

CAS SciFinder Discovery Platform (Academic)

全面高效获取科技信息



刘子露
ZLiu@acs-i.org
美国化学文摘社(CAS)北京代表处

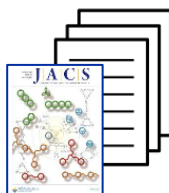
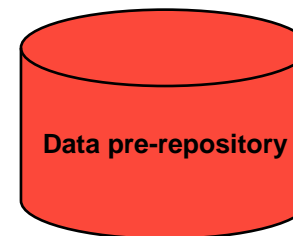
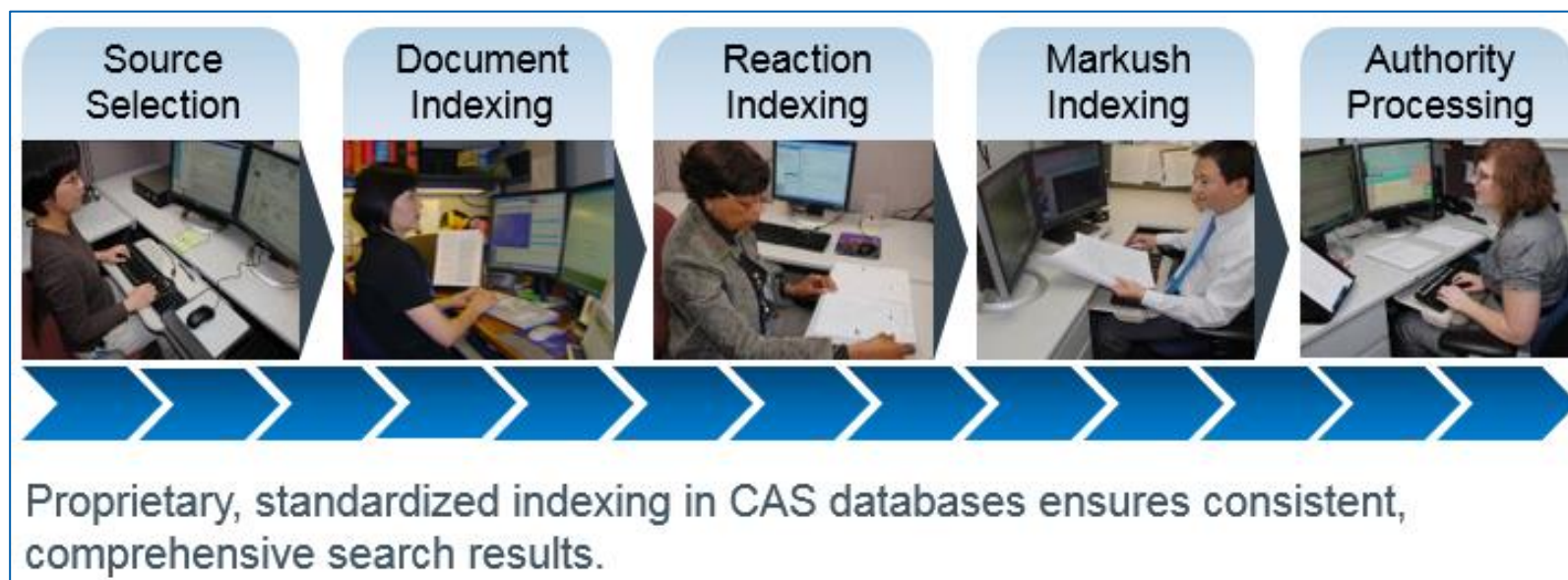


大纲

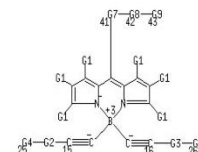
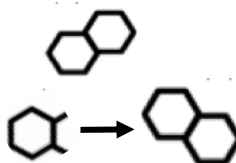
- CAS及CAS SciFinder Discovery Platform (Academic)简介
- 常见检索方式
 - 文献检索
 - 物质检索 (CAS Markush*)
 - 反应检索
 - 逆合成反应路线设计 (CAS Retrosynthesis*)
 - 序列检索*
 - 分析实验方法 (CAS Analytical Methods)
 - 配方/制剂信息检索 (CAS Formula*)
- 常见问题及解答



CAS科学家的智力标引



1990
Smith, M.
anthracene



Androst-4-en-3-one,
17-hydroxy-17-
methyl-, (17β)-

CAS科学家利用人类智慧对公开内容进行揭示，使相关信息更容易被挖掘

CAS 具有最全面的学科连接内容合集



Over
55K
scientific journals
and documents

Over
274
million substances

Over
50
languages
translated

Over
64
patent offices
worldwide

CAS独特的内容合集



来源：

<https://www.cas.org/cas-data>

<https://www.cas.org/about/cas-content>

CAS解决方案与服务



Discovery

CAS SciFinder Discovery Platform™

Get discoveries to market faster and optimize margins by giving researchers the information they need



Intellectual Property

STN IP Protection Suite™

Ensure that your intellectual property is protected and find opportunities to extend into new markets



Custom Solutions

CAS Custom ServicesSM

Customized data, analytics and insights to maximize the value of information assets and fuel digitalization success

CAS SciFinder Discovery Platform (Academic)平台解决方案

CAS SciFinderⁿ——加速科学发现的业界领先的科学工具

业界最领先的相关性搜索引擎，提供和化学相关的各学科的文献、物质、反应和生物序列等检索内容，检索智能、高效、简单。可用于基金申请的文献准备、为新课题制定实验计划、寻求学术合作者、进行逆合成分析以及更多其他的教学和科研活动。


CAS Analytical Methods——借助CAS科学家深度加工的科学方法，提升研究效率

分析方法解决方案涵盖来自期刊中的化学分析方法，提供检索和对比功能，可快速获得能直接在实验室操作的分析方法。可为法医学、食品科学、农学、制药、环境等学科的教学和实验提供帮助。

CAS Formulus——助力开发安全、有效的产品

集成配方（制剂）数据与工作流程的解决方案，提供来自期刊、专利和产品说明中的配方详情。可检索制药、化妆品、食品、农化、油墨、涂料等众多领域中的配方，及其工艺、成分、目标成分的常见配伍成分、设计配方、和探索合规要求等。

CAS SciFinderⁿ 登录网址: <https://SciFinder-n.cas.org>




Log In to SciFinderⁿ

Username or Email Address

Next

[Create an account.](#) | [Can't log in?](#)



Log In to SciFinderⁿ

Welcome, Zilu Liu [Not You?](#)

Password


Log In

☐ Keep me signed in

[Create an account.](#) | [Can't log in?](#)

使用CAS SciFinder账号登录

CAS SciFinder[®]主界面



A division of the American Chemical Society

SCIFINDER DISCOVERY PLATFORM

CAS SciFinder[®]

CAS Analytical Methods

CAS Formulus

STN IP PROTECTION SUITE

STNext

CAS Scientific Patent Explorer

REGULATORY

CAS Chemical Compliance Index

ACCOUNT MANAGEMENT

CAS Profile

CAS SciFinder[®]

Alerts 13

Saved

Zilu Liu

Searching for...

All

Substances

Reactions

References

Suppliers

Sequences

Retrosynthesis

References

Search by Keyword, Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. [Learn More](#)

Antitumor

AND

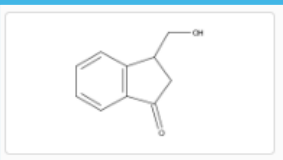
Author Name

Enter last name, first name middle name.

+ Add Advanced Search Field

Launch CAS Lexicon

CAS Lexicon enables you to browse the CAS General Thesaurus to find indexed concepts and substances to build a Reference query with up to 1,000 indexed search terms.



Edit Drawing Remove

Recent Search History

February 8, 2023

References

10:25 AM

CSF-1R inhibitor (371K Results)

Rerun Search

Edit Search

View All Search History

提醒更新的结果
已保存的检索和结果集
账户信息

检索项逻辑关系
文本与结构检索便捷联用

灵活检索选项

查看全部检索历史

重新运行检索式
修改检索式

近期检索历史

大纲

- CAS及CAS SciFinderⁿ简介
- 常见检索方式
 - 文献检索
 - 物质检索 (CAS Markush*)
 - 反应检索
 - 逆合成反应路线设计 (CAS Retrosynthesis*)
 - 生物序列检索*
 - 分析实验方法 (CAS Analytical Methods)
 - 配方/制剂信息检索 (CAS Formulus)
- 常见问题及解答



文献检索

- 文献检索方法
 - 主题词的构建技巧
 - 利用高级检索项自定义组合检索
 - 间接检索：从物质、反应获得文献
- 检索策略推荐
 - 关注某特定领域的文献：主题检索
 - 关注物质有关的文献：先获得物质，再获得文献或文本+结构联合检索
 - 关注某科研人员的文献：作者名检索
 - 关注某机构科研进展：机构名检索

主题词检索

支持使用：主题词、物质名称、CAS登记号、专利号、PubMed ID、文献号、DOI

Searching for...

- All
- Substances
- Reactions
- References**
- Suppliers
- Sequences
- Retrosynthesis

References

Search by Keyword, Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. [Learn More](#)

Seebeck

- Seebeck effect
- Seebeck coefficient
- Seebeck thermoelec. effect
- Seebeck thermoelectric effect
- Thermoelectric Seebeck effect
- Thermoelectric Seebeck coefficient

References

Search by Keyword, Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. [Learn More](#)

seabeck

- Seebeck effect
- Seebeck coefficient
- Seebeck thermoelec. effect
- Seebeck thermoelectric effect
- Thermoelectric Seebeck effect
- Thermoelectric Seebeck coefficient

- 充分利用自动提示检索词
- 充分利用自动纠错功能
- 基于科学家创建的叙词表

使用布尔逻辑运算符，精准构建检索主题

- 布尔逻辑运算符(and, or, not)，默认运算顺序or > and > not
- “ ” 不允许词形变化，但可出现单数或复数；
- () 优先运算，括号中表达式还可以和其他术语交互
- 支持通配符*或?，如 poly*可代表polymer, polymerization, polyethylene等（*代表0或多个字符；? 代表0或1个字符）

The screenshot displays the CAS SciFinder-n search interface. On the left, a sidebar titled 'Searching for...' contains buttons for 'All', 'Substances', 'Reactions', 'References' (which is highlighted in blue), and 'Suppliers'. Below these are buttons for 'Sequences' and 'Retrosynthesis'. The main area is titled 'References' and includes a search bar with the text 'Seebeck effect and "coordination polymer"'. To the right of the search bar are buttons for 'X', 'Draw', and a magnifying glass icon. Below the search bar, there is a dropdown menu set to 'AND', a field for 'Author Name' with the placeholder text 'Enter last name, first name middle name.', and another 'X' button. An example 'Schubert, J A' is shown below the author field. A link 'Learn more about SciFinder[®] Advanced Search.' is also present. At the bottom, there is a blue button labeled 'Launch CAS Lexicon' and a text box explaining that CAS Lexicon enables browsing the CAS General Thesaurus to find indexed concepts and substances to build a Reference query with up to 1,000 indexed search terms.

CAS SciFinder-n Help

使用布尔逻辑运算符，精准构建检索主题

poly* not polyethylene
检索：聚合物，排除聚乙烯

References search for "poly* not polyethylene"

Substances Reactions Citing Knowledge Graph Save and Alert

Filter Behavior

Filter by Exclude

Document Type

- ☐ Journal (12.5M)
- ☐ Patent (5.9M)
- ☐ Review (1M)
- ☐ Biography (1,536)
- ☐ Book (22K)
- [View All](#)

Substance Role

- ☐ Uses (5.5M)
- ☐ Biological Study (2.4M)
- ☐ Properties (2.1M)
- ☐ Process (1.6M)
- ☐ Preparation (1.4M)
- [View All](#)

Language

- ☐ English (11.6M)
- ☐ Chinese (2.8M)
- ☐ Japanese (1.7M)
- [View All](#)

19,203,161 Results Sort: Relevance View: Full Abstract

1

Electrophoretic transfer of proteins from polyacrylamide gels to nitrocellulose sheets: Procedure and some applications
By: Towbin, Harry; Staehelin, Theophil; Gordon, Julian
Proceedings of the National Academy of Sciences of the United States of America (1979), 76(9), 4350-4 | Language: English, Database: CAbplus and MEDLINE

A method was devised for the electrophoretic transfer of proteins from polyacrylamide gels to nitrocellulose sheets. The method results in quant. transfer of ribosomal proteins from gels containing urea. For Na dodecyl sulfate gels, the original band pattern was obtained with no loss of resolution, but the transfer was not quant. The method allows detection of proteins by autoradiog. and is simpler than conventional procedures. The immobilized proteins were detectable by immunol. procedures. All addnl. binding capacity on the nitrocellulose was blocked with excess protein; then, a specific antibody was bound and, finally, a 2nd antibody directed against the 1st antibody. The 2nd antibody was wither radioactively labeled or conjugated to fluorescein or to peroxidase. The specific protein was then detected by either autoradiog., under UV light, or by the peroxidase reaction product, resp. In the latter case, as little as 100 pg of protein was clearly detectable.

Full Text Substances (2) Reactions (0) Citing (28K) Citation Map

2

Polymer photovoltaic cells: enhanced efficiencies via a network of internal donor-acceptor heterojunctions
By: Yu, G.; Gao, J.; Hummelen, J. C.; Wudl, F.; Heeger, A. J.
Science (Washington, D. C.) (1995), 270(5243), 1789-91 | Language: English, Database: CAbplus

The carrier collection efficiency (η_c) and energy conversion efficiency (η_e) of polymer photovoltaic cells were improved by blending of the semiconducting polymer with C₆₀ or its functionalized derivatives Composite films of poly(2-methoxy-5-(2'-ethyl-hexyloxy)-1,4-phenylene vinylene) (MEH-PPV) and fullerenes exhibit η_c of about 29 percent of electrons per photon and η_e of about 2.9 percent, efficiencies that are better by more than two orders of magnitude than those that have been achieved with devices

(poly* not polyethylene) and "conductive device"
检索：聚乙烯以外的聚合物，作导电器件

References search for "(poly* not polyethylene) and \"conductive device\""

Substances Reactions Citing Knowledge Graph Save and Alert

Based on your query, we've returned the most relevant results. Would you like to load the entire result set?
[Learn about result relevance.](#)
[Load More Results](#)

187 Results Sort: Relevance View: Partial Abstract

1

Liquid Metal Droplets Wrapped with Polysaccharide Microgel as Biocompatible Aqueous Ink for Flexible Conductive Devices
By: Li, Xiankai; Li, Mingjie; Zong, Lu; Wu, Xiaochen; You, Jun; Du, Peikang; Li, Chaoyu
Advanced Functional Materials (2018), 28(39), n/a | Language: English, Database: CAbplus

Nanometerization of liquid metal in organic systems can facilitate deposition of liquid metals onto substrates and then recover its conductivity through sintering. Although having broader potential applications, producing stable aqueous inks of liquid metals keeps challenging because of rapid oxidation of liquid metal when exposing to water and oxygen. Here, a biocompatible aqueous ink is produced by encapsulating alloy nanodroplets of gallium and indium (EGaln) into microgels of marine polysaccharides. During sonicating bulk EGaln in aqueous alginate solution, alginate not only facilitates th...

View More

Full Text Substances (4) Reactions (0) Citing (36) Citation Map

2

Conductive polymers and devices
By: Vannikov, A. V.
Vysokomolekulyarnye Soedineniya, Seriya A i Seriya B (2009), 51(4), 547-571 | Language: Russian, Database: CAbplus

A review. Classes of polymeric conductors, mechanisms of conductivity, optical properties, and photophys. properties of thin polymeric films and devices based on them were considered.

Full Text Substances (0) Reactions (0) Citing (9) Citation Map

3

Method of manufacturing a nanoscale conductive device
By: Kabir, Mohammad Shafiqul; Campbell, Eleanor E. B.; Delsing, Per
World Intellectual Property Organization, WO2004096699 A1 2004-11-11 | Language: English, Database: CAbplus

A method of manufacturing a nanoscale conductive device, comprising the steps of providing a substrate, having a top surface provided with at least one surface irregularity, providing an elongated nanoconductor across the at least one surface irregularity,

高级检索—高效实现多项自定义组合检索

References

Search by Keyword, Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. [Learn More](#)

(PVDF or PEDOT) and "wearable device"



Draw



AND

AND

OR

NOT

Publication Name

ACS Applied



Authors

Publication Name

Organization

Title

Abstract/Keywords

Concept

Substances

Publication Year

Document Identifier

Patent Identifier

Publisher

ACS Applied Materials & Interfaces

ACS Applied Energy Materials

ACS Applied Nano Materials

ACS Applied Bio Materials

ACS Applied Polymer Materials

ACS Applied Electronic Materials

ACS Applied Engineering Materials

ACS Applied Optical Materials

文本检索：

关键词、物质名称、CAS RN、DOI等

高级检索：

作者名、期刊名、机构名、题目、摘要、
概念词、物质标识符、出版商

结构检索

* 检索方法可单独使用，也可联用

CAS Lexicon—利用词库选词启发检索

Searching for...

- All
- Substances
- Reactions
- References**
- Suppliers
- Sequences
- Retrosynthesis

References

Search by Keyword, Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. [Learn More](#)

Enter a query...

Author Name Enter last name, first name middle name. Example: Schubert, J A

+ Add Advanced Search Field [Learn more about SciFinder[®] Advanced Search.](#)

Launch CAS Lexicon CAS Lexicon enables you to browse the CAS General Thesaurus to find indexed concepts and substances to build a Reference query with up to 1,000 indexed search terms.

- 在CAS词库层级中浏览CAS标引的概念词（Concepts）和物质
- 建立用于检索文献的检索式（最多可用1000个词）

在CAS Lexicon词库层级中选择适合的主题词：

- Preferred Term
- Narrower Terms
- Broader Terms
- Related Terms

Search CAS Lexicon

Seebeck effect **Search Concept**

Your Query
You may include up to 1,000 terms in a search. [Clear All](#)

Preferred Term

☒ **Seebeck effect**
This will search synonyms: Seebeck coefficient; Seebeck thermoelec. effect; Seebeck thermoelectric effect; Thermoelectric Seebeck coefficient; Thermoelectric Seebeck effect
[View fewer synonyms](#)

Broader Terms (1) [Deselect All](#)

☒ Thermoelectricity

Related Terms (3) [Deselect All](#)

☒ Joule effect
☒ Peltier effect
☒ Thermocouples

Select a boolean operator **OR** [Add Term\(s\)](#) [Learn more about CAS Lexicon searching.](#)

Seebeck effect ×
Seebeck effect - Related Terms (3 Concepts) ×
Thermoelectricity ×

文献结果集—排序与筛选

- 聚类筛选项一目了然
- 直接勾选高效定位所需信息
- 无需逐步二次检索和限定

文献类型
文献语言
研究发展趋势
作者
发表机构
发表年份
CAS标引的技术术语
CAS标引的学科研究方向

二次检索
下载数据分析报告

References search for "(PVDF or PEDOT) and "wearable device""

Substances Reactions Citing Knowledge Graph

Sort: Relevance View: Partial Abstract

687 Results

1

High-Performance Flexible All-Solid-State Supercapacitor from Latent PEDOT/PSS Films

By: Liu, Yuqing; Weng, Bo; Razal, Joselito M.; Xu, Qun; Zhao, Chen; Hou, Yuyang; Seyedin, G.; Chen, Jun

Scientific Reports (2015), 5, 17045 | Language: English, Database: CAPLUS and MEDLINE

Although great attention has been paid to **wearable electronic devices** in recent years, flexible lightweight batteries or supercapacitors with high performance are still not readily available due to the limitations of the flexible electrode inventory. In this work, highly flexible, bendable and conductive rGO-PEDOT/PSS films were prepared using a simple bar-coating method. The assembled device using rGO-PEDOT/PSS electrode could be bent and rolled up without any decrease in electrochem. performance. A relatively high areal capacitance of 448 mF cm⁻² was achieved at a scan rate of 10 mV s⁻¹ using...

View More

Full Text

Substances (13) Reactions (0) Citing (173) Citation Map

2

Highly stretchable multilayer electronic circuits using biphasic gallium-indium

By: Liu, Shanliangzi; Shah, Dylan S.; Kramer-Bottiglio, Rebecca

Nature Materials (2021), 20(6), 851-858 | Language: English, Database: CAPLUS and MEDLINE

Stretchable electronic circuits are critical for soft robots, **wearable technologies** and biomedical applications. Development of sophisticated stretchable circuits requires new materials with stable conductivity over large strains, and low-resistance interfaces between soft and conventional (rigid) electronic components. To address this need, we introduce biphasic Ga-In, a printable conductor with high conductivity (2.06 x 10⁶ S m⁻¹), extreme stretchability (>1,000%), negligible resistance change when strained, cyclic stability (consistent performance over 1,500 cycles) and a reliable interf...

View More

Full Text

Substances (17) Reactions (0) Citing (91) Citation Map

3

A self-powered skin-patch electrochromic biosensor

By: Santiago-Malagon, Sara; Rio-Colin, Diego; Azizkhani, Haniyeh; Aller-Pellitero, Miguel; Guirado, Gonzalo; del Campo, F. Javier

Biosensors & Bioelectronics (2021), 175, 112879 | Language: English, Database: CAPLUS and MEDLINE

| Analytical Methods

One of the limitations of many skin-patch wearable sensors today is their dependence on silicon-based electronics, increasing their complexity and unit cost. Self-powered sensors, in combination with electrochromic materials, allow simplifying the construction of...

排序方式：
相关性
引用次数
收录号
发表时间

CAS标引的学科研究方向

CA Section

By CountAlphanumeric

通过CA Section 纵览并定位学科研究方向

6 Selected

☐ Electrochemical, Radiational, and Thermal Energy Technology (210)

☒ Electric Phenomena (169)

☒ Biochemical Methods (83)

☐ Textiles and Fibers (55)

☐ Plastics Fabrication and Uses (52)

☒ Pharmaceuticals (22)

☐ Plastics Manufacture and Processing (20)

☐ Optical, Electron, and Mass Spectroscopy and Other Related Properties (18)

☐ Unavailable (8)

☒ Electrochemistry (7)

☐ Inorganic Analytical Chemistry (5)

☐ Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes (5)

☒ Surface Chemistry and Colloids (5)

☐ Synthetic Elastomers and Natural Rubber (4)

☐ Air Pollution and Industrial Hygiene (3)

☐ Chemistry of Synthetic High Polymers (3)

☒ Magnetic Phenomena (3)

☐ Coatings, Inks, and Related Products (2)

☐ Physical Organic Chemistry (2)

☐ Thermodynamics, Thermochemistry, and Thermal Properties (2)

☐ Unit Operations and Processes (2)

☐ Apparatus and Plant Equipment (1)

☐ Cement, Concrete, and Related Building Materials (1)

☐ Food and Feed Chemistry (1)

☐ Nonferrous Metals and Alloys (1)

☐ Pharmacology (1)

☐ Toxicology (1)

☐ Water (1)

Apply

Cancel

文献结果集—聚类筛选Concept

Concept

通过Concept纵览并精准定位核心研究点

×

Top Count

Alphanumeric

Search

7 Selected

☐ Wearable devices (501)

☐ Fluoropolymers (343)

☐ Electric conductivity (155)

☐ Electrodes (128)

☒ Surface structure (124)

☐ Homo sapiens (117)

☐ Human (117)

☐ Nanofibers (101)

☐ Electric current-potential relationship (100)

☐ Polyesters (92)

☐ Carbon nanotubes (86)

☒ Flexibility (84)

☐ Stress-strain relationship (83)

☐ Electrospinning (82)

☒ Current density (50)

☒ Hydrogels (50)

☐ Humans (48)

☐ Polymers (48)

☐ Carbon black (47)

☐ Electronics (47)

☒ Nanowires (47)

☐ Electric capacitance (45)

☐ Piezoelectric materials (44)

☐ Electric potential (41)

☐ Electronic device fabrication (40)

☐ Triboelectric nanogenerators (40)

☐ Electric impedance (39)

☒ Coating materials (30)

☐ Electrolytes (29)

☐ Sheet resistance (29)

☐ Surface area (29)

☒ Skin (28)

☐ Supercapacitor electrodes (28)

☐ Cyclic voltammetry (27)

☐ Dielectric loss (26)

☐ Energy storage systems (26)

☐ Lithium-ion secondary batteries (26)

☐ Plastic films (26)

☐ Strain (26)

☐ Surface roughness (26)

☐ Bending (25)

Apply

Cancel

Concept

通过Search精准定位感兴趣的核心研究点

×

Top Count

Alphanumeric

Search

Concept Name

nano*

Search

17 Selected

☒ Carbon nanofibers (14)

☐ Carbon nanotube fibers (4)

☒ Carbon nanotubes (86)

☐ Cellulosic nanofibers (1)

☒ Core-shell nanoparticles (1)

☐ Electric nanogenerators (24)

☒ Metal Nanoparticles (3)

☐ Nanoantennas (1)

☐ Nanocoils (2)

☒ Nanocomposites (63)

☐ Nanocrystals (4)

☐ Nanofibril (2)

☒ Nanofilms (6)

☐ Nanofilters (1)

☒ Nanoflakes (2)

☐ Nanoflowers (2)

☐ Nanohorns (1)

☐ Nanoimprint lithography (1)

☐ Nanoparticles (53)

☐ Nanoparticle size distribution (2)

☐ Nanoplatelets (3)

☒ Nanosheets (23)

☒ Nanospheres (1)

☐ Nanostructured materials (9)

☐ Nanostructures (18)

☐ Nanotechnology (4)

☐ Nanotubes (12)

☐ Nanotubes, Carbon (11)

☒ Nanowires (47)

☐ Pharmaceutical nanocarriers (1)

☐ Pharmaceutical nanocomposites (2)

Apply

Cancel

文献结果集—保存及下载

References search for "(PVDF or PEDOT) and "wearable device""

Substances Reactions Citing Knowledge Graph

Filtering: Concept: Hydrogels X
Excluding: Search Within Results: dop* X

Based on your query, we've returned the most relevant results. Would you like to load the entire result set?
[Learn about result relevance.](#)

Load More Results

41 Results Sort: Relevance View: Partial Abstract

1

Enhancing Strain-Sensing Properties of the Conductive Hydrogel by Introducing PVDF-TrFE
By: Hu, Zhirui; Li, Jie; Wei, Xiaotong; Wang, Chen; Cao, Yang; Gao, Zhiqiang; Han, Jing; Li, Yingchun
ACS Applied Materials & Interfaces (2022), 14(40), 45853-45868 | Language: English, Database: CAPLUS and MEDLINE

Conductive hydrogels have attracted attention because of their wide application in wearable devices. However, it is still a challenge to achieve conductive hydrogels with high sensitivity and wide frequency band response for smart wearable strain sensors. Here, we report a composite hydrogel with piezoresistive and piezoelec. sensing for flexible strain sensors. The composite hydrogel consists of cross-linked chitosan quaternary ammonium salt (CHACC) as the hydrogel matrix, poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT: PSS) as the conductive filler, and poly(vinylidene fluori...

