

CAS SCIFINDER
DISCOVERY PLATFORM™

快速入门 指南

CAS
A division of the
American Chemical Society



目录

- 2 CAS SciFinder® 使用界面
- 2-3 文献检索
- 4 CAS Lexicon
- 5-6 IP Connections——专利检索
- 7-8 Searchsense——智能检索
- 9-10 物质检索
- 11 高级检索
- 12 CAS Roles
- 13-14 CAS Sequences 检索
- 15 CAS Life Sciences——生命科学数据
- 16-17 反应检索
- 18-19 逆合成反应路线设计
- 20 CAS Markush
- 20 CAS PatentPak®
- 21-25 CAS Formulus®
- 26-28 CAS Analytical Methods™
- 29 登录, 培训, 支持

CAS SciFinder

主界面及文献检索

检索界面

The screenshot shows the main interface of CAS SciFinder. At the top, there's a banner with "Good Afternoon" and a search bar with placeholder text "Proton nmr spectral data for C13H13Br". To the right are buttons for "更新结果提醒" (Update Result Reminder), "检索结果管理" (Search Results Management), and "账号设置" (Account Settings). Below the banner are several search categories: "Featured Search" (Prior Art Discovery, CAS词库), "专利 Markush 检索" (Patent Markush, Search CAS Sequences), "高级检索选项" (Advanced Search), "逆合成路线设计" (Retrosynthetic Analysis), and "现有技术探索" (Search CAS Lexicon).

文献结果集界面

您可以输入文本或/和结构，或利用 CAS 词库查询文献，点击 References 选项卡访问文献结果集：

- 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。

This screenshot shows the search results for the query "methanol and (food or candy or \"chewing gum\")". The "References" tab is selected. On the left, there are filters for "All", "Substances", "Reactions", "Citing", "Filter Results", "Behavior", and "Search Within Results". The main area displays a list of results, with the first one being "Steviol glycoside agglomerates and process for producing". It includes details like Assignee: Cargill, Inc., Date: 2011-08-04, and a brief abstract. There are buttons for "View More", "View Full Text", and "View Abstract". To the right, there are sections for "Analyze Results" showing "Top Concepts" (Food, Food analysis, Antioxidants, etc.) and "Top Formulation Purposes" (Food, Dietary supplement, etc.). There are also buttons for "更改结果展示内容" (Change Result Display Content), "更改结果排序" (Change Result Sort), "保存或添加到项目" (Save or Add to Project), and "下载检索结果" (Download Search Results).



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 8 Citation Map 查看文献的引文地图

In this Reference 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 chromatography (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 forced degradation studies. Responses of MTX and TEF were found to be a linear function of concentration over the range 1–50 μg/mL ($r^2 = 0.9976$ 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

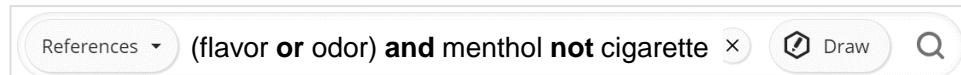
Publication Information * Journal 查看分析方法详情 查看配方/制剂详情 View Less

Source Database Information Company/Organization Publisher Language
Biomedical Chromatography AN: 2018:1864661 Department of Pharmaceutics, School John Wiley & Sons Ltd. English
Volume: 32 CAN: 170:324809 of Pharmaceutical Education and
Issue: 12 PubMed ID: 30133709 Research Jamia Hamdard
Pages: n/a Caplus and MEDLINE New Delhi
Journal: Article India

CODEN: BICHE2 题录信息
E-ISSN: 1099-0801

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。



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 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



首先点击主界面上的 "CAS Lexicon"，输入检索词，然后浏览多层次词库列表。

Search CAS Lexicon

biopesticides

Search Concept

Multiple preferred concepts found. Select one to continue.

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 ⓘ 点击下位词以查看其子类别
 Bionematocides
 Botanical pesticides
 Microbial pesticides ⓘ
 Plant-incorporated protectants ⓘ
 RNA interference pesticides ⓘ

Biological control ...

AND OR NOT

[Add to Query](#)

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格

Biopesticides - Preferred Concept ⓘ

Biopesticides - Narrower Concepts (9)

Biochemical pesticides ⓘ
Biofungicides
Bioherbicides
Bioinsecticides ⓘ
Bionematocides
Botanical pesticides
Microbial pesticides ⓘ
Plant-incorporated protectants ⓘ
RNA interference pesticides ⓘ

执行检索

Clear Query [Search](#)



专利检索

专利文献筛选及可视化分析

在文献结果集中，可以筛选专利状态、专利局、IPC分类号。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

Filtering: Document Type: Patent ▾

Clear All Filters

1 0,645 Results Sort: Relevance ▾ View: Partial Abstract ▾

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

Assignee: Sumitomo Chemical Company, Limited
World Intellectual Property Organization, WO2011062291 A1 2011-05-26 | Language: English, Database: CPlus
Patent Status: Dead Family Members: 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)₂, 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 ▾ 筛选专利局

PatentPak ▾ Full Text ▾ 12 0 7

Preventing and controlling method for rice disease and insect pest

Assignee: Unknown
China, CN10519369 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, monosulfat 80 g and 75% fengdeng (pesticide) 35 g, carrying out foliage-planting seedling, step 5, in heading stage, adopting 500 times

PatentPak ▾ Full Text ▾ 4 0 0

Analyze Results

Top Document Types

Patent

Download 可视化分析

Patent Offices

1 8.853

Other

ARIPO 26 EPO 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

R1-C(=O)-N(R2)-C(=O)-N(R3)-C2=C(C=C(R4)-N(R5)-C(=O)-R6)-C=C2-R7

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 C₅-C₁₀ cycloalkenyl, substituted or unsubstituted C₆-C₂₀ aryl, substituted or unsubstituted C₁-C₂₀ heterocyclyl, OR9, C(=X1)R9, C(=X1)OR9, C(=X1)N(R9)₂, N(R9)R2, N(R9)C(=X1)R9, SR9, S(O)R9, 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)R9, 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 C₅-C₁₀ cycloalkenyl, substituted or unsubstituted C₆-C₂₀ aryl, substituted or unsubstituted C₁-C₂₀ heterocyclyl, OR9, C(=X1)R9, C(=X1)N(R9)₂, N(R9)C(=X1)R9, SR9, S(O)R9, 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)R9, C₆-C₂₀ aryl, or C₁-C₂₀ heterocyclyl, (each of which that can be substituted, may optionally be substituted with R9);

Markush 详情

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

Claims
Classifications
CAS Concepts
Markush Structures

Patent Markush 1

Notes: Patent claim 1 additional isotopic derivatives also claimed View all on Markush Detail

