

CAS SCIFINDER  
DISCOVERY PLATFORM™

# 快速入门 指南

CAS

A division of the  
American Chemical Society





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**CAS SciFinder**

# 页面及文献检索

## 主界面

以下选项可在 CAS SciFinder 的主界面上找到。



## 检索界面

CAS SciFinder拥有简洁的检索界面。



## 检索界面

进行文献检索时, 您可以在一个易于使用的界面中访问完整的检索结果集:

- 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。

The search results interface includes:

- 查看关联物质 (View associated substances)
- 查看关联反应 (View associated reactions)
- 搜索关键词: menthol and (food or candy or "chewing gum")
- 保存检索结果、创建提醒、添加项目、共享检索结果 (Save search results, create reminder, add project, share search results)
- 与已保存的结果集合并 (Merge with saved results)
- Substances, Reactions, Citing, Knowledge Graph buttons
- Filtering: Concept: Flavor (移除已应用的筛选项) (Remove applied filter)
- Excluding: Concept: Antibacterial agents (X) (Remove excluded filter)
- 391 Results (391 Results)
- 点击标题打开文献详细信息 (Click title to open document details)
- Coencapsulation of xylitol and menthol by double emulsion followed by complex coacervation and microcapsule application in chewing gum (By: Santos, Milla G., Carpinteiro, Debora A.; Thomazini, Marcelo; Rocha-Selmi, Gláucia; Christiane E. C.; Favaro-Trindade, Carmen S.)
- 选择 Filter by 或 Exclude, 然后选择筛选项 (Select Filter by or Exclude, then choose filters)
- 更改结果显示方式 (Change result display mode)
- 保存或添加到项目 (Save or add to project)
- 点击访问全文链接 (Click to access full text)
- Full Text dropdown
- Substances (2), Reactions (0), Citing (44), Citation Map buttons
- 获取与该参考文献关联的物质、反应和引文信息 (Get substances, reactions, and citations associated with this reference)
- 在检索结果集中进行二次检索 (Perform a secondary search within the results set)
- Document Type dropdown: Journal (1,321), Patent (1,822), Review (53), Clinical Trial (26)
- 选择筛选项以缩小结果范围 (Select filters to narrow down results)

# 文献详情和检索操作符

## 文献详情

获取 CAS SciFinder 中每篇文献的详细信息。

### Fruit juice-containing food products with refreshing and cooling flavors

46 0 6 Citation Map 查看文献的引文地图 Save

CAS Formulus®, the comprehensive formulations database and workflow solution, is now available for all SciFinder® users. [View content from CAS Formulus® in this document.](#) [Learn more about Formulus®.](#) X

In this Reference By: Shimizu, Toru; Shigeta, Yoshinari; Kunieda, Satomi

- IPC Data
- CAS Concepts
- Substances
- Formulations
- Cited Documents

文献详情快速导览

A fruit juice-containing food product contains, in addition to a fruit component and a sweet base, (a) one or more refreshing substances selected from the group consisting of menthol, menthone, camphor, pulegol, isopulegol, pulegone, cineol, mint oil, peppermint oil, spearmint oil, eucalyptus oil, and fractions thereof, and (b) one or more cool-tasting substances selected from the group consisting of 3-(l-menthoxy)propane-1,2-diol, N-ethyl-p-menthane-3-carboxamide, 3-(l-menthoxy)-2-methylpropane-1,2-diol, p-menthane-3,8-diol, 2-(l-menthoxy)ethanol-1-ol, 3-(l-menthoxy)propan-1-ol, 4-(l-menthoxy)butan-1-ol, cyclic carboxamides, acyclic carboxamides, N,2,3-trimethyl-2-iso-Pr butanamide, a menthoxy alkanol (alkyl group having 2-6 carbons), a menthoxy alkyl ether (alkyl group having 1-6 carbons), and a menthoxy alkanediol (alkyl group having 3-6 carbons). Thus, an orange juice beverage may contain menthol as the refreshing component and 3-(l-menthoxy)-1,2-propanediol as the cool-tasting component.

Keywords: fruit juice flavor food beverage menthol

PatentPak Viewer Get Prior Art Analysis Full Text ▾

查看书目详情

Publication Information Patent 点击获取现有技术分析 View Less

Patent Number WO2005048743	Publication Date 2005-06-02	Application Number WO2004-JP17524	Application Date 2004-11-18	Kind Code A1
Assignee Takasago International Corporation, Japan	Source World Intellectual Property Organization	Database Information AN: 2005:470226 CAN: 143:25602	Language English	专利族和优先权申请信息

Patent Family

Patent	Language	Kind Code	PatentPak Options	Publication Date	Application Number	Application Date
WO2005048743	English	A1	PDF   PDF+   Viewer	2005-06-02	WO2004-JP17524	2004-11-18
JP2005143461	Undetermined	A	PDF: 显示原始专利PDF PDF+: 显示带有标引物质表格的全文 Viewer: 显示带有标引结果的可交互的全文			2003-11-19

## 布尔逻辑运算符

您可以使用布尔逻辑运算符进行文献检索。

使用括号表明对此逻辑运算符进行优先运算，例如使用“OR”连接相关术语，如下所示：

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。



# 物质名称及结构式检索

## 物质检索

可以通过在检索框中输入一个或多个物质名称或标识符来检索物质。还可以通过绘制或编辑结构式进行检索。以下是通过物质名称进行检索的示例选项。

**Streptomycin**

57-92-1

**Streptomycin sulfate**

"**Streptomycin sulfate**" **Streptomycin**

**Sulfoximin\***

**WO2019234160**

检索 Streptomycin 记录

检索使用 CAS Registry Number 作为标识符的物质记录

检索三项记录: Streptomycin, Streptomycin sulfate 和 Sulfate

检索两项记录: Streptomycin sulfate 和 Streptomycin

检索所有以 Sulfoximin 开头的名称

检索该专利的所有标引物质

The screenshot shows the SciFinder interface with various search and drawing tools. At the top, there are tabs for All, Substances (selected), Reactions, References, and Suppliers. A search bar at the top right says "输入化学品名称查询". To the right is a drawing panel with a sulfur atom structure, labeled "点击绘制新的结构" (Click to draw a new structure). Below the search bar are buttons for "Add Advanced Search Field" and "Search CAS Lexicon". A "Retrosynthetic Analysis" section is also visible. On the right, there's a "Search CAS Sequences" section and a "Search Patent Markush" button. A "Edit Drawing" and "Remove" button are located near the drawing panel.

## 物质检索结果

物质检索结果在一个直观的界面中呈现，您将看到与您的检索最相关的结果，包括其关键属性信息和高分辨率结构式图像。

This screenshot shows the results page of the SciFinder interface. On the left, there are several filter options: "Structure Match" (selected), "As Drawn (117)", "Substructure (6.2M)" (highlighted in blue), "Similarity (1,052)", "Analyze Structure Precision", "Chemscape Analysis", "Create Chemscape Analysis", "Filter Behavior", "Filter by", and "Search Within Results". A "结构精度分析" (Structure Precision Analysis) tool is also shown. In the center, search results are listed for compounds like 90357-06-5 (Bicardamide), 80-08-0 (Dapsone), and 149104-88-1 ([4-(Methylsulfonyl)phenyl]boronic acid). Each result includes basic information like CAS RN, CAS Name, References, Reactions, and Suppliers. A detailed view of the third result is expanded, showing its structure (C12H12N2O2S), properties, and related data. On the right, there are buttons for "Edit Structure", "Reset", and "Download".

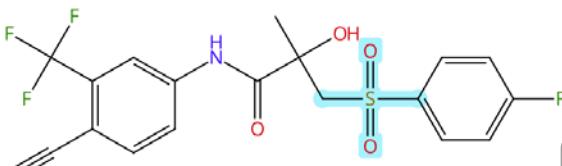
# 物质详情和结构绘制面板

## 物质详情

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

CAS Registry Number: 90357-06-5

4,364 233 116 Save



GHS危害图例，在页面底部选项卡中可查看完整列表

**C<sub>18</sub>H<sub>14</sub>F<sub>4</sub>N<sub>2</sub>O<sub>4</sub>S** 按希爾顺序排列的分子式

Propanamide, N-[4-cyano-3-(trifluoromethyl)phenyl]-3-[(4-fluorophenyl)sulfonyl]-2-hydroxy-2-methyl- (9CI, ACI) 系统名称