View More

Full Text Substances (7) Reaction (1) Citing (1) Citation Map

2

Antifreeze and moisturizing high conductivity PEDOT/PVA hydrogels for wearable motion sensor
By: Peng, Yinjie; Yan, Bin; Li, Yueshan; Lan, Ji; Shi, Lingying; Ran, Rong
Journal of Materials Science (2020), 55(3), 1280-1291 | Language: English, Database: CAPLUS

Conductive hydrogel has shown significant promise in the field of wearable devices. However, the mediocre antifreezing property and relatively low strain sensitivity limit the application of these gels. Herein, we developed a multifunctional hydrogel sensor based on a polyvinyl alc. substrate with poly(3,4-ethylenedioxythiophene) as the conductive filler and a glycerin/water component solvent as the dispersion medium. The resulting optimal sample exhibits attractive combination of high tensile stress (~ 1.0 MPa), large elongation (> 400%), reasonable conductivity (~ 3.5 S m⁻¹), while the g...

View More

Full Text Substances (5) Reaction (1) Citing (40) Citation Map

3

High-Stretchability, Ultralow-Hysteresis ConductingPolymer Hydrogel Strain Sensors for Soft Machines
By: Shen, Zegun; Zhang, Zhilin; Zhang, Ningbin; Li, Jinhao; Zhou, Peiwei; Hu, Fang; Peng, Yur; Lu, Baoyang; Gu, Guoqing

Save Results and Create Alert

Name
EGFR

Save Options
☐ Query Only
☐ Selected Answers
☒ All Answers (Up to 20,000)

Alert Frequency
☒ No Alerts
☐ As Available
☐ Weekly
☐ Monthly

Add Existing Tags (Optional)
No tags defined

New Tag (Optional)
Pharm

Tag Color
Light Green

Save Cancel

支持结果集的:

- 合并、交集和去重
- 下载保存
- 邮件分享
- 设置提醒

可存为格式:

- ris
- PDF
- Rtf
- Excel
- TXT

Search Within Results

Search for up to 3 text strings within the result set.

Enter a query...

Search

Searching for... Clear All

dop* X

文献详情

文献详情界面包括：标题、摘要、重要的技术术语、引文地图、文献中重要的物质、反应、参考文献、原文链接

Enhancing Strain-Sensing Properties of the Conductive Hydrogel by Introducing PVDF-TrFE

Substances (7)

Reaction (1)

Citing (1)

Citation Map

Journal

Source

ACS Applied Materials & Interfaces
Volume: 14
Issue: 40
Pages: 45853-45868
Journal: Article
2022
DOI:
[10.1021/acsami.2c13074](https://doi.org/10.1021/acsami.2c13074)

CODEN: AAMICK
E-ISSN: 1944-8252
ISSN-L: 1944-8244

Database Information

AN: 2022:2510278
CAN: 180:208379
PubMed ID: 36170495
CAPUS and MEDLINE

Company/Organization

School of Materials Science and Engineering
North University of China
Taiyuan 030051
China

Publisher

American Chemical Society

Language

English

By: Hu, Zhirui; Li, Jie; Wei, Xiaotong; Wang, Chen; Cao, Yang; Gao, Zhiqiang; Han, Jing; Li, Yingchun

Conductive hydrogels have attracted attention because of their wide application in wearable devices. However, it is still a challenge to achieve conductive hydrogels with high sensitivity and wide frequency band response for smart wearable strain sensors. Here, we report a composite hydrogel with piezoresistive and piezoelec. sensing for flexible strain sensors. The composite hydrogel consists of cross-linked chitosan quaternary ammonium salt (CHACC) as the hydrogel matrix, poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT: PSS) as the conductive filler, and poly(vinylidene fluoride-co-trifluoroethylene) (PVDF-TrFE) as the piezoelec. filler. A one-pot thermoforming and solution exchange method was used to synthesize the CHACC/PEDOT: PSS/PVDF-TrFE hydrogel. The hydrogel-based strain sensor exhibits high sensitivity (GF: 19.3), fast response (response time: 63.2 ms), and wide frequency range (response frequency: 5-25 Hz), while maintaining excellent mech. properties (elongation at break up to 293%). It can be concluded that enhanced strain-sensing properties of the hydrogel are contributed to both greater change in the relative resistance under stress and wider response to dynamic and static stimulus by adding PVDF-TrFE. This has a broad application in monitoring human motion, detecting subtle movements, and identifying object contours and a hydrogel-based array sensor. This work provides an insight into the design of composite hydrogels based on piezoelec. and piezoresistive sensing with applications for wearable sensors.

Static load time

Dynamic fast response

High sensitivity and wide frequency band response

Piezoresistive hydrogel

Piezoelectric hydrogel

Composite hydrogel

Chemical crosslinking process

Dipolar interaction

Swelling process

Compression process

CHACC

PEDOT:PSS

PVDF-TrFE

Cross-linked bond

Keywords: conductive hydrogel wearable strain piezoelec sensor; composite hydrogels; fast response; high sensitivity; piezoresistive and piezoelectric sensation; wearable sensors

View Source

Full Text

Concepts

Substances

Cited Documents

Expand All | Collapse All

CAS科学家提供的标准技术术语

Electric resistance	Polythiophenes
Elongation at break	Role: Properties; Technical or Engineered Material Use
Hydrogels	Strain sensors
Open circuit potential	Stress-strain relationship
Piezoelectric sensors	Tensile strength
	Wearable devices

原文中重点研究的物质信息

Substances (7)

2839834-68-1

106602-18-0

Image Not Available

ClCC1OC1

(C₃H₅ClO.Unspecified)_x

Role: Properties, Synthetic Preparation, Preparation

1219717-04-0

Image Not Available

Unspecified

Clevios PH 750

Role: Properties, Technical or Engineered Material Use, Uses

126213-51-2

C1=CC=C2C(=C1)OCOC2

(C₆H₆O₂S)_x

Poly(3,4-ethylenedioxythiophene)

Role: Properties, Technical or Engineered Material Use, Uses

Notes: polystyrenesulfonate-doped

106602-18-0

Image Not Available

Unspecified

N-[2-Hydroxy-3-(trimethyl ammonium)propyl]chitosan chloride

Role: Reactant, Reactant or Reagent

50851-57-5

[O-]C(=O)c1ccc(cc1)S(=O)(=O)[O-]

(C₈H₈O₃S)_x

Poly(styrenesulfonic acid)

Role: Properties, Technical or Engineered Material Use, Uses

Notes: PEDOT dopant

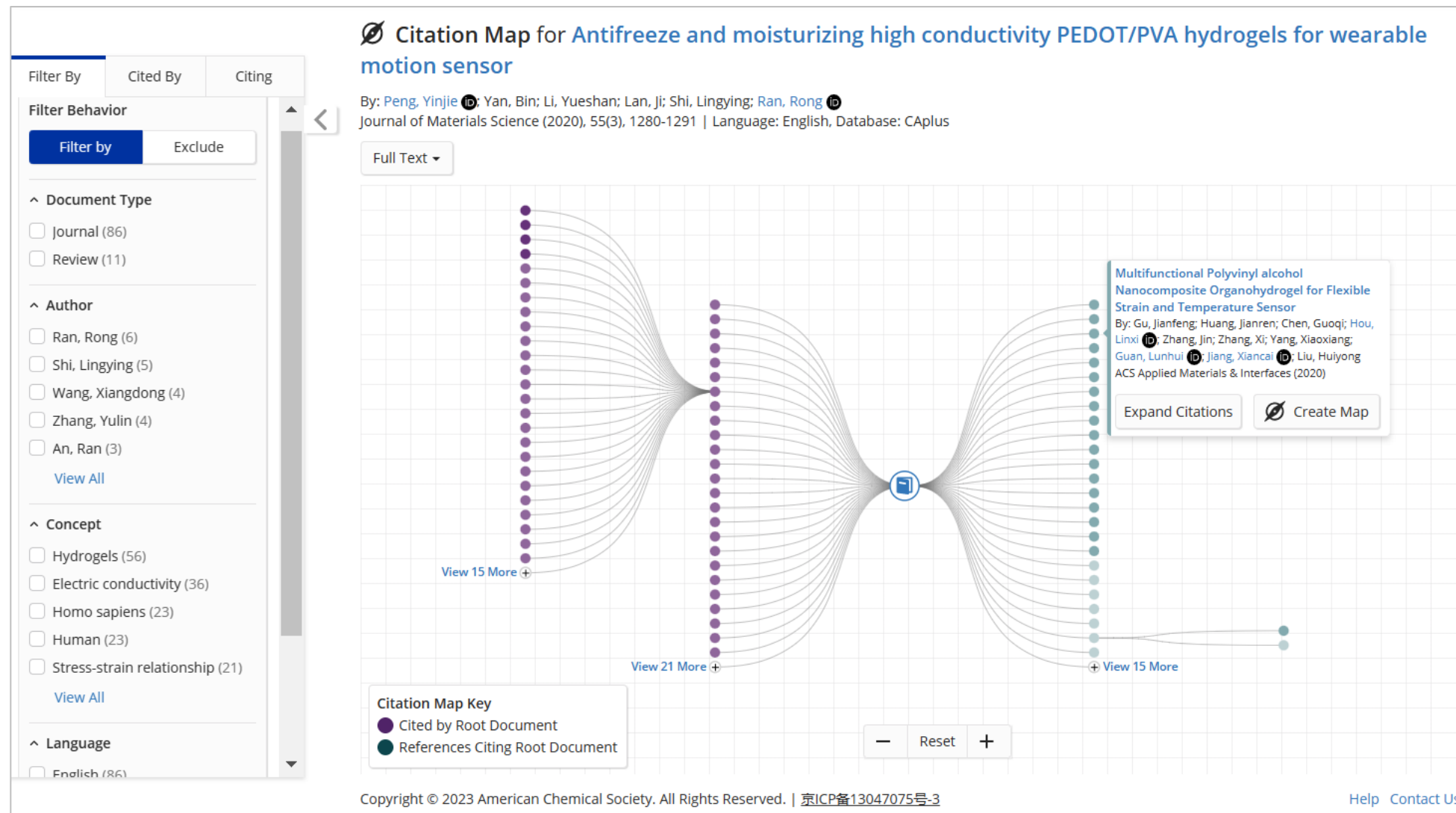
28960-88-5

F/C=C/F

F/C(F)=C/F

物质角色

文献详情—引文地图



引文地图：

- 获取前向引文
- 获取后向引文
- 可通过聚类选项筛选引文

文献检索—主题词+结构联合检索

CAS SciFinder®

References search for "enzyme and reduction" + drawn structure

Substances (8,921)

Structure Match

As Drawn (0)

Substructure (8,921)

Filter Behavior

Filter by Exclude

Document Type

Substance Role

- Biological Study (6,107)
- Uses (1,361)
- Properties (1,035)
- Reactant or Reagent (503)
- Preparation (500)

View All

Language

- English (8,314)
- Chinese (318)
- Undetermined (82)
- Russian (55)
- German (52)

View All

Publication Year

1908 2023

8,921 Results

Sort: Relevance View: Partial Abstract

1

Asymmetric Reduction of Cyclic Imines Catalyzed by a Whole-Cell Biocatalyst Containing an (S)-Imine Reductase

By: Leipold, Friedemann; Hussain, Shahed; Ghislieri, Diego; Turner, Nicholas J. ChemCatChem (2013), 5(12), 3505-3508 | Language: English, Database: CAplus

The authors report the cloning, overexpression and kinetic characterization of the (S)-imine reductase ((S)-IRED) from Streptomyces sp. GF3546. (S)-IRED catalyzes the asym. reduction of imines. The (S)-IRED was also overexpressed in Escherichia coli to yield a whole-cell biocatalyst that is able to utilize glucose for cofactor recycling. (S)-IRED was shown to catalyze the highly enantioselective reduction of 5,6, and seven-membered imines, including dihydro- β -carboline.

Full Text

Substances (60) Reactions (88) Citing (106) Citation Map

2

A novel (R)-imine reductase from Paenibacillus lactis for asymmetric reduction of 3H-indoles

By: Li, Hao; Zhang, Guang-Xiang; Li, Liu-Mei; Ou, Yu-Shi; Wang, Ming-Yang; Li, Chun-Xiu; Zheng, Gao-Wei; Xu, Jian-He ChemCatChem (2016), 8(4), 724-727 | Language: English, Database: CAplus

A novel (R)-imine reductase (I) from P. lactis was heterologously overexpressed in Escherichia coli, purified, and characterized. Purified I exhibited relatively high catalytic efficiency ($k_{cat}/K_m = 1.58 \text{ s}^{-1} \text{ mM}^{-1}$) toward 2,3,3-trimethylindolenine. A panel of 3H-indoles and 3H-indole iodides were reduced by I to yield the corresponding products with good-to-excellent enantioselectivity (66-98% ee). In addition, I also possessed good activity toward other types of imines such as pyrrolidine, tetrahydropyridine, and dihydroisoquinoline, indicating a reasonably broad substrate acceptance. In a 100- μm ...

Full Text

Substances (37) Reactions (18) Citing (30) Citation Map

3

Palladium-mediated stereocontrolled reductive amination of azido sugars prepared from enzymic aldol condensation: a general approach to the synthesis of deoxy aza sugars

By: Kajimoto, Tetsuya; Chen, Lihren; Liu, Kevin K. C.; Wong, Chi Huey Journal of the American Chemical Society (1991), 113(17), 6678-80 | Language: English, Database: CAplus

This paper describes a general strategy for the synthesis of a number of deoxyazasugars based on a combined enzymic aldol condensation and Pd-catalyzed reductive amination. Fructose-1,6-diphosphate aldolase, rhamnulose-1-phosphate aldolase,

Substance Role

By Count Alphanumeric

物质在文献中的研究角色

<input type="checkbox"/> Biological Study (6,035)	<input type="checkbox"/> Food or Feed Use (117)	<input type="checkbox"/> Occurrence, Unclassified (16)
<input type="checkbox"/> Biological Study, Unclassified (4,381)	<input type="checkbox"/> Catalyst Use (116)	<input type="checkbox"/> Bioindustrial Manufacture (15)
<input type="checkbox"/> Uses (1,336)	<input type="checkbox"/> Formation, Non-preparative (92)	<input type="checkbox"/> Cosmetic Use (15)
<input type="checkbox"/> Properties (1,030)	<input type="checkbox"/> Biosynthetic Preparation (86)	<input type="checkbox"/> Miscellaneous (13)
<input type="checkbox"/> Therapeutic Use (714)	<input type="checkbox"/> Analytical Role, Unclassified (68)	<input type="checkbox"/> Natural Product Occurrence (9)
<input type="checkbox"/> Pharmacological Activity (532)	<input type="checkbox"/> Analyte (58)	<input type="checkbox"/> Reagent (9)
<input type="checkbox"/> Reactant or Reagent (493)	<input type="checkbox"/> Occurrence (53)	<input type="checkbox"/> Industrial Manufacture (7)
<input checked="" type="checkbox"/> Preparation (491)	<input checked="" type="checkbox"/> Biochemical Process (41)	<input type="checkbox"/> Byproduct (5)
<input checked="" type="checkbox"/> Reactant (486)	<input type="checkbox"/> Purification or Recovery (41)	<input type="checkbox"/> Prophetic Synthesis or Use (5)
<input type="checkbox"/> Process (464)	<input type="checkbox"/> Diagnostic Use (40)	<input type="checkbox"/> Geological or Astronomical Occurrence (3)
<input type="checkbox"/> Physical, Engineering, or Chemical Process (381)	<input type="checkbox"/> Pharmacokinetics (38)	<input type="checkbox"/> Combinatorial Study (2)
<input checked="" type="checkbox"/> Synthetic Preparation (353)	<input type="checkbox"/> Pollutant (38)	<input type="checkbox"/> Geological or Astronomical Process (2)
<input type="checkbox"/> Analytical Study (275)	<input type="checkbox"/> Formation, Unclassified (30)	<input type="checkbox"/> Analytical Matrix (1)
<input type="checkbox"/> Biological Use, Unclassified (205)	<input type="checkbox"/> Nanoscale (26)	<input type="checkbox"/> Geological or Astronomical
	<input type="checkbox"/> Agricultural Use (25)	

Apply Cancel

思考题：
如何检索含Cs/Sn的钙钛矿(perovskite)相关文献？

文献检索—主题词+结构联合检索

例：如何检索特定（亚）结构相关的有机光伏相关文献？

References

Search by Keyword, Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. [Learn More](#)

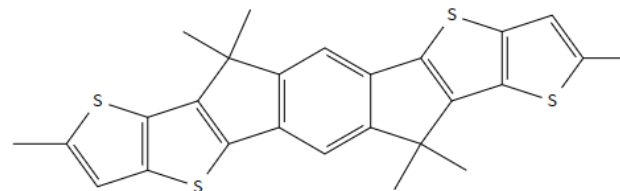
organic photovoltaic

AND Author Name Enter last name, first name middle name.

+ Add Advanced Search Field

[Launch CAS Lexicon](#) CAS Lexicon enables you to browse the CAS General Thesaurus to find indexed concepts and substances to build a Reference query with up to 1,000 indexed search terms.

[Edit Drawing](#) [Remove](#)



例：如何检索含Fe/Ni/Cr/Ti 高熵合金的相关文献？

CAS SciFinder®

References High entropy alloy

References search for "High entropy alloy" + drawn structure

Substances Reactions Citing Knowledge Graph

Structure Match

As Drawn (612)

Substructure (615)

612 Results

1

Phase evolution and magnetic characteristics of TiFeNiCr and TiFeNiCrM (M = M... entropy alloys

By: Mishra, Rajesh K.; Shahi, Rohit R.

[Edit Drawing](#) [Remove](#)

查看Chemzent 来源的文献

- ChemZent是最古老的德国化学文摘的英文版，唯一提供可用英文获取德国化学文摘的解决方案
- 化学研究相关文献可回溯至1830年，可用于追溯化学科学起源时期的研究，丰富化学历史知识

References search for "enzyme and reduction" + drawn structure

Substances Reactions Citing Knowledge Graph Save and Alert

Structure Match: As Drawn (0) Substructure (8,881)

Filter Behavior: Filter by Exclude

Document Type Language Publication Year Available at My Institution Author Publication Name Concept

Database: CAPIUS (8,605) MEDLINE (6,814) **CHEMZENT (31)**

Search Within Results

Filter Content Report: Download filter data from this result set

Filtering: Database: CHEMZENT 31 Results Sort: Relevance View: Partial Abstract

Fabric change of CARB azole in rats and rabbit
By: Johns, S. R.; Wright, S. E.
Chemisches Zentralblatt (1966), 137(5), 01578-01578 | Language: German, Database: CHEMZENT

Machine Translated: After administration of carbazoles is 3-hydroxy carbazole, conjugate with glucuronic acid in the urine separated Hauptstoffwechselprod. in rats and rabbits. The hydroxylation in 3-position is in accordance with the etching oxidizing **enzymes** at the position of greatest electron density. For the investigation of werden carbazole-14 C is used. Experiments: 14C-carbazole (I), Melting Point 242-244° (from benzene) by diazotization and **reduction** of 14C-aniline to 14C-phenylhydrazine (240-245°) with cyclohexanone in 14C-tetrahydrocarbazole is converted. Dehydrogenation to Pd-C gives I. Respect m...

Cobamide and ribo nucleotide reduction. 3. Part The content of the Cobamid-abhängigen Ribonucleosid-triphosphatreduktase in Lactobacillus leichmanii influencing factors
By: Ghambeer, R. K.; Blakley, R. L.
Chemisches Zentralblatt (1968), 139(28), 160-160 | Language: German, Database: CHEMZENT

Machine Translated: Hysic. Res. common. 20 (1965) 20. — the content of ribo nucleoside triphosphate reductase (I) in extracts of L. leichmanii depends on the age of the culture. During the linear growth if I-Geh. with increasing age up to the end of the linear phase on and falls then. Extracts from stationary cells exhibit no significant I-Aktivität. The rapid I-Synth. during the linear growth by chloramphenicol and ActinomycinD inhibited. The decrease of I-Geh. after completion of the linear growth is based not on the presence one increased amount proteolyt. **Enzymes** nor on incomplete release of said **enzyme**. The

Nr. 5-1559 E-6. Pharmakologie, Therapie, Toxikologie, Hygiene 1966

68-74, 1963; Washington, D.C., George Washington Univ., School of Med., Dep. of Pharmacol.; engl.) — Die i.p. Injektion von 1 mg des adeninanalogen Purin-antimetaboliten 4-Aminopyrazolopyrimidin (I) verursachte bei Mäusen einen Anstieg der Gesamtlebertipide innerhalb 24 Std. auf das 3-4fache. Hierin waren an erster Stelle die Neutrallipide, in geringerem Ausmaß auch das Cholesterin (II) beteiligt, während der Phospholipid-(III)-Geh. unverändert blieb. I-Gabe hemmte den in vitro-Einbau von ¹⁴C₁₁-Acetat (IV) in die Lipide von Leberschnitten, hatte aber wenig Einfl. auf die Ox. von IV u. ¹⁴C₁₁-Palmitat (V) in vitro. Die Plasmalipidkonz. sank nach I-Applikation u. war durch einen Abfall der Triglyceride u. des II hervorgerufen. III u. freie Fettsäuren waren nicht beteiligt. V wurde von den Lebern der mit I behandelten Tiere schlechter aufgenommen als von den Lebern der Kontrolltiere. Obgleich der Einbau von ¹⁴C₁₁-Orotsäure in RNS durch I gehemmt wurde, konnte kein verminderter Einbau von ¹⁴C₁₁-Glycin in Leber- u. Plasmaproteine festgestellt werden. Die normalerweise massive Hyperlipidämie nach Gabe von Triton WR-1339 wurde durch I verhindert. VI. schließt aus den Unters., daß I wahrscheinlich die Sekretion von Triglyceriden aus der Leber bremst. H. Zöllner 4607◇

1559 Stoffwechsel des Carbazols in Ratten und Kaninchen. S. R. Johns und S. E. Wright. (J. med. Chem. 7, 158-161, 1964; Sydney, Univ. of Sydney, Dep. of Pharmacy; engl.) — Nach Gabe von Carbazol (I) 3-Hydroxycarbazol, konjugiert mit Glucuronsäure, das im Harn ausgeschiedene Hauptstoffwechselprod. bei Ratten u. Kaninchen. Die Hydroxylierung in 3-Stellung ist in Übereinstimmung mit dem Angriff oxydierender Enzyme an der Stellung mit der größten Elektronendichte. Für die Unters. wurde Carbazol-¹⁴C verwendet.

Versuche: ¹⁴C-Carbazol (I), F. 242-244° (aus Bzl.) durch Diazotierung u. Red. von ¹⁴C-Anilin zu ¹⁴C-Phenylhydrazinhydrochlorid (F. 240-245°), das mit Cyclohexanon in ¹⁴C-Tetrahydrocarbazol übergeführt wird. Dehydrierung an Pd-C ergibt I. Hergestellt Bezugs-substanzen: 1-Hydroxycarbazol, F. 160-162° durch Cyclisierung von Cyclohexan-1,2-dionmonophenylhydrazon (F. 183-185°) in Äthanol. Essigsäure über 1,2,3,4-Tetrahydro-1-oxocarbazol (F. 169°), das an Pd-C dehydriert wird. 3-Hydroxycarbazol (II), F. 260-261° über folgende Stufen: p-Methoxyphenylhydrazinhydrochlorid (III), F. 198-200° (aus A.) durch Diazotierung u. Red. von p-Anisidin. — 6-Methoxy-1,2,3,4-tetrahydrocarbazol (IV), C₁₄H₁₁NO, F. 94-95° (aus A.), durch Rk. von III mit Cyclohexanon in was. Essigsäure (50%ig) bei Ggw. von Natriumacetat. 3-Methoxycarbazol (V) C₁₃H₁₁NO,

N-Butyl-, Äthobromid, DL₅₀ 38,4. Curarisierungswirkg., 30,7, cholinolyt. Aktivität, 0,04; N-Cyclohexyl-, Äthobromid, 33,5/28/0,02; N-Phenyl-, Äthobromid, 17,5/20/0,09; N-Phenyl-, Benzylbromid, 11/13/0,14; N-β-Phen-äthyl-, Äthobromid, 21/22/0,1; N-Octyl-, Äthobromid, 6,8/6,7/1,5; Lauryl-, Äthobromid, 21,5/12,6/16; N-Butyl-, Hydrochlorid, 115/-/0,02; N-Cyclohexyl-, HCl, 75/-/0,02; N-Phenyl-, HCl, 47,5/-/cholinerg.; N-β-Phenäthyl-, HCl, 60/-/0,03; N-Octyl-, HCl, 47/-/0,5; N-Lauryl-, HCl, 37,5/-/1,5; N,N-dialkylcarbaminsäure-β-di-äthylaminoäthylester, Äthobromide: diäthyl-, DL₅₀ 26, Curarisierungswirkg., 26, spasmolyt. Aktivität, 50 (Papaverin = 100), 0,05 (I = 100), Antihistamin-aktivität, — (Promethazin = 100); dibutyl-, 8/11/2100/6/4,3; dicyclohexyl-, 2,2/4,8/2300/2,4/0,05; Diphenyl-, 8,5/11,6/310/0,13/0,03; Di-[β-phenäthyl]-, 6,5/6,5/570/0,38/0,07; Dibutyl-, Benzylbromid, 7,5/5,5/200/0,11/-; Carbazol(II), Äthobromid, 3,3/4,6/730/0,28/0,20; Acridin (III), Äthobromid, 5,8/4,5/770/0,6/0,20; Phenozazin (IV), Äthobromid, 4,0/5,3/1400/1,3/0,5; Phenothiazin (V), Äthobromid, 3,0/4,6/600/8,0/5,0; Hydrochloride: Dibutyl-, 38/-/1000/3,0/3,0; Dicyclohexyl-, 22/-/1130/2,4/0,1; Di-phenyl-, 42,5/-/770/4,5/0,1; Di-[β-phenäthyl]-, 10,3/-/400/0,14/0,2; II, 20/-/280/0,1/0,3; III, 35/-/1800/1/1; IV, 24,5/-/770/0,8/1; V, 25/-/12000/16/30.

