

CAS SCIFINDER
DISCOVERY PLATFORM™

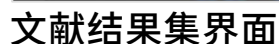
快速入门 指南

学术版

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检索界面



- 文献检索结果按照上一次设置偏好排序。
- 可以使用筛选项进一步缩小检索结果范围。
- 可以保存检索结果，发送链接，设置提醒，或将检索结果添加到项目列表。



文献详情和检索运算符

文献详情

获取 CAS SciFinder 中每篇文献的详细信息。

Development and validation of stability indicating reversed-phase liquid chromatographic method for simultaneous quantification of methotrexate and teriflunomide in nanoparticles and marketed formulation

2

0

8

Citation Map

查看文献的引文地图

Download

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Bookmark

In this Reference

Concepts

Substances

Analytical Methods

Formulations

Cited Documents

By: Pandey, Shweta; Mahtab, Asiya; Singh, Archu; Ahmad, Farhan Jalees; Aqil, Mohd.; Talegaonkar, Sushama

DOI: 10.1002/bmc.4372

Methotrexate (MTX) and teriflunomide (TEF) are the two most effective disease-modifying antirheumatic drugs used as combination therapy for rheumatoid arthritis and no robust high-performance liquid chromatog. (HPLC) method is available for their simultaneous estimation to date. Therefore, we have developed and validated an isocratic reversed-phase HPLC method for simultaneous anal. of MTX and TEF spiked in the form of active pharmaceutical ingredients, tablets and nanoformulations. The best separation was achieved on a BDS, C₁₈, 4.6 × 250 mm, 5 µm anal. column (Thermo Hypersil) with methanol-ethylammonium formate-potassium dihydrogen phosphate buffer (55 mM, pH 3.5; 65:5:30, volume/volume) as mobile phase at a flow rate of 0.8 mL/min. All the samples were subjected to force degradation studies. Responses of MTX and TEF were found to be a linear function of concentration over the range 1-50 µg/mL (r² = 0.9976 and 0.9982). The limits of detection and limit of quantification were 7.74 and 25.82 ng/mL and 10.74 and 35.80 ng/mL, resp. Degradation products produced under the stress studies did not interfere with the detection of MTX and TEF and therefore the developed method can be regarded as stability indicating.

Keywords: reversed phase HPLC methotrexate teriflunomide nanoparticle formulation stability; Teriflunomide; hydroxyapatite nanoparticles; liposomes; methotrexate; nanostructured lipid carriers; reversed-phase HPLC

View Source

Full Text

View in CAS Analytical Methods

View in CAS Formulus

Publication Information • Journal

查看分析方法详情

查看配方/制剂详情

View Less

Source	Database Information	Company/Organization	Publisher	Language
Biomedical Chromatography Volume: 32 Issue: 12 Pages: n/a Journal: Article 2018 DOI: 10.1002/bmc.4372 CODEN: BICHE2 E-ISSN: 1099-0801	AN: 2018:1864661 CAN: 170:324809 PubMed ID: 30133709 CAPus and MEDLINE	Department of Pharmaceutics, School of Pharmaceutical Education and Research Jamia Hamdard New Delhi India	John Wiley & Sons Ltd.	English

题录信息

布尔逻辑运算符

如下所示，您可以使用布尔逻辑运算符进行文献检索，可以通过使用括号对逻辑运算符进行优先运算。

References (flavor or odor) and menthol not cigarette Draw

AND 要求文献结果中同时出现两个术语。

OR 要求文献结果中至少出现其中一个术语或两个术语都出现。

NOT 从检索结果中排除包含NOT后面的词语的文献结果。

使用通配符可在文献检索、物质检索以及二次筛选检索中获得更全面的结果，通配符可用于词中或者词尾。

* 可替换0到多个字符 例如: polymorph* | immunoglobulin*conjugate*

? 可替换0个或者1个字符 例如: benzonorbornen?

包含双引号的短语将作为精确短语进行检索。
例如：搜索 "Programmed cell death protein" 只会找到完全匹配 "Programmed cell death protein" 的结果。

CAS SciFinder Discovery Platform 快速入门指南 | 3

CAS Lexicon

CAS Lexicon 概述

可以通过 CAS Lexicon，在 CAS 总的词库层级中浏览 CAS 科学家标引的概念词或核心研究点，或相关的重要物质，并建立用于文献检索的检索式。

访问和浏览

Search CAS Lexicon

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

biopesticides

Search Concept

Multiple preferred concepts found. Click one to continue.

Biopesticides

RNA interference

Plant-incorporated protectants

Biopesticides

Pesticides based on microorganisms, substances produced by plants, plant-incorporated protectants, or other naturally occurring substances or their synthetic analogs that control pests.

Biopesticides

Search Concept

Preferred Concept

☒ Biopesticides

This will search synonyms: Biocontrol agents (pest); Biological control ...
[View more synonyms](#)

Broader Concepts (2)

Select All

☐ Agricultural biological agents

☐ Pesticides

Narrower Concepts (9)

Select All

☐ Biochemical pesticides

☐ Biofungicides

☐ Bioherbicides

可以通过选择核心研究点并将其添加到右侧的检索窗口，来构建高度精准的 CAS Lexicon 检索。只有选定的 CAS 核心研究点会被检索。

Preferred Concept

☒ Biopesticides

This will search synonyms: Biocontrol agents (pest); Biological control ...
[View more synonyms](#)

Broader Concepts (2)

Select All

☐ Agricultural biological agents

☐ Pesticides

Narrower Concepts (9)

Deselect All

☒ Biochemical pesticides

☒ Biofungicides

☒ Bioherbicides

☒ Bioinsecticides

☒ Bionematocides

☒ Botanical pesticides

☒ Microbial pesticides

☒ Plant-incorporated protectants

Biopesticides - Preferred Concept

Biopesticides - Narrower Concepts (9)

Biochemical pesticides

Biofungicides

Bioherbicides

Bioinsecticides

Bionematocides

Botanical pesticides

Microbial pesticides

Plant-incorporated protectants

RNA interference pesticides

AND OR NOT

Add to Query

Clear Query

Search

用逻辑运算符组合不同的核心研究点

将所选词加入右侧检索窗口

点击下位词以查看其子类别

执行检索

专利检索

专利文献筛选及可视化分析

在文献结果集中，通过 Document Type 选项获得专利文献，支持筛选专利局、IPC 分类号等。在 "Analyze Results" 中对专利布局进行可视化分析。

References search for "(pesticide or "pest control") and rice not pollution"

View Related Results

We are displaying the most relevant results.
Learn about result relevance.
Load All Results

Filter Results

Analyze Results

Behavior

Filter by

Exclude

Search Within Results

Document Type

Patent Office

Patent Status

Language

Publication Year

International Patent Classification (IPC)

Author/Inventor

Organization

Filtering: Document Type: Patent X

10,645 Results

Sort: Relevance View: Partial Abstract

1

Composition of 4-oxo-4-[(2-phenylethyl)amino]-butyric acid and second pesticide, and method for controlling arthropod pests

Assignee: Sumitomo Chemical Company, Limited
World Intellectual Property Organization, WO2011062291 A1 2011-05-26 | Language: English, Database: CPlus

Patent Status: Dead Family Members: JP JP CA AR + 14 more

The present invention provides an arthropod pests control composition comprising, as active ingredients, 4-oxo-4-[(2-phenylethyl)amino]-butyric acid and a compound of formula (I), wherein X¹ represents a C₁-C₃ alkyl group or a hydrogen atom, X² represents a Me group or -CH(CH₃)-cycPr, X³ represents a Me group or a halogen atom, X⁴ represents a Me group, a cyano group or a halogen atom, and X⁵ represents a trifluoromethyl group or a halogen atom; and a method of controlling arthropod pests, which comprises applying effective amounts of 4-oxo-4-[(2-phenylethyl)amino]-butyric acid and a compound.

View More

2

Preventing and controlling method for rice disease and insect pest

Assignee: Unknown
China, CN105519369 A 2016-04-27 | Language: Chinese, Database: CPlus

Patent Status: Dead

Preventing and controlling method for rice disease and insect pest, comprises: step 1, before sowing, basking seeds in sunshine, manually selecting, removing impurity and diseased seed, Step 2, soaking the basked seed in step 1 in clean water for 10-12h, Step 3, adopting the 1500-2000 times solution of 25% prochloraz to soak seeds for 24-35h, carrying out pregermination sowing, and growing seedlings, Step 4, monosultap 80 g and 75% fengdeng (pesticide) 35 g, carrying out foliage-planting seedling, step 5, in heading stage, adopting 500 times...

Analyze Results

Top Document Types

Patent

Download visualization analysis

Patent Offices

1 8,853

World Map

Other

ARIPO 26 EAPO 55 EPO 920

专利权利要求

在专利文献详情页的导航栏中点击 "Claims"，查看专利权利要求。

CAS SciFinder

Pyridinylimidazole

2,094 216 7

In this Patent

Claims

Classifications

CAS Concepts

Markush Structures

Substances

Reactions

Formulations

Claims

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

1 What is claimed is:
A composition comprising a molecule according to Formula One:

Formula One

Chemical Structure

wherein
(a) X is N or CR8;
(b) R1 is H, F, Cl, Br, I, CN, NO2, substituted or unsubstituted C1-C6 alkyl, substituted or unsubstituted C2-C6 alkenyl, substituted or unsubstituted C1-C6 alkoxy, substituted or unsubstituted C2-C6 alkenyloxy, substituted or unsubstituted C3-C10 cycloalkyl, substituted or unsubstituted C3-C10 cycloalkenyl, substituted or unsubstituted C6-C20 aryl, substituted or unsubstituted C1-C20 heterocyclyl, OR9, C(=X1)R9, C(=X1)N(R9), N(R9)2, N(R9)C(=X1)R9, SR9, S(O)OR9, or R9S(O)R9, wherein each said R1, which is substituted, has one or more substituents selected from F, Cl, Br, I, CN, NO2, C1-C6 alkyl, C2-C6 alkenyl, C1-C6 haloalkyl, C2-C6 haloalkenyl, C1-C6 haloalkyloxy, C2-C6 haloalkenyloxy, C3-C10 cycloalkyl, C3-C10 cycloalkenyl, C3-C10 halocycloalkyl, C3-C10 halocycloalkenyl, OR9, S(O)OR9, C6-C20 aryl, or C1-C20 heterocyclyl, each of which that can be substituted, may optionally be substituted with R9;
(c) R2 is H, F, Cl, Br, I, CN, NO2, substituted or unsubstituted C1-C6 alkyl, substituted or unsubstituted C2-C6 alkenyl, substituted or unsubstituted C1-C6 alkoxy, substituted or unsubstituted C2-C6 alkenyloxy, substituted or unsubstituted C3-C10 cycloalkyl, substituted or unsubstituted C3-C10 cycloalkenyl, substituted or unsubstituted C6-C20 aryl, substituted or unsubstituted C1-C20 heterocyclyl, OR9, C(=X1)R9, C(=X1)N(R9), N(R9)2, N(R9)C(=X1)R9, SR9, S(O)OR9, or R9S(O)R9, wherein each said R2, which is substituted, has one or more substituents selected from F, Cl, Br, I, CN, NO2, C1-C6 alkyl, C2-C6 alkenyl, C1-C6 haloalkyl, C2-C6 haloalkenyl, C1-C6 haloalkyloxy, C2-C6 haloalkenyloxy, C3-C10 cycloalkyl, C3-C10 cycloalkenyl, C3-C10 halocycloalkyl, C3-C10 halocycloalkenyl, OR9, S(O)OR9, C6-C20 aryl, or C1-C20 heterocyclyl, each of which that can be substituted, may optionally be substituted with R9;

CAS SciFinder Discovery Platform 快速入门指南 | 5

在 Markush Structures 中查看专利中的马库什结构和详情信息。

权利要求中的物质

在物质检索结果中，可以利用物质研究角色 Substances Claimed 定位专利权利要求中的物质。

现有技术探索

在 CAS SciFinder 主页点击 “Prior Art Discovery”，利用自然语言和结构式（可选），进行 AI 驱动的现有技术探索。

❖ Prior Art Discovery

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

This disclosure is related to the field of processes to produce molecular molecules to control pests. In general, the molecules of Formula One n, butterflies, lice, grasshoppers, locusts, crickets, fleas, thrips, bristletails, formulation can also contain other components. These components include insecticides, drift reduction agents, compatibility agents, and anti-

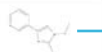
输入不少于200个英文字符的自然语言，进行现有技术探索

Priority Date: 08-12-2025 Edit

自定义日期

Add Structure (Optional)

Edit



输入结构

Edit Drawing Remove

❖ Prior Art Discovery for "This disclosure is related to the field of processes to produce molecules that are useful as pesticides (e..."

