

CAS SciFinder Discovery Platform

全面高效获取科技信息



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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
- 探索反应实验方案与合成相关策略
- 高效获取分析方法及配方制剂信息

常见问题Q&A



CAS 内容合集来源于化学、超越化学

5大类80小类

- 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
- 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

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

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

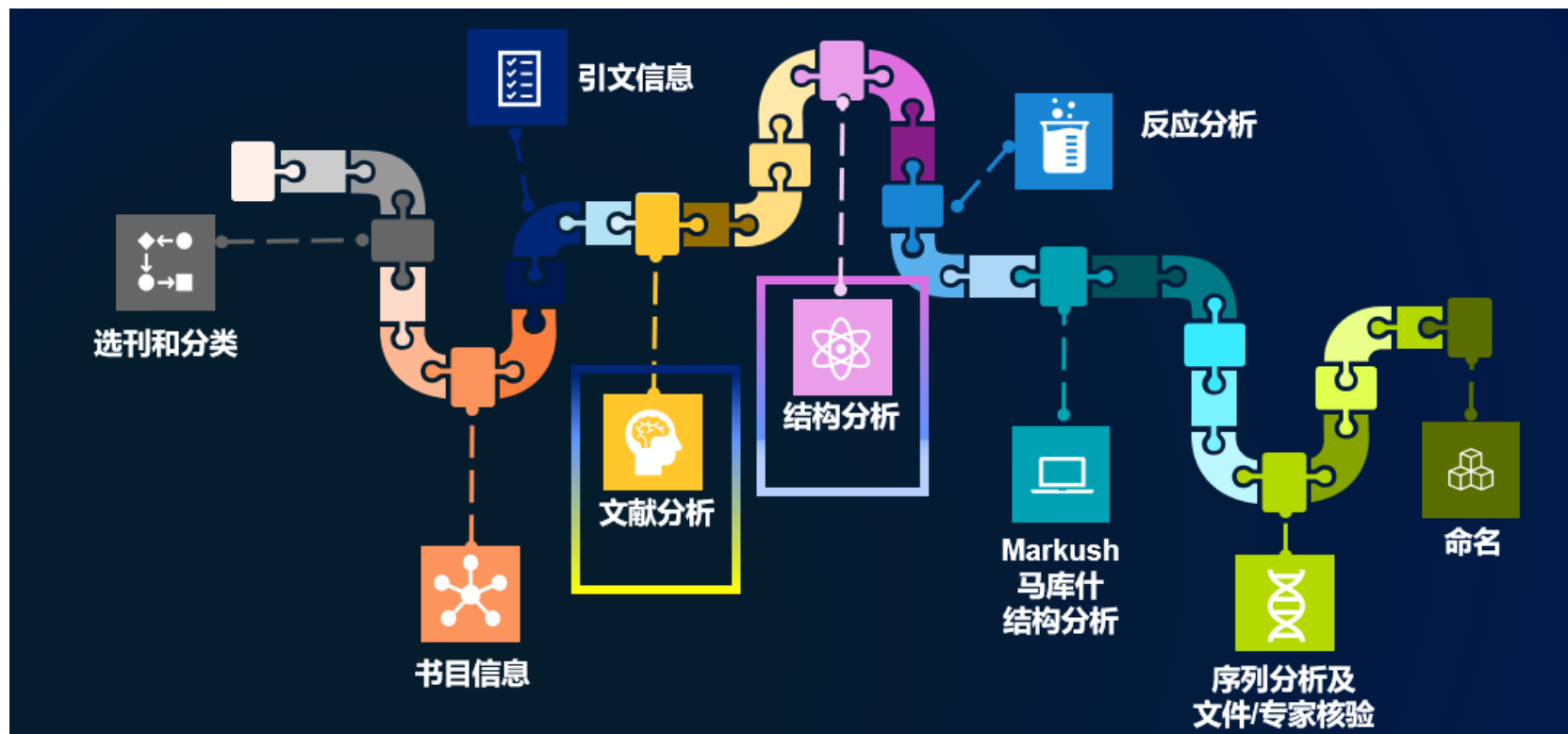


来源：

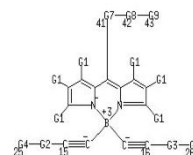
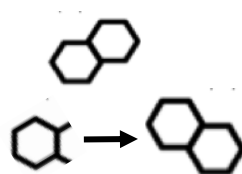
<https://www.cas.org/cas-data>

<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

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



数据库名: SciFinder

说明: 查找您需要的电子资源

数据库导航 常用数据库

外文库

CAS SciFinderⁿ

共1个数据库

中文库

暂无数据

CAS SciFinderⁿ使用说明

最后更新: 2026-09-04 访问量: 24048

- ◆访问方式
校园网直接访问, 校外可通过VPN或设置图书馆代理服务器访问。 [校外访问指南](#)
- ◆数据库网址
CAS SciFinderⁿ网址: <https://scifinder-n.cas.org/>
CAS Analytical Methods 网址: <https://methods.cas.org>
CAS Formulus 网址: <https://formulus.cas.org>

首次使用需注册: [请点击这里注册](#)

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



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使用CAS SciFinder账号登录

清晰简洁的检索界面

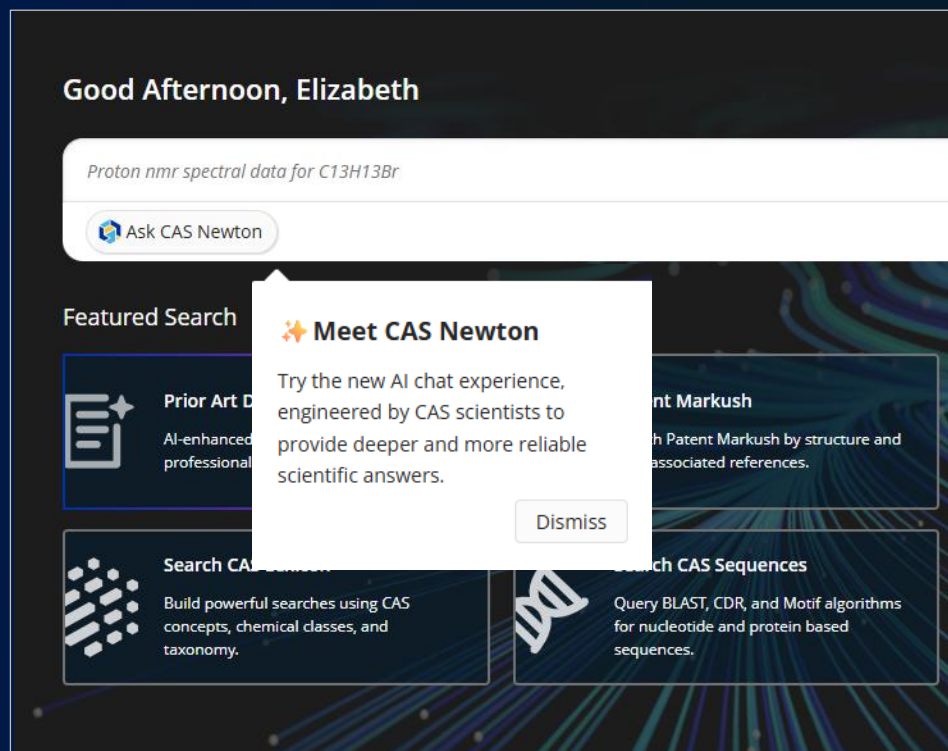
The image shows the CAS SciFinder web interface with several features highlighted by blue callout boxes and yellow annotations:

- 更新结果提醒** (Update Results Reminder): Located in the top right navigation bar.
- 检索结果管理和账号设置** (Search Results Management and Account Settings): A menu on the right side containing links for Projects, History, Saved, Downloads, Settings, Help & Support, and Submit Feedback.
- 结构绘制面板** (Structure Drawing Panel): A button labeled "Draw" in the search bar area.
- 代理AI (Agentic AI)** (Agentic AI): A button labeled "Ask CAS Newton" in the search bar area.
- 现有技术探索** (Existing Technology Exploration): A button for "Prior Art Discovery" in the Featured Search section.
- 专利Markush检索** (Patent Markush Search): A button for "Patent Markush" in the Featured Search section.
- 高级检索选项** (Advanced Search Options): A button for "Advanced Search" in the Featured Search section.
- 逆合成路线设计** (Retrosynthetic Route Design): A button for "Retrosynthetic Analysis" in the Featured Search section.
- CAS词库** (CAS Lexicon): A button for "Search CAS Lexicon" in the Featured Search section.
- CAS序列检索** (CAS Sequence Search): A button for "Search CAS Sequences" in the Featured Search section.
- 近期检索历史** (Recent Search History): A button in the bottom section labeled "Recent Search History".

The interface also includes a left sidebar with navigation links such as LIFE SCIENCES, CAS BioFinder, CAS SCIFINDER DISCOVERY PLATFORM, CAS SciFinder, CAS Analytical Methods, CAS Formulus, STN IP PROTECTION SUITE, CAS STNext, REGULATORY, CAS Chemical Compliance Index, ACCOUNT MANAGEMENT, and CAS Profile.

代理式人工智能——CAS NewtonSM

融合科研信息、专业智慧与高效工具，加速科学发现



CAS Newton 是一款专为科学发现而打造、赋能科研见解的代理型 AI。它通过对话式交互，提供对全球已公开科学数据的便捷访问。CAS Newton 以 CAS 科学家精心标引的科学数据为基础，深度整合 CAS 内容合集（CAS Content CollectionTM）收录的150 余年的文献资源，确保信息准确且科学严谨。

CAS Newton 不止于信息检索，更能进行推理与信息关联，直接为您提供可付诸行动的精准答案。

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
- 探索反应实验方案与合成相关策略
- 高效获取分析方法及配方制剂信息

常见问题Q&A

如何精准构建检索主题？

- 布尔逻辑运算符(and, or, not)，默认运算顺序or > and > not
- “ ” 不允许词形变化，但可出现单数或复数
- () 优先运算，括号中表达式还可以和其他术语交互
- 支持通配符*或?，*代表0或多个字符；? 代表0或1个字符

References search for **"("natural product" not camptothecin) and synthesis"**

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

View Related Results ▾

Filter Results <

Analyze Results

Behavior

Filter by Exclude

Search Within Results

Document Type

Flags

Patent Office

Patent Status

Language

Publication Year

International Patent Classification (IPC)

Sort: Relevance View: Partial Abstract ▾

186,072 Results

1

Synthesis of natural product inspired compound collections

By: Kumar, Kamal; Waldmann, Herbert
Angewandte Chemie, International Edition (2009), 48(18), 3224-3242 | Language: English, Database: CAlus and MEDLINE

A review. **Natural products**, their derivatives, and their analogs are among the most important sources for new drug candidates and tools for chem. biol. and medicinal chem. research. Therefore, there is a need for the development of efficient **synthesis** methods which give access to **natural product** derived and inspired compound collections. To meet this challenge, the requirements of multistep stereoselective **syntheses**, and the logic and methodol. of **natural product** total **synthesis** need to be translated and adapted to the methods and formats for the **synthesis** of compound collections. Recent devel...

View More ▾

Full Text ▾ 0 0 257

2

Natural product synthesis in the age of scalability

natural pro

- 自动提示检索词
- 基于科学家创建的叙词表

Natural product

Natural products

Natural protein fiber

Natural protein fibers

Natural products, chiral

Natural product nomenclature

Natural products, CapsiAlil

Natural products nomenclature

Natural product mol. structure

Natural products, heterocyclic

Relevance

Times Cited

Accession Number: Ascending

Accession Number: Descending

Publication Date: Newest

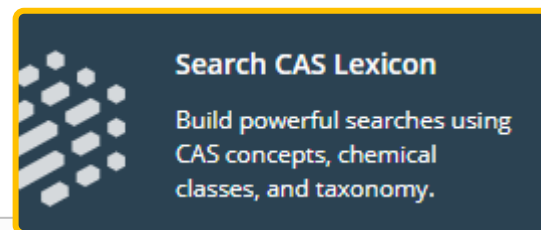
Publication Date: Oldest

排序方式

想要快速探索不熟悉的领域，灵活应对新挑战？

CAS科学家构建标准技术词词库，助力快速开启文献调研，启发信息获取新思路

主题词示例： **organic electroluminescent devices**



Search CAS Lexicon [Learn more about CAS Lexicon searching.](#)

Organic electroluminescent devices

Preferred Concept • 同义词及相关术语

☒ Organic electroluminescent devices
This will search synonyms: Active matrix **organic** light emitting diode; Active-matrix **organic** light-emitting diode; AMOLED; Light emitting **devices**; OLED; Light emitting **devices**; **organic**; OLED; OLEDs; **Organic** LED; **Organic** LEDs; **Organic** light emitting **device**; **Organic** light emitting **devices**; **Organic** light-emitting diode; **Organic** light-emitting diodes; **Org.** LED; **Org.** light-emitting **device**; **Org.** light-emitting **devices**; **Org.** light-emitting diode; **Org.** light-emitting diodes
[View fewer synonyms](#)

Broader Concepts (2) • 上位词 [Select All](#)

☐ Electroluminescent devices
☐ Organic semiconductor devices

Narrower Concepts (1) • 下位词 [Select All](#)

☐ Organic electroluminescent display devices

Related Concepts (1) • 相关词 [Deselect All](#)

☒ Thermally activated delayed fluorescence

Organic electroluminescent devices - Preferred Concept

Organic electroluminescent devices - Related Concept

Thermally activated delayed fluorescence

References search for 2 CAS Lexicon Concepts

51,144 Results Sort: Relevance View: Partial Abstract

☐ 1

Organometallic compound, organic light-emitting device including the same, and electronic apparatus including the organic light-emitting device

Assignee: Samsung Display Co., Ltd.
European Patent Organization, EP4524144 A1 2025-03-19 | Language: English, Database: CAPLUS
Patent Status: ☐ Unknown ☒ KR ☒ US ☒ CN

Formula 1

Provided are macrocyclic platinum cyclometalated aralkylimidazolidine NHC organometallic compounds[(cyclo-Im¹X¹Ar¹OAr²X²Im²X³)Pt] (1, Im¹, Im² = substituted 2-imidazolidine, Ar¹, Ar² = optionally substituted 1,3-phenylene; X¹, X², X³ = CH₂, substituted methylene, 9-fluorenylidene), useful as dopants for light-emitting layers of organic electroluminescent devices (OLEDs) and OLEDs including thereof. The performance of the disclosed compounds 1 was evaluated by assembly of test OLEDs according to standard protocol.