重要参数

Key Physical Properties	Value	Condition
Molecular Weight	430.38	-
Melting Point (Experimental)	190-195 °C (decomp)	-
Boiling Point (Predicted)	650.3±55.0 °C	Press: 760 Torr
Density (Predicted)	Canonical SMILES N#CC1=CC=C(C=C(F)F)NCC(=O)C(O)CCS(=O)(=O)C2=CC=C(F)C=C2 InChI InChI=1S/C18H14F4N2O4S/c1-17(26,10-29(27,28)14-6-3-12(19)4-7-14)16(25)24-13-5-2-11(9-23)18(20,21)22/h2-8,26H,10H2,1H3,(H,24,25) InChI Key LKJPYSCBVHEWIU-UHFFFAOYSA-N 9 Other Names for this Substance N-[4-Cyano-3-(trifluoromethyl)phenyl]-3-[(4-fluorophenyl)sulfonyl]-2-hydroxy-2-methylpropanamide (ACI) Propanamide, N-[4-cyano-3-(trifluoromethyl)phenyl]-3-[(4-fluorophenyl)sulfonyl]-2-hydroxy-2-methyl-, (-)- (ZCI) (±)-4-Cyano-α,α,α-trifluoro-3-[(p-fluorophenyl)sulfonyl]-2-methyl-m-lactotolidide Bicalutamide	

在源文献链接中列出或可获取的物质属性和谱图信息

化学标识符列表，包含SMILES、InChI、系统名称、俗名和商品名

## CAS 结构绘制面板

您可以使用 CAS 结构绘制面板绘制结构式和反应式进行查询。

CAS Draw 导入和导出结构文件 输入 CAS 登记号、SMILES，或 InChI 以创建结构

套索|选框工具 | 元素周期表|常见官能团和保护基 | 可变基团定义工具|R基团定义工具 | 片段结构定义工具|从模板中选择结构 | 添加正电荷|添加负电荷 | 重复结构单元工具|碳链工具 | 可变位置定义工具|环锁定工具 | 原子锁定工具|旋转/翻转片段 | 反应角色定义工具|反应原子标记工具 | 化学键标记工具|反应箭头绘制工具

输入要绘制的元素符号

了解键盘快捷键（例如，快捷绘制杂原子）

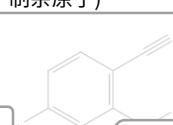
杂原子和氢同位素绘制

绘制化学键. 带有▲符号说明有其他展开选项

绘制环

调整窗口大小

OK Cancel



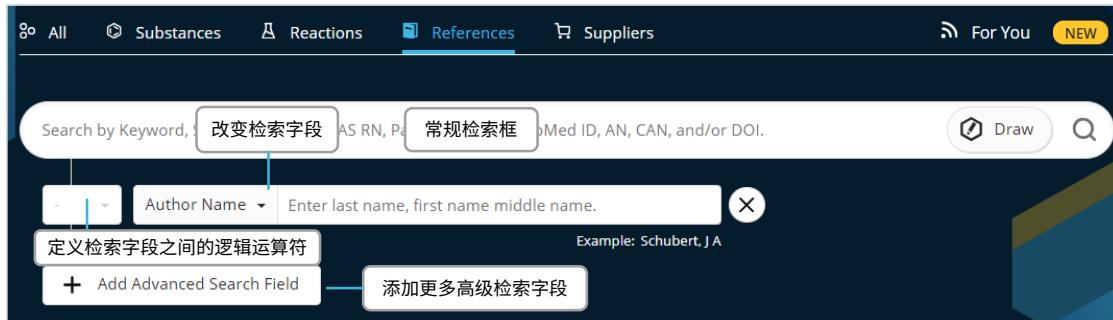


# 高级检索

## 执行高级检索

您可以使用 CAS SciFinder 主搜索界面上的高级检索字段进行特定的文献检索和物质检索。

- 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, 不能使用逻辑运算符
- 允许使用通配符, 例如 peek\*
- 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

"pollution monitoring"

使用逻辑运算符组合检索字段

AND  
Chemical Name  
Polyethylene

OR  
Chemical Name  
Polypropylene

A screenshot of the SciFinder search interface for advanced literature search. It shows a search query "pollution monitoring" and two search fields: one for "Chemical Name" containing "Polyethylene" and another for "Chemical Name" containing "Polypropylene". The operator "AND" is selected between the first field and the second field.

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

### 高级物质检索

Steel

AND  
Tensile Strength (Mpa)  
>0

Search key property values only.

A screenshot of the SciFinder search interface for advanced material search. It shows a search query "Steel" and a search field for "Tensile Strength (Mpa)" with the value ">0". A checkbox for "Search key property values only" is checked.

检索说明:  
检索钢材拉伸强度性能信息

References  
Edit Search  
"pollution monitoring"

A screenshot of the SciFinder search interface showing the "Edit Search" button highlighted in blue.

点击“Edit Search”修改高级检索项

## 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
- 生物活性数据
- 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
- 生物活性数据
- 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，使您可以聚焦将感兴趣的物质与其在文献中的具体Role相关联的文献。

- 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）的使用。

## 物质检索结果中的 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。

Reference Role

By Count Alphanumeric

出现在物质检索结果集中的“reference roles”的例子

该结果集中的具有该Role属性的物质数量

0 Selected

Adverse Effect (15)  Diagnostic Use (3)  Pharmacological Activity (10)  
 Agricultural Use (29)  Food or Feed Use (120)  Physical, Engineering, or Chemical Process (888)  
 Analyte (17)  Formation, Non-preparative

## 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。我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3,661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。

Substances Polypropylene

9003-07-0

(C<sub>3</sub>H<sub>6</sub>)<sub>x</sub>  
Polypropylene

321K References 7,909 Reactions 27 Suppliers

Filter Behavior Filter by Exclude

456,514 Results Sort: Relevance View: Full Abstract

1 Microstructure of polypropylene

By: Busico, Vincenzo; Cipullo, Roberta  
Progress in Polymer Science (2001), 26(3), 443-533 | Language: English, Database: CASplus

A review, with 175 references, on catalyst technologies for manufacture of **polypropylene** with well-controlled microstructure and properties for advanced applications. The development of transition metal catalysts with tunable structure and selectivity is discussed. **Polypropylene** products with novel and well-controlled microstructure are described. The use of high-field <sup>13</sup>C NMR methods to study the stereochemistry of **polypropylene** is also discussed.

Full Text Substance (1) Reactions (0) Citing (385) Citation Map

单击“View All”可以  
选择更多 Roles  
donate nanocomposites  
Jian Xiong; Cheung, Ying Kit  
Polymer (2002), 43(10), 2981-2992 | Language: English, Database: CASplus

Substance Role

By Count Alphanumeric

1 Selected

Uses (268K)  Biological Use, Unclassified (3,793)  
 Technical or Engineered Material Use (191K)  Pollutant (3,661)  
 Polymer in Formulation (81K)  Biological Study (22K)  
 Properties (61K)  Preparation (19K)  
 Process (52K)

View All

Language

Publication Year

Microplastics in marine environment review of methods for identification and quantification  
By: Hidalgo-Ruz, Valeria; Gutow, Lars; Thompson, Richard C.; Thiel, Martin  
Environmental Science & Technology (2012), 46(17), 3005-3017 | Language: English, Database: CASplus and MEDLINE

This review provides a comprehensive overview of methods used for the identification and quantification of microplastics from the marine environment. Three main sampling strategies were identified: selective, volume-reduced, and bulk sampling. Most sediment samples come from sandy beaches at the high tide line, and most seawater samples were taken at the sea surface using neuston nets. Particles were distinguished during sampling by size, shape, and color. This review also found that the use of microtweezers during sampling was one of the most commonly used methods for the identification of microplastics using type, shape, degradation stage, and color as criterial. Chem. and phys. characteristics (e.g., specific d) were also used. The most reliable method to identify the chem. composition of microplastics is by IR spectroscopy. Most studies reported that plastic fragments were present in all samples. The most common methods for quantification are (a) g/m<sup>2</sup> for sediments and sea surface studies and (b) items per m<sup>3</sup> for water column studies. Mean size of sieves and filters used during sampling or sample processing influence abundance estimates. Most studies reported two main size ranges of microplastics: (i) 500 µm, which are retained by a 500 µm sieve, and (ii) 1–500 µm or fractions thereof that are retained on filters. We recommend that future research focus on the development of methods for the identification and quantification of microplastics, but also on standardized sampling procedures which allow the spatiotemporal comparison of microplastic abundance across marine environments.

Full Text Substances (3) Reactions (0) Citing (2,269) Citation Map

3663-53-6  
CAS RN Chemical Name Roles

Kepka, Polyprene

此结果集中的3,661篇参考文献中的每一篇都将聚丙烯作为污染物讨论。

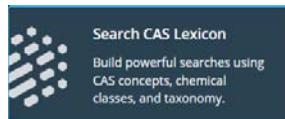


# CAS Lexicon

## 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，以及重要的物质，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，然后浏览多层级词库列表。

biopesticides

Multiple preferred concepts found. Click 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.