专利文献

Patents (93)

非专利文献

Non-Patent Literature (83)

Search Details

Your Inputs

Text

This disclosure is related to the field of processes to produce molecules that are useful...

View All

Priority Date

2025-08-13

Structure



1

Pyridinylimidazoles as pesticidal and processes for preparation and pesticidal composition

Assignee: Dow AgroSciences LLC

US20120110701 A1, Publication Date: 2012-05-03 | Priority Date: 2010-11-03

...to pyridinylimidazoles of **formula I** as **pesticides** useful in pest control. Compounds of **formula I** wherein X is N and XR8; R1, R2, R3, R4 and R8 are independently H, F, Cl, Br, I, CN, etc.; R5 is H, (un)substituted C1-6...

Full Text

2

Sustained-release pesticidal compositions

Assignee: HOMS, LLC

US20080069785 A1, Publication Date: 2008-03-20 | Priority Date: 2004-12-14

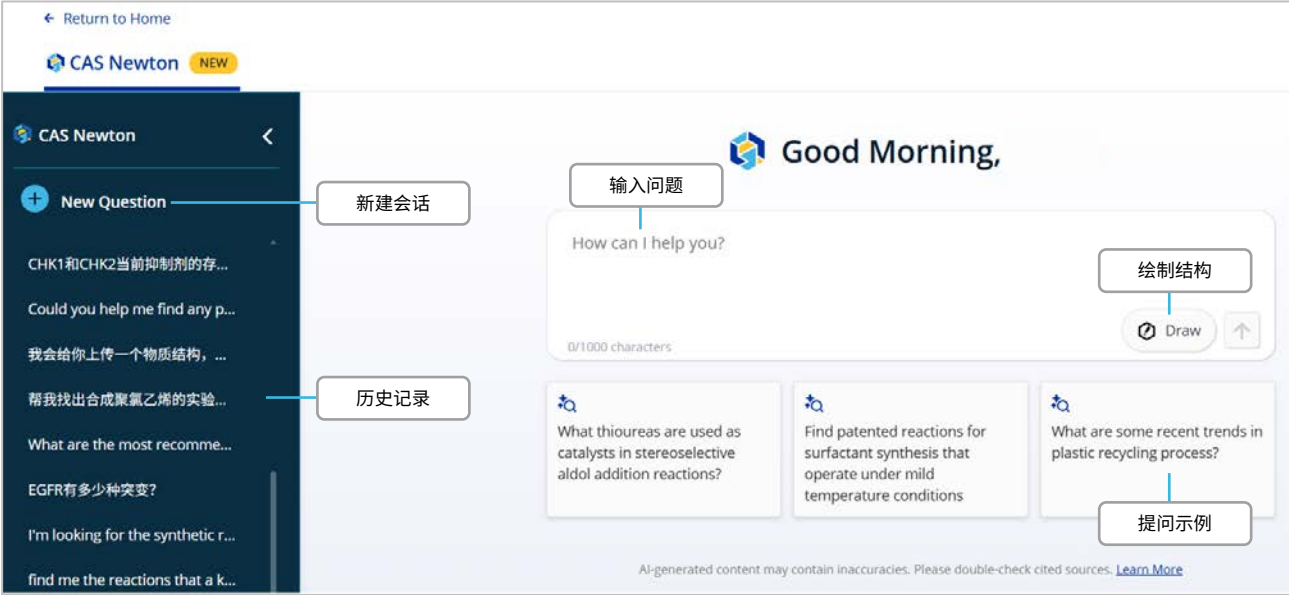
...include aphids, arca, bed bugs, bees, beetles, centipedes, caterpillars, chiggers, cockroaches, crickets, cutworms, earwigs, fleas, flies, fire ants, gnats, grasshoppers, hookworms, Japanese beetles, June bugs, lice, locusts, maggots, mealworms, mealybugs, millipedes, mites, mosquitoes, moths, pillbugs, scorpions, silverfish, spiders, stinkbugs, termites, thrips, ticks...

Full Text



CAS Newton——代理式人工智能

CAS Newton 是一款专为科学发现而打造的、具备科学智能的代理式人工智能。



CAS Newton 依托 CAS 内容合集，将大量参考文献提炼为简明见解，确保信息准确且科学严谨，有效规避 AI 幻觉。支持多轮互动，可连贯上下文，随着问题的深入持续改进方法，大幅降低专业检索门槛。



智能检索

AI Summary

在文献结果页面查看 AI Summary——AI 技术对检索结果进行的提炼和总结，更快理解文献中披露的信息。

AI Summary

Based on the search results, here's a summary of key findings related to crown ether and lithium and salts:

The search results highlight various aspects of crown ether-like lithium salts, including their synthesis, properties, and applications. One study describes the formation of amorphous solid electrolytes using cryptands or crown ethers with lithium salts, while another examines the transport rates of metal cations through bulk liquid membranes containing crown ethers. Additionally, research has been conducted on the design of asymmetric ether-like lithium salts to improve the performance of lithium metal batteries. Another study presents a nanofiltration membrane with crown ether as exclusive Li+ transport channels for efficient extraction of lithium from salt lake brine. Furthermore, the isolation and X-ray structures of lithium crown ether salts of free phenyl carbanions are discussed, along with the computerized conductometric determination of stability constants of complexes of crown ethers with alkali metal salts and neutral molecules in polar solvents.

Key Findings:

查看文献来源

1. Amorphous Solid Electrolytes:

- Amorphous solid electrolytes can be formed by the interaction of cryptands or crown ethers with lithium salts when the cavity size of the macrocycle does not match the diameter of the lithium cation. (1)

2. Metal Cation Transport Rates:

- The transport rates of metal cations through bulk liquid membranes containing crown ethers depend on the cation concentration in the source salt solution phase and the anion type. (2)

3. Lithium Metal Battery Performance:

- Designing an asymmetric ether-like lithium salt can improve the fast-cycling performance of lithium-metal batteries, particularly for practical lithium-metal batteries with high cathode loading. (3)

4. Nanofiltration Membranes:

- A nanofiltration membrane with crown ether as exclusive Li+ transport channels, generated by crown ethers, can efficiently extract lithium from salt lake brines with high Mg2+/Li+ mass ratio. (4)

5. Isolation and X-ray Structures:

- The isolation and X-ray structures of lithium crown ether salts of free phenyl carbanions have been reported, providing insight into the molecular structure of these compounds. (9)

Designing an asymmetric ether-like lithium salt to enable fast-cycling high-energy lithium metal batteries
Nature Energy (2023), 8(9), 934-945
Language: English, Database: CAplus

自然语言检索

您可以通过输入自然语言，查询文献、物质、反应和供应商等多类型的信息。
检索示例：检索 "Raman spectra of luminol"，查看3-氨基-苯二甲酰肼的拉曼谱图。

CAS SciFinder

Raman spectra of luminol

输入自然语言

Draw

45

Results for "Raman spectra of luminol"

All Substances Reactions References Suppliers Patent Markush

Spectrum

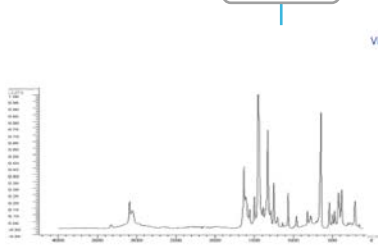
Showing 1 of 1 Result

查看谱图

Experimental

View Spectra Details

521-31-3
Luminol
Viewing 1 of 1



查看所有谱图

View All Spectra

Raman Spectrum

Conditions
No data available.

Spectra Summary

Spectrum ID
SLSRAMAN_000706

Source
Sigma-Aldrich Co. LLC. (Spectr...)

View All

智能检索

输入自然语言，查询物质属性。

检索示例：检索 "boiling point of ethanol"，获取乙醇的沸点信息。

Results for "boiling point of ethanol"

All Substances Reactions References Suppliers Patent Markush

64-17-5
Ethanol

Boiling Point
78.5 °C

Source
"Hazardous Substances Data Bank" data were obtained from the National Library of Medicine (US)

Boiling Point Properties
Showing 5 of 423 Results [View in Detail Page →](#)

Value	Condition	Source
78.5 °C	-	"Hazardous Substances Data Bank" data were obtained fro...
181.27 °C	Press: 15200 Torr	Semenov, I. P.; Theoretical Foundations of Chemical Enginee...
110 °C (approx)	-	Horikoshi, Satoshi; Scientific Reports, (2018), 8(1), 1-10, CAplus
85 °C (approx)	-	Li, H.; Proceedings of the Combustion Institute, (2017), 36(1)...
80 °C	-	Singh, Akhileendra Pratap; Journal of Energy Resources Techn...