PatentPak 109 56 0

Filter Results

Behavior

Search Within Results

Document Type

Patent Office

Patent Status

Language

Publication Year

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 X
Volume (Optional) Issue (Optional) Starting Page (Optional)

AND Publication Year 2020 to 2025 X
+ Add Advanced Search Field

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

AND
OR
NOT

Search

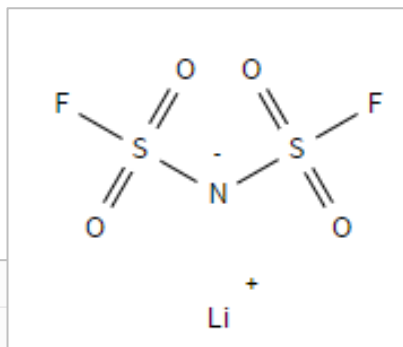
Advanced Search
Select data fields and search operators to create a focused query.

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

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

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)

文献结果的数据关联、筛选与定题追踪

CAS SciFinder herb and medic*

Navigation: All Substances Reactions **References** Suppliers Patent Markush

数据关联 (Data Association): View Related Results

结果集的二次筛选 (Secondary Filtering of Results): Search Within Results

设置定题追踪 (Set Topic Tracking): Alerts (toggle on)

Save Results Dialog:

- 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: ☒ Alerts
- Frequency: As Available
- Add Email(s): Add Recipient(s)
- Buttons: Cancel Save

Analyze Results Panel:

- Top Document Types: Journal (purple), Patent (green)
- Patent Offices: 1 to 18

Search Results:

Filtering: Search Within Results: synthesis or manufacture X Clear All Filters

64 Results Sort: Relevance View: Partial Abstract

Document 1:

Pentacyclic triterpenoids from the medicinal herb, Centella asiatica (L.) Urban

By: James, Jacinda T.; Dubery, Ian A.

Molecules (2009), 14(10), 3922-3941 | Language: English, Database: CAPLUS and MEDLINE

A review. Centella asiatica accumulates large quantities of pentacyclic triterpenoid saponins, collectively known as centellobiosides. These terpenoids include asiaticoside, centelloside, madecassoside, brahmioside, brahmioside, thankuniside, sceleffoside, centelloside, asiatic-, brahm-, centellic- and madecassic acids. The triterpene saponins are common secondary plant metabolites and are synthesized via the isoprenoid pathway to produce a hydrophobic triterpenoid structure (aglycon) containing a hydrophilic sugar chain (glycone). The biol. activity of saponins has been attributed to these charac...

Full Text 6 0 266

Document 2:

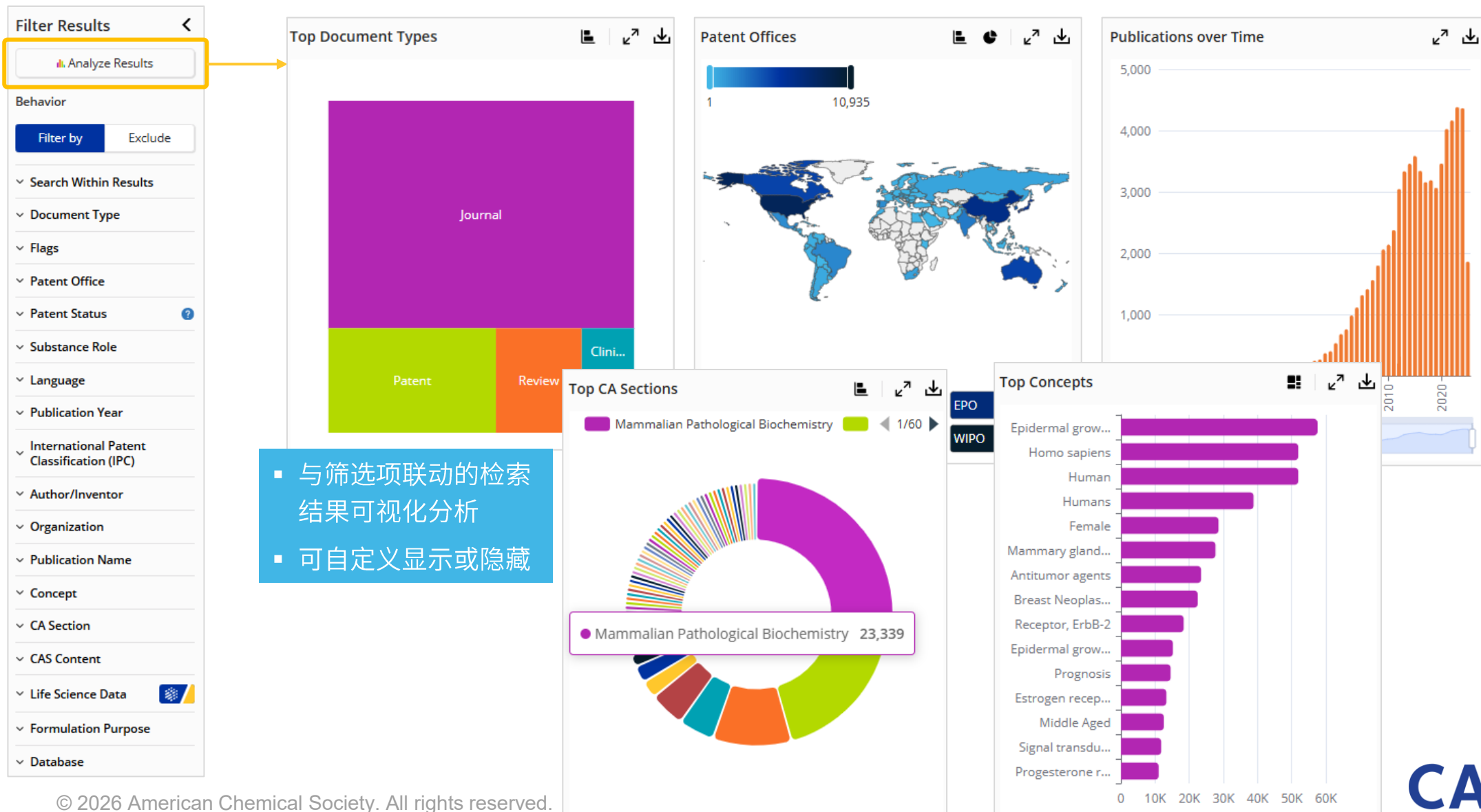
Centelloside accumulation in leaves of Centella asiatica is determined by resource partitioning between primary and secondary metabolism while influenced by supply levels of either nitrogen, phosphorus or potassium

By: Mueller, Viola; Lankes, Christa; Zimmermann, Benno F.; Noga, Georg; Hunsche, Mauricio

Journal of Plant Physiology (2013), 170(13), 1165-1175 | Language: English, Database: CAPLUS and MEDLINE

In the present study we aimed to investigate the relevance of either N, P or K supply for herb and leaf yield and for centelloside concentrations in Centella asiatica L. urban leaves. In this regard, we elucidated the causal relationship between assimilation rate, leaf N, P and K concentrations, herb and leaf

文献结果的筛选与可视化分析



筛选工具 Concept & CA Section

CA Section CAS标引的学科研究方向

By Count | Alphanumeric

0 Selected

- ☐ Pharmacology (223)
- ☐ Pharmaceuticals (81)
- ☐ Plant Biochemistry (53)
- ☐ Pharmaceutical Analysis (51)
- ☐ Food and Feed Chemistry (36)
- ☐ Essential Oils and Cosmetics (10)
- ☐ Biochemical Methods (7)
- ☐ Unavailable (6)
- ☐ Fermentation and Bioindustrial Chemistry (4)
- ☐ Fertilizers, Soils
- ☐ Mammalian Pa
- ☐ Toxicology (3)
- ☐ Carbohydrates
- ☐ Immunochemi
- ☐ Microbial, Algal, and Fungal Biochemistry (2)
- ☐ Agrochemical Bioregulators (1)

Concept CAS标引的核心研究点

Top Count | Alphanumeric | Search

0 Selected

- ☐ Pharmaceutical natural products (218)
- ☐ Homo sapiens (131)
- ☐ Human (131)
- ☐ Animals (118)
- ☐ Triterpenes (118)
- ☐ Saponins (115)
- ☐ Humans (105)
- ☐ Centella asiatica (101)
- ☐ Plant extracts (92)
- ☐ Drugs, Chinese Herbal (87)
- ☐ Signal transduction (84)
- ☐ Flavonoids (77)
- ☐ Chinese medicine (75)
- ☐ Chromatography, High Pressure Liquid (66)
- ☐ Antioxidants (64)
- ☐ Molecular docking (57)
- ☐ Rats (57)
- ☐ Alkaloids (34)
- ☐ Pharmacology (34)
- ☐ Phytochemicals (34)
- ☐ Leaf (33)
- ☐ Medicine, Chinese Traditional (30)
- ☐ Oxidative stress, biological (30)
- ☐ Drug targets (29)
- ☐ HPLC (29)
- ☐ Molecular structure (29)
- ☐ Pharmacokinetics (29)
- ☐ Quality control (29)
- ☐ Rats, Sprague-Dawley (29)
- ☐ Herb (28)
- ☐ Pharmaceutical tablets (28)
- ☐ Proteins (28)
- ☐ Root (28)
- ☐ Epidermal growth factor
- ☐ Bioactive agents (19)
- ☐ Spices (19)
- ☐ Concept
- ☐ Top Count
- ☐ Alphanumeric
- ☐ Search
- ☐ Concept Name
- ☐ deliver*
- ☐ Select All on Page
- ☐ Chewable drug delivery systems (9)
- ☐ Drug delivery systems (14)
- ☐ Infusion drug delivery systems (1)
- ☐ Liquid oral drug delivery systems (2)
- ☐ Nasal drug delivery systems (1)
- ☐ Oral drug delivery systems (27)
- ☐ Solid oral drug delivery systems (1)
- ☐ Topical drug delivery systems (4)
- ☐ Transdermal drug delivery systems (2)
- ☐ Metabolomics (17)
- ☐ p53 (protein) (17)
- ☐ Pharmaceutical analysis (17)

精准定位核心研究点

支持使用通配符

Cancel OK

文献详情：通过CAS科学家的增值标引，快速概览重要信息

Synthesis of madecassic acid derivatives and their cytotoxic activity

27

54

4

Citation Map

引文地图



In this Reference

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

导航速览

By: Van Loc, Tran; Nhu, Vo Thi Quynh; Chien, Tran Van; Ha, Le Thi Thu; Thao, Tran Thi Phuong; Sung, Tran Van

DOI: 10.1515/zn-2017-0172

Fifteen new 28-amide derivatives of madecassic acid, isolated from the tropical **medicinal herb** *Centella asiatica* (Apiaceae), have been synthesized, and their cytotoxicity on three cancer cell lines, KB (carcinoma cancer), HepG2 (liver cancer) and Lu-1 (lung cancer), was evaluated. The results showed that acetylation of the 2,3,23-hydroxyl group and/or amidation of the 28-COOH group strongly increased the cytotoxicity.