K. Maier 4607◇

1561 Wirkung von Chlorcyclizin und anderen Stoffen auf die Toxizität verschiedener Organophosphat-Anticholinesterasen. Richard M. Welch und J. M. Coon. (J. Pharmacol. exp. Therapeut. 148, 192-98, 1964; Philadelphia, Pa., Jefferson Med. Coll., Dep. of Pharmacol.; engl.) — VI. untersuchten verschiedene Substanzen mit bekannter Wirkg. auf die Lebermikrosomen-Enzymsyst. auf deren Wirkg. auf die Toxizität einiger Organophosphatsektizide an Mäusen. Eine Vorbehandlung der Tiere täglich über 4 Tage mit Chlorcyclizin (I), Phenobarbital (II), SKF-525 A (α,α-Diphenyl-α-propyl-essigsäure-β-diäthylaminodithylester - HCl) (III) oder Cyclizin zeigte einen deutlichen Schutz gegen die Toxizität von Malathion, Parathion (IV) u. EPN (p-Nitrophenylthionbenzolphosphoräureäthylester). Eine I-Vorbehandlung erhöhte außerdem wesentlich die orale DL₅₀ von Paraoxon (V), TEPP (Tetraäthylpyrophosphat) u. Physostigmin. Eine a.e.-Dosis von I, II oder III schützte gegen IV. Die Umwandlung von IV in V durch Mäuseleber erfolgte etwa 2mal so schnell, wenn das Tier 4 Tage vorher mit I vorbehandelt wurde. Eine I-Dosis senkte deutlich die Serum-Paraoxonase (VI; A-Esterase), erhöhte aber dagegen gering die Leber-VI. I erhöhte innerhalb von 24 Std. das Verhältnis Lebergew. zu Körpergew. um

专利文献详情

PatentPak:

- 快速理解专利
- 快速定位专利中的物质
- 一键下载原文
- 阅读其他语言撰写的等同专利

References search for "enzyme and reduction" + drawn structure

Substances Reactions Citing Knowledge Graph

Structure Match: As Drawn (0) Substructure (8,921)

Filter Behavior: Filter by Exclude

Document Type: Journal (527) Patent (87) Review (10) Conference (4) Preprint (1)

Substance Role

Language

Publication Year

Available at My Institution

Author

Organization

Publication Name

Concept

CA Section

Filtering: Document Type: Patent X Substance Role: 3 Selected X Clear All Filters

87 Results Sort: Relevance View: Partial Abstract

1

Preparation of azepinoindole compounds as CYP1B1 enzyme inhibitor

By: Wang, Jiang; Xiong, Yuan; Yang, Liangyi; Jia, Aiqun; Ge, Guangbo; Tang, Shi China, CN115073473 A 2022-09-20 | Language: Chinese, Database: CAplus

The invention discloses an azepinoindole compound shown in formula I, wherein R¹=H, Me, OMe, OH, NH₂, SCF₃, F, CF₃, NO₂, tert Bu, Ph, naphthalene, phenanthrene, pyridine, quinoline or pyrene; R²=H, Cl, Me, F; R³=H, Me, F, OMe, Cl, Br. For example, 6-phenyl-5,12-dihydrobenzo[6,7]azepino[3,4-b]indole was prepared by multi-step reaction. The title compound can be used as CYP1B1 enzyme inhibitor.

View More

PatentPak Full Text Substances (170) Reactions (10) Citing (0) Citation Map

2

Nitro-substituted squaraine reporter dyes as reagent for measuring nitroreductase enzyme activity

By: West, Richard Martin; Ismail, Rahman World Intellectual Property Organization, WO2005118839 A1 2005-12-15 | Language: English, Database: CAplus

Disclosed are nitro-substituted squaraine reporter dyes and methods using such dyes for detecting nitroreductase enzyme activity and nitroreductase gene expression in cellular assays. Representative dyes are I (X, Y = O, S, CH₂CH, CH(Me)R²; R¹, R² = C₁₋₄-alkyl, (CH₂)_n, P, ((CH₂)_nO)₂, R³, W; R³, R⁴ = H, NO₂, halogen, SO₃, C₁₋₄-alkoxy, (CH₂)_nCOOR⁵; at least one of groups R¹⁻⁴ comprises at least one NO₂ group; R⁵ = C₁₋₆-alkyl optionally substituted with COOR⁷, SO₃, or OH; R⁶ = Me, Et; R⁷ = H, C₁₋₄-alkyl, CH₂COOR⁸; R⁸ = Me, tBu; P = COOR⁷, SO₃, OH; W = mono- or di-substituted nitrobenzyl; n = 1-11.

View More

PatentPak Full Text Substances (43) Reactions (54) Citing (3) Citation Map

Patent Language Kind Code PatentPak Options

Patent	Language	Kind Code	PatentPak Options
WO2005118839	English	A1	PDF PDF+ Viewer
AU2005250209	English	A1	PDF
CN1993477	Chinese	A	PDF
AU2005250209	English	B2	PDF
JP4838239	Japanese	B2	PDF
EP1749103	English	B1	PDF
US8378120	English	B2	PDF

Key Substances in Patent

Analyst Markup Locations (2)

Page 19

Page 22

CAS RN 1640-39-7

Analyst Markup Locations (2)

Page 20

Page 23

CAS RN 192137-08-9

Analyst Markup Locations (1)

Page 20

CAS RN 252358-63-7

Analyst Markup Locations (2)

Page 21

Page 23

CAS RN 162920-91-4

CAS PatentPak

PAGE 23 / 52 ZOOM DOWNLOAD PDF PDF+

Key Substances in Patent

WO 2005/118839

21

3.2 Preparation of Compound (3)

To 1-(3,5-dinitrobenzyl)-2,3,3-trimethyl-3H-indolium iodide (132mg) was added 3-(5-carboxypentyl)-1,1,2-trimethyl-1H-benzo[e]indolium iodide (114mg), 5 3,4-dihydroxy-3-cyclobuten-1,2-dione (32mg), pyridine (4.5ml), acetic acid (4.5ml) and acetic anhydride (1ml). The mixture was heated to 90°C for 4 hours and the solvent then stripped using rotary evaporation. Silica flash column chromatography was performed (EA/MeOH) and the relevant fractions combined and concentrated. The resulting material was further purified by 10 reverse phase HPLC (CH₃CN / H₂O / TFA) to give 1.7mg. MALDI-TOF (C₄₃H₄₀N₄O₈ requires M⁺ 740) 741.

4. Preparation of 2-(3-ethyl-6-nitro-2-benzothiazolynidenemethyl)-4-(1-(2-(2-methoxyethoxy)ethyl)-3,3-dimethyl-2- 15 indolynidenemethyl)cyclobutenediylum-1,3-diolate (Compound (4))

Compound (4)

4.1 Preparation of 1-(2-(2-methoxyethoxy)ethyl)-2,3,3-trimethyl-3H-indolium bromide

20 To 2,3,3-trimethylindolenine (1.59g) was added 1-bromo-2-(2-methoxyethoxy)ethane (2.75g) and dichlorobenzene (5ml). The mixture was

文献检索小结

1. 检索词的构建：使用布尔逻辑算符及通配符连接主题词，利用CAS Lexicon精准选词
2. 利用高级检索选项进行自定义组合检索
3. 通过聚类筛选工具快速获得目标文献
4. 利用引文地图拓展检索
5. 主题词+结构联合检索快速获得文献
6. 使用PatentPak高效阅读专利

物质检索

- 物质检索方法
 - 物质标识符、文献标识符检索
 - 分子式、物性参数、谱图数据检索
 - 结构式检索
- 检索策略推荐
 - 有机化合物，金属配合物，天然产物：结构检索
 - 无机物，合金：分子式检索
 - 高分子化合物：分子式检索和结构检索

物质检索

- 通过物质标识符、文献标识符检索物质

Searching for...

All

Substances

Reactions

References

Suppliers



Sequences


Retrosynthesis

Substances


Search by Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. [Learn More](#)

Enter a query...

 Draw 

- Molecular Formula 

Examples: C6H6 | (C8H8)_x | C22H26CuN2O5.C2H3N

 Add Advanced Search Field [Learn more about SciFinder[®] Advanced Search.](#)

- 使用结构绘制面板进行结构检索

- 高级检索

物质检索—物质名称、CAS RN、代码

CAS SciFinder[®] Substances Paxlovid 2628280-40-8

Substances search for "Paxlovid 2628280-40-8"

References Reactions Suppliers

Filter Behavior

Filter by Exclude

Reaction Role

Product (1)

Reactant (1)

Reference Role

Adverse Effect (2)

Analyte (2)

Analytical Study (2)

Biological Study (2)

Biological Study, Unclassified (2)

View All

Commercial Availability

Number of Components

Molecular Weight

2 Results

Sort: Relevance View: Partial

1

2628280-40-8

Absolute stereochemistry shown

C23H32F3N5O4
3-Azabicyclo[3.1.0]hexane-2-carboxamide, N-[(1S)-1-cyano-2-[(3S)-2-oxo-3-pyrroli...

319 References 106 Reactions 39 Suppliers

2

2803933-60-8

Absolute stereochemistry shown

C37H48N6O5S2.C23H32F3N5O4
Components: 2
Paxlovid

39 References 0 Reactions 0 Suppliers

- 物质检索框中可同时检索多个物质识别符（物质名称或CAS RN）
- 不同物质使用空格隔开（<2000个字符）

物质检索—文献标识符及结果集排序

CAS SciFinder[®] Substances 10.1126/science.abl4784

Substances search for "10.1126/science.abl4784"

References Reactions Suppliers

Filter Behavior

Filter by Exclude

Reaction Role

- ☐ Product (9)
- ☐ Reactant (7)
- ☐ Reagent (4)
- ☐ Catalyst (2)
- ☐ Solvent (2)

Reference Role

- ☐ Biological Study (10)
- ☐ Biological Study, Unclassified (10)
- ☐ Pharmacokinetics (10)
- ☐ Pharmacological Activity (10)
- ☐ Preparation (10)
- [View All](#)

Bioactivity Data

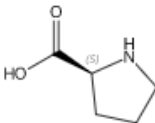
Commercial Availability

- ☐ Available (6)
- ☐ Not Available (4)

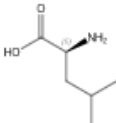
10 Results

Sort: Molecular Formula: Ascending View: Partial

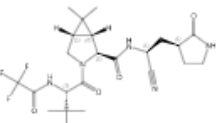
1 147-85-3


Absolute stereochemistry shown, Rotation (-)
C₅H₉NO₂
L-Proline
117K References 48K Reactions 164 Suppliers

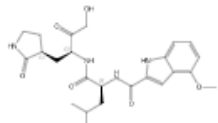
2 61-90-5


Absolute stereochemistry shown, Rotation (+)
C₆H₁₃NO₂
L-Leucine
125K References 6,092 Reactions 154 Suppliers

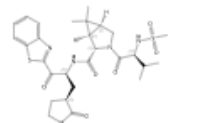
4 2628280-40-8


Absolute stereochemistry shown
C₂₃H₃₂F₃N₅O₄
3-Azabicyclo[3.1.0]hexane-2-carboxamide, N-[(1S)-1-cyano-2-[(3S)-2-oxo-3-pyrroli...

5 870153-29-0


Absolute stereochemistry shown
C₂₄H₃₂N₄O₆
1H-Indole-2-carboxamide, N-[(1S)-1-[[[(1S)-3-hydroxy-2-oxo-1-[[[(3S)-2-oxo-3-pyrroli...

6 2757763-45-2


Absolute stereochemistry shown
C₂₈H₃₇N₅O₆S₂
3-Azabicyclo[3.1.0]hexane-2-carboxamide, N-[(1S)-2-(2-benzothiazolyl)-2-oxo-1-[[...

Relevance
CAS RN: Ascending
CAS RN: Descending
Molecular Formula: Ascending
Molecular Formula: Descending
Molecular Weight: Ascending
Molecular Weight: Descending
Number of References: Ascending
Number of References: Descending
Number of Suppliers

使用文献标识符，迅速获得关注文献中的物质信息

不同物质排序：

- 相关度
- CAS RN
- 分子式
- 分子量
- 文献量
- 供应商数量

物质检索—分子式

- 含碳化合物，C排第一位，H排第二位，其他元素符号按照首字母顺序进行排列
- 不含碳化合物，按照元素符号的首字母顺序进行排列
- 不同组分之间用“.”隔开，如：铁钴镍合金 Co.Fe.Ni
- 无机含氧盐：阳离子和阴离子用点（.）分开；阴离子以氢补齐至电中性 Na₂SO₄: H₂O₄S.2Na

Searching for...

Substances

Search by Substance Name, CAS RN, Patent Number

Enter a query...

- Molecular Formula CH₂O₃

Reactions

References

Searching for...

Substances

Search by Substance Name, CAS RN, Patent Number

Enter a query...

- Molecular Formula Co.Fe.Ni

Reactions

References

适用于分子式检索的物质类型包括：

- 无机化合物：合金，无机表格化合物，多氧簇金属化合物等
- 聚合物

物质检索—Advanced Search

Searching for...

Substances

Search by Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. [Learn More](#)

Enter a query...

Draw

Examples: C6H6 | (C8H8)x | C22H26CuN2O5.C2H3N

[Learn more about SciFinder[®] Advanced Search.](#)

Molecular Formula

- Molecular Formula
- CAS Registry Number >
- Chemical Identifier >
- Document Identifier
- Patent Identifier
- Experimental Spectra >
- Biological >
- Chemical Properties >
- Density >
- Electrical >
- Lipinski >
- Magnetic >
- Mechanical >
- Optical and Scattering >
- Structure Related >
- Thermal >

Recent Search History

February 13, 2023

Substances 157119-63-6 (1 Result)

2:05 PM

Rerun Search

Edit Search

高级检索字段：

- CAS RN（物质、组份）、物质标识符、分子式、文献号、专利号
- 实验谱图： ^1H , ^{13}C , ^{15}N , ^{19}F , ^{31}P NMR
- 化学标识符：化学名称、InChI key
- 生物：生物富集因子、LD50
- 化学：Koc, LogD, LogP、溶解度、分子量、pKa、蒸汽压
- 密度属性：密度、摩尔体积
- 电学：电导/电导率、电阻/电阻率
- Lipinski：自由旋转键、H受体/供体
- 磁：磁力矩
- 机械属性：拉伸强度
- 光散射：旋光性、折射率
- 结构：极性表面积
- 热学：熔点、沸点、闪电、玻璃转化温度、蒸发焓

物质检索—联用检索(1)

查找满足以下属性要求的合金：

1. 密度 $<7\text{g/cm}^3$
2. 拉伸强度 $>1000\text{MPa}$
3. 熔点 >600

Filter Behavior

Filter by Exclude

Reaction Role

Reference Role

Commercial Availability

Number of Components

Element

Substance Class

☒ Alloy (12)

☐ Element (2)

☐ Manual Registration (2)

☐ Organic/Inorganic Small Molecule (1)

Isotopes

Metals

Experimental Property

☐ Density (12)

☐ Melting Point (12)

☐ Tensile Strength (12)

☐ Glass Transition Temperature (11)

Filtering: Substance Class: Alloy X

12 Results

1

56802-58-5

Image Not Available

Unspecified

Aluminum alloy, base, (Duralumin)

2

252664-07-6

Component	Percent
Zr	68
Cu	13
Ni	9.7
Nb	6.1
Al	3.5

Al.Cu.Nb.Ni.Zr

Components: 5

Zirconium alloy, base, Zr,Al,Cu,Nb,Ni (VIT 106)

2,476 References 1 Reaction 0 Suppliers

62 References 0 Reactions 0 Suppliers

4

857638-02-9

Component	Percent
Zr	59

5

253178-50-6

Component	Percent
Zr	66

物质类别中锁定合金Alloy

Substances

Search by Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. [Learn More](#)

Enter a query...

Draw

Density (g/cm³) <7

☒ Include predicted values. Examples: 1.15 | <7.53 | >150 | 9.3 to 15 | 8.9e-2

☐ Search key property values only.

AND Tensile Strength (Mpa) 1000 to 2500

☒ Search key property values only. Examples: 1.15 | <7.53 | >150 | 9.3 to 15 | 8.9e-2

AND Melting Point (°C) >600

☐ Search key property values only. Examples: 1.15 | <7.53 | >150 | 9.3 to 15 | 8.9e-2

Zirconium alloy, base, Zr 59,Cu 39,Al 2.5 (9CI, ACI)

Key Physical Properties	Value	Condition
Melting Point (Experimental)	700-935 °C	-
Density (Experimental)	6.35 g/cm ³	Temp: Room temp; Press: 800 Torr

Experimental Properties

Density	Mechanical	Structure Related	Thermal
Property	Value	Condition	Source
Tensile Strength	1820 MPa (Yield) (approx)	-	(1) CAS
Tensile Strength	1600 MPa (Yield) (approx)	-	(1) CAS
Compressive Strength - 1 Source	See Full Text		(2) CAS
Hardness - 1 Source	See Full Text		(3) CAS
Microhardness - 1 Source	See Full Text		(4) CAS

物质检索—联用检索(2)

- 分子量：220至280之间
- pKa：1.3至1.8之间
- C谱特征峰：114至171之间，96，11.5

Searching for...

Substances

Search by Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. [Learn More](#)

Enter a query...

Draw

Molecular Weight 220 to 280
Predicted values only. Examples: 46.07 | 125 to 350 | >300

AND pKa 1.3 to 1.8
Predicted values only. Examples: -1.77 | <9.25 | >2.4 | 5.25 to 8.25

AND Carbon-13 NMR 114 to 171, 96, 11.5
Allowance of ± 2 ppm. Examples: 152.3, 127.6, 133.1 | 155.02 to 207.59 | 187

+ Add Advanced Search Field [Learn more about SciFinder[®] Advanced Search.](#)

Substances search for 3 Advanced Fields

References Reactions Suppliers

Filtering: Bioactivity Data: 3 Selected X

Clear All Filters

15 Results Sort: Molecular Formula: Ascending View: Partial

1 296262-16-3

2 723-46-6

3 1631737-39-7

4 442571-27-9

5 1927010-88-5

6 697787-29-4

Filter Behavior

Filter by Exclude

Reaction Role

- Product (15)
- Reactant (11)
- Reagent (1)
- Catalyst (1)

Reference Role

- Preparation (15)
- Synthetic Preparation (15)
- Biological Study (14)
- Pharmacological Activity (14)
- Uses (14)

Bioactivity Data

- ☒ Structure Activity Relationships (15)
- ☒ Toxicity (2)
- ☒ Absorption, Distribution, Metabolism, Excretion (1)

Commercial Availability

Number of Components

Molecular Weight

Stereochemistry

物质详情

CAS Registry Number: 723-46-6

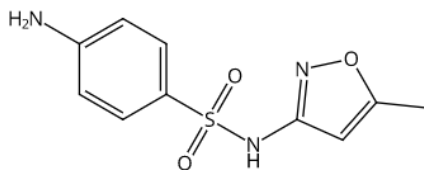
References (24K)

Reactions (961)

Suppliers (120)



Save



$C_{10}H_{11}N_3O_3S$

Benzenesulfonamide, 4-amino-N-(5-methyl-3-isoxazolyl)- (9CI, ACI)

Key Physical Properties	Value	Condition
Molecular Weight	253.28	-
Melting Point (Experimental)	167 °C	-
Boiling Point (Predicted)	482.1±55.0 °C	Press: 760 Torr
Density (Experimental)	1.4895 g/cm ³	-
pKa (Predicted)	5.81±0.50	Most Acidic Temp: 25 °C

Experimental Properties | Spectra

Expand All | Collapse All

Other Names and Identifiers

Experimental Properties

Experimental Spectra

Structure Activity Relationships



Absorption, Distribution, Metabolism, and Excretion Data



Toxicity



Predicted Properties

Predicted Spectra

Bioactivity Indicators

Target Indicators

折叠菜单显示物质各类信息

Experimental Spectra

¹ H NMR	¹³ C NMR	Hetero NMR	IR	Mass	Raman	UV and Visible
Source						
View Proton NMR Spectrum	(1) LC					
View Proton NMR Spectrum	(2) ENAMINE					
View Proton NMR Spectrum	(2) ENAMINE					
View Proton NMR Spectrum	(3) CAS					
View Proton NMR Spectrum	(4) CAS					
View Proton NMR Spectrum	(5) CAS					
View Proton NMR Spectrum	(6) BIORAD					
View Proton NMR Spectrum	(6) BIORAD					
View Proton NMR Spectrum	(7) AIST					
Proton NMR Spectrum - 4 Sources						(8-11) CAS

Sources

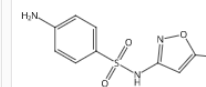
(1) Spectral data were obtained from Life Chemicals

(2) Spectral data were obtained from Enamine Ltd.

(3) Ham, Won Seok; Angewandte Chemie, International Edition, (2019), 58(2), 532-536, CAplus

Proton NMR Spectrum for 723-46-6

723-46-6



$C_{10}H_{11}N_3O_3S$

CAS Name
Sulfamethoxazole

Conditions

Working Frequency

400 MHz

Solvent

[Dimethyl sulfoxide \(67-68-5\)](#)

[Carbon tetrachloride \(56-23-5\)](#)

Temperature

20 °C

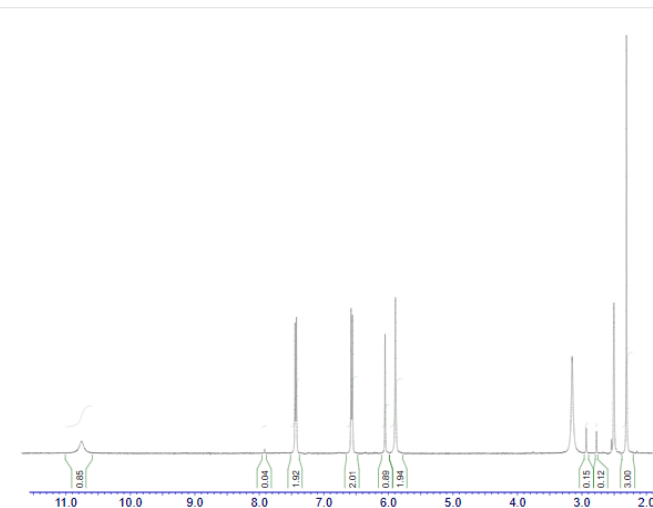
Spectrum Summary

Spectrum ID

F0175-0013

Source

Spectral data were obtained from Life Chemicals



物质详情

Structure Activity Relationships CAS LIFE SCIENCES

Target Function Parameter Disease Organism

Filter Disease

- ☐ Bacterial infection (273)
- ☐ Microbial infection (206)
- ☐ Oxidative stress (76)
- ☐ Toxoplasmosis (46)
- ☐ Bacterial infections

Apply Clear All

Target	Function	Parameter	Disease	Organism	Assay	Source
1132187-M	Inhibitor	Drug ren	-	-	View Detail	(1) CAS
207419-N	Inhibitor	Drug ren	-	-	View Detail	(1) CAS
226605-F	Inhibitor	Drug ren	-	-	View Detail	(1) CAS
A. baumannii	Inhibitor	MIC	Microbial infections	-	View Detail	(2) CAS
Acanthamoeba	Inhibitor	IC50	Acanthamoeba keratitis	-	View Detail	(3) CAS
Acanthamoeba	Inhibitor	IC50	Acanthamoeba keratitis	-	View Detail	(3) CAS

Absorption, Distribution, Metabolism, and Excretion Data CAS LIFE SCIENCES

Target Function Parameter Disease Organism

Filter Parameter

- ☐ Drug concentration (7)
- ☐ Cell uptake (2)
- ☐ Serum concentration (2)
- ☐ fAUC(0-24 h) (2)
- ☐ fCmax (2)
- ☐ t1/2 (2)

Apply Clear All

Target	Function	Parameter	Value	Disease	Organism	Assay	Source
Methicillin-resistant Staphylococcus aureus	-	Drug concentration	217.5 mg x h/L	Bacterial infections	-	View Detail	(1) CAS
Methicillin-resistant Staphylococcus aureus	-	Cell uptake	13 mg/L	Bacterial infections	-	View Detail	(1) CAS
Methicillin-resistant Staphylococcus aureus	-	Serum concentration	10 h	Bacterial infections	-	View Detail	(1) CAS
Methicillin-sensitive Staphylococcus aureus	-	fAUC(0-24 h)	217.5 mg x h/L	Bacterial infections	-	View Detail	(1) CAS

Assay Data CAS LIFE SCIENCES

Target 207419-N

Assay Name -

Assay Type Functional

Procedure Laccase degradation assay

Function Inhibitor

Parameter Drug removal

Value 0.00 %

Ligand Dose -

Disease -

Biological System in vitro

Source Evaluation of bezafibrate, gemfibrozil, indomethacin, sulfamethoxazole, and diclofenac removal by ligninolytic enzymes
By: Camarillo Ravelo, Dante; Loera Corral, Octavio; Gonzalez-Martinez, Ignacio; Chan Cupul, Wilberth; Rodriguez Nava, Celestino Odin
Preparative Biochemistry & Biotechnology (2020), 50(6), 592-597 | Language: English, Database: CAsplus and MEDLINE

