

CAS SCIFINDER
DISCOVERY PLATFORM™

快速入门 指南

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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。



文献详情

 Fruit juice-containing food products with refreshing and cooling flavors

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

In this Reference

By: Shimizu, Toru; Shigeta, Yoshinari; Kunieda, Satomi

- [IPC Data](#)
- [CAS Concepts](#)
- [Substances](#)
- [Formulations](#)
- [Cited Documents](#)

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-(1-menthoxy)propane-1,2-diol, N-ethyl-p-menthane-3-carboxamide, 3-(1-menthoxy)-2-methylpropane-1,2-diol, p-menthane-3,8-diol, 2-(1-menthoxy)ethan-1-ol, 3-(1-menthoxy)propan-1-ol, 4-(1-menthoxy)butan-1-ol, cyclic carboxamides, acyclic carboxamides, N,2,3-trimethyl-2-iso-Pr butanamide, a menthoxy alcohol (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-(1-menthoxy)-1,2-propanediol as the cool-tasting component.

Keywords: fruit juice flavor food beverage menthol

文献详情快速导览

PatentPak [Viewer](#)

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Full Text ▾

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Publication Information • Patent

点击获取现有技术分析

[View Less](#)

Patent Number	Publication Date	Application Number	Application Date	Kind Code
WO2005048743	2005-06-02	WO2004-IP17524	2004-11-18	A1

Assignee	Source	Database Information	Language
Takasago International Corporation, Japan	World Intellectual Property Organization	AN: 2005:470226 CAN: 143:25602	English

专利族和优先权

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 PDF+ Viewer			2003-11-19



专利族和优先权申请信息

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

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

Click to draw new structure

Search by Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. 输入化学品名称查询

+ Add Advanced Search Field

添加高级检索字段

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

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

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

Click to search structure for editing

Edit Drawing Remove

Search Patent Markush

勾选以执行Markush检索

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。

选择结构匹配的类型

Structure Match

As Drawn (117)

Substructure (6.2M)

Similarity (1,052)

Analyze Structure Precision

Chemscape Analysis

结构精度分析

Visually explore structure similarity with a powerful new tool. Learn more about Chemscape.

Create Chemscape Analysis

Filter Behavior

Filter by Exclude

Search Within Results

Search for up to 3 structures within the result set.

Draw

Reference Roles

Preparation (3.1M)

Synthetic Preparation (3M)

6,208,864 Results

1

90357-06-5

Click CAS registration number to view details

2

80-08-0

Click structure to open substance information window

3

67-71-0

Change the display method of detailed information

C₁₂H₁₂N₂O₂
Dapsone

C₂H₆O₂S
Dimethyl sulfone

CAS RN
149104-88-1

CAS Name
[4-(Methylsulfonyl)phenyl]boronic acid

检索与物质相关的数据

Get Substance Details

Get Bioactivity Data

Get Reactions (2,494)

Synthesize (9)

Start Retrosynthetic Analysis

Get References (1,404)

Get Suppliers (103)

在结构绘制面板中打开编辑此物质

下载.sdf或.mol文件,复制Smiles到剪贴板

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

Download

Save

C₁₈H₁₄F₄N₂O₄S

按希尔顺序排列的分子式

系统名称

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)		

Other Names

Experimental Properties

Experimental Spectra

Canonical SMILES

InChI

InChI Key

9 Other Names for this Substance

GHS危害图例，在页面底部选项卡中可查看完整列表

化学标识符列表，包含SMILES、InChI、系统名称、俗名和商品名

重要参数

在源文献链接中列出或可获取的物质属性和谱图信息

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

Enter a CAS Registry Number, SMILES, or InChI...

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

套索|选框工具

绘制原子和化学键|橡皮擦

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

Zoom: 90%

OK

Cancel

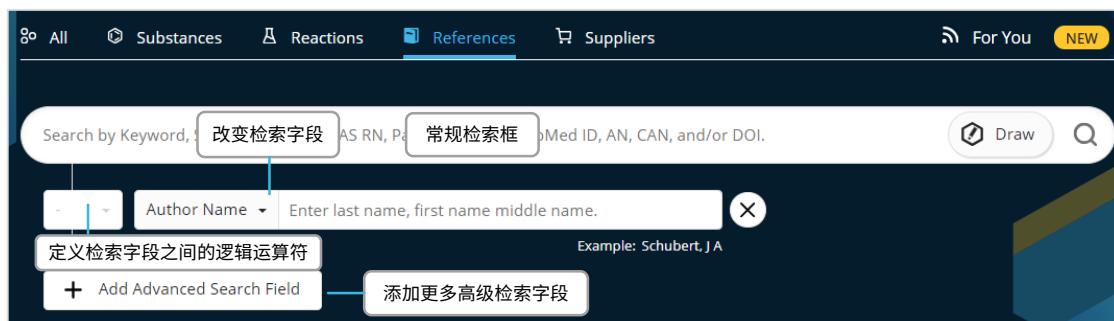


高级检索

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)



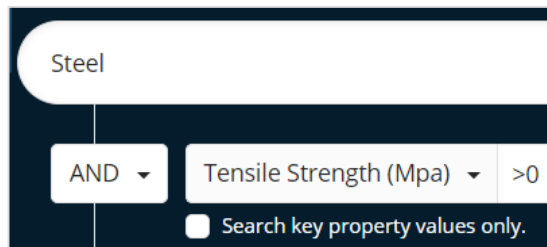
高级检索示例

高级文献检索

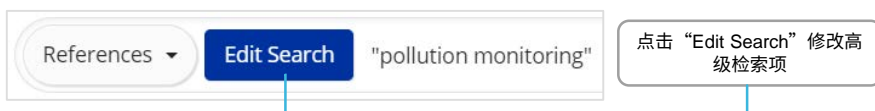


检索说明:
检索“pollution monitoring”以及
(polyethylene or polypropylene)

高级物质检索



检索说明:
检索钢材拉伸强度性能信息



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

C3H6

Polypropylene

321K References

7,909 Reactions

27 Suppliers

Filter Behavior

Filter by

Exclude

Search Within Results

Document Type

Substance Role

Language

Uses (268K)

Properties (61K)

Process (52K)

Biological Study (23K)

Preparation (19K)

View All

Uses (268K)

Properties (61K)

Process (52K)

Biological Use, Unclassified (3,793)

☒ Pollutant (3,661)

Biological Study, Unclassified (2,558)

Miscellaneous (2,444)

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: CAPIUS

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 ¹³C NMR methods to study the stereochem. of polypropylene is also discussed.

