutions. The electrolyte solutions were separately injected into 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., acaricides, insecticides, molluscicides, and nematocides), 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](#) [Search](#)


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

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

347 Results

Sort: Relevance ▾ View: Partial Abstract ▾

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

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 of waste polyurethane can produce polyether polyols with good closed-loop rec...

View All ▾

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 of waste polyurethane can produce polyether polyols with good closed-loop rec...

Key Findings:

- 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)
- 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)
- 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)
- 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

Good Afternoon, [redacted]

Proton nmr spectral data for C13H13Br

Draw

Advanced Search
Select a search type, and then add multiple search fields to build your query.

Substances References Clear All

Search by Substance Name, Functional Group, CAS Registry Number, or DOI.

Molecular Formula

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

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

Draw

Exam

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

Results for "PEG"

Substances

Showing 1 of 619 Results

View All Substances →

Reactions

Showing 1 of 69,931 Results

References

Showing 20 of 650,680 Results

Properties

Boiling Point: 227 °C

Density: 1.2 g/cm³

Temp: 20 °C; Press: 758.54 Torr

Substances search for "PEG"

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

Sort: Relevance View: Partial

1 25322-68-3

HO-[CH2-CH2-O]n-H

(C₂H₄O)_nH₂O

PEG

499K 69K 714

2 1370345-22-4

C1CO1

(C₂H₄O)_x

Oxirane, homopolymer

Preferred RN: 25322-68-3

0 0 0

3 934660-23-8

HO-[CH2-CH2-O]n-[CH2-CH2-O]m-[CH2-CH2-O]n-OH

(C₂H₄O)_n(C₂H₄O)_mC₂H₆O₂

Poly(oxy-1,2-ethanediyl), α,α'-1,2-ethanediylbis[ω-hydroxy-

Preferred RN: 25322-68-3

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. (Russian)

Unspecified

Laurex 9

8 58339-86-9

Image Not Available

Notes: PEG monoalkyl ether (Russian). Indexed also at Surfactants and PEG

Unspecified

9 854918-94-8

Image Not Available

Notes: A blend of PEG castor oil and PEG oleate (Rhodia)

Unspecified

- 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 **Na₂SO₄：H₂O₄S.2Na**

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

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

Filter Results

- Behavior
- Filter by
- Exclude
- Search Within Results
- Reaction Role
- Reference Role
- Commercial Availability
- Number of Components
- Element
- Aromatic Rings
- Substance Class
- Isotopes

14 Results

Sort: Relevance View: Partial

Result 1: 2304767-82-4

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

C.Hf.Nb.Ta.Ti.Zr
Components: 6
Hafnium niobium tantalum titanium zirconium carbide (Hf_{0.2}Nb_{0.2}Ta_{0.2}Ti_{0.2}Zr_{0.2}C)

Result 2: 1427190-21-3

Component	Ratio
Zr	x
Hf	x
C	x
Ti	x
Ta	x
Nb	x

C.Hf.Nb.Ta.Ti.Zr
Components: 6
Hafnium niobium tantalum titanium zirconium carbide

Result 3: 2649374-42-3

Component	Ratio
C	1
Zr	0-1
Hf	0-1
Ti	0-1
Ta	0-1
Nb	0-1

C.Hf.Nb.Ta.Ti.Zr
Components: 6
Hafnium niobium tantalum titanium zirconium carbide ((Hf,Nb,Ta,Ti,Zr)C)

分子式检索： 高效检索聚合物或无机化合物

$(C_2H_4O)_n C_4H_8O$

- $(C_2H_4O)_n C_4H_8O$: 括号中是重复结构单元，括号外为n
- $(C_5H_6O_4.C_4H_6O_2.C_3H_4O_2)_x$: 括号中是单体，括号外为x

$(C_5H_6O_4.C_4H_6O_2.C_3H_4O_2)_x$

Substances search for " $(C_2H_4O)_n C_4H_8O$ "

Filter Results

Behavior

Filter by Exclude

Search Within Results

Reaction Role

Reference Role

Commercial Availability

Number of Components

13 Results

Sort: Relevance View: Partial

31497-33-3

$(C_2H_4O)_n C_4H_8O$
Poly(oxy-1,2-ethanediyl), α -(2-methyl-2-propen-1-yl)- ω -hydroxy-

27252-80-8

$(C_2H_4O)_n C_4H_8O$
Polyethylene glycol allyl methyl ether

85600-94-8

$(C_2H_4O)_n C_4H_8O$
Poly(oxy-1,2-ethanediyl), α -3-buten-1-yl- ω -hydroxy-

Substances search for " $(C_5H_6O_4.C_4H_6O_2.C_3H_4O_2)_x$ "

Filter Results

Behavior

Filter by Exclude

Search Within Results

Reaction Role

Reference Role

Commercial Availability

Number of Components

Molecular Weight

Stereochemistry

Element

Functional Group

Aromatic Rings

Substance Class

6 Results

Sort: Relevance View: Partial

97384-95-7

$(C_5H_6O_4.C_4H_6O_2.C_3H_4O_2)_x$
Components: 3
Butanedioic acid, 2-methylene-, polymer with 2-methyl-2-propenoic acid and 2-pro...

63899-49-0

$(C_5H_6O_4.C_4H_6O_2.C_3H_4O_2)_x$
Components: 3
Butanedioic acid, 2-methylene-, polymer with ethenyl acetate and 2-propenoic aci...

56280-96-7

$(C_5H_6O_4.C_4H_6O_2.C_3H_4O_2)_x$
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

Substances

References

Clear All

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

Advanced Search

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

Draw

-

Molecular Formula

Enter a molecular formula.

Examples: C6H6 | (C8H8)x | C22H26CuN2O5.C2H3N

Search

+ 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

Proton NMR

Carbon-13 NMR

Nitrogen-15 NMR

Fluorine-19 NMR

Phosphorus-31 NMR

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： ^1H , ^{13}C , ^{15}N , ^{19}F , ^{31}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 References Clear All

Search by Substance Name, Functional Group, CAS RN, Patent Number, PubMed

-

Molecular Weight

220 to 280

Predicted values only.

AND

pKa

1.3 to 1.8

Predicted values only.

AND

Carbon-13 NMR

114 to 171, 96, 11.5

Allowance of ± 2 ppm.

+ Add Advanced Search Field

Substances Advanced search for 3 fields

View Related Results

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

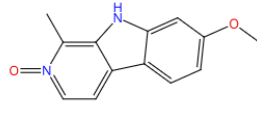
Filtering: Life Science Data: 3 Selected X

13 Results

Sort: Relevance View: Partial

1

57498-78-9

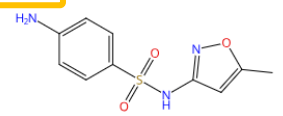


C13H12N2O2
9H-Pyrido[3,4-b]indole, 7-methoxy-1-methyl-, 2-oxide

16 11 2

2

723-46-6

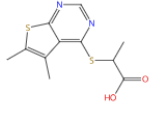


C10H11N3O3S
Sulfamethoxazole

31K 1,090 116

3

442571-27-9

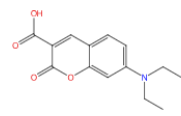


C11H12N2O2S2
2-[(5,6-Dimethylthieno[2,3-d]pyrimidin-4-yl)thio]propionic acid

2 4 31

4

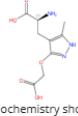
50995-74-9



C14H15NO4
7-Diethylaminocoumarin-3-carboxylic acid

5

1628224-40-7

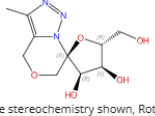


C9H13N3O5
(α S)- α -Amino-3-(carboxymethoxy)-5-methyl-1H-pyrazole-4-propanoic acid

Absolute stereochemistry shown, Rotation (-)