Keywords: madecassic acid preparation anticancer human

View PDF

Full Text

Publication Information • Journal

Source

Zeitschrift fuer Naturforschung, B: A
Journal of Chemical Sciences
Volume: 73
Issue: 2
Pages: 91-98
Journal
2018
DOI:
[10.1515/zn-2017-0172](#)

CODEN: ZNBSEN
ISSN: 0932-0776

题录信息

Database Information

AN: 2018:224092
CAN: 171:394741
CAplus

Company/Organization

Institute of Chemistry
Organic Synthesis
Vietnam Academy of
Technology (VAST)
Ha Noi 10000
Viet Nam

CAS Concepts

核心研究点

Amines

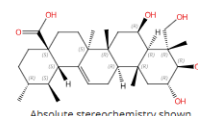
Role: Reactant

Antitumor agents

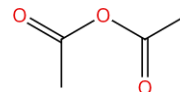
Cancer

Reactions

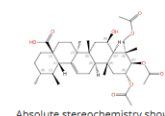
31-355-CAS-20564441



+



→



Steps: 1 Yield: 85%

1,1 Solvents: [Pyridine](#); 12 h, rt

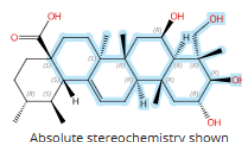
54

Steps: 1

Substances

物质

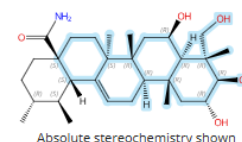
18449-41-7



C₃₀H₄₈O₆
Madecassic acid

Role: Pharmacological Activity, Purification or Recovery, Reactant, Therapeutic Use, Biological Study, Preparation, Reactant or Reagent, Uses

2376279-18-2



C₃₀H₄₉NO₅
(2α,3β,4α,6β)-2,3,6,23-Tetrahydroxyurs-12-en-28-amide

Role: Pharmacological Activity, Synthetic Preparation, Therapeutic Use, Biological Study, Preparation, Uses

物质研究角色

如何快速获取引文信息？——可视化的引文地图

Citation Map

Filter By Cited By Citing

可筛选

Filter Results

Behavior

Filter by Exclude

Document Type

- ☐ Journal (16)
- ☐ Review (1)
- ☐ Preprint (1)

Flags

- ☐ Has DOI (16)
- ☐ Has Related Substances (14)
- ☐ Has Related Reactions (3)

Author/Inventor

- ☐ Dai, Yue (4)
- ☐ Xia, Yufeng (3)
- ☐ Gong, Zhunan (2)

Citation Map for Synthesis of madecassic acid derivatives and their cytotoxic activity

By: Van Loc, Tran; Nhu, Vo Thi Quynh; Chien, Tran Van; Ha, Le Thi Thu; Thao, Tran Thi Phuong; Sung, Tran Van
Zeitschrift fuer Naturforschung, B: A Journal of Chemical Sciences (2018), 73(2), 91-98 | Language: English, Database: CAplus

Full Text

Get References

可链接至对应的文献结果页面

可下载

Developing an Amide-Spacered Triterpenoid Rhodamine Hybrid of Nano-Molar Cytotoxicity Combined with Excellent Tumor Cell/Non-Tumor Cell Selectivity

By: Heise, Niels V. ; Denner, Toni C.; Becker, Selina; Hoenke, Sophie ; Csuk, Rene
Molecules (2023)

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Citation Map Key

- Cited by Root Document
- References Citing Root Document

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?

- Cited By: 被引文献
- Citing: 施引文献

深入专利文献详情

Herbal microparticulate formulation containing Gymnema sylvestre extract and curcumin for diabetes management

14

0

0

Citation Map

Download

Save

Bookmark

In this Patent

Claims

Classifications

CAS Concepts

Substances

Formulations

Inventors: Bhujbal, Santosh S.; Kulkarni, Aditi S.; Chitlange, Sohan S.

The invention relates to an antidiabetic herbal formulation prepared using n microparticulate formulation contains following components: 0.5-5% of each crosslinking agent in water, wherein the polymer matrix is selected from a g maltodextrin, dextrin, microcrystalline cellulose, sodium alginate or combina sodium tripolyphosphate and calcium chloride or combination thereof.

Keywords: Gymnema extract curcumin herbal microparticulate formulation

PatentPak

Get Prior Art Analysis

Full Text

View in CAS Fo

Publication Information

Patent

Patent Number

IN201921045670

Publication Date

2019-11-22

Application Number

IN2019-21045670

Assignee

Dr. D. Y. Patil Institute of Pharmaceutical Sciences & Research, India

Source

India
CODEN: INXXBQ

Database Information

AN: 2019:2203191
CAN: 178:300164
Capius

Language

English

Patent Family

专利家族

Patent	Language	Full Text	Publication Date	Application Number	Application Date	Patent Status	Status Date
IN201921045670 A	English	PatentPak PDF	2019-11-22	IN2019-21045670	2019-11-09	Alive	2025-04-02
IN480297 B	English		2023-12-15	IN2019-21045670	2019-11-09	Alive	2025-04-02

Claims

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

1

What is claimed is:
A novel herbal microparticulate formulation for the management of Diabetes Mellitus, comprising Gymnema sylvestre extract and Curcumin in an amount 0.5-5 % of each, and a polymer matrix in an amount ranging from 1-3% w/v in water for each and cross linking agent in an amount ranging from 1-5% w/v in water for each:
where said polymer matrix is selected from a group comprising of edible starch, soluble starch, cellulose, dextrins, mannitol, cyclodextrins, maltodextrin, dextrin, microcrystalline, cellulose, sodium alginate or combination thereof, where said cross linking agent is selected from a group comprising of barium chloride, aluminium sulphate, sodium tripolyphosphate and calcium chloride or combination thereof.

2

A method of preparing microparticulate formulation comprising Gymnema sylvestre extract and Curcumin, said method comprising steps of:
a) dispersing the Gymnema sylvestre extract in an amount ranging from 0.5 % to 5 % in a polymer matrix in an amount ranging from 1-5% to obtain solution A;
b) adding the solution A, in a solution of crosslinking agent in an amount ranging from 1-5% to obtain solution B;
c) stirring the solution B to obtain the microparticulate of Gymnema sylvestre extract C;
d) dispersing the Curcumin in an amount ranging from 0.5 % to 5 % in a polymer matrix in an amount ranging from 1-5% to obtain solution D;
e) adding the solution D, in a solution of crosslinking agent in an amount ranging from 1-5% to obtain solution E; and
f) stirring the solution E to obtain the microparticulate of Curcumin F.

3

A method of preparing microparticulate formulation comprising Gymnema sylvestre extract and Curcumin, said method comprising steps of:
a) dispersing the Gymnema sylvestre extract in an amount ranging from 0.5 % to 5 % in apolymer matrix in an amount ranging from 1-5% to obtain solution A;
b) adding the solution A, in a solution of crosslinking agent in an amount ranging from 1-5% to obtain solution B;
c) stirring the solution B to obtain the microparticulate of Gymnema sylvestre extract C;
d) dispersing the Curcumin in an amount ranging from 0.5 % to 5 % with a polymer matrix in an amount ranging

Classifications

分类信息

Patent	Classification	Codes
IN201921045670 A	IPC1	A61K
IN480297 B	IPC1	A61K

Patent Status

专利状态

22

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CAS PatentPak: 高效浏览专利

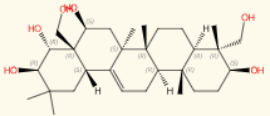
一键定位专利原文中的核心研究物质

CAS PatentPak

PAGE 26 / 56 ZOOM - + DOWNLOAD PDF PDF+

Key Substances in Patent

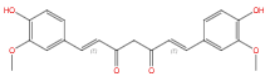
CAS RN 22467-07-8



Analyst Markup Locations (1)

Page 25

CAS RN 458-37-7



Analyst Markup Locations (1)

Page 41

CAS RN 9005-25-8

Starch

Analyst Markup Locations (1)

Page 41

CAS RN 9004-34-6

Cellulose

6. Flavonoids +

7. Carbohydrate +

8. Xanthoprotein +

9. Phenol +

5

Example 2: Identification of gymnemagenin in the *Gymnema sylvestre* extract by Thin Layer Chromatography (TLC)

Standard Gymnemagenin (90%) was procured from market and prepared the standard gymnemagenin solution by dissolving 1 mg of standard Gymnemagenin in 1 ml methanol.

10 10 µl of prepared sample was applied on TLC plates.

Sample preparation: 100 mg of *Gymnema sylvestre* extract was dissolved in 10 ml of methanol and 10 µl of prepared sample was applied on TLC plates.

Solvent system: Isopropyl alcohol: methanol: chloroform: acetic acid (5: 1: 3: 0.5).

Detection by spraying reagent: Modified Vanillin- Sulphuric Acid: 0.5% vanillin in sulfuric

15 acid-ethanol (4:1) v/v (stock solution) reagent, followed by heating in hot air oven at 105°C for 5-8 min

Solvent front: 8 cm

25

?

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

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
- 探索反应实验方案与合成相关策略
- 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, [User Name]

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.

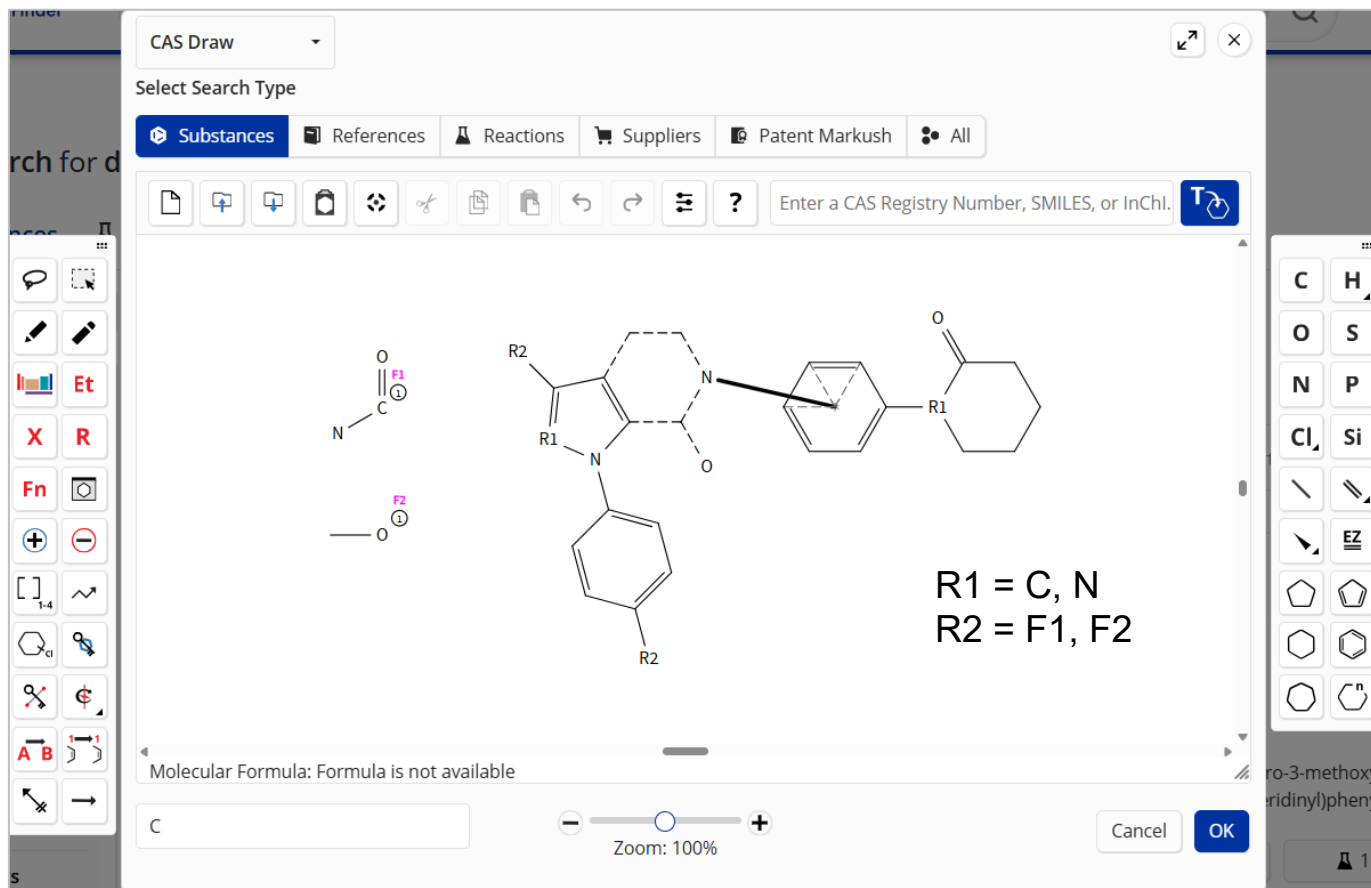
Draw

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

基于分子结构，检索目标物质



R-Group Definitions

R1 R2 R3 R4 R5 R6 R7 R8 R9 R10 R11 R12 >

R2: F2, F1

- > Atoms
- > Variables
- > Shortcuts
- ▼ Fragments

Fragment F1: A carbonyl group with a nitrogen atom attached to the carbonyl carbon.

Fragment F2: A carbonyl group with an oxygen atom attached to the carbonyl carbon.

