

# CAS SciFinder Discovery Platform (Academic)

## 全面高效获取科技信息



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**CAS**  
A division of the  
American Chemical Society

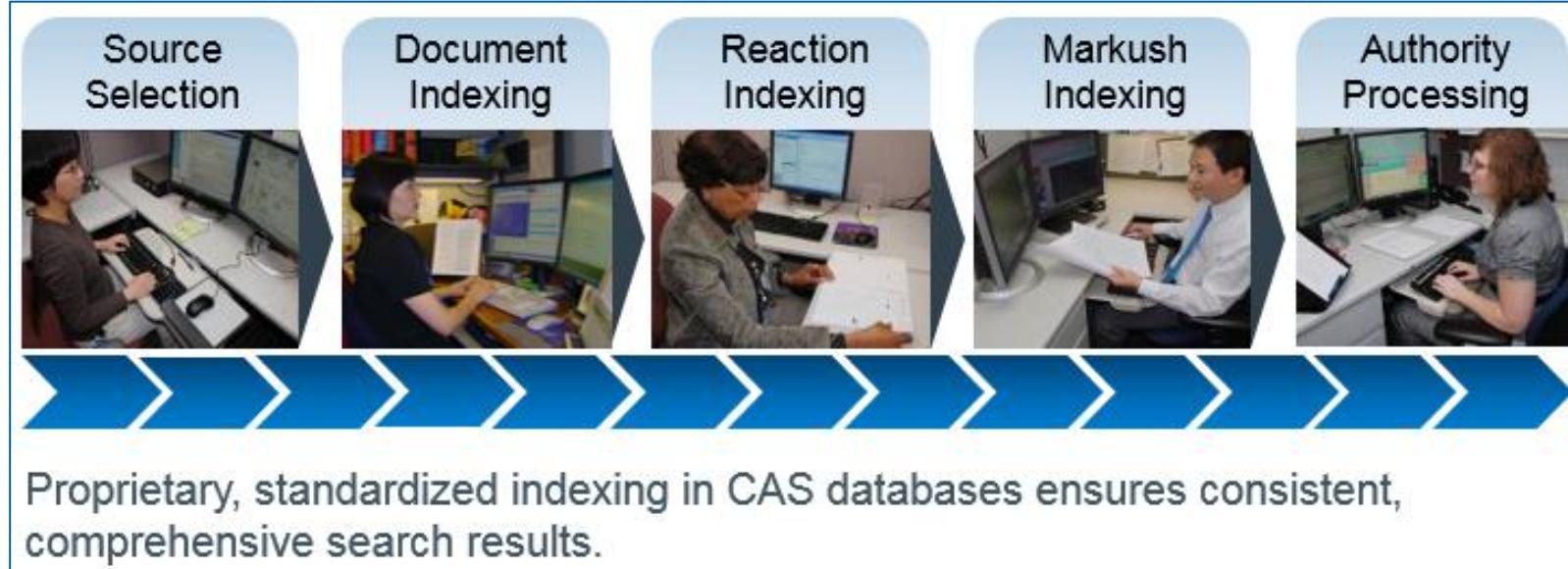


# 大纲

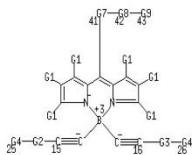
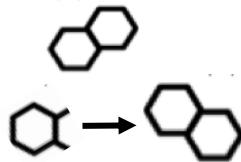
- CAS及CAS SciFinder Discovery Platform (Academic)简介
- 常见检索方式
  - 文献检索
  - 物质检索 (CAS Markush\*)
  - 反应检索
  - 逆合成反应路线设计 (CAS Retrosynthesis\*)
  - 序列检索\*
  - 分析实验方法 (CAS Analytical Methods)
  - 配方/制剂信息检索 (CAS Formulus\*)
- 常见问题及解答



# CAS科学家的智力标引



1990  
Smith, M.  
anthracene



Androst-4-en-3-one,  
17-hydroxy-17-  
methyl-, (17 $\beta$ )-

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 **64** patent offices worldwide
- Over **50** languages translated

# 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™**

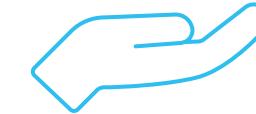
Get discoveries to market faster and optimize margins by giving researchers the information they need



## 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 Services™**

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 SciFinder<sup>n</sup>** —— 加速科学发现的业界领先的科学工具

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

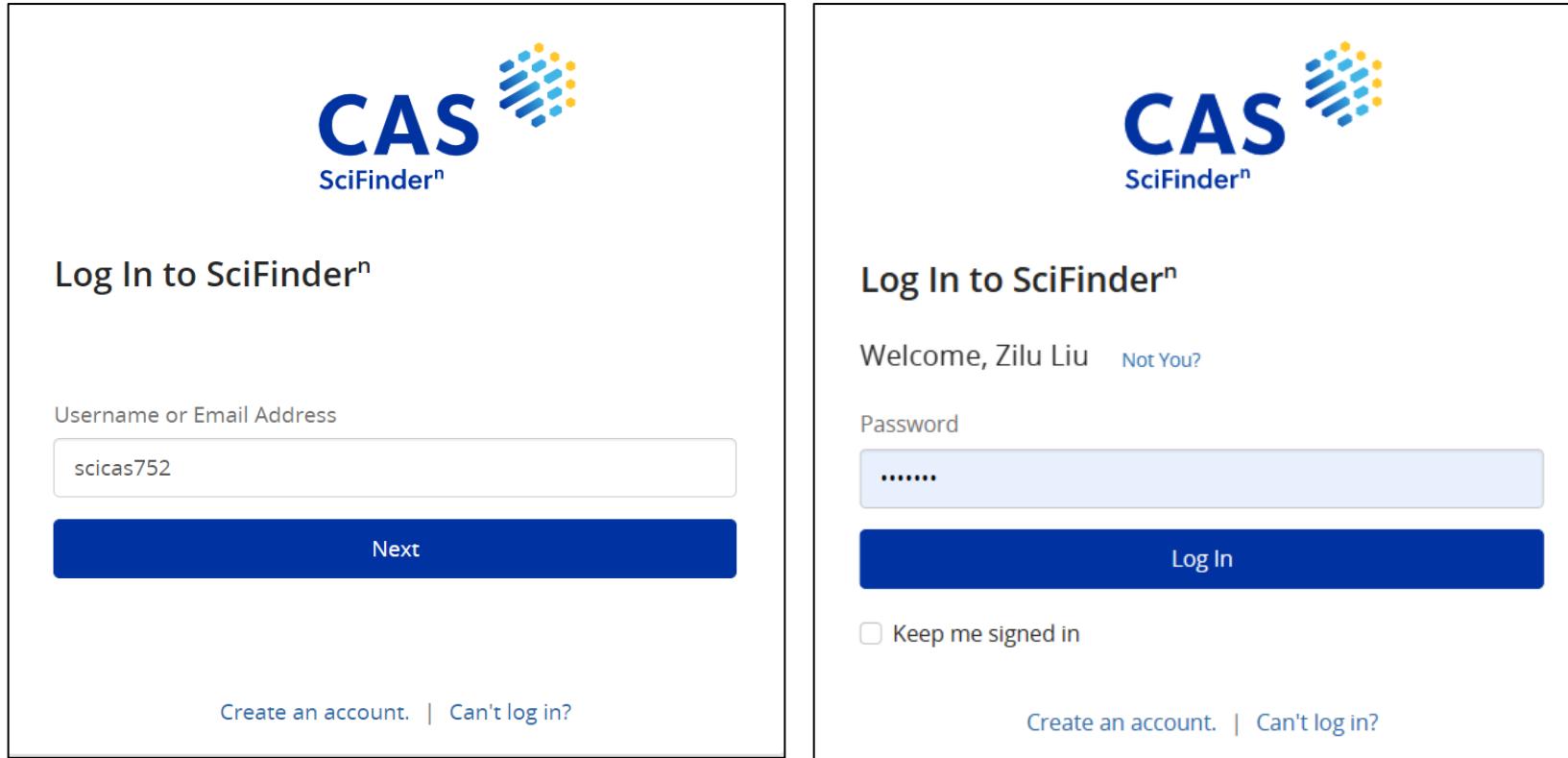
## **CAS Analytical Methods** —— 借助CAS科学家深度加工的科学方法，提升研究效率

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

## **CAS Formulus** —— 助力开发安全、有效的产品

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

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



The image displays two side-by-side screenshots of the CAS SciFinder<sup>n</sup> login interface. Both screenshots feature the CAS SciFinder logo at the top center, consisting of the letters 'CAS' in blue and a blue and yellow circular graphic to its right.

**Left Screenshot (Initial Login Screen):**

- The title "Log In to SciFinder<sup>n</sup>" is centered above the input fields.
- A text input field labeled "Username or Email Address" contains the text "scicas752".
- A large blue rectangular button below the input field is labeled "Next".
- At the bottom, there are links for "Create an account." and "Can't log in?".

**Right Screenshot (After Logging In):**

- The title "Log In to SciFinder<sup>n</sup>" is centered above the input fields.
- A text input field labeled "Password" contains several dots (".....") representing the password.
- A large blue rectangular button below the input field is labeled "Log In".
- To the left of the "Log In" button is a checkbox labeled "Keep me signed in".
- At the bottom, there are links for "Create an account." and "Can't log in?".

使用CAS SciFinder账号登录

# CAS SciFinder<sup>n</sup>主界面

The screenshot shows the main interface of the CAS SciFinder platform. On the left is a sidebar with links to various services: SCIFINDER DISCOVERY PLATFORM (CAS SciFinder<sup>n</sup>, CAS Analytical Methods, CAS Formulus, STN IP PROTECTION SUITE, STNext, CAS Scientific Patent Explorer, REGULATORY, CAS Chemical Compliance Index, ACCOUNT MANAGEMENT, CAS Profile). The main area has a header with the CAS logo, a search bar, and user account info (Alerts, Saved, Zili Liu). A search panel on the right shows a search for "Antitumor" using the "References" option. It includes fields for "Author Name" and a chemical structure input (a tricyclic compound with a hydroxyl group) which is highlighted with a blue box. Below this is a "Launch CAS Lexicon" button and a note about building reference queries. At the bottom, there's a "Recent Search History" section for "February 8, 2023" showing a search for "CSF-1R inhibitor (371K Results)" at 10:25 AM, with "Rerun Search" and "Edit Search" buttons.

灵活检索选项

近期检索历史

查看全部检索历史

重新运行检索式  
修改检索式

提醒更新的结果  
已保存的检索和结果集  
账户信息

检索项逻辑关系  
文本与结构检索便捷联用



# 大纲

- CAS及CAS SciFinder<sup>n</sup>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
  - 利用高级检索项目自定义组合检索
  - 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

The screenshot shows the CAS search interface. On the left, there is a sidebar with the following buttons:

- Searching for...
- All
- Substances
- Reactions
- References** (highlighted in blue)
- Suppliers
- Sequences
- Retrosynthesis

The main search area has a header "References" and a search bar with the placeholder "Search by Keyword, Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. Learn More". Below the search bar, the word "Seebeck" is typed. To the right of the search bar are three buttons: a clear button (X), a "Draw" button, and a magnifying glass search button.

The search results list the following terms:

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

A second search interface window is overlaid on the main one, showing the same search parameters and results for the term "seabeck".

- 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 shows the SciFinder-n search interface. On the left, a sidebar lists search categories: All, Substances, Reactions, References (which is selected and highlighted in blue), Suppliers, Sequences, and Retrosynthesis. The main search area has a header 'Searching for...' and a 'References' section. The search bar contains the query 'Seebeck effect and "coordination polymer"'. Below the search bar are dropdown menus for 'AND' and 'Author Name', and a text input field for 'Enter last name, first name middle name.' with an example 'Schubert, J A'. There is also a link to 'Add Advanced Search Field' and a button to 'Launch CAS Lexicon'. A note at the bottom of the search bar area states: '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.'

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

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: CPlus 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 either 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: CPlus

The carrier collection efficiency ( $\eta_c$ ) and energy conversion efficiency ( $\eta_e$ ) of polymer photovoltaic cells were improved by blending of the semiconducting polymer with  $C_{60}$  or its functionalized derivatives. Composite films of poly[2-methoxy-5-(2'-ethyl-hexyloxy)-1,4-phenylene vinylene] (MEH-PPV) and fullerenes exhibit  $\eta_c$  of about 29 percent of electrons per photon and  $\eta_e$  of about 2.9 percent, efficiencies that are better by more than two orders of magnitude than those that have been achieved with devices

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

(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

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

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, Chaoxu  
Advanced Functional Materials (2018), 28(39), n/a | Language: English, Database: CPlus

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 (EGaIn) into microgels of marine polysaccharides. During sonication bulk EGaIn 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: CPlus

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: CPlus

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 naniconductor 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"



AND  
AND  
OR  
NOT  
[Add A](#)

Publication Name

ACS Applied

Substances

Authors

- 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

Organization

Title

Abstract/Keywords

Concept

Substances

Publication Year

Document Identifier

Patent Identifier

Publisher



文本检索：

关键词、物质名称、CAS RN、DOI等

高级检索：

作者名、期刊名、机构名、题目、摘要、概念词、物质标识符、出版商

结构检索

\* 检索方法可单独使用，也可联用

# CAS Lexicon—利用词库选词启发检索

Searching for...

References

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

Enter a query... Draw 

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.

All Substances Reactions References Suppliers Sequences Retrosynthesis

- 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)

Search CAS Lexicon

Seebeck effect 

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 thermoelectric effect; Seebeck thermoelectric effect; Thermoelectric Seebeck coefficient; Thermoelectric Seebeck effect View fewer synonyms

Broader Terms (1) Deselect All  Thermoelectric

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

在CAS Lexicon词库层级中选择适合的主题词：

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

# 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 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

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

687 Results 知识图谱 Sort: Relevance View: Partial Abstract

1 High-Performance Flexible All-Solid-State Supercapacitor from Large 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: CPlus 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 electrochemical performance. A relatively high areal capacitance of  $448 \text{ mF cm}^{-2}$  was achieved at a scan rate of  $10 \text{ mV s}^{-1}$  using... View More

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

2 Highly stretchable multilayer electronic circuits using biphasic gallium-indium By: Liu, Shanliangzi; Shah, Dylan S.; Kramer-Bottiglio, Rebecca Nature Materials (2021), 20(6), 851-858 | Language: English, Database: CPlus 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 ( $2.06 \times 10^6 \text{ S m}^{-1}$ ), 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: CPlus 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

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标引的学科研究方向

CA Section

通过CA Section 纵览并定位学科研究方向

By Count Alphanumeric

6 Selected

- Electrochemical, Radiational, and Thermal Energy Technology (210)
- Electric Phenomena (169)
- Biochemical Methods (83)
- Textiles and Fibers (55)
- Plastics Fabrication and Uses (52)
- Pharmaceuticals (22)
- Plastics Manufacture and Processing (20)
- Optical, Electron, and Mass Spectroscopy and Other Related Properties (18)
- Unavailable (8)
- Electrochemistry (7)
- Inorganic Analytical Chemistry (5)
- Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes (5)
- Surface Chemistry and Colloids (5)
- Synthetic Elastomers and Natural Rubber (4)
- Air Pollution and Industrial Hygiene (3)
- Chemistry of Synthetic High Polymers (3)
- Magnetic Phenomena (3)
- Coatings, Inks, and Related Products (2)
- Physical Organic Chemistry (2)
- Thermodynamics, Thermochemistry, and Thermal Properties (2)
- Unit Operations and Processes (2)
- Apparatus and Plant Equipment (1)
- Cement, Concrete, and Related Building Materials (1)
- Food and Feed Chemistry (1)
- Nonferrous Metals and Alloys (1)
- Pharmacology (1)
- Toxicology (1)
- Water (1)

**Apply** **Cancel**

# 文献结果集—聚类筛选Concept

通过Concept纵览并精准定位核心研究点

Concept

Top Count Alphanumeric Search

7 Selected

- Wearable devices (501)
- Current density (50)
- Fluoropolymers (343)
- Hydrogels (50)
- Electric conductivity (155)
- Humans (48)
- Electrodes (128)
- Surface structure (124)
- Polymers (48)
- Carbon black (47)
- Electronics (47)
- Nanowires (47)
- Electric capacitance (45)
- Piezoelectric materials (44)
- Electric potential (41)
- Electronic device fabrication (40)
- Triboelectric nanogenerators (40)
- Electric impedance (39)
- Coating materials (30)
- Electrolytes (29)
- Sheet resistance (29)
- Surface area (29)
- Skin (28)
- Supercapacitor electrodes (28)
- Cyclic voltammetry (27)
- Dielectric loss (26)
- Energy storage systems (26)
- Lithium-ion secondary batteries (26)
- Plastic films (26)
- Strain (26)
- Surface roughness (26)
- Bending (25)

Apply Cancel

通过Search精准定位感兴趣的核心研究点

Concept

Top Count Alphanumeric Search

Concept Name

nano\*

Search

17 Selected

- Carbon nanofibers (14)
- Nanofibril (2)
- Carbon nanotube fibers (4)
- Nanofilms (6)
- Carbon nanotubes (86)
- Nanofilters (1)
- Cellulosic nanofibers (1)
- Nanoflakes (2)
- Core-shell nanoparticles (1)
- Nanoflowers (2)
- Electric nanogenerators (24)
- Nanohorns (1)
- Metal Nanoparticles (3)
- Nanoimprint lithography (1)
- Nanoantennas (1)
- Nanoparticles (53)
- Nanocoils (2)
- Nanoparticle size distribution (2)
- Nanocomposites (63)
- Nanoplatelets (3)
- 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  
Excluding: Search Within Results: dop\*

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: Cplus 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 piezoelectric 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)...  
View More

2 Antifreeze and moisturizing high conductivity PEDOT/PVA hydrogels for wearable motion sensor  
By: Peng, Yinfie; Yan, Bin; Li, Yueshan; Lan, Ji; Shi, Lingying; Ran, Rong  
Journal of Materials Science (2020), 55(3), 1280-1291 | Language: English, Database: Cplus  
 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<sup>-1</sup>), while the gl...  
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3 High-Stretchability, Ultralow-Hysteresis ConductingPolymer Hydrogel Strain Sensors for Soft Machines  
By: Shen, Zegun; Zhang, Zhilin; Zhang, Ningbin; Li, Linhai; Zhou, Peiwei; Hu, Enqi; Rong, Yu; Lu, Ruowang; Gu, Guoying

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

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

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

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

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E-ISSN: 1944-8252  
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CAN: 180:208379  
PubMed ID: 36170495  
Catalyst and MEDLINE

Company/Organization  
School of Materials Science and Engineering  
North University of China  
Talyuan 030051  
China

Publisher  
American Chemical Society

Language  
English

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 piezoelectric 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 piezoelectric 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 piezoelectric and piezoresistive sensing with applications for wearable sensors.