6

1631737-39-7



C10H15N3O5
(2R,3R,4S,5R)-4,5-Dihydro-5-(hydroxymethyl)-3'-methylspiro[furan-2(3H),7'(6'H)-]pyran

Absolute stereochemistry shown, Rotation (-)

- 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](#)

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

[View All Patents](#)

Chemical Structure: Cc1cc(NC(=O)Nc2ccc(N)cc2)nn1

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**

Additional Details

Experimental Spectra

¹ H NMR	¹³ C NMR	Hetero NMR
View Proton NMR Spectrum (Image Available)		
View Proton NMR Spectrum (Image Available)		
View Proton NMR Spectrum (Image Available)		
View Proton NMR Spectrum (Image Available)		
View Proton NMR Spectrum (Image Available)		

723-46-6

Chemical Structure: Cc1cc(NC(=O)Nc2ccc(N)cc2)nn1

C₁₀H₁₁N₃O₃S

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

1H NMR Spectrum:

[Reset](#)

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

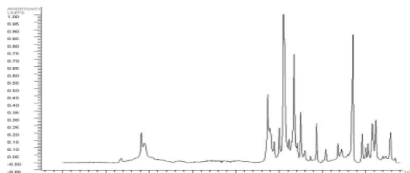
Showing 1 of 1 Result

View All Spectra →

521-31-3

Luminol

Viewing 1 of 1



−

Reset

+

Results for "the proton spectra of ibuprofen"

[All](#) [Substances](#) [Reactions](#) [References](#) [Suppliers](#) [Patent Markush](#)

Spectra

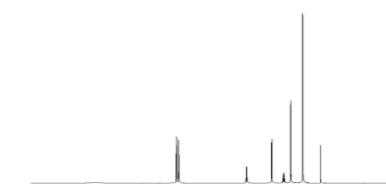
Showing 5 of 28 Results

View All Spectra →

15687-27-1

Ibuprofen

Viewing 1 of 5



−

Reset

+

Experimental

View Spectra Details

Proton NMR Spectrum

Conditions

Working Frequency

300 MHz

Solvent

Chloroform-d (865-49-6)

Results for "What are the hazards of bisphenol A"

[All](#) [Substances](#) [Reactions](#) [References](#) [Suppliers](#) [Patent Markush](#)


GHS Hazard Table

Showing 5 of 62 Results

View in Detail Page →

Regulatory List

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



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 Substances 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

View in Detail Page →

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

Results for "the logP of olaparib"

All Substances 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

View in Detail Page →

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

Results for "pKb of alanine"

All Substances 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

View in Detail Page →

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

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

[]₁₋₄

重复工具

取代位置可变

环锁定工具

原子锁定工具

CAS Draw

Select Search Type

SubstancesReferencesReactionsSuppliersPatent MarkushAll

Enter a CAS Registry Number, SMILES, or InChI.

Draw or change atoms or bonds.

Molecular Formula:

C

Zoom: 100%

CancelOK

直接选择检索类型

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 1,095 Results

Structure Match

- 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

Sort: Number of References: Descending

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

R1

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

2170153-32-7

C30H29BrMnNO2P2
(OC-6-42)-Bromodicarbonyl[2-(diphenylphosphino-κP)-N-[2-(diphenylphosphino-κP)et...]

62 1,297 0

1929551-26-7

C30H53BrMnNO2P2
Stereoisomer of bromodicarbonyl[2-(dicyclohexylphosphino-κP)-N-[2-(dicyclohexylp...

27 54 0

53687-39-1

C42H43CoNP3
Cobalt, [2-(diphenylphosphino)-N,N-bis[2-(diphenylphosphino)ethyl]ethanamine-N,P...

4

1418299-84-9

C32H63CoNP2Si
(SP-4-1)-[2-(Dicyclohexylphosphino-κP)-N-[2-(dicyclohexylphosphino-κP)ethyl]etha...

5

1428439-31-9

C32H64CoNP2Si.C32H12BF24
Components: 2

6

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

Structure Match

As Drawn (1)

Substructure (36K)

Similarity (594K)

Analyze Structure Precision

Behavior

Filter by

Exclude

Search Within Results

Reaction Role

36,710 Results

Sort: Number of References: Descending

View: Partial

1 1415607-60-1

2 1241891-64-4

3 1980037-96-4

可以选取最多六个性质在物质结果上显示

Substance Properties Display

Boiling Point X Density X Molecular Weight X pKa X

4 of 6 properties selected

Reset to

Acoustic

Sound Velocity

Biological

Bioconcentration Factor

Median Lethal Dose

Chemical

Electric Dipole Moment

Ka

Kb

Koc

logD

InoP

Density

Density

Molar Volume

Electrical

Dielectric Constant

Electric Conductance

Electric Conductivity

Electric Resistance

Electric Resistivity

Flow and Diffusion

Viscosity

Lininski

Optical and Scattering

Optical Rotatory Power

Refractive Index

Structure Related

Polar Surface Area

Thermal

Autoignition Temperature

Combustion Enthalpy

Critical Point

Enthalpy of Vaporization

Entropy

View All Settings

Cancel

Save

Substances search for drawn structure

View Related Results ▾

Filter Results

Structure Match

As Drawn (1)

Substructure (36K)

Similarity (594K)

Analyze Structure Precision

Behavior

Filter by

Exclude

Search Within Results

Reaction Role

36,710 Results

Sort: Number of References: Descending

View: Full

1 1415607-60-1

C₃₃H₁₉N₃

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 ³	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)

[View All](#)

聚合物类别

Polymer Class

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

[View All](#)

Aromatic Rings

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

[View All](#)

芳环数量

Functional Group

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

[View All](#)

官能团

LogP

No Min to No Max [Apply](#)

Available Range: -25.829 to 87.223

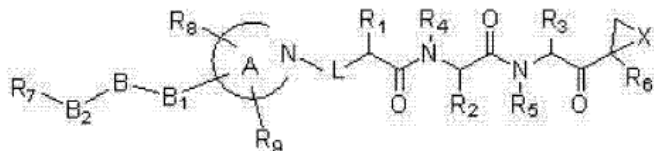
CAS Markush检索，助力结构查新

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

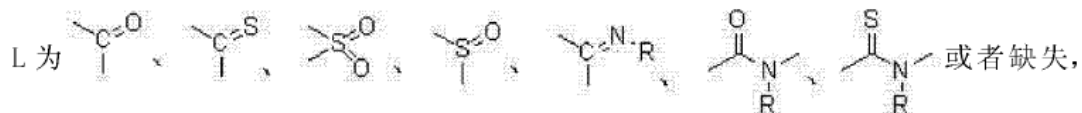
其中：

R_1, R_2, R_3 各自独立选自 H、 C_{1-6} 烷基 -D、卤代的 C_{1-6} 烷基 -D、 C_{1-6} 羟基烷基、 C_{1-6} 巯基烷基、 C_{1-6} 烷氧基烷基、芳基、芳烷基、杂芳基或杂芳烷基；其中：D 为 N(R_a) (R_b) 或缺失， R_a, R_b 各自独立选自 H、OH、 C_{1-6} 烷基、卤代的 C_{1-6} 烷基或 N 末端保护基；

R_4, R_5 各自独立选自 H、OH、 C_{1-6} 烷基、卤代的 C_{1-6} 烷基或芳烷基；

R_6 选自 H、 C_{1-6} 烷基，卤代的 C_{1-6} 烷基， C_{1-6} 羟基烷基， C_{1-6} 烷氧基，卤代的 C_{1-6} 烷氧基， $C(O)O-C_{1-6}$ 烷基， $C(O)NH-C_{1-6}$ 烷基，芳烷基；

X 为 O、S、NH、N- C_{1-6} 烷基或 N- 卤代的 C_{1-6} 烷基；



其中 R 选自 H、 C_{1-6} 烷基或卤代的 C_{1-6} 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_8, R_9 和 B_1 基团取代；