- 选择可变基团
- 自定义R基团
- 片段结构
- 键型键级不确定
- 重复工具
- 取代位置可变

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

View: Partial

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)ethyl]ethanamine-N,P...

62 1,297 0

1929551-26-7

C30H53BrMnNO2P2

Stereoisomer of bromodicarbonyl[2-(dicyclohexylphosphino-κP)-N-[2-(dicyclohexylphosphino-κP)ethyl]ethanamine-N,P...

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]ethanamine-N,P...

5

1428439-31-9

C32H64CoNP2Si.C32H12BF24

Components: 2

6

分子式检索：高效检索高分子化合物或无机化合物

- 含碳化合物，C排第一位，H排第二位，其他元素符号按照首字母顺序进行排列
- 不含碳化合物，按照元素符号的首字母顺序进行排列
- 不同组分之间用“.”隔开，如：高熵碳化物 C.Hf.Nb.Ta.Ti.Zr
- 无机含氧盐：阳离子和阴离子用点（.）分开；阴离子以氢补齐至电中性 Na_2SO_4 : $\text{H}_2\text{O}_4\text{S}.2\text{Na}$

CAS SciFinder

H₂O₄S.2Na

Substances Reactions References Suppliers Patent Markush

View Related Results

Filter Results

Behavior

Filter by Exclude

Search Within Results

Reaction Role

Reference Role

Life Science Data

Commercial Availability

Number of Components

Molecular Weight

9 Results

1 7757-82-6

[O-]S(=O)(=O)[O-]

• 2 Na

H₂O₄S.2Na

Components: 2

Component RN: 7664-93-9

Sodium sulfate

133K 65K 216

2 13759-07-4

[O-]S(=O)(=O)[O-]

• 2 Na

H₂O₄S.2Na

Components: 2

Component RN: 7664-93-9

Thenardite (Na₂(SO₄))

1,025 0 1

3 14262-80-7

[O-]S(=O)(=O)[O-]

• 2 Na

H₂O₄S.2Na

Components: 2

Component RN: 13770-01-9

Sulfuric-³⁵S acid, disodium salt

74 1 3

分子式检索：高效检索聚合物

$(C_2H_4O)_n C_4H_8O$

- $(C_2H_4O)_n C_4H_8O$: 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

1 31497-33-3 $(C_2H_4O)_n C_4H_8O$ Poly(oxy-1,2-ethanediyl), α -(2-methyl-2-propen-1-yl)- ω -hydroxy- 1,905 1,728 13

2 27252-80-8 $(C_2H_4O)_n C_4H_8O$ Polyethylene glycol allyl methyl ether 1,055 588 12

3 85600-94-8 $(C_2H_4O)_n C_4H_8O$ Poly(oxy-1,2-ethanediyl), α -3-buten-1-yl- ω -hydroxy- 45 21 0

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

1 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... 30 5 0

2 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... 7 2 0

3 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... 3 0 1

属性值联用检索目标物质

Substances

References

Clear All

Advanced Search

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

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

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

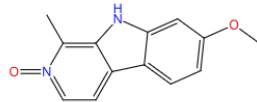
Functional Group

Filtering: Life Science Data: 3 Selected X

13 Results

Sort: Relevance View: Partial

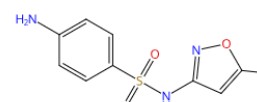
57498-78-9



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

16 11 2

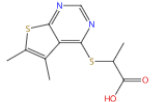
723-46-6



C10H11N3O3S
Sulfamethoxazole

31K 1,090 116

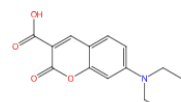
442571-27-9



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

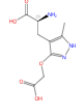
2 4 31

50995-74-9



C14H15NO4
7-Diethylaminocoumarin-3-carboxylic acid

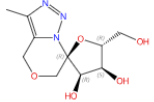
1628224-40-7



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

Absolute stereochemistry shown, Rotation (-)

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

32

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American Chemical Society

快速筛选关键物质，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

^ Substance Class 物质类别

☒ 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

^ Polymer Class 聚合物类别

☐ Polyacrylic (2,224)

☐ Polyether (1,563)

☐ Polyether (1,531)

☐ Polyamide (1,116)

☐ Manual registration (1,080)

View All

^ Aromatic Rings 芳环数量

☐ No aromaticity (208K)

☐ 1 (294K)

☐ 2 (994K)

☐ 3 (799K)

☐ 4 (165K)

View All

^ Functional Group 官能团

☐ Halide (1.6M)

☐ Amide (1.3M)

☐ Imine (1.2M)

☐ Alkene (1.1M)

☐ Alkyl halide (1M)

View All

^ LogP

No Min

to

No Max

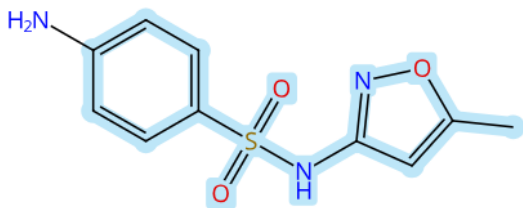
Apply

Available Range: -25.829 to 87.223

聚焦产物属性表征信息，与实验结果进行比对

CAS Registry Number: 723-46-6

33K 1,136 110 View in CAS BioFinder



$C_{10}H_{11}N_3O_3S$
Benzenesulfonamide, 4-amino-*N*-(5-methyl-3-isoxazolyl)- (9CI, ACI)

Properties

- Molecular Weight
- Melting Point (Experimental)
- Boiling Point (Predicted)
- Density (Experimental)

Experimental Properties | Spectra

Other Names and Identifiers

- Experimental Properties
- Experimental Spectra

Patents C

- Iron electrolysis degradation from
- Patent Number: CN
- Publication Date: 20
- Compositions of
- Patent Number: WO
- Publication Date: 20
- Application of Jo
- water treatment
- Patent Number: CN
- Publication Date: 20

Experimental Properties

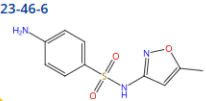
Biological	Chemical	Density	Electrical	Lipinski	Structure Related	Thermal
Property	Value	Condition	Source			
Median Lethal Dose	3662 mg/kg	Organism: mouse; Route: oral	(1) CAS			
Median Lethal Dose	3662 mg/kg	Organism: mouse; Route: oral	(2) APC			
Median Lethal Dose	3500 mg/kg	Organism: mouse; Route: oral	(3) CAS			
ADME (Absorption, Distribution, Metabolism, Excretion) - 5 Sources	See Full Text		(4-8) CAS			
Half-Life (Biological) - 4 Sources	See Full Text		(9-12) CAS			
LC50 - 2 Sources	See Full Text		(13-14) CAS			
Minimum Inhibitory Concentration - 17 Sources	See Full Text		(15-31) CAS			

Experimental Spectra

^1H NMR ^{13}C NMR Hetero NMR IR Mass Raman UV and Visible

View Proton NMR Spectrum (Image Available)

723-46-6



$C_{10}H_{11}N_3O_3S$

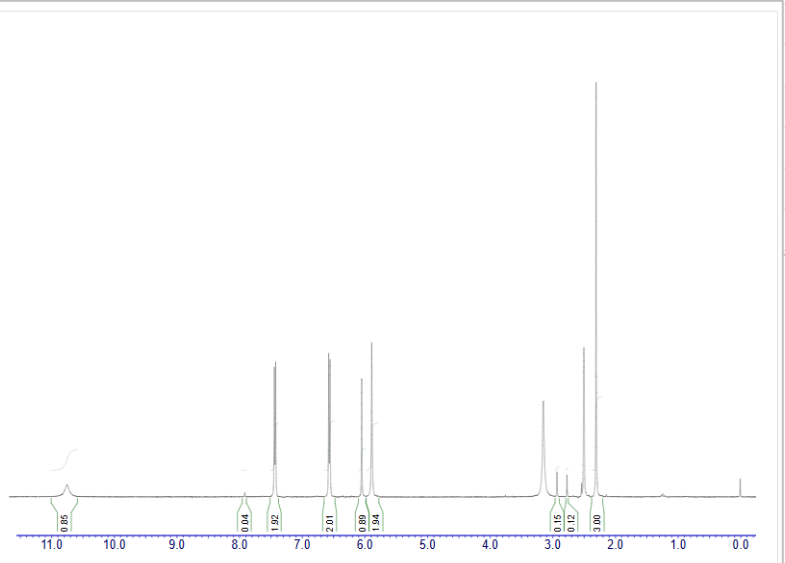
CAS Name
Sulfamethoxazole

Conditions

- Working Frequency
400 MHz
- Solvents
Dimethyl sulfoxide (67-68-5)
Carbon tetrachloride (56-23-5)
- Temperature
20 °C

Spectrum Summary

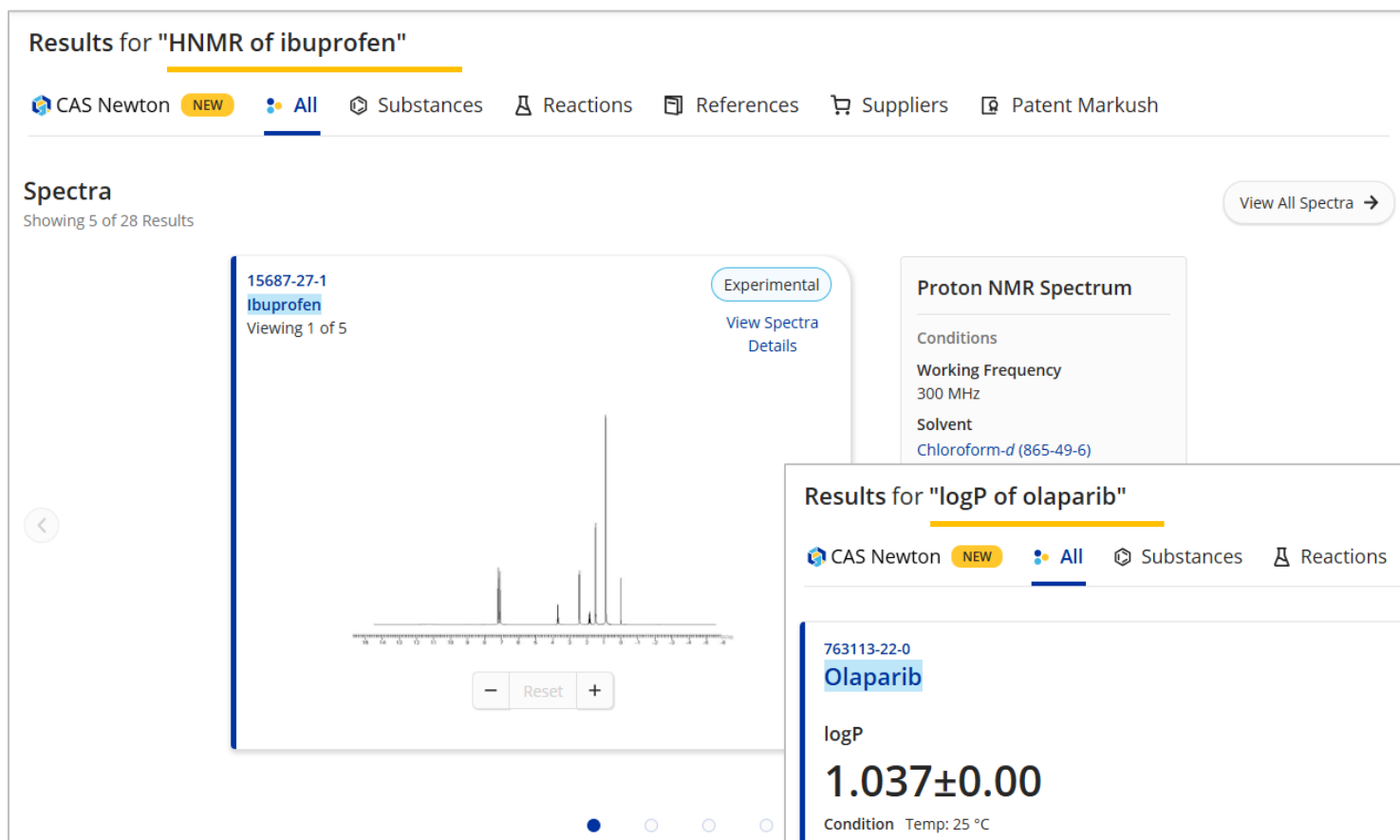
- Spectrum ID
F0175-0013
- Source
Spectral data were obtained from Life Chemicals