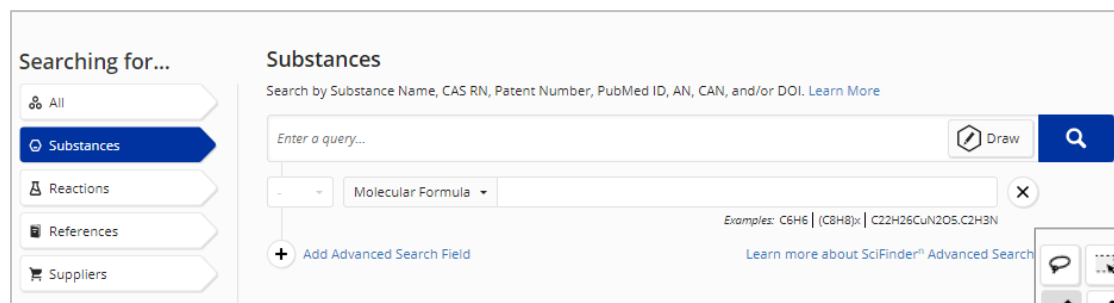
Toxicity CAS LIFE SCIENCES

Parameter

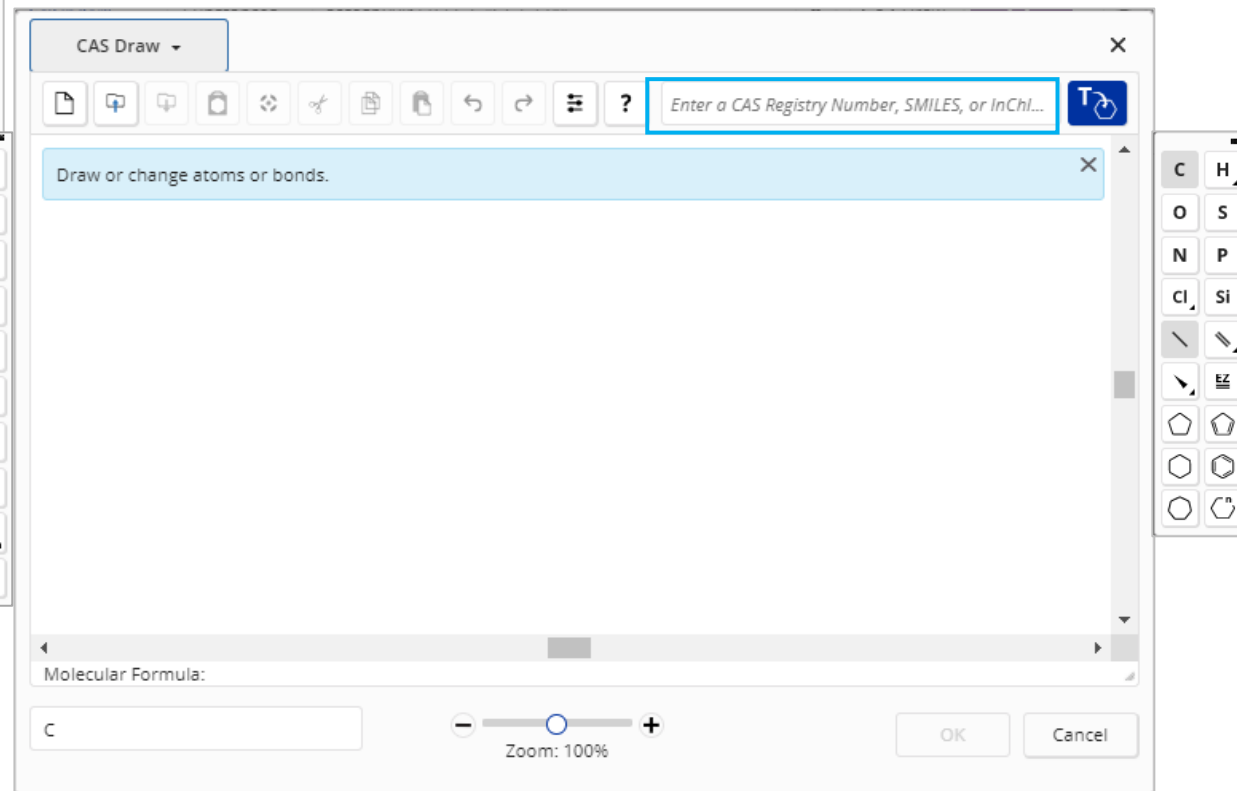
Target	Function	Parameter	Value	Disease	Organism	Assay	Source
-	-	EC50	>12.500 µM	-	-	View Detail	(1) CAS
-	-	EC50	>12.500 µM	-	-	View Detail	(1) CAS
-	-	EC50	>12.500 µM	-	-	View Detail	(1) CAS
-	-	EC50	1.917 µM	-	-	View Detail	(1) CAS
-	-	EC50	>12.500 µM	-	-	View Detail	(1) CAS

(1) Plouffe, David M.; Cell Host & Microbe (2016), 19(1), 114-126, CAsplus and MEDLINE

物质检索—结构检索



	选择可变基团		取代位点可变
	自定义R基团		锁工具
	重复片段工具		片段结构



CAS Draw和ChemDoodle的使用指南

https://scifinder-n.cas.org/help/#t=Drawing_Search_Queries%2FDrawing_Structure_Queries.htm <https://www.cas.org/support/training/scifinder-n/structure-search>

<https://www.cas.org/support/training/scifinder-n/chemdoodle-structure-search>

物质检索—结构检索

结构检索时，无需分步进行，一次检索即可得到As Drawn, Substructure和Similarity结果

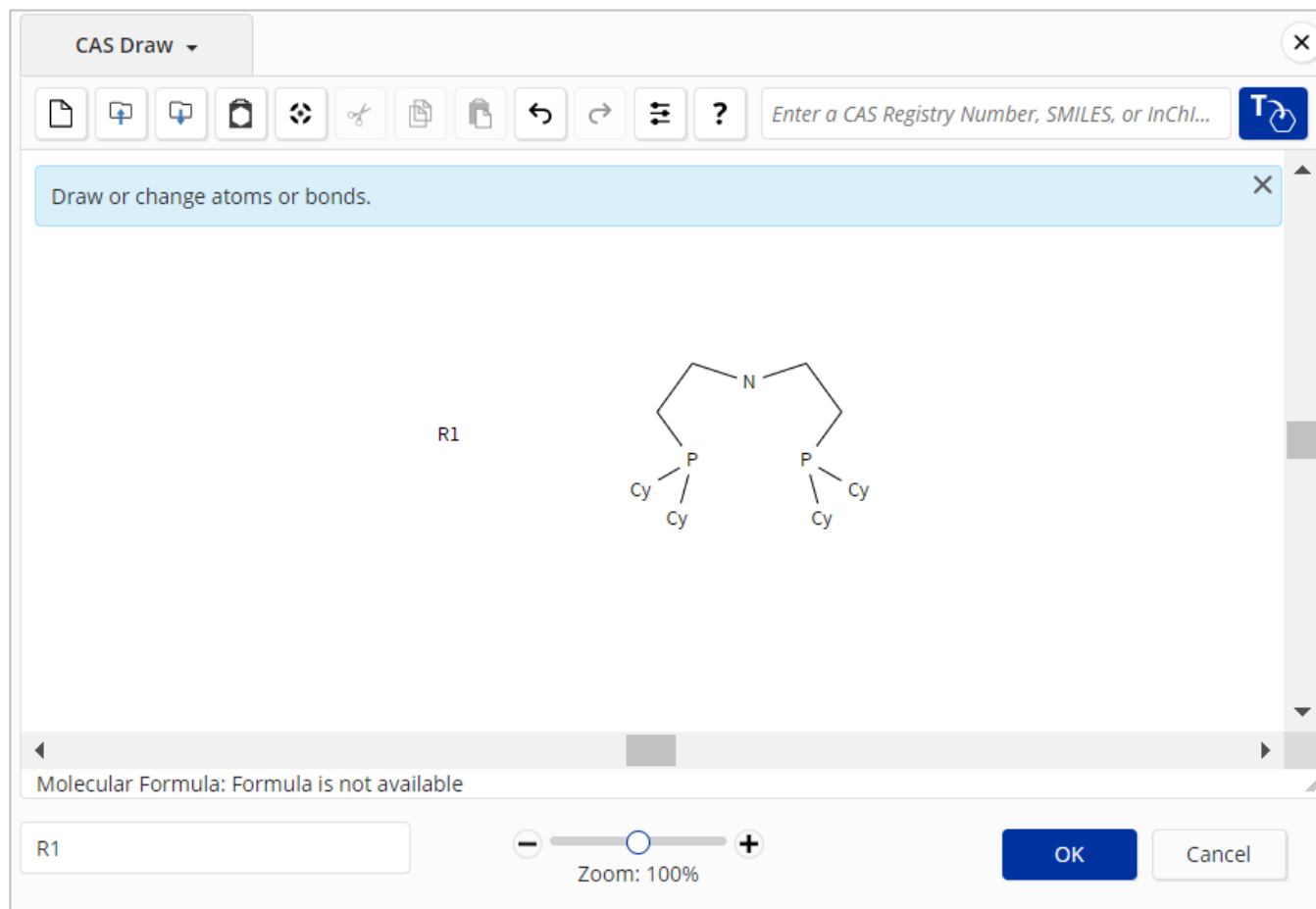
Structure Match

As Drawn (0)

Substructure (732)

Similarity (9)

Analyze Structure Precision



R-Group Definitions

R1 R2 R3 R4 R5 R6 R7 R8 R9 R10 R11 R12

R1: Ni, Cu, Co

Atoms

H															He			
Li	Be												B	C	N	O	F	Ne
Na	Mg												Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr	
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe	
Cs	Ba	*	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn	
Fr	Ra	**																

*Lanthanides: La Ce Pr Nd Pm Sm Eu Gd Tb Dy Ho Er Tm Yb Lu

**Actinides: Ac Th Pa U Np Pu Am Cm Bk Cf Es Fm Md No Lr

Isotopes: D T

物质检索—检索结果集筛选

结构检索类别:

As Drawn

亚结构

相似结构

Chemscape分析

Filter by & Exclude

物质筛选类别:

反应角色

文献角色

立体化学

物质类别

同位素

金属包含

实验物性数据

二次检索.....

Substances search for drawn structure

References Reactions Suppliers

Structure Match

As Drawn (0)

Substructure (732)

Similarity (9)

Analyze Structure Precision

Chemscape Analysis

Visually explore structure similarity with a powerful new tool.

Learn more about Chemscape.

Create Chemscape Analysis

Filter Behavior

Filter by Exclude

Reaction Role

Reference Role

Commercial Availability

Number of Components

Molecular Weight

Stereochemistry

Element

Substance Class

Isotopes

Metals

Experimental Property

Bioactivity Indicator

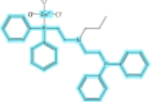
Search Within Results

732 Results

Sort: Relevance View: Partial

1

685504-28-3

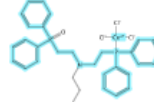


$C_{31}H_{35}Cl_3CoNP_2$
(T-4)-Trichloro[N-[2-(diphenylphosphino- κP)ethyl]-N-[2-(diphenylphosphino)ethyl]...]

0 References 0 Reactions 0 Suppliers

2

807307-30-8

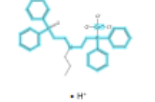


$C_{31}H_{35}Cl_3CoNOP_2$
Cobaltate(1-), trichloro[N-[2-(diphenylphosphino- κP)ethyl]-N-[2-(diphenylphosphino)ethyl]...

0 References 0 Reactions 0 Suppliers

3

635299-07-9

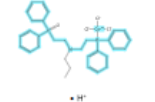


$C_{31}H_{35}Cl_3CoNOP_2 \cdot H^+$
Components: 2
Component RN: 807307-30-8
Cobaltate(1-), trichloro[N-[2-(diphenylphosphino- κP)ethyl]-N-[2-(diphenylphosphino)ethyl]...

0 References 0 Reactions 0 Suppliers

4

635299-08-0

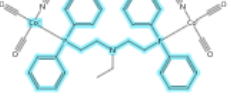


$C_{31}H_{35}Cl_3CoNOP_2 \cdot 2/5 C_2H_6O \dots$
Components: 3
Cobaltate(1-), trichloro[N-[2-(diphenylphosphino- κP)ethyl]-N-[2-(diphenylphosphino)ethyl]...

1 Reference 9 Reactions 0 Suppliers

5

16827-53-5

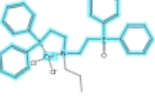


$C_{34}H_{33}Co_2N_5O_6P_2$
Cobalt, [μ -[2,2'-bis(diphenylphosphino)triethylamine]]tetracarbonyldinitrosyldi...

1 Reference 0 Reactions 0 Suppliers

6

635299-09-1



$C_{31}H_{35}Cl_2CoNOP_2$
(T-4)-Dichloro[N-[2-(diphenylphosphino- κP)ethyl]-N-[2-(diphenylphosphino)ethyl]...

1 Reference 3 Reactions 0 Suppliers

物质检索—结构检索

结构检索类别：

- As Drawn

绘制结构中可出现R基团、可变基团；绘制结构中价态未达饱和的原子只能接氢；如有环系，不与其他环稠合或成桥环

- Substructure 亚结构

包括As Drawn检索结果；价态未达饱和的原子可以连接氢以外的其他原子；如有环系，可形成其他环

- Similarity 相似结构

获得片段或整体结构与被检索结构相似的结果，母体结构可以被取代，也可以被改变

注：如果关注相似结构检索结果，请不要绘制通式结构

物质检索-检索结果集筛选: Reaction Role

Substances search for drawn structure

References Reactions Suppliers

Structure Match

As Drawn (0)

Substructure (732)

Similarity (9)

Analyze Structure Precision

Chemscape Analysis

Visually explore structure similarity with a powerful new tool. [Learn more about Chemscape.](#)

Create Chemscape Analysis

Filter Behavior

Filter by Exclude

Reaction Role

Product (216)

Reactant (53)

Reagent (3)

Catalyst (36)

Reference Role

Commercial Availability

Number of Components

Molecular Weight

Filtering: Reaction Role: Catalyst X

36 Results

Sort: Relevance View: Partial

1 2 3 4 5 6

1879110-74-3

C33H39Cl2CoNP2
(T-4)-[N,N-Bis[2-(diphenylphosphino-κP)ethyl]-1-pentanamine]dichlorocobalt

1 Reference 2 Reactions 0 Suppliers

2332371-33-0

C30H33Cl2CoNP2
(T-4)-Dichloro[2-(diphenylphosphino-κP)-N-[2-(diphenylphosphino-κP)ethyl]-N-ethyl...

1 Reference 3 Reactions 0 Suppliers

1879110-75-4

C31H35Cl2CoNP2
(T-4)-[N,N-Bis[2-(diphenylphosphino-κP)ethyl]-2-propanamine]dichlorocobalt

1 Reference 2 Reactions 0 Suppliers

1087216-22-5

C28H29Cl2CoNP2
Dichloro[2-(diphenylphosphino-κP)-N-[2-(diphenylphosphino-κP)ethyl]ethanamine-κN...

8 References 105 Reactions 0 Suppliers

2170923-58-5

C28H29Cl2CoNP2
(7B-5-13)-Dichloro[2-(diphenylphosphino-κP)-N-[2-(diphenylphosphino-κP)ethyl]eth...

1 Reference 32 Reactions 0 Suppliers

1846596-28-8

C28H53Cl2CoNP2
(7B-5-13)-Dichloro[2-(dicyclohexylphosphino-κP)-N-[2-(dicyclohexylphosphino-κP)ethyl]eth...

7 References 13 Reactions 0 Suppliers

利用物质在反应中的角色精准定位相应的物质

物质检索—检索结果集筛选：Reference Role

利用物质的研究角色精准定位相应的物质

Reference Role

By Count

Alphanumeric

5 Selected

☐ Preparation (489)

☒ Synthetic Preparation (488)

☐ Properties (245)

☐ Reactant (98)

☐ Reactant or Reagent (98)

☐ Uses (88)

☒ Catalyst Use (77)

☒ Process (32)

☐ Physical, Engineering, or Chemical Process (31)

☒ Industrial Manufacture (9)

☐ Technical or Engineered Material Use (8)

☐ Formation, Non-preparative (6)

☒ Biological Study (4)

☐ Pharmacological Activity (4)

☐ Therapeutic Use (4)

☐ Analytical Reagent Use (1)

☐ Analytical Study (1)

☐ Formation, Unclassified (1)

Apply

Cancel

Structure Match

As Drawn (0)

Substructure (732)

Similarity (9)

Analyze Structure Precision

Chemscrape Analysis

Visually explore structure similarity with a powerful new tool.
[Learn more about Chemscrape.](#)

Create Chemscrape Analysis

Filter Behavior

Filter by

Exclude

Reaction Role

Reference Role

☐ Preparation (489)

☐ Synthetic Preparation (488)

☐ Properties (245)

☐ Reactant (98)

☐ Reactant or Reagent (98)

☒ Industrial Manufacture (9)

[View All](#)

Commercial Availability

☐ Not Available (9)

Filtering: Reference Role: Industrial Manufacture


Clear All Filters

9 Results

Sort: Relevance View: Partial

1

1087216-22-5



C₂₈H₂₉Cl₂CoNP₂
Dichloro[2-(diphenylphosphino-κP)-N-[2-(diphenylphosphino-κP)ethyl]jethana mine-κN...

8

References

105

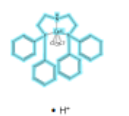
Reactions

0

Suppliers

2

1395056-63-9



C₂₈H₂₉Cl₃CoNP₂.H
Components: 2
Component RN: 1395144-60-1
Cobaltate(1-), trichloro[2-(diphenylphosphino-κP)-N-[2-(diphenylphosphino-κP)ethyl]jethana mine-κN...

3

References

8

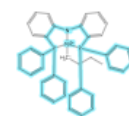
Reactions

0

Suppliers

3

579490-65-6



C₄₀H₃₇NNiP₂
(SP-4-1)-Butyl[2-(diphenylphosphino-κP)-N-[2-(diphenylphosphino-κP)phenyl]benzen...

6

References

20

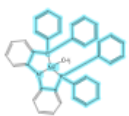
Reactions

0

Suppliers

4

579490-58-7



C₃₇H₃₁NNiP₂
(SP-4-1)-[2-(Diphenylphosphino-κP)-N-[2-(diphenylphosphino-κP)phenyl]benzen amina...

7

References

22


Reactions

0

Suppliers

5

579490-62-3



C₃₈H₃₃NNiP₂
(SP-4-1)-[2-(Diphenylphosphino-κP)-N-[2-(diphenylphosphino-κP)phenyl]benzen amina...

6

References

21


Reactions

0

Suppliers

6

579490-55-4



C₃₆H₂₈ClNNiP₂
(SP-4-3)-Chloro[2-(diphenylphosphino-κP)-N-[2-(diphenylphosphino-κP)phenyl]benze...

8

References

52

Reactions

0

Suppliers

物质检索—检索结果集的保存

References Reactions Suppliers

Structure Match

As Drawn (0)

Substructure (732)

Similarity (9)

Analyze Structure Precision

Chemscape Analysis

Visually explore structure similarity with a powerful new tool.

Learn more about Chemscape.

Create Chemscape Analysis

Filter Behavior

Filter by

Reaction Role

Reference Role

Commercial Availability

Number of Components

Molecular Weight

Element

Filtering: Search Within Results: Drawn Structure X

109 Results

Sort: Relevance View: Partial

1698881-12-7

C58H56N2NiP4S4
(SP-4-1)-Bis[*N,N*-bis[2-(diphenylphosphino)ethyl]carbamodithioato-*κ*S,*κ*S'] nickel

65120-45-8

C34H43N2NiP2S
Nickel(1+), [*N,N*-bis[2-(diphenylphosphino)ethyl]-*N',N'*-diethyl-1,2-ethanediamine...

65120-39-0

C35H45N2NiP2S
Nickel(1+), [*N,N*-bis[2-(diphenylphosphino)ethyl]-*N',N'*-diethyl-1,2-ethanediamine...

1698881-15-0

C87H84CoN3P6S6
(OC-6-11)-Tris[*N,N*-bis[2-(diphenylphosphino)ethyl]carbamodithioato-*κ*S,*κ*S'] cobalt

1698881-21-8

C58H56Au4Cl4N2NiP4S4
Bis[μ_3 -[*N,N*-bis[2-(diphenylphosphino)-*κ*P]ethyl]carbamodithioato-*κ*S,*κ*S']]tetrakis (...)

65120-46-9

O=C([O-])=O

1 Reference 4 Reactions 0 Suppliers

0 References 0 Reactions 0 Suppliers

0 References 0 Reactions 0 Suppliers

0 References 0 Reactions 0 Suppliers

文献信息 反应信息 供应商信息

Save Results and Create Alert

Name

PNP-S

Save Options

☐ Query Only

☐ Selected Answers

☒ All Answers (Up to 20,000)

Alert Frequency

☐ No Alerts

☐ As Available

☐ Weekly

☒ Monthly

Add Existing Tags (Optional)

☒ catalyst

☐ Other fields

☒ Task

☐ Try

New Tag (Optional)

Tag Color

Save Cancel

Download Substance Results

File Type

PDF

Display

☐ Structures Only

☒ Result Summary

☐ Result Details

Select Quantity

☒ All Results

☐ Selected Results

☐ Range (ex. 2 to 20)

File Name

Substance_20221121_1345

Include

☒ Task History

☐ Substance Identifiers

☐ Experimental Spectra

☐ Predicted Spectra

☐ Regulatory Information

☐ Experimental Properties

☐ Predicted Properties

☐ Bioactivity Indicators

☐ Target Indicators

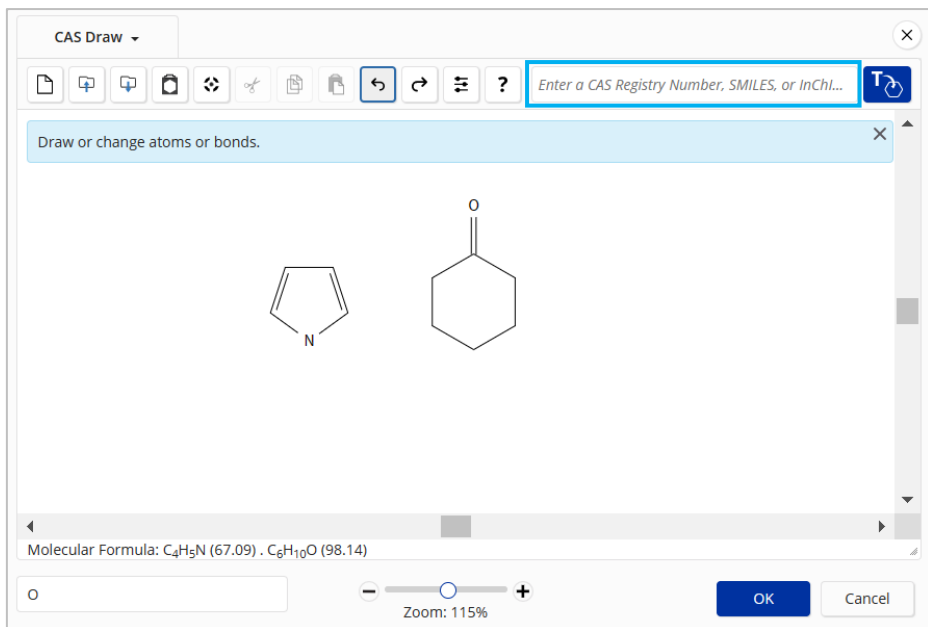
Download Cancel

Learn more about downloads.

物质检索——结构检索综合示例

请思考，已知活性结构片段，如何查找：

1. 所有包含它们的天然产物或药物？
2. 锁定尚未合成的物质？
3. 若结构尚未合成，如何获取逆合成路线？



Reference Role

- ☐ Preparation (23K)
- ☐ Synthetic Preparation (21K)
- ☐ Uses (18K)
- ☐ Biological Study (10K)
- ☐ Therapeutic Use (8,159)
- ☒ Natural Product Occurrence (277)

[View All](#)

Filter Behavior

Filter by **Exclude**

Reaction Role

- ☒ Product (54)
- ☐ Reactant (21)

Structure Match

As Drawn (2)

Substructure (58K)

Similarity (580)

[Analyze Structure Precision](#)

Chemscape Analysis

Visually explore structure similarity with a powerful new tool. [Learn more about Chemscape.](#)

[Create Chemscape Analysis](#)

Filter Behavior

Filter by **Exclude**

Reaction Role

- ☒ Product (54)
- ☐ Reactant (21)

Filtering: Reference Role: Natural Product Occurrence... X Number of Components: 1 X

Excluding: Reaction Role: Product X

223 Results

Sort: Number of References: Ascending View: Partial

1	2	3
2707395-49-9	2699076-84-9	2707395-48-8
<chem>C13H11NO3</chem> 5,6-Dihydro-9,10-dihydroxy-11H-pyrrolo[2,1-b][3]benzazepin-11-one	<chem>C16H9NO4</chem> Benzo[5',6']pentaleno[1',2':3,4]pyrrolo[2,1-b]oxazol-7(11bH)-one, 10,11-dihydroxyl...	<chem>C14H13NO3</chem> 6,11-Dihydro-8,9-dihydroxy-5H-pyrrolo[2,1-b][3]benzazepine-3-carboxaldehyde
1 Reference 0 Reactions 0 Suppliers	1 Reference 0 Reactions 0 Suppliers	1 Reference 0 Reactions 0 Suppliers

4	5	6
2126788-65-4	2126179-96-0	2126179-95-9
4 Reference 0 Reactions 0 Suppliers	5 Reference 0 Reactions 0 Suppliers	6 Reference 0 Reactions 0 Suppliers

——亚结构检索，限定结果为单组份、Natural Product Occurrence，获得含已知活性结构片段的天然产物

——排除物质结果集中，reaction role为product的结果

——通过CAS Retrosynthesis Tool

CAS Markush检索

(19) 中华人民共和国国家知识产权局



(12) 发明专利申请



(10) 申请公布号 CN 104945470 A

(43) 申请公布日 2015.09.30

(21) 申请号 201410122313.4
(22) 申请日 2014.03.30
(71) 申请人 浙江大学
地址 310027 浙江省杭州市西湖区浙大路38号
申请人 中国科学院上海药物研究所

C07K 1/16(2006.01)
C07K 1/06(2006.01)
A61P 38/06(2006.01)
A61P 35/00(2006.01)
A61P 35/02(2006.01)
A61P 25/28(2006.01)
A61P 37/02(2006.01)

(72) 发明人 南永洲 李佳 刘滔 张建康
周宇波 杨波 何俏军 许磊
南小蓓

(74) 专利代理机构 杭州求是专利事务有限公司
代理人 张法高 赵航丽

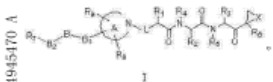
(51) Int. Cl.
C07K 5/087(2006.01)
C07K 5/083(2006.01)

权利要求书3页 说明书24页 附图4页

(54) 发明名称
杂环构建的三肽环氧酮类化合物及制备和应用

(57) 摘要

本发明提供一种杂环构建的三肽环氧酮类化合物,以 Carfilzomib 为先导化合物,经缩合、酸性条件下脱去 Boc 保护基、碱性条件下反应得氨基酸甲酯异氰酸酯、水解、在缩合剂作用下获得。本发明是小分子肽类蛋白酶抑制剂。本发明化合物具有极强的蛋白酶抑制活性及细胞增殖抑制活性,是有前景的蛋白酶抑制剂,为癌症治疗药物的研究提供了新的思路。本发明化合物的合成所需原料易得,路线设计合理,反应条件温和,各步产率高,操作简便,适合工业化生产。具有下述式 I 的结构通式:



具体物质[Specific Substance]:

以具体化学结构陈述的特定物质, 会被分配CAS RN

具体实施方式

[0026] 本发明结合附图和实施例作进一步的说明,以下实施例仅是说明本发明,而不是以任何方式限制本发明。

[0027] 制备实施例 1、4-(吡嗪-2-基氨甲酰基)哌啶-1-甲酸叔丁酯 (1a, 1b)