Search Concept

Biopesticides

**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 ⓘ

**Biopesticides - Preferred Concept ⓘ**

**Biopesticides - Narrower Concepts (9)**

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

**逻辑运算符可以用来组合不同的核心研究点**

**点击 “Add to Query” 将所选词加入右侧窗格**

**点击 “Search” 执行检索。检索结果详情中命中的词将会突出显示**

AND OR NOT

Add to Query

Clear Query

Search

# 检索CAS序列

## 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。
- 充分利用支持的格式，例如：包含由单字母代码表示的残基的序列（例如，在FASTA格式中）。
- 注意，序列输入可支持批量检索。
- 根据需要调整BLAST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 of a DNA double helix. Below it is a sub-header: 'Search CAS Sequences' and 'Query BLAST, CDR, and Motif algorithms for nucleotide and protein based sequences.' On the left, there are three tabs: 'BLAST' (selected), 'CDR', and 'Motif'. A 'Clear Search' button is at the top right. The main search area has a text input field containing a FASTA sequence: '> human insulin sequence\nfvnqhlcgshlveaylvcgergffytpktgiveqcctsicslyqlenycn'. To the right of this is a 'Upload Sequence (.fasta or .txt)' button. Below the sequence input is a 'Sequence Type' section with 'Nucleotide' selected. Under 'Search Within:', both 'Nucleotides' and 'Proteins' are listed, with 'Proteins' selected and a checked checkbox for 'Include NCBI Sequences'. A large blue button at the bottom right says 'Search Sequences'. A callout box labeled '高级参数设置' (Advanced Sequence Search) points to the bottom-left section of the interface, which includes fields for 'Alignment Identity %', 'Match with Gaps?', 'Gap Costs', 'Query Coverage %', 'Word Size', 'Scoring Matrix', 'BLAST Algorithm' (set to 'BLASTp'), 'E-Value' (set to '10'), 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。

Sequences  
1:34 PM

Sequence Type: Protein  
Search Within: Proteins  
NCBI Included: Yes  
BLAST Algorithm: BLASTp  
Alignment Identity: -  
Query Coverage: 90%

> human insulin sequence  
fvnqlcgshlveaylvcgergffytpktgiveqcctsicslyqlenycn

View Results

Edit Search

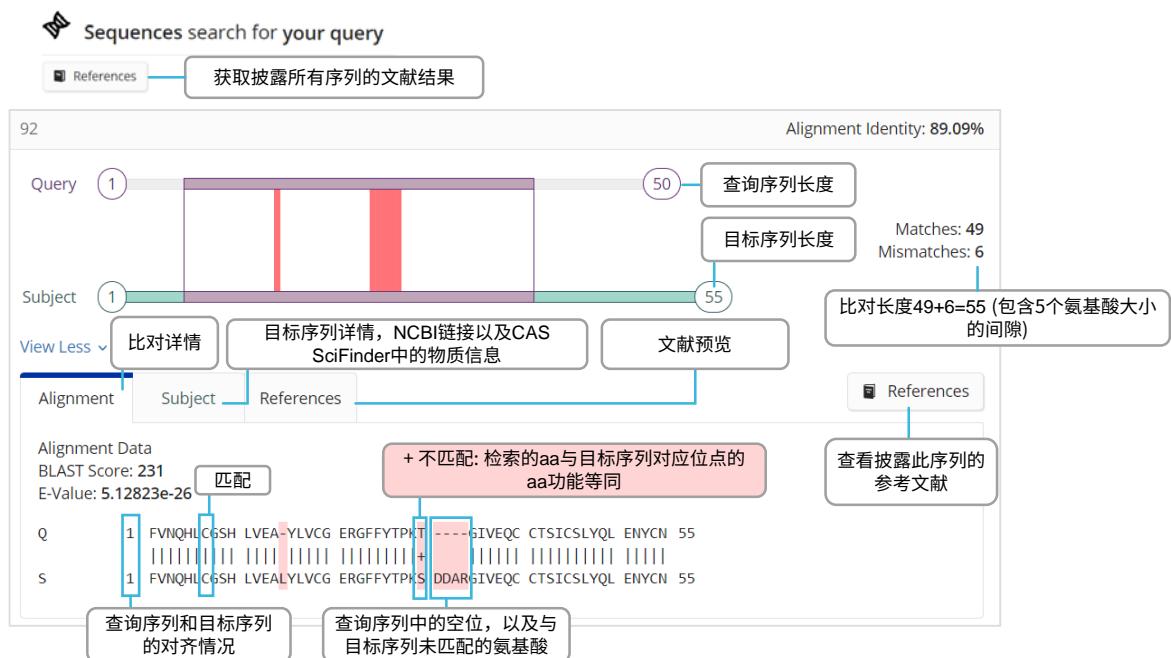
Complete

Results will expire on Oct 31, 2023.

## 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

0 to  $10^6$

Query Coverage %

0 to 100

Subject Coverage %

0 to 100

Alignment Identity %

0 to 100

Sequence Length

26 to 9521

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

查询序列长度

目标序列长度

比对上的序列长度

Organisms

- Homo sapiens (25)  
 Mus musculus (25)

# 生物活性数据

## 检索靶点、配体和疾病

通过物质检索和文献检索的高级检索字段，您可以找到与靶点、配体和疾病相对应的生物活性数据。这将在 CAS Life Sciences 中检索物质和/或文献。

The first screenshot shows a search for substances with bioactivity data, using fields like Molecular Formula, Bioactivity Data (NEW), Target, Ligand, and Disease.

The second screenshot shows a search for literature with bioactivity data, using fields like Author Name, Publication Year, and Document Identifier.

The third screenshot shows a search for substances by keyword, target, and ligand, specifically targeting the Renin receptor ATP6IP2.

A callout box indicates: "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)" (Select target, ligand, or disease (add and combine further bioactivity search fields)).

## 文献检索和物质检索中的生物活性数据筛选项

Left panel: Life Science Data filters include Pharmacological Data (56), ADME (113), and Toxicity (5). A callout box says: "通过药理学数据, ADME和毒性数据文献结果集中进行筛选" (Filter results based on pharmacological data, ADME, and toxicity data).

Middle panel: Formulation Purpose filter.

Right panel: Commercial Availability filter, showing available substances (3,636). A callout box says: "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" (Filter results based on substance pharmacological data, ADME, and toxicity data).

## 物质详情页中的生物活性数据

Top section: Pharmacological Data table showing EC50 values for Toll-like receptor 7 agonists. A callout box says: "显示完整的实验细节" (View full experimental details).

Middle section: ADME table.

Bottom section: Toxicity table.

Right side: Detailed assay graph for Ligand 144875-48-9, showing its chemical structure (C13H22N4O2 Resiquimod) and experimental details.

## 文献详情页中的生物活性数据

Table: Pharmacological Data for Alpha-amylase and Alpha-glucosidase inhibitors, showing IC50 values and diseases.



# 反应检索

## 进行反应检索

可以使用CAS反应登记号、物质名称、CAS 登记号、文献标识符、化学结构或基于文本来进行反应检索。

The screenshot shows the SciFinder interface with a dark blue header. The 'Reactions' tab is selected. A search bar at the top allows searching by CAS Reaction Number, Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. Below the search bar are three main buttons: 'Retrosynthetic Analysis' (with a retrosynthesis icon), 'Search CAS Lexicon' (with a cube icon), and a button for 'Edit Drawing' which shows a chemical reaction scheme.

## 反应检索结果

默认情况下，反应检索结果按照上一次设置进行分组。

The screenshot displays the search results for a drawn structure. On the left, there are filters for 'References', 'Structure Match' (set to 'As Drawn (0)'), 'Substructure (20K)', and 'Similarity (18)'. The main area shows 'Scheme 1 (2 Reactions)' with a reaction scheme involving a substituted benzene ring and a hydroxyl group. The first reaction is detailed with reagents (Triethylamine, Diphenylphosphoryl azide), solvents (Toluene), steps (1), yield (100%), and a reference (31-614-CAS-27240963). The second reaction is also detailed with similar information. To the right, there are buttons for 'Save', 'Print', and 'Share'. At the bottom, a 'Get Similar Reactions' dialog is open, showing a reaction scheme from a benzene derivative to a nitrone and three selection options: 'Broad (107,942) Reaction centers only', 'Medium (21,764) Reaction centers plus adjacent atoms and bonds', and 'Narrow (4,822) Reaction centers plus extended atoms and bonds'. Buttons for 'Get Reactions' and 'Cancel' are at the bottom of the dialog.