Static load time + Dynamic fast response → High sensitivity and wide frequency band response

Chemical crosslinking process: PVDF-TrFE reacts with HACC to form a cross-linked bond.

Dipolar interaction: PEDOT:PSS and PVDF-TrFE interact via dipole-dipole interactions during the stretching and compression processes.

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

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Concepts  
Substances  
Cited Documents

## Concepts

CAS科学家提供的标准技术术语

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



(C<sub>3</sub>H<sub>5</sub>ClO.Unspecified)<sub>x</sub>

Role: Properties, Synthetic Preparation, Preparation

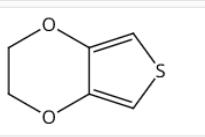
1219717-04-0

Image Not Available

Unspecified  
Clevios PH 750

Role: Properties, Technical or Engineered Material Use, Uses

126213-51-2



(C<sub>6</sub>H<sub>6</sub>O<sub>2</sub>S)<sub>x</sub>  
Poly(3,4-ethylenedioxythiophene)

Role: Properties, Technical or Engineered Material Use, Uses

Notes: polystyrenesulfonate-doped

106602-18-0

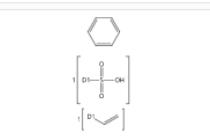
Image Not Available

Unspecified

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

Role: Reactant, Reactant or Reagent

50851-57-5



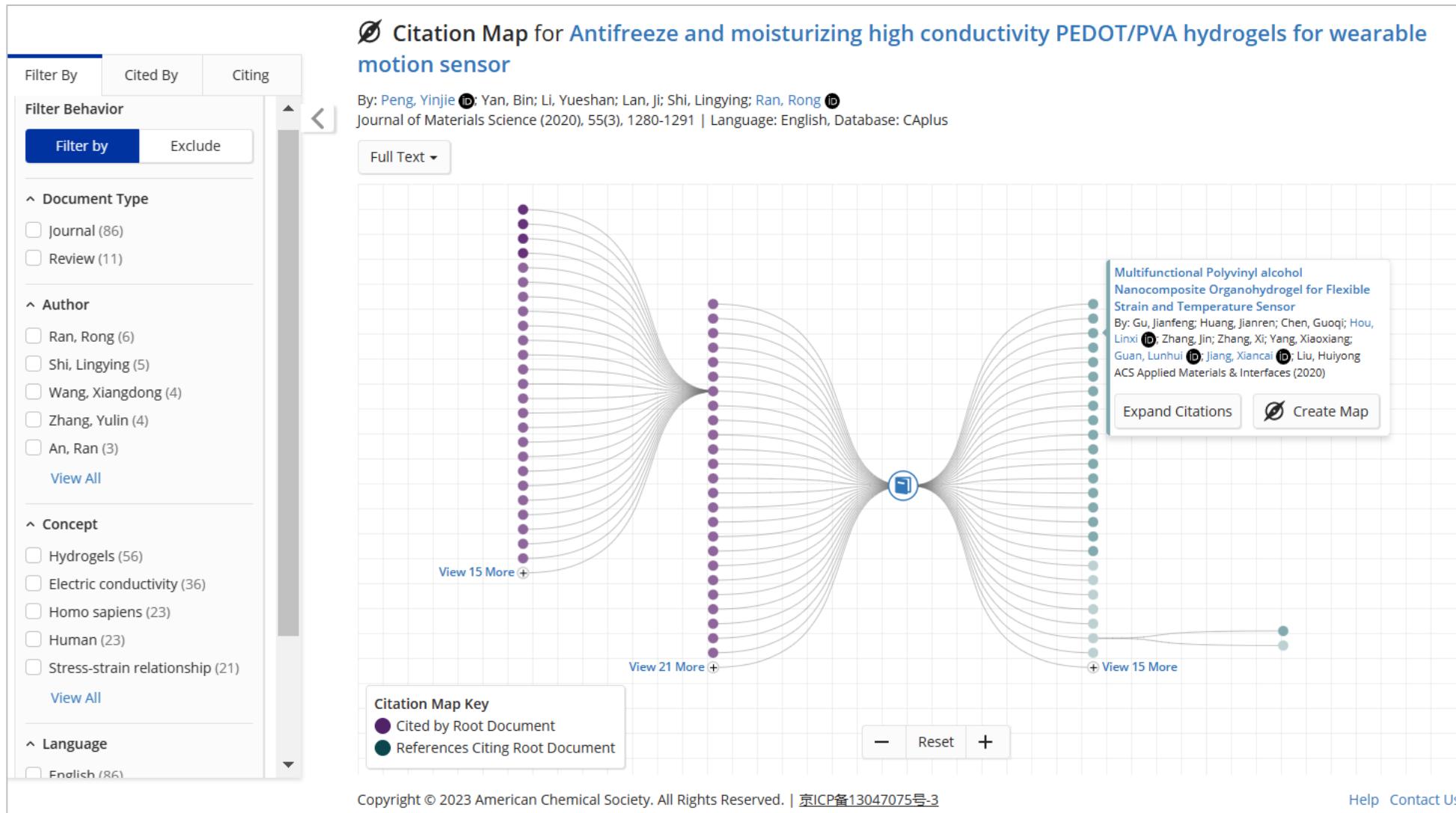
(C<sub>8</sub>H<sub>8</sub>O<sub>3</sub>S)<sub>x</sub>  
Poly(styrenesulfonic acid)

Role: Properties, Technical or Engineered Material Use, Uses

Notes: PEDOT dopant

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Substance Role

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

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Language

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

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Publication Year

1908 2023

8,921 Results Sort: Relevance View: Partial Abstract

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

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

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

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

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

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

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

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

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

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

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

## 物质在文献中的研究角色

Substance Role

By Count Alphanumeric

Biological Study (6,035)  
Biological Study, Unclassified (4,381)  
Uses (1,336)  
Properties (1,030)  
Therapeutic Use (714)  
Pharmacological Activity (532)  
Reactant or Reagent (493)  
Preparation (491)  
Reactant (486)  
Biochemical Process (41)  
Synthetic Preparation (353)  
Analytical Study (275)  
Biological Use, Unclassified (205)

Food or Feed Use (117)  
Catalyst Use (116)  
Formation, Non-preparative (92)  
Biosynthetic Preparation (86)  
Analytical Role, Unclassified (68)  
Analyte (58)  
Occurrence (53)  
Process (464)  
Physical, Engineering, or Chemical Process (381)  
Diagnostic Use (40)  
Pharmacokinetics (38)  
Pollutant (38)  
Formation, Unclassified (30)  
Nanoscale (26)  
Agricultural Use (25)

Occurrence, Unclassified (16)  
Bioindustrial Manufacture (15)  
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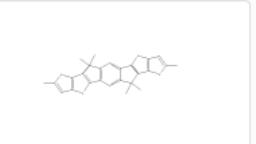
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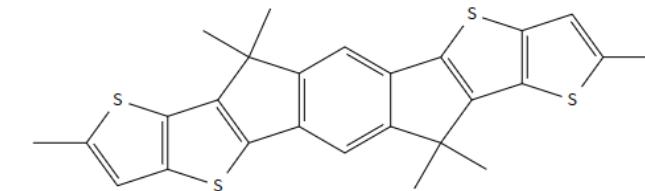
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[Phase evolution and magnetic characteristics of TiFeNiCr and TiFeNiCrM \(M = Mn\) entropy alloys](#)  
By: Mishra, Rajesh K.; Shahi, Rohit R.

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Structure Match Database: CHEMZENT Clear All Filters

Filtering: As Drawn (0) Substructure (8,881)

31 Results Sort: Relevance View: Partial Abstract

1 Fabric change of CARB azole in rats and rabbit

By: Johns, S. R.; Wright, S. E. Chemisches Zentralblatt (1966), 137(5), 01578-01578 | Language: German, Database: CHEMZENT

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

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Substances (14) Reactions (0) Citing (0) Citation Map

2 Cobamide and ribo nucleotide reduction. 3. Part The content of the Cobamid-abhängigen Ribonucleosid-triphosphatreduktase in Lactobacillus leichmanii influencing factors

By: Ghambeer, R. K.; Blakley, R. L. Chemisches Zentralblatt (1968), 139(28), 160-160 | Language: German, Database: CHEMZENT

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

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

3

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

68—74, 1963; Washington, D.C., George Washington Univ., School of Med., Dep. of Pharmacol.; engl.) — Die i.p. Injektion von 1 mg des adeninanalogen Purin-antimetaboliten 4-Aminopyrazolopyrimidin (I) verursachte bei Mäusen einen Anstieg der Gesamtleberlipide innerhalb 24 Std. auf das 3-4fache. Hieraus waren an erster Stelle die Neutrallipide, in geringerem Ausmaß auch das Cholesterin (II) beteiligt, während der Phospholipid-(III)-Geh. unverändert blieb. I-Gabe hemmte den in vitro-Einbau von <sup>14</sup>C<sub>12</sub>-Acetat (IV) in die Lipide von Leberschnitten, hatte aber wenig Einfl. auf die Ox. von IV u. <sup>14</sup>C<sub>12</sub>-Palmitat (V) in vitro. Die Plasmalipidkonz. sank nach I-Applikation u. war durch einen Abfall der Triglyceride u. des II hervorgerufen. III u. freie Fettsäuren waren nicht beteiligt. V wurde von den Lebern der mit I behandelten Tiere schlechter aufgenommen als von den Lebern der Kontrolltiere. Obgleich der Einbau von <sup>14</sup>C<sub>12</sub>-Orotäure in RNS durch I gehemmt wurde, konnte kein verminderter Einbau von <sup>14</sup>C<sub>12</sub>-Glycin in Leber- u. Plasmaproteine festgestellt werden. Die normalerweise massive Hyperlipidämie nach Gabe von Triton WR-1339 wurde durch I verhindert. VI schließt an den Unters., daß I wahrscheinlich die Sekretion von Triglyceriden aus der Leber hemmt. H. Zöllner 4607 ◇

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

Versuch: <sup>14</sup>C-Carbazol (I), F. 242—244° (aus Bzl.) durch Diazotierung u. Red. von <sup>14</sup>C-Anilin zu <sup>14</sup>C-Phenylhydrazinhydrochlorid. (F. 240—245°), das mit Cyclohexanon in <sup>14</sup>C-Tetrahydrocarbazol übergeführt wird. Dehydrierung an Pd-C ergibt I. Hergestellte Bezugssubstanzen: 1-Hydroxykarbazol, F. 160—162° durch Cyclisierung von Cyclohexan-1,2-dien-monophenylhydrazon (F. 183—185°) in Athanol. Essigsäure über 1,2,3,4-Tetrahydro-1-oxocarbazol (F. 169°), das an Pd-C dehydriert wird. 3-Hydroxykarbazol (II), F. 250—261° über folgende Stufen: p-Methoxyphenylhydrazinhydrochlorid (III), F. 198—200° (aus A.) durch Diazotierung u. Red. von p-Anisidin. — 3-Methoxy-1,2,3,4-tetrahydrocarbazol (IV), C<sub>13</sub>H<sub>14</sub>NO, F. 94—95° (aus A.), durch Rk. von III mit Cyclohexanon in wss. Essigsäure (50%;g) bei Ggw. von Natriumacetat. 3-Methoxykarbazol (V) C<sub>13</sub>H<sub>14</sub>NO,

K. Maier 4607 ◇

1561 Wirkung von Chlorycyclizin und anderen Stoffen auf die Toxizität verschiedener Organophosphat-Anticholinesterasen. Richard M. Welch und J. M. Coon. (J. Pharmacol. exp. Therapeut. 148, 192—198, 1964; Philadelphia, Pa., Jefferson Med. Coll., Dep. of Pharmacol.; engl.) — Vi. untersuchten verschiedene Substanzen mit bekannter Wirkg. auf die Lebermikrosomen-Enzymsyst. auf deren Wirkg. auf die Toxizität einiger Organophosphatsinsektizide am Mäuseen. Eine Vorbehandlung der Tiere täglich über 4 Tage mit Chlorycyclizin (I), Phenobarbital (II), SKF-525A (α,α-Diphenyl-α-propyl-essigsäure-β-dithiylaminodithylester · HCl; III) oder Cyclizin zeigte einen deutlichen Schutz gegen die Toxizität von Malathion, Parathion (IV) u. EPN (p-Nitrophenyl-thionobenzolphosphorsäuredithylester). Eine I-Vorbehandlung erhöhte außerdem wesentlich die orale DL<sub>50</sub> von Paraoxon (V), TEPP (Tetraethylpyrophosphat) u. Physostigmin. Eine s.c.-Dosis von I, II oder III schützte gegen IV. Die Umwandlung von IV in V durch Mäuseleber erfolgte etwa 2mal so schnell, wenn das Tier 4 Tage vorher mit I vorbehandelt wurde. Eine I-Dosis senkte deutlich die Serum-Paraoxonase (VI; A-Esterase), erhöhte aber dagegen gering die Leber-VI. I erhöhte innerhalb von 24 Std. das Verhältnis Lebergew. zu Körpergew. um

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References search for "enzyme and reduction" + drawn structure

Substances (8,921)

Filter Behavior: Filter by

Document Type: Patent

Substance Role: 3 Selected

87 Results

Preparation of azepinoindole compounds as CYP1B1 enzyme inhibitor

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

The invention discloses an azepinoindole compound shown in formula I, wherein R<sup>1</sup>=H, Me, OMe, OH, NH<sub>2</sub>, SCF<sub>3</sub>, F, CF<sub>3</sub>, NO<sub>2</sub>, tert Bu, Ph, naphthalene, phenanthrene, pyridine, quinoline or pyrene; R<sup>2</sup>=H, Cl, Me, F, R<sup>3</sup>=H, Me, F, OMe, Cl, Br. For example, 6-phenyl-5,12-dihydrobenzo[6,7]azepino[3,4-b]indole was prepared by multi-step reaction. The title compound can be used as CYP1B1 enzyme inhibitor.

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 = O, S, CH:CH, CH(Me)R); R<sup>1</sup>, R<sup>2</sup> = C<sub>1-4</sub>-alkyl, (CH<sub>2</sub>)<sub>n</sub>-P, [(CH<sub>2</sub>)<sub>2</sub>O]<sub>m</sub>R<sup>6</sup>; R<sup>3</sup> = H, NO<sub>2</sub>, halogen, SO<sub>3</sub><sup>-</sup>, C<sub>1-4</sub>-alkoxy, (CH<sub>2</sub>)<sub>m</sub>COOR<sup>7</sup>; at least one of groups R<sup>1-4</sup> comprises at least one NO<sub>2</sub> group; R<sup>5</sup> = C<sub>1-4</sub>-alkyl optionally substituted with COOR<sup>7</sup>, SO<sub>3</sub><sup>-</sup>, or OH; R<sup>6</sup> = Me, Et; R<sup>7</sup> = H, C<sub>1-4</sub>-alkyl, CH<sub>2</sub>OCOR<sup>8</sup>; R<sup>8</sup> = Me, tBu; P = COOR<sup>7</sup>, SO<sub>3</sub><sup>-</sup>; OH<sup>-</sup>; W = mono-, di-, or bisubstitution nitrobenzene; n = 1-7.

Available at My Institution

Author

Organization

Publication Name

Concept

CA Section

Patent: WO2005118839 | Language: English | Kind Code: A1 | PDF | PDF+ | Viewer

Uses in detection or imaging of

-6 alkyl, etc.; G<sup>a</sup>, G<sup>b</sup> = F, alkyl, alkoxy, etc.; n = 0-4), cyclooctyne-n = 1), and activity-based probes III (L = halo, alkoxy, phenoxy, which form triazolyl products. The provided compounds are Methods for detection and imaging of biomols. using

CAS PatentPak

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Key Substances in Patent

Analyser Markup Locations (2)

Analyst Page 19

Analyst Page 22

CAS RN 1640-39-7

Analyst Markup Locations (2)

Analyst Page 20

Analyst Page 23

CAS RN 192137-08-9

Analyst Markup Locations (1)

Analyst Page 20

CAS RN 252358-63-7

Analyst Markup Locations (2)

Analyst Page 21

Analyst Page 23

CAS RN 162929-91-4

WO 2005/118839

3.2 Preparation of Compound (3)

To 1-(3,5-dinitrobenzyl)-2,3,3-trimethyl-3H-indolium iodide (132mg) was added 3-(5-carboxypentyl)-1,1,2-trimethyl-1H-benzo[e]indolium iodide (114mg),

5 3,4-dihydroxy-3-cyclobuten-1,2-dione (32mg), pyridine (4.5ml), acetic acid (4.5ml) and acetic anhydride (1ml). The mixture was heated to 90°C for 4 hours and the solvent then stripped using rotary evaporation. Silica flash column chromatography was performed (EA/MeOH) and the relevant fractions combined and concentrated. The resulting material was further purified by

10 reverse phase HPLC (CH<sub>3</sub>CN / H<sub>2</sub>O / TFA) to give 1.7mg. MALDI-TOF (C<sub>43</sub>H<sub>40</sub>N<sub>4</sub>O<sub>8</sub> requires M<sup>+</sup> 740) 741.

4. Preparation of 2-(3-ethyl-6-nitro-2-benzothiazolinylideneethyl)-4-(1-(2-(2-methoxyethoxy)ethyl)-3,3-dimethyl-2-indolinylidenemethyl)cyclobutenediylium-1,3-diolate (Compound (4))

15

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

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



# 文献检索小结

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4. 利用引文地图拓展检索
5. 主题词+结构联合检索快速获得文献
6. 使用PatentPak高效阅读专利

# 物质检索

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

# 物质检索

- 通过物质标识符、文献标识符检索物质

The screenshot shows the SciFinder search interface for substances. On the left, there is a sidebar with a navigation menu:

- Searching for... (dropdown: All)
- Substances** (selected)
- Reactions
- References
- Suppliers
- Sequences
- Retrosynthesis

The main search area is titled "Substances" and contains the following fields:

- A search bar with placeholder text "Enter a query..." and a "Draw" button.
- A "Molecular Formula" input field with a dropdown arrow and an "X" button to clear the input.
- Example entries: C6H6 | (C8H8)x | C22H26CuN2O5.C2H3N
- A link to "Learn more about SciFinder® Advanced Search."
- An "Add Advanced Search Field" button.