将 1-(叔丁氧羰基)哌啶-4-甲酸 (2.75g, 12mmol) 置于 50mL 三颈瓶中, N₂ 保护下加入 25mL 无水 CH₂Cl₂, 然后缓缓滴入吡啶 (2.5mL, 30mmol) 和二氯亚砷 (1.1mL, 14mmol), 该反应液置于室温反应半小时。随后, 2-氨基吡嗪 (0.95g, 10mmol) 和三乙胺 (5.7mL, 40mmol) 溶于 15mL CH₂Cl₂ 后缓缓滴入上述反应液, 室温反应 6 小时。反应液加 30mL 饱和食盐水稀释, 分出有机层, 水层 CH₂Cl₂ 提取 (15mL×3), 合并有机层, 无水硫酸钠干燥后减压除去溶剂, 柱层析分离得白色固体 2.3g, 收率 74%。m.p.: 134-136°C; ¹H NMR (500MHz, CDCl₃): δ = 9.55 (s, 1H, pyrazine-H), 8.35 (d, 1H, J=2.0Hz, pyrazine-H), 8.23 (s, 1H, pyrazine-H), 7.97 (s, 1H, NH), 4.20 (m, 2H, CH₂), 2.81 (m, 2H, CH₂), 2.48 (m, 1H, CH), 1.93 (d, 2H, J=12.5Hz, CH₂), 1.76 (m, 2H, CH₂), 1.47 (s, 9H, CH₃) ppm; ESI-MS: m/z = 307 [M+H]⁺。

[0028] 制备实施例 2、4-(吡嗪-2-酰基)哌啶-1-甲酸叔丁酯 (1c, 1d)

吡嗪-2-羧酸 (1.5g, 12mmol) 置于 50mL 反应瓶中, 加入 35mL 无水 CH₂Cl₂ 溶解, 随即加入 1-羟基苯并三氮唑 (1.6g, 12mmol) 和 N-(3-二甲氨基丙基)-N'-乙基碳二亚胺盐酸盐 (3.5g, 18mmol), 室温反应半小时。随后, 哌啶-1-甲酸叔丁酯 (1.9g, 10mmol) 加入反应液中, 室温反应 3 小时。反应液加入 30mL 饱和碳酸氢钠水溶液稀释, 分出有机层, 饱和食盐水

CAS Markush检索

预测性物质[Prophetic Substance]:

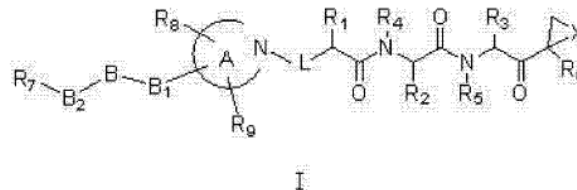
- 使用Markush结构陈述的预测物质，一个Markush可以陈述成百上千，甚至更多的结构
- 被Markush结构包含，但未被实施或呈现在表格、权利要求书或说明书中的结构，不会被CAS分配CAS Registry Number
- Markush检索，能检索到通过Substance可能检索不到的结构

CN 104945470 A

权 利 要 求 书

1/3 页

1. 一种杂环构建的三肽环氧酮类化合物，具有下述结构通式 I：



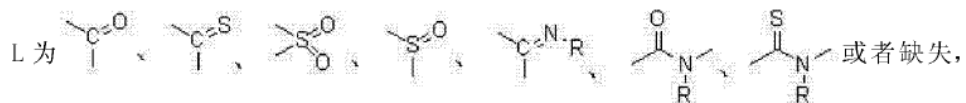
其中：

R_1, R_2, R_3 各自独立选自 H、 C_{1-6} 烷基、 C_{1-6} 烷基-D、卤代的 C_{1-6} 烷基-D、 C_{1-6} 羟基烷基、 C_{1-6} 巯基烷基、 C_{1-6} 烷氧基烷基、芳基、芳烷基、杂芳基或杂芳烷基；其中：D 为 $N(R_0)$ (R_0) 或缺失， R_0, R_0 各自独立选自 H、OH、 C_{1-6} 烷基、卤代的 C_{1-6} 烷基或 N 末端保护基；

R_4, R_5 各自独立选自 H、OH、 C_{1-6} 烷基、卤代的 C_{1-6} 烷基或芳烷基；

R_6 选自 H、 C_{1-6} 烷基、卤代的 C_{1-6} 烷基、 C_{1-6} 羟基烷基、 C_{1-6} 烷氧基、卤代的 C_{1-6} 烷氧基、 $C(O)O-C_{1-6}$ 烷基、 $C(O)NH-C_{1-6}$ 烷基、芳烷基；

X 为 O、S、NH、N- C_{1-6} 烷基或 N- 卤代的 C_{1-6} 烷基；



其中 R 选自 H、 C_{1-6} 烷基或卤代的 C_{1-6} 烷基；

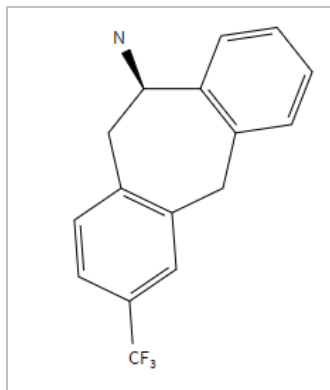
环 A 选自 5 ~ 7 元的饱和脂肪杂环、不饱和杂环、或者有取代的 5 ~ 7 元的饱和脂肪杂环、不饱和杂环，所述的杂环包含 0 ~ 3 个选自 O、N 和 S 的杂原子并任选地被 R_8, R_9 和 B_1 基团取代；

R_8, R_9 分别独立选自 H、OH、 C_{1-6} 烷基、 C_{1-6} 烷氧基、 C_{1-6} 羟基烷基、 C_{1-6} 巯基烷基、 C_{1-6} 烷基-D、芳基、杂环芳基、环烷基和杂环基，这些基团可以被卤素、硝基、氨基、CN、 C_{1-6} 烷基、卤代的 C_{1-6} 烷基、 C_{1-6} 烷氧基或卤代的 C_{1-6} 烷氧基取代，每个基团可与一个或多个芳基或杂环

CAS Markush检索

第一步：物质结构检索

- As drawn结果为0
- Substructure结果为2
- Similarity相似度最高85-89%



Structure Match

As Drawn (0)

Substructure (2)

Similarity (5,664)

Chemscape Analysis

Visually explore structure similarity with a powerful new tool.

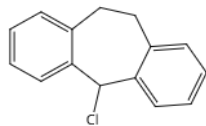
[Learn more about Chemscape.](#)

[Create Chemscape Analysis](#)

Filtering: Number of Components: 1 X Clear All Filters

5,332 Results Sort: Number of References: Descending View: Partial

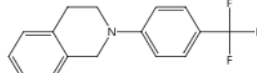
1 61 1210-33-9



C₁₅H₁₃Cl
5-Chlorodibenzosuberane

143 References 130 Reactions 61 Suppliers

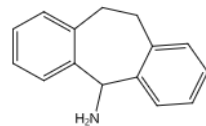
2 64 1057277-76-5



C₁₆H₁₄F₃N
1,2,3,4-Tetrahydro-2-[4-(trifluoromethyl)phenyl]isoquinoline

90 References 121 Reactions 2 Suppliers

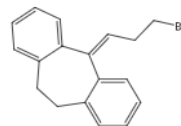
3 68 7005-53-0



C₁₅H₁₅N
IEM 2115

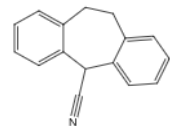
58 References 78 Reactions 14 Suppliers

4 60 3436-04-2



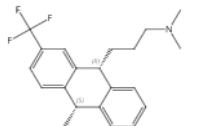
C₁₈H₁₇Br
5-(3-Bromopropylidene)-10,11-dihydro-5H-dibenzo[a,d]cycloheptene

5 62 1729-63-1



C₁₆H₁₃N
10,11-Dihydro-5H-dibenzo[a,d]cycloheptene-5-carbonitrile

6 64 35764-73-9



C₂₁H₂₄F₃N
Fluotracen

Relative stereochemistry shown

[Feedback](#)

Filter Behavior

Filter by Exclude

Similarity

85-89 (1)

80-84 (2)

75-79 (20)

70-74 (140)

65-69 (958)

60-64 (4,211)

Reaction Role

Reference Role

CAS Markush检索

第二步：Markush结构检索
获得四件专利文献

- 直观呈现检索结构与专利原文中Markush匹配部分的结构；
- 标引其在专利中出现的位置；
- 详细的结构取代信息描述

CAS SciFinder®

Substances Enter a query...

Return to Home

Patent Markush search for drawn structure

References

Patent Markush Match

As Drawn (4)

Substructure (33)

Filter Behavior

Filter by Exclude

Patent Office

World Intellectual Property Organization (3)

European Patent Organization (1)

CA Section

Agrochemical Bioregulators (1)

Electric Phenomena (1)

Heterocyclic Compounds (More Than One Hetero Atom) (1)

Pharmacology (1)

Filter Content Report

Download filter data from this result set.

4 Results

1

WO2011025969

Compounds that treat malaria and prevent malaria transmission

By: Su, Xin-Zhuan; Yuan, Jing; Raj, Dipak; Pattaradilokrat, Sittiporn; Johnson, Ron; Huang, Ruili

World Intellectual Property Organization, WO2011025969 A1 2011-03-03 | Language: English, Database: CAplus

Assignee: United States Dept. of Health and Human Services

Patent claim 1

PatentPak Full Text

Patent	Language	Kind Code	PatentPak Options
WO2011025969	English	A1	PDF PDF+ Viewer
CN102595894	Chinese	A	PDF
US20120196882	English	A1	PDF PDF+ Viewer
US9375424	English	B2	PDF
US20160303103	English	A1	PDF

2

EP502788

By: Regnier, Gilbert; Orlandini, Adam; Abassi, Ghannem; Pierre, Adam; Leonce, Stephane

European Patent Organization, EP502788 A1 1992-09-09 | Language: French, Database: CAplus

Assignee: Adir et Cie.

Patent claim 11

Full Text

There are no notes to display for this structure.

为了尽可能完整地获得公开的结构信息，需要同时进行Substance和Markush结构检索

物质检索小结

1. 利用结构绘制工具合理扩大结构检索范围：R基团、可变基团、可变位置取代等
2. 利用结构绘制工具适当限定检索结构：环锁工具、原子锁工具、EZ构型限定等
3. 正确理解As Drawn、Substructure、Similarity检索结果集的意义和范围
4. 充分利用物质筛选项准确定位目标物质：Reaction Role、Reference Role等
5. 利用CAS Markush检索尽可能全面的获得结构的公开信息

反应检索

- 反应检索方法
 - 物质或文献标识符
 - 结构式
 - 关键词与结构联用
- 常用获取方法推荐
 - 已知物质：由物质获取反应
 - 已知文献：从文献中获取反应
 - 精确结构反应检索
 - 亚结构反应检索

反应检索

通过物质或文献标识符进行检索

CAS SciFinder® Reactions Semaglutide

Return to Home

Reactions search for "Semaglutide"

References

Filter Behavior

Filter by Exclude

Substance Role

Product (222)

Reactant (10)

Yield

90-100% (3)

80-89% (5)

70-79% (2)

50-69% (2)

10-29% (1)

View All

Number of Steps

Reaction Mapping

Experimental Protocols

Synthetic Methods (11)

Reaction Type

Stereochemistry

Reagent

Catalyst

Solvent

Commercial Availability

Reaction Notes

Search Within Results

228 Results

Group: By Scheme Sort: Number of Steps: Descending View: Collapsed

Scheme 1 (1 Reaction) Steps: 7

910463-68-2
Image Not Available
Suppliers (28)

Suppliers (98)

Suppliers (64)

Expand Scheme

Scheme 2 (5 Reactions) Steps: 5-7

910463-68-2
Image Not Available
Suppliers (28)

Suppliers (79)

Suppliers (37)

Expand Scheme

Scheme 3 (2 Reactions) Steps: 3-7

910463-68-2
Image Not Available
Suppliers (28)

Suppliers (93)

Suppliers (132)

CAS SciFinder® Reactions 175:621496

Return to Home

Reactions search for "175:621496"

References

Filter Behavior

Filter by Exclude

Yield

90-100% (3)

80-89% (5)

70-79% (2)

50-69% (3)

No Yield Available (120)

Number of Steps

1 (25)

2 (29)

3 (27)

4 (21)

5 (16)

6-10 (15)

Non-Participating Functional Groups

Amide (10)

Carboxylic ester (10)

Carboxylic acid (9)

Ether (5)

Amine (3)

View All

Reaction Mapping

Experimental Protocols

Synthetic Methods (132)

Reaction Type

Stereochemistry

133 Results

Group: By Scheme Sort: Number of Steps: Descending View: Collapsed

Scheme 1 (2 Reactions) Steps: 7-8

204656-20-2
Image Not Available
Suppliers (37)

Suppliers (145)

Suppliers (77)

Expand Scheme

Scheme 2 (1 Reaction) Steps: 8

204656-20-2
Image Not Available
Suppliers (37)

Suppliers (136)

Expand Scheme

Scheme 3 (1 Reaction) Steps: 7

204656-20-2
Image Not Available
Suppliers (37)

Suppliers (32)

Supplier (1)

Expand Scheme

反应检索

Searching for...

Reactions

Search by Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. [Learn More](#)

Enter a query...

Draw

CAS Draw

Draw or change atoms or bonds.

reactant

product

Molecular Formula: Formula is not available

C

Zoom: 100%

OK

Cancel

X = Cl, Br

反应检索—结果集的分组与排序

As drawn结果为32

Reactions search for drawn structure

References

Structure Match

- As Drawn (32)
- Substructure (8,521)
- Similarity (0)

Filter Behavior

Filter by Exclude

Yield

Number of Steps

Non-Participating Functional Groups

Reaction Mapping

Experimental Protocols

- Synthetic Methods (3)
- Experimental Procedure (12)

Reaction Type

Reagent

Catalyst

Solvent

Commercial Availability

Reaction Notes

Search Within Results

Filtering: Reaction Mapping: Mapping Data Available

16 Results

Group: By Scheme

Sort: Yield View: Collapsed

Relevance

Publication Date: Newest

Publication Date: Oldest

Yield

Number of Steps: Ascending

Number of Steps: Descending

Scheme 1 (5 Reactions)

Suppliers (85)

Suppliers (15)

Expand Scheme

Scheme 2 (1 Reaction)

Steps: 1 Yield: 76%

Suppliers (51)

Suppliers (3)

31-614-CAS-28968228 Steps: 1 Yield: 76%

Preparation of heterocyclic compounds as selective subtype alpha 2 adrenergic agents

By: Heidelberg, Todd M.; et al

World Intellectual Property Organization, WO2009091874 A1 2009-07-23

PatentPak Full Text

Experimental Protocols

1.1 Reagents: [O-Methylhydroxylamine hydrochloride](#)
Solvents: [Pyridine](#); rt; 1 h, 50 °C

1.2 Reagents: [\(7-4\)-Trihydro\(tetrahydrofuran\)boron](#)
Solvents: [Tetrahydrofuran](#); rt; 3 h, reflux; reflux → 0 °C

1.3 Reagents: [Sodium hydroxide](#)
Solvents: [Water](#); overnight, reflux; reflux → rt

反应分组：
按类型分组
按文献分组

反应排序：
相关度
公布时间
产率
步数

反应检索—结果集筛选

Substructure结果8521

As Drawn反应检索
亚结构反应检索
相似反应检索

反应筛选类别：
产率、反应步数
不参与反应的官能团
实验步骤
反应类型
立体化学
试剂、催化剂、溶剂
商品信息……

文献筛选类别：
文献类型、语言
出版年份、刊物名

Structure Match

As Drawn (32)

Substructure (8,521)

Similarity (0)

Filter Behavior

Filter by Exclude

Yield

Number of Steps

Non-Participating Functional Groups

Reaction Mapping

Experimental Protocols

Reaction Type

Stereochemistry

Reagent

Catalyst

Solvent

Commercial Availability

Reaction Notes

Search Within Results

Source Reference

Document Type

Language

Publication Year

Organization

Publication Name

CA Section

Filter Content Report

8,521 Results

Group: By Transformation View: Collapsed

1

Acylation of Nitrogen Nucleophiles by Carboxylic Acids

View 1 Related Reaction

$$\text{R}-\text{C}(=\text{O})\text{OH} + \text{R}^1-\text{NH}-\text{R}^1 \longrightarrow \text{R}-\text{C}(=\text{O})\text{N}(\text{R}^1)_2$$

2

Hydrolysis or Hydrogenolysis of Carboxylic Esters or Thioesters

View 1 Related Reaction

$$\text{R}-\text{C}(=\text{O})\text{OR}^1 \xrightarrow{\text{H}_2\text{O}} \text{R}-\text{C}(=\text{O})\text{OH} + \text{R}^1-\text{YH}$$
$$\text{R}-\text{C}(=\text{O})\text{SR}^1 \xrightarrow{\text{H}_2} \text{R}-\text{C}(=\text{O})\text{OH} + \text{R}^1-\text{H}$$

Y = O, S

3

Acylation of Nitrogen Nucleophiles by Acyl/ Thioacyl/ Carbamoyl Halides and Analogs

View 2 Related Reactions

$$\text{R}-\text{C}(=\text{Y})\text{X} + \text{R}^1-\text{NH}-\text{R}^1 \longrightarrow \text{R}-\text{C}(=\text{Y})\text{N}(\text{R}^1)_2$$

Y = O, S, NR'

4

Formation of N/O/S Heterocycles

View 49 Related Reactions

$$\text{Y}'-\text{C}(=\text{Y})-\text{R}^1 \longrightarrow \text{Y}'-\text{C}(=\text{Y})-\text{R}^1$$

2 Results

Group: By Scheme Sort: Relevance View: Collapsed

Scheme 1 (1 Reaction) Steps: 1

$$\text{Cl}-\text{C}_6\text{H}_4-\text{C}(=\text{O})-\text{Cl} + \text{Cl}-\text{C}_6\text{H}_4-\text{C}(=\text{O})-\text{Cl} \longrightarrow \text{Cl}-\text{C}_6\text{H}_4-\text{C}(=\text{O})-\text{N}(\text{C}_6\text{H}_4-\text{C}(=\text{O})-\text{Cl})_2$$

Suppliers (39) Suppliers (63) Suppliers (78)

Absolute stereochemistry shown

Expand Scheme

Scheme 2 (1 Reaction) Steps: 1

$$\text{Cl}-\text{C}_6\text{H}_4-\text{C}(=\text{O})-\text{Cl} + \text{Cl}-\text{C}_6\text{H}_4-\text{C}(=\text{O})-\text{Cl} \longrightarrow \text{Cl}-\text{C}_6\text{H}_4-\text{C}(=\text{O})-\text{N}(\text{C}_6\text{H}_4-\text{C}(=\text{O})-\text{Cl})_2$$

Suppliers (39) Suppliers (63) Suppliers (61)

Absolute stereochemistry shown

31-313-CAS-18612019 Steps: 1

Benzamide compounds as ROR gamma modulators and their preparation

1.1 Reagents: Titanium isopropoxide, (R)-2-Methylpropane-2-sulfonamide
Solvents: Tetrahydrofuran; 18 h, 70 °C

1.2 Reagents: Sodium borohydride; 3 h, rt

1.3 Reagents: Methanol; 0 °C

1.4 Reagents: Hydrochloric acid
Solvents: Diethyl ether, 1,4-Dioxane; 1 h, 0 °C

By: Das, Sanjib; et al
World Intellectual Property Organization, WO2017199103 A1
2017-11-23

PatentPak Full Text

折叠菜单显示：相同反应类型的反应在同一菜单里，方便阅读和筛选

反应检索—结果集筛选：不参与反应官能团

Reactions search for drawn structure

References

Structure Match

- As Drawn (32)
- Substructure (8,521)**
- Similarity (0)

Filter Behavior

Filter by Exclude

Yield

Number of Steps

Non-Participating Functional Groups

- ☒ Halide (290)
- ☐ Phenyl halide (286)
- ☐ Carboximidine (109)
- ☐ Alkene (84)
- ☐ Cyclic alkene (80)
- [View All](#)

Reaction Mapping

Experimental Protocols

Reaction Type

Stereochemistry

Filtering: Non-Participating Functional Groups: Halide X Clear All Filters

290 Results Group: By Scheme Sort: Relevance View: Collapsed

Scheme 1 (1 Reaction) Steps: 1 Yield: 100% Suppliers (107)

Expand Scheme

Scheme 2 (1 Reaction) Steps: 1 Yield: 100% Expand Scheme

Scheme 3 (1 Reaction) Steps: 1 Yield: 100%

不参与反应官能团：
出现在反应前后，但未发生变化的官能团

Non-Participating Functional Groups

By Count Alphanumeric

1 Selected

<input checked="" type="checkbox"/> Halide (282)	<input type="checkbox"/> Diene (45)	<input type="checkbox"/> Acetal (3)
<input type="checkbox"/> Phenyl halide (278)	<input type="checkbox"/> Ether (40)	<input type="checkbox"/> Acyclic alkene (3)
<input type="checkbox"/> Carboximidine (101)	<input type="checkbox"/> Cyclic ketone (29)	<input type="checkbox"/> Carbamate (3)
<input type="checkbox"/> Alkene (84)	<input type="checkbox"/> Urea (16)	<input type="checkbox"/> Carboxylic acid (3)
<input type="checkbox"/> Cyclic alkene (80)	<input type="checkbox"/> Tertiary amine (9)	<input type="checkbox"/> Alcohol (2)
<input type="checkbox"/> Amide (69)	<input type="checkbox"/> Imine (8)	<input type="checkbox"/> Primary alcohol (2)
<input type="checkbox"/> Amine (59)	<input type="checkbox"/> Thiocarbonyl (7)	<input type="checkbox"/> Unsaturated ester (2)
<input type="checkbox"/> Carboxylic ester (53)	<input type="checkbox"/> Acyclic ketone (5)	<input type="checkbox"/> Nitro (1)
<input type="checkbox"/> Secondary amine (50)	<input type="checkbox"/> Alkyl halide (4)	<input type="checkbox"/> Primary amine (1)
<input type="checkbox"/> Ketone (48)	<input type="checkbox"/> Nitrile (4)	<input type="checkbox"/> Unsaturated ketone (1)

Apply Cancel

反应检索—结果集筛选: Synthetic Methods™

Structure Match

As Drawn (32)

Substructure (8,521)

Similarity (0)

Filter Behavior

Filter by

Exclude

Yield

Number of Steps

Non-Participating Functional Groups

Reaction Mapping

Experimental Protocols

☒ Synthetic Methods (40)

☐ Experimental Procedure (83)

Reaction Type

Stereochemistry

Reagent

Catalyst

Solvent

Commercial Availability

Reaction Notes

Search Within Results

Source Reference

Filtering:

Non-Participating Functional Groups: Halide X

Experimental Protocols: Synthetic Methods X

Clear All Filters

40 Results

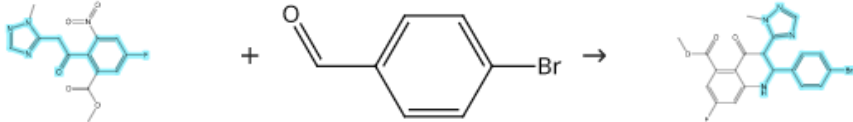
Group: By Scheme

Sort: Relevance

View: Collapsed

Scheme 1 (1 Reaction)

Steps: 1 Yield: 98%



Suppliers (15)

Suppliers (89)

☐ 31-614-CAS-24450288

Steps: 1 Yield: 98%

1.1 Reagents: [Hydrochloric acid](#), [Titanium chloride \(TiCl₃\)](#)
Solvents: [Methanol](#), [Tetrahydrofuran](#), [Water](#); rt; 30 min, rt; 2 h, 30 - 50 °C
1.2 Reagents: [Water](#)

DoE Optimization Empowers the Automated Preparation of Enantiomerically Pure [¹⁸F]Talazoparib and its In Vivo Evaluation as a PARP Radiotracer

By: Bowden, Gregory D. et al
Journal of Medicinal Chemistry (2021), 64(21), 15690-15701

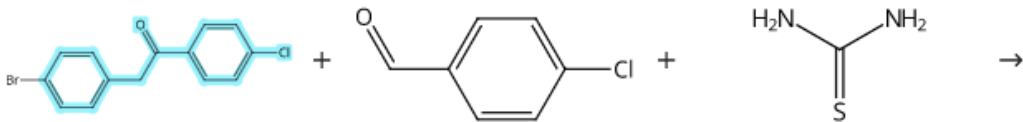
Experimental Protocols

Full Text

Collapse Scheme

Scheme 2 (1 Reaction)

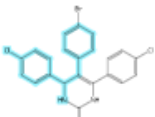
Steps: 1 Yield: 96%



Suppliers (9)


Suppliers (97)

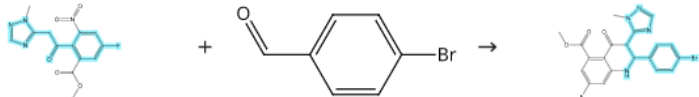
Suppliers (91)



反应检索—结果集筛选: Synthetic Methods™

Synthetic Methods™: 查看文献详情, 分类显示详尽信息, 方便操作

 CAS Reaction Number: 31-614-CAS-24450288



Suppliers (15)

Suppliers (89)



98%

Reaction Overview

Steps: 1 Yield: 98%

JOURNAL

DoE Optimization Empowers the Automated Preparation of Enantiomerically Pure [¹⁸F]Talazoparib and its In Vivo Evaluation as a PARP Radiotracer

By: Bowden, Gregory D. ; et al
[View All](#) 
Journal of Medicinal Chemistry (2021), 64(21), 15690-15701

[View PDF](#) [Full Text](#)

Company/Organization
Werner Siemens Imaging Center,
Department of Preclinical Imaging
and Radiopharmacy
Eberhard Karls University
Tuebingen 72076
Germany

Step 1

Stage	Reagents	Catalysts	Solvents	Conditions
1	Hydrochloric acid Titanium chloride (TiCl₃)	-	Methanol Tetrahydrofuran Water	rt; 30 min, rt; 2 h, 30 - 50 °C
2	Water	-	-	-

[Alternative Steps \(2\)](#)

Experimental Protocols

Synthetic Methods

Products [Methyl 2-\(4-bromophenyl\)-7-fluoro-1,2,3,4-tetrahydro-3-\(1-methyl-1H-1,2,4-triazol-5-yl\)-4-oxo-5-quinolinecarboxylate](#), Yield: 98%

Reactants [4-Bromobenzaldehyde](#)
[Benzoic acid, 5-fluoro-2-\[2-\(1-methyl-1H-1,2,4-triazol-5-yl\)acetyl\]-3-nitro-, methyl ester](#)

Reagents [Hydrochloric acid](#)
[Titanium chloride \(TiCl₃\)](#)
[Water](#)

Procedure

1. Suspend methyl 5-Fluoro-2-(2-(1-methyl-1H-1,2,4-triazol-5-yl)acetyl)-3-nitrobenzoate (8.1 g, 25.2 mmol) and 4-bromobenzaldehyde (8.9 g, 50.5 mmol) in THF (50 mL) and MeOH (10 mL).
2. Add titanium(III) chloride solution [20% wt solution in HCl (2 M), 130 mL, 6 equiv] to the resulting mixture in dropwise fashion over 30 minutes at room temperature.
3. Maintain the reaction temperature between 30 and 50°C for 2 hours.
4. Quench the mixture by the slow addition of water (260 mL).
5. Pour the reaction mixture into a separating funnel.
6. Extract the mixture with ethyl acetate (4 x 140 mL).
7. Pool the organic fractions.
8. Wash the organic fractions with NaHCO₃ (3 x 60 mL) and NaHSO₃ (3 x 100 mL).
9. Dry the organic fractions with sodium sulfate (Na₂SO₄).
10. Concentrate the solvent under reduced pressure to obtain a thick yellow syrup.
11. Wash the residue with aliquots of diethyl ether (3 x 10 mL), carefully.
12. Dry the resulting yellow syrup under high vacuum to obtain product.