R_8, R_9 分别独立选自 H、OH、 C_{1-6} 烷基， C_{1-6} 烷氧基， C_{1-6} 羟基烷基， C_{1-6} 巯基烷基， C_{1-6} 烷

具体物质[Specific Substance]

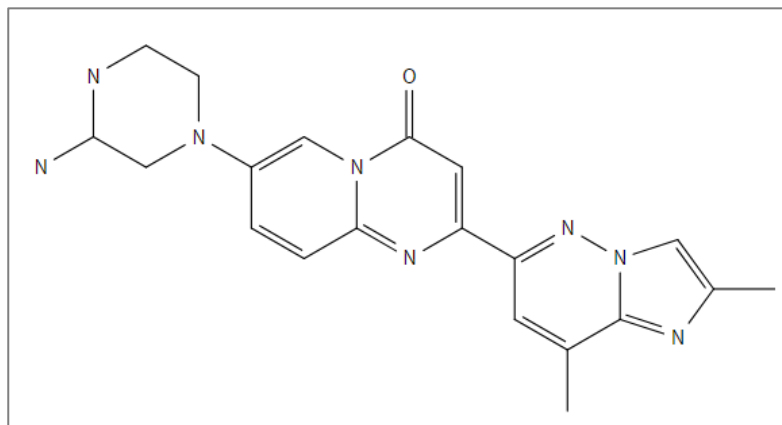
- 以具体化学结构陈述的特定物质，会被分配CAS 登记号

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 × Number of Components: 1 × Clear All Filters

288 Results

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)

Results:

- 1825352-54-2: 2-(2,8-Dimethylimidazo[1,2-b]pyridazin-6-yl)-7-[(3R)-3-methyl-1-piperazinyl]-4H-...
C₂₁H₂₃N₇O
Absolute stereochemistry shown
5 25 1
- 1825352-53-1: 2-(2,8-Dimethylimidazo[1,2-b]pyridazin-6-yl)-7-[(3S)-3-methyl-1-piperazinyl]-4H-...
C₂₁H₂₃N₇O
Absolute stereochemistry shown
5 25 1
- 1825352-79-1: 9-Methyl-2-(2-methylimidazo[1,2-b]pyridazin-6-yl)-7-[(3R)-3-methyl-1-piperazinyl]-...
C₂₁H₂₃N₇O
Absolute stereochemistry shown
5 19 1
- 1825352-78-0: 9-Methyl-2-(2-methylimidazo[1,2-b]pyridazin-6-yl)-7-[(3S)-3-methyl-1-piperazinyl]-...
C₂₁H₂₃N₇O
Absolute stereochemistry shown
5 19 0
- 1825352-52-0: rel-2-(2,8-Dimethylimidazo[1,2-b]pyridazin-6-yl)-7-[(3R,5S)-3,5-dimethyl-1-piperazinyl]-...
C₂₂H₂₅N₇O
Relative stereochemistry shown
4 25 1
- 2097817-67-7: 2-(2,8-Dimethylimidazo[1,2-b]pyridazin-6-yl)-7-[(3S,5S)-3,5-dimethyl-1-piperazinyl]-...
C₂₂H₂₅N₇O
Absolute stereochemistry shown
3 16 1

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 ▾

1 Result

1

Markush详情页

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

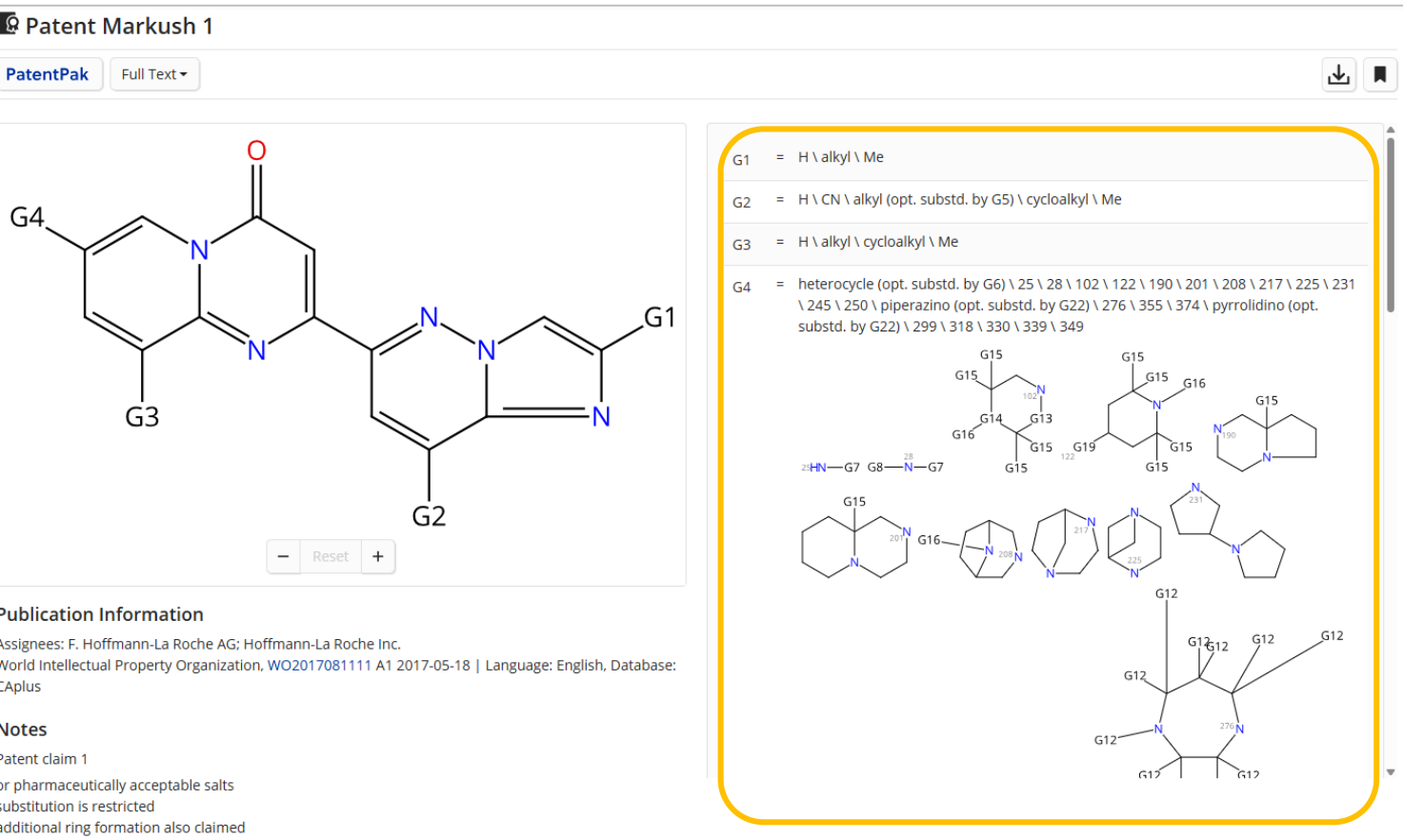
Patent claim 1

PatentPak ▾ Full Text ▾

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

629: opt. substd.