- 高级检索

- 使用结构绘制面板进行结构检索

# 物质检索—物质名称、CAS RN、代码

The screenshot shows the SciFinder search interface. The search bar at the top contains "Paxlovid 2628280-40-8". Below the search bar, there are three buttons: "References", "Reactions", and "Suppliers", all of which are highlighted with a blue border. On the left, a sidebar titled "Filter Behavior" includes sections for "Reaction Role" (Product, Reactant), "Reference Role" (Adverse Effect, Analyte, Analytical Study, Biological Study, Biological Study, Unclassified), and "Commercial Availability", "Number of Components", and "Molecular Weight". The main search results area shows "2 Results". Result 1 is for "2628280-40-8", which is Paxlovid. It shows a chemical structure, the formula C<sub>23</sub>H<sub>32</sub>F<sub>3</sub>N<sub>5</sub>O<sub>4</sub>, and the full name: 3-Azabicyclo[3.1.0]hexane-2-carboxamide, N-[(1S)-1-cyano-2-[(3S)-2-oxo-3-pyrroli...]. Result 2 is for "2803933-60-8", which is a different compound. Both results show their respective chemical structures and formulas. At the bottom of each result panel, there are buttons for "References", "Reactions", and "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

S 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)

Bioactivity Data

Commercial Availability

- Available (6)
- Not Available (4)

10 Results

Sort: Molecular Formula: Ascending View: Partial

1 147-85-3  
61-90-5  
2628280-40-8  
870153-29-0  
2757763-45-2

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

CC(C)C[C@H](N)C(=O)O  
C5H9NO2  
L-Proline

CC(C)C[C@H](N)C(=O)O  
C6H13NO2  
L-Leucine

CC(C)C[C@H]1[C@H]2[C@@H]3[C@H]4[C@H]2[C@H]1C(=O)N3C#N  
C23H32F3N5O4  
3-Azabicyclo[3.1.0]hexane-2-carboxamide, N-[<sup>15</sup>(1)-cyano-2-[(<sup>35</sup>)-2-oxo-3-pyrroli...

CC(C)C[C@H]1[C@H]2[C@@H]3[C@H]4[C@H]5[C@H]2[C@H]1C(=O)N3C(=O)C=C5  
C24H32N4O6  
1H-Indole-2-carboxamide, N-[<sup>15</sup>(1)-[(<sup>15</sup>)-3-hydroxy-2-oxo-1-[(<sup>35</sup>)-2-oxo-3-pyr...

CC(C)C[C@H]1[C@H]2[C@@H]3[C@H]4[C@H]5[C@H]2[C@H]1C(=O)N3C(=O)C=C5  
C28H37N5O6S2  
3-Azabicyclo[3.1.0]hexane-2-carboxamide, N-[<sup>15</sup>(2-2-(benzothiazolyl)-2-oxo-1-...

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 Na<sub>2</sub>SO<sub>4</sub>: H<sub>2</sub>O<sub>4</sub>S.2Na

Searching for...

All

Substances

Reactions

References

Substances

Search by Substance Name, CAS RN, Patent Number

Enter a query...

Molecular Formula ▾ CH<sub>2</sub>O<sub>3</sub>



Searching for...

All

Substances

Reactions

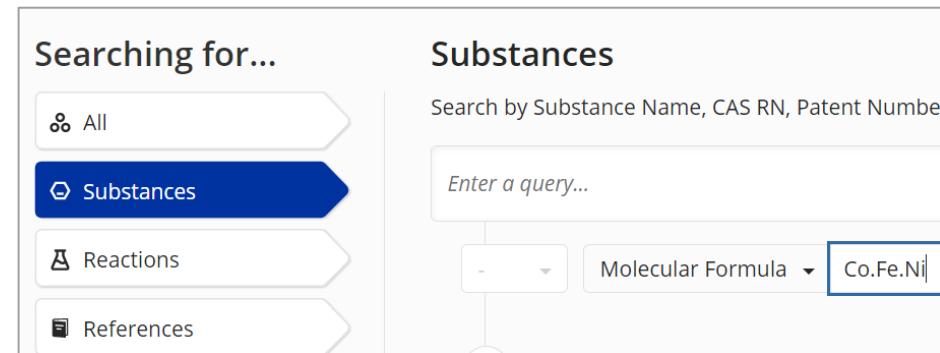
References

Substances

Search by Substance Name, CAS RN, Patent Number

Enter a query...

Molecular Formula ▾ Co.Fe.Ni



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

The screenshot shows the SciFinder Advanced Search interface. On the left, there's a sidebar with a search bar and links for All, Substances, Reactions, References, Suppliers, Sequences, and Retrosynthesis. Below that is a Recent Search History section for February 13, 2023, which lists a search for Substance 157119-63-6 at 2:05 PM. The main area is titled "Substances" and allows searching by Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and DOI. It features a search bar with a "Draw" button and a "Q" search icon. A dropdown menu for "Molecular Formula" is open, showing options like 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, and Thermal. There are also "Add Another" and "View All Search History" buttons.

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

# 物质检索—联用检索(1)

查找满足以下属性要求的合金：

- 密度<7g/cm<sup>3</sup>
- 拉伸强度>1000MPa
- 熔点>600

Filter Behavior

Filtering: Substance Class: Alloy X

12 Results

1 56802-58-5 Image Not Available Unspecified Aluminum alloy, base, (Duralumin)

2 252664-07-6 Component Percent Zr 68 Cu 13 Ni 9.7 Nb 6.1 Al 3.5

Al.Cu.Nb.Ni.Zr Components: 5 Zirconium alloy, base, Zr,Al,Cu,Nb,Ni (VIT 106)

3 857638-02-9 Component Percent Zr 59

4 2,476 References 1 Reaction 0 Suppliers

5 253178-50-6 Component Percent Zr 66

Substance Class: Alloy (12)

Element (2)

Manual Registration (2)

Organic/Inorganic Small Molecule (1)

Isotopes

Metals

Experimental Property

Density (12)

Melting Point (12)

Tensile Strength (12)

Glass Transition Temperature (11)

物质类别中锁定合金Alloy

## Substances

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

Enter a query...

Density (g/cm3) <7  
Include predicted values. Examples: 1.15 | <7.53 | >150 | 9.3 to 15 | 8.9e-2

AND Tensile Strength (Mpa) 1000 to 2500  
Search key property values only. Examples: 1.15 | <7.53 | >150 | 9.3 to 15 | 8.9e-2

AND Melting Point (°C) >600  
Search key property values only. Examples: 1.15 | <7.53 | >150 | 9.3 to 15 | 8.9e-2

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

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

### Experimental Properties

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

# 物质检索—联用检索(2)

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

Searching for... **Substances**

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

Enter a query...

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  $\pm 2$  ppm. Examples: 152.3, 127.6, 133.1 | 155.02 to 207.59 | 187

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

All Substances Reactions References Suppliers Sequences Retrosynthesis

**Substances search for 3 Advanced Fields**

References Reactions Suppliers Save and Alert Clear All Filters

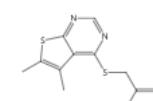
Filter Behavior: Filter by Exclude

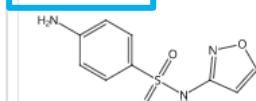
Filtering: Bioactivity Data: 3 Selected X

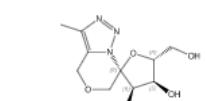
15 Results Sort: Molecular Formula: Ascending View: Partial

1 2 3 4 5 6

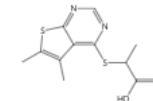
**296262-16-3** 723-46-6 1631737-39-7

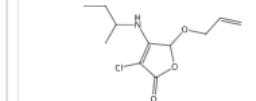
  
C10H10N2O2S2  
2-((5,6-Dimethylthieno[2,3-d]pyrimidin-4-yl)thio)acetic acid

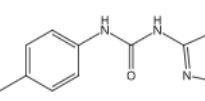
  
C10H11N3O2S  
Sulfamethoxazole

  
C10H15N3O5  
(2R,3R,4S,5R)-4,5-Dihydro-5-(hydroxymethyl)-3-methylspiro[furan-2(3H),7(6H)-]...

**442571-27-9** 1927010-88-5 697787-29-4

  
C11H12N2O2S2  
2-((5,6-Dimethylthieno[2,3-d]pyrimidin-4-yl)thio)propanoic acid

  
C11H16ClNO3  
3-Chloro-4-((1-methylpropyl)amino)-5-(2-propen-1-yloxy)-2(5H)-furanone

  
C12H13N3O2  
N-(5-Methyl-3-isoxazolyl)-N-(4-methylphenyl)urea

View All

5 References 42 Reactions 44 Suppliers 24K References 961 Reactions 120 Suppliers 2 References 22 Reactions 0 Suppliers 1 Reference 3 Reactions 0 Suppliers 3 References 4 Reactions 3 Suppliers

# 物质详情

CAS Registry Number: 723-46-6

References (24K) Reactions (961) Suppliers (120)

Save

CNc1ccc(cc1)S(=O)(=O)Nc2cc(C)c3ocnc3c2

$C_{10}H_{11}N_3O_3S$   
Benzenesulfonamide, 4-amino-N-(5-methyl-3-isoxazolyl)- (9Cl, 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 <sup>3</sup>	-
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 CAS LIFE SCIENCES

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

▼ Toxicity CAS LIFE SCIENCES

▼ Predicted Properties

▼ Predicted Spectra

▼ Bioactivity Indicators

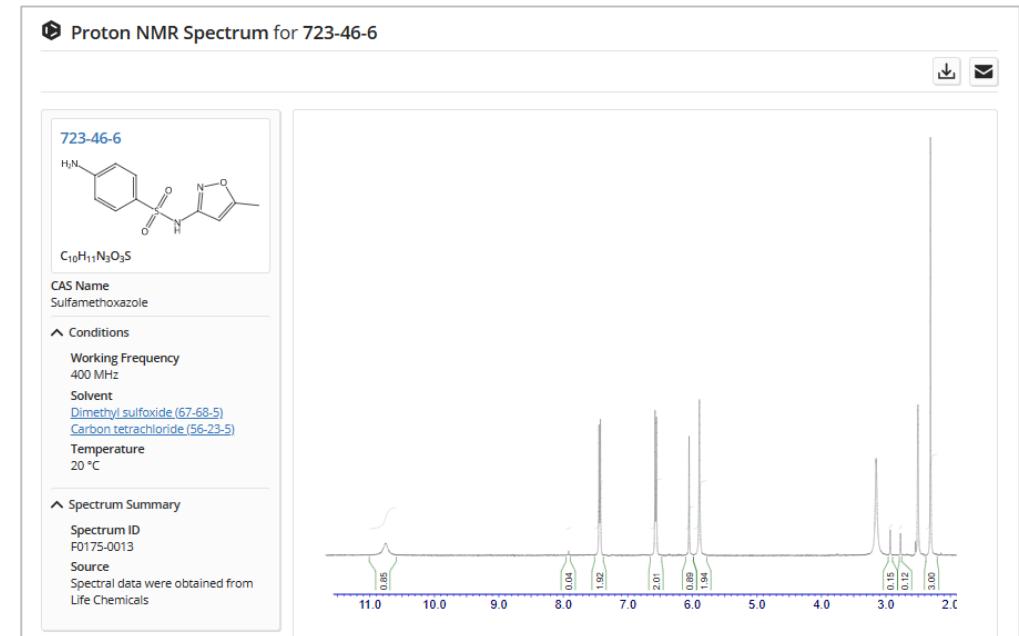
▼ Target Indicators

折叠菜单显示物质各类信息

▲ Experimental Spectra

Source	
<a href="#">View Proton NMR Spectrum</a>	(1) LC
<a href="#">View Proton NMR Spectrum</a>	(2) ENAMINE
<a href="#">View Proton NMR Spectrum</a>	(2) ENAMINE
<a href="#">View Proton NMR Spectrum</a>	(3) CAS
<a href="#">View Proton NMR Spectrum</a>	(4) CAS
<a href="#">View Proton NMR Spectrum</a>	(5) CAS
<a href="#">View Proton NMR Spectrum</a>	(6) BIORAD
<a href="#">View Proton NMR Spectrum</a>	(6) BIORAD
<a href="#">View Proton NMR Spectrum</a>	(7) AIST
<a href="#">Proton NMR Spectrum - 4 Sources</a>	(8-11) CAS

Sources  
(1) Spectral data were obtained from Life Chemicals  
(2) Spectral data were obtained from Enamine Ltd.  
(3) Ham, Won Seo; Angewandte Chemie, International Edition, (2019), 58(2), 532-536, C<sub>A</sub>plus



# 物质详情

**Structure Activity Relationships**

Target	Function	Parameter	Disease	Organism
1132187-M	Inhibitor	Drug removal	<input type="checkbox"/> Bacterial infection (273)	-
207419-N	Inhibitor	Drug removal	<input type="checkbox"/> Microbial infection (206)	-
226605-F	Inhibitor	Drug removal	<input type="checkbox"/> Oxidative stress (76)	-
A. baumannii	Inhibitor	MIC	<input type="checkbox"/> Toxoplasmosis (46)	-
Acanthamoeba	Inhibitor	IC50	<input type="checkbox"/> Bacterial infections	-
Acanthamoeba	Inhibitor	IC50		0.8 ug/mL
Acanthamoeba	Inhibitor	IC50		Acanthamoeba keratitis

**Filter Disease**

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

**CAS LIFE SCIENCES**

**Absorption, Distribution, Metabolism, and Excretion Data**

Target	Function	Parameter	Disease	Organism	Assay	Source
Methicillin-resistant Staphylococcus aureus	-	<input type="checkbox"/> Drug concentration (7)	Bacterial infections	-	<a href="#">View Detail</a> (1) CAS	
Methicillin-resistant Staphylococcus aureus	-	<input type="checkbox"/> Cell uptake (2)	Bacterial infections	-	<a href="#">View Detail</a> (1) CAS	
Methicillin-resistant Staphylococcus aureus	-	<input type="checkbox"/> Serum concentration (2)	Bacterial infections	-	<a href="#">View Detail</a> (1) CAS	
Methicillin-sensitive Staphylococcus aureus	-	<input type="checkbox"/> fAUC(0-24 h) (2)	Bacterial infections	-	<a href="#">View Detail</a> (1) CAS	
Methicillin-sensitive Staphylococcus aureus	-	<input type="checkbox"/> fCmax (2)	Bacterial infections	-	<a href="#">View Detail</a> (1) CAS	
Methicillin-sensitive Staphylococcus aureus	-	<input type="checkbox"/> t1/2 (2)	Bacterial infections	-	<a href="#">View Detail</a> (1) CAS	
Methicillin-sensitive Staphylococcus aureus	-		Bacterial infections	-	<a href="#">View Detail</a> (1) CAS	

**Filter Parameter**

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

**CAS LIFE SCIENCES**

**Assay Data** **CAS LIFE SCIENCES**

Ligand **723-46-6**

Nc1ccc(cc1)S(=O)(=O)Nc2ccoc2  
C<sub>10</sub>H<sub>11</sub>N<sub>3</sub>O<sub>3</sub>S  
Sulfamethoxazole

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, indometacin, sulfamethoxazole, and diclofenac removal by ligninolytic enzymes By: Camarillo Ravelo, Dante; Loera Corral, Octavio <a href="#">(1)</a> ; Gonzalez-Martinez, Ignacio; Chan Cupul, Wilberth; Rodriguez Nava, Celestino Odin Preparative Biochemistry & Biotechnology (2020), 50(6), 592-597   Language: English, Database: CAplus and MEDLINE

**Toxicity**

Target	Function	Parameter	Value	Disease	Organism	Assay	Source
-	-	EC50	>12.500 μM	-	-	<a href="#">View Detail</a> (1) CAS	
-	-	EC50	>12.500 μM	-	-	<a href="#">View Detail</a> (1) CAS	
-	-	EC50	>12.500 μM	-	-	<a href="#">View Detail</a> (1) CAS	
-	-	EC50	1.917 μM	-	-	<a href="#">View Detail</a> (1) CAS	
-	-	EC50	>12.500 μM	-	-	<a href="#">View Detail</a> (1) CAS	

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

# 物质检索—结构检索

The screenshot shows the SciFinder interface. On the left, there's a sidebar with arrows pointing to 'All', 'Substances' (which is selected), 'Reactions', 'References', and 'Suppliers'. The main area has a search bar for 'Substances' with a 'Draw' button and a search icon. Below it is a 'Molecular Formula' dropdown and a text input field with examples like C6H6, (C8H8)x, C22H26CuN2O5.C2H3N. A link to 'Advanced Search' is also present. On the right, a 'CAS Draw' window is open, showing a toolbar with various drawing and selection tools, a text input field for 'Enter a CAS Registry Number, SMILES, or InChI...', and a large workspace for drawing molecules. A legend on the far right lists chemical elements: C, H, O, S, N, P, Cl, Si, with corresponding icons.

X 选择可变基团 Q 取代位点可变

R 自定义R基团

Fn 重复片段工具 Fn 片段结构

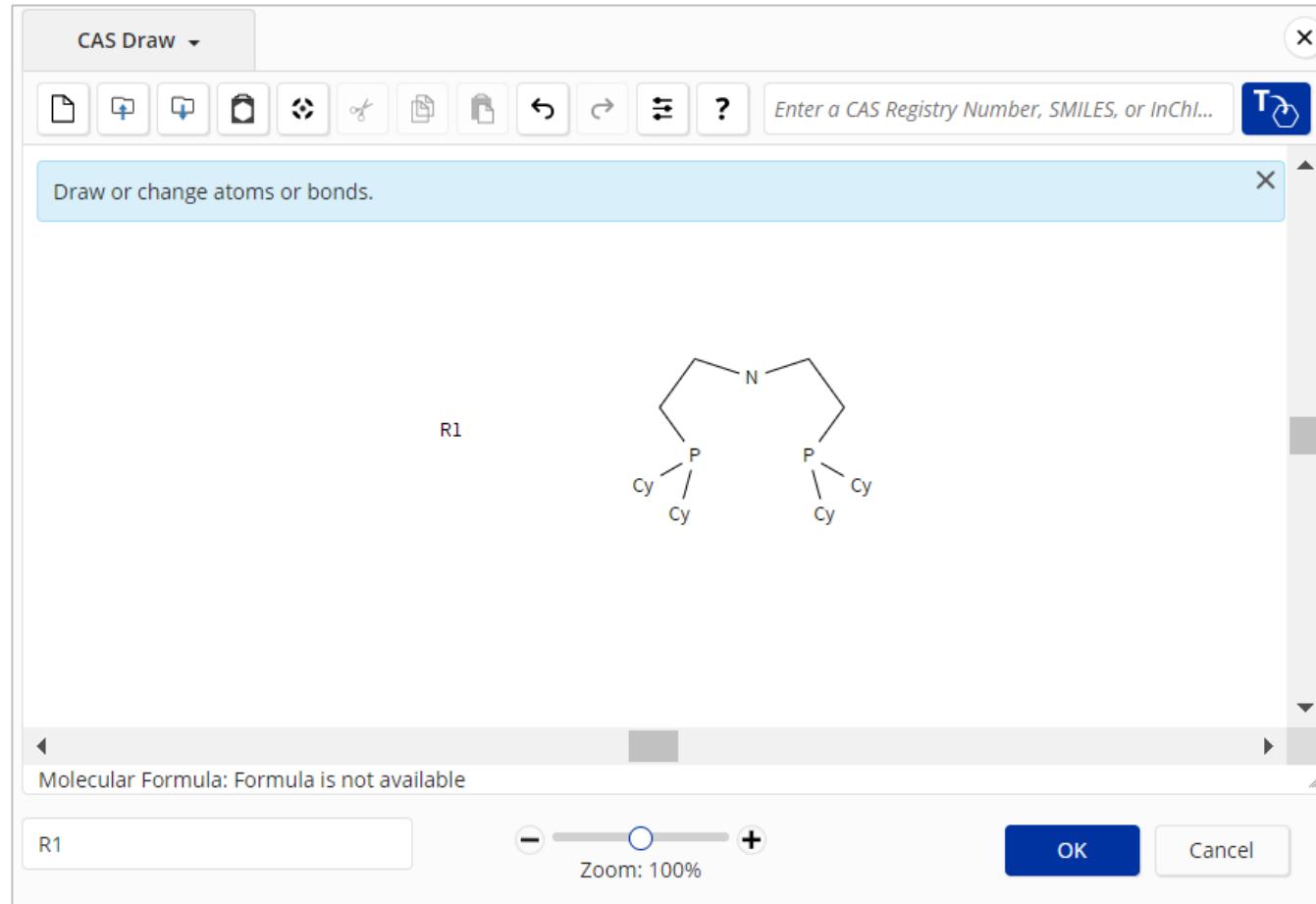
CAS Draw和ChemDoodle的使用指南

[https://scifinder-n.cas.org/help/#t=Drawing\\_Search\\_Queries%2FDrawing\\_Structure\\_Queries.htm](https://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



R-Group Definitions

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

R1: Ni, Cu, Co

Atoms

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

\*Lanthanides

\*\*Actinides

Isotopes

# 物质检索—检索结果集筛选

结构检索类别：  
As Drawn  
亚结构  
相似结构

Chemscape分析

Filter by & Exclude

物质筛选类别：  
**反应角色**  
**文献角色**  
**立体化学**  
**物质类别**  
**同位素**  
**金属包含**  
**实验物性数据**  
**二次检索**.....