Transformation Mannich Reaction/ Mannich-Type Reactions/ Biginelli Condensation
Condensation Reaction between Compounds with Active Hydrogen and Aldehydes or Ketones/
Knoevenagel Reaction
Reduction of Nitro Compounds to Amines

Scale gram

Characterization Data

^ 5-Quinolinecarboxylic acid, 2-(4-bromophenyl)-7-fluoro-1,2,3,4-tetrahydro-3-(1-methyl-1H-1,2,4-triazol-5-yl)-4-oxo-, methyl ester

State yellow amorphous solid

Transformations

1. Mannich Reaction/ Mannich-Type Reactions/ Biginelli Condensation
2. Condensation Reaction between Compounds with Active Hydrogen and Aldehydes or Ketones/ Knoevenagel Reaction
3. Reduction of Nitro Compounds to Amines

CAS Method Number 3-315-CAS-33168860

联合检索—结构与关键词

联用检索提高检索效率

Searching for...

References

Search by Keyword, Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. [Learn More](#)

Friedel-crafts acylation

AND Author Name Enter last name, first name middle name.

+ Add Advanced Search Field [Learn more about Sci](#)

Launch CAS Lexicon CAS Lexicon enables you to browse the CAS General Thesaurus to find indexed concepts and substances to build a Reference query with up to 1,000 indexed search terms.

Edit Drawing Remove

Reactions for AN 2011:601374

References

Filter Behavior

Filter by Exclude

Yield

80-89% (1)

70-79% (8)

50-69% (12)

Number of Steps

1 (21)

Non-Participating Functional Groups

Alkene (21)

Amine (21)

Cyclic alkene (21)

Secondary amine (14)

Tertiary amine (7)

[View All](#)

Reaction Mapping

21 Results

Group: By Scheme Sort: Yield View: Collapsed

Scheme 1 (1 Reaction) Steps: 1 Yield: 82%

Suppliers (84) Suppliers (100) Suppliers (11)

Expand Scheme

Scheme 2 (1 Reaction) Steps: 1 Yield: 78%

Suppliers (90) Suppliers (63) Suppliers (10)

Expand Scheme

References search for "Friedel-crafts acylation" + drawn structure

Substances Reactions Citing Knowledge Graph

1,100 Results Sort: Relevance View: Partial Abstract

As Drawn (1,100)

Substructure (2,270)

Filter Behavior

Filter by Exclude

Document Type

Journal (996)

Patent (68)

Review (31)

Conference (27)

Dissertation (1)

Preprint (8)

Substance Role

Reactant or Reagent (1,067)

Process (34)

Properties (29)

Full Text

Substances (40) Reactions (21) Citing (99) Citation Map

Hexafluoro-2-propanol-Promoted Intermolecular Friedel-Crafts Acylation Reaction

By: Valeriya, Rakesh H.; Aube, Jeffrey

Organic Letters (2016), 18(15), 3534-3537 | Language: English, Database: CAplus and MEDLINE

The intermol. Friedel-Crafts acylation was carried out in hexafluoro-2-propanol to yield aryl and heteroaryl ketones at room temperature without any addnl. reagents.

反应检索小结

1. 通过物质标识符、文献标识符、结构式进行反应信息检索
2. 反应结果集的浏览与筛选
3. 利用Synthetic Methods™查看文献中合成方法详情
4. 关键词与反应式的联合检索

大纲

- CAS Retrosynthesis Tool的使用
 - 获得已知化合物的逆合成反应路线
 - 获得未知化合物的逆合成反应路线



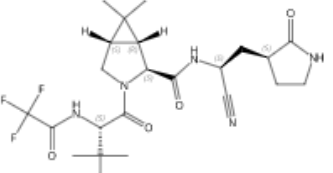
CAS Retrosynthesis Tool—由物质获得

获得已知化合物的逆合成路线（1）：

点击物质结构，弹出的物质菜单中点击 Start Retrosynthetic Analysis

1

2628280-40-8



Absolute stereochemistry shown

$C_{23}H_{32}F_3N_5O_4$

3-Azabicyclo[3.1.0]hexane-2-carboxamide, N-[(1S)-1-cyano-2-[(3S)-2-oxo-3-pyrroli...

236
References

53
Reactions

39
Suppliers

CAS RN
2628280-40-8

CAS Name
3-Azabicyclo[3.1.0]hexane-2-carboxamide, N-[(1S)-1-cyano-2-[(3S)-2-oxo-3-pyrroli...

Substance Detail

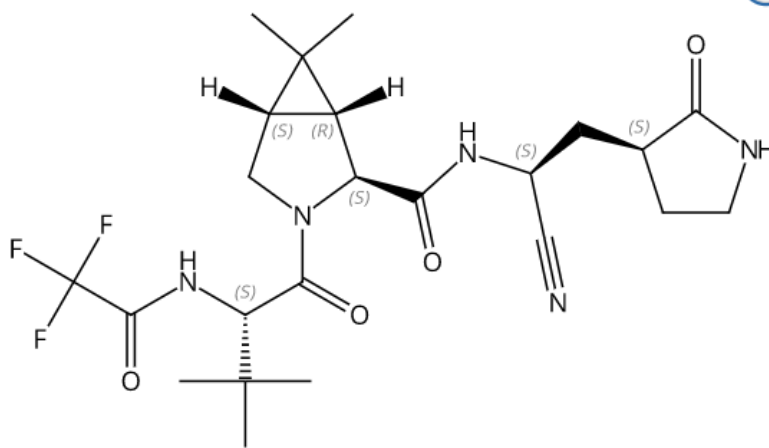
Reactions (53)

Synthesize (52)

Start Retrosynthetic Analysis

References (236)

Suppliers (39)



Absolute stereochemistry shown

Edit Structure

Reset

Download

CAS Retrosynthesis Tool:

- 逆合成反应路线设计功能
- 启发合成实验设计思路
- 高效获取逆合成反应路线

64

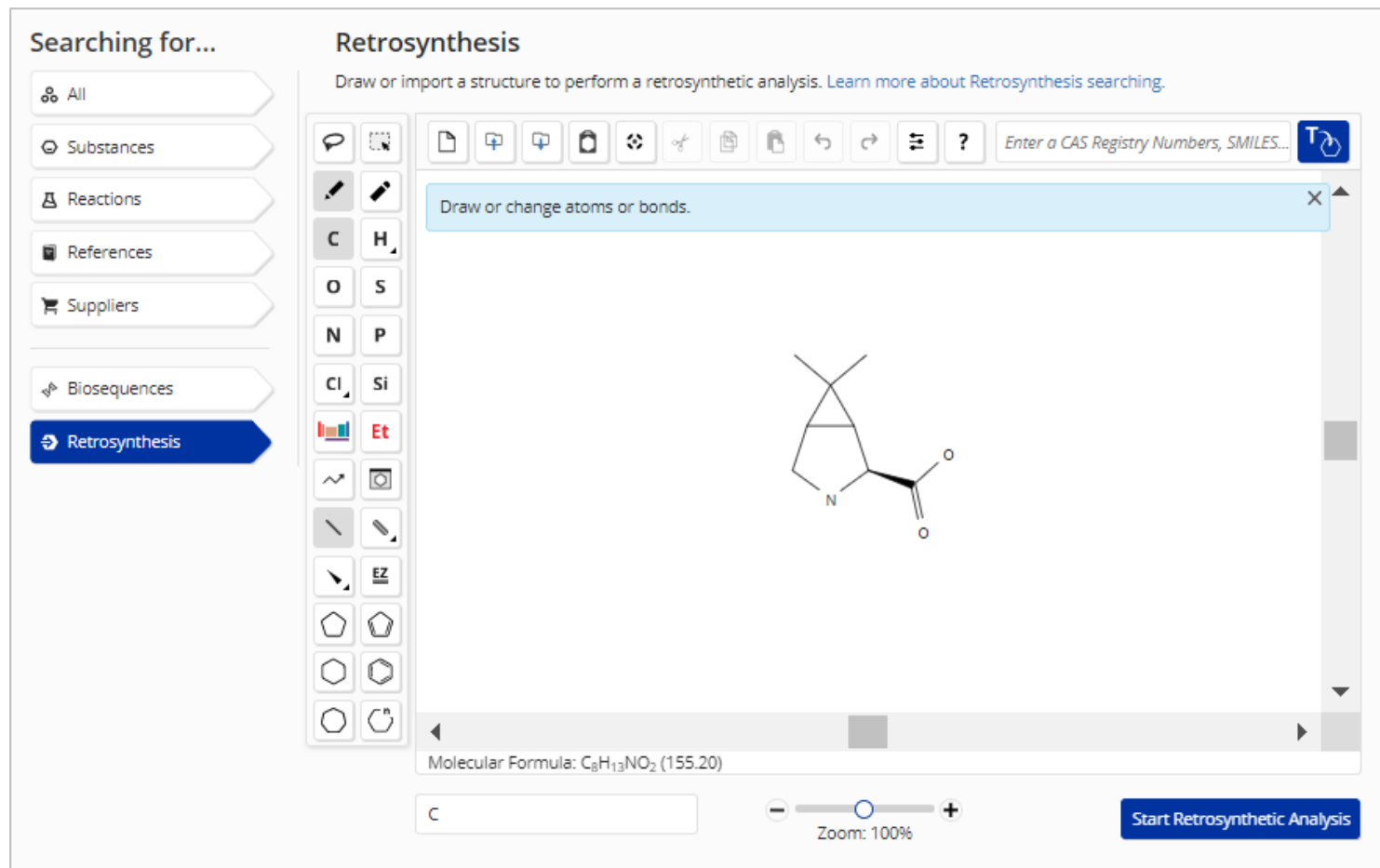
© 2023 American Chemical Society. All rights reserved.

CAS
A division of the
American Chemical Society

CAS Retrosynthesis Tool—直接绘制

获得已知化合物的逆合成路线（2）：

点击Retrosynthesis检索项，打开绘图板，绘制目标化合物，获得实验路线



CAS Retrosynthesis Tool—预设参数

预设反应路线参数：

反应深度

反应规则常见性

起始原料费用

设置断裂键或保护键

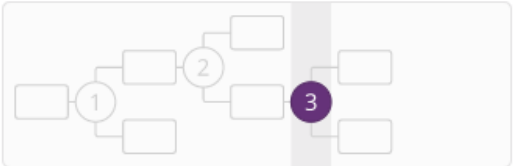
Retrosynthesis Plan Options for drawn structure

Powered by **ChemPlanner®**

Select Synthetic Depth

[Learn more.](#)

☐ 1
☐ 2
☒ 3
☐ 4



Set Rules Supporting Predicted Reactions

[Learn more.](#)

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

Set Starting Materials Cost Limit

[Learn more.](#)

USD/mol ▾

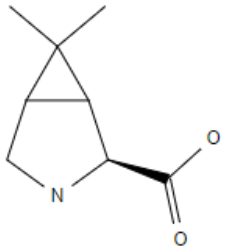
☐ Email me when my plan is complete

[↩ Create Retrosynthesis Plan](#)

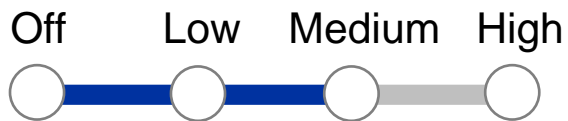
Break and Protect Bonds

[Learn more.](#)

[Clear All Bond Selections](#)



CAS Retrosynthesis Tool—路线概览



Scoring Profiles:

降低每步原料结构的复杂性

逆合成路线中前体的数量

支持预测路线的文献数量多少

预测路线大概成本

每步的产率

每步的原子转化效率

Retrosynthesis Plan for drawn structure

Powered by ChemPlanner®

Overview Steps Predicted Results ON

View Excluded Options

Plan Information 路线概览

Estimated Yield: 49%
Overall Price: \$96.82
(USD per 100 grams)

Commercially Available: A, B, C

Plan Options

Synthetic Depth: 3
Predicted Rules: Common
Break & Protect Bonds: No
Starting Material Cost Limit: \$100.00/mol
Edit Plan Options

Scoring Profiles 调节参数

Complexity Reduction

Convergence

Evidence

Cost

Yield

Retrosynthesis Step Key

Max Yield 97%

Max Yield -

Feedback

CAS Retrosynthesis Tool—路线详情

Reactions (1,181) Group: By Scheme View: Expanded

References

Scheme 1 (1 Reaction) Steps: 1

Reaction 1: 1-Ethyl-3-(2-dimethylaminopropyl)carbodiimide, 1-Hydroxybenzotriazole, Diisopropylethylamine + (S)-1-(cyclohexylmethyl)pyrrolidine-2-carboxamide + 4-Methylmorpholine N-oxide, 7-Azabenzotriazole-1-yl-N,N,N',N'-tetramethyluronium hexafluorophosphate

Reaction Summary

1.1 Reagents: 1-Ethyl-3-(2-dimethylaminopropyl)carbodiimide, 1-Hydroxybenzotriazole, Diisopropylethylamine
Solvents: Dichloromethane; overnight, rt

1.2 Reagents: Zileuton
Solvents: Acetic acid; 30 min, rt

1.3 Reagents: 4-Methylmorpholine N-oxide, 7-Azabenzotriazole-1-yl-N,N,N',N'-tetramethyluronium hexafluorophosphate
Solvents: Dimethylformamide; 16 h, rt

View Reaction Detail | Experimental Protocols

Collapse Scheme

Retrosynthesis Powered by ChemPlanner

Predicted Results ON

Overview Steps

View step specific evidence and alternate steps below or select the node between steps on the plan.

A \Rightarrow B + C + D
Average Yield: 37%
Evidence (1,181)
Alternative Steps (85)

B \Rightarrow E
Maximum Yield: 80%
Evidence (180,876)
Alternative Steps (20)

C \Rightarrow F + G
Maximum Yield: -
Evidence (1)
Alternative Steps (15)

E \Rightarrow H + I
Maximum Yield: -
Evidence (1)
Alternative Steps (24)

View All Alternatives (14)
View Evidence (4,737)
Exclude This Step

Retrosynthesis Step Key
Experimental Steps
Predicted Steps

Reset

- 快速获取最优的逆合成路线
- 可获取预测逆合成路线
- 可查看每步路线的详细条件
- 可自定义选择替代路线

CAS Retrosynthesis Tool—路线详情

点击Alternative Steps查看并选择替换路线，得到自定义的合成路线

Retrosynthesis Plan for drawn structure Powered by ChemPlanner®

Overview **Steps** Predicted Results ☒

View step specific evidence and alternate steps below or select the node between steps on the plan.

A ⇒ B + C + D
Average Yield: 41%
Evidence (1,209)
Alternative Steps (93)

B ⇒ E
Maximum Yield: 80%
Evidence (199,213)
Alternative Steps (15)

C ⇒ F + G
Maximum Yield: -
Evidence (1)
Alternative Steps (13)

D ⇒ H
Maximum Yield: -
Evidence (1)
Alternative Steps (58)

E ⇒ I + J
Maximum Yield: 92%
Evidence (22,464)
Alternative Steps (24)

View Excluded Options

Retrosynthesis Step Key

The diagram illustrates a retrosynthetic pathway starting from a complex molecule (A). It branches into several parallel paths. Path 1: A → B (14 alternatives) → E (3 alternatives) → I (86 alternatives) and J (42 alternatives). Path 2: A → C (0 alternatives) → F (43 alternatives) and G (95 alternatives). Path 3: A → D (103 alternatives) → H (86 alternatives). Each step is represented by a chemical structure and a box containing its maximum yield and the number of alternative steps available. A 'Retrosynthesis Step Key' is provided at the bottom left.

获取替代路线

A ⇒ B + C + D Alternative Steps (93)

Filter by

- Alternative Step Type
 - ☐ Predicted (93)
- Stereochemistry
 - ☐ Non-Selective (93)

1 of 34 Predicted Step

Chemical reaction scheme showing the conversion of a complex starting material to a product, with reagents and conditions indicated.

2 of 34 Predicted Step

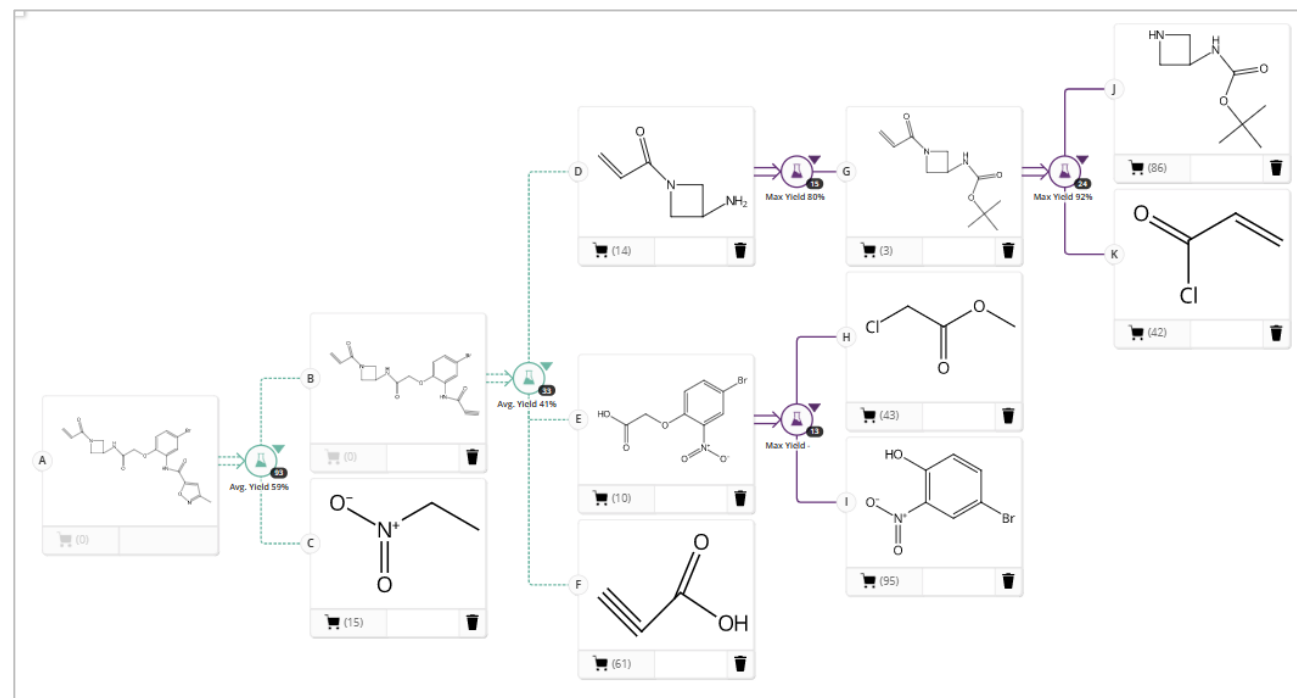
Chemical reaction scheme showing the conversion of a complex starting material to a product, with reagents and conditions indicated.

3 of 34 Predicted Step

Chemical reaction scheme showing the conversion of a complex starting material to a product, with reagents and conditions indicated.

Selected [View 1 similar Alternative](#) [View Evidence \(1,209\)](#) Average Yield: 41%

[Select](#) [View 7 similar Alternatives](#) [View Evidence \(277\)](#) Average Yield: 59%



逆合成路线小结

1. 通过物质结构获取已知化合物的逆合成路线
2. 获取预测的逆合成路线
3. 反应路线参数的预先设定与调节
4. 查看反应路线详情和文献支持，自定义选择替代路线

大纲

- CAS SciFinderⁿ中的序列检索
 - BLAST
 - CDR
 - Motif

视频链接:

https://american-chemical-society.zoom.us/rec/share/JPoebb74K7-dbzGw2Aj8vRqqeddB5zzBnQTV8MYcW2E2QQqq2rkYWoBtkHy_tt2.ag1fUmL880MKBne3?startTime=1647943207000

[下一节：反应检索](#)



Sequences Search™ — Blast检索

Searching for...

All

Substances

Reactions

References

Suppliers

Sequences

Retrosynthesis

Sequences

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

BLAST

CDR

Motif

Upload Sequence

Clear Search

Enter a query or upload a file...

Sequence Type:

Nucleotide

Protein

Search Within:

☐ Nucleotides

☒ Proteins

☒ Include NCBI Sequences

Start Sequence Search

Advanced Sequence Search

可选择是否包含NCBI中的序列

支持四种检索选择：
Protein-Protein
Protein-Nucleotides
Nucleotide-Nucleotides
Nucleotide-Proteins

高级检索—设置相关参数

Sequences

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

BLAST

CDR

Motif

Upload Sequence

Clear Search

AACAACAACATATCAAATCCTACTGGTGCCACAACCTGA

Sequence Type:

Nucleotide

Protein

Search Within:

☒ Nucleotides

☐ Proteins

☒ Include NCBI Sequences

Start Sequence Search

Advanced Sequence Search

Adjust Parameters for Short Sequences | Reset All

Alignment Identity %

Match with Gaps?

Gap Costs

Query Coverage %

Word Size

Reward for Match

Penalty for Mismatch

BLAST Algorithm

E-Value

Exclude Low Complexity Regions

80

☐ Yes

☒ No

Existence 5 Extension 2

90

11

2, -3

BLASTn

10

☐ Yes

☒ No

Query Sequence

Subject Sequence

QQLLVVEE

GG

|||||

QQLLVVEE

IGS

Alignment

Query Coverage (100%) = $\frac{\text{Alignment Length}}{\text{Query Length}} = \frac{10}{10}$

Subject Coverage (91%) = $\frac{\text{Alignment Length}}{\text{Subject Length}} = \frac{10}{11}$

Sequence Identity (90%) = $\frac{\text{Number of Matches}}{\text{Alignment Length}} = \frac{9}{10}$

Recent Search History

View All Search History

February 13, 2023

Sequences

11:26 AM

Sequence Type: Nucleotide

Search Within: Nucleotides

NCBI Included: Yes

BLAST Algorithm: BLASTn

Alignment Identity: 80%

Query Coverage: 90%

AACAACAACATATCAAATCCTACTGGTGCCACAACCTGA

View Results

Edit Options

Searching...

Recent Search History

View All Search History

February 13, 2023

Sequences

11:26 AM

Sequence Type: Nucleotide

Search Within: Nucleotides

NCBI Included: Yes

BLAST Algorithm: BLASTn

Alignment Identity: 80%

Query Coverage: 90%

AACAACAACATATCAAATCCTACTGGTGCCACAACCTGA

View Results

Edit Search

Complete

74

© 2023 American Chemical Society. All rights reserved.

CAS
A division of the
American Chemical Society

BLAST检索结果

- 序列一致性详情
- 目标序列
- 披露序列的专利文献

- 可视化地图

- 结果筛选

Sequences search for your query

References

BLAST Search Details

Sequence Type: Nucleotide
Search Within: Nucleotides
BLAST Algorithm: BLASTn
NCBI Included: Yes
Alignment Identity: 80%
Query Coverage: 90%
E-Value: 10
Match with Gaps?: No
Gap Costs: Existence 5
Extension 2
Word Size: 11

Bioscope Analysis

Visually explore sequence similarity with a new tool.
[Learn more about Bioscope.](#)

Create Bioscope Analysis

Filter by

▼ E-Value

▲ Query Coverage %

0 to 100

▲ Subject Coverage %

0 to 100

▲ Alignment Identity %

0 to 100

▲ Sequence Length

Query Details AACAAACATATCAAATCCTACTGGTGGCACAACCTTGA [View More](#)

170 Results

Sort: Alignment Identity View: Expanded

1 Alignment Identity: 100%

Query 1 39

Subject 1 595

Matches: 39
Mismatches: 0

View Less

Alignment Subject References

Alignment Data
BLAST Score: 78
E-Value: 7.79462e-12

Q 1 AACAAACA TATCAATCC TACTGGTGGC ACAACTTGA 39
S 393 AACAAACA TATCAATCC TACTGGTGGC ACAACTTGA 431

2 Alignment Identity: 100%

Query 1 39

Subject 1 813

Matches: 39
Mismatches: 0

View Less

Alignment Subject References

CAS Registry Number: 325380-52-7
NCBI Identifier: BG319743
Length: 813 nt
Organisms: Zea mays

Sequence

1 AAGAACAAA AGGATCAGCA GCCAGAGATG AGATGTAAGG TACTGATCCC CCATGCGCTT AGCTTAGCTT AACCCATGCC
81 CTAACATCTC GTACCCATAG CATAACAGGA ACACGAGGC AACTACTACA ACAACAAGGA CACGAGCAGC AAATTGTCTG
161 TCAGTCACG TACTAGAAAG AACAAACA TATCAATCC TACTGGTGGC ACAACTTGAC AGAGGGTCTA GAACGAGCTA

Download Sequence Results

File Type

☒ Excel (.xlsx)

☐ FASTA (.fasta)

Select Quantity

☒ All Results

☐ Range (ex. 2 to 20)

File Name

Sequences_20230213_1132

Download Cancel [Learn more about downloads.](#)

下载结果:

- 比对详情
- 序列长度参数
- 相关专利号
- 专利中的序列编号等

(Excel或FASTA格式)

BLAST检索结果

6

Alignment Identity: 100%

Query

1

39

Subject

1

1,060

Matches: 39

Mismatches: 0

View Less

Alignment

Subject

References

CAS Registry Number: 785872-37-9

Length: 1,060 nt

Sequence

1 CATTGGGTAC CTCGAGGCCG GCCGGGAGCT CGCACTCACT CACTCACAAG TCACACAGCC ACACTTGAAC CGTGCCCCG

81 AGCGGAGGGA GCTTGACGG GCCAACGCAC ACATAACACA AGCTCGTCGT CGATGGCGCG GTGGGCTGCG GTGCTGGCGC

161 TGGCCGCGGC CACGGCCATC GCCGTGGCGT CCGTGCGGG CGGCGACATG AACGCGGACA AGACGGAGTG CGCGGACCAG

241 CTGGTGGGCC TGGCGCCGTG CCTGCAGTAC GTGCAAGGGG AGGCCCGCGC GCCCGCGCC GACTGTGCG GCGGCTTGG

321 CCAGGTGCTG GGAAGAGCC CCAAGTGCT GTGCGTGCTC GTCAAGGACA AGGACGACCC CAACCTGGG ATCAAGATCA

Alignment

Subject

References

Nucleic acid molecules and other molecules associated with plants

Assignees: LA ROSA, THOMAS J.; ZHOU, YIHUA; KOVALIC, DAVID K.; CAO, YONGWEI; LIU, JINGDONG; CHEIKH, NORDINE; SHUKLA, HRIDAYABHIRANJAN; RUFF, THOMAS G.; HARDEMAN, KRISTINE J.; EDGERTON, MICHAEL D.; VARAGONA, MARGUERITE; WU, WEI; CONNER, TIMOTHY W.