输入自然语言，查询反应信息。您可以指定多种反应角色，包括：

- "synthesis/preparation/manufacture of..." 连接物质指定目标反应产物
- "from" 连接物质指定反应物或试剂
- "in" 连接物质指定溶剂
- "catalyzed by" 连接物质指定催化剂
- "mediated by" 连接物质指定试剂

检索示例：检索 "synthesis of paclitaxel catalyzed by triphenylphosphine"，获取三苯基膦催化的紫杉醇合成反应。

Reactions search for "synthesis of paclitaxel catalyzed by triphenylphosphine"

All Substances **Reactions** References Suppliers Patent Markush

View Related Results

7,007 Results Group: By Scheme Sort: Relevance View: Expanded

Filter Results

Behavior

Filter by Exclude

Search Within Results

Non-Participating Functional Groups

Alcohol (1)

Scheme 1 (1 Reaction) Steps: 1 Yield: 60% ***

Absolute stereochemistry shown, Rotation (-)

+

Suppliers (82)

→

Absolute stereochemistry shown, Rotation (-)

Suppliers (139)

物质检索

检索物质相关的方式有：1. 物质名称、CAS 登记号等；2. 结构式；3. 官能团（自然语言）；4.文献标识符。

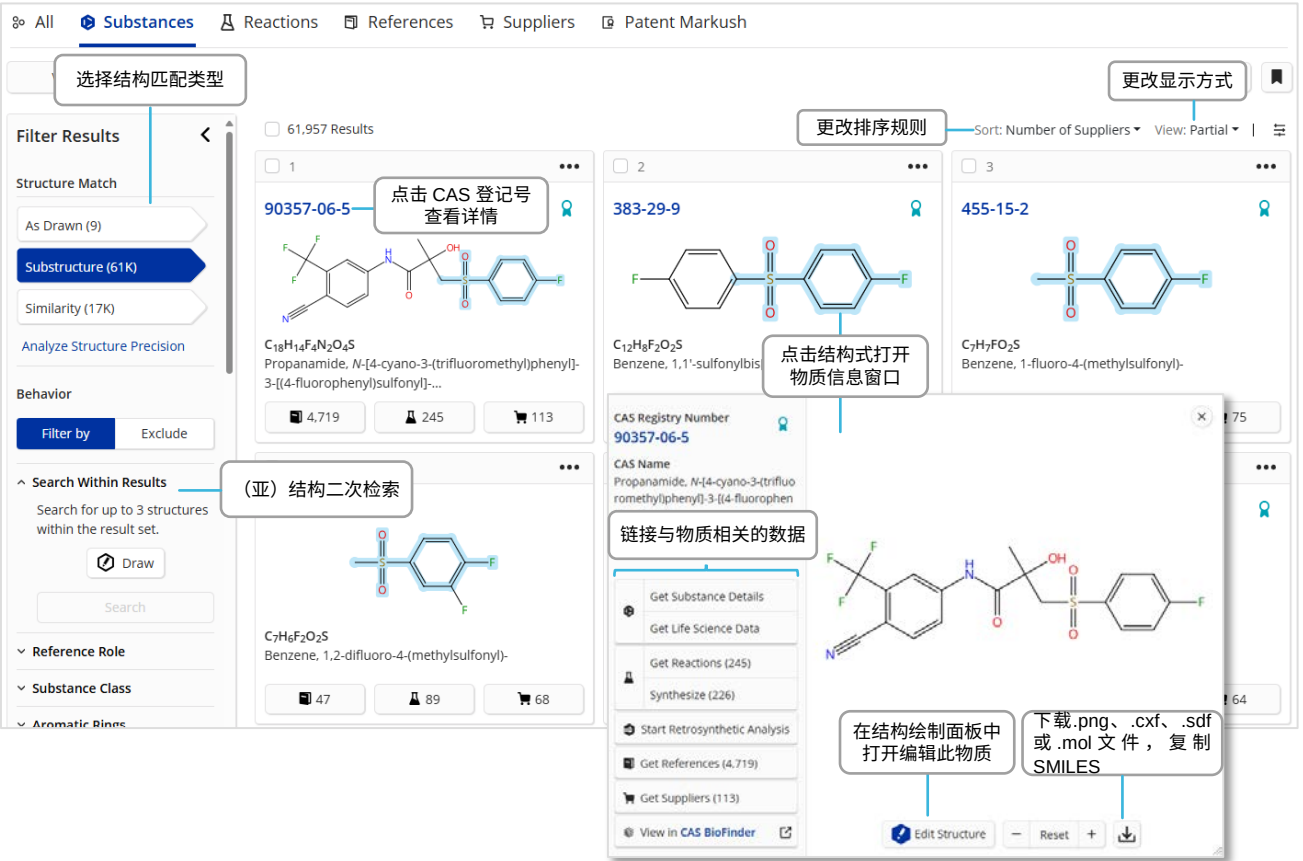
以下是物质检索的示例：

Streptomycin
57-92-1
"Streptomycin sulfate"
Sulfoximin*
WO2019234160



物质检索结果

物质检索结果在一个直观的界面中呈现，包括物质名称、CAS 登记号和高分辨率结构式图像。您可以通过 Sort 选择结果的排序规则，包括相关度、分子量、分子式、关联文献的数量或供应商的数量等。



结构绘制面板和物质详情

CAS 结构绘制面板

如需利用结构检索，您可以使用 CAS 结构绘制面板绘制结构式或反应式进行查询。

The screenshot shows the CAS Draw software interface. Annotations include:

- CAS Draw**: Select Search Type (Substances, References, Reactions, Suppliers, Patent Markush, All).
- 选择检索类型, 物质、文献、反应、供应商、专利 Markush 或一站式检索**: Select Search Type (Substances, References, Reactions, Suppliers, Patent Markush, All).
- 导入和导出结构文件**: Import and Export Structure Files.
- 套索|选框工具**: Lasso/Selection Tool.
- 绘制原子和化学键|橡皮擦**: Draw Atoms and Chemical Bonds | Eraser.
- 元素周期表|常见官能团和保护基**: Periodic Table | Common Functional Groups and Protecting Groups.
- 可变基团定义工具|R基团定义工具**: Variable Group Definition Tool | R-Group Definition Tool.
- 片段结构定义工具|从模板中选择结构**: Fragment Structure Definition Tool | Select Structure from Template.
- 添加正电荷|添加负电荷**: Add Positive Charge | Add Negative Charge.
- 重复结构单元工具|碳链工具**: Repeat Structure Unit Tool | Carbon Chain Tool.
- 可变位置定义工具|环锁定工具**: Variable Position Definition Tool | Ring Locking Tool.
- 原子锁定工具|旋转/翻转片段**: Atom Locking Tool | Rotate/Flip Fragment.
- 反应角色定义工具|反应原子标记工具**: Reaction Role Definition Tool | Reaction Atom Marking Tool.
- 化学键标记工具|反应箭头绘制工具**: Chemical Bond Marking Tool | Reaction Arrow Drawing Tool.
- 了解键盘快捷键 (例如, 快捷绘制杂原子)**: Learn Keyboard Shortcuts (e.g., Quick Drawing of Heteroatoms).
- 可输入系统命名、CAS 登记号、SMILES 或 InChI 以创建结构**: Can enter systematic name, CAS registry number, SMILES, or InChI to create structure.
- 杂原子和氢同位素绘制**: Draw Heteroatoms and Hydrogen Isotopes.
- 绘制化学键, 带有 ▲ 符号说明有其他展开选项**: Draw Chemical Bonds, with ▲ symbol indicating other expandable options.
- 调整窗口大小**: Adjust Window Size.
- 绘制环**: Draw Rings.
- 输入要绘制的元素符号**: Enter the element symbol to be drawn.
- Zoom: 100%**: Zoom level indicator.

物质详情

点击某个物质检索结果的 CAS 登记号时, 会显示该物质的详细信息, 包括结构式、分子式、物质性质及其他信息。

The screenshot shows the CAS Registry Number 90357-06-5 page. Annotations include:

- CAS Registry Number: 90357-06-5**: CAS Registry Number: 90357-06-5.
- 结构被专利保护的系列专利信息**: Structure is protected by a series of patent information.
- Patents Claimed In**: Patents Claimed In.
- Methods for treating prostate cancer with radiopharmaceuticals**: Methods for treating prostate cancer with radiopharmaceuticals.
- Role: Therapeutic Use**: Role: Therapeutic Use.
- Patent Number: WO2025189134**: Patent Number: WO2025189134.
- Publication Date: 2025-09-11**: Publication Date: 2025-09-11.
- Preparation of triazolo[4,5-b]pyridine compounds useful as inhibitors of Werner Syndrome RecQ helicase (WRN)**: Preparation of triazolo[4,5-b]pyridine compounds useful as inhibitors of Werner Syndrome RecQ helicase (WRN).
- Role: Therapeutic Use**: Role: Therapeutic Use.
- Patent Number: WO2025172934**: Patent Number: WO2025172934.
- Publication Date: 2025-08-21**: Publication Date: 2025-08-21.
- Combined use of antibody-drug conjugate and androgen receptor antagonist**: Combined use of antibody-drug conjugate and androgen receptor antagonist.
- Role: Therapeutic Use**: Role: Therapeutic Use.
- Patent Number: WO2025167929**: Patent Number: WO2025167929.
- Publication Date: 2025-08-14**: Publication Date: 2025-08-14.
- View All Patents**: View All Patents.

Other annotations include:

- 按希尔顺序排列的分子式**: Molecular formula arranged by Hill order: $C_{18}H_{14}F_4N_2O_4S$.
- CA 索引名**: CA Index Name: Propanamide, N-(4-cyano-3-(trifluoromethyl)phenyl)-3-[(4-fluorophenyl)sulfonyl]-2-hydroxy-2-methyl-, (9CI, ACI).
- GHS 危害图例**: GHS Hazard Pictograms.
- 重要参数**: Important Parameters.
- 化学标识符列表, 包含 SMILES、InChI、系统名称、俗名和商品名等**: List of chemical identifiers, including SMILES, InChI, systematic name,俗名, and trade names, etc.
- 物质属性、谱图信息和生物活性数据**: Substance properties, spectral information, and biological activity data.

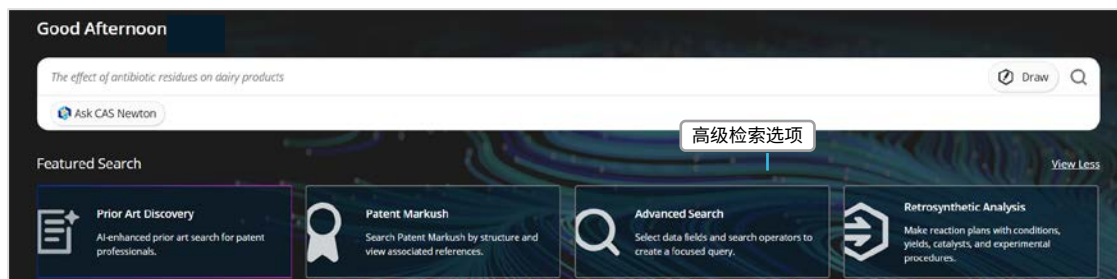
Properties	Value	Condition
Molecular Weight	430.38	-
Melting Point (Experimental)	191.88 °C (form II) (polymorph)	-
Boiling Point (Predicted)	650.308±55.00 °C	Press: 760.00 Torr
Density (Predicted)	1.522±0.10 g/cm ³	Temp: 25 °C; Press: 760 Torr
pKa (Experimental)		

高级检索

执行高级检索

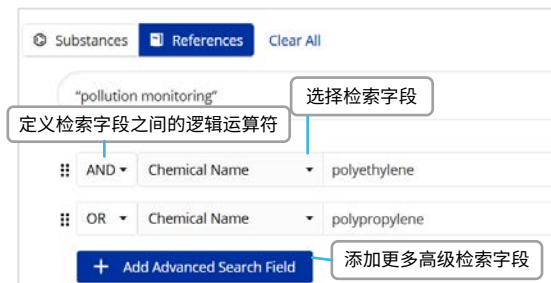
点击 CAS SciFinder 主界面的 Advanced Search，使用高级检索字段进行特定的文献或物质检索。

- 逻辑运算符的处理顺序为：**OR, AND, NOT**
- 仅使用单个高级检索字段时，无需使用逻辑运算符
- 允许使用通配符，例如 pollut*
- 最多使用50个高级检索字段（如果主检索字段也被使用，则为49个）



