

CAS SciFinder Discovery Platform (Academic)

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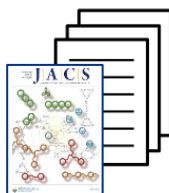
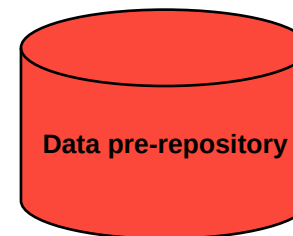
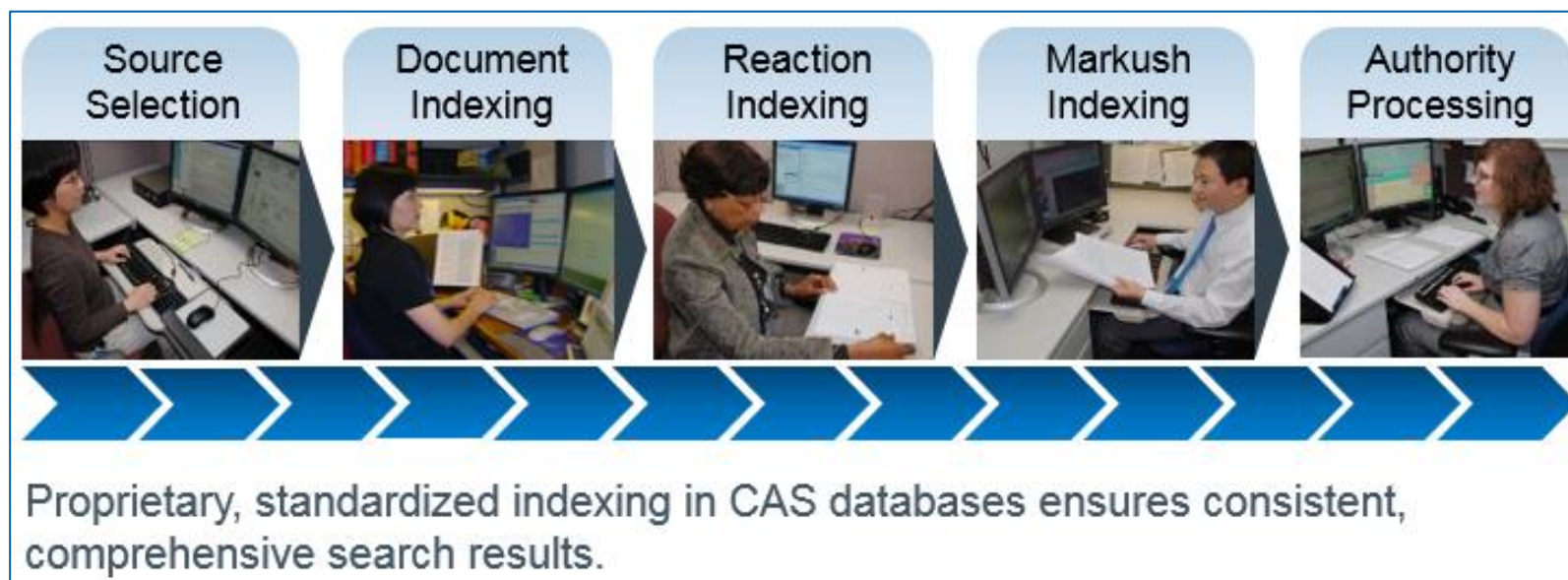
刘子露
ZLiu@acs-i.org
美国化学文摘社(CAS)北京代表处



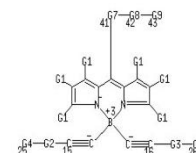
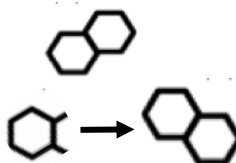
大纲

- 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

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A division of the American Chemical Society

SCIFINDER DISCOVERY PLATFORM

CAS SciFinder[®]

CAS Analytical Methods

CAS Formulus

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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

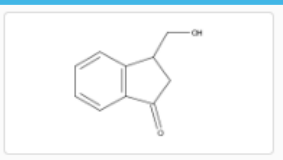
Enter last name, first name middle name.

+ Add Advanced Search Field

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

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
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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', followed by a field for 'Author Name' with the placeholder text 'Enter last name, first name middle name.' and an 'X' button. An example 'Schubert, J A' is shown. Below this is a '+ Add Advanced Search Field' button and a link to 'Learn more about SciFinder[®] Advanced Search.' At the bottom, there is a 'Launch CAS Lexicon' button 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'-ethylhexyloxy)-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

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 usin...

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

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

Database

Search Within Results

Filter Content Report

Download filter data from this result set.

排序方式：
相关性
引用次数
收录号
发表时间

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 ×

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

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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)	☒ Current density (50)	☒ Coating materials (30)
☐ Fluoropolymers (343)	☒ Hydrogels (50)	☐ Electrolytes (29)
☐ Electric conductivity (155)	☐ Humans (48)	☐ Sheet resistance (29)
☐ Electrodes (128)	☐ Polymers (48)	☐ Surface area (29)
☒ Surface structure (124)	☐ Carbon black (47)	☒ Skin (28)
☐ Homo sapiens (117)	☐ Electronics (47)	☐ Supercapacitor electrodes (28)
☐ Human (117)	☒ Nanowires (47)	☐ Cyclic voltammetry (27)
☐ Nanofibers (101)	☐ Electric capacitance (45)	☐ Dielectric loss (26)
☐ Electric current-potential relationship (100)	☐ Piezoelectric materials (44)	☐ Energy storage systems (26)
☐ Polyesters (92)	☐ Electric potential (41)	☐ Lithium-ion secondary batteries (26)
☐ Carbon nanotubes (86)	☐ Electronic device fabrication (40)	☐ Plastic films (26)
☒ Flexibility (84)	☐ Triboelectric nanogenerators (40)	☐ Strain (26)
☐ Stress-strain relationship (83)	☐ Electric impedance (39)	☐ Surface roughness (26)
☐ Electrospinning (82)		☐ Bending (25)

Apply

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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)	☐ Nanofibril (2)	☒ Nanosheets (23)
☐ Carbon nanotube fibers (4)	☒ Nanofilms (6)	☒ Nanospheres (1)
☒ Carbon nanotubes (86)	☐ Nanofilters (1)	☐ Nanostructured materials (9)
☐ Cellulosic nanofibers (1)	☒ Nanoflakes (2)	☐ Nanostructures (18)
☒ Core-shell nanoparticles (1)	☐ Nanoflowers (2)	☐ Nanotechnology (4)
☐ Electric nanogenerators (24)	☐ Nanohorns (1)	☐ Nanotubes (12)
☒ Metal Nanoparticles (3)	☐ Nanoimprint lithography (1)	☐ Nanotubes, Carbon (11)
☐ Nanoantennas (1)	☐ Nanoparticles (53)	☒ Nanowires (47)
☐ Nanocoils (2)	☐ Nanoparticle size distribution (2)	☐ Pharmaceutical nanocarriers (1)
☒ Nanocomposites (63)	☐ Nanoplatelets (3)	☐ Pharmaceutical nanocomposites (2)
☐ Nanocrystals (4)		

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

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

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

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: CAlplus 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...

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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: CAlplus

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 el...

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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, Yir; Lu, Baoyang; Gu, Guoqing

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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

Switching 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

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Full Text

Concepts

Substances

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CAS科学家提供的标准技术术语

Concepts

Electric resistance

Polythiophenes

Role: Properties; Technical or Engineered Material Use

Elongation at break

Strain sensors

Hydrogels

Stress-strain relationship

Open circuit potential

Tensile strength

Piezoelectric sensors

Wearable devices

原文中重点研究的物质信息

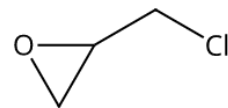
Substances

Substances (7)

2839834-68-1

106602-18-0

Image Not Available



(C₃H₅ClO.Unspecified)_x

Role: Properties, Synthetic Preparation, Preparation

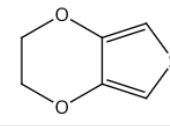
1219717-04-0

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Role: Properties, Technical or Engineered
Material Use, Uses

126213-51-2



(C₆H₆O₂S)_x
Poly(3,4-ethylenedioxythiophene)

Role: Properties, Technical or Engineered
Material Use, Uses

Notes: polystyrenesulfonate-doped

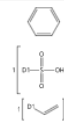
106602-18-0

Image Not Available

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

Role: Reactant, Reactant or Reagent

50851-57-5

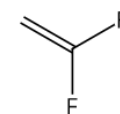
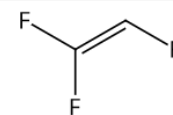


(C₈H₈O₃S)_x
Poly(styrenesulfonic acid)

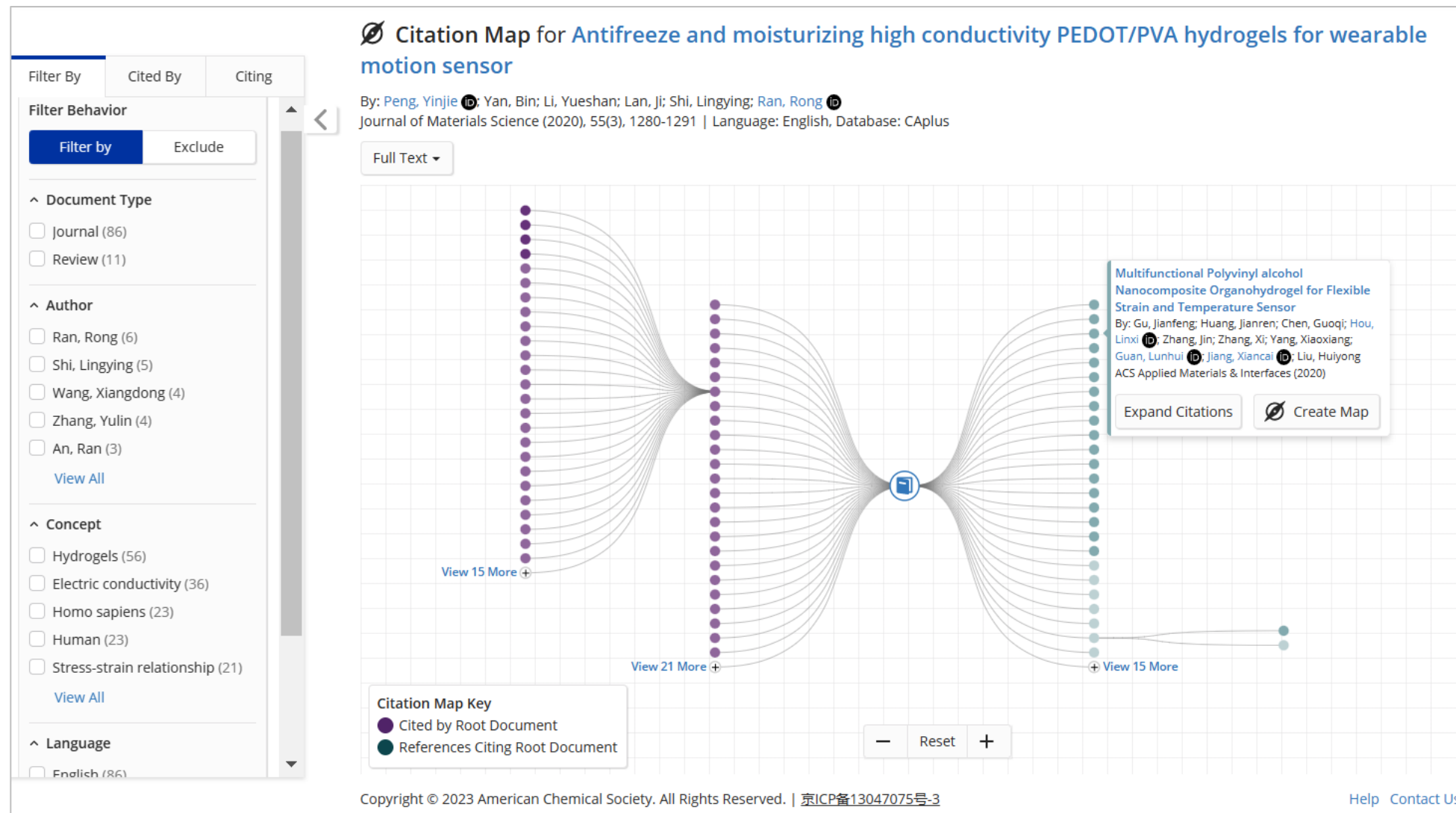
Role: Properties, Technical or Engineered
Material Use, Uses