US20120216318 A1 | Seq ID No: 16999

Nucleic acid molecules and other molecules associated with plants

Assignees: LA ROSA, THOMAS; ZHOU, YIHUA; KOVALIC, DAVID; CAO, YONGWEI; LIU, JINGDONG; CHEIKH, NORDINE; SHUKLA, HRIDAYABHIRANJAN; RUFF, THOMAS; HARDEMAN, KRISTINE; EDGERTON, MICHAEL; VARAGONA, MARGUERITE; WU, WEI; CONNER, TIMOTHY

US20040214272 A1 | Seq ID No: 16999

Nucleic acid molecules and other molecules associated with plants

Substance Detail

Reference (1) Reactions (0) Suppliers (0)

CAS Registry Number
785872-37-9

Image Not Available

Unspecified

DNA (Zea mays clone MRT4577_11549C.1 protein fragment-specifying cDNA) (9CI)

Nucleic Acid Sequence

Sequence Length: 1060

204 a, 336 c, 311 g, 209 t

Sequence Details

Sequence: DNA: linear

1	cattgggtac	ctcgaggccg	gccgggagct	cgcaactact	cactcacaag
51	tcacacagcc	acacttgaac	cgctccccgc	agcggaggga	gcttgacagg
101	gccaacgcac	acataacaca	agctcgtcgt	cgatggcgcg	gtgggctcgc
151	gtgctggcgc	tggccgcggc	cacggccatc	gccgtggcgt	ccgtggcggg
201	cggcgacatg	aacgcggaca	agacggagtg	cgcggaccag	ctggtgggcc
251	tggcgccgtg	cctgcagtac	gtcagggggc	agggccgcgc	gccgccgccc
301	gactgctcgc	gcggcctcgc	ccaggctcgt	gggaagagcc	ccaagtgcct
351	gtcgtgctc	gtcaaggaca	aggacgaccc	caacctgggc	atcaagatca
401	acgccaccct	cgcctcgcgc	ctccccaacg	cctcgggcgc	caccgcgcgc
451	aacgtctccc	actgcgtcca	gtcctcgtcat	attcccccg	gtccaaaga
501	cgccgcgctc	ttcagtcggc	gcagcgacaa	gggctccact	gccgtccag
551	ccaaggacaa	ctcagcgcg	acgacgact	ccgcgcgct	gcaggcgacc
601	accggacgcg	gcgtgtcctc	ctcggcgcg	accggcggtg	ctgcactcac

Other Names and Synonyms

1 Other Name for this Substance

1999: PN: US20040214272

Patent Annotations

Source: Zea mays

Reference: US20040214272. SEQID 16999: claimed

Feature	Location	Description
misc_feature		Clone ID: MRT4577_1154C.1

序列详情及相关的专利文献结果

References from your sequence

Substances

Reactions

Citing

Knowledge Graph

Open

Download

Email

Save

Filter Behavior

Filter by

Exclude

Document Type

☐ Patent (38)

Language

☐ English (38)

Publication Year

2005

2020

No Min

to

No Max

Apply

View Larger

Available at My Institution

Author

Organization

Publication Name

Concept

CA Section

Database

Search Within Results

Filter Content Report

Download filter data from this result set.

Download

38 Results

Sort: Publication Date: Newest

View: Full Abstract

1

Expressing Arabidopsis thaliana genes in plants for low low-nitrogen tolerance

By: Nadzan, Gregory; Schneeberger, Richard; Kim, Han Suk; Dang, David Van-Dinh; Feldmann, Kenneth A.; Pennell, Roger; Kwok, Shing; Zhang, Hongyu; Christensen, Cory; Okamura, Jack; et al
United States, US10815494 B2 2020-10-27 | Language: English, Database: CPlus

Methods and materials for modulating low-nitrogen tolerance levels in plants are disclosed. For example, nucleic acids encoding low nitrogen tolerance-modulating polypeptides are disclosed as well as methods for using such nucleic acids to transform plant cells. Also disclosed are plants having increased_{RLCL21} low-nitrogen tolerance levels and plant products produced from plants having increased low-nitrogen tolerance levels.

PatentPak

Full Text

Substance (1)

Reactions (0)

Citing (0)

Citation Map

2

Functionally-defined, sequence-determined DNA fragments and their use in genetic engineering of plants

By: Alexandrov, Nickolai; Brover, Vyacheslav; Feldmann, Kenneth A.; Makarov, Vladimir; Swaller, Timothy J.; Nadzan, Gregory; Mascia, Peter; Troukhan, Maxim; Rarang, Joel; Burns, James; et al
United States, US20170037422 A1 2017-02-09 | Language: English, Database: CPlus

Libraries of plant genomic fragments that are functionally-defined and sequenced, included identification of open reading frames and gene products, are described for use in plant improvement. Members of the library contain extensive and 5'- and 3'-UTRs that will allow expression in a plant host. The DNA mols. are useful for specifying a gene product in cells, either as a promoter or as a protein coding sequence or as an UTR or as a 3' termination sequence, and are also useful in controlling the behavior of a gene in the chromosome, in controlling the expression of a gene or as tools for genetic mapping, recognizing or isolating identical or related DNA fragments, or identification of a particular individual organism, or for clustering of a group of organisms with a common trait.

PatentPak

Full Text

Substance (1)

Reactions (0)

Citing (0)

Citation Map

Patent	Language	Kind Code	PatentPak Options
US20170037422	English	A1	PDF PDF+ Viewer
US20060107345	English	A1	PDF
US20120159672	English	A1	PDF
US20060150283	English	A1	PDF
US20060048240	English	A1	PDF
US20060168696	English	A1	PDF PDF+ Viewer
US20060066666	English	A1	PDF

77

© 2023 American Chemical Society. All rights reserved.

CAS
A division of the
American Chemical Society

Sequences Search™—Motif检索

Motif中有可变部分，可借助符号来表示：

“[]” 中括号：代表或者，表示出现在该位置的氨基酸或核苷酸是括号中的任意一个

“{ }” 大括号：代表氨基酸或核苷酸的重复次数。其中字段可用逗号开，{2, 6} 表示在大括号左边紧密相连的氨基酸可重复2-6次

Searching for...

All

Substances

Reactions

References

Suppliers

Sequences

Retrosynthesis

Sequences

Enter a protein or nucleotide string. [Learn more about Sequence Search.](#)

BLAST

CDR

Motif

Clear Search

[SG]x{4}GK[DT]

- X代表未指定氨基酸，可以是常见氨基酸、不常见氨基酸
- 对于核苷酸序列：N代表未指定核苷酸

Advanced Sequence Search ^

Reset All

Query Coverage % ⓘ

E-Value ⓘ

Combine Motif Results

90

10

☐

Sequence Type:

Nucleotide

Protein

☒ Include NCBI Sequences

Start Sequence Search

Motif检索结果

Motif Search Details

Sequence Type: Protein
NCBI Included: Yes
Query Coverage: 90%
E-Value: 10

Bioscape Analysis

Visually explore sequence similarity with a new tool.
[Learn more about Bioscape.](#)

Create Bioscape Analysis

Filter by

E-Value

Query Coverage %

Subject Coverage %

Alignment Identity %

Sequence Length

Organisms

☒ Homo sapiens (248)

☐ synthetic construct (23)

☐ unidentified (2)

☐ Mus musculus (1)

Query Details [View More](#)

> Seq 1: 1 SXXXXGKD 8

248 Results

Sort: Alignment Identity View: Expanded

1

Alignment Identity: 75%

Query 1 8

Subject 1 114

Matches: 6
Mismatches: 2

View Less

Alignment Subject References

Alignment Data
BLAST Score: 77
E-Value: 0.00104148

Q 1 SXXXXGKD 8
| | | | | ++
S 94 SXXXXXXD 101

2

Alignment Identity: 75%

Query 1 8

Subject 1 643

Matches: 6
Mismatches: 2

View Less

Alignment Subject References

CAS Registry Number: -
Length: 643 aa
Organisms: Homo sapiens
Sequence
1 MEKSSSCESL GSQPAARPP SVDLSAST SHSENSVHTK SASVVSSDSI STSADNFSPD LRVLRNSNKL AEMEEPPLLP

Sequences Search™—CDR检索

CDR (complementarity—determining regions): 抗体或细胞中的互补决定区

Searching for...

All

Substances

Reactions

References

Suppliers

Sequences

Retrosynthesis

Sequences

Enter a protein string, or upload a .txt or .fasta file. [Learn more about Sequence Search.](#)

BLAST

CDR

Motif

Upload Sequence

Clear Search

CDR1

RASQSVSGSRFTYMH

X

CDR2

YASILES

X

CDR3

QHSWEIPPWT

X

☐ Include NCBI Sequences

Start Sequence Search

支持单个或多个CDR序列检索并用

CDR检索结果

Sequences search for your query

References

CDR Segments

Select a segment below to view individual or intersecting CDR results.

CDR1 CDR2

2,316 2,469 16,182

58 200 44

665 CDR3

Apply

Reset Segments

Bioscape Analysis

Visually explore sequence similarity with a new tool.
[Learn more about Bioscape.](#)

Create Bioscape Analysis

Filter by

E-Value

0 to 10⁶

Query Coverage %

0 to 100

Subject Coverage %

Query Details [View Less](#)

> CDR1
RASQSVSGSRFTYMH

> CDR2
YASILES

> CDR3
QHSWEIPPWT

21,934 Results

Sort: Alignment Identity View: Expanded

1 Alignment Identity: 100%

Subject 1 112

CDR1 1 15

CDR2 1 7

CDR3 1 10

Matches: 32
Mismatches: 0

[View Less](#)

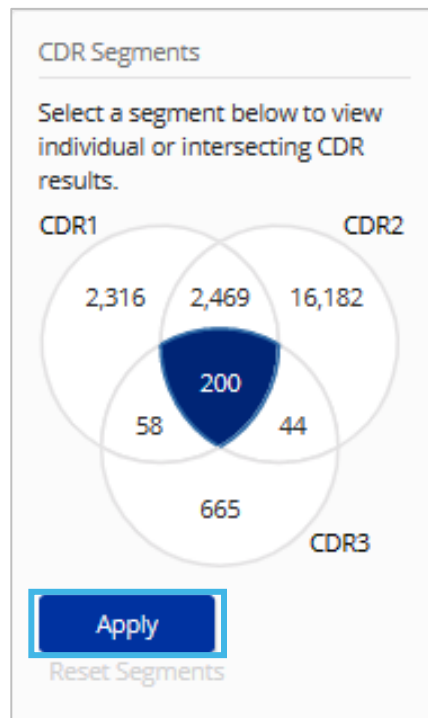
Alignment Subject References

Alignment Data
BLAST Score: 84
E-Value: 7.45568461509489

CDR1	1	RASQSVSGSR	FTYMH	15
S	24	RASQSVSGSR	FTYMH	38
CDR2	1	YASILES		7
S	54	YASILES		60
CDR3	1	QHSWEIPPWT		10
S	93	QHSWEIPPWT		102

References

获取披露该序列的文献



CDR Segments:

- 匹配到一个或者多个CDR的subject序列的序列数量
- 可根据已知信息和需求查看1-3个CDR被包含的序列结果

Reset segments:

- 重新选择查看匹配的序列结果

序列检索小结

- Sequences涵盖期刊、专利、NCBI当中的序列信息
- Sequences可以针对DNA/RNA的核苷酸序列、肽/蛋白的氨基酸序列进行检索
- 生物序列的获取方法：Sequences检索、物质名称/代码/结构式、关键词及文献-物质的数据关联
- Motif适合检索短序列，并支持可变部分输入
 - ✓ X代表未指定氨基酸，N代表未指定核苷酸
 - ✓ []表示出现在该位置的序列是括号里氨基酸/核苷酸中的任意一个
 - ✓ { } 代表氨基酸/核苷酸的重复次数，如重复次数是范围，用逗号将数字隔开，如{2, 6}

大纲

- 分析实验方法
 - 通过文献获得分析方法
 - 主题检索或分类浏览



分析实验方法的获取 (1)

方法一：在CAS SciFinder[®]的文献结果集页面，点击CAS solutions中的 Analytical Methods获得有具体分析实验方法的文献，从文献详情页中链接至分析实验方法

CAS SciFinder[®] References petroleum oil and analysis

References search for "petroleum oil and analysis"

Substances Reactions Citing Knowledge Graph

Based on your query, we've returned the most relevant results. Would you like to load the entire result set? [Learn about result relevance.](#)

Load More Results

Filter Behavior

Filter by Exclude

Document Type

Language

Publication Year

Available at My Institution

Author

Organization

Publication Name

Concept

CA Section

CAS Solutions

☒ Analytical Methods (612)

Formulus (17)

Database

Filtering: CAS Solutions: Analytical Methods

612 Results

Sort: Relevance View: Partial Abstract

1

Screening of soil for alcohol-extracted organic compounds by turbidity analysis

By: Sakai, Hiroyuki; Okada, Akira; Fujita, Takeshi; Wada, Shin-ichiro
Journal of the Faculty of Agriculture, Kyushu University (2011), 56(1), 93-97 | Language: English, Database: CAplus
| Analytical Methods

To quickly detect organic compounds in soil, a low-cost screening method has been developed to use a simple procedure without requiring specific reagents or equipment. This method semi-quant. detects organic compounds and indicates at concentration levels of 2,000 to 15,000 mg kg⁻¹. The indication will be helpful to know where grounds are polluted with organic compounds at a site, especially when tracking organic compounds in soil during remediation work.

Full Text

Substances (2) Reactions (0) Citing (2) Citation Map

2

Sensitivity improvement in ICP MS analysis of fuels and light petroleum matrices using a microflow nebulizer and heated spray chamber sample introduction

By: Caumette, Guilhem; Lienemann, Charles-Philippe; Merdrignac, Isabelle; Paucot, Hugues; Bouyssiere, Brice; Lobinski, Ryszard
Talanta (2009), 80(2), 1039-1043 | Language: English, Database: CAplus and MEDLINE
| Analytical Methods

Reasons for signal suppression during the anal. of light petroleum matrixes by inductively coupled plasma mass spectrometry (ICP MS) were examined. A decrease of the ionization efficiency of the plasma was the principal factor responsible for this loss of sensitivity. Consequently, an interface based on a total consumption micronebulizer and a heated spray chamber was constructed to alleviate this problem. A method based on flow-injection ICP MS using this interface was developed for the direct multielement anal. of undiluted fuels (gasoline, kerosene) and gas condensates offering an increase in sensitivity by at least a factor of 3-4 in comparison with the existing setups.

View More

Full Text

Substance (1) Reactions (0) Citing (56) Citation Map

Sensitivity improvement in ICP MS analysis of fuels and light petroleum matrices using a microflow nebulizer and heated spray chamber sample introduction

Substance (1) Reactions (0) Citing (55) Citation Map

JOURNAL

Source

Talanta
Volume: 80
Issue: 2
Pages: 1039-1043
Journal; Article
2009
DOI:
[10.1016/j.talanta.2009.08.017](https://doi.org/10.1016/j.talanta.2009.08.017)

CODEN: TLNTA2
E-ISSN: 1873-3573
ISSN-L: 0039-9140

Database Information

AN: 2009:1286528
CAN: 152:78583
PubMed ID: 19836594
CAplus and MEDLINE

Company/Organization

UMR 5254, LCABIE, Helioparc,
CNRS
UPPA
Pau 64053

By: Caumette, Guilhem; Lienemann, Charles-Philippe; Merdrignac, Isabelle; Paucot, Hugues; Bouyssiere, Brice; Lobinski, Ryszard

Reasons for signal suppression during the anal. of light petroleum matrixes by inductively coupled plasma mass spectrometry (ICP MS) were examined. A decrease of the ionization efficiency of the plasma was the principal factor responsible for this loss of sensitivity. Consequently, an interface based on a total consumption micronebulizer and a heated spray chamber was constructed to alleviate this problem. A method based on flow-injection ICP MS using this interface was developed for the direct multielement anal. of undiluted fuels (gasoline, kerosene) and gas condensates offering an increase in sensitivity by at least a factor of 3-4 in comparison with the existing setups.

Keywords: gasoline kerosene inductively coupled plasma mass spectrometry sensitivity plasma

View Source Full Text

Expand All Collapse All

Concepts

MEDLINE® Medical Subject Headings

Substances

Analytical Methods

Title	CAS Method Number
Analysis of Titanium in Kerosene by Inductively coupled plasma mass spectrometry	1-135-CAS-84928 ↗

分析实验方法详情

Analysis of Titanium in Kerosene by Inductively coupled plasma mass spectrometry

CAS MN: 1-135-CAS-84928

Method Category: Petroleum Product Analysis
Technique: Inductively coupled plasma mass spectrometry

实验原料

Materials	Role	Image	CAS RN
Cadmium	analyte	View Structure	7440-43-9
Mercury	analyte	View Structure	7439-97-6
Lead	analyte	View Structure	7439-92-1
Silver	analyte	View Structure	7440-22-4
Iron	analyte	View Structure	7439-89-6
Vanadium	analyte	View Structure	7440-62-2
Tin	analyte	View Structure	7440-31-5
Titanium	analyte	View Structure	7440-32-6
Chromium	analyte	View Structure	7440-47-3

Source

Sensitivity improvement in ICP MS analysis of fuels and light petroleum matrices using a microflow nebulizer and heated spray chamber sample introduction

Caumette, Guilhem; Lienemann, Charles-Philippe; Merdrignac, Isabelle; Paucot, Hugues; Bouyssiere, Brice; Lobinski, Ryszard

Talanta (2009), 80 (2), 1039 - 1043. Elsevier B.V.

CODEN: TLNTA2 | ISSN: 00399140 | DOI: 10.1016/j.talanta.2009.08.017 | [View in SciFinderⁿ](#)

Full Text ▾

Abstract ^

Reasons for signal suppression during the anal. of light petroleum matrixes by inductively coupled plasma mass spectrometry (ICP MS) were examined A decrease of the ionization efficiency of the plasma was the principal factor responsible for this loss of sensitivity. Consequently, an interface based on a total consumption micronebulizer and a heated spray chamber was constructed to alleviate this problem. A method based on flow-injection ICP MS using this interface was developed for the direct multielement anal. of undiluted fuels (gasoline, kerosene) and gas condensates offering an increase in sensitivity by at least a factor of 3-4 in comparison with the existing setups.

文献详情

Equipment Used

ICP-MS system, Elan 6000, PE-SCIEX1, PerkinElmer, ON, Canada

Microflow nebulizer

Syringe pump, 140C, Applied Biosystems, Foster City, CA, USA

Pump, Smartline Pump 1000, Knauer, Berlin, Germany

Thermostat, Neslab RTE-111, Thermo Fisher Scientific, Waltham, MA

Conditions

Instrument

RF power: 1300 W; Ar nebulizer gas: 0.8 L/min and auxiliary O₂ flow: 45 mL/min; integration time per isotope: 20 ms

Flow rate: 20 µL/min

Instructions

Sample Preparation

1. Collect petroleum samples (kerosene, gasoline and full range gas condensate).

Standards Preparation

1. Use conostans monoelemental standards in oil (1000 mg/kg) and multielemental S-21 oil (100 mg/kg) as standards.

ICP-MS analysis

1. Analyze the sample using a PerkinElmer Elan 6000 (PE-SCIEX1, ON, Canada).

2. Introduce the sample using microflow nebulizer consisting of a fused silica capillary of 180 µm i.d. (375 µm o.d.) and heated spray chamber (jacketed to allow the

分析仪器

分析条件

操作步骤

Validation

Linearity Range	1 - 250 µg/kg
Limit of Detection	0.8 µg/kg (gasoline), Titanium 0.1 µg/kg (gasoline), Vanadium 5 µg/kg (gasoline), Chromium 7 µg/kg (gasoline), Iron 0.04 µg/kg (gasoline), Silver 0.3 µg/kg (gasoline), Cadmium 0.2 µg/kg (gasoline), Tin 1 µg/kg (gasoline), Mercury 0.1 µg/kg (gasoline), Lead

数据有效性

分析实验方法的获取 (2)

方法二：登录<https://methods.cas.org>

- 主题检索或分类浏览；
- 筛选分析目标物、介质、方法类别、分析技术等

The screenshot shows the CAS Analytical Methods homepage. At the top, there's a search bar with the text "Enter keyword, matrix, analyte, etc." and a magnifying glass icon. Below the search bar, there's a section titled "Browse Method Categories" which lists various categories in a grid. A blue box highlights the "Food Analysis" category. To the right of the categories, there's a section titled "Recent Searches" with a link to "Browse: Pesticide Residue Analysis".

Search

方法分类: 13大类, 45小类

农业应用、生物鉴定、生物分子分离、环境、食品、考古、有机物、药学、毒理学等

Browse Method Categories

- Agricultural Applications / Analysis
- 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

Recent Searches

Browse: Pesticide Residue Analysis

The screenshot shows the search results page for "chromium sulfate". The left sidebar contains filters for Analyte, Matrix, Method Category, Technique, and Year. The main content area displays two search results. The first result is "Analysis of Copper by Solid phase extraction" with CAS MN: 1-142-CAS-235450. The second result is "Analysis of Copper in Seawater by Solid phase extraction" with CAS MN: 1-142-CAS-228765. Both results show details like Analyte, Matrix, Other Materials, Method Category, Technique, Equipment Used, and Source. A blue box highlights the "Add to Compare" button for the second result.

CAS Solutions Analytical Methods

chromium sulfate

Results (20)

Sort Relevance

Compare (2/3)

Remove from Compare

View Details & Instructions

Analyte: Copper; Nickel; Chromium; Trace heavy metals

Other Materials: Reagent: 2,2'-[[1-Methyl-1,2-ethanediyl]bis(nitriloethylidene)]bis[phenol]; Acetonitrile; Sodium dodecyl sulfate; α -Hydroxyacetophenone; Nitric acid; Propylenediamine; Hydrochloric acid; Ethanol; Methanol; Potassium hydroxide

Method Category: Trace Element Analysis; Suboptimal Analysis

Technique: Flame atomic absorption spectroscopy; Solid phase extraction

Equipment Used: pH/Ion meter; Stirrer; Atomic absorption spectrometer; Hollow cathode lamp; Water bath; Mechanical shaker

Source: A preconcentration procedure for copper, nickel and chromium ions in some food and environmental samples on modified Diaion SP-850

Shokrolahi, A.; Ghaedi, M.; Shabani, R.; Montazerzohori, M.; Chehreh, F.; Soylyak, M.; Alipour, S.

Food and Chemical Toxicology (2010), 48 (2), 482-489. Elsevier Ltd.