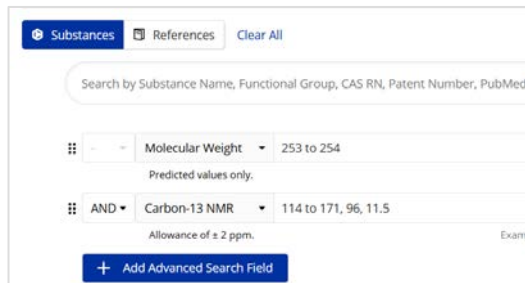
高级检索示例

高级文献检索

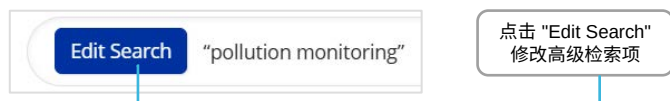


检索说明：检索 "pollution monitoring" 以及 (polyethylene or polypropylene)

高级物质检索



检索说明：检索具有特定分子量和核磁谱图峰值的物质



可用的高级检索字段

您可以在高级检索项中利用多个检索字段和类别，包括：

文献检索

- 作者
- 期刊名称
- 发表机构
- 标题
- 摘要/关键字
- 核心研究点
- 物质
- 生命科学数据
- 出版年份
- 文档标识符
- 专利标识符
- 出版商

物质检索

- 分子式
- CAS 登记号
- 化学标识符
- 文献标识符
- 专利标识符
- 实验谱图
- 生命科学数据
- 生物学数据
- 化学性质
- 密度
- 电学
- Lipinski
- 磁
- 机械属性
- 光学与散射
- 结构相关数据
- 热学



CAS Roles

CAS Roles 概述

Roles与物质相关联，表示反应中物质的作用，或文献中对于物质的研究方向。例如在反应中作为催化剂 (Catalyst)，或在分析研究中物质作为分析物 (Analyte) 使用。

物质及反应检索结果中的Roles

在物质检索结果集中，Roles 的筛选项表示对应物质在文献中的 Role；在反应检索结果集中，则对应物质在反应中的 Role。

Reference Role

By Count

Alphanumeric

1 Selected

☐ Prophetic Synthesis or Use (68K)

☐ Biological Study, Unclassified (53K)

☐ Agricultural Use (50K)

☐ Therapeutic Use (29K)

☐ Pharmacological Activity (27K)

☐ Reactant or Reagent (24K)

☒ Substance Claimed (4,098)

☐ Combinatorial Study (309)

☐ Analyte (307)

☐ Adverse Effect (285)

☐ Analytical Reagent Use (271)

☐ Byproduct (158)

☐ Cosmetic Use (151)

☐ Formation, Non-preparative (140)

☐ Formation, Unclassified (135)

出现在物质检索结果集中的
"Reference Role" 的例子

Substance Role

☐ Product (9)

☐ Reactant (1,113)

☐ Reagent (3,707)

☐ Catalyst (1,140)

☐ Solvent (5)

出现在反应检索结果集中的
"Substance role" 的例子

该结果集中的具有该
Role 属性的物质数量

文献检索结果中的 Roles

每当您检索具有CAS登记号的独特物质的相关文献时，Roles 将作为文献检索结果中的筛选项出现。

示例：找到将聚丙烯作为污染物 (pollutant) 研究的文献

检索聚丙烯相关文献，得到多条记录。其中 Substance role 选项显示了此检索结果集中的聚丙烯的所有适用Roles。其中 Pollutant 这一项 Role 表明有6,165篇文献将聚丙烯作为污染物 (pollutant)研究。

9003-07-0

(C₃H₆)_n
1-Propene, homopolymer

358K 9,326 51

Substance Role

☐ Uses (299K)

☐ Substance Claimed (106K)

☐ Properties (65K)

☐ Process (58K)

☐ Biological Study (25K)

☒ Pollutant (6,165)

View All

Database

Patent Office

Patent Status

358,490 Results

Sort: Publication Date: Newest View: Partial Abstract

1

Co-pyrolysis of polyolefin separators and active materials from lithium batteries: Thermal conversion performance, interaction behaviors, and products
By: Liu, Hui; Han, Jingkun; Gu, Jing; Feng, Yuheng; Liu, Gongqi; Yuan, Haoran
Fuel 2026, 404(8): 136198 | Language: English, Database: Capius

logravitric anal., Fourier transform IR spectroscopy-mass spectrometry (TG-FTIR-MS) and pyrolysis-gas chromatog- (MS) to investigate the thermal degradation behavior of polyolefin separators, focusing on the complex interactions among different polymers and the influence of contaminants such as electrode materials. The results indicate that the pyrolysis temperature range for polyolefin separators is 449.6-510.4°C, with residual mass below 2%. Interactions between polyethylene (PE) and polypropylene (PP) separators elevated the peak temperatures

More

Filtering: Substance Role: Pollutant

Clear All Filters

6,165 Results

Sort: Publication Date: Newest View: Partial Abstract

1

Environmental impact of nurdle spill from MSC ELSA 3 on the Kanyakumari Coast, Southern India
By: Perumal, Karthikeyan; Kalandhasamy, Prabhu; Thavasimuthu, Citarasu
Marine Pollution Bulletin 2026, 222(Part 1): 118615-1 | Language: English, Database: Capius and MEDLINE

a-flagged cargo ship MSC ELSA 3 to capsize on May 25, 2025, while traveling from port of origin to port of destination. The ship was carrying a large amount of plastic pellets (nurdles, <1.5 mm) spilled and started washing up on the coasts of Kanyakumari coast (Kodimunai, Panavilai) showed extensive deposition of nurdles made mostly of polyethylene and polypropylene was detected

View More

Full Text 3

单击 "View All" 可以选择更多 Roles

此结果集中的6,165篇文献中的每一篇都将聚丙烯作为污染物讨论。

CAS 序列检索

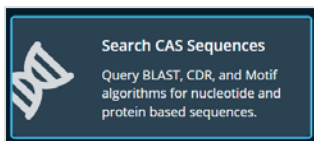
检索选项

可以使用三种不同的方式检索序列：

- BLAST: 检索相似序列
- CDR: 利用 CDR 检索抗体或T细胞受体
- Motif: 检索氨基酸或核苷酸位点可变的序列

要执行序列检索，请按照以下步骤操作：

- 在CAS SciFinder 主界面中打开 CAS Sequences 模块。
- 选择序列检索方式。
- 从文件中加载序列，或粘贴序列到检索窗格中。
- 可用多种格式文件上传序列，如 FASTA、TXT 等。
- 注意，序列输入可支持批量检索。
- 根据需要调整运行参数，然后启动序列检索。



BLAST

CDR

Motif

序列检索选项

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

将序列复制粘贴到这个窗口

上传 FASTA 序列或粘贴到 BLAST 窗格

包含 NCBI 数据库中的序列

高级参数设置

Advanced Sequence Search

Adjust Parameters for Short Sequences | Reset All

Alignment Identity %

Match with Gaps?

Gap Costs

Query Coverage %

Word Size

Scoring Matrix

BLAST Algorithm

E-Value

Exclude Low Complexity Regions

Sequence Type

Search Within

Search Sequences

序列检索结果及详情

访问结果

序列检索结果在最近检索历史 (Recent Search History) 和检索历史 (Search History) 中呈现。 点击 "View Results" 查看序列检索结果。

October 9, 2025

Search

Sequences

4:18 PM

Sequence Type: Protein

Search Within: Proteins

NCBI Included: Yes

BLAST Algorithm: BLASTp

Alignment Identity: -

Query Coverage: 90%

GFSGLGQPPGPPGSPGQGP3GASGPAGPR

View Results

Edit Search

Complete

Results will expire on November 9, 2025.

查看结果

在查看序列结果时：

- 比对结果按序列一致性排序。
- 简化的图形概览显示比对质量。
- 不匹配部分以红线标示。
- 详细比对结果可在 "Alignment" 标签中查看。
- 目标序列详情和相关专利预览可在单独的标签中查看。
- 点击 **References** 可获取相关文献。
- 支持下载 **XLSX** 格式的结果文件。

Sequences search for your query

References

获取披露所有序列的文献结果

5

Query 1

30

查询序列长度

Subject 1

1,464

目标序列长度

Alignment Identity: 96.67%

Matches: 29

Mismatches: 1

比对长度29+1=30

View

比对详情

目标序列详情，NCBI 链接以及 CAS SciFinder 中的物质信息

文献预览

References

查看披露此序列的参考文献

Alignment Data

BLAST Score: 167

E-Value: 1.00099e-15

匹配

+ 错配

Q 1 GFSGLGQPPG PPGSPGQGP SGASGPAGPR 30

S 1112 GFSGLGQPPG PPGSPGQGP SGASGPAGPR 1141

查询序列和目标序列的对齐情况

筛选结果

检索结果会随着筛选项调整而动态改变。

E-Value

0 to 10⁶

E-值（期望值）

Query Coverage %

0 to 100

比对上的序列长度
查询序列长度

Subject Coverage %

0 to 100

比对上的序列长度
目标序列长度

Alignment Identity %

0 to 100

匹配上的氨基酸或碱基对的数量
比对上的序列长度

Sequence Length

30 to 14168

Organisms

Gallus gallus (11)

Rattus norvegicus (7)

synthetic construct (7)

Cygnus olor (5)

Dromaius novaehollandiae (5)

View All

生命科学信息

检索靶点、配体和疾病

通过高级检索中的 Life Science data 字段，进行物质检索或文献检索，您可以找到与靶点、配体和疾病相对应的生命科学信息。

Advanced Search

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

Substances

References

Clear All

检索具有生命科学数据的物质

Molecular Formula

Molecular Formula

CAS Registry Number

Chemical Identifier

Document Identifier

Patent Identifier

Experimental Spectra

Life Science Data

Biological

Chemical Properties

Density

Substances

References

Clear All

检索具有生命科学数据的文献

Author/inventor Name

Authors/inventors

Publication Name

Organization

Title

Abstract/Keywords

Concept

Substances

Life Science Data

Publication Year

Document Identifier

Patent Identifier

Publisher

Advanced Search

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

Substances

References

Clear All

输入靶点

Search by Keyword, Substance/Functional

Target

Renin receptor ATP6IP2

+ Add Advanced Search Field

选择靶点、配体或疾病（可添加和组合进一步的生物活性检索字段）

文献和物质结果集中的 Life Science data 选项

Life Science Data

☒ Biomarkers (359)

☐ Pharmacological Data (1,380)

☐ ADME (216)

☐ Toxicity (87)

筛选有生物标志物，药理学数据，ADME 或毒性数据的文献结果

Life Science Data

☐ Pharmacological Data (1,422)

☐ ADME (60)

☐ Toxicity (9)

通过物质的药理学数据，ADME 和毒性数据，对物质结果进行筛选

Artemisinin

By: Ashley, Eliza

rest of the world

C₃₅H₂₄O₇

2-(2,2-Diphenyl-1,3-benzodioxol-5-yl)-5,7-dihydroxy-3-(phenylmethoxy)-4H-1-benzo...