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  
JOURNAL Development of a Scalable Synthesis of an Azaindolyl-Pyrimidine Inhibitor of Influenza Virus Replication  
By: Liang, Jianyin  
View All ▾  
Organic Process Development (2016), 20(5), 965-969  
View Source Full Text ▾  
Company/Organization Vertex Pharmaceuticals Incorporated Boston, Massachusetts 02210 United States

Absolute stereochemistry shown, Rotation (+)  
[Stage 2] Suppliers (48) Suppliers (149) Suppliers (2)

Absolute stereochemistry shown, Rotation (-)  
85%

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 <sub>3</sub> ) 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] <sup>+</sup> calculated for C <sub>17</sub> H <sub>24</sub> NO <sub>4</sub> 306.1700, found 306.1700
State	sticky solid

CAS Method Number 3-451-CAS-15598720

Transformations 1. Schmidt Reaction 反应转换类型

Reaction Notes scalable 其他重要注释



# 逆合成反应路线设计工具

## 启动工具

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 SciFinder interface with the following elements:

- Top Navigation Bar:** Shows "Good Afternoon, Ilja" and tabs for All, Substances, Reactions (highlighted), References, and Suppliers.
- Search Bar:** "Search by CAS Reaction Number, Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI." with a "Draw" button and a magnifying glass icon.
- Tool Buttons:** Three buttons: "Retrosynthetic Analysis" (with a retrosynthetic icon), "Search CAS Lexicon" (with a search icon), and "Search CAS Sequences" (with a DNA helix icon).
- Central Area:** A large window for "Retrosynthetic Analysis".
  - Left Panel:** Shows a chemical structure of a complex molecule (a methoxy-substituted trifluoromethyl-oxadiazole-thiophene-naphthalene derivative) and a "Start Retrosynthetic Analysis" button.
  - Right Panel:** Shows the same molecule with its CAS RN (2408121-76-4) and CAS Name (2-[Methoxy[5-[5-(trifluoromethyl)-1,2,4-oxadiazol-3-yl]-2-thienyl]methyl]-5-meth...). It also lists options: Get Substance Details, Get Bioactivity Data, Get Reactions (1), Synthesize (1), Start Retrosynthetic Analysis (highlighted with a blue box labeled "2"), Get References (1), and Get Suppliers (0). Buttons for Edit Structure, Reset, and Download are at the bottom.

# 逆合成反应路线设计工具

## 选择方案选项

您可以编辑方案选项以：

- 修改合成深度。
- 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。
- 更改起始原料的成本限制。
- 选择较少文献实例支持的不常见或罕见规则。

设置好了所需的选项后，点击 “Create Retrosynthesis Plan”

更改方案中的合成深度

设置在首次断键中  
要断裂的键

设置在整个方案  
中保护的键

清除已有选择

Powered by ChemPlanner®

Retrosynthesis Plan Options for drawn structure

Select Synthetic Depth

1 2 3 4

Learn more.

Break and Protect Bonds

Break Bond Protect Bond Clear All Bond Selections

Set Rules Supporting Predicted Reactions

Common Uncommon (includes Common Rules) Rare (includes Common and Uncommon Rules)

选择较少文献实例支持的不  
常见或罕见规则

Set Starting Materials Cost Limit

1000 USD/mol

Email me when my plan is complete

更改原料成本上限(USD/mol或USD/g)

Create Retrosynthesis Plan

点击Create Retrosynthesis Plan，开始运行逆合成反应路  
线设计

首次断键中要断裂的键  
受保护的键

The screenshot displays the 'Retrosynthesis Plan Options for drawn structure' interface. At the top, there are three main buttons: '更改方案中的合成深度' (Change synthesis depth in the scheme), '设置在首次断键中要断裂的键' (Set bonds to break in the first cut), '设置在整个方案中保护的键' (Set bonds to protect throughout the scheme), and '清除已有选择' (Clear existing selection). Below these are sections for 'Select Synthetic Depth' (with radio buttons for 1, 2, 3, or 4), 'Set Rules Supporting Predicted Reactions' (with options for 'Common', 'Uncommon (includes Common Rules)', and 'Rare (includes Common and Uncommon Rules)'), and 'Set Starting Materials Cost Limit' (with a field set to '1000' and a dropdown menu for 'USD/mol'). There is also a checkbox for 'Email me when my plan is complete'. On the right side, there is a chemical structure of a target molecule with specific bonds highlighted: one in red for 'Break Bond' and one in green for 'Protect Bond'. Below the structure are two buttons: '首次断键中要断裂的键' (Bonds to break in the first cut) and '受保护的键' (Protected bonds). At the bottom left, a large blue button says 'Create Retrosynthesis Plan'. A note at the bottom left says '点击Create Retrosynthesis Plan，开始运行逆合成反应路  
线设计' (Click Create Retrosynthesis Plan to start running the retrosynthesis route design).



# 逆合成方案和备选路线

## 打开方案

有报道的实验方案通常会在几秒钟内生成。预测的逆合成方案的计算可能需要更长的时间。

Retrosynthesis Plan for drawn structure

查看方案信息

Plan Information

Estimated Yield: 22% Overall Price: \$48.62 (USD per 100 grams)

Scoring Profiles

Complexity Reduction, Convergence, Evidence, Cost, Yield, Atom Efficiency

调整评分选项

显示报道的实验步骤

打开/关闭预测步骤

查看排除的步骤或物质

Powered by ChemPlanner®

下载、分享和保存您的方案

查看方案步骤

查看并选择备选反应路线

蓝色实线表示报道的实验步骤

绿色虚线表示预测的步骤

Avg. Yield 79% Max Yield 79%

Avg. Yield 59% (3)

Avg. Yield 83% (84)

Avg. Yield 47% (10)

Avg. Yield 50% (197)

Avg. Yield 63% (104)

Feedback

## 备选路线

您可以概览所有实验报道的和预测的反应，并将其与反应依据一起作为反应结果集显示。您可以通过以下方式访问这些反应依据：(1)步骤概览中的链接，或(2)备选反应路路线的反应式。

Step Evidence

A → B + C 1.1 Reagents: Butyllithium  
Average Yield: 47% Evidence (16) Alternative Steps

B → D + E 1.1 Reagents: Potassium tert-butoxide Solvents: Tetrahydrofuran View All Experimental Protocols 1

C → F + G 1.1 Reagents: Diisopropylethylamine Ammonium chloride O-(7-Azabenzotriazol-1-yl)-N,N,N',N'-tetramethyluronium hexafluoro phosphate Solvents: Dimethylformamide: 2 d, rt View All Experimental Protocols

D → H + I Predicted Step Only No reaction summary Experimental Protocols

E → J 1.1 Solvents: Carbon tetrachloride Maximum Yield: 83% Evidence (1) Alternative Steps (14)

Filter by

Alternative Step Type: Predicted (48), Stereochemistry: Non-Selective (48)

5 of 15

Predicted Step

55 Results Group: By Scheme Sort: Relevance View: Expanded

Reactions from Retrosynthesis Plan Evidence

References

Filter Behavior

Filter by Exclude

Search Within Results

Yield: 90-100% (2), 80-89% (3), 70-79% (10), 50-69% (15), 30-49% (2), View All

Number of Steps: 1 (55)

Non-Participating Functional Groups

Supplier (49) Supplier (51) Supplier (61)

31-614-CAS-29434160 Steps: 1 1: Solvents: Dichloromethane; rt 1.2 Reagents: Triethylamine; rt 18 h, rt Preparation of piperidine-containing compounds for treating and preventing metabolic and cerebrovascular diseases

Rodriguez, Martha E.; et al. World Intellectual Property Organization, WO2010080854 A1 2010-07-15

预测反应依据

Experimental Protocols PatentPak Full Text

# 逆合成评分选项

## 评分选项

对于包含预测步骤的方案，您可以增加或减少预测步骤和替代反应路线中每个选项中的分数权重，以决定在逆合成方案/替代反应路线中所显示的内容。

- 每个评分项可以设置为 “Off（最左），Low, Medium，或者High（最右）。
- 如下图所示，每个评分项的默认设置为 “Medium” 。

## 评分简介

For plans with predicted steps, you may increase or reduce the score assigned to steps and alternatives by each profile, which determines what is displayed in the plan/alternative steps.

Each scoring profile may be set to **Off** (extreme left), **Low**, **Medium**, or **High** (extreme right); the default setting for each profile is "Medium," as shown below. Moving the slider all the way to the left turns that profile's scoring "Off," and it will not be a factor step selection or alternative ranking.

The screenshot shows a user interface for a retrosynthesis planning tool. On the left, there is a sidebar with "Plan Information" (Estimated Yield: 79%, Overall Price: \$599.28 USD per 100 grams) and "Scoring Profiles" for six categories: Complexity Reduction, Convergence, Evidence, Cost, Yield, and Atom Efficiency. Each category has a horizontal slider with a midpoint labeled "Medium". Below the sliders are "Apply" and "Reset Scoring" buttons. To the right of the interface, detailed descriptions for each category are provided:

- Complexity Reduction**: Reduces the complexity of a step's reactants compared to its product. **In retrosynthesis plans, you typically want high complexity reduction.**
- Convergence**: Determines how "branched" the plan is; **you typically want the plan to be as branched as possible (high convergence)**, rather than linear. **Increasing Convergence displays steps/alternatives with more reactants.**
- Evidence**: Ranks plan steps/alternatives based on the number of evidence examples supporting the particular reaction type. **More evidence examples for a step means that the reaction type has more applications and is more versatile in terms of conditions and substrates**, and hence predictions made based on it are probably more reliable. **Increasing Evidence displays steps/alternatives with more supporting examples.**
- Cost**: Weighs the expenses of the reactions by ranking starting materials based on the lowest price found amongst catalogs.
- Yield**: Applies to the yield of each step in the plan, which contributes to the yield of the target molecule. **Increasing the Yield displays a higher yield target molecule and steps/alternatives.**
- Atom Efficiency**: Reduces reactant parts not included in a plan step's product. **Increasing Atom Efficiency displays steps/alternatives with the least amount of reactant atoms that do not map to the product.**

Clicking the **Apply** button redraws the retrosynthesis plan with the revised scoring profiles; clicking **Reset Scoring** restores the "Medium" default.