直观的 Markush 详情页



Publication Information

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

Notes

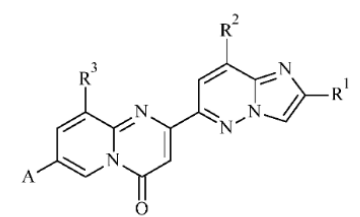
Patent claim 1
or pharmaceutically acceptable salts
substitution is restricted
additional ring formation also claimed

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)



(I)

wherein

5 **R¹** is hydrogen or C₁₋₇-alkyl;

R² is hydrogen, cyano, C₁₋₇-alkyl, C₁₋₇-haloalkyl or C₃₋₈-cycloalkyl;

R³ is hydrogen, C₁₋₇-alkyl, or C₃₋₈-cycloalkyl;

A is N-heterocycloalkyl or NR¹²R¹³, wherein N-heterocycloalkyl comprises 1 or 2 nitrogen ring atoms and is optionally substituted with 1, 2, 3 or 4 substituents selected from R¹⁴;

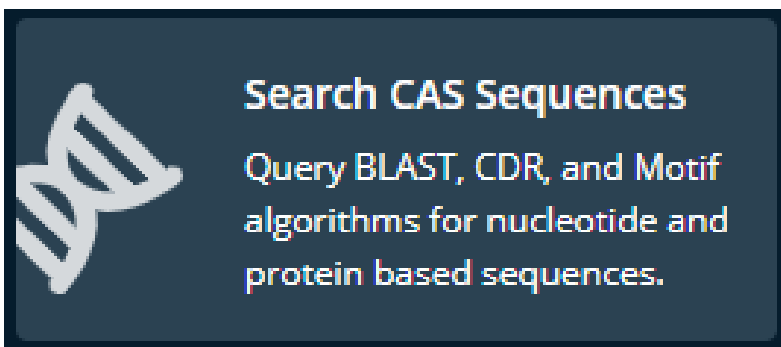
10 **R¹²** is heterocycloalkyl comprising 1 nitrogen ring atom, wherein heterocycloalkyl is optionally substituted with 1, 2, 3 or 4 substituents selected from R¹⁴;

R¹³ is hydrogen, C₁₋₇-alkyl or C₃₋₈-cycloalkyl;

15 **R¹⁴** is independently selected from hydrogen, C₁₋₇-alkyl, amino, amino-C₁₋₇-alkyl, C₃₋₈-cycloalkyl and heterocycloalkyl or two R¹⁴ together form C₁₋₇-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

Reactions search for "Suzuki coupling reaction"

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

1,470 Results

Scheme 1 (5 Reactions)

Suppliers (96)

31-177-CAS-1895561 Steps: 1 Yield: 100%

1.1 Reagents: [Palladate\(6-\)](#), [dichlorobis\(3,3'-\(phosphino\)ferrocene\)dichloropalladium](#) (215K)

Catalysts: [Palladate\(6-\)](#), [dichlorobis\(3,3'-\(phosphino\)ferrocene\)dichloropalladium](#) (215K)

Solvents: [Glycerol](#); 4 h, 80 °C

Experimental Protocols

31-177-CAS-17315362 Steps: 1 Yield: 99%

1.1 Reagents: [Ethylene glycol](#), [Potassium acetate](#)

Catalysts: [Palladium](#)

Solvents: [Dimethyl sulf.](#); 2 h, 120 °C

CAS SciFinder

Suzuki coupling reaction

人名反应智能识别

Reactions search for "Suzuki coupling reaction"

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

Group: By Scheme Sort: Relevance View: Expanded

Scheme 1 (1 Reaction) Steps: 1 Yield: 100%

Supplier (1)

Suppliers (51)

31-179-CAS-11123183 Steps: 1 Yield: 100%

1.1 Reagents: [Potassium carbonate](#)

Catalysts: [Dichloro\[1,1'-bis\(diphenylphosphino\)ferrocene\]palladium](#) (215K)

Solvents: [1,4-Dioxane](#), [Water](#); 60 - 90 min, 120 - 140 °C

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) Steps: 1 Yield: 100%

Suppliers (4)

Suppliers (101)

Suppliers (3)

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

155,676 Results Group: By Scheme Sort: Relevance View: Expanded

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

Scheme 1 (1 Reaction) Steps: 1 Yield: 100%



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

Supplier (1)

31-113-CAS-5796848 Steps: 1 Yield: 100%

1.1 Reagents: [Ammonium formate](#)
Catalysts: [Palladium](#)
Solvents: [Isopropanol](#), [Tetrahydrofuran](#), [Water](#); rt


1.2 Reagents: [Diphenyl ether](#); rt

[Experimental Protocols](#)

[Full Text](#)

[Collapse Scheme](#)

Scheme 2 (1 Reaction) Steps: 1 Yield: 100%



Suppliers (51) Suppliers (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"

🔍 All

📄 Substances

🔬 Reactions

📖 References

🛒 Suppliers

📜 Patent Markush

View Related Results ▾

114,093 Results

Group: By Scheme ▾ Sort: Relevance ▾ View: Expanded ▾

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)

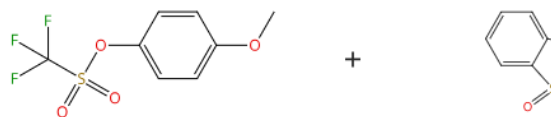
No Scale Provided (33K)

Experimental Protocols

Reaction Type

Stereochemistry

Scheme 1 (1 Reaction)



Suppliers (58)

31-614-CAS-27980971

Steps: 1 Yield: 100%

1.1 Reagents: [Sodium carbonate](#), [Triethyls...](#)


Catalysts: [Palladium diac...](#), [1,1-Bis\(diphenylphosphino\)...](#)

Solvents: [Acetonitrile](#); 16 h, 80 °C

Experimental Protocols

Collapse Scheme ▴

Scheme 2 (1 Reaction)



Reactions search for "Reduction of Ketones to Alcohols catalyzed by Carbonyl reductase"

🔍 All

📄 Substances

🔬 Reactions

📖 References

View Related Results ▾

335,050 Results

Group: By Scheme ▾ Sort: Relevance ▾ View: Expanded ▾

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

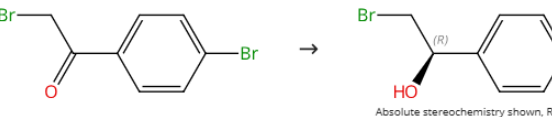
Stereochemistry

Reagent

Catalyst

Scheme 1 (12 Reactions)

Steps: 1 Yield: 97-100% ***



Suppliers (86)

Suppliers (36)

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

Full Text ▾

31-513-CAS-10291418

Steps: 1 Yield: 99% ***

1.1 Solvents: [Ethanol](#); 18 h, 30 °C

Full Text ▾

One-pot chemo-enzymatic synthesis of chiral α-halogenated aryl alcohols

By: Yang, Jingwen; et al

Youji Huaxue (2018), 38(7), 1811-1816

Chiral pharmaceutical intermediates 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.

49

© 2025 American Chemical Society. All rights reserved.

CAS
A division of the
American Chemical Society

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)

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)

Structure 1: Clc1ccc(cc1)C(=O)Cc2ccccc2 → Nc1ccc(cc1)Cc2ccccc2

Suppliers (79) Suppliers (13)

Group: By Scheme Sort: Relevance View: Expanded

By Scheme

By Document

By Transformation

Steps: 1 Yield: 85%

Relevance

Publication Date: Newest

Publication Date: Oldest

Yield

Number of Steps: Ascending

Number of Steps: Descending

Structure 2: Clc1ccc(cc1)C(=O)Cc2ccccc2 → Nc1ccc(cc1)Cc2ccccc2

Suppliers (43) Suppliers (3)

31-614-CAS-28968228 Steps: 1 Yield: 76%

1.1 Reagents: [O-Methylhydroxylamine hydrochloride](#)
Solvents: [Pyridine](#); rt; 1 h, 50 °C

1.2 Reagents: [\(7-4\)-Trihydro\(tetrahydrofuran\)](#)
Solvents: [Tetrahydrofuran](#); rt; 3 h, reflux; reflux → 0 °C

1.3 Reagents: [Sodium hydroxide](#)
Solvents: [Water](#); overnight, reflux; reflux → rt

Experimental Protocols

Preparation of heterocyclic adrenergic agents
Assignee: Allergan, Inc.
World Intellectual Property Organization