物质详情页中的生命科学信息

Pharmacological Data

筛选功能

下载 Excel 文件

Clear All Filters

Knowledge Graph

View Detail (1) CAS

Target	Function	Parameter	Value	Disease	Organism	Assay	Source
Toll-like receptor 7	Agonist	EC50	0.42 μM	cancer	human		(1) CAS
Toll-like receptor 7	Agonist	EC50	1.4 μM				
Toll-like receptor 7	Agonist	EC50	0.42 μM	acute pathogen infection	H		

显示完整的实验细节

Assay Data

CAS LIFE SCIENCES

View Detail

Next

Close

Ligand

144875-48-9

CC1(C)C2=CC=CC=C2N(C1)C3=CC=CC=C3

C₁₇H₁₂N₂O₂

Resiquimod

Target

Toll-like receptor 7

Assay Name

SEAP reporter assay

Procedure

-

Assay Comment

-

Condition

-

Parameter

EC50

Value

0.42 μM

Measurement Remarks

-

Ligand Dose

-

Biological System

Human; HEK cells

Source

Preparation of 6-amino-7,9-dihydro-8H-purin-8-one derivatives as immunostimulant Toll-like receptor 7 agonists
By: Foudel, Yam B.; Gangwar, Sanjeev; Sivaprakasam, Prasanna; Poo, Shoshana L.
World Intellectual Property Organization WO2019036023 A1 2019-02-21 | Language: English, Database: CAPLUS

ADME

Target	Function	Parameter	Value	Disease
Toll-like receptor 8	Agonist	Absorbance	Exhibits greater NIR light absorbance	Neoplasm
Toll-like receptor 7	Agonist	Absorbance	Exhibits greater NIR light absorbance	Neoplasm

Toxicity

Target	Function	Parameter	Value	Disease	Organism	Assay	Source
-	-	Cell killing	More effective at killing cancer cells	-	-	View Detail	(1) CAS

文献详情页中的生命科学信息

Biomarkers

CAS LIFE SCIENCES

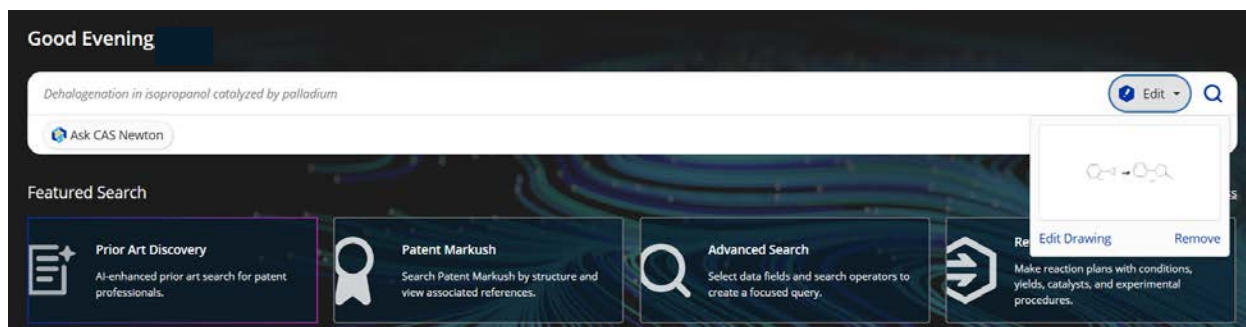
Download

Biomarker	Biomarker Type	Disease	Category	Measurement	Details
SEMA6A (DNA)	Molecular	central nervous system neuroblastoma	Gene-disease association linked with genetic variation	Association score	View Detail
CCL2 (DNA)	Molecular	central nervous system neuroblastoma	Gene-disease association linked with genetic variation	Association score	View Detail



反应检索

可以使用化学结构、自然语言、物质名称、CAS 登记号、文献 DOI 号或专利号等进行反应检索。



反应检索结果

默认情况下，反应检索结果按照上一次的设置进行分组。

对于单步反应，你可以根据相邻原子与特定反应中心的相似性来获取相似反应。

- **Broad:** 获取反应中心一致的反应；
- **Medium:** 获取反应中心一致，相邻原子一致的反应；
- **Narrow:** 获取反应中心一致，相邻原子、拓展原子和键一致的反应。

反应详情

查看反应详情

反应详情页为您提供了从文献及其 Supporting Information 中提取的信息，包括溶剂、催化剂、试剂、反应条件和表征数据等。

Get Similar Reactions

检索相似反应

Reaction Overview

Steps: 1 Yield: 85%

反应文献

Development of a Scalable Synthesis of an Azaindoly-Pyrimidine Inhibitor of Influenza Virus Replication

By: Liang, Jlang

View All

Organic Process Development (2016), 20(5), 965-969

View Source

Full Text

Company/Organization

Vertex Pharmaceuticals Incorporated

Boston, Massachusetts 02210

United States

查看所有作者

查看所有作者

Step 1

Stage

Reagents

Catalysts

Solvents

Conditions

1	Triethylamine Diphenylphosphoryl azide	-	Toluene	2 h, reflux; reflux → 60 °C
2	-	-	-	overnight, 60 °C → 80 °C

查看生成同一产物的其他反应

Alternative Steps (5)

Experimental Protocols

Synthetic Methods

查看详细步骤

Products

Ethyl (1*R*,3*S*)-3-[(benzyloxycarbonyl)amino]cyclohexanecarboxylate, Yield: 85%

Reactants

1-Ethyl (1*R*,3*S*)-1,3-cyclohexanedicarboxylate
Benzyl alcohol

Reagents

Triethylamine
Diphenylphosphoryl azide

Solvents

Toluene

Procedure

1. Add diphenylphosphoryl azide (DPPA) (166 mL, 769 mmol) and triethylamine (107 mL, 769 mmol) to (1*S*, 3*R*)-3-ethoxycarbonylcyclohexanecarboxylic acid (140 g, 700 mmol) in toluene (1.4 L).

Characterization Data

查看表征数据

Ethyl (1*R*,3*S*)-3-[(benzyloxycarbonyl)amino]cyclohexanecarboxylate

Proton NMR Spectrum

(300 MHz, CDCl₃) δ 7.48-7.30 (m, 5H), 5.11 (s, 2H), 4.67 (s, 1H), 4.13 (q, *J* = 7.1 Hz, 2H), 3.55 (s, 1H), 2.42 (t, *J* = 11.8 Hz, 1H), 2.28 (d, *J* = 12.6 Hz, 1H), 2.10-1.79 (m, 3H), 1.50-1.19 (m, 6H), 1.19-1.00 (m, 1H).

Optical Rotatory Power

−33.3° (c = 1 in DCM).

HRMS

(ESI) [M + H]⁺ calculated for C₁₇H₂₄NO₄ 306.1700, found 306.1700

State

sticky solid

CAS Method Number 3-451-CAS-15598720

Transformations

1. Schmidt Reaction

反应转化类型

Reaction Notes

scalable

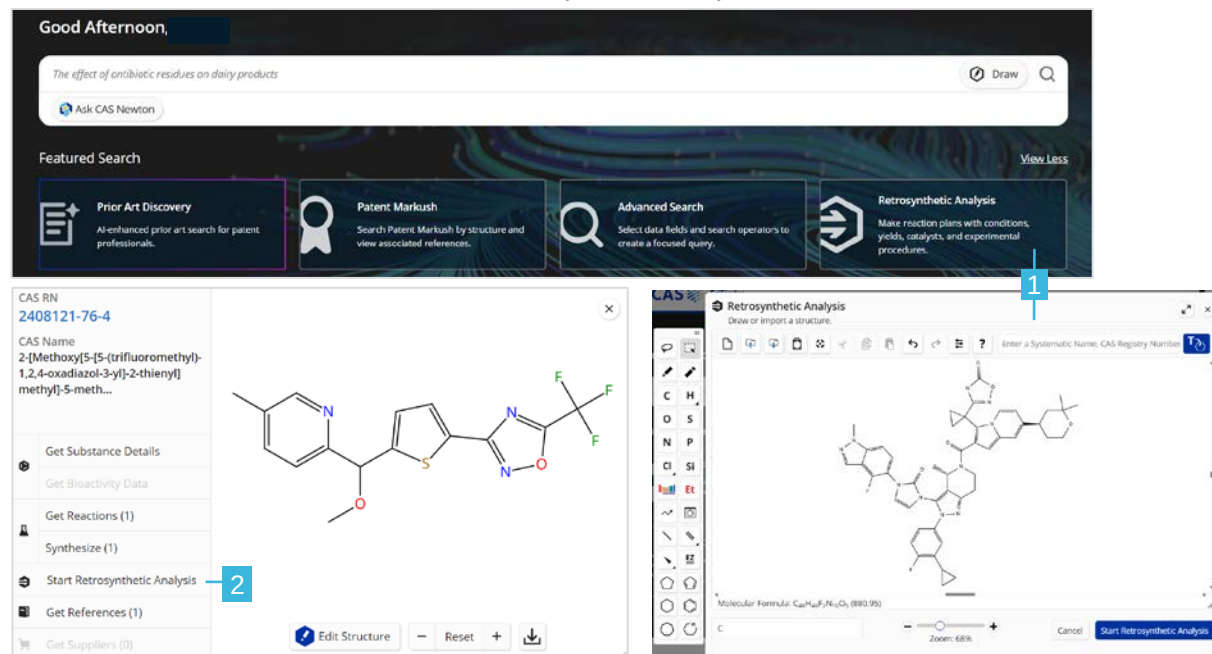
其他重要注释

逆合成反应路线设计工具

开启逆合成设计

在 CAS SciFinder 中启动 "Retrosynthetic Analysis" 主要有两种方式：

1. 点击主界面上的 "Retrosynthetic Analysis" 选项，在绘制窗口中绘制或导入一个结构。绘制的物质可以是一个新颖结构，或无文献报道过合成方法的物质。
2. 在现有物质的弹出窗口上点击 "Start Retrosynthetic Analysis" 选项。