Notes: PEDOT dopant

28960-88-5



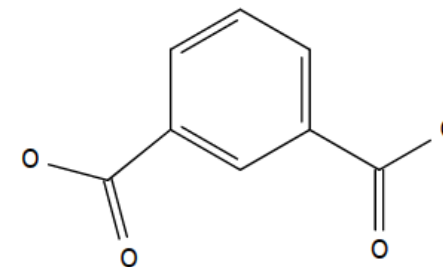
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例1：检索与特定（亚）结构及MOF相关的文献？

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Metal-organic framework

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1

Scalable Green Synthesis and Full-Scale Test of the Metal-Organic Framework CAU-10-H for Use in Adsorption-Driven Chillers

By: Lenzen, Dirk; Bendix, Phillip; Reinsch, Helge; Froehlich, Dominik; Kummer, Harry; Moellers, Marc; Huegenell, Philipp P. C.; Glaeser, Roger; Henninger, Stefan; Stock, Norbert 

Advanced Materials (Weinheim, Germany) (2018), 30(6), n/a | Language: English, Database: CAPus and MEDLINE

The demand for cooling devices has increased during the last years and this trend will continue. Adsorption-driven chillers (ADCs) using water as the working fluid and low temperature waste energy for regeneration are an environmentally friendly alternative to currently used cooling devices and can concurrently help to dramatically decrease energy consumption. Due to the ideal water sorption behavior and proven lifetime stability of $[\text{Al}(\text{OH})(\text{m-BDC})] \cdot x\text{H}_2\text{O}$ ($\text{m-BDC}^{2-} = 1,3\text{-benzenedicarboxylate}$), also denoted CAU-10-H, a green very robust synthesis process under reflux, with high yields $\geq 95\%$ is developed.

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Full Text

Substances (6)

Reactions (0)

Citing (104)

Citation

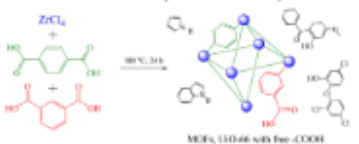
2

UiO-66-Type Metal-Organic Framework with Free Carboxylic Acid: Versatile Adsorbents via H-bond for Both Aqueous and Nonaqueous Phases

By: Song, Ji Yoon; Ahmed, Imteaz; Seo, Pill Won; Jhung, Sung Hwa

ACS Applied Materials & Interfaces (2016), 8(40), 27394-27402 | Language: English, Database: CAPus and MEDLINE

Versatile Adsorbents in Aqueous and Non-aqueous Media



The metal-organic framework (MOF) UiO-66 was synthesized in one step from zirconium chloride and isophthalic acid (IPA), together with the usual link material, terephthalic acid (TPA). UiO-66 with free -COOH can be obtained in a facile way by replacing up to 30% of TPA with IPA. However, the chem. and thermal stability of the synthesized MOFs decrease with increasing IPA content used in the syntheses, suggesting an increase in the population of imperfect bonds in the MOFs because of the asym. structure of IPA. The obtained MOFs with free -COOH were applied in liquid-phase adsorptions from...

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Substances (7)

Reactions (0)

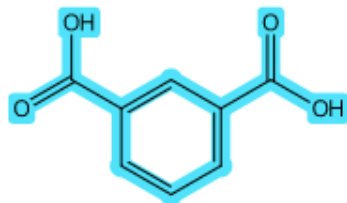
Citing (98)

Citation Map

Substances

Substances (7)

121-91-5

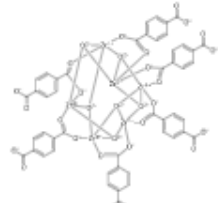


$\text{C}_8\text{H}_6\text{O}_4$
Isophthalic acid

Role: Reactant, Reactant or Reagent

Notes: hydrogen bonding complex with UiO-66, triclosan, oxybendazole, indole and pyrrole; ligand exchange with UiO-66

1072413-80-9



$\text{C}_{48}\text{H}_{24}\text{O}_{30}\text{Zr}_6$
Hexakis[μ-[1,4-benzenedicarboxylato(2-)-κO¹:κO¹]]hexa-μ₃-oxohexazirconium

Role: Properties, Synthetic Preparation, Preparation

Notes: hydrogen bonding complex with triclosan, oxybendazole, indole and pyrrole

文献检索—主题词+结构联合检索

例2：如何检索含Fe/Ni/Cr/Ti 高熵合金的相关文献？

The screenshot shows the CAS SciFinder interface. The search query is "High entropy alloy". The left sidebar includes filters for "Substance Role" (Properties, Process, Uses, Preparation, Nanoscale) and "Publication Year" (2002 to 2023). The main search results area shows two results. The first result is "Phase evolution and magnetic characteristics of TiFeNiCr and TiFeNiCrM (M = Mn, Co) high entropy alloys" by Mishra, Rajesh K.; Shahi, Rohit R. The second result is "Microstructures and properties of high-entropy alloys" by Zhang, Yong; Zuo, Ting Ting; Tang, Zhi; Gao, Michael C.; Dahmen, Karin A.; Liaw, Peter K.; Lu, Zhao Ping. A blue box highlights the "Substances (3)" filter in the second result, with a callout box containing the elements Fe, Ni, Cr, and Ti, and the text "由文献获得物质" (Material obtained from literature).

Substance Role 物质在文献中的研究角色

The Substance Role filter panel shows a list of roles with checkboxes and counts. The roles are: Properties (417), Industrial Manufacture (112), Physical, Engineering, or Chemical Process (387), Synthetic Preparation (37), Process (387), Modifier or Additive Use (14), and Uses (387). The "Properties (417)" and "Industrial Manufacture (112)" roles are selected.

The Concept filter panel shows a list of concepts with checkboxes and counts. The concepts are: Stress-strain relationship (95), Yield strength (82), Vickers hardness (81), Annealing (70), Heat treatment (65), Grain size (62), Mechanism (15), Ball mill (15), Precipitation hardening (34), Solid solutions (34), Temperature (34), Face-centered cubic crystals (32), Tensile strength (32), X-ray diffraction (32), Atomization, physical (16), Corrosion (16), Grain refinement (16), Mixing enthalpy (16), Particle size distribution (16), and Crystal dislocations (15). The "Solid solutions (34)" and "Fracture toughness (16)" concepts are selected.

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- 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 "solar cell"

Substances ▾

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Database: CHEMZENT X

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☐ 1

Experiments over the photoelectric fatigue of alkali metals

By: Bergwitz, K.

Chemisches Zentralblatt (1907), 78 Book 2(6), 439-439 | Language: German, Database: CHEMZENT

Machine Translated: Periodically ELSTER and GEITEL produced Na-, K- und Rb-Zellen (cathode solid alkali metal anode Al in a water fabric vacuum of 0.33) can be in exposure to visible light no fatigue determining nor to one cell with liquid K-Na-Legierung, the surface of which in the vacuum renew it. In one **photoelectric cell** by exposure induced current by a sensitive telephone are detected.

CheMZent

Full Text ▾

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

☐ 2

Light electric cell

By: H., Polyphos Elektrizitäts-Gesellschaft m. b.

Chemisches Zentralblatt (1908), 79 Book 2(14), 1223-1223 | Language: German, Database: CHEMZENT

Machine Translated: Light electrical cell. For photo electric cells the deposition of photoelectric active particles to the anode to prevent aims at the anode of those on the deposited particles to free, is the anode with one heating device provided by, for forming the to be heated anode of a platinum wire, by unite electric current heated so that the anode itself as heating device. Wherein **photoelectric cells**, the electrodes being in a diluted gas filled space, can be for example the cathode comprises rubidium and the anode of a platinum wire, which latter at two sites to the glass wall is sealed so that the pla...

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439

liefern, kann P_2S_5 in Zündmassen, z. B. Streichhölzern (man zieht 200—300 von Holz befreite Streichholzköpfe mit CS_2 aus), durch B. der Jodverb. nachgewiesen werden. (Chem.-Ztg. **31**. 640. 26/6.) GROSCHUPF.

John Theodore Hewitt und Thomas Field Winmill, Arsenidjodid. Das von BAMBERGER und PHILIPP (Ber. Dtsch. Chem. Ges. **14**. 2643) beschriebene Arsenidjodid hat das nach LANDSBERGER in CS_2 bestimmte Mol.-Gew. As_2J_4 . K., konz. H_2SO_4 wirkt auf die Verb. nicht ein; ebenso scheint k., rauchende HNO_3 nur wenig zu reagieren, während beim Erwärmen Oxydation erfolgt. Pyridin zers. die Substanz unter Abscheidung von As und Auflösen von AsJ_3 . Sd. Essigsäureanhydrid löst ebenfalls; beim Abkühlen scheidet sich eine gelbe, nicht homogene Substanz ab, welche wahrscheinlich zum größten Teil ein Derivat des AsJ_3 ist. Fügt man feingepulvertes AsJ_3 zu 4 Mol. Magnesiumphenylbromid in Ä., so erhält man ein unl. Öl, welches bei der Zers. mit verd. H_2SO_4 Triphenylarsin, $As(C_6H_5)_3$ (PFEIFFER, Ber. Dtsch. Chem. Ges. **37**. 4620; C. **1905**. I. 147), farblose Nadeln aus verd. A., F. 160°, liefert. Demnach erfolgt der Übergang des Dijodids in Arsen-trijodid so leicht, daß man es kaum zur direkten Synthese von Kakodylverb. verwenden können wird. (Proceedings Chem. Soc. **23**. 150. 30/5.; Journ. Chem. Soc. London **91**. 962—64. Juni. East London Coll.) FRANZ.