Substances search for drawn structure

Structure Match: As Drawn (0) Substructure (732) Similarity (9) Analyze Structure Precision

732 Results

Sort: Relevance View: Partial

Rank	Chemical ID	Chemical Name	Chemical Structure	References	Reactions	Suppliers
1	685504-28-3	<chem>C31H35Cl3CoNP2</chem> (T-4)-Trichloro[N-[2-(diphenylphosphino- $\kappa^P$ ethyl)-N-[2-(diphenylphosphino)ethyl]...		0	0	0
2	807307-30-8	<chem>C31H35Cl3CoNOP2</chem> Cobaltate(1-), trichloro[N-[2-(diphenylphosphino- $\kappa^P$ ethyl)-N-[2-(diphenylphosphino)ethyl]...		0	0	0
3	635299-07-9	<chem>C31H35Cl3CoNOP2.H</chem> Components: 2 Component RN: 807307-30-8 Cobaltate(1-), trichloro[N-[2-(diphenylphosphino- $\kappa^P$ ethyl)-N-[2-(diphenylphosphino)ethyl]...		0	0	0
4	635299-08-0	<chem>C31H35Cl3CoNOP2.2/5C2H6O....</chem> Components: 3 Cobaltate(1-), trichloro[N-[2-(diphenylphosphino- $\kappa^P$ ethyl)-N-[2-(diphenylphosphino)ethyl]...	 OH	1	9	0
5	16827-53-5	<chem>C34H33Co3N3O6P2</chem> Cobalt, [ $\mu$ -[2,2'-bis(diphenylphosphino)triethylamine]]tetracarbonyldinitrosylid...		1	0	0
6	635299-09-1	<chem>C31H35Cl2CoNOP2</chem> (T-4)-Dichloro[N-[2-(diphenylphosphino- $\kappa^P$ ethyl)-N-[2-(diphenylphosphino)ethyl]...		1	3	0

# 物质检索—结构检索

结构检索类别：

- As Drawn

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

- Substructure 亚结构

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

- Similarity 相似结构

获得片段或整体结构与被检索结构相似的结果，母体结构可以被取代，也可以被改变

**注：如果关注相似结构检索结果，请不要绘制通式结构**

# 物质检索—检索结果集筛选：Reaction Role

利用物质在反应中的角色精准定位相应的物质

Substances search for drawn structure

References Reactions Suppliers Save and Alert

Structure Match As Drawn (0) Substructure (732) Similarity (9) Analyze Structure Precision Chemscape Analysis Visually explore structure similarity with a powerful new tool. Learn more about Chemscape. Create Chemscape Analysis Filter Behavior Filter by Reaction Role Product (216) Reactant (53) Reagent (3) Catalyst (36) Reference Role Commercial Availability Number of Components Molecular Weight

Filtering: Reaction Role: Catalyst X Clear All Filters Sort: Relevance View: Partial

36 Results

Rank	Chemical ID	Chemical Structure	Chemical Name	Reactions	Suppliers
1	1879110-74-3		$C_{33}H_{39}Cl_2CoNP_2$ (T-4)-[N,N-Bis[2-(diphenylphosphino- $\kappa P$ )ethyl]-1-pentanamine]dichlorocobalt	1 Reference 2 Reactions 0 Suppliers	
2	2332371-33-0		$C_{30}H_{33}Cl_2CoNP_2$ (T-4)-Dichloro[2-(diphenylphosphino- $\kappa P$ )-N-[2-(diphenylphosphino- $\kappa P$ )ethyl]-2-propanamine]dichlorocobalt	1 Reference 3 Reactions 0 Suppliers	
3	1879110-75-4		$C_{31}H_{35}Cl_2CoNP_2$ (T-4)-[N,N-Bis[2-(diphenylphosphino- $\kappa P$ )ethyl]-2-propanamine]dichlorocobalt	1 Reference 2 Reactions 0 Suppliers	
4	1087216-22-5		$C_{28}H_{29}Cl_2CoNP_2$ Dichloro[2-(diphenylphosphino- $\kappa P$ )-N-[2-(diphenylphosphino- $\kappa P$ )ethyl]ethanamine- $\kappa N$ ...	8 References 105 Reactions 0 Suppliers	
5	2170923-58-5		$C_{28}H_{29}Cl_2CoNP_2$ (T8-5-13)-Dichloro[2-(diphenylphosphino- $\kappa P$ )-N-[2-(diphenylphosphino- $\kappa P$ )ethyl]eth...	1 Reference 32 Reactions 0 Suppliers	
6	1846596-28-8		$C_{28}H_{53}Cl_2CoNP_2$ (T8-5-13)-Dichloro[2-(dicyclohexylphosphino- $\kappa P$ )-N-[2-(dicyclohexylphosphino- $\kappa P$ )e...	7 References 13 Reactions 0 Suppliers	

# 物质检索—检索结果集筛选：Reference Role

利用物质的研究角色精准定位相应的物质

Reference Role

By Count Alphanumeric

5 Selected

<input type="checkbox"/> Preparation (489)	<input checked="" type="checkbox"/> Process (32)	<input checked="" type="checkbox"/> Biological Study (4)
<input checked="" type="checkbox"/> Synthetic Preparation (488)	<input type="checkbox"/> Physical, Engineering, or Chemical Process (31)	<input type="checkbox"/> Pharmacological Activity (4)
<input type="checkbox"/> Properties (245)	<input checked="" type="checkbox"/> Industrial Manufacture (9)	<input type="checkbox"/> Therapeutic Use (4)
<input type="checkbox"/> Reactant (98)	<input type="checkbox"/> Technical or Engineered Material Use (8)	<input type="checkbox"/> Analytical Reagent Use (1)
<input type="checkbox"/> Reactant or Reagent (98)		<input type="checkbox"/> Analytical Study (1)
<input type="checkbox"/> Uses (88)		<input type="checkbox"/> Formation, Non-preparative (6)
<input checked="" type="checkbox"/> Catalyst Use (77)		<input type="checkbox"/> Formation, Unclassified (1)

Apply Cancel

Structure Match

As Drawn (0)

Substructure (732) **Similarity (9)**

Analyze Structure Precision

Chemscape Analysis

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

Create Chemscape Analysis

Filter Behavior

Filter by Exclude

Reaction Role

Reference Role

- Preparation (489)
- Synthetic Preparation (488)
- Properties (245)
- Reactant (98)
- Reactant or Reagent (98)
- Industrial Manufacture (9)

View All

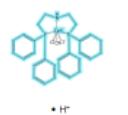
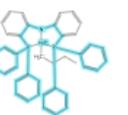
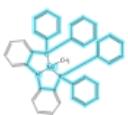
Commercial Availability

Not Available (9)

Filtering: Reference Role: Industrial Manufacture

Clear All Filters

Sort: Relevance View: Partial

9 Results	1	2	3
<input type="checkbox"/> 1087216-22-5	<input type="checkbox"/> 1395056-63-9	<input type="checkbox"/> 579490-65-6	
			
C <sub>28</sub> H <sub>29</sub> Cl <sub>2</sub> CoNP <sub>2</sub> Dichloro[2-(diphenylphosphino- $\kappa$ P)-N-[2-(diphenylphosphino- $\kappa$ P)ethyl]ethanamine- $\kappa$ N...	C <sub>28</sub> H <sub>29</sub> Cl <sub>3</sub> CoNP <sub>2</sub> -H Components: 2 Component RN: 1395144-60-1 Cobaltate(1-), trichloro[2-(diphenylphosphino- $\kappa$ P)-N-[2-(diphenylphosphino- $\kappa$ P)ethyl]benzen...	C <sub>40</sub> H <sub>37</sub> NNiP <sub>2</sub> ( <i>SP</i> -4-1)-Butyl[2-(diphenylphosphino- $\kappa$ P)-N-[2-(diphenylphosphino- $\kappa$ P)phenyl]benzen...	
<input type="checkbox"/> 8 References <input type="checkbox"/> 105 Reactions <input type="checkbox"/> 0 Suppliers	<input type="checkbox"/> 3 References <input type="checkbox"/> 8 Reactions <input type="checkbox"/> 0 Suppliers	<input type="checkbox"/> 6 References <input type="checkbox"/> 20 Reactions <input type="checkbox"/> 0 Suppliers	
4	5	6	
<input type="checkbox"/> 579490-58-7	<input type="checkbox"/> 579490-62-3	<input type="checkbox"/> 579490-55-4	
			
C <sub>37</sub> H <sub>31</sub> NNiP <sub>2</sub> ( <i>SP</i> -4-1)-[2-(Diphenylphosphino- $\kappa$ P)-N-[2-(diphenylphosphino- $\kappa$ P)phenyl]benzenamina...	C <sub>38</sub> H <sub>33</sub> NNiP <sub>2</sub> ( <i>SP</i> -4-1)-[2-(Diphenylphosphino- $\kappa$ P)-N-[2-(diphenylphosphino- $\kappa$ P)phenyl]benzenamina...	C <sub>36</sub> H <sub>28</sub> CINNIP <sub>2</sub> ( <i>SP</i> -4-3)-Chloro[2-(diphenylphosphino- $\kappa$ P)-N-[2-(diphenylphosphino- $\kappa$ P)phenyl]benze...	
<input type="checkbox"/> 7 References <input type="checkbox"/> 22 Reactions <input type="checkbox"/> 0 Suppliers	<input type="checkbox"/> 6 References <input type="checkbox"/> 21 Reactions <input type="checkbox"/> 0 Suppliers	<input type="checkbox"/> 8 References <input type="checkbox"/> 52 Reactions <input type="checkbox"/> 0 Suppliers	

# 物质检索—检索结果集的保存

References ▾ Reactions ▾ Suppliers ▾

Structure Match  
As Drawn (0)  
**Substructure (732)**  
Similarity (9)

Analyze Structure Precision

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

Filter Behavior  
**Filter by** 文献信息 反应信息 供应商信息

Reaction Role  
Reference Role  
Commercial Availability  
Number of Components  
Molecular Weight  
Element

109 Results

Sort: Relevance ▾ View: Partial ▾

Rank	Chemical ID	Chemical Name	Chemical Structure	References	Reactions	Suppliers
1	1698881-12-7	<chem>C58H56N2NiP4S4</chem> ( <i>SP</i> -4-1)-Bis[ <i>N,N</i> -bis[2-(diphenylphosphino)ethyl]carbamodithioato- <i>K5,K5'</i> ]nickel		1 Reference	4 Reactions	0 Suppliers
2	65120-45-8	<chem>C34H43N2NiP2S</chem> Nickel(1+), [ <i>N,N</i> -bis[2-(diphenylphosphino)ethyl]- <i>N,N'</i> -diethyl-1,2-ethanediamine...		0 References	0 Reactions	0 Suppliers
3	65120-39-0	<chem>C35H45N2NiP2S</chem> Nickel(1+), [ <i>N,N</i> -bis[2-(diphenylphosphino)ethyl]- <i>N,N'</i> -diethyl-1,2-ethanediamine...		0 References	0 Reactions	0 Suppliers
6	65120-46-9	<chem>C58H56Au4Cl4N2NiP4S4</chem> Bis[μ <sub>3</sub> -[ <i>N,N</i> -bis[2-(diphenylphosphino)ethyl]carbamodithioato- <i>K5,K5'</i> ]]tetrakis(...)		0 References	0 Reactions	0 Suppliers

Save and Alert

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  
Select Quantity  
 All Results  
 Selected Results  
 Range (ex. 2 to 20)  
Display  
 Structures Only  
 Result Summary  
 Result Details

File Name Substance\_20221121\_1345

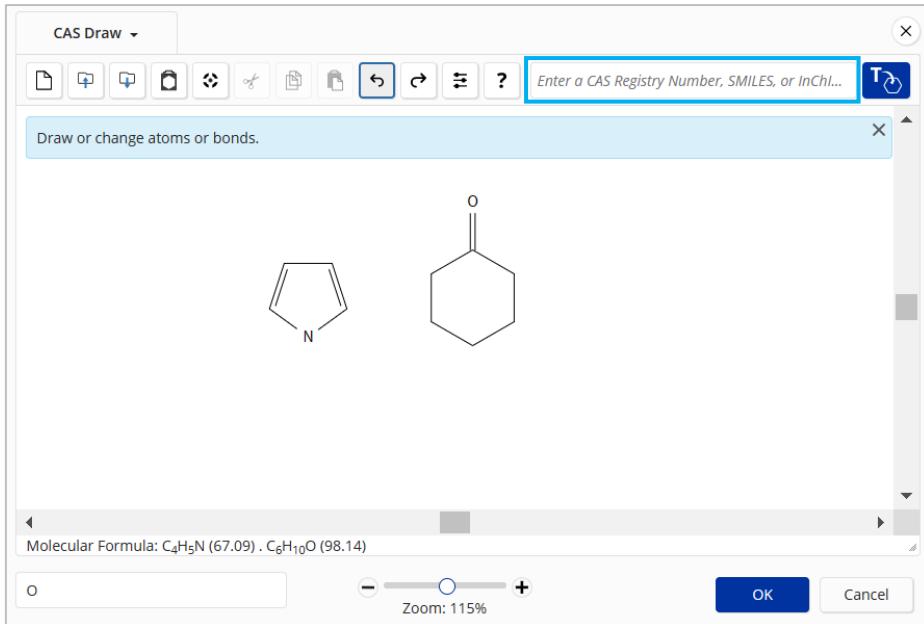
Include  
 Task History  
 Substance Identifiers  
 Experimental Spectra  
 Predicted Spectra  
 Bioactivity Indicators  
 Regulatory Information

Download Cancel Learn more about downloads.

# 物质检索——结构检索综合示例

请思考，已知活性结构片段，如何查找：

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



Reference Role

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

[View All](#)

Filter Behavior

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

Reaction Role

- Product (54)
- Reactant (21)

Structure Match

As Drawn (2) Substructure (58K) Similarity (580) Analyze Structure Precision

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

Create Chemscape Analysis

Filter Behavior Filter by Exclude

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

Excluding: Reaction Role: Product X

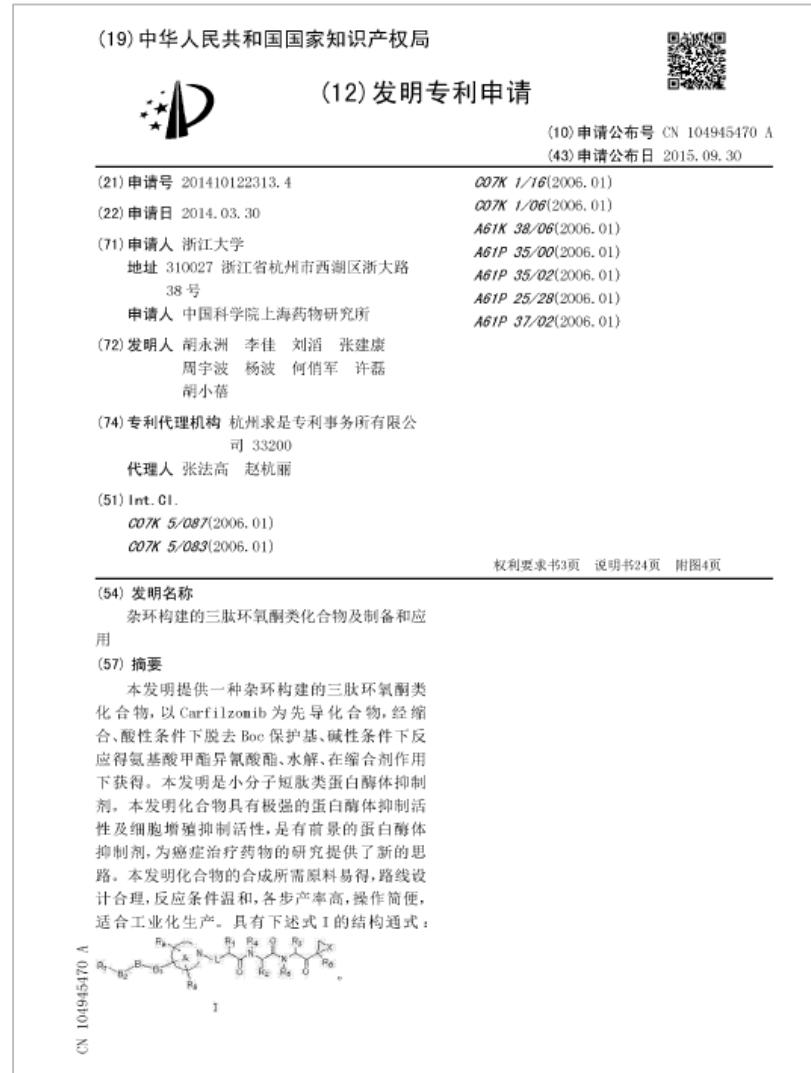
223 Results

Sort: Number of References: Ascending View: Partial

Number	Chemical Structure	Chemical Name	Chemical Formula	Notes
1		2707395-49-9	C <sub>13</sub> H <sub>11</sub> NO <sub>3</sub>	5,6-Dihydro-9,10-dihydroxy-11H-pyrrolo[2,1-b][3]benzazepin-11-one
2		2699076-84-9	C <sub>16</sub> H <sub>9</sub> NO <sub>4</sub>	Benzo[5,6]pentaleno[1',2':3,4]pyrrolo[2,1-b][3]benzazepin-7(11bH)-one, 10,11-dihydro...
3		2707395-48-8	C <sub>14</sub> H <sub>13</sub> NO <sub>3</sub>	6,11-Dihydro-8,9-dihydroxy-5H-pyrrolo[2,1-b][3]benzazepine-3-carboxaldehyde
4		2126788-65-4		
5		2126179-96-0		
6		2126179-95-9		