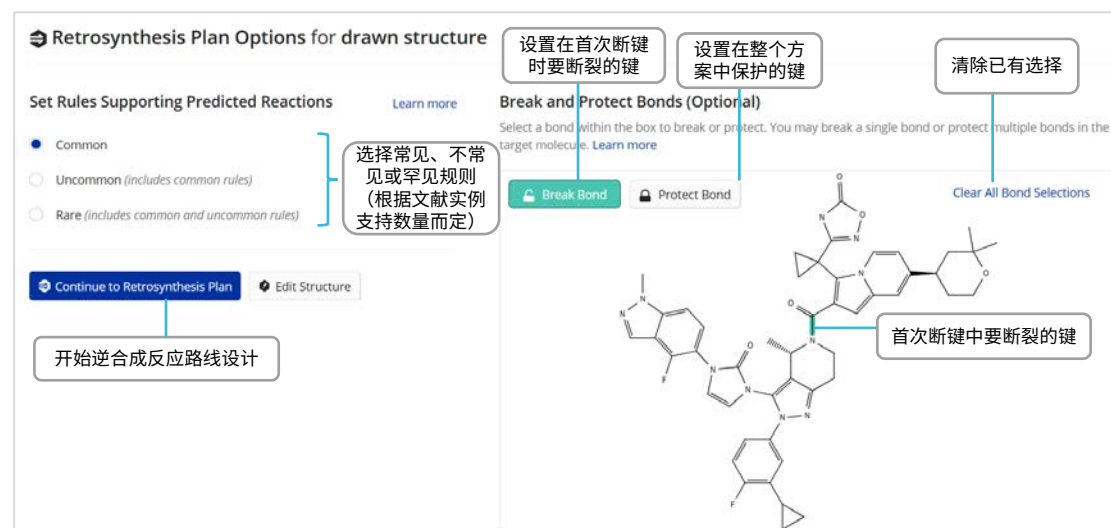


参数设置

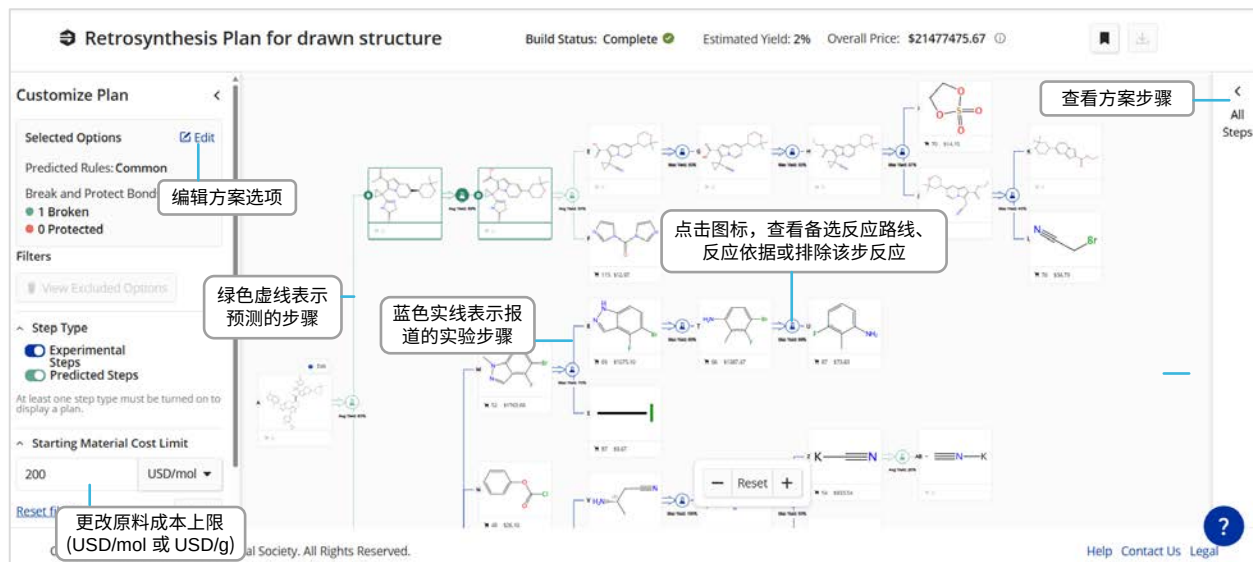
您可以编辑方案选项以：

- 在整个合成路线保护指定的化学键。
- 定义在首次断键中要断裂的键。
- 选择预测反应的反应规则

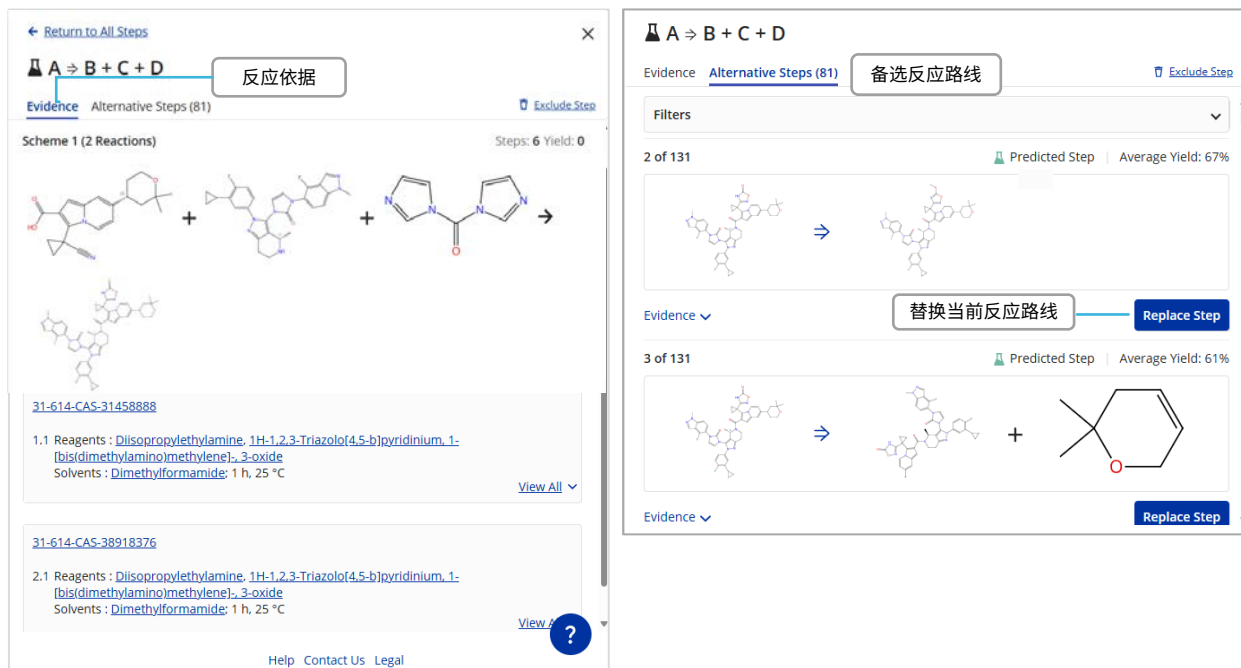
设置好了所需的选项后，点击 "Continue to Retrosynthesis Plan"



逆合成方案和备选路线



反应依据和备选路线



Patent Markush 检索及 CAS PatentPak

Patent Markush 检索

点击主界面上或 CAS Draw 中的“Patent Markush”选项，执行 Markush 结构检索。

Patent Markush

Search Patent Markush by structure and view associated references.

进行 Markush 检索

结构匹配度

命中的 Markush 结构

筛选受理专利局

专利中重要的 Markush 详情信息

跳转至专利文献详情页面

展开专利家族列表，跳转至 CAS PatentPak，下载 PDF 原文

View Related Results

Filter Results

Patent Markush Match

As Drawn (0)

Substructure (5)

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Patent Office

World Intellectual Property Organization (4)

China (1)

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Patent Markush Details

1,3-Benzoxazine-2,4(3H)-dione derivative and its synthetic method and application for treating Alzheimer's disease

Assignee: Central South University

China, CN108570012 A 2018-09-25 | Language: Chinese, Database: CPlus

Patent Status: Alive

Patent claim 1

PatentPak

Full Text

CAS PatentPak

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CAS 科学家标引的重要物质定位标记

Key Substances in Patent

CAS RN 3108317-86-5

Analyst Markup Locations (3)

Page 132 - Claim

Page 30

Page 61

CAS RN 3111024-43-9

Analyst Markup Locations (3)

Page 132 - Claim

Page 30

Page 64

定位到专利中物质所在位置

专利中被标引的核心物质

WO 2025/261486

PCT/CN2025/102372

- 130 -

thereof, wherein, in Formula I-3, I-3-a, I-3-b, I-3-c, I-3-d, I-3-e, I-3-f, I-3-g, I-3-h, I-3-i, I-3-j, I-3-k, I-3-l, I-3-m, or I-3-n, J⁷ is CR²⁶ and J⁸ is CR²⁸, wherein R²⁶ and R²⁸ together with the carbon atoms they are attached to represent a 5-7 membered ring, preferably, a 6-membered ring, such as a phenyl, carbocyclic or heterocyclic ring, which is optionally substituted, for example, (or) etc., when substituted, the 5-7-membered ring can be typically substituted with 1-3 substituents each independently selected from halogen or C₁₋₄ alkyl optionally substituted with F, such as methyl.

注释：点击物质的定位标记符，即可跳转至专利全文中该物质出现的位置

36. A compound selected from the compounds shown in Examples section or any of the compounds shown in Table herein, or a pharmaceutically acceptable salt thereof.

37. A pharmaceutical composition comprising the compound according to any one of claims 1-36 or a pharmaceutically acceptable salt thereof.

CAS SciFinder Discovery Platform 快速入门指南 | 21

CAS Formulus

检索制剂或配方

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American Chemical Society

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PLATFORM

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CAS SciFinder

Good Evening

Proton nmr spectral data for C13H13Br

Featured Search

Prior Art Discovery
Discover prior art in patents and non-

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Help & Support

Alerts

Saved

Good Morning,

Formulations Ingredients

Search by Formulations

可输入制剂或配方的原料、用途、物理形态、功能或文献识别符（包括专利号、DOI号等）

Q

Formulation Designer
Design custom formulation
templates based on selections
and ingredients

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

浏览并选择检索项

All Fields

Form

Function

Ingredient

Purpose

Route

Target

添加新的检索项

Return to Home

Advanced Formulations Search

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

Search For

Ingredient

Operator

Optional

Required

Optional

Excluded

Enter one term

Ex: caffeine, sodium, 50-00-0

Add Another Term

Q Search

单击执行检索

清除所有内容

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点击下拉菜单，浏览并设置运算符



Formulations search for "celecoxib"

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Filter by

选择筛选项，精准获得配方或制剂结果

Industry

- ☒ Pharmaceutical
☐ Unclassified

Purpose

- ☐ Drug delivery systems (111)
☒ Analgesics (85)
☐ Anti-inflammatory agents (80)
☐ Antiarthritics (57)
☐ Pharmaceutical formulations (33)

View All

Physical Form

- ☐ Capsules (102)
☒ Tablets (85)
☐ Solutions (54)
☐ Suspensions (31)
☐ Liquids (17)

View All

State of Matter

Delivery Route

- ☒ Oral drug delivery systems (85)
☐ Controlled-release drug delivery systems (11)
☐ Topical drug delivery systems (5)
☐ Parenteral drug delivery systems (4)
☐ Inhalation drug delivery systems (2)

View All

Information Included

- ☒ Component Amount (84)
☐ Process (64)
☒ Experimental Activity (49)
☐ Effective Dose (5)

Document Type

Organization

Language

Publication Year



No Min to No Max Apply

Pharmaceutical Dosage Form Containing Celecoxib for Relieving Pain: Drug Delivery Systems or Analgesics--Controlled-Release Drug Delivery Systems

Location: Example, DF-3, IRG-3, SRG-1, Table 1, 6, 8, 13

Purpose: Analgesics, Drug delivery systems

Target: celecoxib, Homo sapiens, Pain

Delivery Route: Oral drug delivery systems

Physical Form: Tablets

制剂或配方成分，功能及用量

Component	Function	Amount Reported
Group: immediate release granulation	-	200 mg
Celecoxib	Analgesics	126 g
Hydroxypropyl methyl cellulose	-	126 g
Cellulose	Disintegrants	26.22 wt %
Poly(vinylpyrrolidone)	Disintegrants	

查看或下载专利全文

Additional group components reported

Group: sustained release granulation	-	333.3 mg
Celecoxib	Analgesics	2515.1 g
Magnesium stearate	Lubricants	0.5 wt %
Hydroxypropyl methyl cellulose acetate succinate	Film-forming agents , Coating materials , Binders	2484.9 g
Methocel K100LV premium CR	-	30.00 wt %

