

CAS SCIFINDER
DISCOVERY PLATFORM™

快速入门 指南

学术版

目录

2	<u>CAS SciFinder®使用界面</u>
2-3	<u>文献检索</u>
4	<u>CAS Lexicon</u>
5-6	<u>物质检索</u>
7	<u>高级检索</u>
8	<u>CAS Roles</u>
9-10	<u>CAS Sequences检索</u>
11	<u>生命科学数据</u>
12-13	<u>反应检索</u>
14-15	<u>逆合成反应路线设计</u>
16	<u>Markush</u>
16	<u>CAS PatentPak®</u>
17-21	<u>CAS Formulus®</u>
22-24	<u>CAS Analytical Methods™</u>
25	<u>登录，培训，支持</u>

CAS SciFinder

主界面及文献检索



检索界面

CAS SciFinder拥有简洁的检索界面。



文献结果集界面

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

查看文献的引文地图

In this Reference

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

文献详情快速浏览

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

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)ethan-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-(1-menthoxy)-1,2-propanediol as the cool-tasting component.

Keywords: fruit juice flavor food beverage menthol

PatentPak Viewer

Get Prior Art Analysis

Full Text ▾

View in CAS Formulus

获取现有技术分析

Publication Information • Patent

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 CODEN: PIXXD2	Database Information AN: 2005:470226 CAN: 143:25602 CAplus	Language English	题录信息

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			JP2003-389758	2003-11-19

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

专利族和优先权申请信息

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



- AND** 要求文献结果中同时出现两个术语。
- OR** 要求文献结果中至少出现其中一个术语或两个术语都出现。
- NOT** 从检索结果中排除包含NOT后面的词语的文献结果。

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

- | | | |
|---|-------------|--|
| * | 可替换0到多个字符 | 例如: polymorph* immunoglobulin*conjugate* |
| ? | 可替换0个或者1个字符 | 例如: benzonorbornen? |

包含双引号的短语将作为精确短语进行检索。

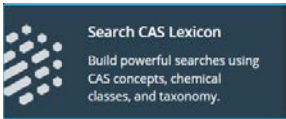
例如：搜索“Programmed cell death protein”只会找到完全匹配“Programmed cell death protein”的结果。