Full Text

Substance (1)

Reactions (0)

Citing (395)

Citation Map

Carbonate nanocomposites

By: Jan Xiong, Chung, Ying Kit

Polymer (2002), 43(10), 2991-2992 | Language: English, Database: CAPIUS

Substance Role

Uses (262K)

Properties (50K)

Process (50K)

Biological Study (22K)

Preparation (19K)

☒ Pollutant (3,217)

View All

Language

Publication Year

1974 to 2023

Apply

Microplastics in marine environment review of methods for identification and quantification

By: Hidalgo-Ruz, Victoria; Gutow, Luis; Thompson, Richard C.; Threl, Martin

Environmental Science & Technology (2012), 46(4), 3045-3075 | Language: English, Database: CAPIUS and MEDLINE

This review of 68 studies compares the methodologies 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 came from sandy beaches, at the high tide line, and most seawater samples were taken at the sea surface using neuston nets. Four steps were distinguished during sample processing: 1. separation, filtration, sieving, and visual sorting of microplastics. Visual sorting was one of the most commonly used methods for the identification of microplastics using type, shape, degradation stage, and color as criteria. Chem. and phys. characteristics (e.g., specific $\delta_{13}C$) 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 polyethylene and polypropylene polymers. Units commonly used for abundance estimates are "items per m³" for sediment and sea surface studies and "items per m³" for water column studies. Mesh 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 μ m - 5 mm, which are retained by a 500 μ m sieve, and (ii) 1-500 μ m, or fractions thereof that are retained on filters. We recommend that future programs of monitoring continue to distinguish these size fractions, but we suggest standardised sampling procedures which allow the spatiotemporal comparison of microplastic abundance across marine environments.

Full Text

Substances (0)

Reactions (0)

Citing (2,296)

Citation Map

Substances

Substances (0)

Chemical Name

Role

9003-07-0

Polypropylene

单击“View All”可以选择更多 Roles

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。

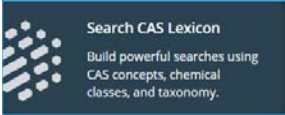


CAS Lexicon

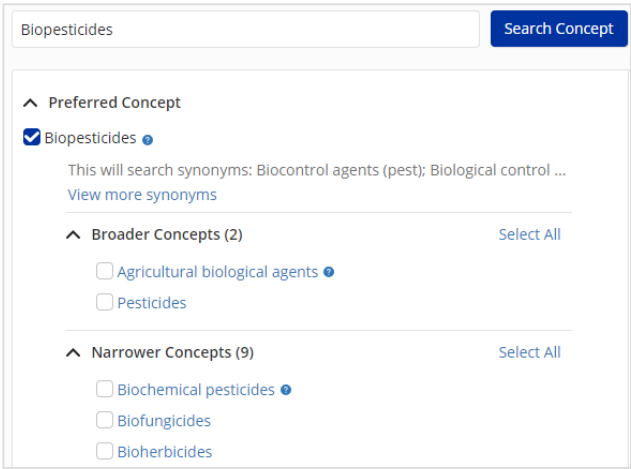
CAS Lexicon概述

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。

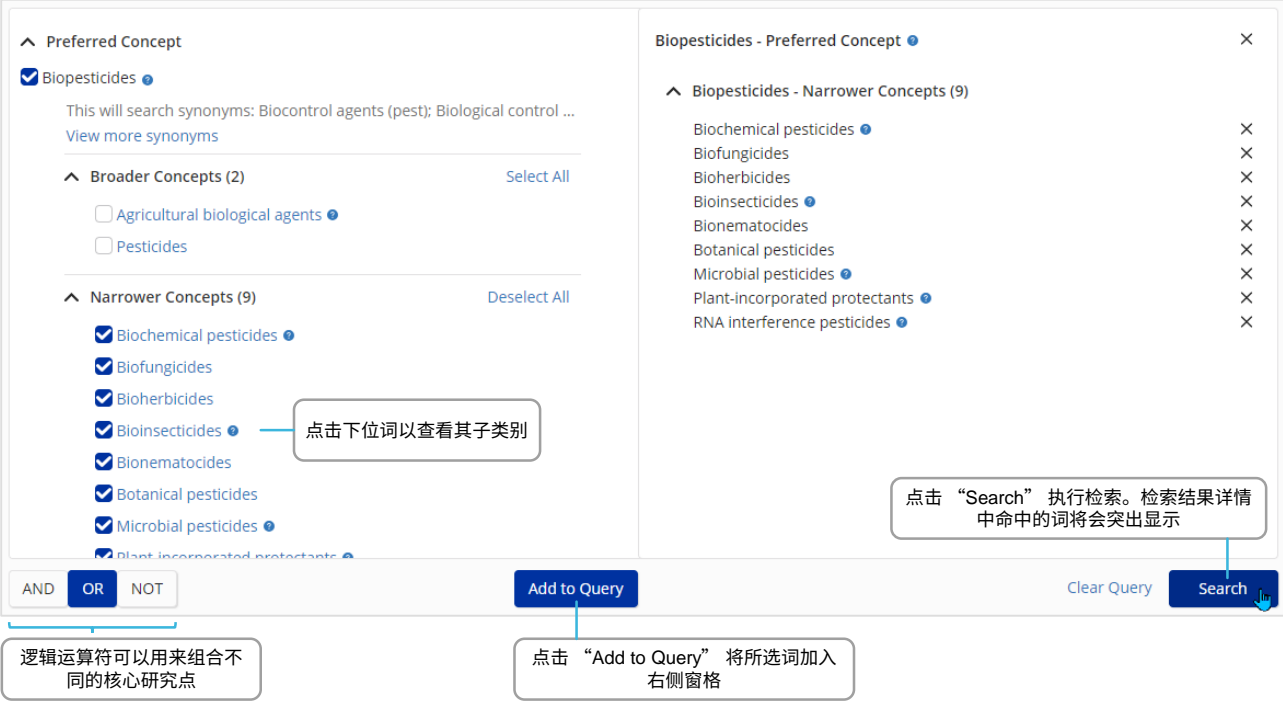
访问和浏览



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



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



检索CAS序列

检索选项

可以使用三种不同的方式检索序列：

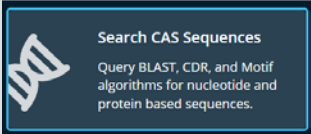
- BLAST：检索相似序列
- CDR：利用 CDR 检索抗体或T细胞受体
- Motif：检索氨基酸或核苷酸位点可变的序列