查看Markush 结构详情

Publication Information: Assignee: Dow AgroSciences LLC United States, US20120110701 A1 2012-05-03 | Language: English, Database: Cplus

Notes: Patent claim 1

CAS 科学家解读的马库什结构详情

G1 = N(=O)C(=O)G2
G2 = H1.F(C1Br)CN1NO2\alkyl(opt., subst.)\alkenyl(opt., subst.)\alkoxy(opt., subst.)\alkenyl oxy(opt., subst.)\cycloalkyl(opt., subst.)\cycloalkenyl(opt., subst.)\arylp(opt., subst.)\heterocycle(opt., subst.)\OH\23\28\NH2\143\SH\46\151\113\63\167\Me

G3 = CH\alkyl(opt., subst.)\alkenyl(opt., subst.)\alkoxy(opt., subst.)\alkenyl oxy(opt., subst.)\cycloalkyl(opt., subst.)\cycloalkenyl(opt., subst.)\arylp(opt., subst.)\heterocycle(opt., subst.)\dialkylamino\G4\G5

G4 = S1S(O)\SO2

G5 = alkyl

G6 = H\CN\alkyl(opt., subst.)\alkenyl(opt., subst.)\alkoxy(opt., subst.)\alkenyl oxy(opt., subst.)\cycloalkyl(opt., subst.)\cycloalkenyl(opt., subst.)\arylp(opt., subst.)\heterocycle(opt., subst.)\30\dialkylamino\OH\32\NH2\G4\G5\G8\G9

G7 = O\LS

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。

Behavior: Filter by Exclude

Search Within Results: Reference Role: Substance Claimed

专利 Claims 中的物质

108 Results: 120068-37-3, 302578-96-7, 302578-97-8

CAS Registry Number: 120068-37-3

C₁₂H₄Cl₂F₆N₄O₅
1H-Pyrazole-3-carbonitrile, 5-amino-1-(trifluoromethylphenyl)-4-

在权利要求中保护该物质的系列专利

Stable synergistic insecticidal composition of fipronil, spinosad and pyriproxyfen
Role: Agricultural Use
Patent Number: IN20241100065 WO202514665
Publication Date: 2025-07-18

Bacillus strains having pesticidal activity and use thereof
Role: Agricultural Use
Patent Number: WO2025134164
Publication Date: 2025-06-26

Pesticidal mixtures comprising an ethylsulfone compound
Role: Agricultural Use
Patent Number: WO2025159019
Publication Date: 2025-06-19

View All Patents

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

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

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)

输入结构

Search Details: Your Inputs Text

This disclosure is related to the field of processes to produce molecules that are useful as pesticides (e.g., herbicides, insecticides, fungicides, nematicides, etc.).

Priority Date: 2025-08-13

Structure

Patents (93) Non-Patent Literature (83) 非专利文献

Select All on Page

1 Pyridinylimidazoles as pesticidal and processes for preparation and pesticidal composition
Assignee: Dow AgroSciences LLC, 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 R8; R1, R2, R3, R4 and R8 are independently H, F, Cl, Br, I, CN, etc.; R5 is H, (un)substituted C1-6.

2 Sustained-release pesticidal compositions
Assignee: HOMS LLC, Publication Date: 2008-03-20 | Priority Date: 2004-12-14
...include aphids, ants, bed bugs, bees, beetles, centipedes, caterpillars, chiggers, cockroaches, crickets, cutworms, earwigs, fleas, flies, fire ants, gnats, grasshoppers, hoolworms, Japanese beetles, June bugs, lice, locust, maggots, mealworms, mealybugs, millipedes, mites, mosquitoes, moths, pillbugs, scorpions, silverfish, spiders, stinkbugs, termites, thrips, ticks...



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。

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 Membrane:
• A nanofiltration membrane with a Mg²⁺/Li⁺ mass ratio of 1:1 can enable fast-cycling high-energy lithium metal batteries. (4)

5. Isolation and X-ray Structures:
• The isolation and X-ray structures of free phenyl carbanions have been reported, providing insight into the molecular structure of these compounds. (5)

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。

Raman spectra of luminol [输入自然语言](#)

Results for "Raman spectra of luminol"

All Substances Reactions References Suppliers Patent Markush

Spectrum Showing 1 of 1 Result

521-31-3 Luminol Viewing 1 of 1

查看谱图

Experimental View Spectra Details

Raman Spectrum

Conditions
No data available.

Spectra Summary
Spectrum ID SLSRAMAN_000706

Source Sigma-Aldrich Co. LLC. (Spectr... View All

View All Spectra →

Results for "HNMR of luminol"

All Substances Reactions References Suppliers Patent Markush

Spectra Showing 1 of 6 Results

521-31-3 Luminol Viewing 1 of 5

Experimental View Spectra Details

Proton NMR Spectrum

Conditions
Working Frequency 300 MHz
Solvent CDCl₃-D₂O (70:27:1)
Standard Tetramethylsilane (TMS)
Temperature 24 °C

Spectra Summary
Spectrum ID CC-1-H-NMR8-1704
Spectrometer BRUKER WH 300
Source Spectral data were obtained fr... View All

View All Spectra →

检索示例：检索 "HNMR of luminol"，查看3-氨基-苯二甲酰肼的核磁共振氢谱。

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

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, CPlus

View in Detail Page →

Results for "hazards of bisphenol a"

All Substances Reactions References Suppliers Patent Markush

GHS Hazard Table for Bisphenol A
Showing 5 of 62 Results

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

View Full Table →

Regulatory List
View in Detail Page →

AIC, ARIIC, CANL, DSL, ECL, EINECS, ENCS, FDA, HAP, HHAZ, HTU, IECSC, INSG, ITC, IUR, JDATA, NDNC, PICCS, PI, PROP, REACH, RTR, S313, SDS, State_CA, PROPS, State_MA, State_MN, State_NJ, State_OR, State_PA, State_VT, State_WA, STOR, STY, TCS, TDCA, TSCA, VNECL VOC, WGK

Confidential Business Information: Public

Regulatory Synonyms (3)

Details by Country/International & Other Lists

检索示例：检索 "hazards of bisphenol a"，获取双酚A的GHS危险信息。

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 ▾

Filter Results

Behavior

Filter by Exclude

Search Within Results

Non-Participating Functional Groups

Alcohol (1)

7.007 Results

Scheme 1 (1 Reaction)

Absolute stereochemistry shown, Rotation (-)

+

Cl

Suppliers (82)

Absolute stereochemistry shown, Rotation (-)

Steps: 1 Yield: 60% ⚡

Suppliers (139)

检索示例：检索 "suzuki coupling reactions"，获取 Suzuki偶联反应。

Reactions search for "suzuki coupling reactions"

All Substances Reactions References Suppliers Patent Markush

View Related Results ▾

Filter Results

Behavior

Filter by Exclude

Search Within Results

Non-Participating Functional Groups

Experimental Protocols

1,473,931 Results

Scheme 1 (1 Reaction)

Absolute stereochemistry shown

Supplier (1)

Absolute stereochemistry shown

Suppliers (50)

Absolute stereochemistry shown

Steps: 1 Yield: 100% ⚡



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）。

以下是物质检索的示例：

Streptomycin

57-92-1

"Streptomycin sulfate"

Sulfoximin*

WO2019234160

The screenshot shows the SciFinder interface with a search bar containing "Proton nmr spectral data for C13H13Br". Below the search bar are three main search categories: "Prior Art Discovery", "Patent Markush", and "Advanced Search". A callout box highlights the "Search Patent Markush" button, which is associated with a drawing tool icon and a checkbox labeled "勾选以执行 Markush 检索" (Check to execute Markush search). Other interface elements include a "Good Morning" greeting, a "Featured Search" section, and a drawing panel on the right.