CAS Lexicon

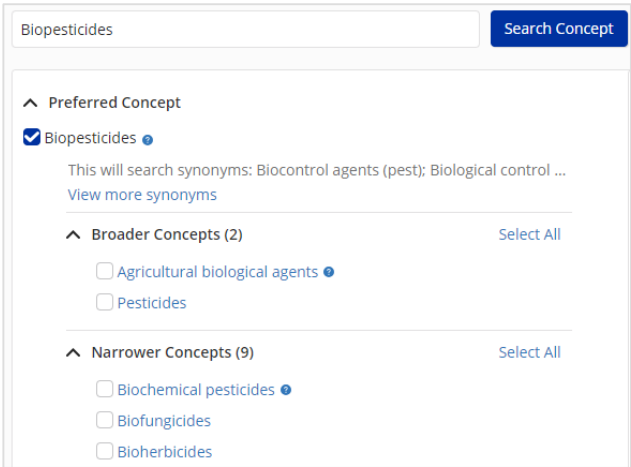
CAS Lexicon概述

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

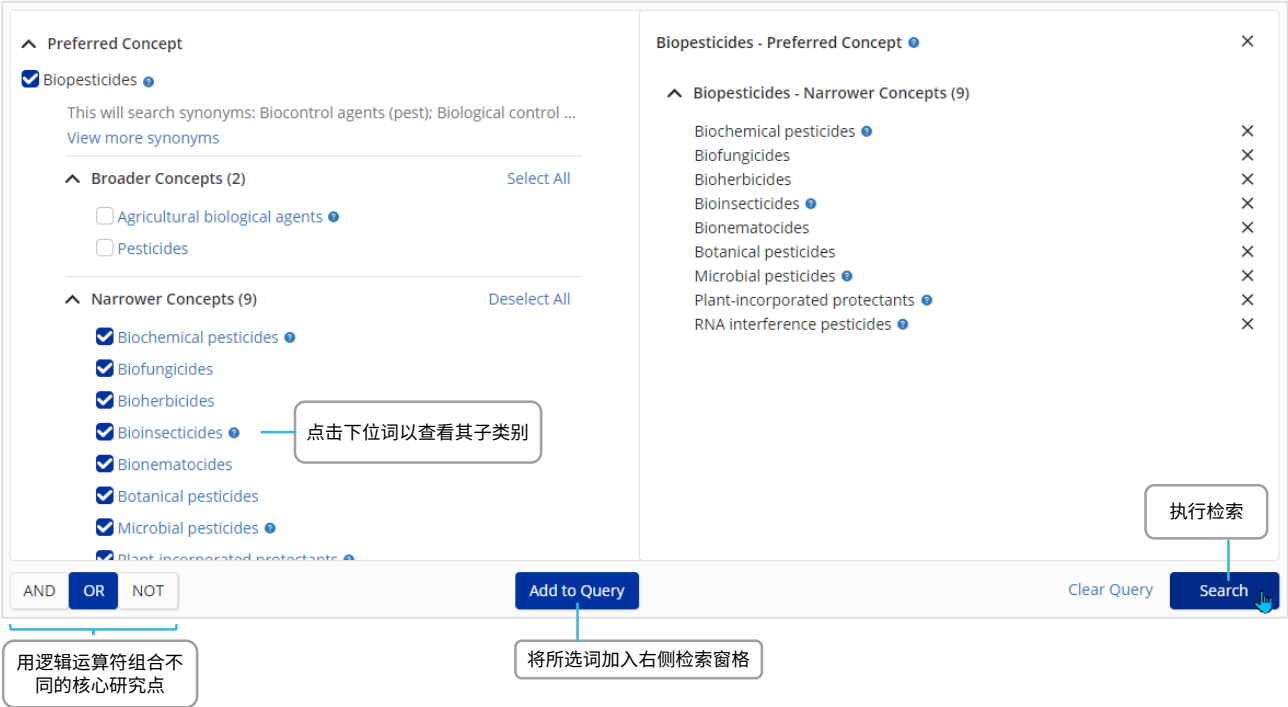
访问和浏览



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。



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。以下是物质检索的示例：

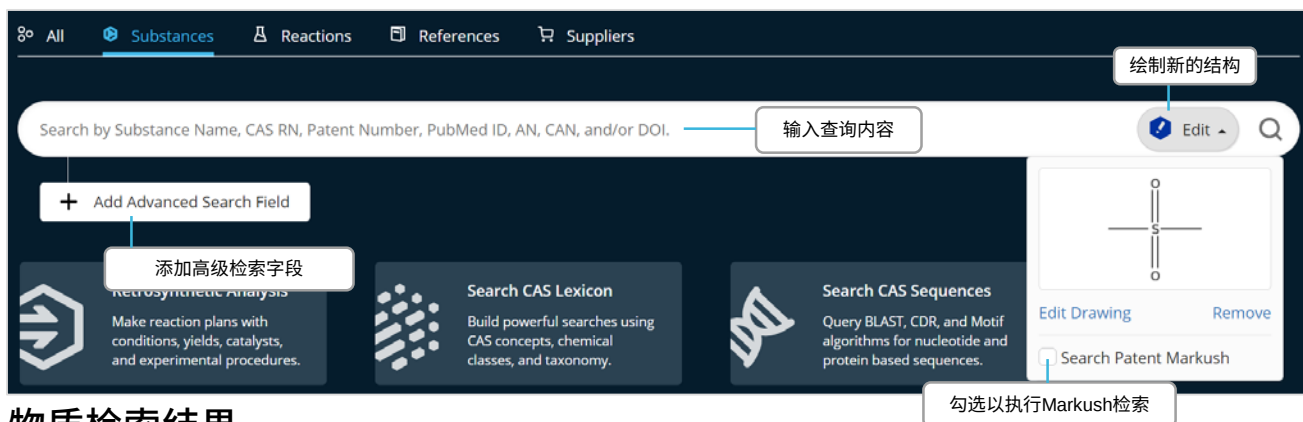
Streptomycin

57-92-1

"Streptomycin sulfate"

Sulfoximin*

WO2019234160



物质检索结果

物质检索结果在一个直观的界面中呈现，您将看到与您的检索最相关的结果，包括物质名称、CAS登记号和高分辨率结构式图像。

物质详情和结构绘制面板

物质详情

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

CAS Registry Number: 90357-06-5

4,364

233

116

Download

Save

C₁₈H₁₄F₄N₂O₄S

按希尔顺序排列的分子式

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

CA索引名

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

物质属性和谱图信息

重要参数

Chemical identifier list, including SMILES, InChI, systematic names, common names, and trade names

Canonical SMILES
N#CC1=CC=C(C=C1C(F)(F)F)NC(=O)C(C)(O)C(S(=O)(=O)C2=CC=C(C(F)=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)15(8-13)18(20,21)22/h2-8,26H,10H2,1H3,(H,24,25)

InChI Key
LKJPYSCBVHEWU-UHFFFAOYSA-N

9 Other Names for this Substance
N-[4-Cyano-3-(trifluoromethyl)phenyl]-3-[[4-(4-fluorophenyl)sulfonyl]-2-hydroxy-2-methyl]propanamide (ACI)
Propanamide, N-[4-cyano-3-(trifluoromethyl)phenyl]-3-[[4-(4-fluorophenyl)sulfonyl]-2-hydroxy-2-methyl-, (±)- (ZCI)
(±)-4'-Cyano-α,α,α-trifluoro-3-[[p-(4-fluorophenyl)sulfonyl]-2-methyl-m-lactoluidide
Bicalutamide

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...

select objects. Ctrl-click to select or deselect individual objects.

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

Zoom: 90%

OK

Cancel

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

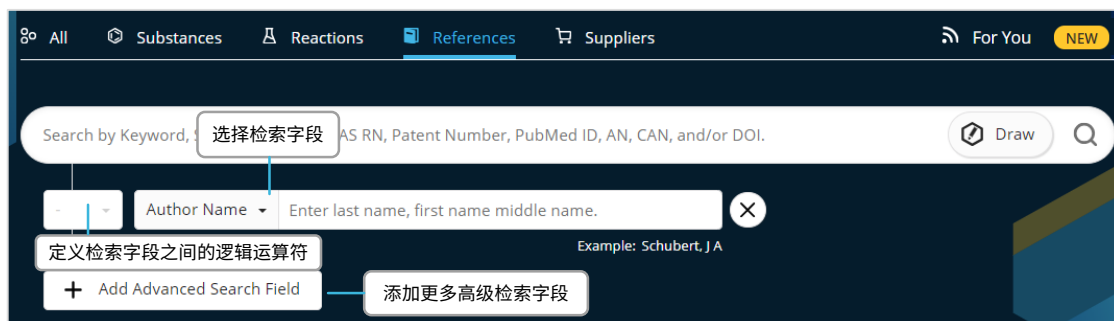


高级检索

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, 无需使用逻辑运算符
- 允许使用通配符, 例如 pollut*
- 最多使用50个高级检索字段 (如果主检索字段也被使用, 则为49个)