Henri Louis Dejust, Über einige oxydierende und entfärbende Eigenschaften des Graphits. Graphit entfärbt bekanntlich Lackmustinktur, Rotwein und Indigoschwefelsäure. Um die Entfärbungskraft des Graphits zu messen, hat Vf. 1 g Graphit mit 42 ccm einer Lackmustinktur, welche 9,8 g Trockenextrakt im l enthielt, je 30 Sekunden lang geschüttelt, die Fl. filtriert und die Farbe der Filtrate verglichen. Untersucht wurde ungereinigter, pulverisierter Graphit mit 79 % C-Gehalt und ein gereinigter Graphit mit 93,1 % C-Gehalt. Die Entfärbung der Lackmustinktur war im letzteren Falle eine weniger intensive. Durch 5 g Graphit wurden 100 ccm der Lackmustinktur völlig entfärbt. Die Rk. der zu entfärbenden Fl. war bei dem gereinigten Graphit einflußlos, während sie bei Tierkohle einen großen Einfluß auf die Entfärbung besaß. — Der Graphit besitzt eine oxydierende Wrkg., analog derjenigen der Tierkohle. So nimmt eine p-Phenylendiaminlsg. an der Luft in Ggw. von Graphit eine braune Färbung an. Andererseits kann der Graphit ohne direkte Mitwirkung der Luft entfärbend wirken. (C. r. d. l'Acad. des sciences **144**. 1264—65. [10/6.*]) DÜSTERBEHN.

K. Bergwitz, Versuche über die lichtelektrische Ermüdung an Alkalimetallen. An den von ELSTER und GEITEL hergestellten Na-, K- und Rb-Zellen (Kathode festes Alkalimetall, Anode Al in einem Wasserstoffvakuum von 0,33 mm) läßt sich

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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: CPlus

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, CH:CH, CH(Me)R⁵; R¹, R² = C₁₋₄-alkyl, (CH₂)_n-P, ((CH₂)₂O)_n-R⁶, W; R³, R⁴ = H, NO₂, halogen, SO₃⁻, C₁₋₄-alkoxy, (CH₂)_mCOOR⁷; 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, CH₂OCOR⁸; R⁸ = Me, tBu; R = COOR⁷, SO₃⁻, OH; W = mono- or di-substituted nitrobenzyl; n = 1-1...

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Key Substances in Patent

WO 2005/118839

3.2 Preparation of Compound (3)

To 1-(3,5-dinitrobenzyl)-2,3,3-trimethyl-3H-indolene (1.59g) was added 3-(5-carboxypentyl)-1,1,2-trimethyl-3,4-dihydroxy-3-cyclobuten-1,2-dione (3.45ml) and acetic anhydride (1ml). The mixture was stirred for 24 hours and the solvent then stripped using rotary evaporation. Column chromatography was performed (EA/MeOH) and the relevant fractions combined and concentrated. The resulting material was further purified by 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-benzothiazolylidenemethyl)-4-(1-(2-methoxyethoxy)ethyl)-3,3-dimethyl-2-indolylidenemethyl)cyclobutenediylum-1,3-diolate (Compound (4))

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

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

CAS RN 1640-39-7
CAS Name 2,3,3-Trimethylindolenine

Chemical Structure: 2,3,3-Trimethylindolenine

Chemical Structure: Compound (4)

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
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 - 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

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

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- 高级检索

物质检索—物质名称、CAS RN、代码

The screenshot displays the CAS SciFinder search results page. At the top, the search bar contains 'Paxlovid 2628280-40-8'. Below the search bar, the results are organized into two columns. The left column shows results for '2628280-40-8', including a chemical structure and the text 'Absolute stereochemistry shown'. The right column shows results for '2803933-60-8', also including a chemical structure and the text 'Absolute stereochemistry shown'. On the left side of the page, there is a 'Filter Behavior' section with options for 'Reaction Role' (Product, Reactant) and 'Reference Role' (Adverse Effect, Analyte, Analytical Study, Biological Study, Biological Study, Unclassified). Below this, there are sections for 'Commercial Availability', 'Number of Components', and 'Molecular Weight'. At the bottom of the results, there are buttons for 'References', 'Reactions', and 'Suppliers' for each result. The 'References' button for the first result is highlighted with a red box.

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

$C_{23}H_{32}F_3N_5O_4$

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

319 References 106 Reactions 39 Suppliers

2

2803933-60-8

Absolute stereochemistry shown

$C_{37}H_{48}N_6O_5S_2 \cdot C_{23}H_{32}F_3N_5O_4$

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

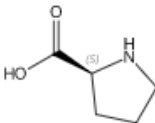
Commercial Availability

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

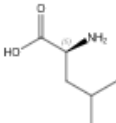
10 Results

Sort: Molecular Formula: Ascending View: Partial

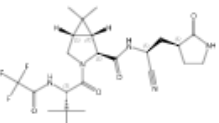
1 147-85-3


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

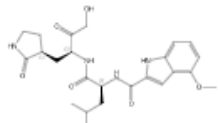
2 61-90-5


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

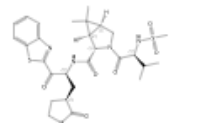
4 2628280-40-8


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-pyrr...

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(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

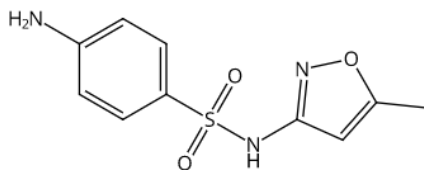
References (24K)

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

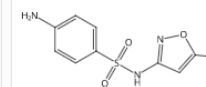
(1) Spectral data were obtained from Life Chemicals

(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

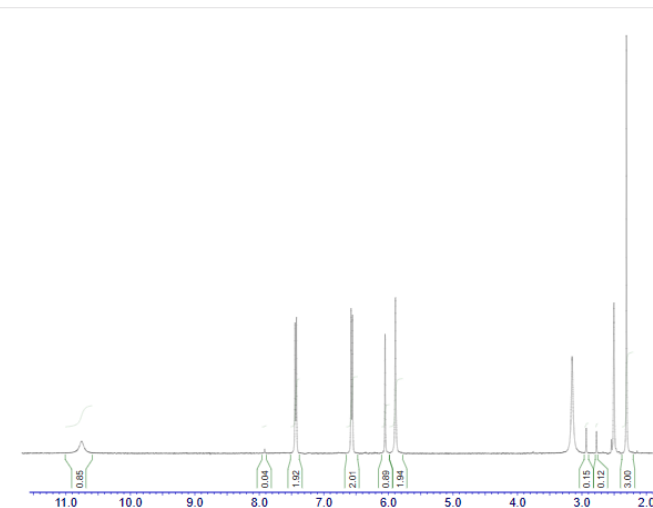
Spectrum Summary

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

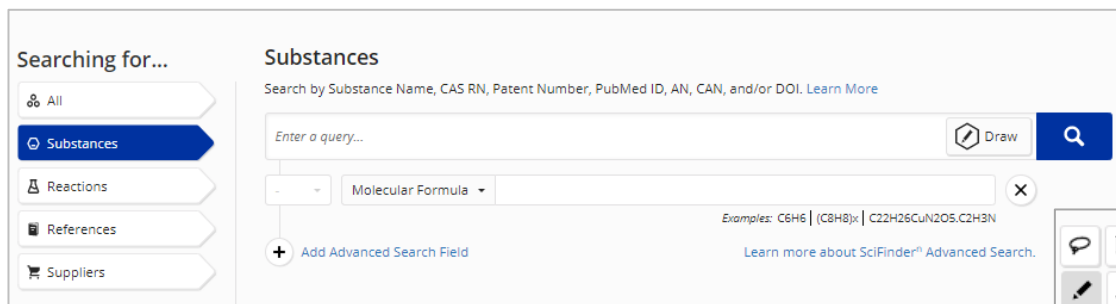
Toxicity CAS LIFE SCIENCES

Parameter

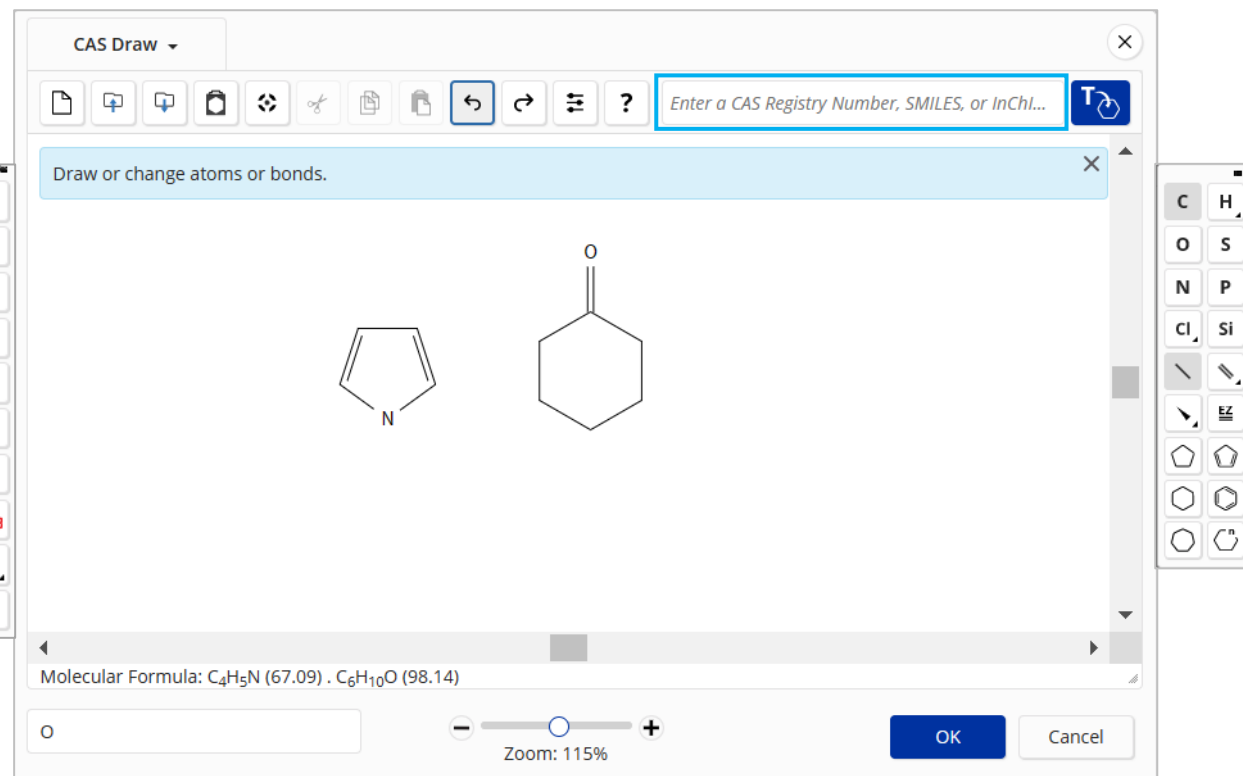
Target	Function	Parameter	Value	Disease	Organism	Assay	Source
-	-	EC50	>12.500 µM	-	-	View Detail	(1) CAS
-	-	EC50	>12.500 µM	-	-	View Detail	(1) CAS
-	-	EC50	>12.500 µM	-	-	View Detail	(1) CAS
-	-	EC50	1.917 µM	-	-	View Detail	(1) CAS
-	-	EC50	>12.500 µM	-	-	View Detail	(1) CAS