# CAS Markush 检索及 CAS PatentPak

## CAS Markush 检索

在物质检索模式下，可以使用“Search Patent Markush”选项执行Markush结构检索。

The screenshot shows the SciFinder interface with the following elements:

- Top Bar:** CAS SciFinder, Substances, Enter a query..., Edit, Search, Save.
- Left Sidebar:** Return to Home, Patent Markush search for drawn structure, References, Patent Markush Match (As Drawn 96), Substructure (119), Filter Behavior (Filter by, Exclude), Patent Office (World Intellectual Property Organization (55), United States (25), European Patent Organization (8), China (3), United Kingdom (2), View All).
- Center Area:** 96 Results, Markush structure search type,命中了的组装Markush结构, Patent claim 1, PatentPak, Full Text, There are no notes to display for this structure, 跳转至 CAS PatentPak Viewer, Preparation of deuterated dihydrofuranones for the treatment of irritation symptoms of joint degeneration, as well as of acute pain, and dysmenorrhea, Assignee: Berolina Drug Development AB, Germany, DE10162120.A1 2003-06-18 | Language: German, Patent claim 1, Markush在专利中的位置, Heterocycle derivatives and methods of use, Assignee: The University of Texas System, World Intellectual Property Organization, WO2001094369 A2 2001-12-13 | Language: English.
- Right Area:** 进行Markush检索 (Perform Markush search) button.

## CAS PatentPak

在 CAS PatentPak 中有三种查看专利PDF的方式：

- PDF:** 仅提供支持文本搜索的专利PDF文件
- PDF+:** 附有标引关键物质专利全文PDF文件
- Viewer:** 附有标引关键物质定位符（见下）的专利PDF

The screenshot shows the CAS PatentPak viewer interface with the following elements:

- Top Bar:** PAGE (14), ZOOM, DOWNLOAD PDF / PDF+, 下载 PDF (Download PDF), CAS Key Substances in Patent.
- Left Sidebar:** Analyst Markup Locations (1), CAS RN 33454-82-9, Li+, CAS RN 14263-07-9, Li+, CAS RN 21324-40-3, Li+.
- Center Content:** Patent claim 12, description of the lithium secondary battery, chemical structure of Lithium trifluoromethanesulfonate, Get Substance Details, Get Reactions (2,637), Synthesize (102), Start Retrosynthetic Analysis, Get References (9,440), Get Suppliers (92), Edit Structure, Reset, 添加注释: 点击物质的定位标记符, 即可跳转至专利全文中改物质出现的位置, 定位到专利中物质所在位置, 跳转至相关信息.
- Right Content:** Ni, Co, and Mn, and the second positive active material shows a peak of Co, or the first positive active material shows peaks of Ni and Mn, and the second positive active material shows a peak of Mn, CAS科学家标引的重要物质定位标记, 12. The lithium secondary battery according to claim 9, wherein the electrolyte comprises at least one organic solvent, 13. The lithium secondary battery according to claim 12, wherein the charging and discharging is performed at a charge rate between 0.2 and 2.0 C and a discharge rate between 0.1 and 2.0 C, 14. The lithium secondary battery according to claim 16, wherein the charging and discharging is performed at a charge current density between 0.1 and 5.0 mA/cm<sup>2</sup> and a discharge current density between 0.1 and 5.0 mA/cm<sup>2</sup>, 15. The lithium secondary battery according to claim 18, wherein the charging and discharging is performed at a charge current density between 0.2 and 4.0 mA/cm<sup>2</sup> and a discharge current density between 0.2 and 4.0 mA/cm<sup>2</sup>, 16. The lithium secondary battery according to claim 16, wherein the charging and discharging is performed at a charge rate between 0.2 and 1.5 C and a discharge rate between 0.2 and 1.5 C, 17. The lithium secondary battery according to claim 17, wherein the charging and discharging is performed at a charge rate between 0.2 and 1.5 C and a discharge rate between 0.2 and 1.5 C, 18. The lithium secondary battery according to claim 18, wherein the charging and discharging is performed at a charge current density between 0.1 and 5.0 mA/cm<sup>2</sup> and a discharge current density between 0.1 and 5.0 mA/cm<sup>2</sup>, 19. The lithium secondary battery according to claim 19, wherein the charging and discharging is performed at a charge current density between 0.2 and 4.0 mA/cm<sup>2</sup> and a discharge current density between 0.2 and 4.0 mA/cm<sup>2</sup>, 20. The lithium secondary battery according to claim 20, wherein the charging and discharging is performed for 1 to 300 times, 21. The lithium secondary battery according to claim 20, wherein the charging and discharging is performed for 1 to 99 times, 22. The lithium secondary battery according to claim 20, wherein the battery is in a charged or discharged condition after the battery is charged and discharged, 23. The lithium secondary battery according to claim 20, wherein the battery is in a condition of being charged or discharged after the battery is charged and discharged, 24. The lithium secondary battery according to claim 20, wherein the battery has an open circuit voltage (OCV) in the range of 1.0 to 5.5V after the battery is charged and discharged, 25. The lithium secondary battery according to claim 24, wherein the battery has an open circuit voltage (OCV) in the range of 1.5 to 4.5V after the battery is charged and discharged.

专利中被标引的核心物质

# 供应商检索及 ChemDoodle

## 供应商检索

供应商检索允许您根据化学结构、名称或其他标识符查找化学品供应商信息。

The screenshot shows the Suppliers search interface. At the top, it says "Suppliers search for '7664-93-9'". Below this is a filter panel on the left with sections for "Preferred Suppliers" (checkboxes for "Preferred" and "No Preference"), "Supplier" (checkbox for "信息的最新更新时间" - Newest Update), "Purity" (checkboxes for "≥99%" (8), "95-98%" (132), "90-94%" (9), and "<90%" (14)), and "View All". In the center, there's a table with columns: Supplier, Substance, Purity, and Purchasing Details. One row is highlighted for "Oakwood Chemical" with "7664-93-9 Sulfuric Acid, ACS Grade" and "95-98%". To the right of the table is a sidebar with sorting options: Relevance, Price: Low to High, Price: High to Low, Supplier: A to Z, Supplier: Z to A, Ships Within, and Purity. Below the table, a modal window titled "Oakwood Chemical Product List" provides detailed information about the supplier and the substance.

Supplier	Substance	Purity	Purchasing Details
Oakwood Chemical Oakwood Chemical Product List United States Last Updated: 1 Mar 2024	7664-93-9 Sulfuric Acid, ACS Grade	95-98%	Order From Supplier 100 ml, USD 25 1 L, USD 40.00 2.5 L, USD 80.00

**Oakwood Chemical Product List**

Preferred Supplier:

Web: <https://www.oakwoodchemical.com>

Email: sales@oakwoodchemical.com

Phone: 1-800-467-3386

Item Details

Chemical Name: Sulfuric Acid, ACS Grade

Order Number: 25494

Purity: 98%

Quantity, Price: 100 ml, USD 25.00  
1 L, USD 40.00  
2.5 L, USD 80.00

Bulk Available

Stock Status: Maintained in stock

Pricing Information: Last Updated 1 Mar 2024

Order From Supplier:

Substance Information

CAS Registry Number: 7664-93-9

CAS Name: Sulfuric acid

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## ChemDoodle

ChemDoodle 是除了标准的CAS结构绘制面板之外，另一个可选的结构编辑器。ChemDoodle非常适用于平板电脑等移动设备。

The screenshot shows the ChemDoodle interface. At the top, there are toolbar buttons: 选择 (Select), 居中 (Center), 翻转片段 (Flip Fragment), 剪切 | 复制 | 粘贴 (Cut | Copy | Paste), 清除 (Clear), 橡皮擦 (Erase), 撤销 | 恢复 (Undo | Redo), 模板 (Template), 打开 | 保存 (Open | Save), and 缩放 (Zoom). On the left is a vertical toolbar with various drawing tools: 标签 (Label), 绘制键 (Draw Bond), 绘制环 (Draw Ring), 添加电荷 (Add Charge), 碳链工具 (Carbon Chain Tool), 重复结构单元 (Repeat Unit), 可变位置定义工具 (Variable Position Definition Tool), 原子锁定 / 链锁定 / 环锁定工具 (Atom Lock / Chain Lock / Ring Lock Tool), 片段结构定义工具 (Fragment Structure Definition Tool), 反应箭头绘制工具 (Reaction Arrow Drawing Tool), 反应原子标记工具 (Reaction Atom Marking Tool), and 化学键标记工具 (Chemical Bond Marking Tool). The main workspace shows a chemical structure of a molecule with atoms labeled F, N, O, and C, and bonds drawn between them. The ChemDoodle logo is in the bottom right corner.