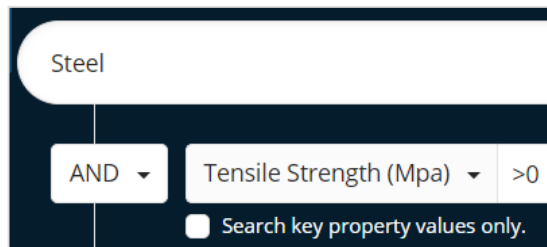
高级检索示例

高级文献检索



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

高级物质检索



检索说明:
检索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
- 生命科学数据
- 出版年份
- 文档标识符
- 专利标识符
- 出版商

物质检索

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

CAS Roles

CAS Roles 概述

Roles与物质相关联，您可以聚焦感兴趣的物质及其特定研究角色相关的文献。

- Super roles 是广泛的类别，包括所有相关的具体的Role。例如分析研究（Analytical Study）。
- Specific roles 更为精确，比如分析研究中物质作为分析物（Analyte）使用。

物质检索结果中的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。

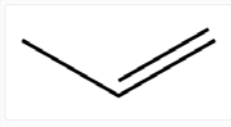
示例：我对（海洋）污染这一课题很感兴趣，怎样才能找到专门将聚丙烯描述为污染物（pollutant）的文献？

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5,475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)_x

Polypropylene

348K

References

8,952

Reactions

36

Suppliers

Author

Document Type

Substance Role

☐ Uses (291K)

☐ Properties (64K)

☐ Process (56K)

☐ Biological Study (25K)

☐ Preparation (20K)

View All

Database

Organization

Author

Document Type

Substance Role

☐ Uses (291K)

☐ Properties (64K)

☐ Process (56K)

☐ Biological Study (25K)

☐ Preparation (20K)

☒ Pollutant (5,475)

View All

Database

348,066 Results

Sort: Relevance

View: Partial Abstract

1

Preparation and Mechanical Properties of Polypropylene-Clay Hybrids

By: Kawasumi, Masaya; Hasegawa, Naoki; Kato, Makoto; Usuki, Arimitsu; Okada, Akane

Macromolecules (1997), 30(20), 6333-6338 | Language: English, Database: CPlus

Polypropylene (PP)-clay hybrids (PPCH) were prepared by simple melt-mixing of 3 components, i.e., PP, maleic anhydride-modified polypropylene oligomers (PP-MA), and clays intercalated with stearylammmonium. The dispersibility of 10 Å thick silicate layers of the clays in the hybrids was investigated using a transmission electron microscope and X-ray diffractometer. There are 2 important

exfoliated and homogeneous dispersion of the layers in the hybrids: (1) the intercalation capability of the

and (2) the miscibility of the oligomers with PP. Almost

Full Text

Substances (3)

Reactions (0)

Citing (1,430)

Citation Map

Filtering: Substance Role: Pollutant

Clear All Filters

5,475 Results

Sort: Relevance

View: Partial Abstract

1

Life in the "Plastisphere": Microbial Communities on Plastic Marine Debris

By: Zettler, Erik R.; Mincer, Tracy J.; Amaral-Zettler, Linda A.

Environmental Science & Technology (2013), 47(13), 7137-7146 | Language: English, Database: CPlus and MEDLINE



Plastics are the most abundant form of marine debris, with global production rising and documented impacts in some marine environments, but the influence of plastic on open ocean ecosystems is poorly understood, particularly for microbial communities. Plastic debris (PMD) collected at multiple locations in the North Atlantic was analyzed with next-generation sequencing to characterize the attached microbial communities. The microbial community of heterotrophs, autotrophs, predators, and symbionts was

community referred to as the Plastisphere. Bio-visualized in

Full Text

Substances (2)

Reactions (0)

Citing (1,743)

Citation Map

此结果集中的5,475篇文献中的每一篇都将聚丙烯作为污染物讨论。

单击“View All”可以选择更多 Roles



检索CAS序列

检索选项

可以使用三种不同的方式检索序列：

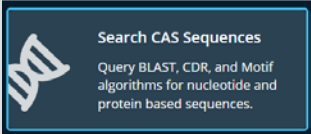
- BLAST：检索相似序列
- CDR：利用 CDR 检索抗体或T细胞受体
- Motif：检索氨基酸或核苷酸位点可变的序列

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

将序列复制粘
贴到这个窗口

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

Q Search Sequences

Advanced Sequence Search ^

Adjust Parameters for Short Sequences | Reset All

Alignment Identity %

Match with Gaps?