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、关联的文献或供应商的数量等。

The screenshot displays the search results for substances. On the left, there is a sidebar for filtering results by structure type (e.g., Substructure, Similarity) and behavior. The main area shows three search results:

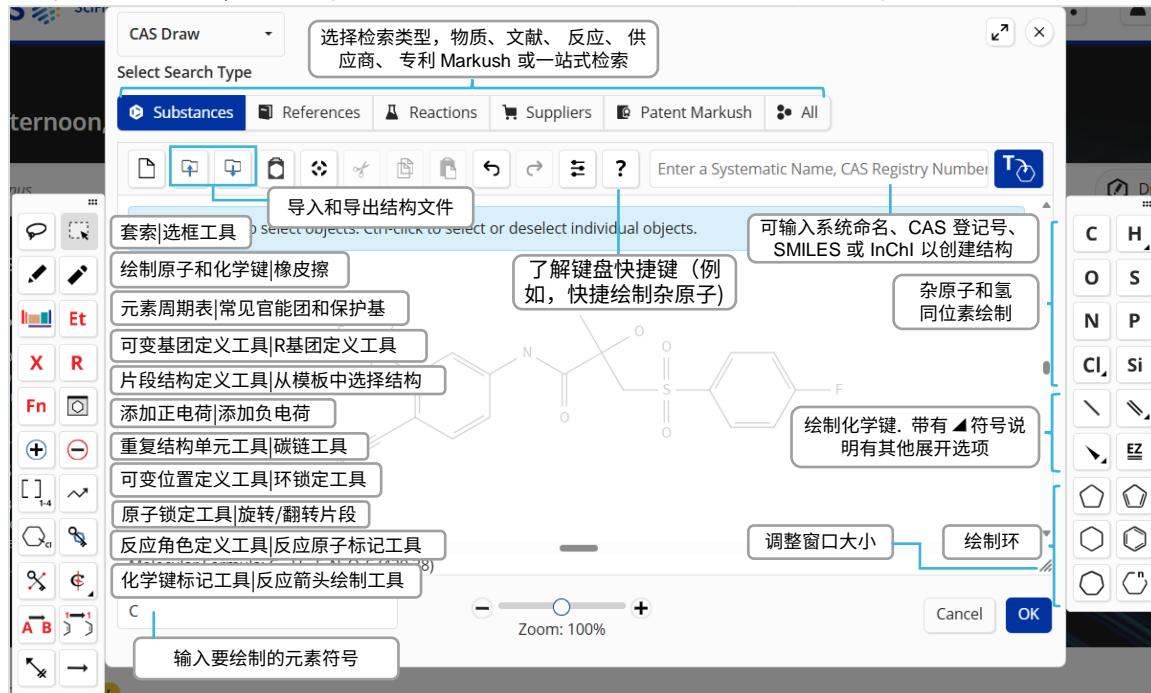
- Result 1:** CAS Registry Number 90357-06-5. Structure: C18H14F4N2O4S. Description: Propanamide, N-[4-cyano-3-(trifluoromethyl)phenyl]-3-[(4-fluorophenyl)sulfonyl]-.
Statistics: 4,719 (Downloads), 245 (Reactions), 113 (Suppliers).
- Result 2:** CAS Registry Number 383-29-9. Structure: C12H8F2O2S. Description: Benzene, 1,1-sulfonylbis-.
Statistics: 75 (Downloads).
- Result 3:** CAS Registry Number 455-15-2. Structure: C7H7FO2S. Description: Benzene, 1-fluoro-4-(methylsulfonyl)-.
Statistics: 64 (Downloads).

Each result card includes a "点开 CAS 登记号 查看详情" (Open CAS Registry Number to view details) button and a "点击结构式 打开 物质信息窗口" (Open substance information window by clicking the structure) button. The bottom right corner shows a drawing panel with a SMILES input field and a "在结构绘制面板中 打开编辑此物质" (Open edit for this substance in the structure drawing panel) button. There is also a note about "下载.png、.cxf、.sdf 或 .mol 文件，复制 SMILES" (Download .png, .cxf, .sdf or .mol files, copy SMILES).

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。



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。

This screenshot shows the detailed information page for substance 90357-06-5. At the top, it displays the CAS Registry Number, 4.714 publications, 245 reactions, and 113 suppliers. The main feature is the chemical structure, which is a complex molecule with a nitrile group, a sulfonamide group, and a hydroxyl group. Below the structure, its molecular formula is given as C₁₈H₁₄F₄N₂O₄S, and its systematic name is Propanamide, N-[4-cyano-3-(trifluoromethyl)phenyl]-3-[(4-fluorophenyl)sulfonyl]-2-hydroxy-2-methyl-. The page also includes a GHS hazard pictogram section, properties table, and a 'Patents Claimed In' section listing three patent documents. A 'Chemical Identifiers' section at the bottom lists SMILES, InChI, and other names. A sidebar on the right contains sections for 'Important Parameters' and 'CAS LIFE SCIENCES'.

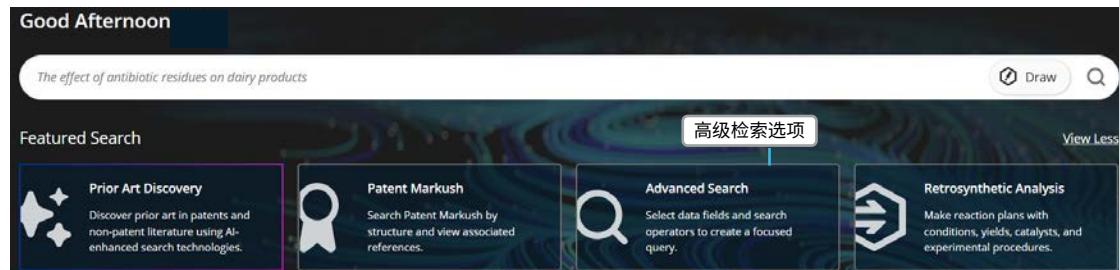


高级检索

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

Substances References Clear All

"pollution monitoring" 选择检索字段

定义检索字段之间的逻辑运算符

AND Chemical Name polyethylene

OR Chemical Name polypropylene

+ Add Advanced Search Field 添加更多高级检索字段

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

Edit Search "pollution monitoring"

点击 "Edit Search" 修改高级检索项

高级物质检索

Substances References Clear All

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

Molecular Weight 253 to 254 Predicted values only.