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。



BLAST

CDR

Motif

序列检索选项

Clear Search

> human insulin sequence
fvnqhlcgshlveaylvcgergffytptkgiveqcctcsicslyqlenycn

上传FASTA序列或粘贴到BLAST窗格

Upload Sequence (.fasta or .txt)

Sequence Type:

Nucleotide

Protein

Search Within:

Nucleotides

Proteins

☒ Include NCBI Sequences

包含NCBI数据库中的序列

Search Sequences

将序列复制粘贴到这个窗口

Advanced Sequence Search

Adjust Parameters for Short Sequences | Reset All

Alignment Identity %

Match with Gaps?

Gap Costs

Existence 11 Extension 1

Query Coverage %

Word Size

Scoring Matrix

BLOSUM62

BLAST Algorithm

E-Value

Exclude Low Complexity Regions

Yes

No

高级参数设置



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

fvnqhlcgshlveaylvcgergfftytpktgiveqcctsiclslyqlenycn

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 References 可获取相关文献。
- 支持下载 XLSX 格式的结果文件。

Sequences search for your query

References

获取披露所有序列的文献结果

92

Alignment Identity: 89.09%

Query

1

50

查询序列长度

Subject

1

55

目标序列长度

Matches: 49

Mismatches: 6

比对长度49+6=55 (包含5个氨基酸大小的间隙)

View Less

比对详情

目标序列详情, NCBI链接以及CAS SciFinder中的物质信息

文献预览

Alignment

Subject

References

Alignment Data

BLAST Score: 231

E-Value: 5.12823e-26

匹配

+ 不匹配: 检索的aa与目标序列对应位点的aa功能等同

Q

1

FVNQHLGSH LVEA-YLVCG ERGFFYTPKT ----GIVEQC CTSICSLYQL ENYCN 55

S

1

FVNQHLGSH LVEALYLVCGERGFFYTPKSDDARGIVEQC CTSICSLYQL ENYCN 55

查询序列和目标序列的对齐情况

查询序列中的空位, 以及与目标序列未匹配的氨基酸

References

查看披露此序列的参考文献

筛选结果

检索结果会随着筛选项调整而动态改变。

E-Value

0 to 10⁶

E-值（期望值）

Query Coverage %

0 to 100

比对上的序列长度
查询序列长度

Subject Coverage %

0 to 100

比对上的序列长度
目标序列长度

Alignment Identity %

0 to 100

匹配上的氨基酸或碱基对的数量
比对上的序列长度

Sequence Length

26 to 9521

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。

检索具有生物活性数据的物质

Molecular Formula

Molecular Formula

CAS Registry Number

Chemical Identifier

Document Identifier

Patent Identifier

Experimental Spectra

Bioactivity Data

Biological

Chemical Properties

Density

检索具有生物活性数据的文献

Search by Keyword, Sub

Author Name

Publication Name

Organization

Title

Abstract/Keywords

Concept

Substances

Bioactivity Data

Publication Year

Document Identifier

Patent Identifier

Search by Keyword, Sub

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物活性数据筛选

Life Science Data

Pharmacological Data (56)

ADME (113)

Toxicity (5)

Formulation Purpose

growth factor level

angiogenesis. Imm

Full Text

Life Science Data

Pharmacological Data (1,422)

ADME (60)

Toxicity (9)

Commercial Availability

Available (3,636)

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

C35H24O7

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

物质详情页中的生物活性数据

Pharmacological Data

筛选功能

靶点、配体和疾病的可视化

下载Excel文件

显示完整的实验细节

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

Assay Data

C11H20N4O2

Resiquimod

Target

Toil-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: Fouad, Yam B.; Gangwar, Sanjeev; Sivaprakasam, Prasanna; Pooj, Shoshana L.
World Intellectual Property Organization WO2019036023
At: 2019-02-21 | Language: English, Database: CAPUS

文献详情页中的生物活性数据

Pharmacological Data

Clear All Filters

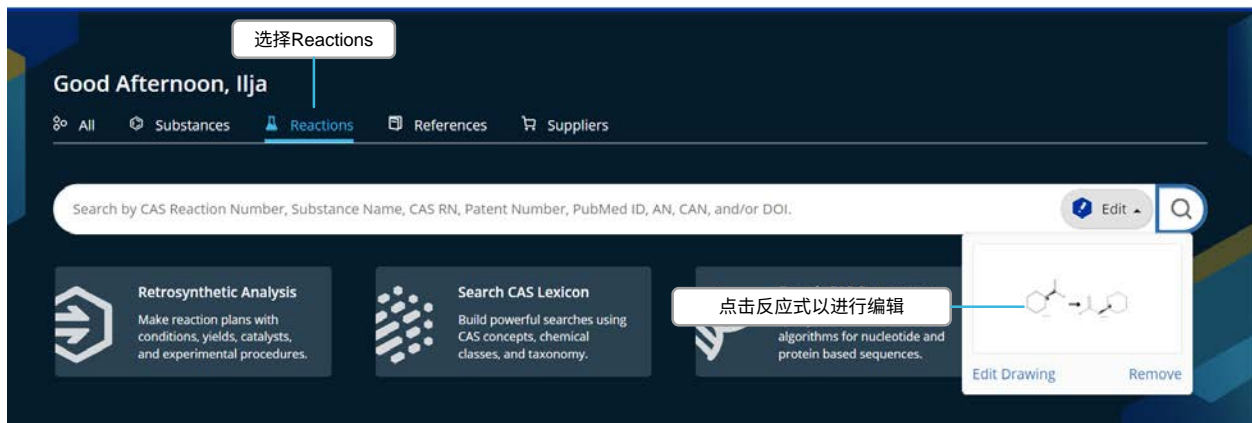
Ligand	Target	Function	Parameter	Value	Disease	Organism	Assay
621-82-9	Alpha-amylase	Inhibitor	IC50	1.017 μM	Metabolic syndrome	Human	View Detail
621-82-9	Alpha-glucosidase	Inhibitor	IC50	0.75 μM	Metabolic syndrome	Human	View Detail



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。



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。

对于单步反应，你可以根据相邻原子与特定反应中心的相似性来获取相似反应。

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

反应详情

查看反应详情

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

Get Similar Reactions

检索相似反应

Reaction Overview

Steps: 1 Yield: 85%

反应文献

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

By: Liang, Jianglin et al.