Gap Costs

Query Coverage %

Word Size

Scoring Matrix

BLAST Algorithm

E-Value

Exclude Low Complexity Regions

-

☐ Yes

☒ No

Existence 11 Extension 1

90

3

BLOSUM62

BLASTp

10

☐ 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

fvnqhlcgshlveaylvcgergffytptktgiveqcctsiclyqlenycn

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: 检索的氨基酸与目标序列对应位点的氨基酸功能等同

Q

1

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

S

1

FVNQHLGSH LVEALYLVCG ERGFFYTPKSDDARGIVEQC 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)



生命科学数据

检索靶点、配体和疾病

在 CAS Life Sciences 中利用高级检索字段进行物质检索或文献检索，您可以找到与靶点、配体和疾病相对应的生命科学数据。

检索具有生命科学数据的物质

Molecular Formula

CAS Registry Number

Chemical Identifier

Document Identifier

Patent Identifier

Experimental Spectra

Life Science Data

Biological

Chemical Properties

Density

检索具有生命科学数据的文献

Author Name

Publication Name

Organization

Title

Abstract/Keywords

Concept

Substances

Life Science Data

Publication Year

Document 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命科学数据筛选

Life Science Data

Biomarkers (359)

Pharmacological Data (1,380)

ADME (216)

Toxicity (87)

筛选有生物标志物，药理学数据，ADME或毒性数据的文献结果

Life Science Data

Pharmacological Data (1,422)

ADME (60)

Toxicity (9)

通过物质的药理学数据，ADME和毒性数据，对物质结果进行筛选

Artemisinin

By: Ashley, Eliza

rest of the world

C₃₅H₂₄O₇

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

物质详情页中的生命科学数据

Pharmacological Data

筛选功能

Target	Function	Parameter	Value	Disease	Organism	Assay	Source
Toil-like receptor 7	Agonist	EC50	0.42 μM	cancer	Human	View Detail	(1) CAS
Toil-like receptor 7	Agonist	EC50	1.4 μM	-	-	View Detail	(2) CAS
Toil-like receptor 7	Agonist	EC50	0.42 μM	acute pathogen infection	-	-	-

ADME

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

Toxicity

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

下载Excel文件

显示完整的实验细节

Chemical Structure

C₁₇H₂₂N₂O₂

Resiquimod

Assay Data

Ligand

144875-48-9

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, Yim B.; Gangwar, Sanjeev; Sivaprakasam, Prasanna; Pooj, Shoshana L.

World Intellectual Property Organization WO2019036023

AI: 2019-02-21 | Language: English, Database: CAPUS

文献详情页中的生命科学数据

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

进行反应检索

选择 Reactions

Good Afternoon

All

Substances

Reactions

References

Suppliers

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

Edit

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.

Click on reaction to edit

algorithms for nucleotide and protein based sequences.

Edit Drawing

Remove

反应检索结果

Reactions search for drawn structure

将分组更改为“By Document”或“By Transformation”

References ▾

Structure Match
As Drawn (0)
Substructure (20K)
Similarity (18)

按结构匹配度查看物质结果

Filter Behavior
Filter by Exclude

▼ Search Within Results

Yield

- ☐ 90-100% (428)
- ☐ 80-89% (263)
- ☐ 70-79% (295)
- ☐ 50-69% (379)
- ☐ 30-49% (207)

View All

Number of Steps

- ☐ 1 (2,455)

Scheme 1 (2 Reactions)

点击结构查看物质信息

Absolute stereochemistry shown, Rotation (+)

Suppliers (48) 查看供应商

Suppliers (484)

Group: By Scheme ▾ Sort: Yield ▾ View: Expanded ▾

发送到 CAS 结构绘制面板

保存、提醒和共享选项

Steps: 1 Yield: 100%

反应结果集筛选项

查看反应详情

Experimental Protocols

31-614-CAS-27240963 Steps: 1 Yield: 100%

1.1 Reagents: Triethylamine, Diphenylphosphoryl azide
Solvents: Toluene

查看参考文献

Stereoselective process for preparing isoxazoloquinoline-substituted cyclohexyl derivatives

Assignee: Eli Lilly and Company
World Intellectual Property Organization, WO2002024705 A1
2002-03-28

PatentPak ▾ Full Text ▾ 访问专利全文

31-614-CAS-27633989 Steps: 1 Yield: 100%

1.1 Reagents: Triethylamine, Diphenylphosphoryl azide
Solvents: Toluene; 40 - 50 °C; 1 h, 110 °C; 110 °C → 70 °C
1.2 70 °C; overnight, 70 °C → 85 °C

Preparation of N-(isoxazoloquinolinyl)cyclohexylcarboxamides and analogs as MRP1 inhibitors

Assignees: Eli Lilly and Co.; Wang, Qiuping; et al.
World Intellectual Property Organization, WO2001046199 A1
2001-06-28

- **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。

查找相似反应

Get Similar Reactions

Set Reaction Similarity

☒ Broad (107,942)
Reaction centers only

☐ Medium (21,764)
Reaction centers plus adjacent atoms and bonds

☐ Narrow (4,822)
Reaction centers plus extended atoms and bonds

Get Reactions Cancel



反应详情

查看反应详情

反应详情页为您提供从文献及其 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) δ 7.48-7.30 (m, 5H), 5.11 (s, 2H), 4.67 (s, 1H), 4.13 (q, J = 7.1 Hz, 2H), 3.55 (s, 1H), 2.42 (t, J = 11.8 Hz, 1H), 2.28 (d, J = 12.6 Hz, 1H), 2.10-1.79 (m, 3H), 1.50-1.19 (m, 6H), 1.19-1.00 (m, 1H).