(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



问题1：已知活性结构片段，查找所有包含它们的天然产物？

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 (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

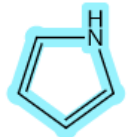
Product (1)

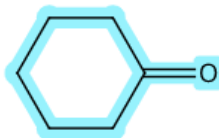
2 Results

Sort: Number o

1

17508-06-4





$C_6H_{10}O.C_4H_5N$

Components: 2

Cyclohexanone, compd. with 1H-pyrrole (1:1)

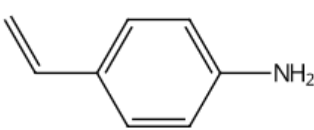
1 Reference

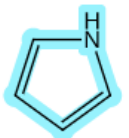
0 Reactions

0 Suppliers

2

1810859-50-7





$(C_8H_9N.C_6H_{10}O.C_4H_5N.CH_2O)...$

Components: 4

Formaldehyde, polymer with cyclohexanone, 4-ethenylbenzenamine and 1H-pyrrole, b...

1 Reference

1 Reaction

0 Suppliers

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

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.....

物质检索—检索结果集筛选：Reference Role

Reference Role: 利用物质的研究角色精准定位相应的物质

Filter Behavior

Filter by Exclude

Reaction Role

Reference Role

☐ Preparation (23K)

☐ Synthetic Preparation (21K)

☐ Uses (18K)

☐ Biological Study (10K)

☐ Therapeutic Use (8,159)

☒ Natural Product Occurrence (277)

View All

Bioactivity Data

Commercial Availability

Number of Components

☒ 1 (277)

☐ 2 (13)

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

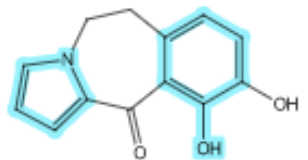
Filter by Exclude

Filtering: Reference Role: Natural Product Occurrenc... X Number of Components: 1 X Clear All Filters

277 Results Sort: Number of References: Ascending View: Partial

☐ 1

2707395-49-9



C₁₃H₁₁NO₃
5,6-Dihydro-9,10-dihydroxy-11H-pyrrolo
[2,1-b][3]benzazepin-11-one

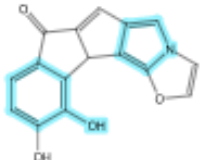
1 Reference

0 Reactions

0 Suppliers

☐ 2

2699076-84-9



C₁₆H₉NO₄
Benzo[5',6']pentaleno[1',2':3,4]pyrrolo[2,
1-b]oxazol-7(11bH)-one, 10,11-
dihydrox...

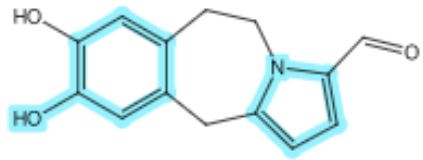
1 Reference

0 Reactions

0 Suppliers

☐ 3

2707395-48-8



C₁₄H₁₃NO₃
6,11-Dihydro-8,9-dihydroxy-5H-pyrrolo
[2,1-b][3]benzazepine-3-carboxaldehyde

1 Reference

0 Reactions

0 Suppliers

☐ 4

☐ 5

☐ 6

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

42

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CAS
A division of the
American Chemical Society

物质检索—检索结果集的保存

Substances search for drawn structure

References ▾ Reactions ▾ Suppliers ▾

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

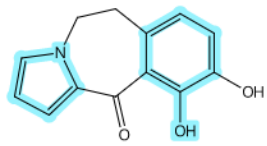
Filtering: Reference Role: Natural Product Occurrenc... X Number of Components: 1 X Clear All Filters

Excluding: Reaction Role: Product X

223 Results Sort: Number of References: Ascending View: Partial

1

2707395-49-9

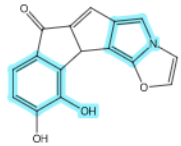


C₁₃H₁₁NO₃
5,6-Dihydro-9,10-dihydroxy-11H-pyrrolo[2,1-b][3]benzazepin-11-one

1 Reference 0 Reactions 0 Suppliers

2

2699076-84-9

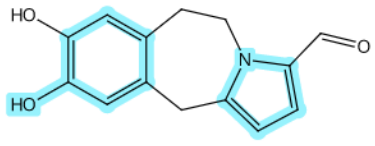


C₁₆H₉NO₄
Benzo[5',6']pentaleno[1',2':3,4]pyrrolo[2,1-b]oxazol-7(11bH)-one, 10,11-dihydrox...

1 Reference 0 Reactions 0 Suppliers

3

2707395-48-8



C₁₄H₁₃NO₃
6,11-Dihydro-8,9-dihydroxy-5H-pyrrolo[2,1-b][3]benzazepine-3-carboxaldehyde

1 Reference 0 Reactions 0 Suppliers

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

例：已知单体，如何查找所有包含它的聚合物？

Edit

Edit Drawing

Remove

☐ Search Patent Markush

Number of Components

☐ 1 (23)

☐ 2 (285)

☒ 3 (92)

☐ 4 (12)

☐ 5 or more (11)

Molecular Weight

Stereochemistry

Element

Substance Class

☒ Polymer (92)

☐ Coordination Compound (42)

☐ Salt and Compound With (9)

☐ General Derivative (3)

Isotopes

4

849402-50-2

$(C_4H_8O.C_4H_4S)_x.xCH_4O$

Components: 3

Furan, tetrahydro-, polymer with thiophene, methyl ether, graft

1

Reference

0

Reactions

0

Suppliers

5

62306-29-0

$(C_6H_6O.C_4H_4S.CH_2O)_x$

Components: 3

Formaldehyde, polymer with phenol and thiophene

2

References

0

Reactions

0

Suppliers

6

183238-72-4

$(C_8H_8.C_6H_6S.C_4H_4S)_x$

Components: 3

Thiophene, ethenyl-, polymer with ethenylbenzene and thiophene, graft

1

Reference

0

Reactions

0

Suppliers

7

202329-42-8

$C_{42}H_{42}Au_3Br_3NP_3$

Tribromo[μ_3 -[2-(diphenylphosphino- κP)- N,N -bis[2-(diphenylphosphino- κP)ethyl] etha...

0

References

0

Reactions

0

Suppliers

8

1698944-23-8

$C_{29}H_{28}NP_2PtS_2$

[N,N -Bis[2-(diphenylphosphino)ethyl] carbamodithioato- $\kappa S, \kappa S'$]platinum(1+)

0

References

0

Reactions

0

Suppliers

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

C07K 1/16(2006.01)

(22) 申请日 2014.03.30

C07K 1/06(2006.01)

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A61P 35/00(2006.01)

38 号

A61P 35/02(2006.01)

申请人 中国科学院上海药物研究所

A61P 25/28(2006.01)

A61P 37/02(2006.01)

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(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。本发明是小分子短肽类蛋白酶抑制

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

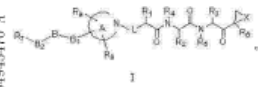
抑制剂,为癌症治疗药物的研究提供了新的思

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℃; 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

CAS Markush检索

预测性物质[Prophetic Substance]:

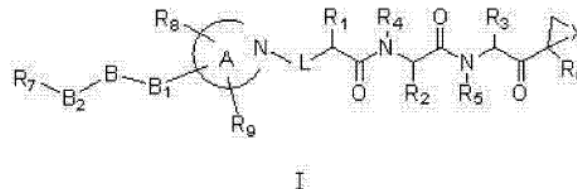
- 使用Markush结构陈述的预测物质，一个Markush可以陈述成百上千，甚至更多的结构
- 被Markush结构包含，但未被实施或呈现在表格、权利要求书或说明书中的结构，不会被CAS分配CAS Registry Number
- Markush检索，能检索到通过Substance可能检索不到的结构

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:



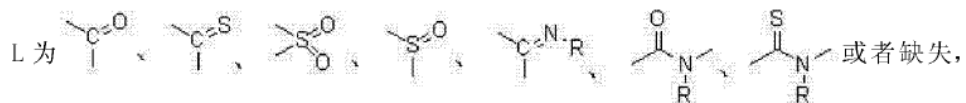
其中：

R_1, R_2, R_3 各自独立选自 H、 C_{1-6} 烷基 -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_a) (R_b) 或缺失， R_a, R_b 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；

R₄, R₅ 各自独立选自 H、OH、C₁₋₆ 烷基、卤代的 C₁₋₆ 烷基或芳烷基；

R₅ 选自 H, C₁₋₆ 烷基, 卤代的 C₁₋₆ 烷基, C₁₋₆ 羟基烷基, C₁₋₆ 烷氧基, 卤代的 C₁₋₆ 烷氧基, C(0)O-C₁₋₆ 烷基, C(0)NH-C₁₋₆ 烷基, 芳烷基;

X 为 O、S、NH、N-C₁₋₆ 烷基或 N- 卤代的 C₁₋₆ 烷基；



其中 R 选自 H、C₁₋₆ 烷基或卤代的 C₁₋₆ 烷基；

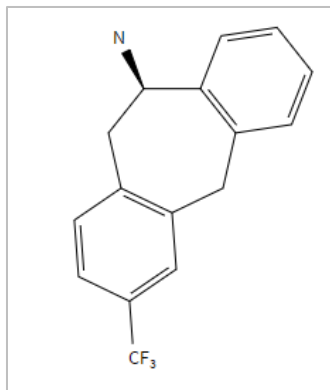
环A选自5~7元的饱和脂肪杂环、不饱和杂环、或者有取代的5~7元的饱和脂肪杂环、不饱和杂环,所述的杂环包含0~3个选自O、N和S的杂原子并任选地被R₈、R₉和B₁基团取代;

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

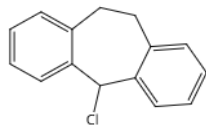
Filtering: Number of Components: 1 X Clear All Filters

Sort: Number of References: Descending View: Partial

5,332 Results

1 61

1210-33-9



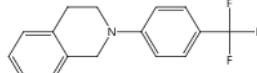
C₁₅H₁₃Cl

5-Chlorodibenzosuberane

143 References 130 Reactions 61 Suppliers

2 64

1057277-76-5



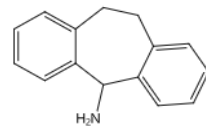
C₁₆H₁₄F₃N

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

90 References 121 Reactions 2 Suppliers

3 68

7005-53-0



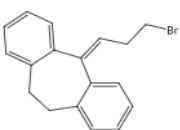
C₁₅H₁₅N

IEM 2115

58 References 78 Reactions 14 Suppliers

4 60

3436-04-2

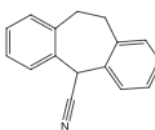


C₁₈H₁₇Br

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

5 62

1729-63-1

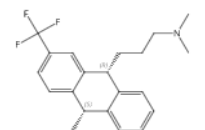


C₁₆H₁₃N

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

6 64

35764-73-9



C₂₁H₂₄F₃N

Fluotracen

Relative stereochemistry shown

Feedback

Structure Match

As Drawn (0)

Substructure (2)

Similarity (5,664)

Analyze Structure Precision

Chemscape Analysis

Visually explore structure similarity with a powerful new tool.