PatentPak

Filter Results <

8,161 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

1

Reductive Alkylation of Ammonia or Amines
View 121 Related Reactions

R-C(=O)-R + R^1-NH-R^1 -> R-CH(R)-N(R^1)-R^1

2

Formation of N/O/S Heterocycles
View 54 Related Reactions

Y'-C(=Y)-R + R^1-C(=Y)-Y' -> Y'-C(R)-N(R^1)-Y'

聚焦反应类型

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

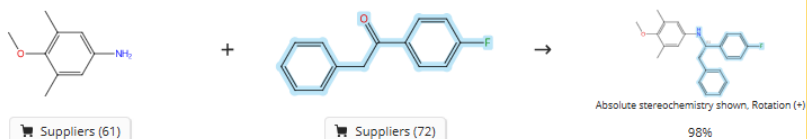
Experimental Protocols

☒ Synthetic Methods (449)

☐ Experimental Procedure (5,678)

CAS Reaction Number: 31-614-CAS-41195127

Get Similar Reactions



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

Procedure

1. Add aniline (0.2 mmol), ketone (0.1 mmol), $\text{Ti}(\text{OiPr})_4$ (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 $\text{Ni}(\text{NTf}_2)_2$ (3.1 mg, 0.005 mmol, 5 mol%), (R)-Ph-BPE (3.1 mg, 0.006 mmol, 6 mol%) and GC standard $n\text{-C}_{12}\text{H}_{26}$ (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.

清晰的实验操作

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_3): 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, $J = 7.9, 6.0$ Hz, 1H), 3.90 (br s, 1H), 3.61 (s, 3H), 3.07 (dd, $J = 13.8, 6.0$ Hz, 1H), 2.99 (dd, $J = 13.8, 7.9$ Hz, 1H), 2.13 (s, 6H)
Carbon-13 NMR	(100 MHz, CDCl_3): δ 162.0 (d, $J_{\text{C-F}} = 243.0$ Hz), 149.2, 143.3, 139.5 (d, $J_{\text{C-F}} = 3.0$ Hz), 137.7, 131.3, 129.4, 128.7, 128.1 (d, $J_{\text{C-F}} = 8.0$ Hz), 126.9, 115.5 (d, $J_{\text{C-F}} = 21.0$ Hz), 113.8, 60.0, 59.2, 45.5, 16.4
Fluorine-19 NMR	(376.6 MHz, CDCl_3): δ -116.0
Optical Rotatory Power	$[\alpha]_D^{25} = +5.6^\circ$ ($c = 1.0$, CHCl_3)
Enantiomeric Excess	90%
HRMS	(ESI ⁺): Calcd for $\text{C}_{23}\text{H}_{25}\text{FNO}$ $[\text{M}+\text{H}]^+$: 350.1915; found: 350.1916
State	yellow oil

产物表征

Reaction Notes

stereoselective (ee = 90%)

反应注释

获取相似反应，拓展实验设计思路

Scheme 4 (15 Reactions) Steps: 1 Yield: 60% ...

Absolute stereochemistry shown Absolute stereochemistry shown, Rotation (-)

Suppliers (120) Suppliers (75)

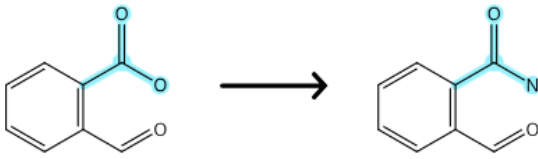
31-614-CAS-42267257 Steps: 1 ... Method and system for the

1.1 Solvents: [Methanol](#), [Water](#); 2.4 MPa, 179 °C; 183.8 °C

Get Similar Reactions

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

Reactions similar to 31-614-CAS-42267257

References

Filter 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

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% ...

1.1 Reagents: [Hexamethyldisilazane](#)
Solvents: [Acetonitrile](#); 40 h, rt → reflux
1.2 Solvents: [Methanol](#); 0 °C; 30 min, rt

Pyrrolidinone urea fpr2 agonists treating atherosclerosis
Assignee: Bristol-Myers Squibb Company
World Intellectual Property Organization, WO2024220482 A1 2024-10-24

PatentPak Full Text

31-367-CAS-21603883 Steps: 1 Yield: 78% ...

1.1 Reagents: [Hexamethyldisilazane](#)
Solvents: [Acetonitrile](#); 40 h, rt → reflux
1.2 Solvents: [Methanol](#); 0 °C; 30 min, rt

Preparation of phenylpyrrolidinone formyl peptide 2 receptor agonists
Assignee: Bristol-Myers Squibb Company
United States, US20190270704 A1 2019-09-05

PatentPak Full Text

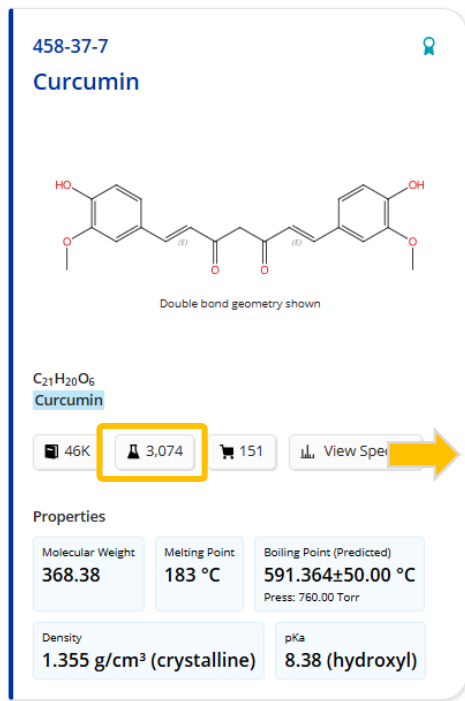
31-367-CAS-19142997 Steps: 1 ...

1.1 Reagents: [Hexamethyldisilazane](#)
Solvents: [Acetonitrile](#); rt → reflux; 48 h, reflux

Preparation of sulfonamides compound as cccDNA inhibitor for treating hepatitis B
Assignees: Chia Tai Tianqing Pharmaceutical Group Co., Ltd.; 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

Behavior

Filter by Exclude

Search Within Results

Substance Role

- ☒ Product (341)
- ☐ Reactant (2,661)
- ☐ Reagent (19)
- ☐ Catalyst (63)

Yield

Number of Steps

Non-Participating Functional Groups

Reaction Mapping

Reaction Scale

- ☐ Milligram (7)
- ☐ Gram (12)
- ☐ No Scale Provided (322)

Experimental Protocols

Reaction Type

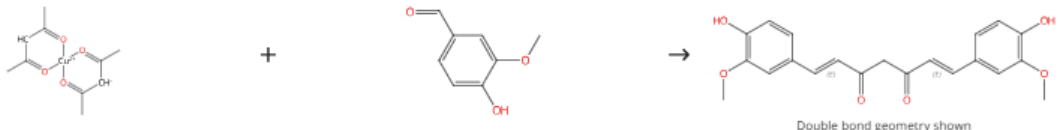
Stereochemistry

Filtering: Substance Role: Product X

341 Results

Group: By Scheme Sort: Relevance View: Expanded

Scheme 1 (1 Reaction) Steps: 1 Yield: 94%



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

PatentPak Full Text

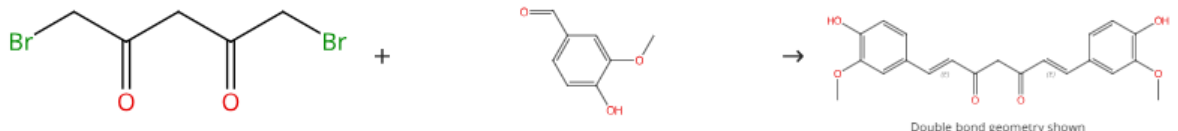
1.1 Reagents: Trimethyl borate
Catalysts: Butylamine
Solvents: Dimethylformamide; 50 min, 60 - 70 °C; 1.5 h, 60 - 70 °C

1.2 Reagents: Sulfuric...
Solvents: Methanol; neutralized

1.3 Reagents: Hydrochloric...
Solvents: Methanol, Water; 2 h, 60 - 70 °C

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

联用检索提高检索效率

Friedel-Crafts acylation

Featured Search

- Prior Art Discovery**
Discover prior art in patents and non-patent literature using AI-enhanced search technologies.
- Patent Markush**
Search Patent Markush by structure and view associated references.
- Advanced Search**
Select data fields and search operators to create a focused query.

