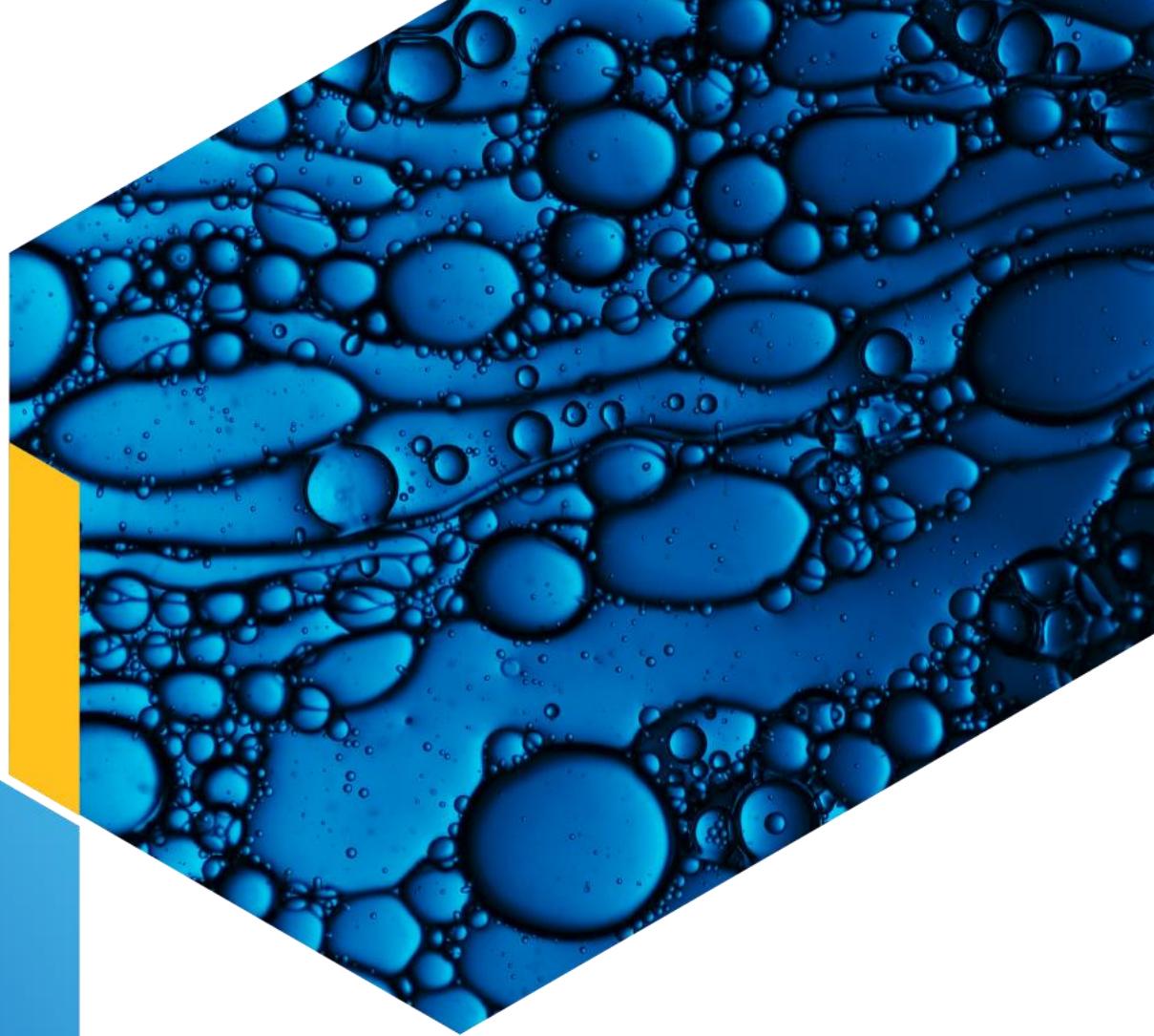


# 利用CAS SciFinder<sup>n</sup> 获取科技信息

朱传娴 [hzhu@acs-i.org](mailto:hzhu@acs-i.org)  
2022.4



# 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检索)
  - 生物序列检索
  - 反应检索
  - 逆合成反应路线设计 (CAS Retrosynthesis Tool)
  - 检索信息的管理
  - 分析方法的获取 (Analytical Methods)
- 常见问题及解决