Optical Rotatory Power

=-33.3° (c = 1 in DCM).

HRMS

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

State

sticky solid

CAS Method Number 3-451-CAS-15598720

Transformations

1. Schmidt Reaction

反应转化类型

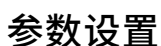
Reaction Notes

scalable

其他重要注释

开启逆合成设计

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。



- 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 “Continue to Retrosynthesis Plan”



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

下载、分享和保存您的方案

Key

Experimental Steps

Predicted Steps

编辑方案选项

Edit Structure

View Excluded Options

Save

查看方案步骤

显示报道的实验步骤

打开/关闭预测步骤

蓝色实线表示报道的实验步骤

绿色虚线表示预测的步骤

点击图标，查看备选反应路线、反应依据或排除该步反应

View all alternatives (67)

View evidence

Exclude this step

?

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反应依据：(1)步骤概览中的链接，或(2)备选反应路线的反应式。

Step

Evidence

A ⇒ B + C

Average Yield: 66%

Evidence

Alternative steps (70)

1.1 Reagents: Hydrochloric acid

Solvents: Dichloromethane, 1,4-Dioxane; 14 h, rt

View All

B ⇒ D + E

Maximum Yield: 92%

Evidence

Alternative steps (25)

1.1 Reagents: Sodium bicarbonate, Sodium carbonate

Solvents: Dichloromethane, Ethyl acetate, Water; 1 h, pH 8, 0 °C

C ⇒ F + G

Average Yield: 63%

Evidence

Alternative steps (67)

1.1 Reagents: Acetic acid, Iron

Solvents: Ethanol; 2 h, reflux; cooled

View All

D ⇒ H

Maximum Yield: 100%

Evidence

Alternative steps (8)

1.1 Reagents: Hydrogen

Catalysts: Palladium

Solvents: Ethanol; 2 h, rt

Experimental Protocols

F ⇒ I

Maximum Yield: 96%

1.1 Reagents: Tetramethylammonium hydroxide

2 of 11

Predicted Step

展开相似反应分组

Select

View 2 similar Alternatives

View evidence

Average yield: 72%

518 Results

反应依据

Group: By Scheme

Sort: Relevance

View: Collapsed

Scheme 1 (2 Reactions)

Steps: 1 Yield: 92%

Suppliers (76)

Suppliers (44)

Suppliers (3)

31-614-CAS-31432345

Steps: 1 Yield: 92%

1.1 Reagents: Sodium bicarbonate

Solvents: Tetrahydrofuran; 0 °C; 0.5 h, 25 °C

Nitrogen heterocyclic compounds and methods of use

Assignee: Black Diamond Therapeutics, Inc.

World Intellectual Property Organization, WO2021127397 A1

2021-06-24

PatentPak

Full Text

CAS Markush 检索

CAS SciFinder

Substances Enter a query...

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

96 Results

结构匹配度

命中的Markush结构

专利授权机构筛选

进行Markush检索

跳转至专利文献详情页面

Markush在专利中的位置

展开专利家族列表，下载PDF原文，或跳转至 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 | Database: CAS

Patent claim 1

PatentPak Full Text

There are no notes to display for this structure.

Heterocycle derivatives and methods of use

Assignee: The University of Texas System
World Intellectual Property Organization: WO2001094369 A2 2001-12-13 | Language: English

在 CAS PatentPak 中有三种查看专利PDF的方式:

- 下载 PDF, 包括标引的物质和注释列表**

下载 PDF

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

专利中被标引的核心物质

12. The lithium secondary battery according to claim 9, wherein the electrolyte comprises at least one organic solvent, a lithium salt, and a lithium trifluoromethanesulfonate (LiTFSI) salt.

13. The lithium secondary battery according to claim 12, wherein the lithium salt is a lithium hexafluoroantimonate (LiSbF₆) salt.

14. The lithium secondary battery according to claim 1, wherein the electrolyte comprises a supporting salt at a concentration of 0.1 to 2.0M.

15. The lithium secondary battery according to claim 1, wherein as a result of SEM-EDX measurement of the

16. The lithium secondary battery according to claim 15, wherein the charging and the discharging is performed at a charge rate between 0.1 and 2.0 C.

17. The lithium secondary battery according to claim 16, wherein the charging and the 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 15, wherein the charging and the discharging is performed at a charge current density between 0.1 and 5.0 mA/cm² and a discharge current density between 0.1 and 5.0 mA/cm².

19. The lithium secondary battery according to claim 18, wherein the charging and the discharging is performed at a charge current density between 0.2 and 4.0 mA/cm² and a discharge current density between 0.2 and 4.0 mA/cm².

20. The lithium secondary battery according to claim 15, wherein the charging and the discharging is performed for 1 to 300 times.

21. The lithium secondary battery according to claim 20, wherein the charging and the discharging is performed for 1 to 99 times.

22. The lithium secondary battery according to claim 15, wherein the battery is in a charged or discharged condition after the battery is charged and discharged.