# 现有技术分析

## 回顾现有技术

在专利文献详情页中，提供了“Get Prior Art Analysis”的选项。其结果也会呈现在检索历史中。其工作原理如下：

- 提供基于人工智能的相关性预测。
- 以单一专利文件作为分析起点。
- 包括对 CAS 核心研究点、标引的物质、IPC专利分类号和专利题目、摘要等内容的分析。
- 生成一份按照相关性排序的已知文献列表，涵盖专利文献和非专利文献。

Aqueous dendritic amine coatings containing dendritic poly(amido)amine (PAMAM)

13 0 1 Citation Map Save

In this Reference By: Wang, Shaofeng; Li, Hairong; Seow, Swee How

• IPC Data  
• CAS Concepts  
• Substances

The present invention relates to a water-based emulsion coating composition, e.g. paint composition, comprising a hyper-branched or dendritic poly(amido)amine, at least one isothiazolone biocide, and a binder.

Keywords: aqueous dendritic amine coatings containing dendritic poly(amido)amine (PAMAM)

PatentPak Viewer Get Prior Art Analysis Full Text ▾

References Prior Art Analysis (195) View Results 1:52 PM Aqueous dendritic amine coatings containing dendritic poly(amido)amine (PAMAM) Complete 在检索历史记录中查看结果

# **CAS Formulus**

# 检索制剂或配方

The screenshot shows the CAS Formulus homepage. At the top, there are links for 'Help & Support' (with a question mark icon), 'Alerts' (with a bell icon showing 9 notifications), 'Saved' (with a bookmark icon), and a user profile icon. The main header says 'Good Afternoon, Liu'. Below the header, there are two tabs: 'Formulations' (selected) and 'Ingredients'. A search bar contains the text 'celecoxib' and a placeholder '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），单击放大镜执行检索'. Below the search bar are two buttons: 'Formulation Designer' (with a dropper icon) and 'Advanced Search' (with a magnifying glass icon).

This screenshot shows the 'Advanced Formulations Search' interface. On the left, a sidebar lists search fields: All Fields, Form, Function, Ingredient, Purpose, Route, and Target. A button '浏览并选择检索项' (Browse and select search items) is highlighted with a blue box. Below the sidebar, a button '添加新的检索项' (Add new search item) is also highlighted. The main search area has three search criteria defined:

- Search For: Ingredient, Operator: Required, Value: Celecoxib. A tooltip '输入检索词或物质' (Enter search term or substance) points to the input field, and a button '删除此项内容' (Delete this item) is shown next to it.
- Search For: Purpose, Operator: Required, Value: Analgesics. A tooltip 'Ex: herbicide, fertilizer, bakery product' is shown below the input field.
- Search For: Form, Operator: Required, Value: Tablets. A tooltip '点击下拉菜单，浏览并设置运算符' (Click the dropdown menu to browse and set operators) points to the operator dropdown, and a button '清除所有内容' (Clear all) is shown next to it.

A 'Search' button is at the bottom left, and a 'Clear All' button is at the bottom right. A tooltip '单击执行检索' (Click to execute search) points to the 'Search' button.

[下载结果为PDF或Excel文件](#)

**Formulations search for "celecoxib"**

Get Additional References 获得结果集对应的文献

Filter by 选择筛选项，精准获得配方或制剂结果

Sort: Relevance Group: By Family

1

**Pharmaceutical Tablets Containing Celecoxib: Antiinflammatory Agents or Analgesics**

Location: Comparative Example 2B, Table 2, 5  
Purpose: Analgesics, Anti-inflammatory agents  
Target: Homo sapiens, Lower back pain, Osteoarthritis, Rheumatoid arthritis, cervical shoulder arm syndrome, shoulder periarthritis  
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: granulated celecoxib	Formulation active agents	1008 g
Celecoxib	Nonsteroidal anti-inflammatory agents <sup>①</sup>	1200 g
D-Glucose, 4-O-β-D-galactopyranosyl-, hydrate (1:?)	Formulation excipients	264 g
Hydroxypropyl cellulose	Disintegrants	...
Cellulose, carboxymethyl ether	Disintegrants	102 g
Additional group components reported		
Magnesium stearate	Lubricants	12 g

① Predicted value

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PATENT

Pharmaceutical tablet containing celecoxib as anti-inflammatory and analgesic agent  
Assignee: Ohara Pharmaceutical Co., Ltd.  
JP2019089758  
Language: Japanese

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

[在CAS SciFinder中查看文献详情](#)

View Formulation Detail [查看制剂或配方详情](#)

11 Similar Formulations - View All [查看相似的制剂或配方](#)

2

**Oral Pulsatile Drug Delivery System of Celecoxib: Antiinflammatory Agents or Analgesics--Controlled Release Drug Delivery Systems for Pharmaceutical Formulation**

Location: Article Page 1, 3, 4, Table 1  
Purpose: Analgesics, Anti-inflammatory agents  
Delivery Route: Oral drug delivery systems  
Physical Form: Tablets

[Add to Compare](#)

Component	Function	Amount Reported
Group: celecoxib granules	Formulation active agents	-
Celecoxib	Nonsteroidal anti-inflammatory agents	-
Mannitol	...	-

[点击蓝色原料名称，查看详情](#)

JOURNAL

Formulation and evaluation of pulsatile drug delivery system of celecoxib  
World Journal of Pharmaceutical Research  
Language: English

[View in CAS SciFinder](#)



# 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



Component	Function	Amount Reported	Optionality
▲ Group: granulated celecoxib	Formulation active agents	1008 g	Mandatory
Celecoxib	Nonsteroidal anti-inflammatory agents <sup>(@)</sup>	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 system...  
Physical Form: Sachets, Tablets, disinte...

Antiarthritic Pharmaceutical Composition  
Purpose: Antiarthritis  
Target: Arthritis, Homo sapiens  
Delivery Route: Oral drug delivery system...  
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

### 专利来源

#### 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

# 检索原料

The screenshot shows the CAS Formulus platform interface. At the top, there's a navigation bar with 'Help & Support', 'Alerts' (with a count of 9), 'Saved', and a user profile icon. The main header says 'Good Afternoon, Liu' and has a '选择Ingredients' (Select Ingredients) button. Below the header, there are tabs for 'Formulations' and 'Ingredients', with 'Ingredients' being active. A search bar contains the text 'propylene glycol' and a magnifying glass icon. To the right of the search bar are buttons for '通过电子邮件发送结果' (Send results via email), '保存结果并设置提醒' (Save results and set reminders), and 'Save'.

The main content area is titled 'Ingredients search for "propylene glycol"'. It shows a list of results with 1 selected and 3 total. The first result is '(±)-Propylene glycol' (Propylene glycol). It displays its chemical structure (C3H8O2) and key physical properties: Molecular Weight (76.09), Melting Point (Experimental) (-59 °C), Boiling Point (Experimental) (188.2 °C), and Density (Experimental) (1.036 g/cm³). It also lists common uses as solvents and humectants. Below this, there are sections for 'Experimental Properties' (including biological, density, and thermal data), 'Sources' (with links to Gotochik et al., 1981 and Ansel, 1963), and 'Commonly Formulated With' (links to ANMAT, Cosmetic Ingredient Inventory, Drug Master File List, and EMA Excipients List).

On the left side, there's a sidebar with 'Filter by' options for Industry (Pharmaceutical is checked), Regulatory Information (REACH, Cosing, EPA Pesticide, FDA Inactive Ingredients Database are checked), Experimental Properties, Commercial Availability, and 'Commonly Formulated With' (which is expanded to show a table of ingredients like Water, Glycerin, Ethanol, etc.).

Annotations highlight various features: '选择筛选项，精准获得原料结果' (Select filters to get precise results), '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), and '查看制剂或配方中，与该原料同时使用的其它配伍成分' (View other co-formulated ingredients used with this raw material).



# 查看原料供应商信息

选择筛选项，精准获得供应商信息

下载结果为Excel文件

Filter by

- Grade
  - Reagent Grade (5)
  - Molecular Biology Grade (4)
  - ACS reagent (2)
  - pharmaceutical primary standard (2)
  - 10mM in DMSO (1)
- [View All](#)

- Certificate of Analysis
  - Available (10)
- [View All](#)

- Bulk Availability
  - Available (40)

- Supplier
  - Thermo Fisher Scientific - Laboratory Chemicals (16)
  - Sigma-Aldrich (15)
  - FUJIFILM Wako Pure Chemical Corporation (14)
  - LGC Standards (12)
  - KANTO CHEMICAL CO., INC. (9)
- [View All](#)

- Supplier-Reported Properties
  - Molecular Weight (42)
  - Product Category (32)
  - Storage (24)
  - Boiling Point (23)
  - Melting Point (23)
- [View All](#)

- Order from Supplier
  - Available (56)

**Suppliers (160)**

Results for ( $\pm$ )-Propylene glycol  
CAS RN: 57-55-6

Aaron Chemicals LLC		点击查看供应商联系方式、货运详情及分销商信息		点击打开来自供应商的购买页面			
View Details		Product Information		Quantity Information		Ordering & Shipping	
Name:	1,2-Propanediol	Molecular Weight:	76.0944	Available Amounts:	500 g USD 5.00	Order from Supplier	Ships Within: 1 week
Weight:				100 g	USD 4.00	Status: Maintained in stock	
				1000 g	USD 7.00		