Additional group components reported

U.S. Pharmacopeia

美国药典信息

View Formulation Detail

查看制剂或配方详情

8 Similar Formulations - View All

查看相似的制剂或配方

Pharmaceutical Composition for Relieving Pain: Analgesics

Location: Example 2-1, Table 15, 16, 25

Purpose: Analgesics

Target: Homo sapiens, Pain

Delivery Route: Oral drug delivery systems

Physical Form: Tablets

Component	Function	Amount Reported
Group: celecoxib mixture	-	-
Celecoxib		200 mg/tablet

点击蓝色原料名称，查看详情

Compare

对比选中的制剂或配方

PATENT

Dosage forms comprising celecoxib providing both rapid and sustained pain relief

Assignee: Pfizer Products Inc.
WO2009063367
Language: English

Patent PDF

View in CAS SciFinder

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中查看文献详情

Compare

PATENT

Pharmaceutical compositions containing celecoxib and tramadol

Assignee : Yooyoung Pharmaceutical Co., Ltd.
KR2017008923
Language: Korean

制剂或配方详情

结果导出为 PDF 格式文件

Pharmaceutical Tablets Containing Celecoxib: Antiinflammatory Agents or Analgesics

结果保存

View

Purpose	Target	Delivery Route	Physical Form
Analgesics, Anti-inflammatory agents	Homo sapiens, Lower back pain, Osteoarthritis, Rheumatoid arthritis, cervical shoulder arm syndrome, shoulder periarthritis	Oral drug delivery systems	Tablets

Predicted value

Formulation Ingredients

制剂或配方原料

Expand All Groups | Collapse All Groups

Feedback

Component	Function	Amount Reported	Optionality
Group: granulated celecoxib	Formulation active agents	1008 g	Mandatory
Celecoxib	Nonsteroidal anti-inflammatory agents	1200 g	Mandatory
D-Glucose, 4-O-β-D-galactopyranosyl-, hydrate (1:7)	Formulation excipients	264 g	Mandatory
Hydroxypropyl cellulose	Disintegrants	384 g	Mandatory
Cellulose, carboxymethyl ether	Disintegrants	102 g	Mandatory
Poly(vinyl alcohol)	Binders	42 g	Mandatory
Sodium dodecyl sulfate	Surfactants	24 g	Mandatory
Magnesium stearate	Lubricants	12 g	Mandatory

More Formulations like this...

相似的制剂或配方

Celecoxib Tablet Composition: Antiarthritics Purpose: Antiarthritics Target: Arthritis, Homo sapiens Delivery Route: Oral drug delivery syst... Physical Form: Tablets

Celecoxib Tablet: Antiarthritics Purpose: Antiarthritics Target: Homo sapiens, Osteoarthritis, ... Delivery Route: Physical Form: Tablets

Pharmaceutical Composition: Antiarthritics-Immediate Release Purpose: Antiarthritics Target: Homo sapiens Delivery Route: Oral drug delivery syst... Physical Form: Sachets, Tablets, disinte...

Antiarthritic Pharmaceutical Composition Purpose: Antiarthritics Target: Arthritis, Homo sapiens Delivery Route: Oral drug delivery syst... Physical Form: Tablets

Process

制备工艺

celecoxib, lactose hydrate, low-substituted hydroxypropyl cellulose and carmellose were added into a high-speed stirring granulator to obtain a mixture. polyvinyl alcohol and sodium lauryl sulfate were dissolved in purified water to obtain a solution. the obtained solution was added dropwise or sprayed over the mixture obtained above and wet granulated to a particle diameter of 4 mm in a crusher. the granulated product was put into a fluid bed dryer supplied with air at a temperature of 85 °C and dried at 40 °C. the dried product was further crushed to obtain granulated celecoxib of diameter 1 mm. the obtained celecoxib granulated product was mixed with magnesium stearate and tableted at 600 kgf pressure to obtain a circular tablet of 340 mg and 9.5 mm diameter.

Experimental Activity

制剂或配方实验评估

Descriptor	Notes	Details
dissolution rate of celecoxib	after 15 minutes	27.6 %
dissolution rate of celecoxib	after 30 minutes	75.1 %
dissolution rate of celecoxib	after 45 minutes	88.7 %
dissolution rate of celecoxib	after 60 minutes	93 %

Source Patent

来源文献

Pharmaceutical tablet containing celecoxib as anti-inflammatory and analgesic agent

Assignee : Ohara Pharmaceutical Co., Ltd.
JP2019089758
Language: Japanese
Location: Comparative Example 2B, Table 2, 5

Patent PDFView in CAS SciFinder

检索配方/制剂成分



Ingredients search for "propylene glycol"

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选择筛选选项，精准获得原料结果

1 Selected 3 Results

选择使用该原料的制剂或配方

查看原料供应商信息

查看实验属性

查看管控信息及清单

查看制剂或配方中，与该原料同时使用的其它配伍成分

将原料添加至 Formulation Designer

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Filter by

- Industry
 - ☐ Agrochemical
 - ☐ Cleaning & Surfactant Products
 - ☐ Cosmetics & Personal Care
 - ☐ Food & Related
 - ☐ Inks, Paints, & Coatings
 - ☒ Pharmaceutical
- Regulatory Information
 - ☐ REACH (6)
 - ☐ Cosing: Cosmetic Ingredient Inventory (3)
 - ☐ EPA Pesticide Inactive Ingredients (3)
 - ☒ FDA Inactive Ingredients Database (3)
 - ☐ Drug Master File List (2)
- Experimental Properties
- Commercial Availability

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View Details

CAS RN: 57-55-6

(z)-Propylene glycol

Key Physical Properties

Property	Value	Condition
Molecular Weight	76.09	-
Melting Point (Experimental)	-59 °C	-
Boiling Point (Experimental)	188.2 °C	-
Density (Experimental)	1.036 g/cm³	-

Commonly Used As: Solvents; Humectants; Pl

Similar Ingredients with Regulatory Information

- Propylene glycol monolaurate
- Propylene glycol butyl ether
- Propylene glycol monopropyl ether

View 14 More

Commonly Formulated With | Regulatory Information | Experimental Properties

Experimental Properties

Property	Value	Density	Condition	Source
Neonatal Lethal Dose	1700 mg/kg	-	Organism: mouse; Route: subcutaneous	[1] CAS
Maternal Lethal Dose	1300 mg/kg	-	Organism: rat; Route: intravenous	[1] CAS
Neonatal Lethal Dose	6200 mg/kg	-	Organism: mouse; Route: injection	[2] CAS

Sources: [1] Gossard, V. M.; Katsikakou, H. *Formulation*, 178(1), 8, 46-5, Cpl/yr; [2] Anon, *Gilbert*, 22(4)200, 1763, Dylus.

Commonly Formulated With

Ingredient	CAS RN/CAS SCN	As Active Ingredients	As Inactive Ingredients	As Any Role
Water	7732-18-5	View Formulations	View Formulations	View Formulations
Glycerol	56-81-5	View Formulations	View Formulations	View Formulations
Ethanol	64-17-5	View Formulations	View Formulations	View Formulations
Carb. acid	7732-18-5	View Formulations	View Formulations	View Formulations
Sodium hydroxide	1310-73-2	View Formulations	View Formulations	View Formulations
Octic acid	113-80-1	View Formulations	View Formulations	View Formulations
Dodecyl ethylenebis(ester)acetate	139-33-3	View Formulations	View Formulations	View Formulations
Sodium sulfate	7757-83-7	View Formulations	View Formulations	View Formulations
Dodecyl glycol monomethyl ether	111-90-0	View Formulations	View Formulations	View Formulations
[3-Amino-2-hydroxypropyl]dimethylammoniumacetate	36578-66-0	View Formulations	View Formulations	View Formulations
Karbitan	11138-66-2	View Formulations	View Formulations	View Formulations
Alcohol, C ₁₂ -12, ethylenebis	68131-39-0	View Formulations	View Formulations	View Formulations
Isopropyl	67-63-0	View Formulations	View Formulations	View Formulations
Polyethylene glycol monomethyl ether	9004-96-2	View Formulations	View Formulations	View Formulations
Hydrogen peroxide	7721-84-1	View Formulations	View Formulations	View Formulations
Polyethylene glycol	2532-46-5	View Formulations	View Formulations	View Formulations
Triacetin	13463-47-7	View Formulations	View Formulations	View Formulations
Methylparaben	99-76-3	View Formulations	View Formulations	View Formulations
Ammonia	7664-41-7	View Formulations	View Formulations	View Formulations
Ethanolamine	141-43-5	View Formulations	View Formulations	View Formulations

Get Formulations | **Get Suppliers** | **Add to Formulation Designer**

Inventory Lists

Ingredient is on the following Inventory Lists:

Acronym	Inventory List	Country
ABC	Australian Inventory of Industrial Chemicals	Australia
AREC	South Korean Act on the Registration and Evaluation of Chemicals	Korea (Republic of)

设计制剂或配方

Formulation Designer

选择应用领域

Pharmaceutical

Cosmetics & Personal Care

Agrochemical

Cleaning & Surfactant Products

Inks, Paints, & Coatings

Food & Related

选择用途

Drug delivery systems

Pharmaceutical formulations

Antitumor agents

Anti-inflammatory agents

Analgesics

Antibacterial agents

Ophthalmic agents

Antidiabetic agents

Antiviral agents

Antihypertensives

- View More Purposes -

选择物理形态

Tablets

Capsules

Solutions

Gels

Liquids

Pharmaceutical ointments

Cream preparations

Suspensions

Sprays

Powders

- View More Physical Forms -

最多添加 5 种成分

Celecoxib

Polyethylene glycol

+ Add Another Ingredient

添加成分

删除成分

Create Template

执行检索

Formulation Designer

重新编辑

结果导出为 Excel 文件

结果保存

Save

Go

Clear

Your Template

Unit Size

mg

Go

Clear

Function	Ingredient	Regulatory Lists	Top Alternatives	Amounts
Active or Featured Ingredient:	Celecoxib	Drug Master File List; EMA EPARS; FDA Orange Book; Japanese Approved Drugs List; NMPA	-	Amount not available
Active or Featured Ingredient:	Polyethylene glycol	ANMAT; Cosing: Cosmetic Ingredient Inventory; Drug Master File List; EPA Pesticide Inactive Ingredients; EPA Safer Chemical Ingredients; FDA GRAS (Part 181, Subpart B); FDA Inactive Ingredients Database	-	Amount not available
Lubricants	Talc (Mg ₃ H ₂ (SiO ₃) ₄)	Cosing: Cosmetic Ingredient Inventory; Drug Master File List; EPA Pesticide Inactive Ingredients; FDA Color Additives;	Sodium dodecyl sulfate; Glyceryl tribehenate; Sodium stearyl fumarate; Magnesium stearate;	Approximate Range: 3 - 4%
Binders	Butyl methacrylate-dimethylaminoethyl methacrylate-methyl methacrylate copolymer	Cosing: Cosmetic Ingredient Inventory; Drug Master File List; EPA Pesticide Inactive Ingredients; EPA Safer Chemical Ingredients; FDA Inactive Ingredients Database	Sodium dodecyl sulfate; Glyceryl tribehenate; Sodium stearyl fumarate; Magnesium stearate;	Approximate Range: 3 - 4%
Disintegrants	Croscarmellose sodium	Cosing: Cosmetic Ingredient Inventory; Drug Master File List; EPA Pesticide Inactive Ingredients; FDA Inactive Ingredients Database	Silica; Starch; Sodium carboxymethyl cellulose; Poly(vinylpyrrolidone); Hydroxypropyl cellulose	Approximate Range: 4 - 5%
Diluents	Magnesium oxide	Cosing: Cosmetic Ingredient Inventory; Drug Master File List; EPA Pesticide Inactive Ingredients; EPA Safer Chemical Ingredients;	Talc (Mg ₃ H ₂ (SiO ₃) ₄); Butyl methacrylate-dimethylaminoethyl methacrylate-methyl methacrylate copolymer	Approximate Range: 8 - 16%