Learn more about Chemscape.

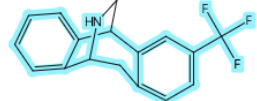
Create Chemscape Analysis

2 Results

Sort: Number of R

1

146364-17-2



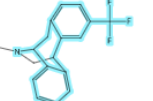
C₁₇H₁₄F₃N

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

1 Reference 1 Reaction 0 Suppliers

2

146364-18-3



C₁₈H₁₆F₃N

10,5-(iminomethano)-5H-dibenzo[a,d]cycloheptene, 10,11-dihydro-12-methyl-3-(trifluoromethyl)-

1 Reference 1 Reaction 0 Suppliers

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

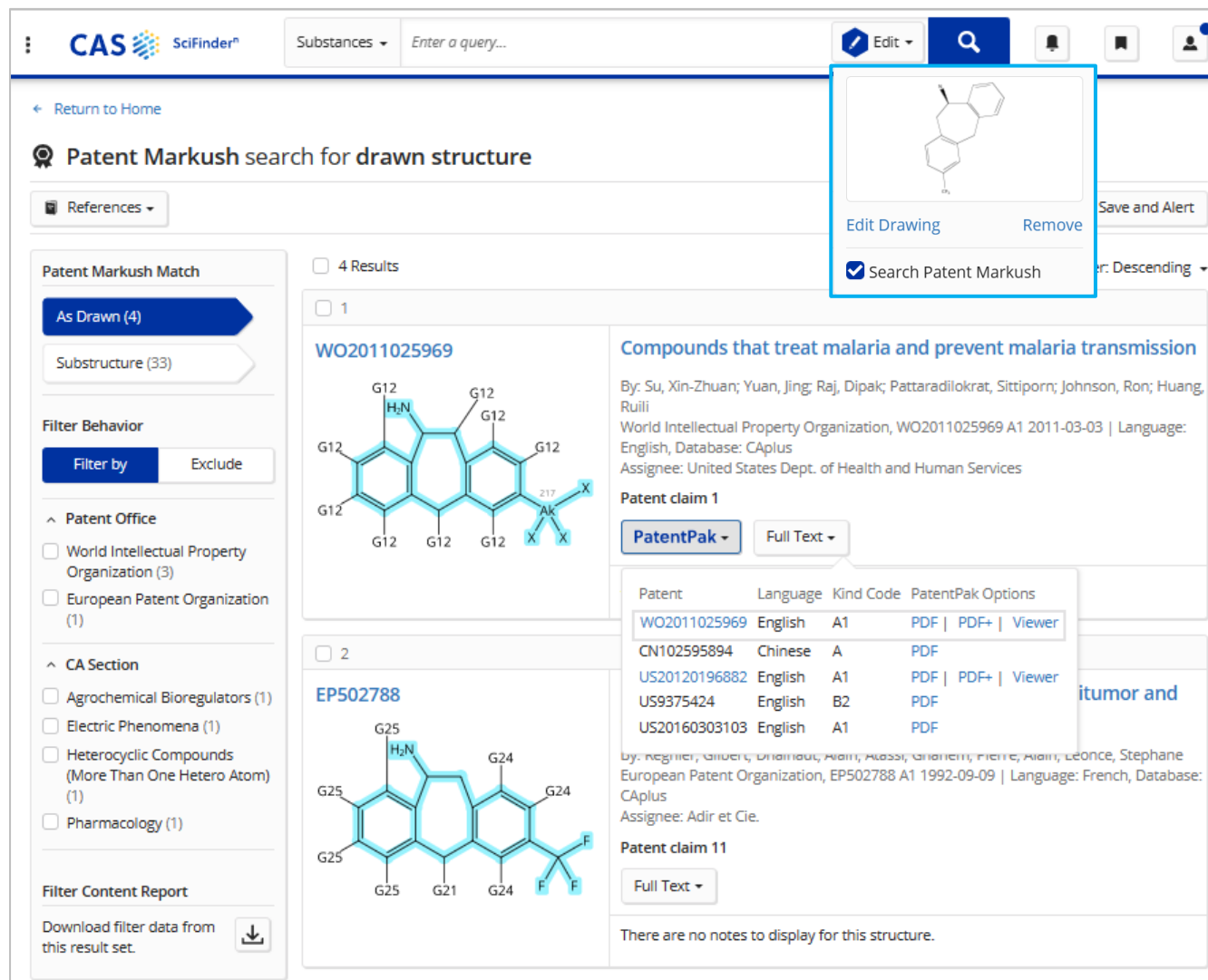
Reference Role

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

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



The screenshot shows the CAS SciFinder interface for a Markush search. The search criteria are set to "Patent Markush search for drawn structure". The search results show 4 results, with the first result being WO2011025969. The chemical structure of the query is displayed, and the search results are listed in a table.

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

Chemical structure of the query:

Nc1ccc2c(c1)c(c3cc(N)cc(N3)c2)c4ccccc4

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

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

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.

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

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

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

Clear All Filters

16 Results

Group: By Scheme

Sort: Yield

View: Collapsed

By Scheme

By Document

By Transformation

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: Heidelbaugh, 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: [\(T-4\)-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

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

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

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

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

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

Benzamide compounds as ROR gamma modulators and their preparation

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)
- ☐ Carboxamidine (109)
- ☐ Alkene (84)
- ☐ Cyclic alkene (80)
- [View All](#)

Reaction Mapping

Experimental Protocols

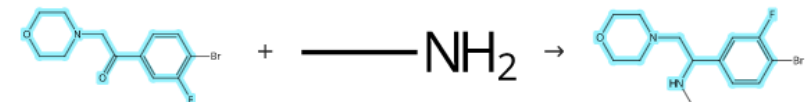
Reaction Type

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)

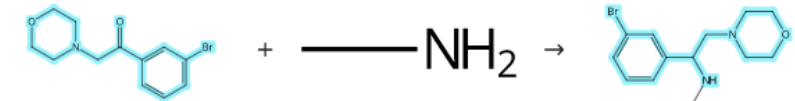
Expand Scheme

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

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

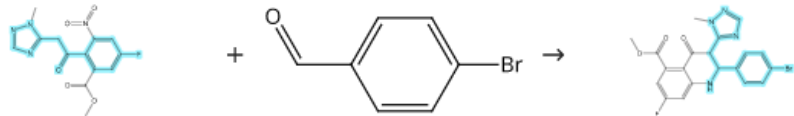
Source Reference

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

Experimental Protocols: Synthetic Methods X

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

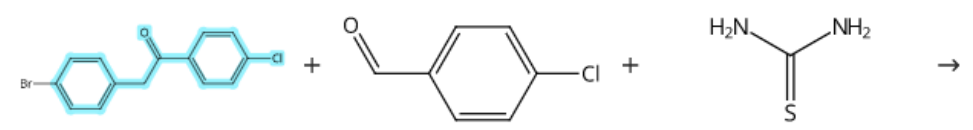
By: Bowden, Gregory D. et al
Journal of Medicinal Chemistry (2021), 64(21), 15690-15701

Full Text

Experimental Protocols

Collapse Scheme

Scheme 2 (1 Reaction) Steps: 1 Yield: 96% ...

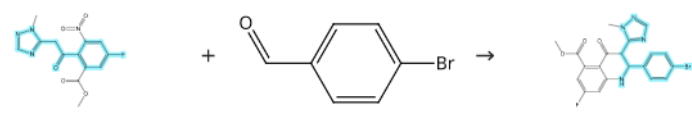


Suppliers (9) Suppliers (97) Suppliers (91)

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

 98%

Suppliers (15) Suppliers (89)

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
Tübingen 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

Searching for...

References

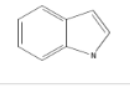
Search by Keyword, Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. [Learn More](#)

Friedel-crafts acylation

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

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

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

联用检索提高检索效率

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)

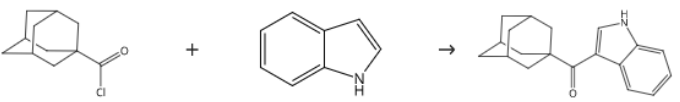
[View All](#)

Reaction Mapping

21 Results

Group: By Scheme Sort: Yield View: Collapsed

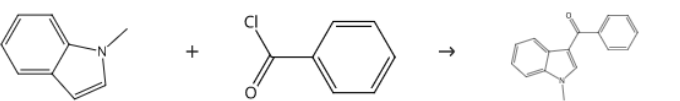
Scheme 1 (1 Reaction) Steps: 1 Yield: 82%



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: Vekariya, Rakesh H.; Aube, Jeffrey

Organic Letters (2016), 18(15), 3534-3537 | Language: English, Database: CAlus 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.