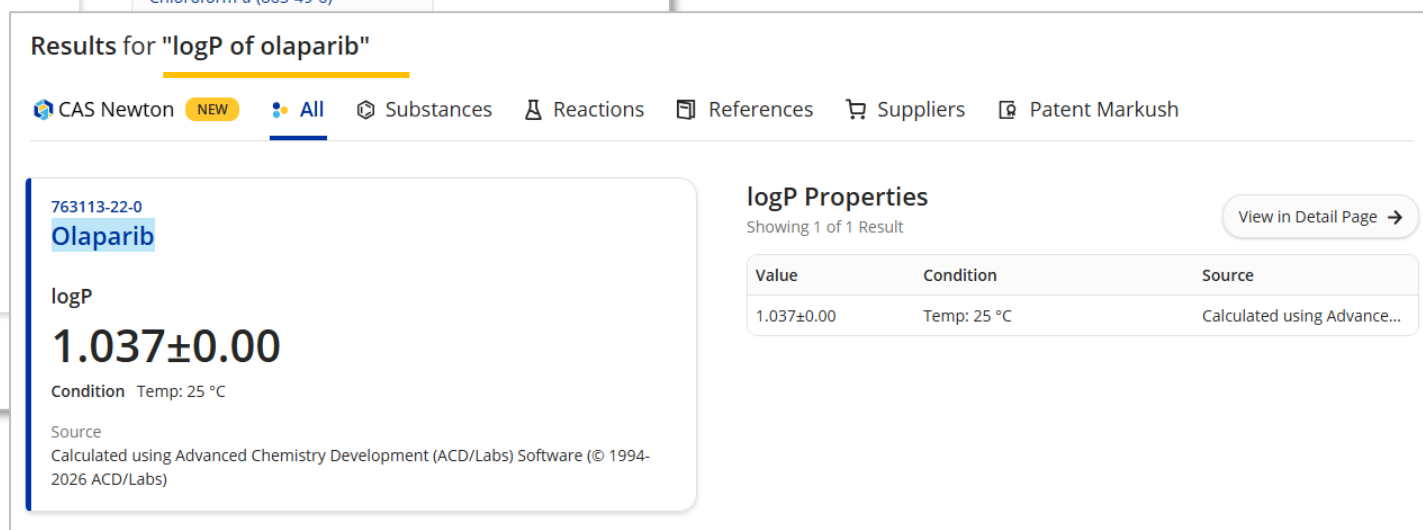
11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0

0.05 0.04 1.92 2.01 0.88 1.94 0.15 0.12 3.00

自然语言直接检索物质谱图、属性，直观高效



无需多次点击和跳转，核磁谱图与物质属性即查即得



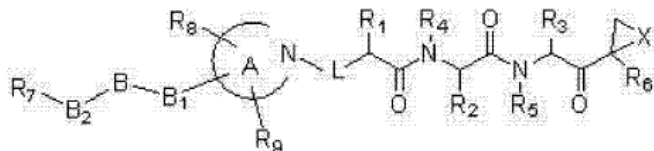
CAS Markush检索，助力结构查新

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

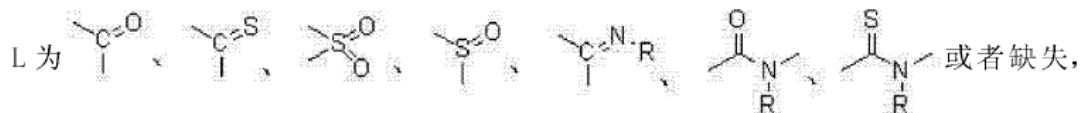
其中：

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]

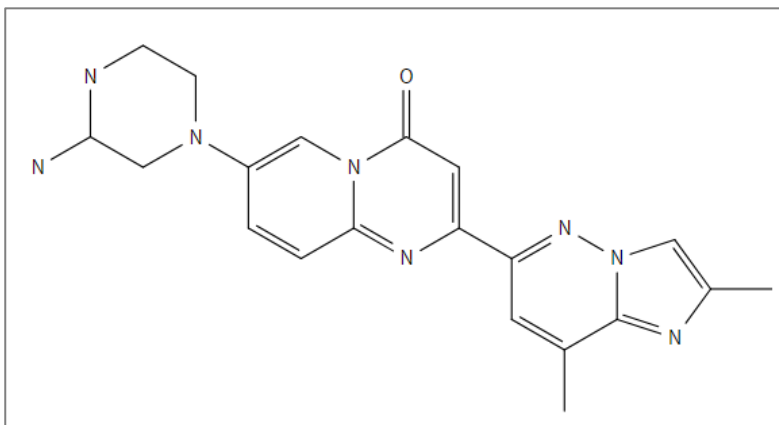
- 以具体化学结构陈述的特定物质，会被分配CAS 登记号

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

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

View Related Results ▾

Filter Results

Analyze Results

Structure Match

As Drawn (0)

Substructure (0)

Similarity (117K)

Behavior

Filter by Exclude

Search Within Results

Similarity

95-98 (2)

90-94 (54)

85-89 (232)

80-84 (265)

75-79 (313)

View All

Reaction Role

Product (255)

Reactant (21)

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

288 Results

Sort: Relevance View: Partial |

1 95 ***

1825352-54-2

Absolute stereochemistry shown

C₂₁H₂₃N₇O

2-(2,8-Dimethylimidazo[1,2-b]pyridazin-6-yl)-7-[(3R)-3-methyl-1-piperazinyl]-4H...

2 95 ***

1825352-53-1

Absolute stereochemistry shown

C₂₁H₂₃N₇O

2-(2,8-Dimethylimidazo[1,2-b]pyridazin-6-yl)-7-[(3S)-3-methyl-1-piperazinyl]-4H...

3 94 ***

1825352-79-1

Absolute stereochemistry shown

C₂₁H₂₃N₇O

9-Methyl-2-(2-methylimidazo[1,2-b]pyridazin-6-yl)-7-[(3R)-3-methyl-1-piperazinyl]...

4 94 ***

1825352-78-0

Absolute stereochemistry shown

C₂₁H₂₃N₇O

9-Methyl-2-(2-methylimidazo[1,2-b]pyridazin-6-yl)-7-[(3S)-3-methyl-1-piperazinyl]...

5 94 ***

1825352-52-0

Relative stereochemistry shown

C₂₂H₂₅N₇O

rel-2-(2,8-Dimethylimidazo[1,2-b]pyridazin-6-yl)-7-[(3R,5S)-3,5-dimethyl-1-piperazinyl]...

6 94 ***

2097817-67-7

Absolute stereochemistry shown

C₂₂H₂₅N₇O

2-(2,8-Dimethylimidazo[1,2-b]pyridazin-6-yl)-7-[(3S,5S)-3,5-dimethyl-1-piperazinyl]...

CAS Markush检索



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

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

CAS SciFinder Enter a query...

Return to Home

Patent Markush search for drawn structure

All Substances Reactions References Suppliers Patent Markush

View Related Results

Filter Results

Patent Markush Match

As Drawn (1)

Substructure (1)

Behavior

Filter by Exclude

Patent Office

World Intellectual Property Organization (1)

CA Section

Heterocyclic Compounds (More Than One Hetero Atom) (1)

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

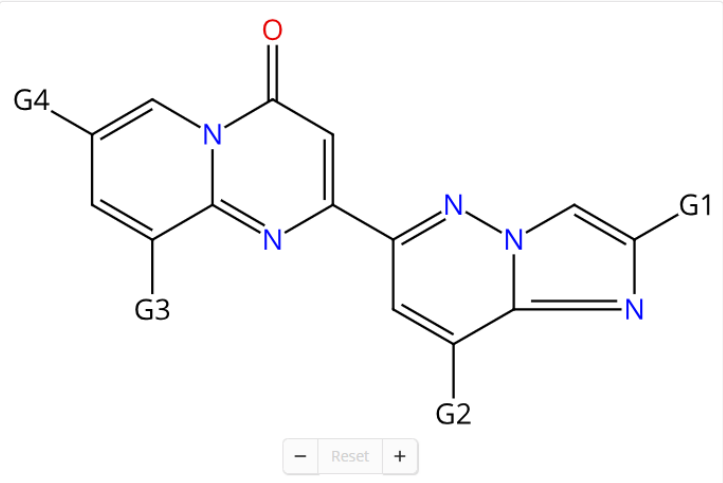
453,454,455,456,457: opt. substd. by G22

629: opt. substd.

直观的 Markush 详情页

Patent Markush 1

PatentPak Full Text

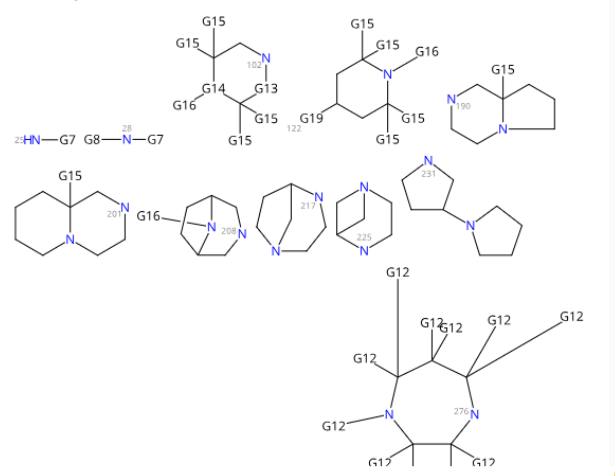


Publication Information
 Assignees: F. Hoffmann-La Roche AG; Hoffmann-La Roche Inc.
 World Intellectual Property Organization, WO2017081111 A1 2017-05-18 | Language: English, Database: CAplus

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

Legend:

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

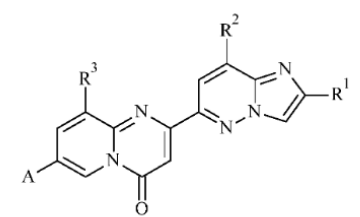


清晰直观展示原文中复杂Markush结构的拆解与解读，助力发现专利文件中隐藏的结构保护信息

原文中Markush结构

Claims

1. The compound of formula (I)



(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;

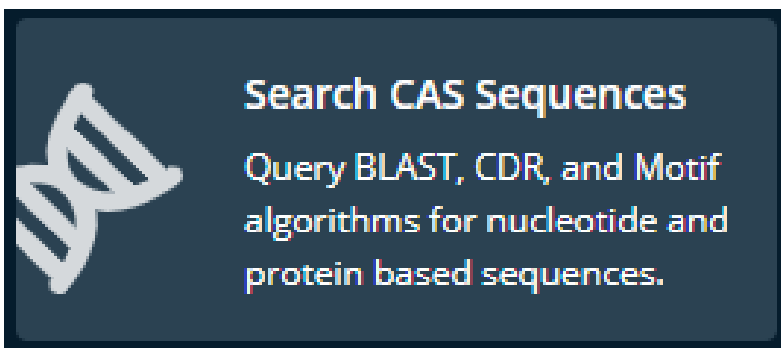
10 **R¹²** is heterocycloalkyl comprising 1 nitrogen ring atom, wherein heterocycloalkyl is optionally substituted with 1, 2, 3 or 4 substituents selected from R¹⁴;

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

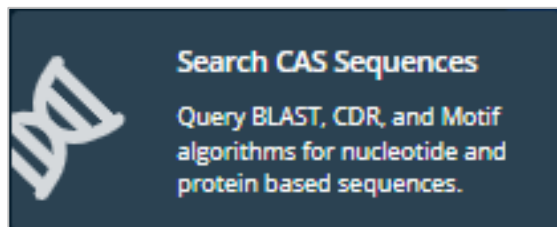
15 **R¹⁴** is independently selected from hydrogen, C₁₋₇-alkyl, amino, amino-C₁₋₇-alkyl, C₃₋₈-cycloalkyl and heterocycloalkyl or two R¹⁴ together form C₁₋₇-alkylene;

CAS SciFinder 中的序列检索

- BLAST
- CDR
- Motif



CAS Sequences——序列检索



支持四种检索选择：
Protein-Protein
Protein-Nucleotides
Nucleotide-Nucleotides
Nucleotide-Proteins

Search CAS Sequences CAS LIFE SCIENCES

Enter a protein or nucleotide string, or upload a .txt or .fasta file. [Learn more about CAS Sequences.](#)

检索方式
BLAST
CDR
Motif

Clear Search

Upload Sequence (.fasta or .txt)

Sequence Type:
☒ Nucleotide ☐ Protein

Search Within:
☒ Nucleotides ☐ Proteins

☒ Include NCBI Sequences

Search Sequences

Advanced Sequence Search

上传fasta或txt格式序列

包括来自期刊、专利和来自NCBI中的序列

Your sequence search has been submitted. You can view the status of your query in your [Recent Search History](#) and on the [History Page](#).

Recent Search History [View All Search History](#)

August 1, 2024

Sequences 4:08 PM	Sequence Type: Nucleotide Search Within: Nucleotides NCBI Included: Yes BLAST Algorithm: BLASTn Alignment Identity: 80% Query Coverage: 90%	AACAACAACATATCAAATCCTACTGGTGCCACAACCTTGA	View Results Edit Options Searching..
----------------------	--	--	---

Results will expire on September 1, 2024.

Recent Search History [View All Search History](#)

August 1, 2024

Sequences 4:08 PM	Sequence Type: Nucleotide Search Within: Nucleotides NCBI Included: Yes BLAST Algorithm: BLASTn Alignment Identity: 80% Query Coverage: 90%	AACAACAACATATCAAATCCTACTGGTGCCACAACCTTGA	View Results Edit Search Complete
----------------------	--	--	---

Results will expire on September 1, 2024.