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

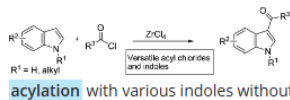
1,364 Results

1

ZrCl₄-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: CAlus 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 aroyl, heteroaryl, alkenoyl, and alkanoyl chlorides un 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: CAlus and MEDLINE

21 Results

View: Expanded ▾

Scheme 1 (1 Reaction) Steps: 1 Yield: 82% ***

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

31-091-CAS-3260537 Steps: 1 Yield: 82% ***

1.1 Catalysts: Zirconium chloride
Solvents: 1,2-Dichloro...; 0 °C; 0 °C → 30 °C; 3.5 h, 30 °C
1.2 Reagents: Water
Experimental Protocols

ZrCl₄-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) Steps: 1 Yield: 78% ***

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

31-091-CAS-6828122 Steps: 1 Yield: 78% ***

1.1 Catalysts: Zirconium chloride
Solvents: 1,2-Dichloro...; 0 °C; 0 °C → 30 °C; 4 h, 30 °C
1.2 Reagents: Water
Experimental Protocols

ZrCl₄-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) Steps: 1 Yield: 77% ***

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

31-091-CAS-12409550 Steps: 1 Yield: 77% ***

ZrCl₄-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

Retrosynthetic Analysis

Make reaction plans with conditions, yields, catalysts, and experimental procedures.



Retrosynthetic Analysis
Draw or import a structure.

Enter a CAS Registry Number, SMILES, or InChI.

Select and draw structures with templates.

Molecular Formula: C₁₉H₁₉BrN₄O₅ (463.29)

Zoom: 80%

Cancel Start Retrosynthetic Analysis

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](#)

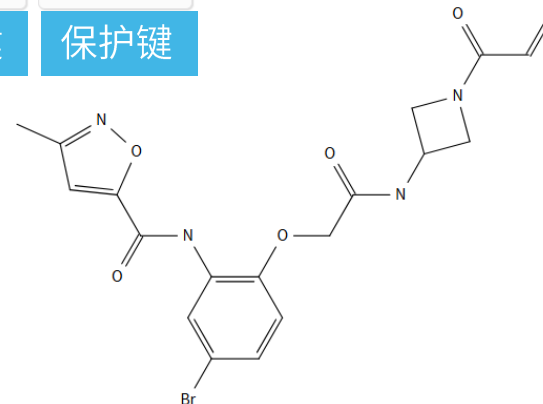
Break Bond

Protect Bond

[Clear All Bond Selections](#)

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](#) [Apply](#)

起始原料价格

可自由拖动、缩放的路线图

已知反应

预测反应

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

起始原料价格

步骤纵览

Viewing All Steps

A ⇒ B + C	Avg Yield: 70%
1.1 Reagents : 1-Ethyl-3-(3'-dimethylaminopropyl)carbodiimide , 1-Hydroxybenzotriazole , Diisopropylethylamine	
Solvents : Dichloromethane ; 16 h, rt	
Evidence Alternative Steps Exclude	
B ⇒ D + E	Avg Yield: 63%
1.1 Reagents : Ethyl acetate , Diisopropylethylamine	
Solvents : Dichloromethane ; rt	
Evidence Alternative Steps Exclude	
C ⇒ O	Max Yield: 50%
No Evidence Summary	
Alternative Steps Exclude	
D ⇒ F	Max Yield: 50%

Help Contact Us Legal

CAS
A division of the American Chemical Society

查看关注步骤的设计依据、可替换路线

57

© 2025 American Chemical Society. All rights reserved.

了解其他反应路线，拓宽实验设计思路

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

Replace Step

Close

31-367-CAS-9390816

1.1 Reagents : Diisopropylethylamine, Phosphorus(1+), bromotri-1-pyrrolidinyl-, (T-4)-
Solvents : Dimethylformamide;

Get Experimental Protocols

Help Contact Us Legal

58

© 2025 American Chemical Society. All rights reserved.

CAS
A division of the
American Chemical Society

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 displays the CAS SciFinder search results for "ciprofloxacin". The interface is divided into several sections:

- Top Navigation:** CAS SciFinder logo, search bar with "ciprofloxacin", and tabs for All, Substances, Reactions, References, Suppliers, and Patent Markush.
- Filter Results (Left Sidebar):** Includes "Analyze Results" button, "Behavior" section with "Filter by" and "Exclude" buttons, and a "Search Within Results" section with various filters. The "CAS Content" section is highlighted, showing "Analytical Methods (3,595)" selected.
- Filtering:** A button labeled "CAS Content: Analytical Methods" is shown, indicating the current filter.
- Results List:** Displays two results. The first result, "Enzymatic rotating biosensor for ciprofloxacin determination", is highlighted. The second result, "High-performance liquid chromatographic determination of ciprofloxacin in plasma samples", is also highlighted. A yellow arrow points from the "Analytical Methods" link in the second result to the "Analytical Methods" section in the detailed view.
- Detailed View (Right Panel):** Shows the full text of the article "High-performance liquid chromatographic determination of ciprofloxacin in plasma samples". It includes the title, authors (Vybirlova, Z.; Nobilis, M.; Zoulova, J.; Kvetina, J.; Petr, P.), DOI (10.1016/j.jpba.2004.09.034), and abstract. The "Analytical Methods" section is highlighted, showing the method title "Analysis of Ciprofloxacin in Blood plasma by Solid phase extraction". The "Substances" section is also highlighted, showing the chemical structure of ciprofloxacin (C₁₇H₁₈FN₃O₃) and its role as an analyte, pharmacokinetic, therapeutic use, analytical study, biological study, and 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

1-101-CAS-44938

Method Category

Active Pharmaceutical Ingredient and Metabolite Analysis

Technique

UV-visible spectroscopy; HPLC

Analyte

Ciprofloxacin

Matrix

Blood plasma

Material

Silanized glass tube
Eppendorf tube
Glass syringe
ACE 5 C18 column (250 mm × 4.6 mm, 5 μm)
[View All](#)

Reagent

Acetonitrile
Methanol
Phosphate-buffered saline solutions

Biological Reagent

-

Source

JOURNAL

A simple HPLC-UV method for the determination of ciprofloxacin in human plasma

Vella, Janis; Busuttill, Francesca; Bartolo, Nicolette Sammut; Sammut, Carmel; Ferrito, Victor; Serracino-Inglott, Anthony; Azzopardi, Lilian M.; LaFerla, Godfrey

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

[View Abstract](#) [Full Text](#)

Equipment Used

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

Conditions

Instrument

column: reversed phase ACE 5 C18 column (250 mm × 4.6 mm, 5 μm); guard column: Agilent Pursuit 5 C18 Meta guard column (10 mm × 4.6 mm, 5 μm); injection sample loop volume: 50 μL; gradient: isocratic
detection wavelength: 277 nm

Validation

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

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 μL of plasma with ciprofloxacin to 1.5 mL Eppendorf tubes.
2. Add 30 μL of internal standard (IS, sulfadimidine sodium) working solution in water (100 μg/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 μL 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 μL 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

63

© 2025 American Chemical Society. All rights reserved.