First Scientific LLC		View Details			
Product Information		Quantity Information		Ordering & Shipping	
Name:	1,2-Propanediol	Molecular Weight:		Available Amounts:	500 g USD 8.00
Weight:				100 g	USD 6.00
SDS Availability:		Shipping:	25 g	25 g	USD 5.00
Code: EN300-21726		Storage:			

Enamine US Inc.		View Details			
Product Information		Quantity Information		Ordering & Shipping	
Name:	propane-1,2-diol	Molecular Weight:	76.09	Available Amounts:	2.5 g USD 27.00
Weight:				50 g	USD 50.00
SDS Availability:	https://enamine.enamine.net/pub/msds?code=EN300-21726&&senderid=0&&lang=en	Shipping:		5 g	USD 29.00
Code: EN300-21726		Storage:		250 mg	USD 19.00
				100 mg	USD 19.00
				100 g	USD 67.00
				10 g	USD 32.00
				1 g	USD 26.00
				500 mg	USD 21.00
				25 g	USD 38.00

## 设计制剂或配方

**Formulation Designer**

浏览并选择物理形态

Clear All Selections

最多添加5种原料进行检索

Add up to 5 Ingredients

删除该原料

添加另一种原料

Create Template

单击执行检索

浏览并选择用途

Physical Form

Industries

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 -

浏览更多选项

浏览并选择应用领域

## Formulation Designer

[Clear All Selections](#)

Industry	Purpose	Physical Form	Active or Featured Ingredient
Pharmaceutical	Analgesics	Tablets	Celecoxib Polyethylene glycol

[Edit Selections](#)

点击，可重新编辑制剂或配方的应用领域、用途、物理形态及原料

[结果保存](#)

[Save](#)



结果导出为Excel文件

### 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 <a href="#">x</a>
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 <a href="#">x</a>
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% <a href="#">x</a>
Binders	Butyl methacrylate-dimethylaminoethyl methacrylate-methyl methacrylate copolymer	View More Alternatives	Alternative Ingredients (Showing all 10)  Select the ingredient you would like to use: Sodium dodecyl sulfate      Stearic acid      Polyethylene glycol Glyceryl tribehenate      Silica      Glycerol behenate Sodium stearyl fumarate      Polyoxyethylene sorbitan monooleate Magnesium stearate      Calcium stearate	
Disintegrants	Croscarmellose sodium	View More Alternatives	Silica; Starch; Sodium carboxymethyl cellulose; Poly(vinylpyrrolidone); Hydroxypropyl cellulose	Approximate Range: 4 - 5% <a href="#">x</a>
Diluents	Magnesium oxide	View More Alternatives	Talc ( $Mg_3H_2(SiO_3)_2$ ); Butyl methacrylate-dimethylaminoethyl methacrylate	Approximate Range: 8 - 16% <a href="#">x</a>
<a href="#">+ Add Function</a>		点击可添加用途	添加用途后，点击获得新的制剂或配方设计结果	
<input type="text" value="Function"/> <input type="text" value="Anti-inflammatory agents"/>				<a href="#">Add Function</a> <a href="#">Cancel</a>



# **CAS Analytical Methods**

# 分析方法检索

The screenshot shows the homepage of the CAS Analytical Methods website. At the top right, there are links for 'Support', 'Saved' (with a bookmark icon), and a user profile with options like 'My CAS Profile', 'Help', and 'Log Out'. A blue line highlights the 'Saved' link. Below the header, a greeting 'Good Afternoon, Liu' is displayed. A search bar contains the text 'blood plasma', with a blue line highlighting it. To the right of the search bar is a magnifying glass icon. On the left, there are two buttons: 'Explore Methods' (with binoculars icon) and 'Advanced Search' (with magnifying glass icon). A blue line highlights the 'Explore Methods' button. Below these buttons are two boxes: '浏览方法分类, 查看相关方法' (Browse method categories, view related methods) and '高级检索' (Advanced search). A blue line highlights the '高级检索' button. At the bottom left, there is a 'Recent Searches' section with the entry 'crocin', and a blue line highlights this entry. To the right of the recent searches is a text box containing the placeholder '点击历史检索重新运行检索, 点击X删除检索历史' (Click history search to run again, click X to delete search history), with a blue line highlighting the placeholder text.

## 高级检索

The screenshot shows the 'Advanced Search' interface. On the left, there is a sidebar with buttons for 'AND', 'OR', and 'NOT', and a box for '逻辑运算符: and, or, not' (Logical operators: and, or, not). A blue line highlights the '逻辑运算符' box. Below this is a button for '增加检索条件' (Add search criteria), with a blue line highlighting it. The main search area has a dropdown for 'Analyte' set to 'palmitic acid'. Below it is another dropdown for 'Matrix' set to 'blood plasma'. Between these dropdowns is a dropdown for 'AND'. A blue line highlights the 'AND' dropdown. There is also a 'Delete search condition' button with a blue line highlighting it. At the bottom of the sidebar is a list of search criteria: 'Keyword', 'Analyte', 'Matrix' (which is bolded), 'Method Category', 'Technique', 'CAS Method Number', and 'Publication Name'. A blue line highlights the 'Matrix' item in the list. A large callout box on the right side of the search area 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, CAS方法号, 出版物名称' (Search conditions include: Keyword, Analyte, Matrix, Method Category, Technique, CAS Method Number, Publication Name).



# 分析方法的分类检索

Explore N 浏览并选择方法分类及子分类

Category	Category Name	可输入关键词	Clear all selections
Agricultural Applications / <b>Bioassays</b>	Bioassay Bioassay Synthetic Probes Biomarker Biological Process Biomarker Cell Assay Biomarker Medicine Assay Biomedicine Material Analysis <b>Biomolecule Isolation Assay</b>	Palmitic acid	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	Bioorganism Isolation Assay Genetic Analysis Nanomaterial Analysis	+ 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 Custom query 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:
  - Palmitic acid (7)
  - Stearic acid (7)
  - Linoleic acid (6)
  - Oleic acid (5)
  - Arachidonic acid (4)
- Matrix:
  - Blood plasma (7)
  - Hazelnut oil (1)
- Method Category:
  - Technique:
    - Gas chromatography (82)
    - Extraction (49)
    - Solvent extraction (48)
    - Flame ionization detectors (39)
    - Gas chromatography-mass spectrometry (26)
  - HPLC (7)
- Year

1 Selected 7 Results Sort: Relevance ▾ Group: By Method ▾

1 选中方法, 导出或保存

**Analysis of Myristic acid in Blood plasma by Solvent extraction**

By: Furukawa, Eri; Chen, Zhen; Ueshiba, Hiroki; Wu, Yue; Chiba, Hitoshi; Yanagawa, Yojiro; Katagiri, Seiji; Nagano, Masashi; Hui, Shu-Ping  
Postpartum cows showed high oocyte triacylglycerols concurrently with high plasma free fatty acids  
Theriogenology (2021), 176, 174-182. Elsevier Inc.

Analyte: cis-Octadecenoic acid; (Z)-Hexadecenoic acid; cis-Octadecadienoic acid; **Palmitic acid**; Myristic acid; Stearic acid  
Matrix: Blood plasma  
Other Materials: Reagent: Chloroform; Methanol  
Material: Atlantic T3 C18 column (2.1 × 150 mm, 3 µm); Ethylenediaminetetraacetic acid-loaded vacuum tubes  
Method Category: Fatty Acid Analysis  
     在CAS SciFinder中查看文献详情

2 选择感兴趣的方法进行对比

**Analysis of Palmitic acid in Blood plasma by Solvent extraction**

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

# 分析方法详情

结果保存

## Analysis of Myristic acid in Blood plasma by Solvent extraction

结果导出



Save

CAS Method Number  
1-122-CAS-534418

Method Category

Technique

Mass spectrometry; HPLC; Solvent extraction

分析方法中的分析物、基质、材料、试剂等分类展示

Analyte
cis-Octadecenoic acid
(Z)-Hexadecenoic acid
cis-Octadecadienoic acid
<b>Palmitic acid</b>
Myristic acid

Matrix
<b>Blood plasma</b>

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

分析方法操作步骤

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 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.