CAS Sequences——BLAST检索结果

Sequences search for your query

References ▾

BLAST Search Details

Sequence Type: Nucleotide
Search Within: Nucleotides
BLAST Algorithm: BLASTn
NCBI Included: Yes
Alignment Identity: 80%
Query Coverage: 90%
E-Value: 10
Match with Gaps?: No
Gap Costs: Existence 5
Extension 2
Word Size: 11

Bioscope Analysis

Visually explore sequence similarity with a new tool.
[Learn more about Bioscope.](#)

Create Bioscope Analysis

Filter by

^ E-Value

0 to 10⁶

^ Query Coverage %

0 to 100

^ Subject Coverage %

0 to 100

^ Alignment Identity %

0 to 100

Query Details AACAACAACATATCAATCTACTGGTGGCACAACCTTGA View More

170 Results Sort: Alignment Identity View: Expanded

1 Alignment Identity: 100%

Query 1 39

Subject 1 528

Matches: 39
Mismatches: 0

View Less ▾

Alignment Subject References

Alignment Data
BLAST Score: 78
E-Value: 7.79206e-12

Q 1 AACAACAACATATCAATCTACTGGTGGCACAACCTTGA 39
|||||
S 23 AACAACAACATATCAATCTACTGGTGGCACAACCTTGA 61

2 Alignment Identity: 100%

Query 1 39

Subject 1 455

Matches: 39
Mismatches: 0

View Less ▾

Alignment Subject References

Alignment Data
BLAST Score: 78
E-Value: 7.79206e-12

Q 1 AACAACAACATATCAATCTACTGGTGGCACAACCTTGA 39
|||||
S 393 AACAACAACATATCAATCTACTGGTGGCACAACCTTGA 431

结果筛选

- 序列一致性详情
- 目标序列
- 披露序列的专利文献

Download Sequence Results

File Type

☒ Excel (.xlsx)
☐ FASTA (.fasta)

Select Quantity

☒ All Results
☐ Range (ex. 2 to 20)

File Name

Sequences_20240801_1638

Download Cancel

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检索结果下载:

- 比对详情
 - 序列长度参数
 - 相关专利号
 - 专利中的序列编号等
- 支持Excel或FASTA格式

CAS Sequences——BLAST检索结果

Query ① 39

Subject ① 929

Matches: 39
Mismatches: 0

View Less ▾

目标序列

Alignment Subject References

CAS Registry Number: 661510-85-6

Length: 929 nt

Organisms: Zea mays

Sequence

```
1  CACAAGTCAC ACAGCCACAC TTGAACCGCA GCCCGCAGCG GAGGGAGCTT GCAC
81  CGTCGTCGAT GGC GCGGTGG GCTGCGGTGC TGGCGCTGGC CGCGGCCACG GCCAT
161 GACATGAACG CGGACAAGAC GGAGTGCGCG GACCAGCTGG TGGGCTGGC GCCG
241 CCGCGCGCCG CCGCCCGACT GCTGCGGCGG CCTGCGCCAG GTGCTGGGGA AGAG
321 AGGACAAGGA CGACCCCAAC CTGGGCATCA AGATCAACGC CACCCTCGCG CTCG
401 CGCGCCAACG TCTCCCACTG CGCTCAGCTC CTGCATATTC CCCC GGGCTC CAAAC
481 CGACAAGGGG TCCACTGCCG CTCCAGCCAA GGACAACCTG ACGGCGACGA CCGAC
561 GACGCGGCGT GTCCTCCTCG GCGGCGACCG CCGGTGCTGC ACTACGGTG CTGCT
641 CCAGAGCTGT CGCTAGCTC GTTCTAGACC CTCTGTCAAG TTGTGCCACC AGTAG
721 AGTACGTGAC GTGACAGACA ATTTGCTGCT GGTGTCCTTG TTGTTGTAGT AGTTG
```

可直接链接到文献结果集

披露序列的专利文献

References

Nucleic acid molecules and other molecules associated with plants and uses thereof for plant improvement
Assignees: LIU, JINGDONG; ZHOU, YIHUA; KOVALIC, DAVID; SCREEN, STEVEN; TABASKA, JACK; CAO, YONGWEI
US20070011783 A1 | Seq ID No: 25627

Nucleic acid molecules and other molecules associated with plants and uses thereof for plant improvement
Assignees: LIU, JINGDONG; ZHOU, YIHUA; KOVALIC, DAVID; SCREEN, STEVEN; TABASKA, JACK; CAO, YONGWEI; ANDERSEN, SCOTT; EDGERTON, MICHAEL; FINCHER, KAREN; HAMMOND-KOSACK, KIM; LA ROSA, THOMAS; MASUCCI, JAMES; URBAN, MARTIN; XIAO, JINHUA; ZIEGLER, TODD
US20070283460 A9 | Seq ID No: 25627

序列详情及相关序列

 CAS Registry Number: 2417899-77-3

Image Not Available

Unspecified

RNA (recombinant 5'-[1,2-[(3'-O-methyl)m⁷G-(5'→5')-ppp-Am]]-capped all uridine→N¹-methylpseudouridine-substituted severe acute respiratory syndrome coronavirus 2 secretory signal peptide contg. spike glycoprotein S1S2-specifying plus 5'- and 3'-untranslated flanking region-contg. poly(A)-tailed messenger BNT162b2), inner salt (ACI)

Nucleic Acid Sequence
Sequence Length: 4284
1106 a, 1315 c, 1062 g, 801 u
modified

 Related Sequences (2)

获取序列一致、修饰不同或
来自不同文献的相关序列

Sequence Details **序列详情**

Sequence: RNA; linear

151	accagaggcg	uguaucucc	cgacaaggug	uucagaucca	gcuugcugca
201	cucacccag	gaccugucc	ugccuuucu	cagcaacgug	accugguucc
251	acgcaucca	cguguccggc	accaauggca	ccaagagauu	cgaacacccc
301	gugcugcccu	ucaacgacgg	ggugauuuu	gccagcaccg	aggaguccaa
351	caucaucaga	ggcuggaucu	ucggcaccac	acuggacagc	aagaccacga
401	gccugcugau	cgugaacaac	gccaccaacg	uggucaucua	agugugcgag
451	uuccaguuu	gcaacgaccc	cuuccugggc	gucuacuacc	acaaggaaca
501	caagagcugg	auggaaagcg	aguuccgggu	guacagcagc	gccacaacuu
551	gcaccuucca	guacgugucc	cagccuuucc	ugauggaccu	ggaaaggcaag
601	caggggcaacu	ucaagaaccu	gcgcgaguuu	guguuaaaga	acaucgacgg
651	cuacuacaag	aucuacagca	agcacacccc	uaucaaccuc	ugcggggauu
701	ugccucaggg	cuucucugcu	cuggaacccc	ugguuggaucu	gcccaucggc
751	aucaacauca	ccceuuuca	gacacuecug	gcccuecaca	gaagcuaccu

Sequence Modifications **序列修饰详情**

Type	Description
modified base	guanosine-1 3'-me
modified base	guanosine-1 m7g
modified base	adenosine-2 am
uncommon link	guanosine-1 to adenosine-2 5'→5' triphosphate

Pharmacological Data 

Bioactivity Indicators

Target Indicators

Regulatory Information

CAS Sequences——Motif检索结果

 Search CAS Sequences 

Enter a protein or nucleotide string. [Learn more about CAS Sequences.](#)

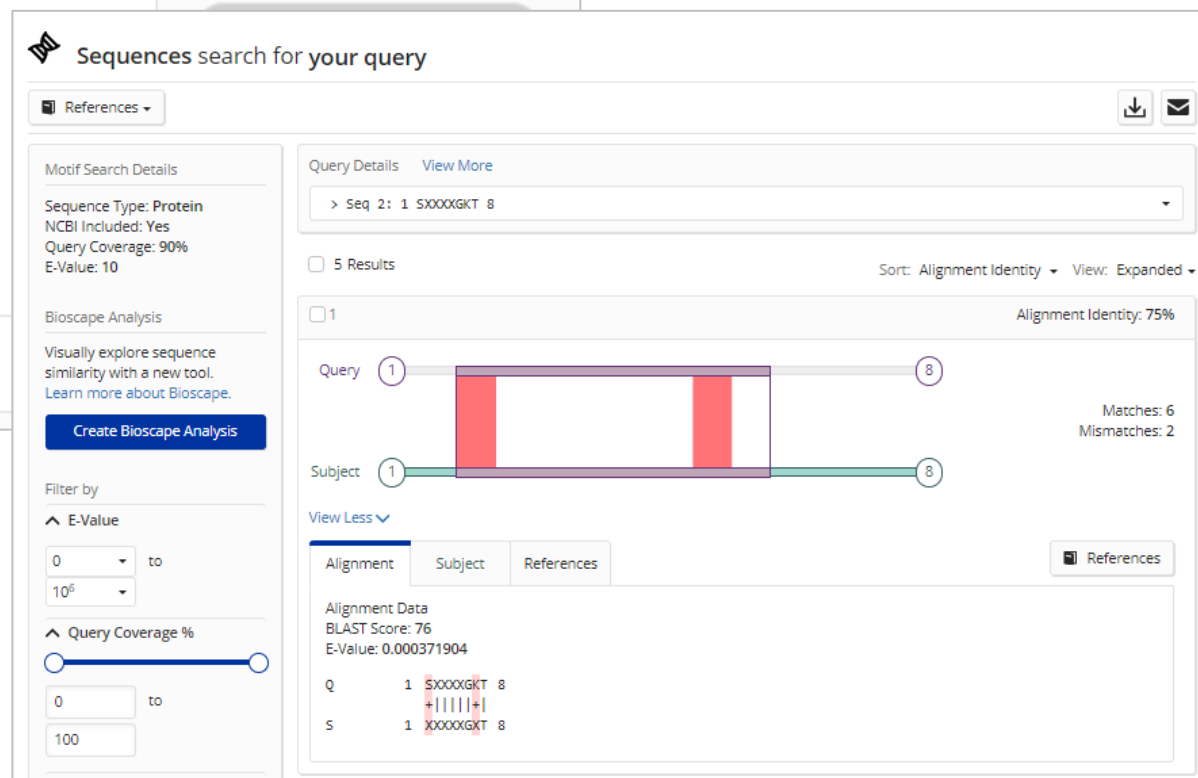
BLAST CDR **Motif** [Clear Search](#)

[SG]X{4}GK[DT]

Sequence Type:

- X代表未指定氨基酸，可以是常见或不常见氨基酸
- 对于核苷酸序列：N代表未指定核苷酸

[Advanced Sequence Search](#) ▼

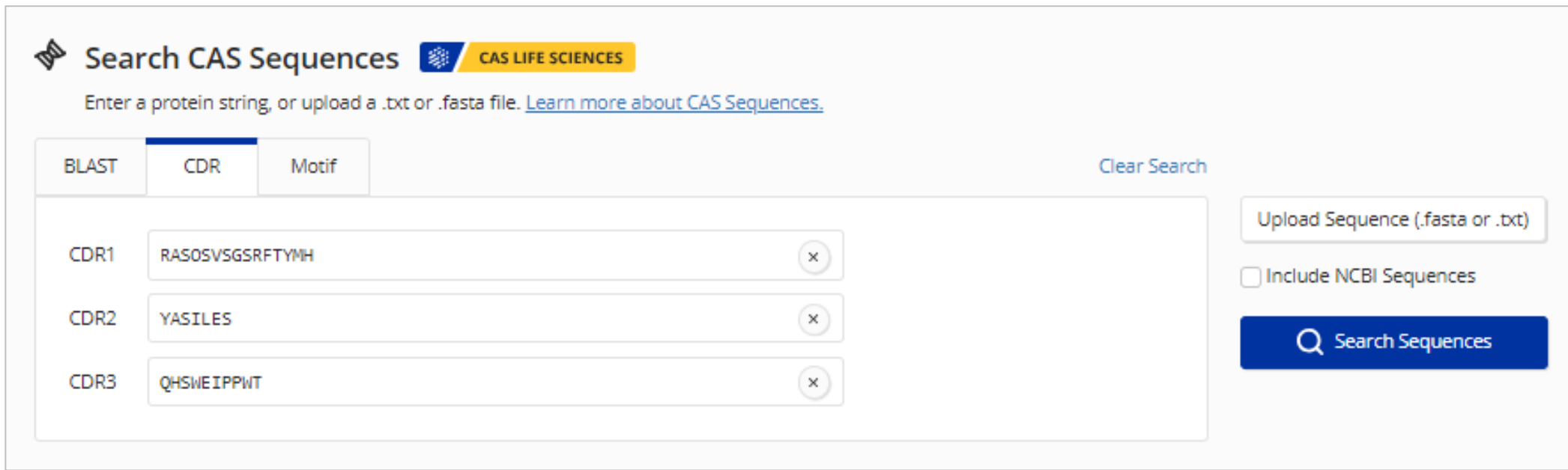


Motif中有可变部分，可借助符号来表示：

- “[]” 中括号：代表或者，表示出现在该位置的氨基酸或核苷酸是括号中的任意一个
- “{ }” 大括号：代表氨基酸或核苷酸的重复次数。其中字段可用逗号隔开，{2,6}表示在大括号左边紧密相连的氨基酸可重复2-6次