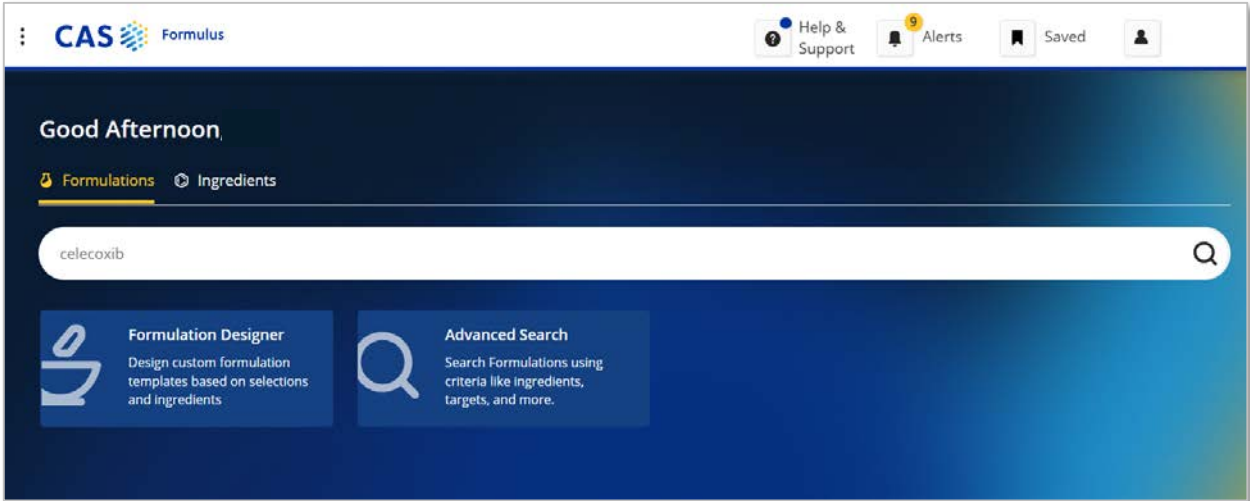
23. The lithium secondary battery according to claim 20, wherein the battery is in a condition of being charged or discharged after the battery is charged and discharged.

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.

CAS Formulus

检索制剂或配方



下载结果为PDF或Excel文件

获得结果集对应的文献



选择筛选项，精准获得配方或制剂结果

Group: By Family ▾

 Compare

对比选中的制剂或配方

制剂或配方成分, 功能及用量

Physical Form: Tablets

在CAS SciFinder
中查看文献详情

[查看制剂或配方详情](#)[查看相似的制剂或配方](#)

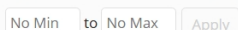
2

 Compare

Physical Form: Tablets

View in CAS SciFinder

点击蓝色原料名称，查看详情



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

Predicted value

Formulation Ingredients

制剂或配方原料

Expand All Groups | Collapse All Groups

Feedback

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

More Formulations like this...

相似的制剂或配方

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

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

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

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

Process

制备工艺

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

Experimental Activity

制剂或配方实验评估

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

Source Patent

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

CAS SciFinder Discovery Platform 快速入门指南 | 19

检索配方成分

CAS

Formulus

Help & Support

Alerts

Saved

Good Afternoon

选择Ingredients

Formulations

Ingredients

propylene glycol

可输入原料名称、CAS登记号或功能信息进行检索

Ingredients search for "propylene glycol"

通过邮件发送结果

保存结果并设置提醒

选择筛选选项，精准获得原料结果

1 Selected 3 Results

1

CAS RN: 57-55-6

View Details

HO

CH2

OH

C3H8O2

(±)-Propylene glycol

View Details

Key Physical Properties

Value

Condition

Molecular Weight

76.09

-

Melting Point (Experimental)

-59 °C

-

Boiling Point (Experimental)

188.2 °C

-

Density (Experimental)