View All

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

View Source

Full Text

Company/Organization

Vertex Pharmaceuticals Incorporated

Boston, Massachusetts 02210

United States

查看所有作者

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, CDCl₃) δ7.48-7.30 (m, 5H), 5.11 (s, 2H), 4.67 (s, 1H), 4.13 (q, J = 7.1 Hz, 2H), 3.55 (s, 1H), 2.42 (t, J = 11.8 Hz, 1H), 2.28 (d, J = 12.6 Hz, 1H), 2.10-1.79 (m, 3H), 1.50-1.19 (m, 6H), 1.19-1.00 (m, 1H).

Optical Rotatory Power

=-33.3° (c = 1 in DCM).

HRMS

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

State

sticky solid

CAS Method Number 3-451-CAS-15598720

Transformations

1. Schmidt Reaction

反应转换类型

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。

Good Afternoon, Ilja

🔍 All 📦 Substances ⚗️ Reactions 📄 References 🏪 Suppliers

Search by CAS Reaction Number, Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. 🎨 Draw 🔍

Retrosynthetic Analysis

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

Search CAS Lexicon

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

Search CAS Sequences

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

Retrosynthetic Analysis

Draw or import a structure.

Click and drag to select objects. Ctrl-click to select or deselect individual objects.

Molecular Formula: $C_{13}H_{17}F_3N_2O_5$ (355.34)

Start Retrosynthetic Analysis Cancel

CAS RN
2408121-76-4

CAS Name
2-[Methoxy[5-{5-(trifluoromethyl)-1,2,4-oxadiazol-3-yl]-2-thienyl}methyl]-5-meth...

- Get Substance Details
- Get Bioactivity Data
- Get Reactions (1)
- Synthesize (1)**
- Start Retrosynthetic Analysis
- Get References (1)
- Get Suppliers (0)

Edit Structure Reset Download

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”

The screenshot displays the 'Retrosynthesis Plan Options for drawn structure' interface, powered by ChemPlanner. The interface includes several configuration sections:

- Select Synthetic Depth:** Radio buttons for depths 1, 2, 3 (selected), and 4. An annotation '更改方案中的合成深度' points to this section.
- Set Rules Supporting Predicted Reactions:** Radio buttons for 'Common' (selected), 'Uncommon (includes Common Rules)', and 'Rare (includes Common and Uncommon Rules)'. An annotation '选择较少文献实例支持的不常见或罕见规则' points to the 'Uncommon' and 'Rare' options.
- Set Starting Materials Cost Limit:** A text input field with '1000' and a dropdown menu set to 'USD/mol'. An annotation '更改原料成本上限(USD/mol或USD/g)' points to the input field.
- Break and Protect Bonds:** Buttons for 'Break Bond', 'Protect Bond' (highlighted in red), and 'Clear All Bond Selections'. Annotations '设置在首次断键中要断裂的键' and '设置在整个方案中保护的键' point to these buttons respectively.
- Clear All Bond Selections:** A button with an annotation '清除已有选择' pointing to it.

On the right, a chemical structure of a complex molecule is shown. Two specific bonds are highlighted with annotations: '首次断键中要断裂的键' (the bond to be broken in the first disconnection) and '受保护的键' (the bond to be protected).

At the bottom left, a blue button labeled 'Create Retrosynthesis Plan' is shown. An annotation '点击Create Retrosynthesis Plan, 开始运行逆合成反应路线设计' points to this button.



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

Apply

Reset Scoring

显示报道的实验步骤

打开/关闭预测步骤

调整评分选项

查看并选择备选反应路线

查看排除的步骤或物质

下载、分享和保存您的方案

查看方案步骤

蓝色实线表示报道的实验步骤

绿色虚线表示预测的步骤

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

1.1 Reagents: Butyllithium

Average Yield: 47%

Evidence (16)

Alternative Steps

1.1 Reagents: Potassium *tert*-butoxide

Solvents: Tetrahydrofuran

View All

Experimental Protocols

1.1 Reagents: Diisopropylethylamine

Ammonium chloride

O-(7-Azabenzotriazol-1-yl)-N,N,N',N'-tetramethyluronium hexafluoro phosphate

Solvents: Dimethylformamide; 2 d, rt

Experimental Protocols

Predicted Step Only

No reaction summary

Experimental Protocols

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

Select

View 8 similar Alternatives

View Evidence

Average Yield: 63%

展开相似反应分组

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

55 Results

Group: By Scheme

Sort: Relevance

View: Expanded

Scheme 1 (1 Reaction)

Steps: 1

Suppliers (49)

Suppliers (51)

Suppliers (61)

31-614-CAS-29434160

Steps: 1

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

By: Rodríguez, Maricha E.; et al

World Intellectual Property Organization, WO201008064 A1 2010-07-15

PatentPak

Full Text

预测反应依据

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.



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.

For a given step, the more precursors there are, and the closer their relative sizes are, the more it's considered convergent.

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

Weights 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 CAS SciFinder interface for a Patent Markush search. The search results are displayed in a list, with the first result selected. The detailed view of the selected patent claim is shown on the right. The interface includes a search bar, a list of results, and a detailed view of a specific patent claim. The search results are displayed in a list, with the first result selected. The detailed view of the selected patent claim is shown on the right. The interface includes a search bar, a list of results, and a detailed view of a specific patent claim.

进行Markush检索

Markush结构检索类型

命中的组装Markush结构

专利机构筛选

Markush在专利中的位置

跳转至专利文献详情页面

跳转至 CAS PatentPak Viewer

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 interface for a patent document. The document is displayed in a list, with the first result selected. The detailed view of the selected patent claim is shown on the right. The interface includes a search bar, a list of results, and a detailed view of a specific patent claim.