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

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数据有效性

Validation

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



# 分析方法详情对比

Compare up to 3 Methods

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删除所有方法方法

Analysis of Palmitic acid in Blood plasma by Solvent extraction Analyte(s): Palmitoleic acid; <b>Palmitic acid</b> ; Elaidic... Matrix: <b>Blood plasma</b> Method Category: Biomolecule Isolation Assay	Analysis of Fatty acids in Blood plasma by HPLC Analyte(s): Stearic acid; Linoleic acid; <b>Palmitic...</b> Matrix: <b>Blood plasma</b> Method Category: Fatty Acid Analysis	Analysis of Lauric acid in Blood plasma by Electrochemiluminescence Analyte(s): <b>Palmitic acid</b> ; Stearic acid; Myristoleic... Matrix: <b>Blood plasma</b> Method Category: Fatty Acid Analysis
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Comparing your 3 selected Methods

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	Method 1	Method 2	Method 3
CAS Method Number	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
Method Category	2-114-CAS-225380	1-122-CAS-96286	1-122-CAS-3193044
Technique	Biomolecule Isolation Assay	Fatty Acid Analysis	Fatty Acid Analysis
Analyte	Time-of-flight mass spectrometry; HPLC; Electrospray ionization mass spectrometry; Solvent extraction	Electrochemical analysis; Atmospheric precipitation; HPLC	Electrochemiluminescence; HPLC
Matrix	Palmitoleic acid; <b>Palmitic acid</b> ; Elaidic acid; Linoleic acid; Stearic acid; Arachidonic acid; Docosahexaenoic acid	Stearic acid; Linoleic acid; <b>Palmitic acid</b> ; Arachidonic acid; Oleic acid; Fatty acids	<b>Palmitic acid</b> ; Stearic acid; Myristoleic acid; Palmitoleic acid; Lauric acid; Arachidonic acid; Oleic acid; Linoleic acid; Linolenic acid; Myristic acid; Fatty acids
Other Materials	Blood plasma	Blood plasma	Blood plasma
Equipment Used	tert-Butyl methyl ether; Chloroform; Formic acid; Methanol; Ethyl acetate; Hydrochloric acid; Sodium chloride; Glass vial; Zorbax Eclipse plus C <sub>18</sub> column (2.1 × 100 mm, 1.8 μm)	Alloxan; Acetonitrile; Lithium perchlorate; 3,5-Di-tert-butyl-1,2-benzoquinone; Maltose; Diethyl ether; Reverse-phase C30 microbore column (250 mm × 1.0 mm i.d.); Membrane filter (pore size, 0.45 μm); Glucose meter (Glucocard)	1-Pyrrolidinepropanamine; 3,4-Dihydro-9-methyl-2H-pyrido[1,2-a]pyrimidin-2-one; Phosphoric acid; Sodium hydroxide; Acetic acid; Acetonitrile; Boric acid (H <sub>3</sub> BO <sub>3</sub> ); 2-Bromo-1-ethylpyridinium tetrafluoroborate; Chloroform; Heptane; Phosphate-buffered saline solutions; Photomultiplier tube; TSK-gel Octyl-80TS (4.6 × 150 mm, Tosoh) column; Cosmosil 5C18-MS (4.6 × 250 mm) column
Conditions	Instrument: column: Zorbax Eclipse plus C <sub>18</sub> column (2.1 × 100 mm, 1.8 μm); column temperature: 40 °C; mobile phase A: 0.2% formic acid and 10 mM ammonium formate in water; mobile phase B: 0.2% formic acid	Instrument: Column: reverse-phase C30 microbore column (Develosil C30-UG-3, 250 mm × 1.0 mm i.d., Nomura Chemical, Aichi, Japan); mobile phase: acetonitrile-ethanol (90:10, v/v) mixture and one containing 6	Instrument: column: TSK-gel Octyl-80TS (4.6 × 150 mm, Tosoh) column; mobile phase: 50 mM BR buffer (pH 2.5) containing 50% acetonitrile and reagent solution of 0.8 mM Ru(bpy) <sub>3</sub> Cl <sub>2</sub> in 10 mM H <sub>2</sub> SO <sub>4</sub> ; flow rate:

# 保存的结果集

The screenshot shows a search interface for 'blood plasma'. A search bar at the top contains the text 'blood plasma'. Below it, a section titled 'Saved (2)' lists two items:

Name	Date	Actions
blood plasma	30 July 2024	<a href="#">查看保存的结果集</a> Saved 4 Results
Analysis of Formaldehyde in Air by Amperometry	11 August 2023	<a href="#">复制链接, 共享检索结果; 或删除保存项</a> Saved 1 Result

A blue callout box highlights the 'Copy Link' and 'Delete' buttons for the second item. Another callout box highlights the 'Saved 4 Results' link for the first item. A third callout box highlights the search term 'blood plasma' in the search bar.

Left sidebar buttons: Return to Home, Saved (2)

Top right buttons: Search icon, Bookmarks icon, Profile icon

Table columns: Name, Date, Actions

Action buttons: Copy Link, Delete



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Chemisches Zentralblatt (1933), 104 Book 2(8), 1217-1217 | Language: German, Database: CHEMZENT

Machine Translated: Chem. FABR. DR. J. wiérnik U. CO. A.-G., Berlin-Waidmannslust; tablets with each 12.5 mg sodium cholate and 2-oxo-3.3 with (p-oxyphenyl)-indolin. The evacuant with effect on Dün-n-u. Thick intestine. — Lygal (DR. Georg Henning, Berlin-Tempelhof): compound of 50% phenyl quinolinecarboxylic acid Ca (or Na) 29% dimethyl amino phenazone and 21% Coffein-Natriumsalicylat. Antiarthritis. — Pantaplant (chemical. Structures KOLBERG G. mass forming H., Kolberg): fluid extracts from pansy, case stalk, feverfew, arnica, hamamelis, ratanhia, and somewhat ZnO and Peru gum in Euceringrundlage. With noni!

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Katagel-Kreidl (Herst. ders.): giftfreie Spezialtrockenbeize für Saatgut. — Medoform (Herst. ders.): Liqui. Formaldehydi saponat. — Meissol (ANT. MEISZL's NACHE., Wien): Ungeziefervertigungsmittel. — Oma (OMA-NÄHRSTOFF-GES., St. Veit a. d. Glan, Kärnten): Kindernährmittel. — Oma-Kinder- u. Wundpulver (Herst. ders.): peledol-(Pellidol? Ref.) haltiger Fettpuder. — Pommette (POMMETTE-KELLEREI, Wien XI): naturreiner Apfelsaft. (Pharmaz. Mh. 14. 42—44, Febr. 1933.) HARMs.

—, Neue Arzneimittel. Spezialitäten und Geheimmittel. Anustypsalbe u. Anustyp-zäpfchen (BÄREN-APOTHEKE, ROB. RADITZ, Wien II): Hämorrhoidalpräparate mit Tannalin, Ichthyol u. Bi-Salzen. — Gynosupp (Herst. ders.): Vaginal-, Kugeln" in Form eines gerade abgestutzten Kegels mit Milchsäure, Bor-Salicylsäure u. Hydarg. salicylicum. Anticoncipiens usw. Auch mit 10% Ichthyol als Gynosupp cum Ichtyolo. (Pharmaz. Mh. 14. 63—66, März 1933.) HARMs.

F. Zernik, Neue pharmazeutische Präparate in Deutschland. Douchin (Dr. R. u. Dr. O. WEIL, Frankfurt a. M.): Cacheits mit 0,2 g Pyrasulf (C. 1933. I. 2278), 0,2 g Chinin „Weil“ (C. 1931. II. 1599), 0,4 g Somnaectin (C. 1931. I. 2223) u. 0,00033 g Scopolamin. Zur Schmerzlinderung in der Austreibungsperiode. (Manufactur. Chemist pharmac. Cosmet. Perfum. Trade J. 4. 50—52, Febr. 1933.) HARMs.

F. Zernik, Neue pharmazeutische Präparate in Deutschland. Intramin pervesival (Dr. GEORG HENNING, Berlin-Tempelhof): neuer Name für Intramin (C. 1931. I. 484). — Intramin intravenös (Herst. ders.): diiodmethansulfosäures Na in 40%ig. wss. Lsg. zur Röntgendärst. der Harnwege. — Stomachylat Bürger (YSATFABRIK G. M. B. H., Wernigerode): Extrakte von Artemisia Absinthium, Achillea millefolium, Gnaphalium arenarium u. Rheum palmatum. Gegen Magenstörungen. — Progynon oleosum (SCHERING-KAHLEBAUM A.-G., Berlin): ölige Lsg. des Follikulinbenzoats. Die 1-cm-Ampulle enthält 10000 Mäuseeinheiten. 1 × wöchentlich intramuskular als Depot. (Manufactur. Chemist pharmae. Cosmetic Perfum. Trade J. 4. 146—48, Mai 1933.) HARMs.

Zernik, Neu eingeführte Arzneimittel und pharmazeutische Spezialitäten. Laxovit (CHEM. FABR. DR. J. WIERNIK U. CO. A.-G., Berlin-Waidmannslust): Tabletten mit je 12,5 mg. Natriumcholat u. 2-Oxo-3,3-bis-(p-oxyphenyl)-indolin. Abführmittel mit Wrkg. auf Dün-n- u. Dickdarm. — Lygal (DR. GEORG HENNING, Berlin-Tempelhof): Verb. von 50% phenylquinolinecarboxylic acid Ca (bzw. Na), 29% Dimethylaminophenazon u. 21% Coffein-Natriumsalicylat. Antiarriticum. — Pantaplant (CHEM. WERKE

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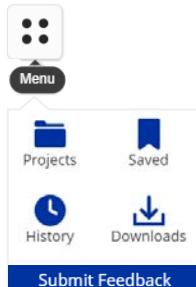
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