AND Carbon-13 NMR 114 to 171, 96, 11.5 Allowance of ± 2 ppm.

+ Add Advanced Search Field

检索说明：检索具有特定分子量和核磁共振图峰值的物质

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，您可以聚焦感兴趣的物质及其特定研究角色相关的文献。

- Super roles 是广泛的类别，包括所有相关的具体的Role。例如分析研究 (Analytical Study)。
- Specific roles 更为精确，比如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。

The screenshot shows two side-by-side filter panels. The left panel, titled 'Reference Role', has tabs for 'By Count' and 'Alphanumeric'. It lists various roles like Prophetic Synthesis or Use, Biological Study, etc., with counts from 29K to 4,098. A checked checkbox for 'Substance Claimed (4,098)' is highlighted. A callout box points to this checkbox with the text '该结果集中的具有该Role属性的物质数量' (Number of substances in the result set with this role attribute). The right panel, titled 'Substance Role', also has tabs for 'By Count' and 'Alphanumeric'. It lists roles like Product, Reactant, Reagent, Catalyst, and Solvent, with counts from 9 to 1,113. A callout box points to the 'Reactant (1,113)' entry with the text '出现在反应检索结果集中的"Substance role"的例子' (Example of "Substance role" in reaction search results).

文献检索结果中的 Roles

每当您的检索信息命中物质的标引信息部分，也就是说，通过检索物质名称，或进行基于物质检索之后的关联检索时，Roles 将作为文献检索结果中的筛选项出现。

示例：我对（海洋）污染这一课题很感兴趣，怎样才能找到专门将聚丙烯描述为污染物 (pollutant) 的文献？

检索聚丙烯会得到许多文献结果。其中 Substance role 窗口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篇文献将聚丙烯描述为污染物 (pollutant)。通过二次检索功能，或通过核心研究点筛选，可将检索结果限定于海洋污染。

The screenshot shows a search interface for 'polypropylene'. On the left, there's a sidebar with filters for 'Substance Role' (Uses, Substance Claimed, Properties, Process, Biological Study), 'Database', and 'Patent Office'. A callout box points to the 'Pollutant (6,165)' option under 'Substance Role' with the text '单击 "View All" 可以选择更多 Roles' (Click "View All" to select more Roles). The main search results area shows a list of publications. One result is highlighted: 'Co-pyrolysis of polyolefin separators and active materials from lithium batteries: Thermal conversion performance, interaction behaviors, and products'. Another result shown is 'Environmental impact of nurdle spill from MSC ELSA 3 on the Kanyakumari Coast, Southern India'. A callout box points to the 'Pollutant (6,165)' entry in the sidebar with the text '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' (Every one of the 6,165 articles in this result set discusses polypropylene as a pollutant).



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

BLAST 相似性检索

BLAST 可用于检索相似的核苷酸或氨基酸序列。序列比对结果以直观的图形布局显示，并提供便捷的精确筛选功能，可根据比对一致性和覆盖率百分比进行筛选。可以直接查看命中序列的关联文献。

要执行 BLAST 搜索，请按照以下步骤操作：

- 在CAS SciFinder 主界面中打开 CAS Sequences 模块。
- 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 BLAST 运行参数，然后启动序列检索。

The screenshot shows the 'Search CAS Sequences' interface. At the top left is a logo with a stylized 'S' and the text 'Search CAS Sequences'. Below it is a sub-instruction: 'Query BLAST, CDR, and Motif algorithms for nucleotide and protein based sequences.' The main search area has a title 'Search CAS Sequences' with a 'CAS LIFE SCIENCES' badge. A text input field says 'Enter a protein or nucleotide string, or upload a .txt or .fasta file.' Below it are three tabs: 'BLAST' (selected), 'CDR', and 'Motif'. To the right of the tabs is a button labeled '序列检索选项' (Sequence Search Options). Further right are 'Clear Search' and 'Upload Sequence (.fasta or .txt)' buttons. A sequence string 'GPGGLQGGPPGPPGCGPGBQGPSCASGPAGPR' is shown. Below the tabs is a box containing the text '将序列复制粘贴到这个窗口' (Copy and paste the sequence into this window). To the right is a 'Sequence Type' section with 'Nucleotide' and 'Protein' buttons, and a checked 'Include NCBI Sequences' checkbox. At the bottom right is a large blue 'Search Sequences' button. A bracket on the right side groups several controls under the heading '高级参数设置' (Advanced Parameters): '包含 NCBI 数据库中的序列' (Include sequences from the NCBI database), 'Search Within' (radio buttons for 'Nucleotides' and 'Proteins'), and the 'Search Within' checkbox. At the very bottom left is an 'Advanced Sequence Search' section with various parameters like 'Alignment Identity %', 'Match with Gaps?', 'Gap Costs', 'Query Coverage %', 'Word Size', 'Scoring Matrix', 'BLAST Algorithm', 'E-Value', and 'Exclude Low Complexity Regions'.

BLAST 结果分析

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: 90% Query Coverage: 90%

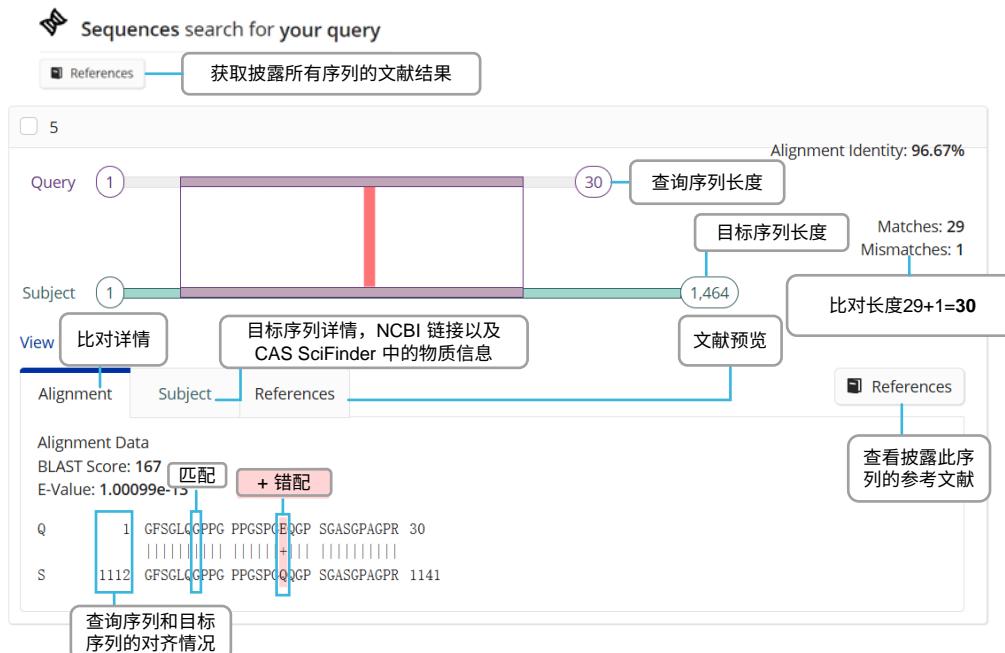
Results will expire on November 9, 2025.