——亚结构检索，限定结果为单组份、Natural Product Occurrence，获得含已知活性结构片段的天然产物  
——排除物质结果集中，reaction role为product的结果  
——通过CAS Retrosynthesis Tool

# CAS Markush检索



**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-基氨基甲酰基)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， $N_2$  保护下加入 25mL 无水  $CH_2Cl_2$ ，然后缓缓滴入吡嗪 (2.5mL, 30mmol) 和二氯亚砜 (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  $CH_2Cl_2$  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  $CH_2Cl_2$  提取 (15mL × 3)，合并有机层，无水硫酸钠干燥后减压除去溶剂，柱层析分离得白色固体 2.3g，收率 74%。m.p. : 134–136°C； $^1H$  NMR (500MHz,  $CDCl_3$ ) :  $\delta$  = 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,  $CH_2$ ), 2.81 (m, 2H,  $CH_2$ ), 2.48 (m, 1H, CH), 1.93 (d, 2H,  $J$ =12.5Hz,  $CH_2$ ), 1.76 (m, 2H,  $CH_2$ ), 1.47 (s, 9H,  $CH_3$ ) ppm; ESI-MS: m/z = 307 [M+H]<sup>+</sup>。

[0028] 制备实施例 2、4-(吡嗪-2-酰基)哌嗪-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  $CH_2Cl_2$  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，哌嗪-1-甲酸叔丁酯 (1.9g, 10mmol) 加入反应液中，室温反应 3 小时。反应液加入 30mL 饱和碳酸氢钠水溶液稀释，分出有机层，饱和食盐

# CAS Markush检索

## 预测性物质[Prophetic Substance]:

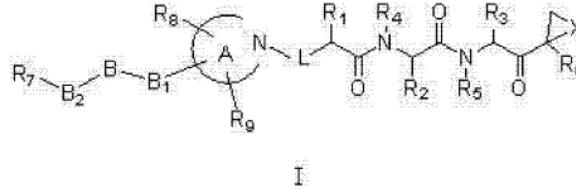
- 使用Markush结构陈述的预测物质，一个Markush可以陈述成百上千，甚至更多的结构
- 被Markush结构包含，但未被实施或呈现在表格、权利要求书或说明书中的结构，不会被CAS分配CAS Registry Number
- Markush检索，能检索到通过Substance可能检索不到的结构

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：



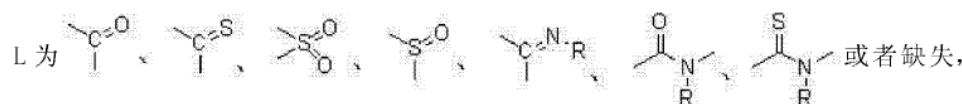
其中：

R<sub>1</sub>, R<sub>2</sub>, R<sub>3</sub>各自独立选自H、C<sub>1-6</sub>烷基-D、卤代的C<sub>1-6</sub>烷基-D、C<sub>1-6</sub>羟基烷基、C<sub>1-6</sub>巯基烷基、C<sub>1-6</sub>烷氧基烷基、芳基、芳烷基、杂芳基或杂芳烷基；其中：D为N(R<sub>a</sub>)(R<sub>b</sub>)或缺失，R<sub>a</sub>, R<sub>b</sub>各自独立选自H、OH、C<sub>1-6</sub>烷基、卤代的C<sub>1-6</sub>烷基或N末端保护基；

R<sub>4</sub>, R<sub>5</sub>各自独立选自H、OH、C<sub>1-6</sub>烷基、卤代的C<sub>1-6</sub>烷基或芳烷基；

R<sub>6</sub>选自H, C<sub>1-6</sub>烷基, 卤代的C<sub>1-6</sub>烷基, C<sub>1-6</sub>羟基烷基, C<sub>1-6</sub>烷氧基, 卤代的C<sub>1-6</sub>烷氧基, C(O)O-C<sub>1-6</sub>烷基, C(O)NH-C<sub>1-6</sub>烷基, 芳烷基；

X为O、S、NH、N-C<sub>1-6</sub>烷基或N-卤代的C<sub>1-6</sub>烷基；



其中R选自H、C<sub>1-6</sub>烷基或卤代的C<sub>1-6</sub>烷基；

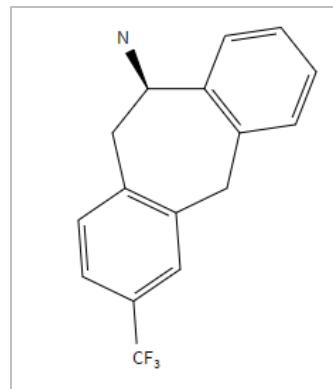
环A选自5~7元的饱和脂肪杂环、不饱和杂环、或者有取代的5~7元的饱和脂肪杂环、不饱和杂环，所述的杂环包含0~3个选自O、N和S的杂原子并任选地被R<sub>8</sub>、R<sub>9</sub>和B<sub>1</sub>基团取代；

R<sub>8</sub>, R<sub>9</sub>分别独立选自H、OH, C<sub>1-6</sub>烷基, C<sub>1-6</sub>烷氧基, C<sub>1-6</sub>羟基烷基, C<sub>1-6</sub>巯基烷基, C<sub>1-6</sub>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<sub>1-6</sub>烷基、卤代的C<sub>1-6</sub>烷基, C<sub>1-6</sub>烷氧基或卤代的C<sub>1-6</sub>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)

Analyze Structure Precision

Chemscape Analysis

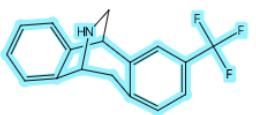
Visually explore structure similarity with a powerful new tool.

Learn more about Chemscape.

Create Chemscape Analysis

Sort: Number of References

2 Results

1 146364-17-2   
C17H14F3N  
10,5-(iminomethano)-5H-dibenzo[a,d]cycloheptene, 10,11-dihydro-3-(trifluoromethyl)...

2 146364-18-3   
C18H16F3N  
10,5-(iminomethano)-5H-dibenzo[a,d]cycloheptene, 10,11-dihydro-12-methyl-3-(trifluoromethyl)...

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

Filtering: Number of References: Descending  Sort: Number of References: Descending  View: Partial

Clear All Filters 

索引	分子式	名称	参考文献数	反应数	供应商数
1	<chem>C15H13Cl</chem>	5-Chlorodibenzosuberane	61	143	130
2	<chem>C16H14F3N</chem>	1,2,3,4-Tetrahydro-2-[4-(trifluoromethyl)phenyl]isoquinoline	64	90	121
3	<chem>C15H15N</chem>	IEM 2115	68	58	78
4	<chem>C18H17Br</chem>	5-(3-Bromopropylidene)-10,11-dihydro-5H-dibenzo[a,d]cycloheptene	60	3436-04-2	62
5	<chem>C16H13N</chem>	10,11-Dihydro-5H-dibenzo[a,d]cycloheptene-5-carbonitrile	62	1729-63-1	64
6	<chem>C21H24F3N</chem>	Fluotracen	64	35764-73-9	

# 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

Screenshot of the CAS SciFinder interface showing a Patent Markush search for a drawn structure. The search results page displays four patent documents:

- WO2011025969**: Compounds that treat malaria and prevent malaria transmission. By: Su, Xin-Zhuan; Yuan, Jing; Raj, Dipak; Pattradilokrat, Sittiporn; Johnson, Ron; Huang, Ruili. World Intellectual Property Organization, WO2011025969 A1 2011-03-03 | Language: English, Database: Cplus. Assignee: United States Dept. of Health and Human Services. Patent claim 1: \*c1ccc(cc1)N(\*)c2cc(\*)c3c(\*)c(\*)c(\*)c3cc2X.  
Full Text: [PatentPak](#) | [PDF](#) | [PDF+](#) | [Viewer](#)
- EP502788**: by: Regnier, Gérard; Dramidou, Alain; Hassi, Ghannem; Pierre, Alain; Léonce, Stéphane. European Patent Organization, EP502788 A1 1992-09-09 | Language: French, Database: Cplus. Assignee: Adir et Cie. Patent claim 11: \*c1ccc(cc1)N(\*)c2cc(\*)c3c(\*)c(\*)c(\*)c3cc2F.  
Full Text: [Full Text](#)

The search interface includes a drawing tool where a complex polycyclic aromatic hydrocarbon structure is drawn, and a search bar with the placeholder "Enter a query...". Other features include "Edit Drawing", "Save and Alert", and "Search Patent Markush".

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

# 物质检索小结

1. 利用结构绘制工具合理扩大结构检索范围：R基团、可变基团、可变位置取代等
2. 利用结构绘制工具适当限定检索结构：环锁工具、原子锁工具、EZ构型限定等
3. 正确理解As Drawn、Substructure、Similarity检索结果集的意义和范围
4. 充分利用物质筛选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

Return to Home

## Reactions search for "Semaglutide"

References ▾ Save and Alert

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

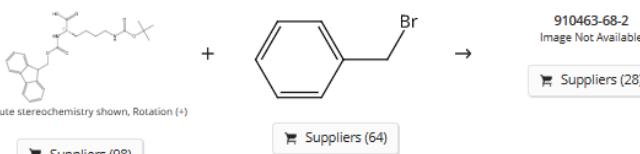
Reactions ▾ Semaglutide

228 Results Group: By Scheme ▾ Sort: Number of Steps: Descending ▾ View: Collapsed ▾

Scheme 1 (1 Reaction)

Steps: 7

Absolute stereochemistry shown, Rotation (+)

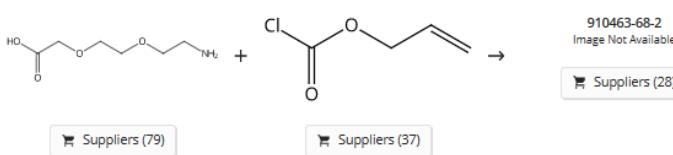


[Suppliers \(98\)](#) [Suppliers \(64\)](#)

[Expand Scheme](#)

Scheme 2 (5 Reactions)

Steps: 5-7



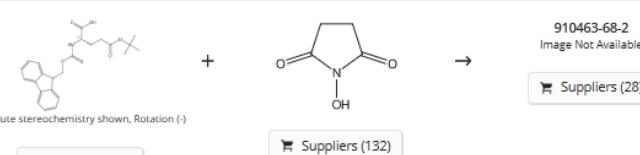
[Suppliers \(79\)](#) [Suppliers \(37\)](#)

[Expand Scheme](#)

Scheme 3 (2 Reactions)

Steps: 3-7

Absolute stereochemistry shown, Rotation (-)



[Suppliers \(93\)](#) [Suppliers \(132\)](#)

Reactions 175:621496

Return to Home

## Reactions search for "175:621496"

References

Filter Behavior

Filter by Exclude

Yield

- 90-100% (3)
- 80-89% (5)
- 70-79% (2)
- 50-69% (3)
- No Yield Available (120)

Number of Steps

- 1 (25)
- 2 (29)
- 3 (27)
- 4 (21)
- 5 (16)
- 6-10 (15)

Non-Participating Functional Groups

- Amide (10)
- Carboxylic ester (10)
- Carboxylic acid (9)
- Ether (5)
- Amine (3)

View All

Reaction Mapping

Experimental Protocols

- Synthetic Methods (132)

Reaction Type

Stereochemistry

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

Scheme 1 (2 Reactions) Steps: 7-8

204656-20-2 Image Not Available

Absolute stereochemistry shown

Suppliers (37)

Suppliers (145)

Suppliers (77)

Expand Scheme

Scheme 2 (1 Reaction) Steps: 8

204656-20-2 Image Not Available

Absolute stereochemistry shown

Suppliers (37)

Suppliers (136)

Expand Scheme

Scheme 3 (1 Reaction) Steps: 7

204656-20-2 Image Not Available

Absolute stereochemistry shown

Absolute stereochemistry shown

Suppliers (37)

Suppliers (32)

Supplier (1)

Expand Scheme

# 反应检索

通过结构式进行检索

Searching for... Reactions

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

Enter a query... Draw Search

CAS Draw

Draw or change atoms or bonds.

reactant → product

Molecular Formula: Formula is not available

OK Cancel

Zoom: 100%

X = Cl, Br

All Substances Reactions References Suppliers

Et R Fn Cy A B

C H O S N P Cl Si EZ

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# 反应检索—结果集的分组与排序

As drawn结果为32

Reactions search for drawn structure

References ▾

Structure Match

As Drawn (32)  

Substructure (8,521)

Similarity (0)

Filter Behavior

Filter by   Exclude

Yield

Number of Steps

Non-Participating Functional Groups

Reaction Mapping

Experimental Protocols

Synthetic Methods (3)

Experimental Procedure (12)

Reaction Type

Reagent

Catalyst

Solvent

Commercial Availability

Reaction Notes

Search Within Results

Filtering: Reaction Mapping: Mapping Data Available X Clear All Filters

16 Results

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

Scheme 1 (5 Reactions)

By Scheme  
By Document  
By Transformation

Relevance  
Publication Date: Newest  
Publication Date: Oldest  
Yield  
Number of Steps: Ascending  
Number of Steps: Descending

Supplier (85) Supplier (15)

Expand Scheme ▾

Scheme 2 (1 Reaction)

Steps: 1 Yield: 76% \*\*\*

Supplier (51) Supplier (3)

31-614-CAS-28968228 Steps: 1 Yield: 76% Preparation of heterocyclic compounds as selective subtype alpha 2 adrenergic agents

1.1 Reagents: O-Methylhydroxylamine hydrochloride Solvents: Pyridine; rt; 1 h, 50 °C  
1.2 Reagents: (Tetrahydrofuran)boron Solvents: Tetrahydrofuran; rt; 3 h, reflux; reflux → 0 °C  
1.3 Reagents: Sodium hydroxide Solvents: Water; overnight, reflux; reflux → rt

Experimental Protocols PatentPak Full Text ▾

The screenshot shows a search interface for reaction schemes based on a drawn structure. The results are filtered to show 16 reactions. The first two schemes are displayed:

**Scheme 1 (5 Reactions):** This scheme shows a reaction where a substituted benzene ring reacts with a substituted phenyl group to form a product. Suppliers for this scheme include 85 companies.

**Scheme 2 (1 Reaction):** This scheme shows a reaction where a substituted benzene ring reacts with a substituted pyridine ring to form a product. Suppliers for this scheme include 51 companies.

A specific reaction from Scheme 2 is highlighted, detailing its experimental protocol:

**Reaction:** Preparation of heterocyclic compounds as selective subtype alpha 2 adrenergic agents

**Protocol:**

- 1.1 Reagents: O-Methylhydroxylamine hydrochloride Solvents: Pyridine; rt; 1 h, 50 °C
- 1.2 Reagents: (Tetrahydrofuran)boron Solvents: Tetrahydrofuran; rt; 3 h, reflux; reflux → 0 °C
- 1.3 Reagents: Sodium hydroxide Solvents: Water; overnight, reflux; reflux → rt

反应分组：  
按类型分组  
按文献分组

反应排序：  
相关度  
公布时间  
产率  
步数

# 反应检索—结果集筛选

Substructure结果8521

As Drawn反应检索  
亚结构反应检索  
相似反应检索

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

**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

2 Hydrolysis or Hydrogenolysis of Carboxylic Esters or Thioesters

View 1 Related Reaction

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

View 2 Related Reactions

4 Formation of N/O/S Heterocycles

View 49 Related Reactions

2 Results

Group: By Scheme Sort: Relevance View: Collapsed

Scheme 1 (1 Reaction)

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

Absolute stereochemistry shown

Expand Scheme

Scheme 2 (1 Reaction)

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

Absolute stereochemistry shown

31-313-CAS-18612019 Steps: 1

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

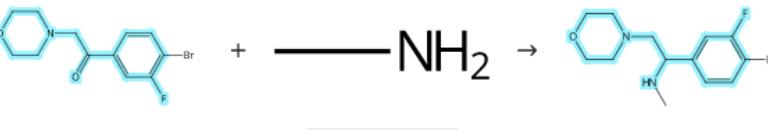
Filtering: Non-Participating Functional Groups: Halide X

Clear All Filters

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

Scheme 1 (1 Reaction)

Steps: 1 Yield: 100% ⚙

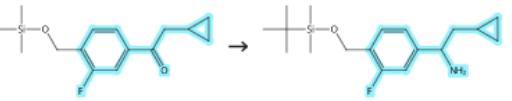


[Suppliers \(107\)](#)

Expand Scheme ▾

Scheme 2 (1 Reaction)

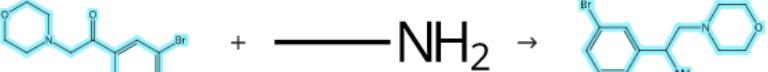
Steps: 1 Yield: 100% ⚙



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)

Primary alcohol (2)

Carboxylic ester (53)

Acyclic ketone (5)

Unsaturated ester (2)

Secondary amine (50)

Alkyl halide (4)

Nitro (1)

Ketone (48)

Nitrile (4)

Primary amine (1)

Unsaturated ketone (1)

Apply Cancel

# 反应检索—结果集筛选：Synthetic Methods™

Structure Match

As Drawn (32)

**Substructure (8,521)**

Similarity (0)

Filter Behavior

Filter by     Exclude

Yield

Number of Steps

Non-Participating Functional Groups

Reaction Mapping

Experimental Protocols

Synthetic Methods (40)

Experimental Procedure (83)

Reaction Type

Stereochemistry

Reagent

Catalyst

Solvent

Commercial Availability

Reaction Notes

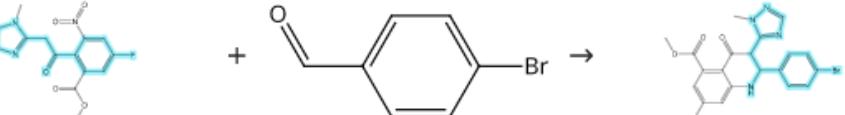
Search Within Results

Source Reference

Filtering: Non-Participating Functional Groups: Halide X    Experimental Protocols: Synthetic Methods X    Clear All Filters