1.036 g/cm³

-

Commonly Used As: Solvents; Humectants; Pl

-

-

Similar Ingredients with Regulatory Information

View 14 More

Propylene glycol monolaurate

Propylene glycol butyl ether

Propylene glycol monopropyl ether

Commonly Formulated With | Regulatory Information | Experimental Properties

Experimental Properties

Property

Value

Condition

Source

Median Lethal Dose

1150 mg/kg

Organism: mouse Route: subcutaneous

11 CAS

Median Lethal Dose

1300 mg/kg

Organism: rat Route: intravenous

11 CAS

Median Lethal Dose

6000 mg/kg

Organism: mouse Route: injection

11 CAS

Sources

(1) Gossard, V. M.; Kraschinsky H;Hormelstein, T;Rett, S.;Hilg, C;Giles

(2) Anon.; Gibert; Q2162302; 1763; D;Jalen

查看原料供应商信息

查看使用该原料的制剂或配方

查看实验属性

查看管控信息及清单

将原料添加至 Formulation Designer

查看制剂或配方中，与该原料同时使用的其它配伍成分

Commonly Formulated With

Ingredient

CAS RN/CAS CN

As Active Ingredients

As Inactive Ingredients

As Any Role

Water

7732-18-5

View Formulations

View Formulations

View Formulations

Glycerol

56-81-5

View Formulations

View Formulations

View Formulations

Ethanol

64-17-5

View Formulations

View Formulations

View Formulations

Carb. acid

7732-18-5

View Formulations

View Formulations

View Formulations

Sodium hydroxide

1310-73-2

View Formulations

View Formulations

View Formulations

Oct. acid

113-80-1

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

Dodecyl glycol monomethyl ether

111-90-0

View Formulations

View Formulations

View Formulations

(3-Amino-2-hydroxypropyl)dimethylammoniumacetate

30574-66-0

View Formulations

View Formulations

View Formulations

Karbitan

11138-96-2

View Formulations

View Formulations

View Formulations

Alcohol, C12-14 ethylhexadecyl

68131-39-0

View Formulations

View Formulations

View Formulations

Isopropylal

67-63-0

View Formulations

View Formulations

View Formulations

Polyethylene glycol monomethyl ether

9004-96-2

View Formulations

View Formulations

View Formulations

Hydrogen peroxide

7721-84-1

View Formulations

View Formulations

View Formulations

Polyethylene glycol

25502-68-5

View Formulations

View Formulations

View Formulations

Triacet

13463-47-7

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

Ethylalcohol

141-43-5

View Formulations

View Formulations

View Formulations

1/23 2/23 3/23 4/23 5/23 Next >

ANMAT

Cosmetics Ingredients Inventory

Drug Master File List

EMA Excipients List

Original Name (translation)

Applicant Name

Event Date

Category

Packaging

Strength

Form

PROYLENGLYCOL *

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 VHM

Source

Marketing Authorizations for Medicines is produced by Argentine 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)



设计制剂或配方

Formulation Designer

Industry

Pharmaceutical

Cosmetics & Personal Care

Agrochemical

Cleaning & Surfactant Products

Inks, Paints, & Coatings

Food & Related

Purpose

Drug delivery systems

Pharmaceutical formulations

Antitumor agents

Anti-inflammatory agents

Analgesics

Antibacterial agents

Ophthalmic agents

Antidiabetic agents

Antiviral agents

Antihypertensives

- View More Purposes -

Physical Form

Tablets

Capsules

Solutions

Gels

Liquids

Pharmaceutical ointments

Cream preparations

Suspensions

Sprays

Powders

- View More Physical Forms -

Add up to 5 Ingredients

Celecoxib

Polyethylene glycol

+ Add Another Ingredient

删除原料

添加原料

Create Template

执行检索

选择应用领域

选择用途

选择物理形态

最多添加5种原料

浏览更多选项

Formulation Designer

Industry

Pharmaceutical

Purpose

Analgesics

Physical Form

Tablets

Active or Featured Ingredient

Celecoxib

Polyethylene glycol

结果导出为Excel文件

Edit Selections

重新编辑

结果保存

Save

Unit Size

mg

Go

Clear

Your Template

Function	Ingredient	Regulatory Lists	Top Alternatives	Amounts
Active or Featured Ingredient:	Celecoxib	Drug Master File List; EMA EPARS; FDA Orange Book; Japanese Approved Drugs List; NMMPA	-	Amount not available
Active or Featured Ingredient:	Polyethylene glycol	ANMAT; Cosing: Cosmetic Ingredient Inventory; Drug Master File List; EPA Pesticide Inactive Ingredients; EPA Safer Chemical Ingredients; FDA GRAS (Part 181, Subpart B); FDA Inactive Ingredients Database	-	Amount not available
Lubricants	Talc ($Mg_3H_2(SiO_3)_4$)	Cosing: Cosmetic Ingredient Inventory; Drug Master File List; EPA Pesticide Inactive Ingredients; FDA Color Additives;	Sodium dodecyl sulfate; Glycerol tribehenate; Sodium stearyl fumarate; Magnesium stearate;	Approximate Range: 3 - 4%
Binders	Butyl methacrylate-dimethylaminoethyl methacrylate-methyl methacrylate copolymer	Cosing: Cosmetic Ingredient Inventory; Drug Master File List; EPA Pesticide Inactive Ingredients; EPA Safer Chemical Ingredients; FDA Inactive Ingredients Database	Sodium dodecyl sulfate; Glycerol tribehenate; Sodium stearyl fumarate; Magnesium stearate;	Approximate Range: 3 - 4%
Disintegrants	Croscarmellose sodium	Cosing: Cosmetic Ingredient Inventory; Drug Master File List; EPA Pesticide Inactive Ingredients; FDA Inactive Ingredients Database	Silica; Starch; Sodium carboxymethyl cellulose; Poly(vinylpyrrolidone); Hydroxypropyl cellulose	Approximate Range: 4 - 5%
Diluents	Magnesium oxide	Cosing: Cosmetic Ingredient Inventory; Drug Master File List; EPA Pesticide Inactive Ingredients; EPA Safer Chemical Ingredients;	Talc ($Mg_3H_2(SiO_3)_4$); Butyl methacrylate-dimethylaminoethyl methacrylate-methyl methacrylate copolymer	Approximate Range: 8 - 16%

查看原料详情

查看原料管制信息

查看可替代的原料选项

添加用途后，点击获得新的制剂或配方设计结果

+ Add Function

点击可添加用途

Function

Anti-inflammatory agents

Add Function

Cancel

CAS Analytical Methods

分析方法检索

查看保存的结果

检索历史

账号管理

CAS Analytical Methods

Support

Saved

History

Good Morning

Search for keywords, matrices or analyte. 输入关键词或者分析物等进行检索

Explore Methods

Search methods using criteria like method categories and subcategories.

浏览方法分类，查看相关方法

Advanced Search

Search methods using criteria like keywords, analytes, matrices and more.