Full Text View in CAS SciFinder

Abstract

Add to Compare

分析方法的对比

Compare Methods		
<div>Expand All Collapse All</div>		
	1	2
Title	Analysis of Chromium in Barium sulfate by Electrothermal atomic absorption spectroscopy	Analysis of Chromium in Barium sulfate by Electrothermal atomic absorption spectroscopy
CAS Method Number	1-142-CAS-3223998	1-142-CAS-3186641
Method Category	Trace Element Analysis; Active Pharmaceutical Ingredient and Metabolite Analysis	Trace Element Analysis; Active Pharmaceutical Ingredient and Metabolite Analysis
Technique	Electrothermal atomic absorption spectroscopy	Acid digestion; Electrothermal atomic absorption spectroscopy
Analyte	Chromium	Chromium
Matrix	Barium sulfate	Barium sulfate
Other Materials	Nitric acid; Pyrolytic coated graphite tubes	Nitric acid
Equipment Used	Atomic absorption spectrometer, AAS ZEEit 60, Analytik Jena, Jena, Germany; Solid sampling system, SSA-5, Analytik Jena, Jena, Germany; Microbalance, M2P, Sartorius, View All	Atomic absorption spectrometer, AAS ZEEit 60, Analytik Jena, Jena, Germany; Microbalance, M2P, Sartorius, Gottingen, Germany; Sub-boiling system, duoPUR 2.01 E, View All
Conditions	Instrument: hollow cathode lamp power: 4 mA; wavelength: 357.9 nm; spectral bandpass: 0.8 nm; integration time: 12 s; atomization temperature: 2400 °C; pyrolysis temperature: View All	Instrument: hollow cathode lamp power: 4 mA; wavelength: 357.9 nm; spectral bandpass: 0.8 nm

Source	Chromium determination in pharmaceutical grade barium sulfate by solid sampling electrothermal atomic absorption spectrometry with Zeeman-effect background View All	Chromium determination in pharmaceutical grade barium sulfate by solid sampling electrothermal atomic absorption spectrometry with Zeeman-effect background View All
Preparation	<p>Collection and preparation of samples</p> <ol style="list-style-type: none"> Obtain the powdered pharmaceutical grade BaSO₄ samples from pharmaceutical industries and dry them in a conventional oven at 105 °C × 2 h. Spike the samples by addition of chromium reference solutions of 0.48 µg/g. <p>Preparation of standard solutions</p> <ol style="list-style-type: none"> Prepare the reference solutions daily by serial dilutions of stock chromium (Cr) solutions (1 g/L Cr in 2% HNO₃). <p>View Less</p>	<p>Preparation of nitric acid solution</p> <ol style="list-style-type: none"> Doubly distill the concentrated nitric acid in a Milestone sub-boiling system (model duoPUR 2.01 E, Bergamo, Italy) and use this for sample digestion/extraction. <p>Collection and preparation of samples</p> <ol style="list-style-type: none"> Obtain the powdered pharmaceutical grade BaSO₄ samples from pharmaceutical industries and dry them in a conventional oven at 105 °C × 2 h. <p>Preparation of standard solutions</p> <ol style="list-style-type: none"> Prepare the reference solutions daily by serial dilutions of stock chromium (Cr) solutions (1 g/L Cr in 2% HNO₃). <p>View Less</p>
Method	Direct solid sampling (DSS) - electrothermal-atomic absorption spectrometric (ETAAS) analysis 1. Carry out the chromium determinations using a model View All	Acid digestion procedure using nitric acid 1. Perform sample acid digestion (extraction) in closed quartz vessels using a high pressure model Multiwave View All
Linearity Range	100 - 1800 pg	
Limit of Detection	2.4 pg	
Recovery	98% - 103% in 0.48 µg/g spiked concentration	
Concentration	0.45 ± 0.04 µg/g (sample data)	0.32 ± 0.04 µg/g (sample data)

分析实验方法小结

1. 通过CAS SciFinderⁿ中的文献结果集获得关联的分析方法
2. 在Analytical Methods平台中，直接通过主题检索或分类浏览获取分析实验方法
3. 查看分析实验方法操作详情，筛选分析目标物、介质、分析方法

大纲

- 配方/制剂信息检索
 - 通过检索式检索配方/制剂
 - 通过文献获得配方/制剂信息



获取配方或制剂

方法（1）：在CAS SciFinder[®]的文献结果集页面，点击CAS solutions中的 Formulus 获得有具体配方或制剂信息的文献，从文献详情页中链接获取

References search for "encapsulat* and "resistant starch""

Substances Reactions Citing Knowledge Graph

Based on your query, we've returned the most relevant results. Would you like to load the entire result set?
[Learn about result relevance.](#)
[Load More Results](#)

Filter Behavior
[Filter by](#) [Exclude](#)

Document Type
Substance Role
Language
Publication Year
Available at My Institution
Author
Organization
Publication Name
Concept
CA Section
CAS Solutions
Bioactivity Data
Formulation Purpose

857 Results
Sort: Relevance View: Partial Abstract

1
Resistant starch from high-amylose maize increases insulin sensitivity in overweight and obese men
By: Maki, Kevin C.; Pelkman, Christine L.; Finocchiaro, E. Terry; Kelley, Kathleen M.; Lawless, Andrea L.; Schild, Arianne L.; Rains, Tia M. Journal of Nutrition (2012), 142(4), 717-723 | Language: English, Database: CAlus and MEDLINE
This study evaluated the effects of 2 levels of intake of high-amylose maize type 2 **resistant starch** (HAM-RS2) on insulin sensitivity (S_i) in participants with waist circumference ≥89 (women) or ≥102 cm (men). Participants received 0 (control starch), 15, or 30 g/d (double-blind) of HAM-RS2 in random order for 4-wk periods separated by 3-wk washouts. Minimal model S_i was assessed at the end of each period using the insulin-modified i.v. glucose tolerance test. The efficacy evaluable sample included 11 men and 22 women (mean ± SEM) age 49.5 ± 1.6 y, with a BMI of 30.6 ± 0.5 kg/m² and waist circ...
[View More](#)
Full Text Substances (9) Reactions (0) Citing (131) Citation Map

2
Conserved and variable responses of the gut microbiome to resistant starch type 2
By: Bendiks, Zachary A.; Knudsen, Knud E. B.; Keenan, Michael J.; Marco, Maria L. Nutrition Research (New York, NY, United States) (2020), 77, 12-28 | Language: English, Database: CAlus and MEDLINE
A review. **Resistant starch** type 2 (RS2), a dietary fiber comprised solely of glucose, has been extensively studied in clin. trials and animal models for its capacity to improve metabolic and systemic health. Because the health modulatory effects of RS2 and other dietary fibers are thought to occur through modification of the gut microbiome, those studies frequently include assessments of RS2-mediated changes to intestinal microbial composition and function. In this review, we identify the conserved responses of the gut microbiome among 13 human and 35 animal RS2 intervention studies. Consisten...
[View More](#)
Full Text Substance (1) Reactions (0) Citing (37) Citation Map

3
Impact of dietary intake of resistant starch on obesity and associated metabolic profiles in human: a systematic review of the literature

CAS Solutions

☒ Formulus (37)

☐ Analytical Methods (4)

Formulation Purpose

By Count Alphanumeric

定位配方或制剂的功能目标

4 Selected

<input checked="" type="checkbox"/> Food (7)	<input type="checkbox"/> Antibacterial agents (1)	<input type="checkbox"/> Gastrointestinal protective agents (1)
<input checked="" type="checkbox"/> Antidiabetic agents (6)	<input type="checkbox"/> Antihypertensives (1)	<input type="checkbox"/> Oral rehydration solutions (1)
<input type="checkbox"/> Dietary supplements (5)	<input checked="" type="checkbox"/> Antioxidants (1)	<input type="checkbox"/> Pharmaceutical adjuvants (1)
<input type="checkbox"/> Diet (3)	<input type="checkbox"/> Antitumor agents (1)	<input type="checkbox"/> Snack food (1)
<input checked="" type="checkbox"/> Drug delivery systems (3)	<input type="checkbox"/> Bakery products (1)	
<input type="checkbox"/> Antimicrobial agents (2)	<input type="checkbox"/> Beverages (1)	

[Apply](#) [Cancel](#)

获取制剂或配方相关信息

Resistant Starch Film-Coated Microparticles for an Oral Colon-Specific Polypeptide Delivery System and Its Release Behaviors

Substances (3) Reactions (0) Citing (42) Citation Map

JOURNAL

Source

Journal of Agricultural and Food Chemistry
Volume: 62
Issue: 16
Pages: 3599-3609
Journal: Evaluation Study; Article; Research Support, Non-U.S. Gov't
2014
DOI:
[10.1021/jf500472b](https://doi.org/10.1021/jf500472b)

CODEN: JAFCAU
E-ISSN: 1520-5118
ISSN-L: 0021-8561

Database Information

AN: 2014:519911
CAN: 160:534190
PubMed ID: 24684664
Capius and MEDLINE

Company/Organization

Ministry of Education Engineering Research Centre of Starch and Protein Processing, Guangdong Province Key Laboratory for Green Processing of Natural Products and Product Safety
South China University of Technology
Guangzhou 510640
China

Publisher

American Chemical Society

Language

English

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

By: Situ, Wenbei; Chen, Ling; Wang, Xueyu; Li, Xiaoxi

For the delivery of bioactive components to the colon, an oral colon-specific controlled release system coated with a resistant starch-based film through aqueous dispersion coating process was developed. Starch was modified by a high-temperature-pressure reaction, enzymatic debranching, and retrogradation, resulting in a dramatic increase in the resistibility against enzymic digestion (meaning the formation of resistant starch, specifically RS3). This increase could be associated with an increase in the relative crystallinity, a greater amount of starch mol. aggregation structure, and the formation of a compact mass fractal structure, resulting from the treatment. The microparticles coated with this RS3 film showed an excellent controlled release property. In streptozotocin (STZ)-induced type II diabetic rats, the RS3 film-coated insulin-loaded microparticles exhibited the ability to steadily decrease the plasma glucose level initially and then maintain the plasma glucose level within the normal range for total 14-22 h with different insulin dosages after oral administration; no hypoglycemia or glycemic fluctuation was observed. Therefore, the potential of this new RS3 film-coated microparticle system has been demonstrated for the accurate delivery of bioactive polypeptides or protein to the colon.

Keywords: starch film coated microparticle colon polypeptide delivery insulin

View PDF Full Text

Expand All Collapse All

- Concepts
- MEDLINE® Medical Subject Headings
- Substances
- Formulations**

Formulations

Resistant Starch (RS 3)Film-Coated Microparticles: Drug Delivery Systems--Controlled Release Drug Delivery Systems

[View CAS Formulus® Detail](#)

Location: SI Page 3 Article Page 2 Figure 1S

Purpose: Drug delivery systems

Target: 5-aminosalicylic acid

Component	成分	Function	功能	Amount Reported	用量
Group: bioactive component-loaded microparticle core		model active agent		-	
	5-Aminosalicylic acid	-		20 %	
	Cellulose	additives		Ratio: 3	
	Starch	excipients		Ratio: 1	
Group: RS3-based aqueous coating dispersion		coating materials		-	
	Starch	release control agent		-	
	(±)-Propylene glycol	plasticizers		10 %	
	Water	Solvents		-	

检索配方或制剂 <https://formulus.cas.org>

方法（2）：

- 登录CAS Formulus主页
- 在检索框输入检索式，如制剂或配方的原料、用途、物理形态、功能或文献识别符（包括专利号、DOI号和CA入库号）进行检索
- 支持高级检索

Searching for...

🔍 Formulations

🔍 Ingredients

🔍 Formulation Designer

Design custom formulations templates based on selections and ingredients.

Formulations

Search for Formulations by Ingredient, Purpose, Form, Function, etc.

orthopedic and implant

🔍

Try [Advanced Search](#) for a more precise search experience

- 制药、化妆品、食品、农化、油墨、涂料等多领域中的配方
- 工艺、成分、目标成分的常见配伍成分、设计配方、探索合规要求等

配方/制剂结果集

- 利用聚类项精简结果：
行业、配方/制剂用途、物理形式、物质状态、递送方式、涵盖信息、文献类型、发表机构、发表年份
- 可查看制剂或配方成分，功能及用量
- 可查看原料详情
- 支持对比选中的制剂或配方
- 支持查看或下载专利全文
- 可查看制剂或配方详情

Formulations search for "orthopedic and implant"

Get Additional References

Compare (0/3) [icon] [icon] [icon] Save

1,064 Results Sort: Relevance

Filter by

- Industry
 - ☐ Cosmetics & Personal Care
 - ☒ Pharmaceutical
 - ☐ Unclassified
- Purpose
 - ☐ Drug delivery systems (296)
 - ☐ Antitumor agents (107)
 - ☐ Pharmaceutical formulations (81)
 - ☐ Ophthalmic agents (73)
 - ☐ Antipsychotics (65)
- Physical Form
 - ☒ Pharmaceutical implants (1,064)
 - ☐ Tablets (315)
 - ☐ Capsules (226)
 - ☐ Powders (207)
 - ☐ Suspensions (154)
- State of Matter
- Delivery Route
- Information Included
 - ☐ Component Amount (1,393)
 - ☒ Process (1,064)
 - ☐ Experimental Activity (721)
 - ☐ Effective Dose (164)
- Document Type
 - ☐ Journal (309)
 - ☐ Article (309)
 - ☐ Patent (755)

View All

1

Implants: Antitumor Agents

Location: Article page 3, 6, 7, 8, 9

Purpose: Antitumor agents

Physical Form: **implant**

Add to Compare

Component	Function	Amount Reported
Group: Ti-TNTs wire implants	implant	-
Ti wires	additives	-
Acetone	Solvents	-
Ethanol	Solvents	-
Perchloric acid	additives	1

Additional group components reported

Trail aqueous solution - 2 mg/mL

View Formulation Detail

2

Composition for Promoting Bone Formation

Location: Claim 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41

Purpose: promoting bone formation

Target: Amphibia, Ape, Aves, Bos taurus, Canis familiaris, Capra, Cavia porcellus, Equus caballus, Felis catus, Fish, Gerbil, Hamster, Homo sapiens, Monkey, Mus musculus, Oryctolagus cuniculus, Ovis aries, Rattus, Reptilia, Swine

Delivery Route: Intraosseous prosthetic implants, intramedullary application

Physical Form: **pharmaceutical implants**

Add to Compare

Component	Function	Amount Reported
Group: surgical implant	-	-
Dental implants	-	-
Plates	-	-
pin	-	-
screw	-	-

Additional group components reported

JOURNAL

Titanium wire implants with nanotube arrays: A study model for localized cancer treatment

Biomaterials

Language: English

Full Text View in CAS SciFinder

PATENT

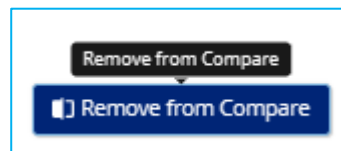
Use of pro-inflammatory compounds for promoting bone formation

Assignee: Imperial Innovations Limited


WO2011007135



Language: English

Patent PDF View in CAS SciFinder



查看制剂或配方详情

 **Implants: Antitumor Agents**


  Save

Purpose	Target	Delivery Route	Physical Form	Source
Antitumor agents	-	-	implant	View

Formulation Ingredients [Expand All Groups](#) | [Collapse All Groups](#)

Component	Function	Amount Reported	Optionality
^ Group: Ti-TNTs wire implants	implant	-	Mandatory
Ti wires	additives	-	Mandatory
Acetone	Solvents	-	Mandatory
Ethanol	Solvents	-	Mandatory
Perchloric acid	additives	1	Mandatory
butanol	Solvents	6	Mandatory
ethylene glycol electrolyte	solid support material	9	Mandatory
Water	Solvents	-	Mandatory
Trail aqueous solution	-	2 mg/mL	Mandatory

More Formulations like this... **NEW**




Ha-NP with HASE: Antitumor Agents
Purpose: Antitumor agents
Target: -
Delivery Route: -
Physical Form: Particles

CIPRODEX: Antibacterial
Purpose: Antibacterial agents
Target: Haemophilus influenzae, Hom...
Delivery Route: AURICULAR (otic)
Physical Form: Liquids, Suspensions

CIPRODEX Ciprofloxacin and Dexamethasone Suspension/ Drops: Antibacterial Agents or...
Purpose: Antibacterial agents, corticos...
Target: Haemophilus influenzae, Hom...
Delivery Route: AURICULAR (optic)...
Physical Form: Liquids, Suspensions

Ha-NP-Loaded Microneedle Patch: Antitumor Agents
Purpose: Antitumor agents
Target: Neoplasm
Delivery Route: skin absorption
Physical Form: Pharmaceutical patches



Process

stage 1: Ti-TNTs wire implants were loaded overnight with 2 mg/mL Trail aqueous solution for in-vitro, ex-vivo and in-vivo studies. prior to loading, implants were cleaned with ethanol, dried under sterile conditions and placed in a 30 mL drops of Trail solutions placed on a parafilm strip. after overnight drug loading, implants were dabbed with a soft tissue and dried and placed in PBS solution to monitor drug release profile at 37 °C, over a range of selected time points.

- 制剂或配方原料
- 相似的制剂或配方
- 制备工艺
- 制剂或配方实验评估
- 专利来源

Experimental Activity

Descriptor	Notes	Details
Ex-vivo study	-	no caspase-3 activity was observed for PBS-TNTs samples
cell death	-	highest cell death was observed in Trail-TNTs
drug release	-	45 %
in-vitro cytotoxicity	-	luciferase activity confirmed 100% cell death in Trail-TNTs
loading amount	-	12.63 µg

Source Journal

Titanium wire implants with nanotube arrays: A study model for localized cancer treatment

Biomaterials
Language: English
Location: Article page 3, 6, 7, 8, 9

[Full Text](#) [View in CAS SciFinder®](#)

94

© 2023 American Chemical Society. All rights reserved.

CAS
A division of the
American Chemical Society

不同制剂或配方信息的对比

Comparing your Formulations			P Predicted value
	Formulation 1	Formulation 2	
Title	Implants: Antitumor Agents	Composition for Promoting Bone Formation	
Purpose	Antitumor agents	promoting bone formation	
Target	-	Amphibia, Ape, Aves, Bos taurus, Canis familiaris, Capra, Cavia porcellus, Equus caballus, Felis catus, Fish, Gerbil, Hamster, Homo sapiens, Monkey, Mus musculus, Oryctolagus cuniculus, Ovis aries, Rattus, Reptilia, Swine	
Delivery Route	-	Intraosseous prosthetic implants, intramedullary application	
Physical Form	implant	pharmaceutical implants	
Experimental Activity	Available	Not Available	
Components	<p>Group: Ti-TNTs wire implants Function: implant Amount Reported: Optionality: Mandatory</p> <p>Ti wires Function: additives Amount Reported: - Optionality: -</p> <p>Acetone Function: Solvents Amount Reported: - Optionality: -</p> <p>Ethanol Function: Solvents Amount Reported: - Optionality: -</p> <p>Perchloric acid Function: additives Amount Reported: 1 Optionality: -</p> <p>Trail aqueous solution Function: - Amount Reported: 2 mg/mL Optionality: -</p>	<p>Group: surgical implant Function: Amount Reported: Optionality: Mandatory</p> <p>Dental implants Function: - Amount Reported: - Optionality: -</p> <p>Plates Function: - Amount Reported: - Optionality: -</p> <p>pin Function: - Amount Reported: - Optionality: -</p> <p>screw Function: - Amount Reported: - Optionality: -</p> <p>Group: pro-inflammatory compound Function: bone formation promoters Amount Reported: Optionality: Mandatory</p> <p>1-Methyl-L-tryptophan Function: dioxygenase 1 inhibitors, 3, indoleamine 2</p>	

- 选择感兴趣的制剂或配方进行对比
- 一次最多可以比较三种不同制剂或配方的信息详情

高级检索

[← Return to Home](#)

Advanced Formulations Search

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

At least two search terms are required.

Search For	Operator	Enter one term
Function ▼	Optional ▼	Anticorrosion
Ex: binder, surfactant, carrier		

Search For	Operator	Enter one term
All Fields ▼	Optional ▼	coating
General search of all fields		

Add Another Term

 Search

- All Fields ▼
- All Fields
- Form
- Function
- Ingredient
- Purpose
- Route
- Target

- Optional ▼
- Required
- Optional
- Excluded

Clear All

检索原料

Searching for...

Formulations

Ingredients

Ingredients

Search by Ingredient Name, CAS Registry Number, or Function

propylene glycol

Q

Ingredients search for "propylene glycol"

Filter by

Industry

☐ Agrochemical

☐ Cleaning & Surfactant Products

☐ Cosmetics & Personal Care

☐ Food & Related

☐ Inks, Paints, & Coatings

☒ Pharmaceutical

View All

Regulatory Information

☐ REACH (5)

☐ Cosing: Cosmetic Ingredient Inventory (3)

☐ EPA Pesticide Inactive Ingredients (3)

☒ FDA Inactive Ingredients Database (3)

☐ ANMAT (1)

View All

Experimental Properties

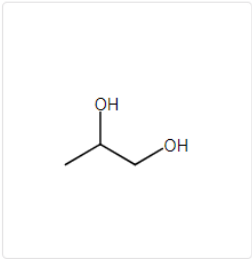
☐ Boiling Point (3)

2 Selected 3 Results

1

CAS RN: 57-55-6

View Details



C₃H₈O₂

(±)-Propylene glycol

Propylene glycol

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/cm ³	Temp: 25 °C

Commonly Used As: Solvents; Carriers; Plasticizers; Humectants; Antifreeze...

Similar Ingredients with Regulatory Information

27194-74-7

Propylene glycol monolaurate

29387-86-8

Propylene glycol butyl ether

30136-13-1

Propylene glycol monopropyl ether

View 14 More

Commonly Formulated With | Regulatory Information | Experimental Properties

Formulations

Suppliers

Add to Designer

- 使用该原料的制剂或配方
- 原料供应商信息
- 可将原料添加至Formulation Designer

- 制剂或配方中，与该原料同时使用的其它配伍成分
- 管控信息及清单
- 实验属性

设计制剂或配方

Searching for...

 Formulations

 Ingredients

 Formulation Designer

Formulations

Search for Formulations by Ingredient, Purpose, Form, Function, etc.



Try [Advanced Search](#) for a more precise search experience

设计配方/制剂

Formulation Designer

* All fields are required

Industry

Cosmetics & Personal Care ▾

Pharmaceutical

Cosmetics & Personal Care

Agrochemical

Cleaning & Surfactant Products

Food & Related

Inks, Paints, & Coatings

Purpose

Skin care products

▾

Physical Form

Gels

▾

Active or Featured Ingredient

Enter one term

Vitamin A

×

Enter one term

polyethylene glycol

×

At least 1 and up to 5 ingredients can be added.

Add Another Ingredient

Create!

Clear All

Purposes (Showing top 100)

Top Count

Alphanumeric

Search

Select the purpose you would like to use:

Cosmetics and Personal care products	Skin care products	Antiarthritics
Skin conditioners	Analgesics	Bath preparations
Hair dyes	Antitumor agents	Transdermal drug delivery systems
Sunscreens	Allergy inhibitors	Insecticides
Hair preparations	Wetting agents	Hair care products
Antiperspirants	Wound healing promoters	Astringents
Cleaning compositions	Dyes	Semiconductor materials
Skin-lightening cosmetics	Fungicides	Insect repellents
Skin cleansers	Stabilizing agents	Sunless tanning products
Oral hygiene products	Whitening agents	Immunostimulants
Shampoos	Depilatories	Anti-Alzheimer agents
Makeup	Skin-darkening agents	Preservatives
Cosmetic fragrance products	Coating materials	Fabric softeners
Deodorants	Permeation enhancers	Food

Cancel

Physical Forms (Showing all 53)

Top Count

Alphanumeric

Search

Select the physical form you would like to use:

Emulsions	Sprays	Cosmetic sticks
Cream preparations	Pharmaceutical ointments	Eyeshadows
Cosmetic lotions	Powders	Films
Cosmetic packs	Cosmetic ointments	Hair conditioners
Gels	Essences	Lipsticks
Liquids	Hydrogels	Mascaras
Nanospheres	Oils	Milk
Solutions	Particles	Paper towels
Capsules	Effervescent materials	Pharmaceutical carriers
Pastes	Foundation cosmetics	Pharmaceutical lotions
Tablets	Pharmaceutical suppositories	Pharmaceutical pastes
Aerosols	Skin moisturizers	Skin cleansers
Foams	Freeze-dried drug delivery systems	Skin conditioners
Cosmetic gels	Coating materials	Skin toners





Cancel

查看制剂或配方设计结果详情

Base Selections

Industry	Purpose	Physical Form	Active or Featured Ingredient
Cosmetics & Personal Care	Skin care products	Gels	Vitamin A polyethylene glycol
Edit	Edit	Edit	Edit

Template

Function	Ingredient	Regulatory 	Top Alternatives	Amounts
Active or Featured Ingredient:	Vitamin A	ANMAT	-	Amount not available 
Active or Featured Ingredient:	polyethylene glycol	ANMAT; CosIng: Cosmetic Ingredient Inventory; Drug Master File List; EPA Pesticide Inactive Ingredients; FDA GRAS (Part 181, Subpart B); FDA Inactive Ingredients Database	-	Amount not available 
Function: Carriers	Polyethylene glycol View More Alternatives	ANMAT; CosIng: Cosmetic Ingredient Inventory; Drug Master File List; EPA Pesticide Inactive Ingredients; FDA GRAS (Part 181, Subpart B); FDA Inactive Ingredients Database	Water; Ethylene glycol	Approximate Range: 3 - 4% 
Function: Skin conditioners	Glycerol View More Alternatives	ANMAT; CosIng: Cosmetic Ingredient Inventory; Drug Master File List; EMA Excipients List; EPA Pesticide Inactive Ingredients; FDA GRAS (Part 182,	Allantoin; Ethylene glycol; 1,2-Octanediol; Tricaprin; Palm-oil glycerides, monoglycerides, diglycerides and triglycerides, hydrogenated	Approximate Range: 3 - 11%

Alternati

Select the

Allant

Ethyle

1,2-O

- 原料详情
- 原料管制信息
- 可替代的原料选项

Alternative Ingredients (Showing all 7)

Select the ingredient you would like to use:

[Allantoin](#)
[Ethylene glycol](#)
[1,2-Octanediol](#)

[Tricaprin](#)
[Palm-oil glycerides, monoglycerides,
diglycerides and triglycerides,](#)

[hydrogenated](#)
[Glyceryl polyacrylate](#)
[N-\(2-Hydroxyethyl\)acetamide](#)

配方/制剂信息检索小结

1. 通过检索原料、用途、物理形态、功能或文献识别符获得配方/制剂信息
2. 检索原料
3. 配方或制剂的设计
4. 通过文献结果集获得关联的配方/制剂信息
5. 查看配方/制剂详情
6. 对比不同配方/制剂信息

大纲

- CAS及CAS SciFinderⁿ简介
- 常见检索方式
 - 文献检索
 - 物质检索 (CAS Markush*)
 - 反应检索
 - 生物序列检索*
 - 逆合成反应路线设计 (CAS Retrosynthesis*)
 - 分析实验方法 (CAS Analytical Methods)
 - 配方/制剂信息检索 (CAS Formulus)
- 常见问题及解答

如何获取CAS SciFinderⁿ账号

（登录贵校图书馆网站，查看注册相关的链接和说明）

--CONTACT INFORMATION--

First Name:

Last Name:

Email:

Confirm Email:

Phone Number:

Fax Number:

Area of Research:

Job Title:

--USERNAME AND PASSWORD--

Username: [Tips](#)

Password:

Re-enter Password:

--SECURITY INFORMATION--

Security Question:

Answer: [Why?](#)

请注意：

- 1.必须输入真实姓名和**学校**邮箱。
- 2.用户名必须是唯一的，且包含 5-15 个字符。它可以只包含字母或字母组合、数字和/或以下特殊字符：
 - -（破折号）
 - _（下划线）
 - .（句点）
 - @（表示“at”的符号）
- 3.密码必须包含 7-15 个字符，并且至少包含**三种以下字符**：
 - 字母
 - 混合的大小写字母
 - 数字
 - 非字母数字的字符（例如 @、#、%、&、*）例：abc@123
- 4.从下拉列表选择一个密码提示问题并给出答案。
单击 Register（注册）。

Registration Already Complete

You have already completed your registration. For assistance with accessing SciFinder, consult the key contact for your organization.

点击激活链接后注册成功；之后直接点击<https://SciFinder-n.cas.org>访问。

CAS SciFinderⁿ检索浏览器推荐

浏览器推荐：

- Windows (7, 8.1, 10): Chrome 60及更高版本, Firefox 55及更高版本, Firefox 52 (ESR)、Edge 15及更高版本
- Mac OS X (10.11, 10.12, 10.13): Safari 9.3及更高版本, Chrome 60及更高版本, Firefox 55及更高版本, Firefox 52 (ESR)
- 不建议使用360浏览器，相关功能或插件会被自动拦截

使用注意事项

- 一人注册一个帐号
- 实名注册，需提供真实姓名信息（中文名用汉语拼音全拼）
- 不得过量下载（<https://www.cas.org/legal/infopolicy>）
- 不得账号分享
- 不得将账号用于非学术研究

常见问题

Unauthorized IP Address

User registration is available only from IP addresses specified by the key contact at your organization. Please try to register again from an authorized location.

- 检查注册链接是否正确
- 确认连入校园网，且不是通过VPN连接
- 如果链接正确，且在校园内，请联系图书馆或china@acs-i.org

常见问题



There was a problem verifying your account.

Try Again

Contact Us

Or [Log Out](#) and try again.

Reference Id: GU75LMf9IZnhTq8mymUog

- 确认账号密码是否正确
- 如果账号密码正确，请填写问题报告后联系图书馆或china@acs-i.org

学习资源



CAS SciFinder®学习中心



预告: 2023 CAS SciFinder Discovery Platform 论坛



<https://mp.weixin.qq.com/s/TGX0QrkeYySH76nBx1QSaw>

回顾: 2022 CAS SciFinder®论坛合集



THANK YOU!



美国化学文摘社北京代表处

ACS International, Ltd. – Representing CAS
Unit 1010, Tower B, Raycom InfoTech Park
2 Kexueyuan Nanlu, Haidian District, Beijing, China
+86-10-6250 8026/7
cas.org