40 Results    Group: By Scheme ▾ Sort: Relevance ▾ View: Collapsed ▾

Scheme 1 (1 Reaction)    Steps: 1 Yield: 98% ⋮



Suppliers (15)     Suppliers (89)

31-614-CAS-24450288    Steps: 1 Yield: 98%    DoE Optimization Empowers the Automated Preparation of Enantiomerically Pure [<sup>18</sup>F]Talazoparib and its In Vivo Evaluation as a PARP Radiotracer

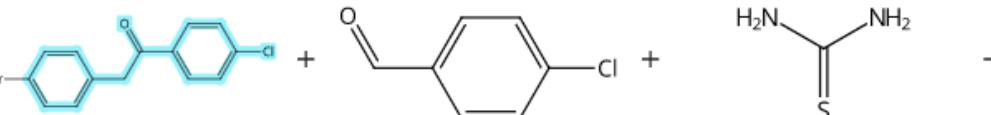
1.1 Reagents: Hydrochloric acid, Titanium chloride ( $TiCl_3$ )  
Solvants: Methanol, Tetrahydrofuran, Water; rt; 30 min, rt; 2 h, 30 - 50 °C  
1.2 Reagents: Water

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

Experimental Protocols     Full Text ▾

Collapse Scheme ▾

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



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



# 反应检索—结果集筛选：Synthetic Methods™

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

CAS Reaction Number: 31-614-CAS-24450288

Reaction Overview  
Steps: 1 Yield: 98%

JOURNAL  
DoE Optimization Empowers the Automated Preparation of Enantiomerically Pure [<sup>18</sup>F]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

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

Chemical reaction scheme:  
  
+   
→   
98%

Suppliers (15) Suppliers (89)

Save

Step 1

Stage	Reagents	Catalysts	Solvents	Conditions
1	Hydrochloric acid Titanium chloride (TiCl <sub>3</sub> )	-	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](#)  
[Benzonic acid, 5-fluoro-2-\(2-\(1-methyl-1H-1,2,4-triazol-5-yl\)acetyl\)-3-nitro-, methyl ester](#)

Reagents: [Hydrochloric acid](#)  
[Titanium chloride \(TiCl<sub>3</sub>\)](#)  
[Water](#)

Procedure

- 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).
- 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.
- Maintain the reaction temperature between 30 and 50°C for 2 hours.
- Quench the mixture by the slow addition of water (260 mL).
- Pour the reaction mixture into a separating funnel.
- Extract the mixture with ethyl acetate (4 x 140 mL).
- Pool the organic fractions.
- Wash the organic fractions with NaHCO<sub>3</sub> (3 x 60 mL) and NaHSO<sub>3</sub> (3 x 100 mL).
- Dry the organic fractions with sodium sulfate (Na<sub>2</sub>SO<sub>4</sub>).
- Concentrate the solvent under reduced pressure to obtain a thick yellow syrup.
- Wash the residue with aliquots of diethyl ether (3 x 10 mL), carefully.
- 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

CAS Method Number 3-315-CAS-33168860

Transformations

- 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

# 联合检索—结构与关键词

联用检索提高检索效率

Searching for...

References

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

Friedel-crafts acylation

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

Add Advanced Search Field

Learn more about Sci

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

Edit Drawing Remove

All Substances Reactions References Suppliers Sequences Retrosynthesis

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)

Reactants: Indole derivative (84), Indole (100), Indole (11)

Products: Acylated indole (1)

Steps: 1 Yield: 82%

Expand Scheme

Scheme 2 (1 Reaction)

Reactants: Indole derivative (90), Benzoyl chloride (63), Benzoyl chloride (10)

Products: Acylated indole (1)

Steps: 1 Yield: 78%

Expand Scheme

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

Substances Reactions Citing Knowledge Graph Save and Alert

Structure Match 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)

1,100 Results Sort: Relevance View: Partial Abstract

1

ZrCl<sub>4</sub>-Mediated Regio- and Chemoselective Friedel-Crafts Acylation of Indole

By: Guchhait, Sankar K; Kashyap, Maneesh; Kamble, Harshad  
Journal of Organic Chemistry (2011), 76(11), 4753-4758 | Language: English, Database: Cplus and MEDLINE

An efficient method for regio- and chemoselective Friedel-Crafts acylation of indoles using acyl chlorides in the presence of ZrCl<sub>4</sub> has been discovered. It minimizes/eliminates common competing reactions that occur due to high and multiamion-nucleophilic character of indole. In this method, a wide range of aryl, heteroaryl, alkenoyl, and alkanoyl chlorides undergo smooth acylation with various indoles without NH protection and afford 3-acylindoles in good to high yields.

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

2

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

By: Velurya, Rakesh H; Aube, Jeffrey  
Organic Letters (2016), 18(15), 3534-3537 | Language: English, Database: Cplus 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

The screenshot shows the CAS Retrosynthesis Tool interface. On the left, there is a sidebar with a search bar containing '2628280-40-8', a 'References' button (236), a 'Reactions' button (53), and a 'Suppliers' button (39). The main area displays the substance details for CAS RN 2628280-40-8. The substance name is 3-Azabicyclo[3.1.0]hexane-2-carboxamide, N-[(1S)-1-cyano-2-[(3S)-2-oxo-3-pyrroli...]. It shows the chemical structure with absolute stereochemistry indicated by (S) and (R) labels. Below the structure are buttons for 'Substance Detail', 'Reactions (53)', 'Synthesize (52)', 'Start Retrosynthetic Analysis' (which is highlighted with a blue box), 'References (236)', and 'Suppliers (39)'. At the bottom are buttons for 'Edit Structure', 'Reset', and 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

# 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

The screenshot shows the CAS Retrosynthesis Tool interface. On the left, there is a sidebar with search filters: All, Substances, Reactions, References, Suppliers, Biosequences, and Retrosynthesis. The Retrosynthesis option is highlighted with a blue arrow. Below the sidebar is a toolbar with various drawing and selection tools. The main workspace has a text input field "Enter a CAS Registry Numbers, SMILES..." and a button "Draw or change atoms or bonds.". A chemical structure of a bicyclic amide is drawn in the workspace. At the bottom, the molecular formula "C<sub>8</sub>H<sub>13</sub>NO<sub>2</sub> (155.20)" is displayed, along with a zoom slider set to 100% and a "Start Retrosynthetic Analysis" button.

# 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.

Break and Protect Bonds

Learn more.

Set Rules Supporting Predicted Reactions

Learn more.

Set Starting Materials Cost Limit

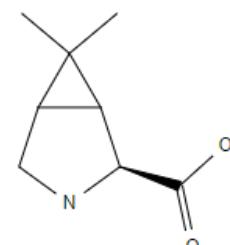
Learn more.

Break Bond    Protect Bond    Clear All Bond Selections

100 USD/mol

Email me when my plan is complete

Create Retrosynthesis Plan



# 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®

View Excluded Options

Plan Information 路线概览

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

Commercially Available: A, B, C

Plan Options

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

Scoring Profiles 调节参数

Complexity Reduction

Convergence

Evidence

Cost

Yield

Retrosynthesis Step Key

A → B → C

Max Yield 97%  
Max Yield -  
Max Yield -

(45) (105) (78)

- Reset +

Feedback

# CAS Retrosynthesis Tool—路线详情

### Reactions (1,181)

Scheme 1 (1 Reaction)

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

Reaction Summary  
Steps: 1 Preparation of N-heteroarylcarbonyl amino acid amide compounds useful as matrix metalloproteinase 13 (MMP-13) inhibitors  
By: Farrow, Neil Alexander; et al  
World Intellectual Property Organization, WO2010056585 A2  
2010-05-20  
PatentPak Full Text

1.1 Reagents: 1-Ethyl-3-(3-dimethylaminopropyl)carbodiimide, 1-Hydroxybenzotriazole, Diisopropylethylamine  
Solvents: Dichloromethane; overnight, rt  
1.2 Reagents: ZnCl<sub>2</sub>  
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®

Overview Steps Predicted Results ON

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

B  $\Rightarrow$  E  
Maximum Yield: 80% Evidence (10,876) 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

Avg. Yield 37%

Retrosynthesis Step Key  
Experimental Steps Predicted Steps

# 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 ON

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

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

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

C  $\Rightarrow$  F + G  
Maximum Yield: -  
Evidence (1)  
Alternative Steps (13)

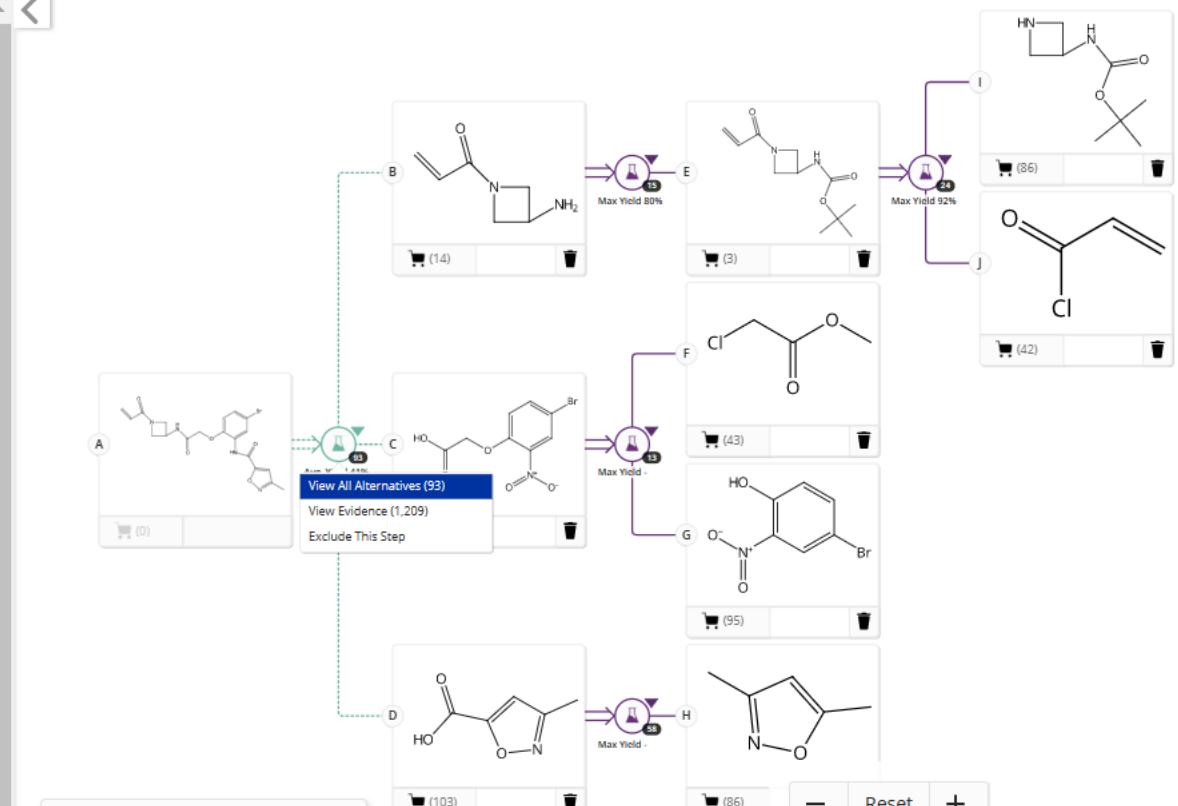
D  $\Rightarrow$  H  
Maximum Yield: -  
Evidence (1)  
Alternative Steps (58)

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

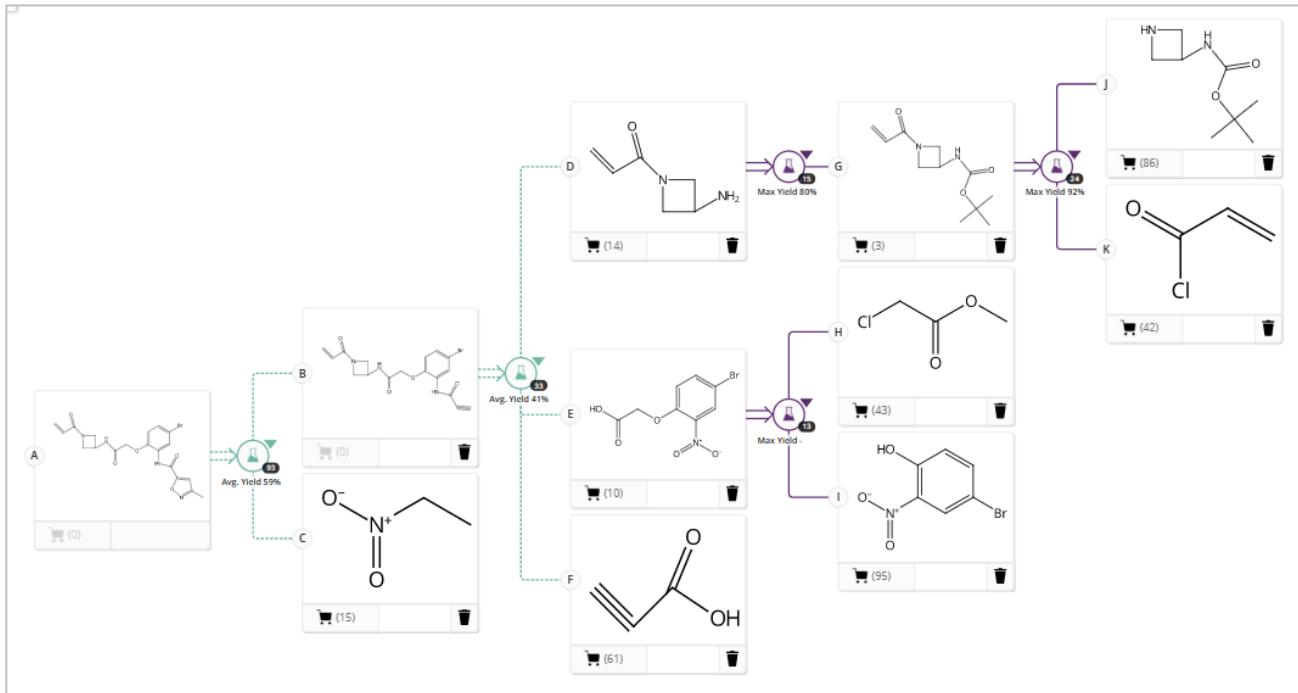
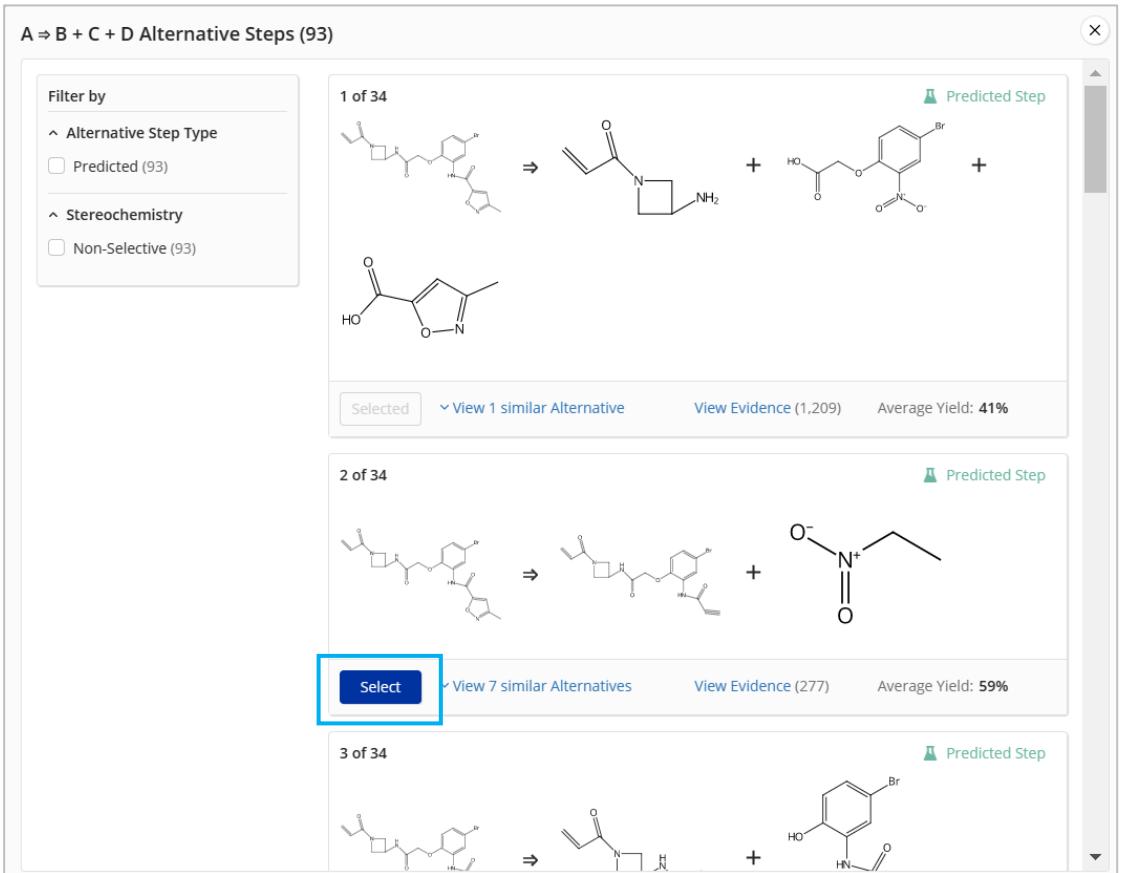
View Excluded Options   Save

Atom M. 1,4-EPE View All Alternatives (93) View Evidence (1,209) Exclude This Step

Retrosynthesis Step Key



## 获取替代路线



# 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 SciFinder®中的序列检索
  - BLAST
  - CDR
  - Motif



视频链接:

[https://american-chemical-society.zoom.us/rec/share/JPoebb74K7-dbzGw2Aj8vRqqeddGB5zzBnQTV8MYcW2E2QQqq2rkYWoBtkHy\\_tt2.ag1fUmL880MKBne3?startTime=1647943207000](https://american-chemical-society.zoom.us/rec/share/JPoebb74K7-dbzGw2Aj8vRqqeddGB5zzBnQTV8MYcW2E2QQqq2rkYWoBtkHy_tt2.ag1fUmL880MKBne3?startTime=1647943207000)

## 下一节：反应检索

# Sequences Search™ — Blast检索

The screenshot shows the 'Sequences' search interface. On the left, a sidebar lists categories: All, Substances, Reactions, References, Suppliers, Sequences (which is selected and highlighted in blue), and Retrosynthesis. The main area has a title 'Sequences' and instructions to 'Enter a protein or nucleotide string, or upload a .txt or .fasta file.' Below this are tabs for BLAST, CDR, Motif, Upload Sequence, and Clear Search. A text input field says 'Enter a query or upload a file...'. To the right, there are options for 'Sequence Type' (Nucleotide is selected), 'Search Within' (Proteins is selected), and a checked checkbox for 'Include NCBI Sequences'. A large blue button at the bottom right says 'Start 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

# 高级检索一设置相关参数

## Sequences

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

BLAST  CDR  Motif Upload Sequence

AACAAACATATCAAATCCTACTGGTGGCACAACTTGA

Sequence Type:  Nucleotide  Protein

Search Within:  Nucleotides  Proteins  
 Include NCBI Sequences

**Advanced Sequence Search ▾** [Adjust Parameters for Short Sequences](#) | [Reset All](#)

Alignment Identity % <input type="text" value="80"/>	Match with Gaps? <input type="radio"/> Yes <input checked="" type="radio"/> No	Gap Costs <input type="radio"/> Existence 5 Extension 2
Query Coverage % <input type="text" value="90"/>	Word Size <input type="text" value="11"/>	Reward for Match <input type="radio"/> Penalty for Mismatch <input type="radio"/> 2, -3
BLAST Algorithm <input type="radio"/> BLASTn	E-Value <input type="text" value="10"/>	Exclude Low Complexity Regions <input type="radio"/> Yes <input checked="" type="radio"/> No

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

Query Sequence: QQLLVVEEGG  
Subject Sequence: |||I|||I|||I|QQLLVVEEIGS  
Alignment

### 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%	AACAAACATATCAAATCCTACTGGTGGCACAACTTGA	<input type="button" value="View Results"/> <input type="button" value="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%	AACAAACATATCAAATCCTACTGGTGGCACAACTTGA	<input type="button" value="View Results"/> <input type="button" value="Edit Search"/> Complete
--------------------	--	---------------------------------------	---

Results will expire on Mar 15, 2023.