Full Text

Substances (50) Reactions (24) Citing (82) Citation Map

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

C₂₃H₃₂F₃N₅O₄

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

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-2-yl]ethyl]

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

62

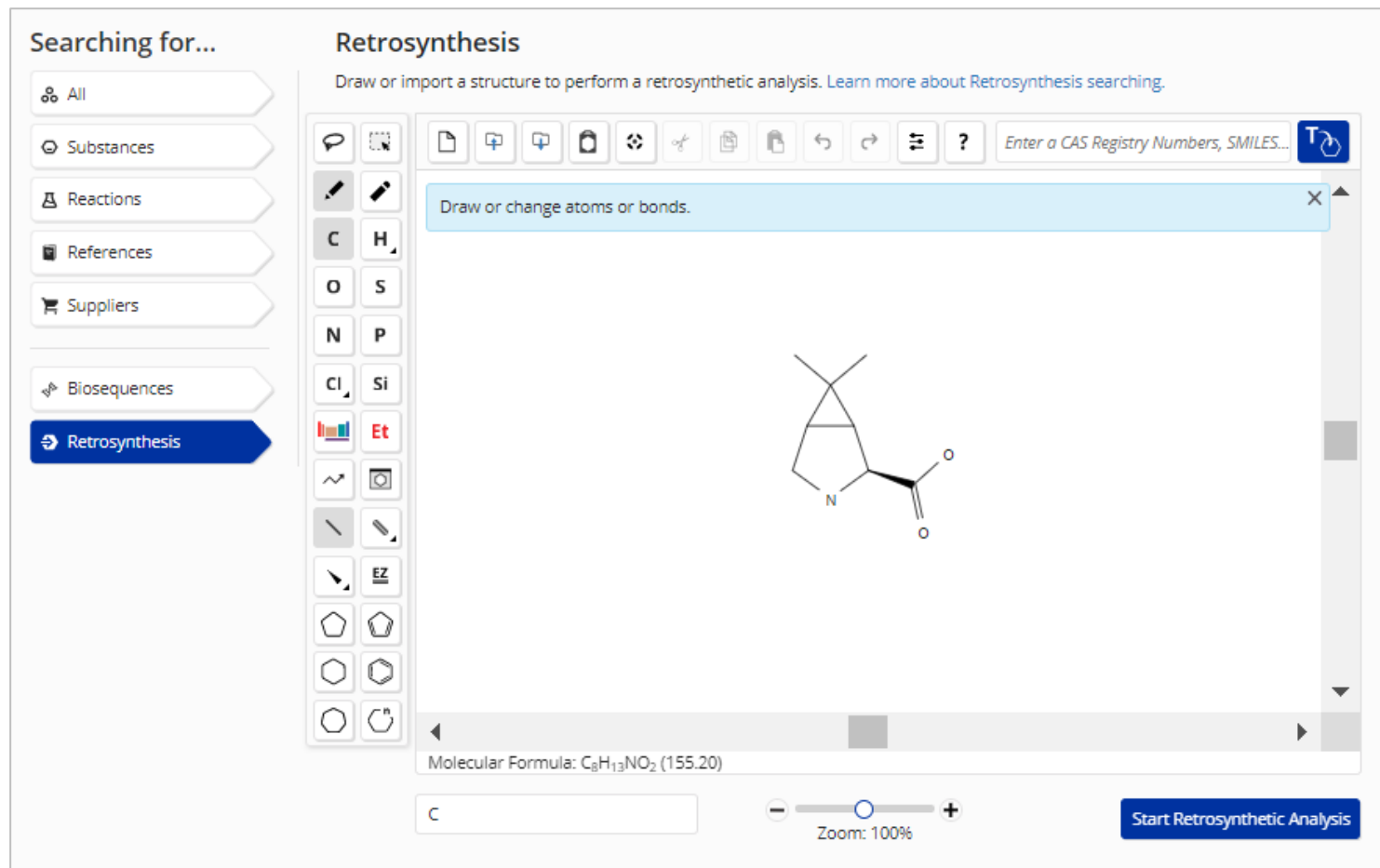
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CAS
A division of the
American Chemical Society

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.](#)

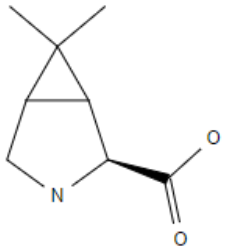
☐ Email me when my plan is complete

[Create Retrosynthesis Plan](#)

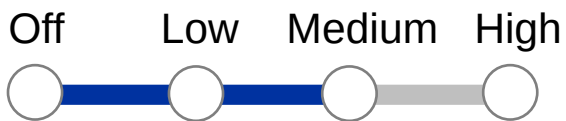
Break and Protect Bonds

[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

Download Email Save

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: CC1(C)CC(C)CC(C)CC1C(=O)N + CC1(C)CC(C)CC(C)CC1C(=O)N + CC1(C)CC(C)CC(C)CC1C(=O)N

Supplier (1) Suppliers (3) Suppliers (103)

Reaction Summary Steps: 1

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, O-(7-Azabenzotriazol-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

Retrosynthesis Step Key

获取替代路线

A ⇒ B + C + D Alternative Steps (93)

Filter by

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

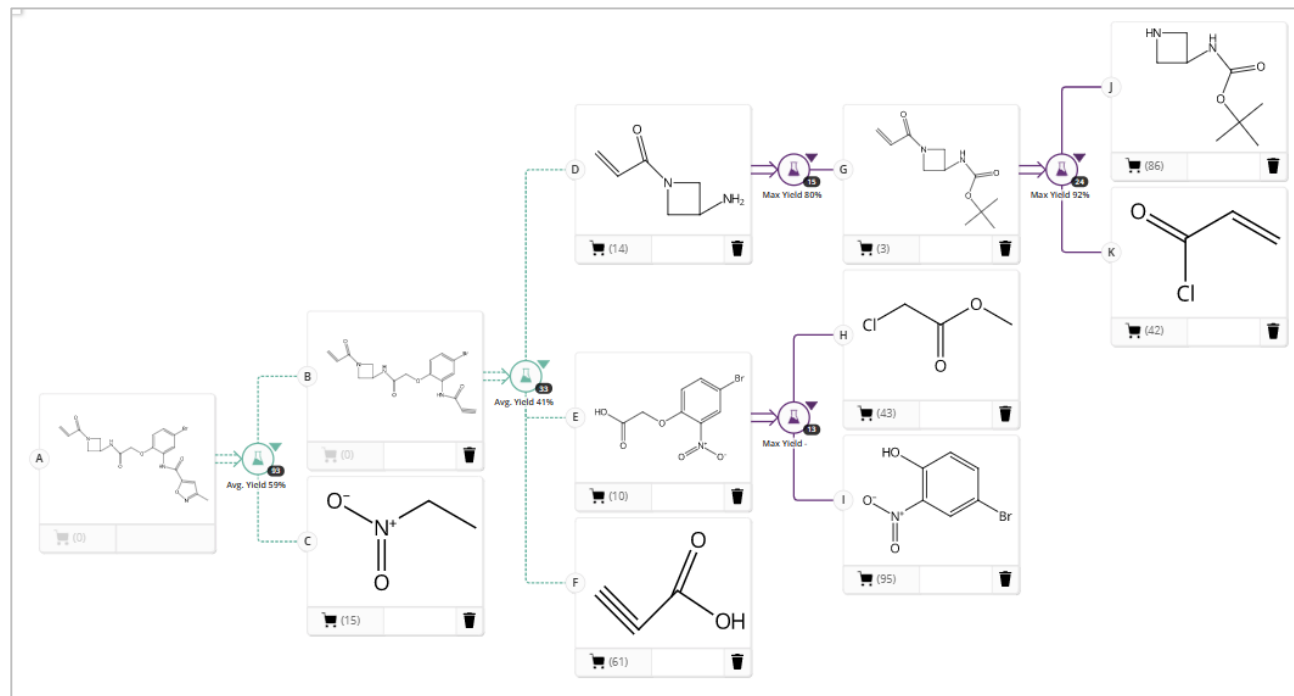
1 of 34 Predicted Step

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

2 of 34 Predicted Step

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

3 of 34 Predicted Step



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



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

QQLLVVEE|GG

Subject Sequence

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...

Results will expire on Mar 15, 2023.

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

Results will expire on Mar 15, 2023.

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

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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 AACAACAACATATCAAATCCTACTGGTGGCACAACCTTGA 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 AACAACAACA TATCAAATCC TACTGGTGGC ACAACTTGA 39
|||||
S 393 AACAACAACA TATCAAATCC 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 CACCAGCAGC AAATTGTCTG
161 TCACGTCAAG TACTAGAAAG AACAACAACA TATCAAATCC 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

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- 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 CGTGCCCGC

81 AGCGGAGGGA GCTTGACGG GCCAACGCAC ACATAACACA AGCTCGTCGT CGATGGCGCG GTGGGCTGCG GTGCTGGCGC

161 TGGCCGCGGC CACGGCCATC GCCGTGGCGT CCGTGCGGG CGGCGACATG AACGCGGACA AGACGGAGTG CGCGGACCAG

241 CTGGTGGGCC TGGCGCCGTG CCTGCAGTAC GTGCAGGGG AGGCCCGCG GCCCGGCC GACTGTGCG GCGGCTGCG

321 CCAGGTGCTG GGAAGAGCC CCAAGTGCT GTGCGTGCT 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	cgctgccgcg	agcggagggg	gcttgacagg
101	gccaacgcac	acataacaca	agctcgtcgt	cgatggcgcg	gtgggctcgc
151	gtgctggcgc	tggccgcgcc	cacggccatc	gccgtggcgt	ccgtggcggg
201	cgcgacatg	aacgcggaca	agacggagtg	cgcgaccag	ctggtggccc
251	tggcgccgtg	cctgcagtac	gtcagggggc	agggccgcgc	gccgccgccc
301	gactgctcgc	gcggcctcgc	ccaggctcgt	gggaagagcc	ccaagtgcct
351	gtcgtgctc	gtcaaggaca	aggacgaccc	caacctgggc	atcaagatca
401	acgccaccct	cgctctcgcg	ctccccaacg	cctcgggcgc	caccgcgcc
451	aacgtctccc	actgcgtcca	gtcctcgtcat	atcccccgg	gtccaaaga
501	cgccgcgctc	ttcagtcggc	gcagcgacaa	gggctccact	gccgtccag
551	ccaaggacaa	ctcagcgccg	acgaccgact	ccgcgcgct	gcaggcgacc
601	accggacgcg	gcgtgtcctc	ctcggcgccg	accgcgggtg	ctgcactcac

Other Names and

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

74

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序列详情及相关的专利文献结果

References from your sequence

Substances

Reactions

Citing

Knowledge Graph

Open

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Filter Behavior

Filter by

Exclude

Document Type

☐ Patent (38)

Language

☐ English (38)

Publication Year



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

75

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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

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Create Bioscape Analysis

Filter by

E-Value

Query Coverage %

Subject Coverage %

Alignment Identity %

Sequence Length

Organisms

0

 to

100

0

 to

100

8

 to

2060

☒ 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

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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](#)