高级检索

Recent Search History

celastrol

点击历史检索重新运行检索，点击X删除检索历史

10 April 2025

View all Search History

高级检索

AND
OR
NOT

逻辑运算符：and, or, not

增加检索条件

Advanced Search

Analyte palmitic acid

AND Matrix blood plasma

Add Search Criteria

清除

删除检索条件

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

Keyword

Analyte

Matrix

Method Category

Technique

CAS Method Number

Publication Name



分析方法的分类检索

Explore Methods

浏览并选择方法分类及子分类

Category

Agricultural Applications /
Bioassays
Biomolecule Isolation
Environmental Analysis
Food Analysis
Fuels / Geology / Biofuels
Historical Analysis / Dating
Miscellaneous
Organic Compound Analysis
Organometallics / Inorganics
Pharmacology / Toxicology
Polymer Analysis
Water Analysis

Category Name

Bioassay
Bioassay Synthetic Probes
Biomarker Biological Process
Biomarker Cell Assay
Biomarker Medicine Assay
Biomedicine Material Analysis
Biomolecule Isolation Assay
Bioorganism Isolation Assay
Genetic Analysis
Nanomaterial Analysis

Include Keywords (Optional)

Palmitic acid

+ Add Another Keyword

可输入关键词

增加关键词

Clear all selections

清除所有条件

检索分析方法

Search Methods

分析方法结果集

Results for Biomolecule Isolation Assay +1 Keyword

结果保存

结果导出

按照分析物、基质、方法分类、技术手段、公开年份等条件筛选结果

1 Selected 3 Results

选中方法，导出或保存

Sort: Relevance

Group: By Method

Filter By

Analyte

Matrix

☒ Blood plasma (3)

Method Category

Technique

☒ HPLC (3)

☐ Electrospray ionization mass spectrometry (2)

☐ Electrospray ionization tandem mass spectrometry (1)

☐ Quadrupole tandem mass spectrometry (1)

☐ Saponification (1)

View All

Validation

☐ Concentration (4)

☐ Linearity Range (3)

☒ Retention Time (3)

☐ Limit of Detection (2)

☐ Limit of Quantitation (1)

1

Analysis of Palmitic acid in Blood plasma by Solvent extraction

查看方法信息详情

JOURNAL

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

Analyte

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

Matrix

Blood plasma

Other Materials

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

Method Category

Biomolecule Isolation Assay

Technique

Electrospray ionization mass spectrometry; HPLC; Electrospray ionization mass spectrometry; Solvent extraction

Equipment

HPLC system; Time of flight mass spectrometer

展示摘要

获得全文链接

View Abstract

Full Text

View in CAS SciFinder

在CAS SciFinder中查看文献详情

选择感兴趣的方法进行对比

Compare

2

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

JOURNAL

Compare

分析方法详情及结果对比

Analysis of Myristic acid in Blood plasma by Solvent extraction

结果导出

↓

Save

结果保存

CAS Method Number

1-122-CAS-534418

Method Category

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

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.

来源文献题录信息

Source

JOURNAL

Postpartum cows showed high oocyte triacylglycerols concurrently with high plasma free fatty acids

Furukawa, Eri; Chen, Zhen; Ueshiba, Hiroki; Wu, Yue; Chiba, Hitoshi; Yanagawa, Yojiro; Katagiri, Seiji; Nagano, Masashi; Hui, Shu-Ping

Theriogenology (2021), 176, 174 - 182. Elsevier Inc.

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

View Abstract ▾

Full Text ▾

展示摘要

获得全文链接

Validation

数据有效性

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

Comparing your 3 selected Methods

删除方法

下载方法比较结果为pdf或excel格式

Method 1

Method 2

Method 3

Analysis of Palmitic acid in Blood plasma by Solvent extraction

Analysis of Fatty acids in Blood plasma by HPLC

Analysis of Lauric acid in Blood plasma by Electrochemiluminescence

CAS Method Number

2-114-CAS-225380

1-122-CAS-96286

1-122-CAS-3193044

Method Category

Biomolecule Isolation Assay

Fatty Acid Analysis

Fatty Acid Analysis

Technique

Time-of-flight mass spectrometry; HPLC; Electrospray ionization mass spectrometry; Solvent extraction

Electrochemical analysis; Atmospheric precipitation; HPLC

Electrochemiluminescence; HPLC

Analyte

Palmitoleic acid; Palmitic acid; Elaidic acid; Linoleic acid; Stearic acid; Arachidonic acid; Docosahexaenoic acid

Stearic acid; Linoleic acid; Palmitic acid; Arachidonic acid; Oleic acid; Fatty acids

Palmitic acid; Stearic acid; Myristoleic acid; Palmitoleic acid; Lauric acid; Arachidonic acid; Oleic acid; Linoleic acid; Linolenic acid; Myristic acid; Fatty acids

登录，培训，支持

登录详情

请访问 scifinder-n.cas.org 登录

使用您现有的CAS SciFinder用户名和密码。

培训

即将举行的活动和网络研讨会：

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

过往活动和网络研讨会录像：

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

培训内容：

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

支持

如需获取有关 CAS SciFinder 使用的其他帮助，请联系 CAS 中国代表处。

电话：010-62508026/7

电子邮箱：china@acs-i.org

网址：<https://www.cas.org/contact>

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

联系我们请访问 cas.org。



010.62508026/7 | china@acs-i.org

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



ACS
International

CAS
A division of the
American Chemical Society