下载 PDF，包括标引的物质和注释列表

下载 PDF

跳转至相关信息

CAS科学家标引的重要物质定位标记

定位到专利中物质所在位置

添加注释：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

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。

Suppliers search for "7664-93-9"

Filter Behavior

Filter by Exclude

Preferred Suppliers

Preferred (52)

No Preference (438)

Supplier

信息的最新更新
更新时间

Hayashi Pure Chemical Products Catalog (106)

Thermo Fisher Scientific Product List (66)

KANTO CHEMICAL (43)

Aladdin Scientific Product Listing (37)

FUJIFILM Wako Chemicals Europe GmbH Product List (37)

View All

Purity

≥99% (8)

95-98% (132)

90-94% (9)

<90% (14)

490 Results

首选/非首选供应商标签

排序选项

Sort: Relevance

Relevance

Price: Low to High

Price: High to Low

Supplier: A to Z

Supplier: Z to A

Ships Within

Purity

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

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

OH

O

S

O

OH

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。

选择 居中 翻转片段 剪切 | 复制 | 粘贴

ChemDoodle

从 CAS 登记号导入结构

清除 橡皮擦

撤销 | 恢复

模板

打开 | 保存

缩放

标签

绘制键

绘制环

添加电荷

碳链工具

重复结构单元

可变位置定义工具

原子锁定/链锁定/环锁定工具

片段结构定义工具

反应箭头绘制工具

反应原子标记工具

化学键标记工具

ChemDoodle®

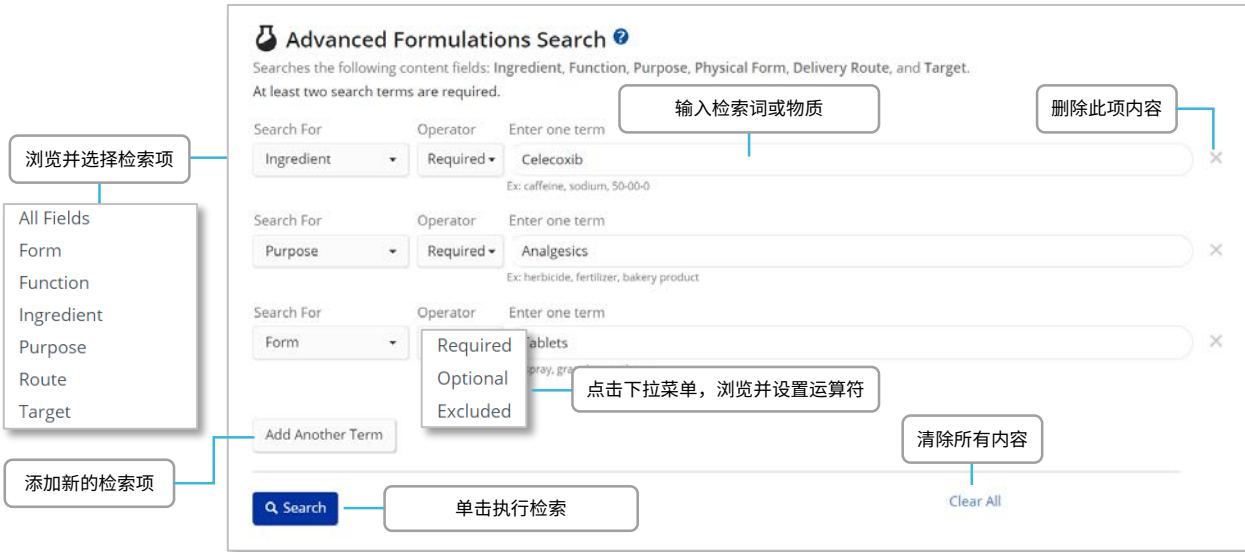
回顾现有技术

- 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。

SciFinder Discovery Platform 快速入门指南 | 21

CAS Formulus

检索制剂或配方



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

Compare (2/3)

Save

Sort: Relevance

Group: By Family

对比选中的制剂或配方

保存结果并设置提醒

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 (108)

☒ Analgesics (81)

☐ Anti-inflammatory agents (80)

☐ Antiarthritics (57)

☐ Pharmaceutical formulations (31)

Physical Form

☐ Capsules (85)

☒ Tablets (81)

☐ Solutions (54)

☐ Suspensions (31)

☐ Liquids (17)

State of Matter

Delivery Route

☒ Oral drug delivery systems (81)

☐ Controlled-release drug delivery systems (11)

☐ Topical drug delivery systems (5)

☐ Parenteral drug delivery systems (4)

☐ Inhalation drug delivery systems (2)

Information Included

☒ Component Amount (80)

☐ Process (59)

☒ Experimental Activity (49)

☐ Effective Dose (5)

Document Type

Organization

Language

Publication Year

1999

2020

No Min to No Max Apply

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	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		
Group: Additional ingredients	-	-
Magnesium stearate	Lubricants	12 g

Ⓢ Predicted value

[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

↓ Save

结果保存

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

② 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 (1:7)	Formulation excipients	264 g	Mandatory
Hydroxypropyl cellulose	Disintegrants	384 g	Mandatory
Cellulose, carboxymethyl ether	Disintegrants	102 g	Mandatory
Poly(vinyl alcohol)	Binders	42 g	Mandatory
Sodium dodecyl sulfate	Surfactants	24 g	Mandatory
Magnesium stearate	Lubricants	12 g	Mandatory

More Formulations like this...