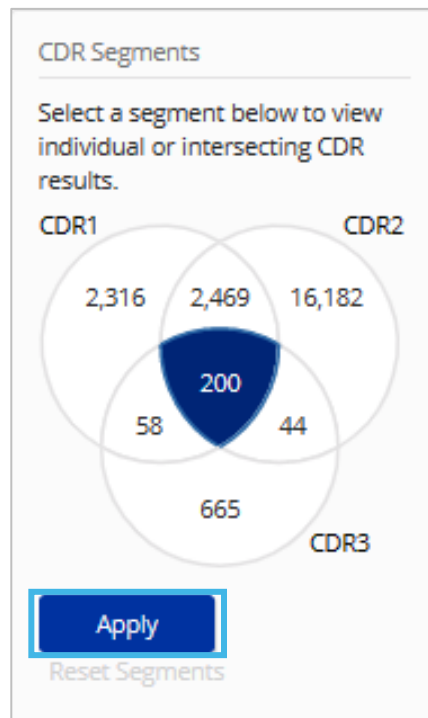
Alignment Subject References

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

References search for "steel and impurity"

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?
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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

☒ Analytical Methods (23)

☐ Formulus (9)

Filtering: CAS Solutions: Analytical Methods

23 Results

Sort: Relevance View: Partial Abstract

1

Validation of an HPLC method for analysis of nifedipine residues on stainless-steel surfaces in the manufacture of pharmaceuticals

By: Milenovic, D. M.; Lazic, M. L.; Veljkovic, V. B.; Todorovic, Z. B.
Acta Chromatographica (2008), 20(2), 183-194 | Language: English, Database: CPlus
[Analytical Methods](#)

A simple, sensitive, and convenient HPLC method has been developed, validated, and applied to anal. of nifedipine residues on the stainless-steel surfaces of equipment used in drug manufacture Cotton swabs moistened with methanol were used to remove residues of the drug from the surfaces; recoveries were 82.26, 86.88, and 88.95% for 25, 125, and 250 µg per swab. The precision of the results, as relative standard deviation (RSD), was <5%. The method was validated over the concentration range 3-50 µg mL⁻¹. Small quantities of residues of the drug and its main impurities were determined by HPLC.

[View More](#)

Full Text

Substances (2) Reactions (0) Citing (10) Citation Map

2

A novel laser-based approach for cleaning contaminated metallic surfaces coupled with rapid residue analysis

By: Fox, Robert V.; Roberts, Lauren; De Lucia, Frank C. Jr.; Miziolek, Andrzej W.; Whitehouse, Andrew I.
Proceedings of SPIE (2013), 8726, 87260N/1-87260N/16 | Language: English, Database: CPlus
[Analytical Methods](#)

We are developing a novel approach for cleaning and confirming contaminated metallic surfaces that is based on laser ablation to clean the surfaces followed closely in time and space by laser anal. of the degree of cleanliness. Laser-based surface cleaning is a well-established technol. and is com. available (e.g., Adapt-Laser). The new development involves the integration of a LIBS (Laser Induced Breakdown Spectroscopy) surface anal. capability to analyze the surface before and right after the laser cleaning step for the presence or absence of unwanted residues. This all-laser approach is bei...

[View More](#)

^ CAS Solutions

☒ Analytical Methods (23)

☐ Formulus (9)

The determination of alloying and impurity elements was performed from a stainless steel matrix and inclusions in process samples. An electrolytic extraction method was applied for the separation of inclusions using two different but commonly used electrolytes, 10% HCl and 10% acetylacetone in methanol. The elemental analyses were performed using at. absorption spectrometry. The elements of interest were aluminum, arsenic, copper, vanadium, titanium and chromium. The aluminum containing inclusions were imaged using a field emission scanning electron microscope. The results for copper and chromium in both electrolytes, vanadium in 10% HCl electrolyte and arsenic in 10% acetylacetone electrolyte were in good agreement with industrial data. Titanium and aluminum were measured from the dissolved steel matrix but titanium was also detected in the inclusions. It was concluded that the anal. results for titanium and aluminum measured using an optical emission spectrometer is affected by the inclusions within the stainless steel.

Keywords: double stabilized stainless steel alloying impurity element inclusion

[Open Access](#)

Full Text

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Concepts

Substances

Analytical Methods

Title	CAS Method Number
Analysis of Aluminum in Stainless steel by Electrochemical extraction	1-119-CAS-285768 ↗
Analysis of Aluminum in Stainless steel by Electrochemical extraction	1-119-CAS-286264 ↗
Analysis of Vanadium in Stainless steel by Electrochemical extraction	1-119-CAS-286328 ↗
Analysis of Vanadium in Stainless steel by Electrochemical extraction	1-119-CAS-286333 ↗
Analysis of Arsenic in Stainless steel by Electrochemical extraction	1-119-CAS-286759 ↗
Analysis of Copper in Stainless steel by Electrochemical extraction	1-119-CAS-286842 ↗
Analysis of Arsenic in Stainless steel by Electrochemical extraction	1-119-CAS-287300 ↗

分析实验方法详情

Analysis of Vanadium in Stainless steel by Electrochemical extraction

CAS MN: 1-119-CAS-286328

Method Category: Element Detection

Technique: Electrothermal atomic absorption spectroscopy; Decomposition; Electrochemical extraction

实验原料

Materials	Role	Image	CAS RN
Vanadium	analyte	View Structure	7440-62-2
Stainless steel	matrix		12597-68-1
Al ₂ O ₃ cutting wheel	material		
SiC grinding paper	material		
0.05 µm pore size polycarbonate filter	material		
Standard calomel reference electrode	material		
Platinum ring counter electrode	material		
Hollow cathode lamps	material		
Electrodeless discharge lamp	material		
THGA graphite tubes	material		
Nitric acid	reagent	View Structure	7697-37-2
Hydrofluoric acid	reagent	View Structure	7664-39-3
Acetylacetone	reagent	View Structure	123-54-6
Chromium	reagent	View Structure	7440-47-3
Methanol	reagent	View Structure	67-56-1
Tetramethylammonium chloride	reagent	View Structure	75-57-0

Source

Determination of alloying and impurity elements from matrix and inclusions from a process sample of a double stabilized stainless steel

Sipola, Teija; Alatarvas, Tuomas; Fabritius, Timo; Peramaki, Paavo

ISIJ International (2016), 56 (8), 1445 - 1451. Iron and Steel Institute of Japan

CODEN: IINTEY | ISSN: 09151559 | DOI: 10.2355/isijinternational.isijint-2016-071

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[Abstract ↗](#)

The determination of alloying and impurity elements was performed from a stainless steel matrix and inclusions in process samples. An electrolytic extraction method was applied for the separation of inclusions using two different but commonly used electrolytes, 10% HCl and 10% acetylacetone in methanol. The elemental analyses were performed using at. absorption spectrometry. The elements of interest were aluminum, arsenic, copper, vanadium, titanium and chromium. The aluminum containing inclusions were imaged using a field emission scanning electron microscope. The results for copper and chromium in both electrolytes, vanadium in 10% HCl electrolyte and arsenic in 10% acetylacetone electrolyte were in good agreement with industrial data. Titanium and aluminum were measured from the dissolved steel matrix but titanium was also detected in the inclusions. It was concluded that the anal. results for titanium and aluminum measured using an optical emission spectrometer is affected by the inclusions within the stainless steel.

分析仪器

Equipment Used

Cutting machine, Secotom-10, Struers

Ultrasonic cleaning unit, P 30 H, Elmasonic

Grinding machine, Labopol-6, Struers

Potentiostat, SP-150, BioLogic

Vacuum pump, BUSCHI

Graphite furnace atomic absorption spectrometer, AAnalyst 600, PerkinElmer

Autosampler, AS-800, PerkinElmer

Conditions

Instrument

internal gas flow rate: 250 mL/min (non-atomization), 0 mL/min (atomization); current: 15 mA; wavelength: 318.4 nm; slit width: 0.7 nm; injection volume: 10 µL

分析条件

Instructions

Preparation of stainless steel process samples

1. Cut stainless steel pieces from a corner piece of different slabs using a Struers Secotom-10 cutting machine with an Al₂O₃ cutting wheel.
2. Grind and polish the steel samples using a Struers Labopol-6 grinding machine with SiC grinding paper to a size of approximately 15 x 10 x 5 mm.
3. Clean the sample from grinding paper traces using an Elmasonic P 30 H ultrasonic cleaning unit (frequency 37 kHz, room temperature).
4. Clean all glassware in an acid bath, rinse with ultrapure water and methanol sequentially.

Electrolytic extraction of stainless steel using 10% acetylacetone

1. Perform electrolytic extraction on a BioLogic SP-150 potentiostat.
2. Use 10% acetylacetone (10 v/v% acetylacetone, 1 w/v% tetramethylammonium chloride and methanol) as the electrolyte.
3. Use the sample as the working electrode and set the potential to 0.150 V vs. the standard calomel electrode (SCE).
4. Suspend the sample in the electrolyte in a platinum basket and use a platinum ring as a counter electrode.
5. Filter the electrolyte through a 0.05 µm pore size polycarbonate filter with the help of a BUSCHI vacuum pump.
6. Expose the sample to ultrasound in methanol and filter the methanol with the electrolyte.

Decomposition of inclusions

1. Dry the polycarbonate filter containing the extracted inclusions overnight in a desiccator.
2. Place the dry filter in a PTFE container with 5 mL concentrated nitric acid and 2 mL HF and close gently.
3. Perform decomposition for 30 minutes at 120 °C (393.15 K).
4. Cool the containers to room temperature, remove the filter and dilute to the volume with water.
5. Prepare a blank sample similarly by filtering a fresh electrolyte through a polycarbonate filter.

Quantification of inclusions using graphite furnace atomic absorption spectrometry (GFAAS) with Cr as a matrix modifier

1. Perform GFAAS on a PerkinElmer AAnalyst 600 graphite furnace atomic absorption spectrometer equipped with an AS-800 autosampler and PerkinElmer THGA graphite tubes (standard platform B0504033).
2. Use a hollow cathode lamp (HCL) as the radiation source.
3. Use the following furnace program: ramp for 10 s to 110 °C, hold for 30 s; ramp for 10 s to 140 °C, hold for 30 s; ramp for 10 s to 1300 °C, hold for 20 s; perform atomization at 2400 °C for 6 s; ramp for 1 s to 2500 °C and hold for 5 s.
4. Set the instrument parameters as follows: internal gas flow rate: 250 mL/min (non-atomization), 0 mL/min (atomization); current: 15 mA; wavelength: 318.4 nm; slit width: 0.7 nm.
5. Add 0.05 µg Cr as a matrix modifier.
6. Inject 10 µL of the sample and perform measurements.

Validation

Linearity Range	0-400 µg/L
Concentration	< 1 µg

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

CAS Solutions

CAS Analytical Methods

★ Saved

Account

Search

Enter keyword, matrix, analyte, etc.