CAS Sequences——CDR检索结果

CDR (complementarity—determining regions): 抗体或细胞中的互补决定区



Search CAS Sequences CAS LIFE SCIENCES

Enter a protein string, or upload a .txt or .fasta file. [Learn more about CAS Sequences.](#)

BLAST **CDR** Motif [Clear Search](#)

CDR1 RASOSVSGSRFTYMH ×

CDR2 YASILES ×

CDR3 QHSWEIPPWT ×

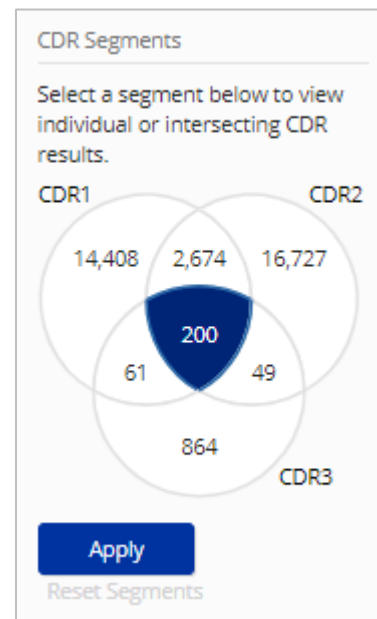
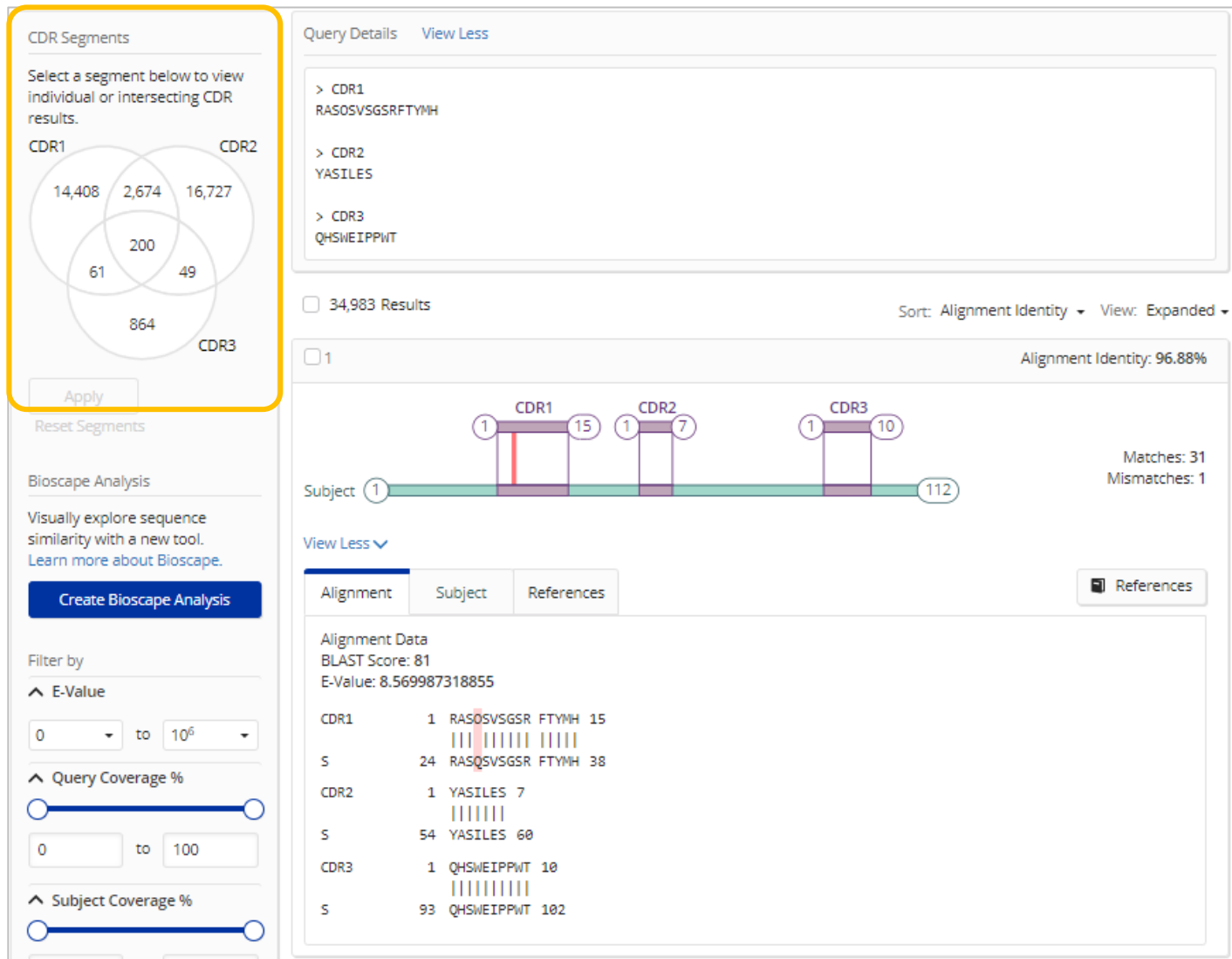
[Upload Sequence \(.fasta or .txt\)](#)

☐ Include NCBI Sequences

[Search Sequences](#)

支持单个或多个CDR序列检索并用

CAS Sequences——CDR检索结果



CDR Segments:

- 匹配到一个或者多个CDR的subject序列的序列数量
- 可根据已知信息和需求查看1-3个CDR被包含的序列结果

Reset segments:

- 重新选择查看匹配的序列结果

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
- 探索反应实验方案与合成相关策略
- 高效获取分析方法及配方制剂信息

常见问题Q&A



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)

Suppliers (79)

Suppliers (13)

By Scheme

By Document

By Transformation

Group: By Scheme Sort: Relevance View: Expanded ▾

Steps: 1 Yield: 85% ...

Relevance

Publication Date: Newest

Publication Date: Oldest

Yield

Number of Steps: Ascending

Number of Steps: Descending

Structure 2 (1 Reaction)

Suppliers (43)

Suppliers (3)

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

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

1.2 Reagents: [\(7-4\)-Trihydro\(tetrahydrof...](#)
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 ▾ Full Text ▾

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

8,161 Results

Group: By Transformation Sort: Reaction Count: Descending View: Expanded ▾

1

Reductive Alkylation of Ammonia or Amines
[View 121 Related Reactions](#)

2

Formation of N/O/S Heterocycles
[View 54 Related Reactions](#)

反应结果的筛选

筛选/排除，二次检索

Filter Behavior

[Filter by](#) [Exclude](#)

^ Search Within Results

Search for up to 3 structures within the result set.

 Draw

试剂

^ Reagent

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

[View All](#)

反应规模

^ Reaction Scale

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

催化剂

^ Catalyst

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

[View All](#)

不参与反应官能团

^ Non-Participating Functional Groups

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

[View All](#)

溶剂

^ Solvent

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

[View All](#)

反应注释

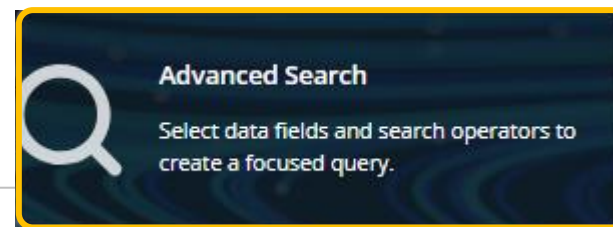
^ Reaction Notes

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

[View Fewer](#)

聚焦特定反应条件

Substance Role >
Reaction Condition >
Reaction Notes
Transformation Name
Document Identifier
Patent Identifier >
Author/Inventor >
Publication Name
Publication Year >



通过反应条件、类型、来源等，精确聚焦需要的反应

Advanced Search

Select a search type, and then add multiple search fields to build a query. ?

Substances Reactions References

- Time > 2h

Examples: 2 h | 30 min | 2h 30 min | 2h-3h | 2-3h | >2h | <30 min

AND Temperature (°C) rt

Examples: 20 | 20-50 | 20 to 50 | rt | >60 | <0

AND Catalyst Enter one substance identifier (chemical name, molecular formula etc.) or structure.

Examples: Pd/C | K2CO3

Edit Structure | Remove

AND Solvent 1,4-Dioxane

Examples: H2O | EtOH

Add Structure

AND Transformation Name Suzuki Coupling

Examples: Diels-Alder | Wittig | Grignard

+ Add Advanced Search Field Clear All

Search

支持绘制结构

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

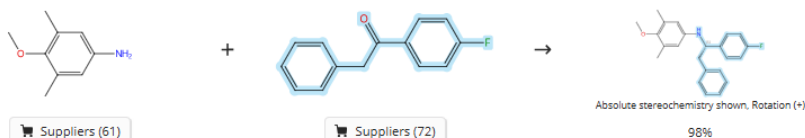
☒ Synthetic Methods (449)

☐ Experimental Procedure (5,678)

CAS Reaction Number: 31-614-CAS-41195127

Get Similar Reactions

获取相似反应



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), Ti(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 Ni(NTf₂)₂ (3.1 mg, 0.005 mmol, 5 mol%), (R)-Ph-BPE (3.1 mg, 0.006 mmol, 6 mol%) and GC standard n-C₁₂H₂₆ (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 _{C,F} = 243.0 Hz), 149.2, 143.3, 139.5 (d, J _{C,F} = 3.0 Hz), 137.7, 131.3, 129.4, 128.7, 128.1 (d, J _{C,F} = 8.0 Hz), 126.9, 115.5 (d, J _{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	[α] _D ²⁵ = +5.6° (c = 1.0, CHCl ₃)
Enantiomeric Excess	90%
HRMS	(ESI ⁺): Calcd for C ₂₃ H ₂₅ FNO [M+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 (-)

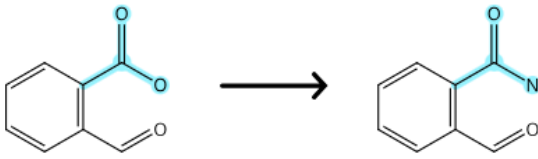
Suppliers (120) Suppliers (75)

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

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

Retrosynthetic Analysis——拓展反应路线设计思路

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

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

查看关注步骤的设计依据、可替换路线

Retrosynthetic Analysis

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

All Steps

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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

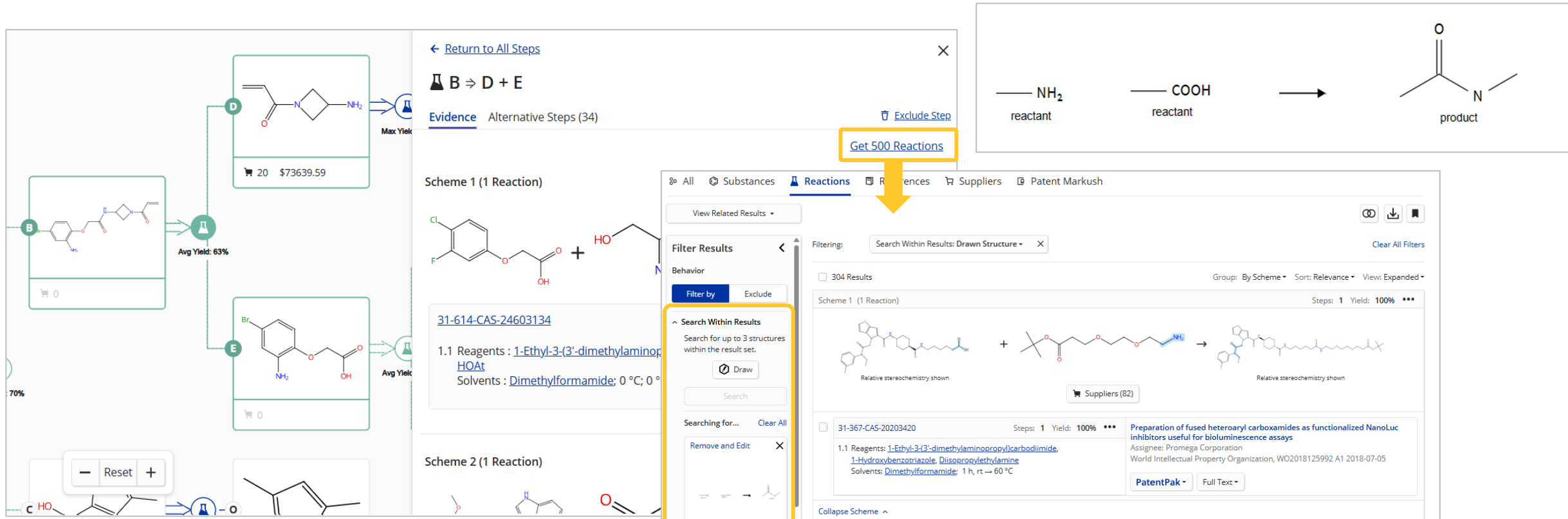
1.1 Reagents : Diisopropylethylamine, Phosphorus(1+), bromotri-1-pyrrolidinyl-, (T-4)-
Solvents : Dimethylformamide;
Get Experimental Protocols

56

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设计该步反应的依据从何而来?