相似的制剂或配方

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

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

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

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

Process

制备工艺

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

Experimental Activity

制剂或配方实验评估

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

Source Patent

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

SciFinder Discovery Platform 快速入门指南 | 25

检索原料

CAS

Formulus

Help & Support

Alerts

Saved

Good Afternoon, Liu

选择Ingredients

FormulationsIngredients

propylene glycol

输入原料名称、CAS登记号或功能信息，单击放大镜执行检索

Ingredients search for "propylene glycol"

通过电子邮件发送结果

保存结果并设置提醒

选择筛选项，精准获得原料结果

1 Selected 3 Results

1

Filter by

Industry

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Cleaning & Surfactant Products

Cosmetics & Personal Care

Food & Related

Inks, Paints, & Coatings

Pharmaceutical

Regulatory Information

REACH (6)

Cosing: Cosmetic Ingredient Inventory (3)

EPA Pesticide Inactive Ingredients (3)

FDA Inactive Ingredients Database (3)

Experimental Properties

Commercial Availability

CAS RN: 57-55-6

View Details

CC(O)CO

C₃H₈O₂

(±)-Propylene glycol

Key Physical Properties

Molecular Weight

76.09

Melting Point (Experimental)

-59 °C

Boiling Point (Experimental)

188.2 °C

Density (Experimental)

1.036 g/cm³

Commonly Used As: Solvents; Humectants; Pl

Similar Ingredients with Regulatory Information

Propylene glycol monolaurate

Propylene glycol butyl ether

Propylene glycol monopropyl ether

View 14 More

Commonly Formulated With | Regulatory Information | Experimental Properties

Get Formulations

Get Suppliers

Add to Formulation Designer

查看原料供应商信息

查看实验属性

查看使用该原料的制剂或配方

查看管制信息及清单

查看制剂或配方中，与该原料同时使用的其它配伍成分

将原料添加至 Formulation Designer

Commonly Formulated With

Ingredient

CAS RN/CAS SCN

As Active Ingredients

As Inactive Ingredients

As Any Role

Water

7132-18-5

View Formulations

View Formulations

View Formulations

Glycerol

56-81-5

View Formulations

View Formulations

View Formulations

Ethanol

64-17-5

View Formulations

View Formulations

View Formulations

Carbamide

77-06-6

View Formulations

View Formulations

View Formulations

Sodium hydroxide

1310-73-2

View Formulations

View Formulations

View Formulations

Oleic acid

112-80-1

View Formulations

View Formulations

View Formulations

Dodecyl ethylhexadecylacetate

139-33-3

View Formulations

View Formulations

View Formulations

Sodium sulfate

7757-83-7

View Formulations

View Formulations

View Formulations

Diphenyl glycol monomethyl ether

111-90-0

View Formulations

View Formulations

View Formulations

(S)-Nonylphenylmethoxymethylacetate

30578-66-0

View Formulations

View Formulations

View Formulations

Karbitol

11138-96-2

View Formulations

View Formulations

View Formulations

Alcohol, C₁₂-14, ethoxylated

68531-39-0

View Formulations

View Formulations

View Formulations

Isopropyl

67-63-0

View Formulations

View Formulations

View Formulations

Polyethylene glycol monomethyl ether

9004-96-2

View Formulations

View Formulations

View Formulations

Hydrogen peroxide

7722-84-1

View Formulations

View Formulations

View Formulations

Polyethylene glycol

25522-68-5

View Formulations

View Formulations

View Formulations

Triacetin

12463-47-7

View Formulations

View Formulations

View Formulations

Methylparaben

99-75-3

View Formulations

View Formulations

View Formulations

Ammonia

7664-41-7

View Formulations

View Formulations

View Formulations

Ethanolamine

141-43-5

View Formulations

View Formulations

View Formulations

ANMAT

Cosing: Cosmetic Ingredients Inventory

Drug Master File List

EMA Excipients List

Original Name (translation)

Applicant Name

Event Date

Category

Packaging

Strength

Form

PROPLENGLYCOL* (PROPYLENE GLYCOL)

ALCON LABORATORIOS ARGENTINA S.A.

March 2019

EYE LUBRICANT

1 Dropper Bottle of 10 ml

0.6 g/100 ml

OPHTHALMIC SOLUTION

* SEE PROSPECTUS IN VVM

Source

Marketing Authorizations for Medicines is produced by Argentina National Administration of Medicines, Food and Medical Technology

Inventory Lists

Ingredient is on the following Inventory Lists:

Acronym

Inventory List

Country

ABC

Australian Inventory of Industrial Chemicals

Australia

AREC

South Korean Act on the Registration and Evaluation of Chemicals

Korea (Republic of)

查看原料供应商信息

选择筛选项，精准获得供应商信息

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)

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 (1)-Propylene glycol

CAS RN: 57-55-6

Aaron Chemicals LLC

View Details

查看供应商联系方式、货运详情及分销商信息

点击查看来自供应商的购买页面

Product Information		Quantity Information		Ordering & Shipping
Name:	1,2-Propanediol	Available Amounts:		Order from Supplier
Molecular Weight:	76.0944	500 g	USD 5.00	Ships Within: 1 week
		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	Available Amounts:		Order from Supplier
		500 g	USD 8.00	Ships Within: 1 week
		100 g	USD 6.00	Status: Maintained in stock
		25 g	USD 5.00	

Enamine US Inc.

View Details

Product Information		Quantity Information		Ordering & Shipping
Name:	propane-1,2-diol	Available Amounts:		Order from Supplier
Molecular Weight:	76.09	2.5 g	USD 27.00	Ships Within: 1 week
		50 g	USD 50.00	Status: Maintained in stock
Weight:		5 g	USD 29.00	
SDS Availability:	https://enamine.enamine.net/pub/msds?code=EN300-21726&&senderid=0&&lang=en	250 mg	USD 19.00	
		100 mg	USD 19.00	
Shipping:	Room temperature	100 g	USD 67.00	
Storage:	Room temperature	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

Industry

Pharmaceutical

Cosmetics & Personal Care

Agrochemical

Cleaning & Surfactant Products

Inks, Paints, & Coatings

Food & Related

浏览并选择应用领域

浏览并选择用途

Drug delivery systems

Pharmaceutical formulations

Antitumor agents

Anti-inflammatory agents

Analgesics

Antibacterial agents

Ophthalmic agents

Antidiabetic agents

Antiviral agents

Antihypertensives

- View More Purposes -

浏览更多选项

浏览并选择物理形态

Tablets

Capsules

Solutions

Gels

Liquids

Pharmaceutical ointments

Cream preparations

Suspensions

Sprays

Powders

- View More Physical Forms -

添加最多5种原料

Celecoxib

Polyethylene glycol

+ Add Another Ingredient

添加另一种原料

删除该原料

Create Template

单击执行检索

SciFinder Discovery Platform 快速入门指南 | 27

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
Active or Featured Ingredient:	Polyethylene glycol	ANMAT; Cosing: Cosmetic Ingredient Inventory; Drug Master File List; EPA Pesticide Inactive Ingredients; EPA Safer Chemical Ingredients; FDA GRAS (Part 181, Subpart B); FDA Inactive Ingredients Database	-	Amount not available
Lubricants	Talc (Mg ₃ H ₂ (SiO ₃) ₄) View More Alternatives	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 View More Alternatives	Alternative Ingredients (Showing all 10) Select the ingredient you would like to use: Sodium dodecyl sulfate Glyceryl tribehenate Sodium stearyl fumarate Magnesium stearate Stearic acid Silica Polyoxyethylene sorbitan monooleate Calcium stearate Polyethylene glycol Glycerol behenate		
Disintegrants	Croscarmellose sodium View More Alternatives	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 View More Alternatives	Cosing: Cosmetic Ingredient Inventory; Drug Master File List; EPA Pesticide Inactive Ingredients; EPA Safer Chemical Ingredients;	Talc (Mg ₃ H ₂ (SiO ₃) ₄); Butyl methacrylate-dimethylaminoethyl methacrylate	Approximate Range: 8 - 16%