[View Results](#) [Edit Search](#) [Complete](#)

查看结果

在查看 BLAST 序列相似性结果时：

- 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 可获取相关文献。
- 支持下载 XLSX 格式的结果文件。



筛选结果

检索结果会随着筛选项调整而动态改变。

E-Value <input max="10<sup>6</sup>" min="0" type="range" value="0"/>	Query Coverage % <input max="100" min="0" type="range" value="0"/>	Subject Coverage % <input max="100" min="0" type="range" value="0"/>	Alignment Identity % <input max="100" min="0" type="range" value="0"/>	Sequence Length <input max="14168" min="30" type="range" value="30"/>
E-值 (期望值)	比对上的序列长度	比对上的序列长度	匹配上的氨基酸或碱基对的数量	Organisms
	查询序列长度	目标序列长度	比对上的序列长度	<input type="checkbox"/> Gallus gallus (11) <input type="checkbox"/> Rattus norvegicus (7) <input type="checkbox"/> synthetic construct (7) <input type="checkbox"/> Cygnus olor (5) <input type="checkbox"/> Dromaius novaehollandiae (5)
				View All



生命科学数据

检索靶点、配体和疾病

在 CAS Life Sciences 中利用高级检索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数据。

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 Enter a molecular formula

CAS Registry Number Multiple entries must be separated by commas

Chemical Identifier Document Identifier Multiple entries must be separated by commas

Patent Identifier

Experimental Spectra Enter chemical name

Life Science Data Target

Biological Properties Density

Substances

Author/Inventor Name Enter last name

Publication Name Enter Keywords

Title Abstract/Keywords

Concept Substances

Publication Year Target

Document Identifier Ligand

Patent Identifier Disease

Publisher

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）

文献检索和物质检索中的生命科学数据筛选项

Life Science Data

Biomarkers (359)

Pharmacological Data (1,380)

ADME (216)

Toxicity (87)

Artemisinin By: Ashley, Elizabeth

筛选有生物标志物，药理学数据，ADME 或毒性数据的文献结果

rest of the world

Pharmacological Data (1,422)

ADME (60)

Toxicity (9)

Commercial Availability

Available (3,636)

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数据

Pharmacological Data

筛选功能

Target	Function	Parameter	Value	Disease	Organism	Assay	Source
Toll-like receptor 7	Agonist	EC50	0.42 μM	Cancer	Human	View Detail (1) CAS	bioactive compounds
Toll-like receptor 7	Agonist	EC50	1.4 μM	-	-	-	-
Toll-like receptor 7	Agonist	EC50	0.42 μM	acute pathogen infection	Human	View Detail (1) CAS	bioactive compounds

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	-

显示完整的实验细节

Ligand 144875-48-9

C₁₇H₂₄N₂O₂ 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 Poudel, Yam B.; Gangwar, Sanjeev; Sivaprakasam, Prasanna; Posy, Shoshana L.

World Intellectual Property Organization WO2019036023 A1 2019-02-21 | Language: English, Database: CAPIUS

文献详情页中的生命科学数据

Biomarkers

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。

The screenshot shows the SciFinder interface with a dark blue header. The 'Good Morning' greeting is at the top left, followed by a search bar containing 'Pauling, Linus'. On the right is an 'Edit' button and a magnifying glass icon. Below the header are four search categories: 'Prior Art Discovery', 'Patent Markush', 'Advanced Search', and a drawing tool for 'Reaction Drawing'. The 'Reaction Drawing' tool has a 'Make yield' button, an 'Edit Drawing' button, and a 'Remove' button.

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。

The screenshot shows the SciFinder interface with a search query 'synthesis of aspirin from sodium bicarbonate' entered. The results are grouped by scheme. A callout box points to the 'Group' dropdown menu with the text '将分组更换为 "By Document" 或 "By Transformation"'. Another callout box points to the 'Send to CAS Reaction Drawing Board' button with the text '发送到 CAS 结构绘制面板'. The results list includes reaction schemes with chemical structures, supplier information, and detailed reaction conditions. A 'Get Similar Reactions' button is also visible.

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。

This dialog box allows setting reaction similarity. It shows a reaction scheme with a starting material (2,2-dihydro-1H-chromene) reacting to form a product (chromone). Three radio button options are available:

- Broad (107,942) Reaction centers only
- Medium (21,764) Reaction centers plus adjacent atoms and bonds
- Narrow (4,822) Reaction centers plus extended atoms and bonds

A 'Get Reactions' button and a 'Cancel' button are at the bottom.



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
JOURNAL Development of a Scalable Synthesis of an Azaindolyl-Pyrimidine Inhibitor of Influenza Virus Replication
By: Liang, Jian... View All **查看所有作者**
Organic Process Development (2016), 20(5), 965-969
View Source Full Text

Absolute stereochemistry shown, Rotation (+) + [Stage 2] Absolute stereochemistry shown, Rotation (-) → 85%
Suppliers (48) Suppliers (149) Suppliers (2)

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 (1R,3S)-3-[(benzyloxycarbonyl)amino]cyclohexanecarboxylate , Yield: 85%
Reactants	1-Ethyl(1R,3S)-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 (1S, 3R)-3-ethoxycarbonylcyclohexanecarboxylic acid (140 g, 700 mmol) in toluene (1.4 L).