查看成分详情

查看成分管制信息

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添加用途后，点击获得新的制剂或配方设计结果

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Function

Anti-inflammatory agents

Add Function

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CAS Analytical Methods

分析方法检索

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Prior Art Discovery

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History

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输入关键词或者分析物等进行检索

Q

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Advanced Search

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高级检索

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10 April 2025

X

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高级检索

AND
OR
NOT

逻辑运算符：and, or, not

增加检索条件

Advanced Search

Analyte

palmitic acid

AND

Matrix

blood plasma

Keyword

Analyte

Matrix

Method Category

Technique

Validation

CAS Method Number

Publication Name

删除检索条件

检索条件包括：关键词、分析物、基质、方法分类、技术手段、数据验证、CAS 方法号、出版物名称

分析方法的分类检索

Explore Methods

浏览并选择方法分类及子分类

Category

Agricultural Applications /

Bioassays

Biomolecule Isolation

Environmental Analysis

Food Analysis

Fuels / Geology / Biofuels

Historical Analysis / Dating

Miscellaneous

Organic Compound Analysis

Organometallics / Inorganics

Pharmacology / Toxicology

Polymer Analysis

Water Analysis

Category Name

Bioassay

Bioassay Synthetic Probes

Biomarker Biological Process

Biomarker Cell Assay

Biomarker Medicine Assay

Biomedicine Material Analysis

Biomolecule Isolation Assay

Bioorganism Isolation Assay

Genetic Analysis

Nanomaterial Analysis

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+ Add Another Keyword

增加关键词

检索分析方法

Search Methods

分析方法结果集

Results for Biomolecule Isolation Assay +1 Keyword

结果保存

结果导出

按照分析物、基质、方法分类、技术手段、公开年份等条件筛选结果

1 Selected 3 Results

选中方法，导出或保存

Sort: Relevance

Group: By Method

Filter By

Analyte

Matrix

Blood plasma (3)

Method Category

Technique

HPLC (3)

Electrospray ionization mass spectrometry (2)

Electrospray ionization tandem mass spectrometry (1)

Quadrupole tandem mass spectrometry (1)

Saponification (1)

View All

Validation

Concentration (4)

Linearity Range (3)

Retention Time (3)

Limit of Detection (2)

Limit of Quantitation (1)

Analysis of Palmitic acid in Blood plasma by Solvent extraction

查看方法信息详情

JOURNAL

Compare

选择感兴趣的方法进行对比

By: Forest, Anik; Ruiz, Matthieu; Bouchard, Bertrand; Boucher, Gabrielle; Gingras, Olivier; Daneault, Caroline; Robillard Frayne, Isabelle; Rhainds, David; Tardif, Jean-Claude; Rioux, John D.; Des Rosiers, Christine
Comprehensive and Reproducible Untargeted Lipidomic Workflow Using LC-QTOF Validated for Human Plasma Analysis
Journal of Proteome Research (2018), 17 (11), 3657-3670. American Chemical Society

Analyte

Palmitic acid; Linoleic acid; Palmitoleic acid; Arachidonic acid; Docosahexaenoic acid

Matrix

Blood plasma

Other Materials

Reagent: Hydrochloric acid; Ethyl acetate; Chloroform; Formic acid; Methanol; Sodium chloride; tert-Butyl methyl ether
Material: Glass vial; Zorbax Eclipse plus C₁₈ column (2.1 × 100 mm, 1.8 μm)

Method Category

Biomolecule Isolation Assay

展示摘要

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Full Text

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ss spectrometry; HPLC; Electrospray ionization mass spectrometry; Solvent extraction
HPLC system; Time of flight mass spectrometer

2

Analysis of Butyric acid in Blood plasma by Electrospray ionization tandem mass spectrometry

JOURNAL

Compare

分析方法详情及结果对比

Analysis of Myristic acid in Blood plasma by Solvent extraction

结果导出

Save

CAS Method Number
1-122-CAS-534418

Method Category
Fatty Acid Analysis

Technique
Mass spectrometry; HPLC; Solvent extraction

结果保存

分析物、基质、材料、试剂等分类展示

Analyte
cis-Octadecenoic acid
(Z)-Hexadecenoic acid
cis-Octadecadienoic acid
Palmitic acid
Myristic acid

Matrix
Blood plasma

Material
Atlantic T3 C18 column (2.1
× 150 mm, 3 μm)
Ethylenediaminetetraacetic
acid-loaded vacuum
tubes

Reagent
Chloroform
Methanol

Biological Reagent

所用仪器信息

Equipment Used
HPLC system, Prominence, Shimadzu Corp,
Kyoto, Japan
Mass spectrometer, LTQ Orbitrap, Thermo-
Fisher Scientific Inc, San Jose, CA, USA

操作步骤

Instructions
Preparation of blood plasma sample
1. Collect blood by caudal venipuncture using ethylenediaminetetraacetic acid-loaded vacuum tubes (Terumo Co., Tokyo, Japan) at oocyte sampling and store on ice.
2. Separate plasma by centrifugation within 4 h of collection and transfer 100 mL of plasma to a 1.5-mL microcentrifuge tube and store at -80 °C until the lipidomic analysis.
Solvent extraction
1. Extract 100-μL plasma sample with 800 μL of ice-cold chloroform/methanol 1:1 (v/v, with internal standard (IS)) twice.
2. Dry extracted lipids under a vacuum, dissolve in methanol and filter to remove any insoluble material prior to the LC/MS injection.
3. Perform the extraction procedure within 1 h to avoid lipid degradation and auto-oxidation.
High performance liquid chromatography-mass spectrometry in negative mode
1. Perform analysis using Shimadzu Prominence HPLC system (Shimadzu Corp., Kyoto, Japan) coupled to an LTQ Orbitrap mass spectrometer (Thermo-Fisher Scientific Inc., San Jose, CA, USA) with an electrospray ionization (ESI) source.
2. Perform separation using an Atlantic T3 C18 column (2.1 × 150 mm, 3 μm, Waters, Milford, MA, USA).
3. Maintain column at 40 °C.
4. Perform LC elution using the mobile phase consisting of 5 mM aqueous ammonium acetate (as mobile phase A), isopropanol (as mobile phase B) and methanol (as mobile phase C).
5. Program the elution gradient as follows: at 0 min: 25% A; 40% B, 35% C; at 1 min: 5% A; 60% B, 35% C; at 27 min: 0% A; 65% B, 35% C; at 28 min: 25% A; 40% B, 35% C; at 30 min: 25% A; 40% B, 35% C.
6. Set the flow rate at 200 μL/min.
7. Maintain sample tray at 4 °C.
8. Perform MS data acquisition under electrospray ionization negative mode.
9. Set MS parameters as follows: MS capillary voltage: 3.0 kV; sheath gas (nitrogen) flow: 50 psi; auxiliary gas (nitrogen): 5 psi; resolving power for high-resolution MS: 60,000; scan speed: 2 Hz; scan ranges: 220-1650 m/z for the negative mode; MS/MS collision energy: 35.0; activation Q value: 0.25; activation time: 30 ms.

来源文献题录信息

Source
JOURNAL
Postpartum cows showed high oocyte triacylglycerols concurrently with high plasma free fatty acids
Furukawa, Eri; Chen, Zhen; Ueshiba, Hiroki; Wu, Yue; Chiba, Hitoshi; Yanagawa, Yojiro; Katagiri, Seiji; Nagano, Masashi; Hui, Shu-Ping
Theriogenology (2021), 176, 174 - 182.
Elsevier Inc.
CODEN : THGNBO | ISSN : 0093691X | DOI : 10.1016/j.theriogenology.2021.09.034
View Abstract ▾ Full Text ▾
展示摘要 获得全文链接

Validation

数据验证

Retention Time
7.53 min, Tetradecanoic acid
9.91 min, Hexadecanoic acid
8.35 min, n-Hexadecenoic acid
11.85 min, Octadecanoic acid
10.5 min, Octadecenoic acid (Z)-
9.25 min, Octadecadienoic acid
Concentration
0.26 ± 0.11 nmol/100 μL (sample data), Tetradecanoic acid
3.68 ± 1.04 nmol/100 μL (sample data), Hexadecanoic acid
0.66 ± 0.28 nmol/100 μL (sample data), n-Hexadecenoic acid
5.34 ± 0.79 nmol/100 μL (sample data), Octadecanoic acid
7.57 ± 2.25 nmol/100 μL (sample data), Octadecenoic acid (Z)-
1.14 ± 0.24 nmol/100 μL (sample data), Octadecadienoic acid

Comparing your 3 selected Methods

删除方法

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	Method 1	Method 2	Method 3
	Analysis of Palmitic acid in Blood plasma by Solvent extraction	Analysis of Fatty acids in Blood plasma by HPLC	Analysis of Lauric acid in Blood plasma by Electrochemiluminescence
CAS Method Number	2-114-CAS-225380	1-122-CAS-96286	1-122-CAS-3193044
Method Category	Biomolecule Isolation Assay	Fatty Acid Analysis	Fatty Acid Analysis
Technique	Time-of-flight mass spectrometry; HPLC; Electrospray ionization mass spectrometry; Solvent extraction	Electrochemical analysis; Atmospheric precipitation; HPLC	Electrochemiluminescence; HPLC
Analyte	Palmitoleic acid; Palmitic acid ; Elaidic acid; Linoleic acid; Stearic acid; Arachidonic acid; Docosahexaenoic acid	Stearic acid; Linoleic acid; Palmitic acid ; Arachidonic acid; Oleic acid; Fatty acids	Palmitic acid ; Stearic acid; Myristoleic acid; Palmitoleic acid; Lauric acid; Arachidonic acid; Oleic acid; Linoleic acid; Linolenic acid; Myristic acid; Fatty acids

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登录，培训，支持及学习资源

登录详情

请访问 scifinder-n.cas.org 登录。

登录方式请查看所在机构图书馆网站说明。

培训

即将举行的活动和网络研讨会：

<https://www.cas.org/cas-webinars?attendance=Coming+soon>

过往活动和网络研讨会录像：

<https://www.cas.org/cas-webinars?attendance=On+demand>

培训内容：

<https://www.cas.org/training/platform/cas-scifinder-discovery-platform>

支持

如需获取有关 CAS SciFinder Discovery Platform 使用的其他帮助，请联系 CAS 美国化学文摘社北京代表处。

电话：010-62508026/7

电子邮箱：china@acs-i.org

网址：<https://www.cas.org/contact>

欢迎微信扫码随时联系 CAS 客服中心

工作时间: 8:30-17:30 (工作日周一至周五)



哔哩哔哩网站资源

<https://space.bilibili.com/630784162>

CAS 学习中心



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