Advanced Search

Browse Method Categories

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

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

除草剂、农药残留、土壤分析

Herbicide Analysis

Pesticide Residue Analysis

Soil Analysis

分析实验方法的获取 (2)

支持筛选：

- ✓ 分析目标物
- ✓ 介质
- ✓ 方法类别
- ✓ 分析技术
- ✓ 发表年份

The screenshot shows the CAS Analytical Methods search interface. The search term 'steel and sulfur' is entered in the top search bar. The left sidebar contains filters for Analyte, Matrix, Method Category, Technique, and Year. The main results area displays two entries for 'Analysis of Carbon in Steel by Laser induced breakdown spectroscopy'. The first entry is selected and its details are shown, including the analyte (Sulfur; Carbon), matrix (Steel), and method (Laser induced breakdown spectroscopy). The second entry is partially visible below.

Search Results: steel and sulfur

Filters:

- Analyte:** Sulfur (13), Carbon (9), Manganese (4), Aluminum (3), Chromium (3), View All
- Matrix:** Steel (13), Reinforced concrete (1), View All
- Method Category:** Element Detection (13), View All
- Technique:** Laser induced breakdown spectroscopy (10), Liquid scintillation counting (3), Neutron activation analysis (3), Time-of-flight mass spectrometry (2), Atomic emission spectrometry (1), View All
- Year:**

Results (13) Sort Relevance

Entry 1: Analysis of Carbon in Steel by Laser induced breakdown spectroscopy
CAS MN: 1-119-CAS-267238
View Details & Instructions
Analyte: Sulfur; Carbon
Matrix: Steel
Other Materials: Material: Continuum Surelite laser
Method Category: Element Detection
Technique: Laser induced breakdown spectroscopy
Equipment Used: Laser-induced breakdown spectrometer; Laser pulse generation system (two synchronized lasers); optical system; Ablation chamber; Spectrometer; CCD camera; Gas environment controls
Source: Double-pulse laser induced breakdown spectroscopy with ambient gas in the vacuum ultraviolet: Optimization of parameters for detection of carbon and sulfur in steel
Jiang, X.; Hayden, P.; Costello, J. T.; Kennedy, E. T.
Spectrochimica Acta, Part B: Atomic Spectroscopy (2014), 101, 106-113. Elsevier B.V.
Full Text | View in CAS SciFinder

Entry 2: Analysis of Carbon in Steel by Laser induced breakdown spectroscopy
CAS MN: 1-119-CAS-265816
View Details & Instructions
Analyte: Carbon; Sulfur

分析方法的对比

Compare Methods

			Expand All	Collapse All
			1	2
Title	Analysis of Carbon in Steel by Laser induced breakdown spectroscopy	Analysis of Silver in Steel by Glow discharge mass spectrometry		
CAS Method Number	1-119-CAS-267238	1-119-CAS-101987		
Method Category	Element Detection	Element Detection		
Technique	Laser induced breakdown spectroscopy	Time-of-flight mass spectrometry; Glow discharge mass spectrometry		
Analyte	Sulfur ; Carbon	Titanium; Chromium; Antimony; Magnesium; Lead; Silicon; Cobalt; Sulfur ; Niobium; Tin; Nickel; Manganese; Vanadium; Boron; Molybdenum; Phosphorus; Silver; Tungsten; Copper; View All		
Matrix	Steel	Steel		
Other Materials	Continuum Surelite laser	Grimm-type chamber (with a 4 mm diameter anode and a 2.5 mm inner diameter flow tube)		
Equipment Used	Laser-induced breakdown spectrometer; Laser pulse generation system (two synchronized lasers); optical system; Ablation chamber; Spectrometer, VM-521, Acton View All	Orthogonal time-of-flight mass spectrometer, Tofwerk, Thun, Switzerland; Dry pump, Triscroll 300, Varian Inc., Palo Alto, USA; Radio frequency glow discharge orthogonal time- View All		

Source	Double-pulse laser induced breakdown spectroscopy with ambient gas in the vacuum ultraviolet: Optimization of parameters for detection of carbon and sulfur in steel View All	A comparison of non-pulsed radiofrequency and pulsed radiofrequency glow discharge orthogonal time-of-flight mass spectrometry for analytical purposes View All
Method	Laser-induced breakdown spectroscopic analysis using nitrogen as ambient gas in double pulse mode 1. Perform the analysis using LIBS setup containing the View All	Glow discharge orthogonal time-of-flight mass spectrometry in pulsed mode 1. Collect the NIST 1262b certified reference steel . View All
Limit of Detection	2.9 ppm, Carbon, 1.5 ppm, Sulfur	0.3 µg/g, Boron, 0.2 µg/g, Magnesium, 0.3 µg/g, Aluminum, 1.9 µg/g, Silicon, 1.6 µg/g, Phosphorus, 1.0 µg/g, Sulfur , 2.3 µg/g, Titanium, 1.1 µg/g, Vanadium, 1.0 µg/g, Chromium, 5.5 View All
Precision		12% (RSD, reproducibility), Boron, 28% (RSD, reproducibility), Magnesium, 2% (RSD, reproducibility), Aluminum, 6% (RSD, reproducibility), Silicon, 5% (RSD, View All
Sensitivity		6 - 165 cps/(µg/g)

Method	Laser-induced breakdown spectroscopic analysis using nitrogen as ambient gas in double pulse mode 1. Perform the analysis using LIBS setup containing the laser pulse generation system (two synchronized lasers), the optical system (lenses, mirrors, polarizer and half-wave plate), an ablation chamber, spectrometer, detection system (CCD camera and computer) and finally the gas environment controls (needle valve, gauge, pressure meters). 2. Use the Q-switched Nd:YAG lasers to create the plasmas in double-pulse mode by Continuum Surelite (model III-10), operating at the fundamental wavelength of 1.06 µm with a pulse width of 6 ± 1 ns and maximum output energy of 800 mJ. 3. Operate the laser at a repetition rate of 10 Hz.. 4. Insert the optical combination of a half-wave plate and a polarizer into the Surelite laser beam to vary the pulse energy incident on the sample. 5. Focus the approximately 10-mm-diameter beams produced by Surelite laser onto the steel samples by plano-convex lenses of 125 mm and 150 mm focal	Glow discharge orthogonal time-of-flight mass spectrometry in pulsed mode 1. Collect the NIST 1262b certified reference steel . 2. Determine the performance of the pulsed RFGD-TOFMS. 3. The radiofrequency glow discharge orthogonal time-of-flight mass spectrometer (RFGD-TOFMS) includes a RFGD bay unit (RF generator, matching box, RF connector, refrigerator disc and sample mounting system with a pneumatic piston to press the sample against the source) (GD Profiler HR instrument (Horiba Jobin Yvon, Longjumeau, France)). 4. Use the GD source of a copper-based modified Grimm-type chamber with a 4 mm diameter anode and a 2.5 mm inner diameter flow tube (EMPA, Switzerland). 5. Extract the ions originating from the source at pressure of 800 Pa through a sampler of 500 µm diameter and a 1 mm diameter skimmer. 6. The following interface region includes electrostatic focusing and deflecting components and couples the
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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?
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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: CAPLUS 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: CAPLUS 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...
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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

☒ Food (7)	☐ Antibacterial agents (1)	☐ Gastrointestinal protective agents (1)
☒ Antidiabetic agents (6)	☐ Antihypertensives (1)	☐ Oral rehydration solutions (1)
☐ Dietary supplements (5)	☒ Antioxidants (1)	☐ Pharmaceutical adjuvants (1)
☐ Diet (3)	☐ Antitumor agents (1)	☐ Snack food (1)
☒ Drug delivery systems (3)	☐ Bakery products (1)	
☐ Antimicrobial agents (2)	☐ Beverages (1)	

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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

CODEN: JAFCAU

E-ISSN: 1520-5118

ISSN-L: 0021-8561

Database Information

AN: 2014:519911

CAN: 160:534190

PubMed ID: 24684664

CAPLUS 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

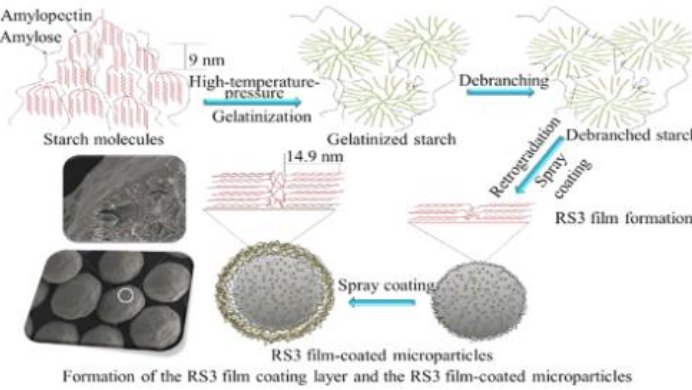
Language

English

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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.



Amylopectin Amylose

9 nm High-temperature-pressure Gelatinization

Starch molecules

Gelatinized starch

14.9 nm Debranching

Debranched starch

Retrogradation Spray coating

RS3 film formation

RS3 film-coated microparticles

Formation of the RS3 film coating layer and the RS3 film-coated microparticles

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		-	

90

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检索配方或制剂 <https://formulus.cas.org>

方法（2）：

- 登录CAS Formulus主页
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- 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) [Download] [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**

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
------------------------	---	---------

JOURNAL

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

Biomaterials

Language: English

Full Text View in CAS SciFinder®

Remove from Compare

Remove from Compare

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**

Component **Function** **Amount Reported**

Group: surgical implant	-	-
Dental implants	-	-
Plates	-	-
pin	-	-
screw	-	-

Additional group components reported

PATENT

Use of pro-inflammatory compounds for promoting bone formation

Assignee: Imperial Innovations Limited

WO2011007135

Language: English

Patent PDF View in CAS SciFinder®

Add to Compare

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 IngredientsExpand 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®](#)

不同制剂或配方信息的对比

Comparing your Formulations			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	Group: Ti-TNTs wire implants Function: implant Amount Reported: Optionality: Mandatory Ti wires Function: additives Amount Reported: - Optionality: - Acetone Function: Solvents Amount Reported: - Optionality: - Ethanol Function: Solvents Amount Reported: - Optionality: - Perchloric acid Function: additives Amount Reported: 1 Optionality: - Trail aqueous solution Function: - Amount Reported: 2 mg/mL Optionality: -	Group: surgical implant Function: Amount Reported: Optionality: Mandatory Dental implants Function: - Amount Reported: - Optionality: - Plates Function: - Amount Reported: - Optionality: - pin Function: - Amount Reported: - Optionality: - screw Function: - Amount Reported: - Optionality: - Group: pro-inflammatory compound Function: bone formation promoters Amount Reported: Optionality: Mandatory 1-Methyl-L-tryptophan Function: dioxygenase 1 inhibitors, 3, indoleamine 2	

- 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

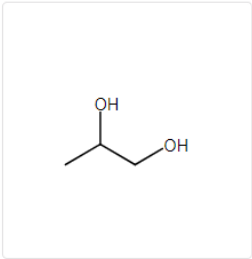
☐ Boiling Point (3)

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: GU75LMf9IZnhTq6mymUog

- 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!



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