Characterization Data **查看表征数据**

^ [Ethyl \(1R,3S\)-3-\[\(benzyloxycarbonyl\)amino\]cyclohexanecarboxylate](#)

Proton NMR Spectrum	(300 MHz, CDCl ₃) 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 C ₁₇ H ₂₄ NO ₄ 306.1700, found 306.1700
State	sticky solid

CAS Method Number 3-451-CAS-15598720

Transformations **反应转化类型**
1. Schmidt Reaction

Reaction Notes **其他重要注释**
scalable

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（无文献报道过合成方法）。
2. 在现有物质的弹出窗口上点击 "Start Retrosynthetic Analysis" 选项。

The screenshot shows the CAS SciFinder software interface. At the top, there's a banner with "Good Afternoon" and a search bar for "Proton nmr spectral data for C13H13Br". Below the banner are four main search options: "Prior Art Discovery", "Patent Markush", "Advanced Search", and "Retrosynthetic Analysis". A blue callout labeled "1" points to the "Retrosynthetic Analysis" option. Another blue callout labeled "2" points to the "Start Retrosynthetic Analysis" button on the left side of the main panel.

The main panel displays a chemical structure of a complex molecule with a molecular formula of C29H40F5N6O10. On the left, there are several buttons for "Get Substance Details", "Get Bioactivity Data", "Get Reactions (1)", "Synthesise (1)", "Start Retrosynthetic Analysis", and "Get References (1)". Below these buttons are "Edit Structure", "Reset", and "+" buttons. The right side of the panel shows the "Retrosynthetic Analysis" interface with a toolbar, a drawing area with the target molecule, and a "Start Retrosynthetic Analysis" button at the bottom right.

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"

This screenshot shows the "Retrosynthesis Plan Options for drawn structure" dialog box. It includes sections for "Set Rules Supporting Predicted Reactions" (with radio buttons for "Common", "Uncommon (includes common rules)", and "Rare (includes common and uncommon rules)"), "Break and Protect Bonds (Optional)" (with buttons for "Break Bond" and "Protect Bond"), and "Clear All Bond Selections". There are also buttons for "Continue to Retrosynthesis Plan" and "Edit Structure".

A callout labeled "开始逆合成反应路线设计" points to the "Continue to Retrosynthesis Plan" button. Another callout labeled "选择常见、不常见或罕见规则 (根据文献实例支持数量而定)" points to the "Set Rules Supporting Predicted Reactions" section. A third callout labeled "首次断键中要断裂的键" points to the "Break Bond" button in the "Break and Protect Bonds (Optional)" section. A fourth callout labeled "设置在首次断键时要断裂的键" points to the "Break Bond" button. A fifth callout labeled "设置在整个方案中保护的键" points to the "Protect Bond" button. A sixth callout labeled "清除已有选择" points to the "Clear All Bond Selections" button.



逆合成方案和备选路线

逆合成路线接近即时生成。

Retrosynthesis Plan for drawn structure

Build Status: Complete Estimated Yield: 2% Overall Price: \$21477475.67

Customize Plan

Selected Options Predicted Rules: Common Break and Protect Bond 1 Broken 0 Protected

Filters View Excluded Options Step Type Experimental Steps Predicted Steps Starting Material Cost Limit 200 USD/mol

更改原料成本上限 (USD/mol 或 USD/g)

编辑方案选项

绿色虚线表示预测的步骤 蓝色实线表示报道的实验步骤

点击查看方案步骤

点击图标, 查看备选反应路线、反应依据或排除该步反应

Reset + ? Help Contact Us Legal

反应依据和备选路线

Return to All Steps

A \Rightarrow B + C + D 反应依据 Evidence Alternative Steps (81) Exclude Step

Scheme 1 (2 Reactions) Steps: 6 Yield: 0

31-614-CAS-31458888

1. Reagents : Diisopropylethylamine, 1H-1,2,3-Triazolo[4,5-b]pyridinium, 1-[bis(dimethylamino)methylene], 3-oxide Solvents : Dimethylformamide; 1 h, 25 °C View All ?

31-614-CAS-38918376

2. Reagents : Diisopropylethylamine, 1H-1,2,3-Triazolo[4,5-b]pyridinium, 1-[bis(dimethylamino)methylene], 3-oxide Solvents : Dimethylformamide; 1 h, 25 °C View All ?

A \Rightarrow B + C + D 备选反应路线 Evidence Alternative Steps (81) Exclude Step

2 of 131 Predicted Step Average Yield: 67%

3 of 131 Predicted Step Average Yield: 61%

替換当前反应路线 Replace Step

Help Contact Us Legal

CAS Markush 检索及 CAS PatentPak

CAS 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。

进行 Markush 检索

Patent Markush

Search Patent Markush by structure and view associated references.

View Related Results

Filter Results

结构匹配度

命中了的 Markush 结构

专利中重要的 Markush 详情信息

CN108570012 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

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

Substructure (5)

Behavior

Filter by

Exclude

筛选受理专利局

World Intellectual Property Organization (4)

China (1)

All Substances Reactions References Suppliers Patent Markush

Sort: Relevance

CAS PatentPak

Key Substances in Patent

CAS RN 2248004-96-6

Analyst Markup Locations (1)

Page 9

定位到专利中物质所在位置

CAS RN 100-00-5

Analyst Markup Locations (1)

Page 9

CAS RN 110-91-8

Analyst Markup Locations (1)

Page 9

下载 PDF

说明书

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

[0040] 实施例

[0041] 4-((2,4-二酮-2H-[1,3]苯并噁唑基)甲基)-N-(4-吗啉苯基)苯甲酰胺(I4)的制备

[0042] (1) 4-(4-硝基苯基)吗啉的制备

[0043] 取3.16g (0.02mol) 对硝基氯苯于100mL圆底烧瓶中, 加入25mL二甲基亚砜溶解, 加入2.62g (0.03mol) 吗啉, 于油浴下控温100℃反应, TLC跟踪反应至终点, 稍冷后, 剧烈搅拌下缓慢加入30mL蒸馏水, 析出大量黄色固体, 抽滤, 用冷水洗涤滤饼, 干燥, 得到4.04g黄色固体, 熔点: 149-150℃, 收率97%。

[0044] (2) 4-(4-吗啉基)苯胺的制备

[0045] 于100mL圆底烧瓶中加入4g铁粉, 30mL水和0.5mL冰醋酸, 加热至回流 10min, 然后加入3.12g (0.015mol) 4-(4-硝基苯基)吗啉溶于20mL甲醇的溶液, 搅拌反应, TLC跟踪反应至终点, 加入少量无水亚硫酸钠, 冷却之后用10%的碳酸钠溶液调节pH至8-9, 用硅藻土过滤, 滤饼用热的乙醇洗涤, 滤液旋蒸部分溶剂之后, 用乙酸乙酯萃取, 依次用饱和碳酸钠溶液和饱和氯化钠溶液洗涤, 有机相用无水硫酸钠干燥, 浓缩得到1.96g黄色固体, 收率139%。