74

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CAS  
A division of the  
American Chemical Society

# BLAST检索结果

- 序列一致性详情
- 目标序列
- 披露序列的专利文献
- 可视化地图
- 结果筛选

Sequences search for your query

Query Details: ACAACAACATATAAATCTACTGGTGGCACAACTTGA View More

Sort: Alignment Identity View: Expanded

170 Results

1 Alignment Identity: 100%

Query [1] Subject [1] Length: 395

Subject [1] Length: 595

Matches: 39 Mismatches: 0

Alignment Data

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

Q 1 ACAACAACATAAATCC TACTGGTGGCACAACTTGA 39

S 393 ACAACAACATAAATCC TACTGGTGGCACAACTTGA 431

2 Alignment Identity: 100%

Query [1] Subject [1] Length: 813

Subject [1] Length: 813

Matches: 39 Mismatches: 0

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

1 AAGAACAAA AGGATCAGCA GCCAGAGATG AGATGTAAGG TACTGATCCC CCATGCCCTT AGCTTAGCTT AACCCATGCC  
81 CTAACATCTC GTACCCATAG CATAACAGGA ACACGCAGGC AACTACTACA ACAACAAGGA CACCGCAGC AAATTGCTG  
161 TCACGTCACTG TACTGAGAAG ACAACAACATAAATCC TACTGGTGGCACAACTTGA AGAGGGTCTA GAACGAGCTA

Download Sequence Results

Select Quantity

All Results

FASTA (.fasta)

File Name: Sequences\_20230213\_1132

Download Cancel Learn more about downloads.

- 下载结果:
- 比对详情
  - 序列长度参数
  - 相关专利号
  - 专利中的序列编号等
- (Excel或FASTA格式)