+ Add Function

点击可添加用途

Function

Anti-inflammatory agents

Add Function

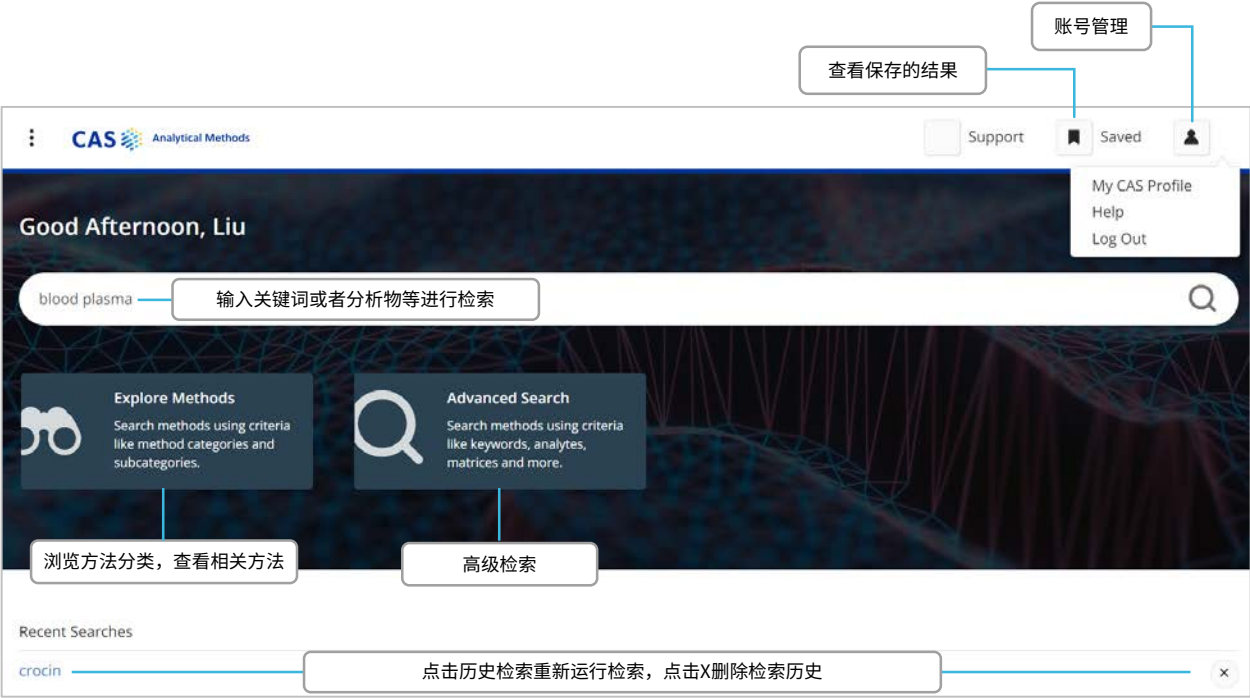
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添加用途后，点击获得新的制剂或配方设计结果



CAS Analytical Methods

分析方法检索



高级检索



分析方法的分类检索

Explore

浏览并选择方法分类及子分类

可输入关键词

Clear all selections

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Category

Agricultural Applications /

Bioassays

Biomolecule Isolation

Environmental Analysis

Food Analysis

Fuels / Geology / Biofuels

Historical Analysis / Dating

Miscellaneous

Organic Compound Analysis

Organometallics / Inorganics

Pharmacology / Toxicology

Polymer Analysis

Water Analysis

Category Name

Bioassay

Bioassay Synthetic Probes

Biomarker Biological Process

Biomarker Cell Assay

Biomarker Medicine Assay

Biomedicine Material Analysis

Biomolecule Isolation Assay

Bioorganism Isolation Assay

Genetic Analysis

Nanomaterial Analysis

Include Keywords (Optional)

Palmitic acid

+ 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

结果保存

结果导出

1 Selected 7 Results

Sort: Relevance

Group: By Method

Filter By

Analyte

☐ Palmitic acid (7)

☐ Stearic acid (7)

☐ Linoleic acid (6)

☐ Oleic acid (5)

☐ Arachidonic acid (4)

View All

Matrix

☐ Blood plasma (7)

☐ Hazelnut oil (1)

Method Category

☐ Gas chromatography (82)

☐ Extraction (49)

☐ Solvent extraction (48)

☐ Flame ionization detectors (39)

☐ Gas chromatography-mass spectrometry (26)

☒ HPLC (7)

View All

Year

选中方法，导出或保存

查看方法信息详情

JOURNAL

Compare

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

展示摘要

获得全文链接

View Abstract

Full Text

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在CAS SciFinder中查看文献详情

选择感兴趣的方法进行对比

2

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

JOURNAL

Compare

分析方法详情

结果保存

结果导出

↓

Save

Analysis of Myristic acid in Blood plasma by Solvent extraction

CAS Method Number

1-122-CAS-534418

Method Category

分析方法中的分析物、基质、材料、试剂等分类展示

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 × 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