CAS

A division of the American Chemical Society

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 displays the CAS Analytical Methods website. The top navigation bar includes the CAS logo, 'Analytical Methods', and links for 'Support' and 'Saved'. A search bar is present with the placeholder text 'Search for keywords, matrices or analyte.' Below the search bar, there are two main sections: 'Explore Methods' and 'Advanced Search'. The 'Explore Methods' section is highlighted with a yellow box and an arrow pointing to it. It features a list of categories on the left, including 'Agricultural Applications / Analysis', 'Bioassays', 'Biomolecule Isolation', 'Environmental Analysis', 'Food Analysis', 'Fuels / Geology / Biofuels', 'Historical Analysis / Dating', 'Miscellaneous', 'Organic Compound Analysis', 'Organometallics / Inorganics', 'Pharmacology / Toxicology' (which is selected), 'Polymer Analysis', and 'Water Analysis'. On the right, there is a 'Category Name' list with 'Active Pharmaceutical Ingredient' selected. Below this, there is a section for 'Include Keywords (Optional)' with a search bar and a '+ Add Another Keyword' button. A 'Search Methods' button is at the bottom right of the 'Explore Methods' section. An arrow points from the 'Search Methods' button to the search results on the right. The search results are titled 'Results for Active Pharmaceutical Ingredient and Metabolite Analysis' and show 114,515 results. Two results are displayed: 1. 'Analysis of Ketoconazole by Cyclic voltammetry' by Alagumalai, Krishnapandi; Muthukutty, Balamurugan; Sivakumar, Mani; Lee, Daeho; Kim, Seong-Cheol. 2. 'Analysis of Rabeprazole in Blood serum by Ion mobility spectrometry' by Mazidi, Fatemeh; Shalbani, Ali; Shishehbore, M. Reza. Each result includes a 'Compare' button and links to 'View Abstract', 'Full Text', and 'View in CAS SciFinder'.

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

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

Category Name

- Active Pharmaceutical Ingredient**
- Addictive Drug Assay
- Forensic Analysis
- Genetic Analysis
- Nanomaterial Analysis
- Organic Compound Analysis
- Toxicity Assay
- Toxin Assay

Include Keywords (Optional)

Enter a keyword...

+ Add Another Keyword

Search Methods

Results for Active Pharmaceutical Ingredient and Metabolite Analysis

114,515 Results

Sort: Relevance Group: By Method

1

Analysis of Ketoconazole by Cyclic voltammetry **JOURNAL**

By: Alagumalai, Krishnapandi; Muthukutty, Balamurugan; Sivakumar, Mani; Lee, Daeho; Kim, Seong-Cheol

Surface-grafted MoS₂ for ketoconazole sensing in biological and aqua samples

Colloids and Surfaces, A: Physicochemical and Engineering Aspects (2025), 706, -. Elsevier B.V.

Analyte Ketoconazole

Other Materials Reagent: Hydrochloric acid; Phosphate; β -Cyclodextrin; Molybdenum sodium oxide; Thiourea; Sodium hydroxide; Acetic acid

Material: Glassy carbon electrodes; Saturated KCl-based silver/silver chloride (Ag/AgCl) electrode; Platinum

Method Category Active Pharmaceutical Ingredient and Metabolite Analysis

Technique Cyclic voltammetry

Equipment Used Electrochemical workstation; Potentiostat/galvanostat

View Abstract **Full Text** **View in CAS SciFinder**

2

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

By: Mazidi, Fatemeh; Shalbani, Ali; Shishehbore, 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

Analyte Rabeprazole

Matrix Blood serum

Other Materials Reagent: Trichloroacetic acid; Ammonium carbonate; Ethanol; Trisodium citrate; Chloroauric acid; Methanol; Thiourea; Cadmium chloride; Ammonia

Material: Gold nanoparticles-cadmium sulfide quantum dots polyethylene column

Method Category Active Pharmaceutical Ingredient and Metabolite Analysis

Technique Atmospheric precipitation; Ion mobility spectrometry; Solid phase extraction

Equipment Used Ion mobility spectrometer

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

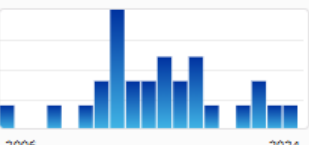
技术&仪器

实验验证

年份

Results for Custom query

Filter By

- ^ Analyte
 - ☒ Lapatinib (28)
 - ☐ Erlotinib (13)
 - ☐ Imatinib (12)
 - ☐ Sorafenib (12)
 - ☐ Dasatinib (10)
 - [View All](#)
- ^ Matrix
 - ☐ Blood plasma (28)
- ^ Method Category
 - ☐ Active Pharmaceutical Ingredient and Metabolite Analysis (27)
 - ☐ Biomolecule Isolation Assay (1)
- ^ Technique
 - ☐ Electrospray ionization tandem mass spectrometry (10)
 - ☐ HPLC-tandem mass spectrometry (7)
 - ☐ Ultra-performance liquid chromatography (7)
 - ☐ Atmospheric precipitation (6)
 - ☐ Quadrupole tandem mass spectrometry (6)
 - [View All](#)
- ^ Validation
 - ☐ Precision (28)
 - ☐ Accuracy (25)
 - ☐ Linearity Range (25)
 - ☐ Limit of Quantitation (24)
 - ☐ Recovery (18)
 - [View All](#)
- ^ Year
 - 
 - No Min to No Max [Apply](#)

28 Results Sort: Relevance Group: By Method

1 [Click title, can enter analysis method details.](#)

Analysis of Lapatinib in Blood plasma by HPLC-tandem mass spectrometry [JOURNAL](#) [Compare](#)

By: Wu, Jianmei; Wiegand, Richard; LoRusso, Patricia; Li, Jing
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
Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences (2013), 941, 100-108. Elsevier B.V.

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](#)

By: Karbownik, Agnieszka; Poraoka, Joanna; Luczak, Anna; Teoyk, Artur; Grabowski, Tomasz; Wolc, Anna; Grzekowiak, Edmund; Szalek, Edyta
Pharmacokinetic interaction after oral coadministration of clarithromycin and the tyrosine kinase inhibitor lapatinib in rats
Acta Polonicae Pharmaceutica (2019), 76 (4), 645-651. Polish Pharmaceutical Society

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

可同时对比3种分析方法

可链接至SciFinder，查看文献详情页

对照多个感兴趣的分析方法详情

	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	2.50 - 1000 ng/mL
Method Category	Active Pharmaceutical Ingredient and Metabolite Analysis	Active Pharm	Limit of Quantitation	5 ng/mL	2.50 ng/mL (LLOQ)
Technique	HPLC-tandem mass spectrometry	HPLC-tandem spectrometry	Recovery	43% ± 14%, 42% ± 10% and 48% ± 12% (recovery), for 5, 15, 800 and 4000 ng/mL spiked sample, respectively.	81, 87 and 87% in 5.00, 100 and 800 ng/mL spiked concentrations, respectively
Analyte	Lapatinib	Lapatinib	Accuracy	102.1%, 98.6%, 102.5% and 98.3% (recovery), for 5, 15, 800 and 4000 ng/mL QC sample, respectively.	107% (inter-assay) in 2.50 ng/mL concentration
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, respectively.	3.03% (RSD, inter-assay) in 2.50 ng/mL concentration
Other Materials	Formic acid; Methanol; Ethyl acetate; XBridge C18 column (3.5 µm, 50 mm × 2.1 mm i.d.)	Acetonitrile; Atmospheric precipitation Security guard	Source	<p>JOURNAL</p> <p>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</p> <p>By: Wu, Jianmei; Wiegand, Richard; LoRusso, Patricia; Li, Jing</p> <p>Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences (2013), 941, 100 - 108.</p> <p>Full Text ▾</p>	<p>JOURNAL</p> <p>A sensitive LC-MS-MS assay for the determination of lapatinib in human plasma in subjects with end-stage renal disease receiving hemodialysis</p> <p>By: Kocan, GERALYN P.; Huang, Mike; Li, Fumin; Pai, Sudhakar</p> <p>Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences (2018), 1097-1098, 74 - 82.</p> <p>Full Text ▾</p>
Equipment Used	LC system., Alliance2695, Waters, Milford, MA, USA; Triple quadrupole mass spectrometer, Quattro Micromass, Waters	HPLC system, Shimadzu, Kyoto, Japan; Sciex, Ontario			
Conditions	<p>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 µm, 50 mm × 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.</p>	<p>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 µm, 50 mm × 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.</p>			