# BLAST检索结果

6 Alignment Identity: 100%

Query (1) Subject (1) Matches: 39 Mismatches: 0

Subject Length: 1,060 nt

CAS Registry Number: 785872-37-9

Sequence

```
1 CATTGGGTAC CTCGAGGCCG GCCGGGAGCT CGCACTCACT CACTCACAAG TCACACAGCC ACACTTGAAC CGCTGCCGC  
81 AGCGGAGGGA GCTTGACCGG CCACACGCAC ACATAACACA AGCTCGTGT CGATGGCGCG GTGGGCTCGG GTGCTGGCGC  
161 TGGCCGCGGC CACGGCCATC CCGTGGCGG CGCGACATG AACCGGACA AGACGGAGTG CGCGGACAG  
241 CTGGTGGGCC TGGCGCCGTG CCTGCAGTAC GTGCAGGGGC AGGCCCGCGC GCCGCGCCGC GACTGCTCGG GCGGCCCTGCG  
321 CCAGGTGCTG GGGAAAGGCC CCAAGTGCCT GTGCGTCTC GTCAAGGACA AGGACGACCC CAACCTGGGC 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	cgcaactca	cactcacaag
51	tcacacacgc	acatcttgaac	cgctgcccgc	agcgggggaa	gtttgcacgg
101	gccaacgcac	acataacaca	agctcgctgt	cgatggcgcc	gtgggctgcg
151	gtgctggcgcc	tggccgcgc	cacggccatc	gccccggcg	ccgtggcgcc
201	cggcgcatg	aacgcggaca	agacggagtg	cgccggaccag	ctggggggcc
251	tggccgcgtg	cttcgcgtac	gtgcaggggc	aggccggcgc	gccggccccc
301	gactgtcgcc	gcccgcgtc	ccagggtgtc	ggggaaagagcc	ccaagtgcct
351	gtggctgtgc	gtcaaggaca	aggaggaccc	caacccggcc	atcaaagatca
401	acgcacacct	cgcgcgtcg	ctccccaaag	cctgcggcgc	cacccggcc
451	aacgtctccc	actgcgccta	gctcctgcata	atccccccgg	gctccaaaga
501	cgccggcgcc	ttcagttcccg	gcagcgacaa	gggttccact	gccgtccag
551	ccaaaggacaa	ctcgacggcg	acgaccgact	ccccgcgcgt	gcaggcgacc
601	accggacgcg	gcgtgtccct	ctcgccggcg	accggccgtg	ctgcactcac

Other Names and References

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_11549C.1

# 序列详情及相关的专利文献结果

References from your sequence

Substances Reactions Citing Knowledge Graph Save

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

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; Okamoto, Jack; et al  
United States, US10815494 B2 2020-10-27 | Language: English, Database: CAplus

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<sub>[RCL2]</sub> 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; Trouhan, Maxim; Rarang, Joel; Burns, James; et al  
United States, US20170037422 A1 2017-02-09 | Language: English, Database: CAplus

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

n tolerance levels in plants

h; Feldmann, Kenneth A.; Pennell, Roger; Kwok, Shing; Zhang, Hongyu; Christensen, Cory; Okamoto, Jack; et al plus

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<sub>[RCL2]</sub> low-nitrogen tolerance levels and plant products produced from plants having increased low-nitrogen tolerance levels.

# Sequences Search™—Motif检索

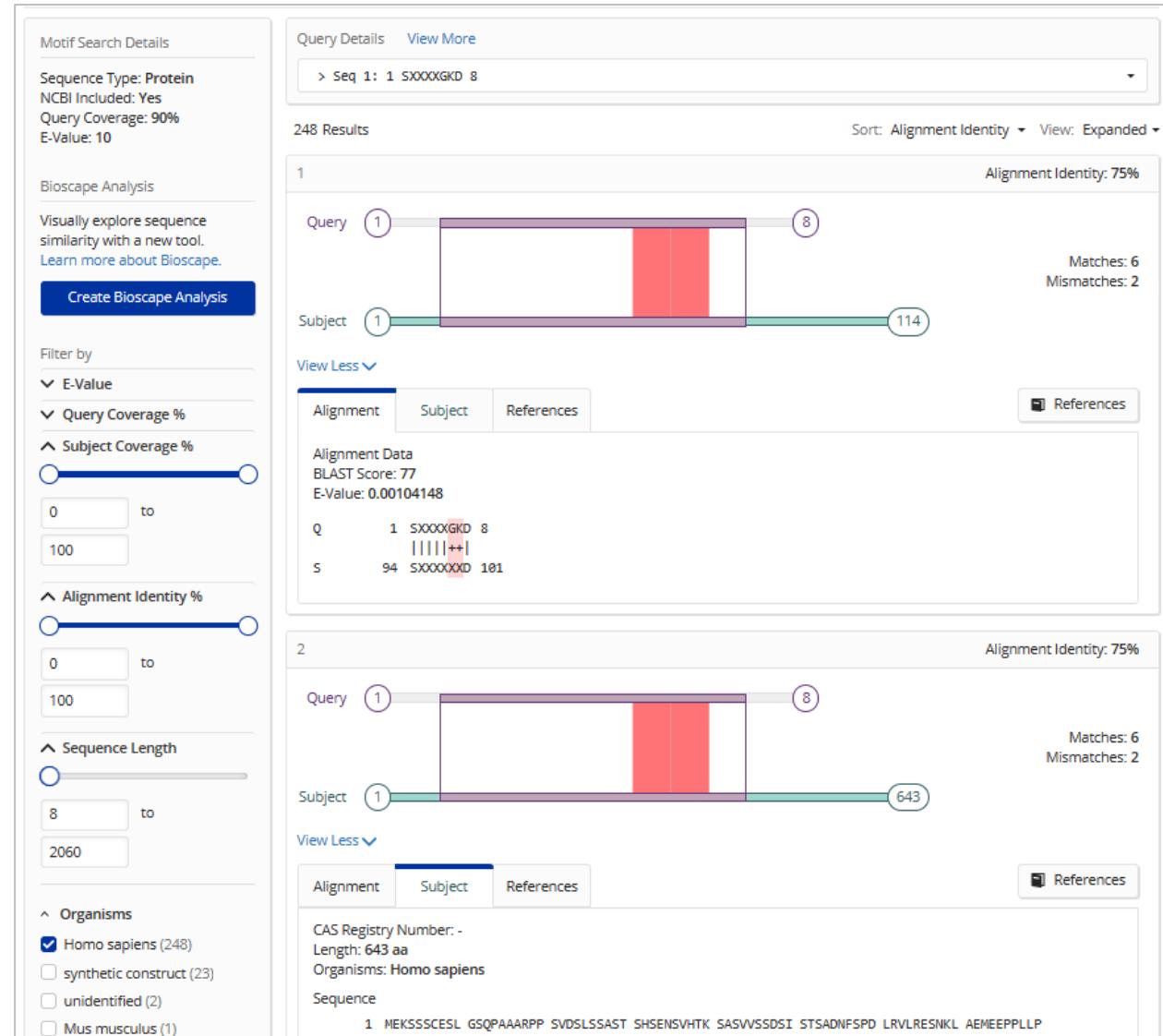
Motif中有可变部分，可借助符号来表示：

“[ ]” 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

The screenshot shows the Sequence Search interface. On the left, there's a sidebar with links: All, Substances, Reactions, References, Suppliers, Sequences (which is highlighted in blue), and Retrosynthesis. The main search area has a title "Sequences" and a search bar with placeholder text "Enter a protein or nucleotide string." Below the search bar are tabs: BLAST, CDR, and Motif (which is also highlighted in blue). The search term "[SG]x{4}GK[DT]" is entered in the search bar. To the right of the search bar are buttons for "Clear Search" and "Sequence Type:" (set to Protein). There's also a checked checkbox for "Include NCBI Sequences" and a large blue "Start Sequence Search" button. At the bottom of the search area are "Advanced Sequence Search" and "Reset All" buttons, along with input fields for "Query Coverage %" (90) and "E-Value" (10), and a checkbox for "Combine Motif Results".

# Motif检索结果



# 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

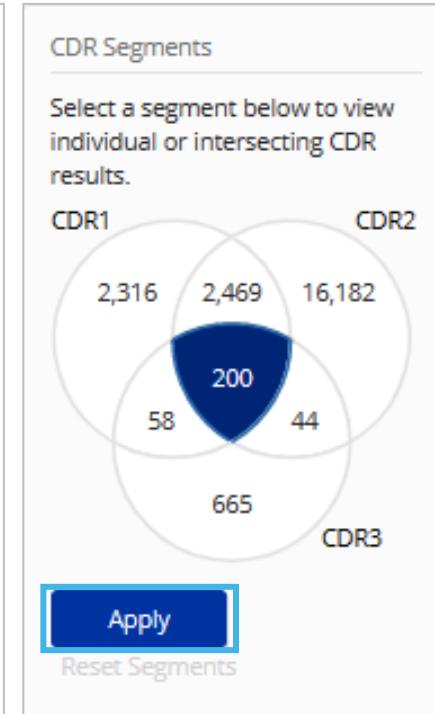
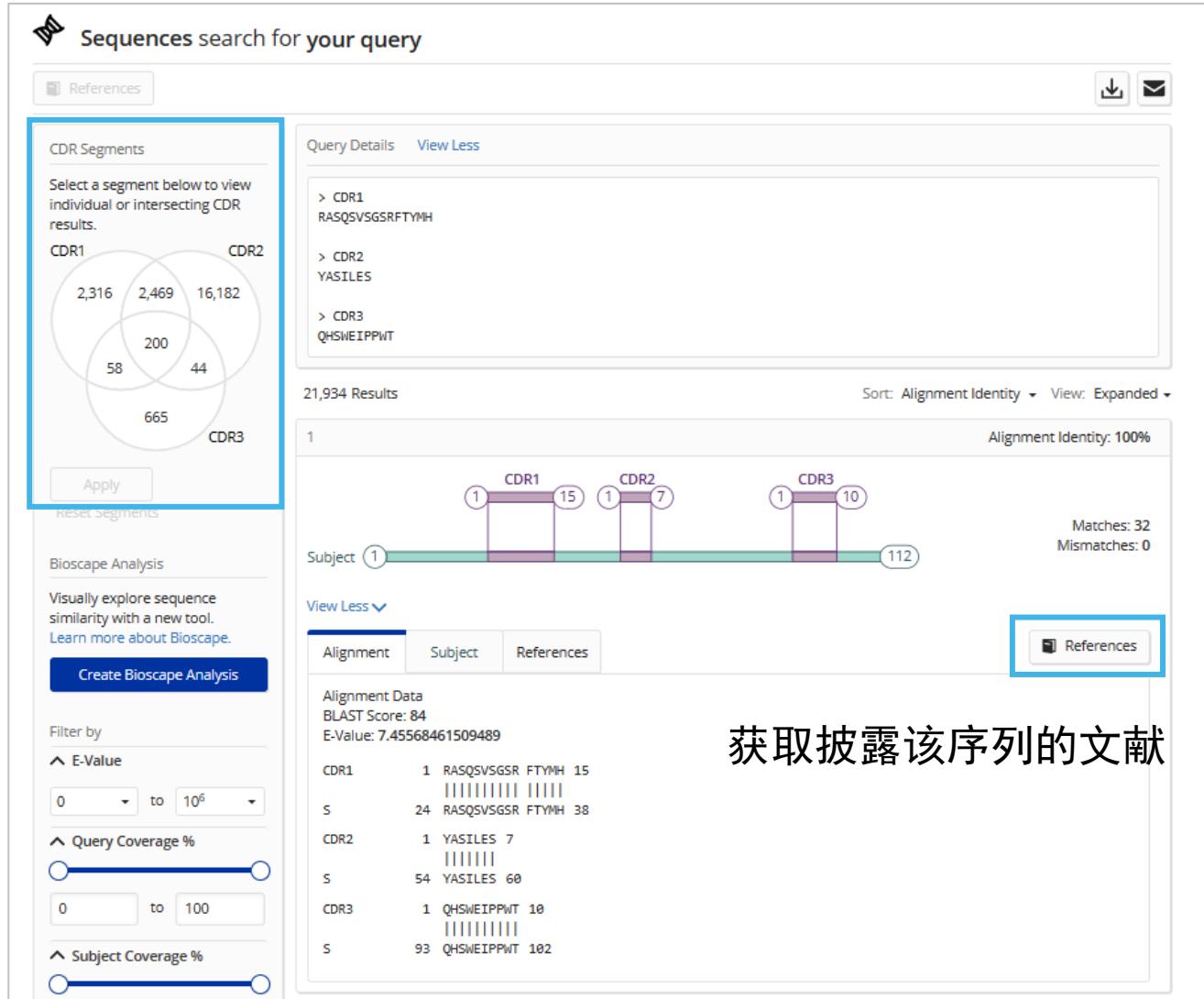
CDR3 QHSWEIIPPWT X

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



## CDR Segments：

- 匹配到一个或者多个CDR的subject序列的数量
- 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<sup>n</sup>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

The screenshot displays two main sections of the CAS SciFinder interface.

**Left Panel (Search Results):**

- Header: CAS SciFinder<sup>n</sup>, References, petroleum oil and analysis, Draw, Search, Notifications, User Profile.
- Section Title: References search for "petroleum oil and analysis".
- Filtering: CAS Solutions: Analytical Methods (selected).
- Results: 612 Results.
- Sort: Relevance, View: Partial Abstract.
- Article Preview 1: Screening of soil for alcohol-extracted organic compounds by turbidity analysis. By: Sakai, Hiroyuki; Okada, Akira; Fujita, Takeshi; Wada, Shin-ichiro. Journal of the Faculty of Agriculture, Kyushu University (2011), 56(1), 93-97 | Language: English, Database: Cplus | Analytical Methods.
- Article Preview 2: Sensitivity improvement in ICP MS analysis of fuels and light petroleum matrices using a microflow nebulizer and heated spray chamber sample introduction. By: Caumette, Guilhem; Lienemann, Charles-Philippe; Merdrignac, Isabelle; Paucot, Hugues; Bouyssiere, Brice; Lobinski, Ryszard. Talanta (2009), 80(2), 1039-1043 | Language: English, Database: Cplus and MEDLINE | Analytical Methods.
- Filter Behavior: Document Type, Language, Publication Year, Available at My Institution, Author, Organization, Publication Name, Concept, CA Section, CAS Solutions (selected), Analytical Methods (612) (highlighted).

**Right Panel (Article Detail):**

- Section Title: Sensitivity improvement in ICP MS analysis of fuels and light petroleum matrices using a microflow nebulizer and heated spray chamber sample introduction.
- Subsections: Substance (1), Reactions (0), Citing (55), Citation Map.
- Author: Caumette, Guilhem; Lienemann, Charles-Philippe; Merdrignac, Isabelle; Paucot, Hugues; Bouyssiere, Brice; Lobinski, Ryszard.
- Journal: Talanta, Volume: 80, Issue: 2, Pages: 1039-1043, Journal; Article, 2009, DOI: 10.1016/j.talanta.2009.08.017.
- Coden: TLNTA2, E-ISSN: 1873-3573, ISSN-L: 0039-9140.
- Database Information: AN: 2009:1286528, CAN: 152:78583, PubMed ID: 19836594, Cplus and MEDLINE.
- Company/Organization: UMR 5254, LCABIE, Helioparc, CNRS, UPPA, Pau 64053.
- Keywords: gasoline kerosene inductively coupled plasma mass spectrometry sensitivity plasma.
- Links: View Source, Full Text.
- Concepts, MEDLINE® Medical Subject Headings, Substances, Analytical Methods.
- Table: Title (Analysis of Titanium in Kerosene by Inductively coupled plasma mass spectrometry), CAS Method Number (1-135-CAS-84928).

# 分析实验方法详情

## Analysis of Titanium in Kerosene by Inductively coupled plasma mass spectrometry

CAS MN: 1-135-CAS-84928

Method Category: Petroleum Product Analysis

Technique: Inductively coupled plasma mass spectrometry

## 实验原料

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

## 分析仪器

### Equipment Used

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

Microflow nebulizer

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

Pump, Smartline Pump 1000, Knauer, Berlin, Germany

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

## 分析条件

### Conditions

#### Instrument

RF power: 1300 W; Ar nebulizer gas: 0.8 L/min and auxiliary O<sub>2</sub> flow: 45 mL/min; integration time per isotope: 20 ms

Flow rate: 20 µL/min

### Instructions

#### Sample Preparation

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

#### Standards Preparation

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

#### ICP-MS analysis

1. Analyze the sample using a PerkinElmer Elan 6000 (PE-SCIEX1, ON, Canada).
2. Introduce the sample using microflow nebulizer consisting of a fused silica capillary of 180 µm i.d. (375 µm o.d.) and heated spray chamber (jacketed to allow the

## 操作步骤

### Source

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

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

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

CODEN: TLNTA2 | ISSN: 00399140 | DOI: 10.1016/j.talanta.2009.08.017 | [View in SciFinder<sup>n</sup>](#)

[Full Text ▾](#)

### Abstract ^

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

## 文献详情

## 数据有效性

### Validation

Linearity Range 1 - 250 µg/kg

Limit of Detection 0.8 µg/kg (gasoline), Titanium

0.1 µg/kg (gasoline), Vanadium

5 µg/kg (gasoline), Chromium

7 µg/kg (gasoline), Iron

0.04 µg/kg (gasoline), Silver

0.3 µg/kg (gasoline), Cadmium

0.2 µg/kg (gasoline), Tin

1 µg/kg (gasoline), Mercury

0.1 µg/kg (gasoline), Lead

# 分析实验方法的获取 (2)

方法二：登录`https://methods.cas.org`

- 主题检索或分类浏览；
- 筛选分析目标物、介质、方法类别、分析技术等

The screenshot shows the homepage of the CAS Analytical Methods website. At the top, there is a search bar with placeholder text "Enter keyword, matrix, analyte, etc." and a "Advanced Search" link. Below the search bar, the text "方法分类: 13大类, 45小类" is displayed. A large blue box highlights the "Browse Method Categories" section, which lists 13 major categories: Agricultural Applications / Analysis, Bioassays, Biomolecule Isolation, Environmental Analysis, Food Analysis, Fuels / Geology / Biofuels, Historical Analysis / Dating, Miscellaneous, Organic Compound Analysis, Organometallics / Inorganics, Pharmacology / Toxicology, Polymer Analysis, Water Analysis, and a "View All" link. At the bottom left, there is a "Recent Searches" section with a link to "Pesticide Residue Analysis".

The screenshot shows the search results page for "chromium sulfate" on the CAS Analytical Methods website. The search bar at the top contains the query "chromium sulfate". The results are listed under the heading "Results (20)". The first result is "Analysis of Copper by Solid phase extraction" (CAS MN: 1-142-CAS-235450). This entry includes details such as Analyte (Copper; Nickel; Chromium; Trace heavy metals), Matrix (Soils, Allium cepa, Brassica napus, Grease, Leaf), Method Category (Trace Element Analysis), Technique (Flame atomic absorption spectroscopy; Solid phase extraction), Equipment Used (pH/Ion meter; Stirrer; Atomic absorption spectrometer; Hollow cathode lamp; Water bath; Mechanical shaker), Source (A preconcentration procedure for copper, nickel and chromium ions in some food and environmental samples on modified Diaion SP-850 by Shokrolahi, A.; Ghaedi, M.; Shabani, R.; Montazerzohori, M.; Chehreh, F.; Soylak, M.; Alipour, S.), and a reference (Food and Chemical Toxicology (2010), 48 (2), 482-489. Elsevier Ltd.). Buttons for "View Details & Instructions" and "Remove from Compare" are present. The second result is "Analysis of Copper in Seawater by Solid phase extraction" (CAS MN: 1-142-CAS-228765), with similar detailed information. A "Compare (2/3)" button is located at the top right of the results area.

# 分析方法的对比

## Compare Methods

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

Source	<a href="#">Chromium determination in pharmaceutical grade barium sulfate by solid sampling electrothermal atomic absorption spectrometry with Zeeman-effect background</a> <a href="#">View All ▾</a>	<a href="#">Chromium determination in pharmaceutical grade barium sulfate by solid sampling electrothermal atomic absorption spectrometry with Zeeman-effect background</a> <a href="#">View All ▾</a>
Preparation	<p>Collection and preparation of samples</p> <ol style="list-style-type: none"> <li>Obtain the powdered pharmaceutical grade BaSO<sub>4</sub> samples from pharmaceutical industries and dry them in a conventional oven at 105 °C × 2 h.</li> <li>Spike the samples by addition of chromium reference solutions of 0.48 µg/g.</li> </ol> <p>Preparation of standard solutions</p> <ol style="list-style-type: none"> <li>Prepare the reference solutions daily by serial dilutions of stock chromium (Cr) solutions (1 g/L Cr in 2% HNO<sub>3</sub>).</li> </ol> <a href="#">View Less ^</a>	<p>Preparation of nitric acid solution</p> <ol style="list-style-type: none"> <li>Doubly distill the concentrated nitric acid in a Milestone sub-boiling system (model duoPUR 2.01 E, Bergamo, Italy) and use this for sample digestion/extraction.</li> </ol> <p>Collection and preparation of samples</p> <ol style="list-style-type: none"> <li>Obtain the powdered pharmaceutical grade BaSO<sub>4</sub> samples from pharmaceutical industries and dry them in a conventional oven at 105 °C × 2 h.</li> </ol> <p>Preparation of standard solutions</p> <ol style="list-style-type: none"> <li>Prepare the reference solutions daily by serial dilutions of stock chromium (Cr) solutions (1 g/L Cr in 2% HNO<sub>3</sub>).</li> </ol> <a href="#">View Less ^</a>
Method	Direct solid sampling (DSS) - electrothermal-atomic absorption spectrometric (ETAAS) analysis <a href="#">View All ▾</a>	Acid digestion procedure using nitric acid <ol style="list-style-type: none"> <li>Perform sample acid digestion (extraction) in closed quartz vessels using a high pressure model Multiwave</li> </ol> <a href="#">View All ▾</a>
Linearity Range	100 - 1800 pg	
Limit of Detection	2.4 pg	
Recovery	98% - 103% in 0.48 µg/g spiked concentration	
Concentration	0.45 ± 0.04 µg/g (sample data)	0.32 ± 0.04 µg/g (sample data)

# 分析实验方法小结

1. 通过CAS SciFinder<sup>n</sup>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<sup>n</sup>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 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

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: CPlus 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  $\geq 89$  (women) or  $\geq 102$  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  $\pm$  SEM) age  $49.5 \pm 1.6$  y, with a BMI of  $30.6 \pm 0.5$  kg/m $^2$  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: CPlus 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. Consistent...

View More

Full Text Substance (1) Reactions (0) Citing (37) Citation Map

3

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

CAS Solutions

Formulus (37)

Analytical Methods (4)

Formulation Purpose

By Count Alphanumeric

4 Selected

Food (7)  Antibacterial agents (1)  
 Antidiabetic agents (6)  Antihypertensives (1)  
 Dietary supplements (5)  Antioxidants (1)  
 Diet (3)  Antitumor agents (1)  
 Drug delivery systems (3)  Bakery products (1)  
 Antimicrobial agents (2)  Beverages (1)

Gastrointestinal protective agents (1)  
Oral rehydration solutions (1)  
Pharmaceutical adjuvants (1)  
Snack food (1)

Apply Cancel

定位配方或制剂的功能目标

# 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 Save

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

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

Database Information  
AN: 2014;519911  
CAN: 160534190  
PubMed ID: 24684664  
Cplus and MEDLINE

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

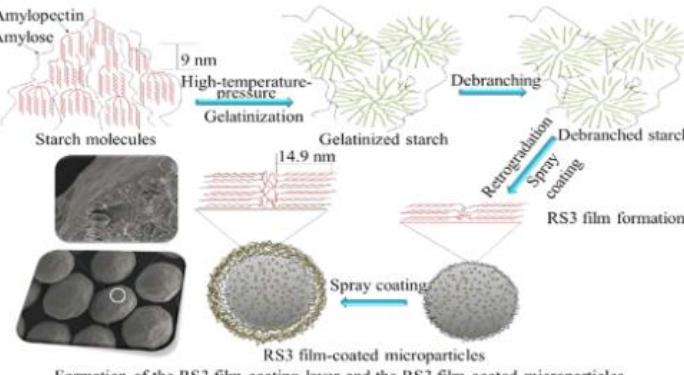
Publisher  
American Chemical Society

Language  
English

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

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

For the delivery of bioactive components to the colon, an oral colon-specific controlled release system coated with a resistant starch-based film through aqueous dispersion coating process was developed. Starch was modified by a high-temperature-pressure reaction, enzymic 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 glycopenia 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.



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		-	

# 检索配方或制剂 <https://formulus.cas.org>

## 方法（2）：

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

The screenshot shows the CAS Formulus homepage. On the left, there's a sidebar with buttons for 'Formulations' (highlighted in blue), 'Ingredients', and 'Formulation Designer'. The main area has a search bar with the placeholder 'Searching for...'. Below it, the word 'Formulations' is displayed in large letters, followed by a sub-instruction: 'Search for Formulations by Ingredient, Purpose, Form, Function, etc.' A search input field contains the text 'orthopedic and implant', and a blue search button with a magnifying glass icon is to its right. Below the search bar, a link says '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) Save 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: Solid, Liquid, Gas

Delivery Route: Ophthalmic drug delivery systems (177), Subcutaneous drug delivery systems (138), Intramuscular injections (81), Pharmaceutical injections (74), Pharmaceutical implants (61)

Information Included: Component Amount (1,393), Process (1,064), Experimental Activity (721), Effective Dose (164)

Document Type: Journal (309), Article (309), Patent (755)

1,064 Results

1 Implants: Antitumor Agents

Location: Article page 3, 6, 7, 8, 9  
Purpose: Antitumor agents  
Physical Form: implant

Add to Compare

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

JOURNAL  
Titanium wire implants with nanotube arrays: A study model for localized cancer treatment  
Biomaterials  
Language: English  
Full Text View in CAS SciFinder

View Formulation Detail

2 Composition for Promoting Bone Formation

Location: Claim 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41  
Purpose: promoting bone formation  
Target: Amphibia, Ape, Aves, Bos taurus, Canis familiaris, Capra, Cavia porcellus, Equus caballus, Felis catus, Fish, Gerbil, Hamster, Homo sapiens, Monkey, Mus musculus, Oryctolagus cuniculus, Ovis aries, Rattus, Reptilia, Swine  
Delivery Route: Intraosseous prosthetic implants, intramedullary application  
Physical Form: pharmaceutical implants

Add to Compare

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

PATENT  
Use of pro-inflammatory compounds for promoting bone formation  
Assignee: Imperial Innovations Limited  
WO2011007135  
Language: English  
Patent PDF View in CAS SciFinder

Remove from Compare Remove from Compare

# 查看制剂或配方详情

## Implants: Antitumor Agents

Purpose	Target	Delivery Route	Physical Form	Source
Antitumor agents	-	-	implant	<a href="#">View</a>

**Formulation Ingredients**

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 or...  
Purpose: Antibacterial agents, corticos...  
Target: Haemophilus influenzae, Hom...  
Delivery Route: AURICULAR (otic)  
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 <b>Implants: Antitumor Agents</b>	<b>Composition for Promoting Bone Formation</b>
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 <b>implant</b>	<b>pharmaceutical implants</b>
Experimental Activity Available	Not Available
Components	<b>Group: Ti-TNTs wire implants</b> Function: <b>implant</b> Amount Reported: Optionality: <b>Mandatory</b>  <b>Ti wires</b> Function: <b>additives</b> Amount Reported: - Optionality: -  <b>Acetone</b> Function: <b>Solvents</b> Amount Reported: - Optionality: -  <b>Ethanol</b> Function: <b>Solvents</b> Amount Reported: - Optionality: -  <b>Perchloric acid</b> Function: <b>additives</b> Amount Reported: 1 Optionality: -  <b>Trail aqueous solution</b> Function: - Amount Reported: <b>2 mg/mL</b> Optionality: -
	<b>Group: surgical implant</b> Function: Amount Reported: Optionality: <b>Mandatory</b>  <b>Dental implants</b> Function: - Amount Reported: - Optionality: -  <b>Plates</b> Function: - Amount Reported: - Optionality: -  <b>pin</b> Function: - Amount Reported: - Optionality: -  <b>screw</b> Function: - Amount Reported: - Optionality: -  <b>Group: pro-inflammatory compound</b> Function: <b>bone formation promoters</b> Amount Reported: Optionality: <b>Mandatory</b>  <b>1-Methyl-<math>\alpha</math>-tryptophan</b> Function: <b>dioxygenase 1 inhibitors, 3, indoleamine 2</b>

- 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  Anticorrosion  
Ex: binder, surfactant, carrier

Search For  Operator  Enter one term

All Fields  coating  
General search of all fields

Add Another Term

- 
- 
- 
- 
- 
- 
- 

- 
- 
- 

Clear All

# 检索原料

Searching for...

Formulations

Ingredients

Ingredients

Search by Ingredient Name, CAS Registry Number, or Function

propylene glycol

Search

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

(±)-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 <sup>3</sup>	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

**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	Antiarthritis
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
Dandruff	Deformation enhancers	Enrol

[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	<a href="#">Edit</a>	

Template					
Function	Ingredient	Regulatory	Top Alternatives	Amounts	
Active or Featured Ingredient:	Vitamin A	ANMAT	-	Amount not available <a href="#">X</a>	
Active or Featured Ingredient:	polyethylene glycol	ANMAT; Cosing: Cosmetic Ingredient Inventory; Drug Master File List; EPA Pesticide Inactive Ingredients; FDA GRAS (Part 181, Subpart B); FDA Inactive Ingredients Database	-	Amount not available <a href="#">X</a>	
Function: Carriers	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	Water; Ethylene glycol	Approximate Range: 3 - 4% <a href="#">X</a>	
	<a href="#">View More Alternatives</a>				
Function: Skin conditioners	Glycerol	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%	<a href="#">View More Alternatives</a>

- 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 SciFinder<sup>n</sup>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 SciFinder<sup>n</sup>账号

(登录贵校图书馆网站，查看注册相关的链接和说明)

The registration form consists of three main sections:

- Contact Information:** Fields for First Name, Last Name, Email, Confirm Email, Phone Number, Fax Number, Area of Research (dropdown), and Job Title (dropdown).
- Username and Password:** Fields for Username, Password, and Re-enter Password.
- Security Information:** Fields for Security Question (dropdown) and Answer.

At the bottom are two buttons: "Register>>" and "Clear All".

请注意：

- 必须输入真实姓名和学校邮箱。
  - 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)
  - 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
- 从下拉列表中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 SciFinder<sup>n</sup>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, 请提供真实姓名信息 (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

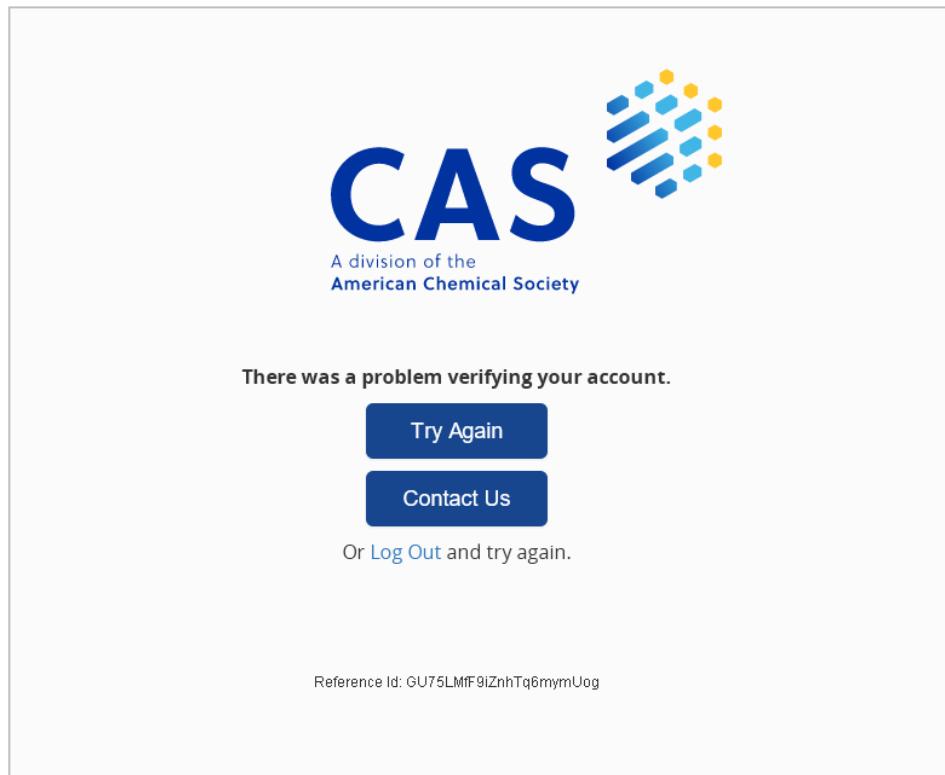
# 常见问题

## 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



- 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



订阅号



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Thursday 11:06

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2023年CAS SciFinder Discovery Platform论坛直...

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2023年CAS SciFinder Discovery Platform论坛直播来了!

Original CAS ACS美国化学会 2023-02-23 11:06 Posted on 北京

CAS SCIFINDER DISCOVER PLATFORM™  
关注直播, 掌握科研利器!

新学期, 科研神器SciFinder升级了! 今年的直播将详细讲解CAS SciFinder Discovery Platform的新功能、检索技巧和科研应用, 为您的学业和科研生涯全程助力!

每次直播时间是18:00-19:00, 欢迎您带上问题, 我们将现场解答; 观看直播还有机会获得幸运纪念品!

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

## 回顾: 2022 CAS SciFinder®论坛合集



# THANK YOU!



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