书目信息

JOURNAL

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

CODEN : THGNBO | ISSN : 0093691X | DOI : 10.1016/j.theriogenology.2021.09.034

View Abstract

Full Text

展示摘要

获得全文链接

Validation

数据有效性

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

点击X删除方法

删除所有方法方法

Clear all

Compare

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

一次最多可以比较三种不同方法，所有方法信息详情的内容都可以进行对比

Comparing your 3 selected Methods

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	Method 1	Method 2	Method 3
	Analysis of Palmitic acid in Blood plasma by Solvent extraction	Analysis of Fatty acids in Blood plasma by HPLC	Analysis of Lauric acid in Blood plasma by Electrochemiluminescence
CAS Method Number	2-114-CAS-225380	1-122-CAS-96286	1-122-CAS-3193044
Method Category	Biomolecule Isolation Assay	Fatty Acid Analysis	Fatty Acid Analysis
Technique	Time-of-flight mass spectrometry; HPLC; Electrospray ionization mass spectrometry; Solvent extraction	Electrochemical analysis; Atmospheric precipitation; HPLC	Electrochemiluminescence; HPLC
Analyte	Palmitoleic acid; Palmitic acid; Elaidic acid; Linoleic acid; Stearic acid; Arachidonic acid; Docosahexaenoic acid	Stearic acid; Linoleic acid; Palmitic acid; Arachidonic acid; Oleic acid; Fatty acids	Palmitic acid; Stearic acid; Myristoleic acid; Palmitoleic acid; Lauric acid; Arachidonic acid; Oleic acid; Linoleic acid; Linolenic acid; Myristic acid; Fatty acids
Matrix	Blood plasma	Blood plasma	Blood plasma
Other Materials	tert-Butyl methyl ether; Chloroform; Formic acid; Methanol; Ethyl acetate; Hydrochloric acid; Sodium chloride; Glass vial; Zorbax Eclipse plus C ₁₈ 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 ₃ BO ₃); 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
Equipment Used	Vortexer, Glas-Col, Terre-Haute, IN, USA; Centrifuge, RVC 2-25, Christ, Osterode, Germany; HPLC system, 1290 Infinity, Agilent Technologies Inc., Santa Clara, CA, USA; Time of flight mass spectrometer, 6550, Agilent Technologies Inc., Santa Clara, CA, USA	HPLC system; Degasser, DG-980-50, Jasco, Tokyo, Japan; HPLC pumps, 301M, Flom, Tokyo, Japan; Sample injector, 7725, Rheodyne, Cotati, CA, USA; Electrochemical detector, LC-4C, BAS, Tokyo, Japan; Electrochemical cell (Radial flow cell), BAS; Electrochemical recorder, 807-IT, Jasco	Degasser, DGU-10B, Shimadzu, Japan; Degasser, DGU-3A, Shimadzu, Japan; Pump, LC-10AD, Shimadzu; Autosampler, SIL-6A, Shimadzu; Chemiluminescence detector, CLD-10A, Shimadzu; HPLC system
Conditions	Instrument: column: Zorbax Eclipse plus C ₁₈ 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) ₃ Cl ₂ in 10 mM H ₂ SO ₄ ; flow rate:

保存的结果集

CAS

Analytical Methods

blood plasma

Q

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Saved (2)

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

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ChemZent追溯学科早期的研究

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Concept

Publication Name

Language

☐ German (3)

Author

Database

☐ CAPUS (63K)

☐ MEDLINE (45K)

☒ CHEMZENT (3)

Filtering: Database: CHEMZENT

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By: Zernik

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Machine Translated: Chem. FABR. DR. J. WIERNIK 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 Dünn-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. Antiarthriticum. — Pantaplant (chemical. Structures KOLBERG G. mass forming H., Kolberg): fluid extracts from

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Katagel-Kreidl (Herst. ders.): gifftfreie Spezialtrockenbeize für Saatgut. — Medoform (Herst. ders.): Liqu. Formaldehydi saponat. — Meissol (ANT. MEISZL'S NACHF., Wien): Ungezieferverteilungsmittel. — Oma (OMA-NÄHRSTOFF-GES., St. Veit a. d. Glan, Kärnten): Kindernährmittel. — Oma-Kinder- u. Wundpulver (Herst. ders.): peledol (Pellidol? Ref.) haltiger Fettpuder. — Pommelte (POMMETTE-KELLEREI, Wien XI): naturreiner Apfelsaft. (Pharmaz. Mh. 14. 42—44. Febr. 1933.) HARMS.

—, Neue Arzneimittel, Spezialitäten und Geheimmittel. Anustypsalbe u. Anustypzäpfchen (BÄREN-APOTHEKE, ROB. RADITZ, Wien II): Hämorrhoidalpräparate mit Tannalbin, Ichthyol u. Bi-Salzen. — Gynosupp (Herst. ders.): Vaginal-„Kugeln“ in Form eines gerade abgestutzten Kegels mit Milchsäure, Bor-Salicylsäure u. Hydrarg. salicylicum. Anticoncipiens usw. Auch mit 10% Ichthyol als Gynosupp cum Ichthyolo. (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.): Cachets mit 0,2 g Pyrasulf (C. 1933. I. 2278), 0,2 g Chinin „Weil“ (C. 1931. II. 1599), 0,4 g Somnacetin (C. 1931. I. 2223) u. 0,00033 g Scopolamin. Zur Schmerzlinderung in der Austreibungsperiode. (Manufactur. Chemist pharmac. Cosmetic 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.): diiodmethansulfosaures Na in 40%ig. wss. Lsg. zur Röntgendarst. der Harnwege. — Stomachysatum Bürger (YSATFABRIK G. M. B. H., Wernigerode): Extrakte von Artemisia Absinthium, Achillea millefolium, Gnaphalium arenarium u. Rheum palmatum. Gegen Magenstörungen. — Progynon oleosum (SCHERING-KAHLBAUM A.-G., Berlin): ölige Lsg. des Follikulinbenzoats. Die 1-ccm-Ampulle enthält 10000 Mäuseeinheiten. 1 × wöchentlich intramuskulär als Depot. (Manufactur. Chemist pharmac. 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 Dünn- u. Dickdarm. — Lygal (DR. GEORG HENNING, Berlin-Tempelhof): Verb. von 50% phenylquinolinecarbonsaurem Ca (bzw. Na), 29% Dimethylaminophenazon u. 21% Coffein-Natriumsalicylat. Antiarthriticum. — Pantaplant (CHEM. WERKE

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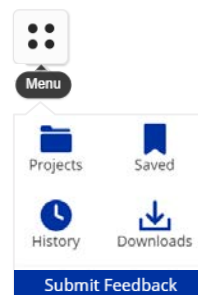
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