下载 PDF, 包括标引的物质和注释列表

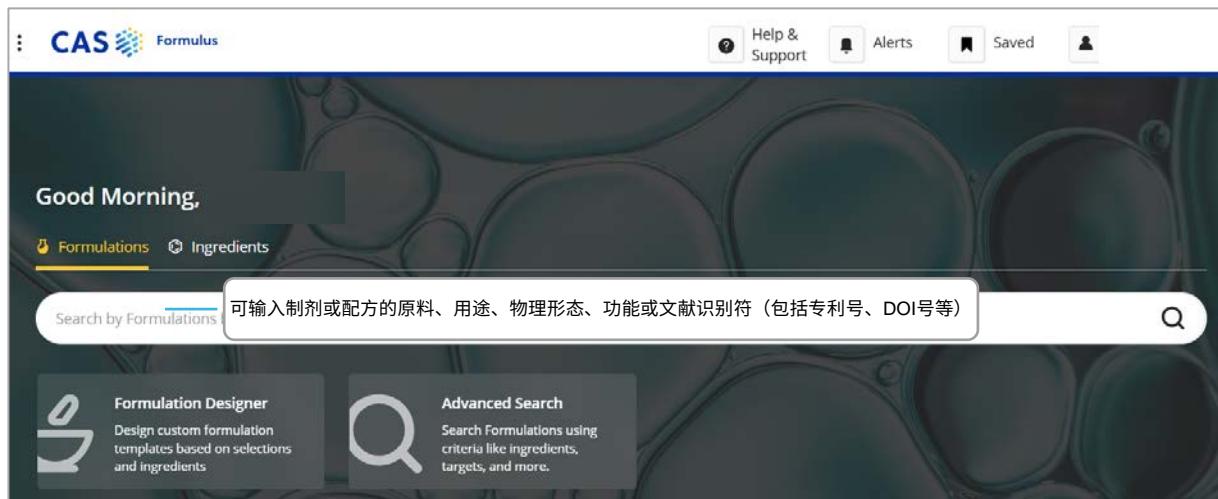
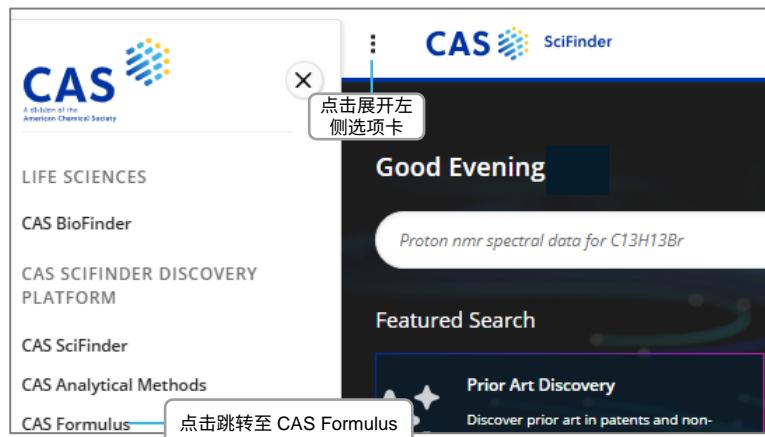
CAS 科学家标引的重要物质定位标记

5/8 页



CAS Formulus

检索制剂或配方



This screenshot shows the 'Advanced Formulations Search' interface. At the top, there is a button to 'Return to Home'. The search form is titled 'Advanced Formulations Search' with a question mark icon. It instructs users to search for content fields: Ingredient, Function, Purpose, Physical Form, Delivery Route, and Target. The search form includes fields for 'Search For' (set to 'Ingredient'), 'Operator' (with dropdown options: Optional, Required, Optional, Excluded), and 'Enter one term' (example: Ex: caffeine, sodium, 50-00-0). There is also a 'Add Another Term' button. To the right of the search form, there is a 'Clear All' button and a '清除所有内容' (Clear all content) button. On the left, there is a sidebar with a 'Browse and select search items' heading and a list of categories: All Fields, Form, Function, Ingredient, Purpose, Route, and Target. A callout box points to the 'All Fields' option with the text '添加新的检索项' (Add new search item). Another callout box points to the 'Optional' dropdown with the text '点击下拉菜单, 浏览并设置运算符' (Click the dropdown menu, browse and set operators).

Formulations search for "celecoxib"

下载结果为 PDF 或 Excel 文件

保存结果并
设置提醒

Get Additional References

获得结果集对应的文献



Save

Filter by 选择筛选选项，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



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	点击蓝色原料名称，查看详情	200 mg/tablet

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](#)

在 CAS SciFinder 中查看文献详情

Compare



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

Save

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



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:?)	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:
Antiarthritis
Purpose: Antiarthritis
Target: Arthritis, Homo sapiens
Delivery Route: Oral drug delivery system...
Physical Form: Tablets

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

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

Antiarthritic Pharmaceutical Composition
Purpose: Antiarthritis
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 PDF

View in CAS SciFinder

检索配方/制剂成分

The screenshot shows the CAS Formulus interface. At the top, there's a navigation bar with 'Good Morning,' 'Help & Support', 'Alerts', 'Saved', and user profile icons. Below the header, there are tabs for 'Formulations' and 'Ingredients', with 'Ingredients' being the active tab. A search bar at the top right contains the placeholder 'Search by ingredient Name, CAS Registry Number, or Function' and a magnifying glass icon.

The main content area displays a search result for 'propylene glycol'. On the left, a sidebar titled 'Filter by' includes sections for 'Industry' (checkboxes for Agrochemical, Cleaning & Surfactant Products, Cosmetics & Personal Care, Food & Related, Inks, Paints, & Coatings, and Pharmaceutical), 'Regulatory Information' (checkboxes for REACH, Cosmetic Ingredient Inventory, EPA Pesticide Inactive Ingredients, FDA Inactive Ingredients Database, and Drug Master File List), and 'Experimental Properties' and 'Commercial Availability'. The 'Pharmaceutical' checkbox under Industry is checked.

The search results show one result: '(±)-Propylene glycol' (CAS RN: 57-55-6). It features a chemical structure diagram (OCC(O)CO) and its IUPAC name, C₃H₈O₂. Key physical properties listed include Molecular Weight (76.09), Melting Point (Experimental) (-59 °C), Boiling Point (Experimental) (188.2 °C), and Density (Experimental) (1.036 g/cm³). The page also lists 'Commonly Used As' (Solvents; Humectants; Plastics; Lubricants; Antifreeze; Anticorrosives; Antiseptics; Preservatives; and Humectants) and 'Similar Ingredients with Regulatory Information'.