进一步明确底物/产物的结构特征
筛选最感兴趣的合成路线

利用自然语言检索反应，降低检索难度

使用CAS数据训练的AI，智能识别检索意向，提供最相关反应检索结果

Reactions search for "Dehalogenation in isopropanol catalyzed by palladium"

All Substances **Reactions** References Suppliers Patent Markush

View Related Results

Filter Results

Behavior

Filter by Exclude

Search Within Results

Yield

Number of Steps

Non-Participating Functional Groups

Reaction Mapping

Reaction Scale

Experimental Protocols

Reaction Type

Stereochemistry

Reagent

Catalyst

Solvent

Commercial Availability

Reaction Notes

155,676 Results

Group: By Scheme Sort: Relevance View: Expanded

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%

Cobalt-Catalyzed Asymmetric Hydrogenation of 1,1-Diarylethenes
By: Chen, Jianhui; et al
Organic Letters (2016), 18(7), 1594-1597

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

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

Experimental Protocols

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"

乙酸钯催化合成醛类化合物

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)

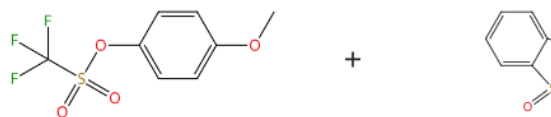
No Scale Provided (33K)

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"

羰基还原酶催化还原酮为醇类化合物

All Substances Reactions References Suppliers Patent Markush

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

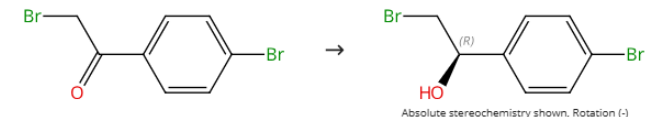
Reaction Type

Stereochemistry

Reagent

Catalyst

Scheme 1 (12 Reactions)



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

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

By: Yang, Jingwen; et al

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

Full Text

31-513-CAS-10291418

Steps: 1 Yield: 99% ***

1.1 Solvents: Ethanol; 18 h, 30 °C

Chiral pharmaceutical intermediaries obtained by reduction of 2-Halo-1-(4-substituted phenyl)-ethanones mediated by Geotrichum candidum CCT 1205 and Rhodotorula glutinis CCT 2182

By: Fardelone, Lucidio C.; et al

Enzyme Research (2011), 976368, 8 pp.

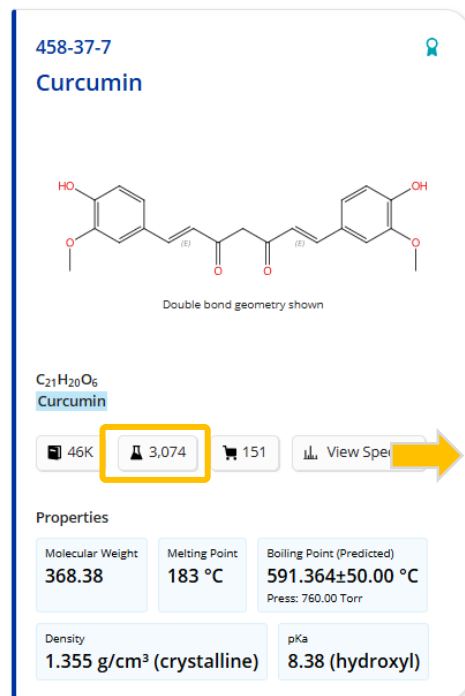
Full Text

59

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从目标物质出发，可拓展的合成实验



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

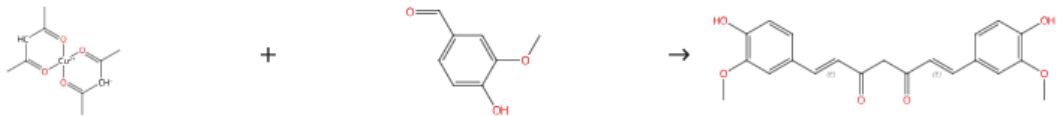
Stereochemistry

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

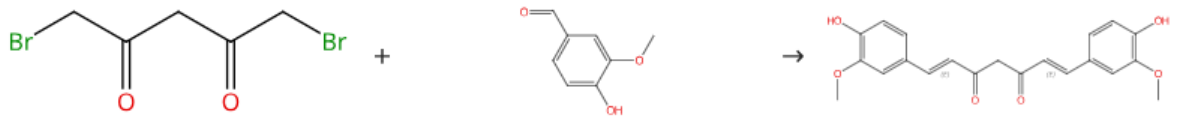
1.1 Reagents: Trimethyl borate
Catalysts: Butylamine
Solvents: Dimethylformamide; 50 min, 60 - 70 °C; 1.5 h, 60 - 70 °C

1.2 Reagents: Sulfuric acid
Solvents: Methanol; neutralized

1.3 Reagents: Hydrochloric acid
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

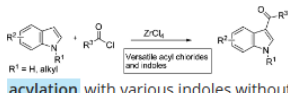
1,364 Results

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 nucleophilic character of indole. In this method, a wide range of aryl, heteroaryl, alkenyl, and alkanoyl chlorides undergo acylation with various indoles without NH protection and afford 3-acylindoles in good to high yields.

Full Text ▾

40

21

108

🔍

2

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

By: Vekariya, Rakesh H.; Aube, Jeffrey

Organic Letters (2016), 18(15), 3534-3537 | Language: English, Database: 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-Dichloroethane; 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-Dichloroethane; 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

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
- 探索反应实验方案与合成相关策略
- 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 like Document Type, Flags, Substance Role, Language, Publication Year, Author/Inventor, Organization, Publication Name, Concept, and CA Section. The 'CAS Content' section is highlighted, showing 'Analytical Methods (3,595)' and 'Formulations (2,495)'.
- Main Results List:** Displays search results for 'ciprofloxacin'. The first result is 'Enzymatic rotating biosensor for ciprofloxacin determination' by Torriero, Angel A. J.; Ruiz-Diaz, Juan J. J.; Salinas, Eloy; Marchevsky, Eduardo J.; Sanz, Maria I.; Talanta (2006), 69(3), 691-699. The second result is 'High-performance liquid chromatographic determination of ciprofloxacin in plasma samples' by Vybiralova, Z.; Nobilis, M.; Zoulova, J.; Kvetina, J.; Petr, P. Journal of Pharmaceutical and Biomedical Analysis (2005), 37(5), 851-858. A yellow arrow points to the 'Analytical Methods' link in the second result's title.
- Article Detail View (Right):** Shows the full text of the article 'High-performance liquid chromatographic determination of ciprofloxacin in plasma samples'. It includes the authors, DOI (10.1016/j.jpba.2004.09.034), abstract, keywords, and a 'Substances' section. The 'Substances' section lists '85721-33-1' and 'C₁₇H₁₈FN₃O₃ Ciprofloxacin' with its chemical structure. The role is listed as 'Analyte, Pharmacokinetics, Therapeutic Use, Analytical Study, Biological Study, Uses'.

CAS科学家增值标引的分析方法详情

Analysis of Ciprofloxacin in Blood plasma by HPLC

CAS Method Number
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

CAS

A division of the American Chemical Society

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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 prompts users to 'Search for keywords, matrices or analyte.' Below this, two main search options are highlighted: 'Explore Methods' (searching by criteria like method categories and subcategories) and 'Advanced Search' (searching by keywords, analytes, matrices, etc.).

The 'Explore Methods' section is expanded, showing a list of categories on the left and a list of category names on the right. The 'Pharmacology / Toxicology' category is selected, leading to the 'Active Pharmaceutical Ingredient' category name. A search bar for 'Include Keywords (Optional)' is also present.

On the right, the 'Results for Active Pharmaceutical Ingredient and Metabolite Analysis' are displayed. Two results are shown:

- Analysis of Ketoconazole by Cyclic voltammetry**
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
- Analysis of Rabeprazole in Blood serum by Ion mobility spectrometry**
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

分析方法检索结果的分析与精炼

分析物

基质

方法分类

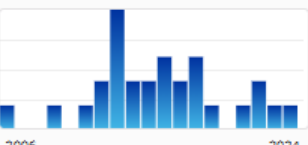
技术&仪器

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 点击标题，可进入分析方法详情。

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

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](#) [Compare](#)

2

Analysis of Lapatinib in Blood plasma by Solvent extraction [JOURNAL](#)

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)

[Compare](#)

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; / precipitation Security guar	Source	JOURNAL A stable isotope-labeled internal standard is essential for correcting for the interindividual variability in the recovery of lapatinib from cancer patient plasma in quantitative LC-MS/MS analysis By: Wu, Jianmei; Wiegand, Richard; LoRusso, Patricia; Li, Jing Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences (2013), 941, 100 - 108. Full Text ▾	JOURNAL A sensitive LC-MS-MS assay for the determination of lapatinib in human plasma in subjects with end-stage renal disease receiving hemodialysis By: Kocan, GERALYN P.; Huang, Mike; Li, Fumin; Pai, Sudhakar Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences (2018), 1097-1098, 74 - 82. Full Text ▾
Equipment Used	LC system., Alliance2695, Waters, Milford, MA, USA; Triple quadrupole mass spectrometer, Quattro Micromass, Waters	HPLC system, Shimadzu, Ky Kyoto, Japan; Sciex, Ontario			
Conditions	Instrument: ionization mode-Positive; heated nebulized probe- 350 °C; pressure of collision gas (Argon) (mbar)- 5.92E-003, 5.92E-003 and 5.92E-003 for lapatinib, lapatinib-d3 and zileuton; dwell time (s)- 0.5, 0.5 and 0.5, for lapatinib, lapatinib-d3 and zileuton; cone voltage (V)- 60, 60 and 22 for lapatinib, lapatinib-d3 and zileuton; collision energy (eV)- 34, 34 and 12, for lapatinib, lapatinib-d3 and zileuton; transition- 581.4>364.96, 584.1>366 and 237.43>161.09, for lapatinib, lapatinib-d3 and zileuton.Chromatographic: XBridge C18 column (3.5 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.	Instrument: and security g 10 mM amm acetonitrile; C supply 2: 80 a V; source gas declustering potential: 102 V and collision energy: 50 V for both lapatinib and internal standard			

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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'. The 'Advanced Search' section is highlighted with an orange arrow pointing to a detailed 'Advanced Formulations Search' dropdown menu. This menu includes a 'Search For' dropdown set to 'Ingredient', an 'Operator' dropdown set to 'Required', and a text input field with an example 'Ex: caffeine, sodium, 50-00-0'. A list of search fields (All Fields, Form, Function, Ingredient, Purpose, Route, Target) is shown below the input field. To the right of the list, there are checkboxes for 'Required', 'Optional', and 'Excluded'. A 'Search' button and a 'Clear All' link are also visible.

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

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)

Language

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

Publication Year

Filter by

Industry

☐ Inks, Paints, & Coatings
☐ Unclassified

Purpose

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

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)

Formulations search for "photoresists"

Get Additional References

188 Results

Sort: Relevance Group: By Family

1

点击标题，可进入制剂/配方详情。

Compare

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	-	-

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

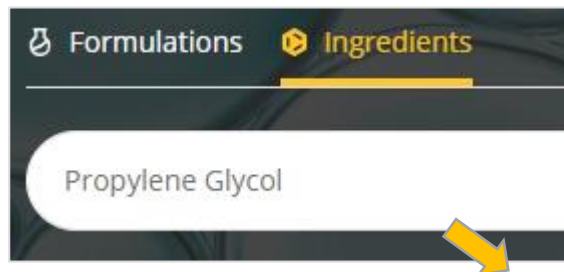
preparation of positive photosensitive anionic electrodeposition coating composition: mix vinyl copolymer (place 10.0 parts of isopropanol and 10.0 parts of butyl cellosolve in a 3-liter four-necked flask equipped with a stirrer, a reflux condenser and a nitrogen inlet tube, and heat to 90 °C. separately,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

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[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

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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'"

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- ☐ Analytical Methods (9)
- ☐ Formulations (3)

▼ Life Science Data

^ Formulation Purpose

- ☐ Cardiovascular agents (3)

▼ Databases

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1

Prevention and treatment of chronic heart failure

By: Jia, Qiujin; Wang, Lirong; Zhang, Xiaonan; Ding, Pharmacological Research (2020), 151, 104552 | L

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

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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 ...

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

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- 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)
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and progress **are**
connections that
matter

谢谢!

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