Format
☒ PDF
☐ XLS
Download Cancel

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 displays the CAS Formulus website. At the top, the CAS logo and 'Formulus' text are visible. Navigation links for 'Formulations' and 'Ingredients' are present, with 'Ingredients' highlighted. A search bar prompts users to 'Search by Ingredient Name, CAS Registry Number, or Function'. Below this, two main sections are shown: 'Formulation Designer' and 'Advanced Search'. An orange arrow points from the 'Advanced Search' section to a detailed view of the search interface. This view includes a title 'Advanced Formulations Search' and a description of the search fields. The search criteria are set to 'Ingredient' and 'Required'. A dropdown menu for 'Ingredient' lists various fields: All Fields, Form, Function, Ingredient, Purpose, Route, and Target. A 'Required' dropdown menu lists 'Required', 'Optional', and 'Excluded'. A 'Search' button is at the bottom left, and a 'Clear All' link is at the bottom right. A text box on the right explains the search capabilities.

Good Evening, [User Name]

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

Search

All Fields
Form
Function
Ingredient
Purpose
Route
Target

Required
Optional
Excluded

Clear All

Recent Search History

针对形式、功能、成分、用途、途径或目标进行精确检索

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

Document Type

☐ Patent (188)
☐ Claim (23)
☐ Comparative Example (9)
☐ Example (156)

Organization

☐ Vantico A.-G. (50)
☐ Shipley Co. LLC (41)
☐ Changzhou Tronly Advanced Electronic Materials Co., Ltd. (22)
☐ Changzhou Tronly New Electronic Materials Co., Ltd. (22)
☐ Sumitomo Chemical Co., Ltd. (18)

View All

Language

☐ English (126)
☐ Chinese (30)
☐ Japanese (22)
☐ Korean (10)

Publication Year

Formulations search for "photoresists"

Get Additional References

188 Results

Sort: Relevance Group: By Family

Filter by

Industry

☐ Inks, Paints, & Coatings
☐ Unclassified

Purpose

☐ Cleaning compositions (2,694)
☐ Coating materials (643)
☐ Detergents (290)
☐ Polishing materials (275)
☒ Photoresists (188)

View All

Physical Form

☐ Liquids (4)
☐ Disperse systems (2)
☐ Solutions (1)

State of Matter

Delivery Route

☐ Coating materials (1)

Information Included

☐ Component Amount (168)
☐ Experimental Activity (143)
☐ Process (117)
☐ Effective Dose (3)

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

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

Compare

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

可同时对比3种制剂/配方

可链接至SciFinder，查看文献详情页

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	View

Formulation Ingredients

配方成分

[Expand All Gr](#)

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	-	444.4 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](#)[Feedback](#)

无需阅读原文
即可获取配方详情

Process

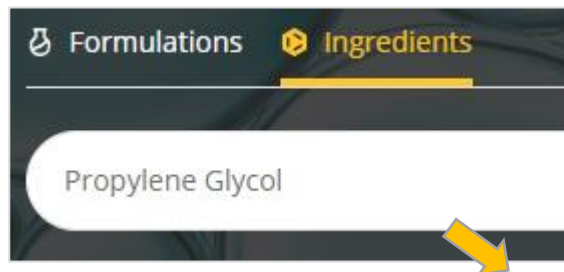
preparation of positive photosensitive anionic electrodeposition coating composition: mix vinyl copolymer (place 10.0 parts of isopropanol and 10.0 parts of butyl cellosolve in a 3-liter four-necked flask equipped with a stirrer, a reflux condenser and a nitrogen inlet tube, and heat to 90 °C. separately, 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]bisphenol 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	Results
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

[Feedback](#)

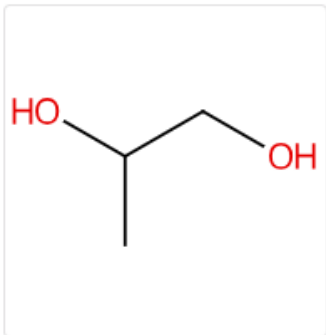
制剂、配方主要成分检索




- 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](#)



C₃H₈O₂

(±)-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 ³	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



Formulation Designer

Industry	Purpose	Physical Form	Add up to 5 Ingredients
Pharmaceutical	Coating materials	Liquids	9050-06-0
Cosmetics & Personal Care	Adhesives	Varnishes	
Agrochemical	Jet-printing inks	Fluids	+ Add Another Ingredient
Cleaning & Surfactant Products	Water-thinned coating materials	Solutions	
Inks, Paints, & Coatings	Printing inks	Paints	
Food & Related	Powder coating materials		
	Paints		
	Antifouling coating materials		
	Anticorrosive coating materials		
	Photocurable coating materials		
	Light-sensitive coating materials		
	Photoactive coating materials		
	Lithographic inks		
	- View More Purposes -		Create Template

Formulation Designer

Clear All Selections

Industry	Purpose	Physical Form	Active or Featured Ingredient
Inks, Paints, & Coatings	Light-sensitive coating materials Lithographic inks Photoactive coating materials	Liquids Paints Varnishes	9050-06-0

Edit Selections Save Download

Your Template Unit Size mg Go Clear

Function	Ingredient	Regulatory Lists	Top Alternatives	Amounts
Active or Featured Ingredient:	Ethanol, homopolymer, 3-phenyl-2-propenoate	-	-	Amount not available
Solvents	Methyl ethyl ketone	EPA Safer Chemical Ingredients; FDA Inactive Ingredients Database	Isopropanol; N-Methyl-2-pyrrolidone	Approximate Range: 20 - 25%
	View More Alternatives			
Photopolymerization catalysts	1H-Imidazole, 2-(2-chlorophenyl)-4,5-diphenyl-, dimer	-	4,4-Bis(diethylamino)benzophenone; 2-(Dimethylamino)-2-(4-methylbenzyl)-1-[(4-morpholin-4-yl)phenyl]-1-butanone; Bis(2,4,6-trimethylbenzoyl)phenylphosphine oxide; Poly(oxy-1,2-ethanediyl), α,α'-1,2,3-propanetriyltris[ω-[[phenyl(2,4,6-trimethylbenzoyl)phosphinyloxy]-; Acrylic acid-butyl acrylate-styrene copolymer	Approximately 1%
	View More Alternatives			

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

583 Results

1

Prevention and treatment of chronic heart failure

By: Jia, Qiujin; Wang, Lirong; Zhang, Xiaonan; Ding, Pharmacological Research (2020), 151, 104552 | Language: English, Database: CAPLUS and MEDLINE

A review. In recent years, although the concept and mortality rate are still high. At present, there is evidence that improving heart function and improving metabolism is expected to become a potential new disease. improving heart function, and improving metabolism.

View More ▾

Full Text ▾

0 0 77

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

In this Patent

- [Claims](#)
- [Classifications](#)
- [CAS Concepts](#)
- [Formulations](#)

Inventors: Zhang, Minyu; Guo, Feifei; Wu, Hongwei; Yang, Hongjun; Wei, Junying; Wu, Sha

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

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: CAPLUS 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 CHF.

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、跨学科研发创新
- 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



There was a problem verifying your account.

Try Again

Contact Us

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

Reference Id: GU75LMF9IZnhTq6mymUog

- 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

使用注意事项

- 一人注册一个帐号
- 实名注册，需提供真实姓名信息（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

CAS SciFinder 学习中心



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>



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