On the right side of the search results, there are several callout boxes with blue arrows pointing to specific features:

- '通过邮件发送结果' (Send results via email)
- '保存结果并设置提醒' (Save results and set reminders)
- '下载结果为 Excel 文件' (Download results as an Excel file)
- '查看原料供应商信息' (View supplier information)
- '查看实验属性' (View experimental properties)
- '查看管控信息及清单' (View regulatory information and lists)
- '将原料添加至 Formulation Designer' (Add ingredient to Formulation Designer)
- '查看使用该原料的制剂或配方' (View formulations containing this ingredient)
- '查看制剂或配方中, 与该原料同时使用的其它配伍成分' (View co-formulants used with this ingredient)

At the bottom of the search results, there's a table titled 'Commonly Formulated With' showing other ingredients like Water, Glycerin, Ethanol, etc., along with their CAS numbers and links to view formulations.

The bottom right corner shows a preview of the 'Formulation Designer' tool, which includes tabs for ANMAT (Argentina), Cosmetic Ingredient Inventory, Drug Master File List, and EMA Excipients List, and a table for adding ingredients.



设计制剂或配方

Formulation Designer

选择应用领域

Industry	Purpose	Physical Form	操作
Pharmaceutical	Drug delivery systems Pharmaceutical formulations Antitumor agents Anti-inflammatory agents Analgesics Antibacterial agents Ophthalmic agents Antidiabetic agents Antiviral agents Antihypertensives - View More Purposes -	Tablets Capsules Solutions Gels Liquids Pharmaceutical ointments Cream preparations Suspensions Sprays Powders - View More Physical Forms -	Add up to 5 Ingredients Celecoxib Polyethylene glycol + Add Another Ingredient 删除成分 添加成分 Create Template 执行检索

Formulation Designer

选择用途

Industry	Purpose	Physical Form	Active or Featured Ingredient
Pharmaceutical	Analgesics	Tablets	Celecoxib Polyethylene glycol 结果导出为 Excel 文件

重新编辑

Edit Selections

结果保存

Save

Clear All Selections

Your Template

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 ($Mg_3H_2(SiO_3)_2$)	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; FDA Color Additives;	Sodium dodecyl sulfate Glyceryl tribehenate Silica Polyoxyethylene sorbitan monooleate Magnesium stearate	Polyethylene glycol Glycerol behenate
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 ($Mg_3H_2(SiO_3)_2$); Butyl methacrylate-dimethylaminoethyl methacrylate	Approximate Range: 8 - 16%

+ Add Function

点击可添加用途

查看成分详情

查看成分管制信息

查看可替代的成分选项

Function
Anti-inflammatory agents
Add Function
Cancel

Select the ingredient you would like to use:
Sodium dodecyl sulfate
Glyceryl tribehenate
Silica
Polyoxyethylene sorbitan monooleate
Magnesium stearate

添加用途后，点击获得新的制剂或配方设计结果

CAS Analytical Methods

分析方法检索

The screenshot shows the main interface of the CAS Analytical Methods website. At the top, there's a sidebar with links to 'LIFE SCIENCES', 'CAS BioFinder', 'CAS SCIFINDER DISCOVERY PLATFORM', 'CAS SciFinder', and 'CAS Analytical Methods'. A callout points to 'CAS Analytical Methods' with the text '点击跳转至 CAS Analytical Methods'. The main content area has a dark background with a 'Good Evening' greeting and a 'Featured Search' for 'Proton nmr spectral data for C13H13Br'. Below this is a 'Prior Art Discovery' section. On the right, there are buttons for '查看保存的结果', '检索历史', and '账号管理'. At the bottom, there's a search bar with placeholder text 'Search for keywords, matrices or analyte.' and a magnifying glass icon. To the left of the search bar are two buttons: 'Explore Methods' (with a grid icon) and 'Advanced Search' (with a magnifying glass icon). Callouts point to these with the text '浏览方法分类, 查看相关方法' and '高级检索'. Below the search bar is a 'Recent Search History' section with a list containing 'celastro' and a timestamp '10 April 2025'. Buttons for 'View all Search History' and '删除历史记录' (Delete History) are also present.

高级检索

This screenshot shows the 'Advanced Search' interface. On the left, there's a sidebar with buttons for 'AND', 'OR', and 'NOT', and a note '逻辑运算符: and, or, not'. Below this is a button '增加检索条件' (Add Search Criteria) with a plus sign icon. The main search area has fields for 'Analyte' (set to 'palmitic acid'), 'Matrix' (set to 'blood plasma'), and a dropdown menu currently showing 'Keyword'. A callout points to 'Keyword' with the text '增加检索条件'. A large callout at the bottom right contains the text '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'. There's also a '删除检索条件' (Delete Search Condition) button with a minus sign icon.



分析方法的分类检索

Explore Method 浏览并选择方法分类及子分类

Category	Category Name	Include Keywords (Optional)	Clear all selections
Agricultural Applications / Bioassays	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	可输入关键词 Palmitic acid + Add Another Keyword 增加关键词	清除所有条件
Biomolecule Isolation			
Environmental Analysis			
Food Analysis			
Fuels / Geology / Biofuels			
Historical Analysis / Dating			
Miscellaneous			
Organic Compound Analysis			
Organometallics / Inorganics			
Pharmacology / Toxicology			
Polymer Analysis			
Water Analysis			

检索分析方法
Search Methods

分析方法结果集

Results for Biomolecule Isolation Assay +1 Keyword

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

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)

1 Selected 3 Results 选中方法, 导出或保存

Sort: Relevance ▾ Group: By Method ▾

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 View Abstract ▾ 获得全文链接 Full Text ▾ 在 CAS SciFinder 中查看文献详情 View in CAS SciFinder

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

结果保存

CAS Method Number: 1-122-CAS-534418

Method Category: Fatty Acid Analysis

Technique: Mass spectrometry; HPLC; Solvent extraction

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

Matrix: Blood plasma

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

Reagent: Chloroform, Methanol

Biological Reagent: -

分析物、基质、材料、试剂等分类展示

操作步骤

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

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

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 x 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 15 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.

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 下载方法比较结果为 PDF 或 Excel 格式

	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



登录，培训，支持

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>

欢迎微信扫码咨询



美国化学文摘社 (CAS) 链接全球科学知识加速科学突破，以实现改善人们生活的愿景。CAS助力全球创新者在当今复杂的数据环境中高效定位，在创新之旅的每个阶段做出自信的决策。作为科学知识管理专家，CAS建立了全球权威的人工标引科学数据合集，提供不可或缺的信息解决方案、定制服务和专业资源。不同行业的科学家、专利专业人士和商业领袖信赖CAS，从而发现机会、降低风险、解锁共享知识，更快地获得灵感实现创新。CAS是美国化学会分支机构。

联系我们请访问 cas.org。



010.62508026/7 | china@acs-i.org

© 2025 American Chemical Society. All rights reserved.
SCIACDENGREF101245240414-A4