# CAS致力于提高创新效率

CAS的数据和服务是基于对以往知识经验的回顾，对当代前沿研究的洞察，以及对未来发展趋势的前瞻



## HINDSIGHT

Connecting past discoveries  
to build a better future

连接前人的发现，建设更美好的未来

## INSIGHT

Revealing unseen relationships that spark ideas and speed  
discovery

揭示能激发想法和加速发现的，未预见的联系

## FORESIGHT

Identifying trends and emerging opportunities to accelerate  
growth

确定加速增长的趋势和新机遇



# CAS具有最全面的学科连接内容合集



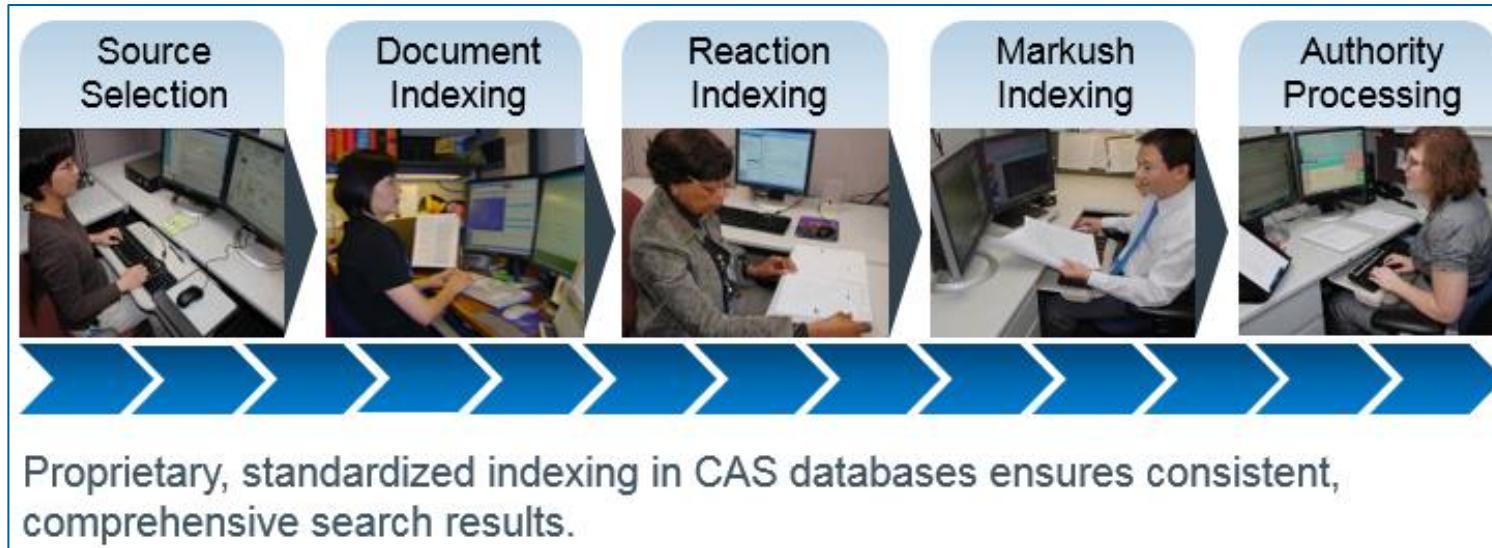
Over  
**50K**  
scientific journals  
and documents

Over  
**250**  
million  
substances

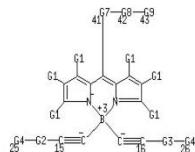
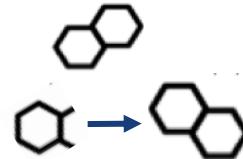
Over  
**50**  
languages  
translated      **64**  
patent offices  
worldwide



# CAS科学家的智力标引



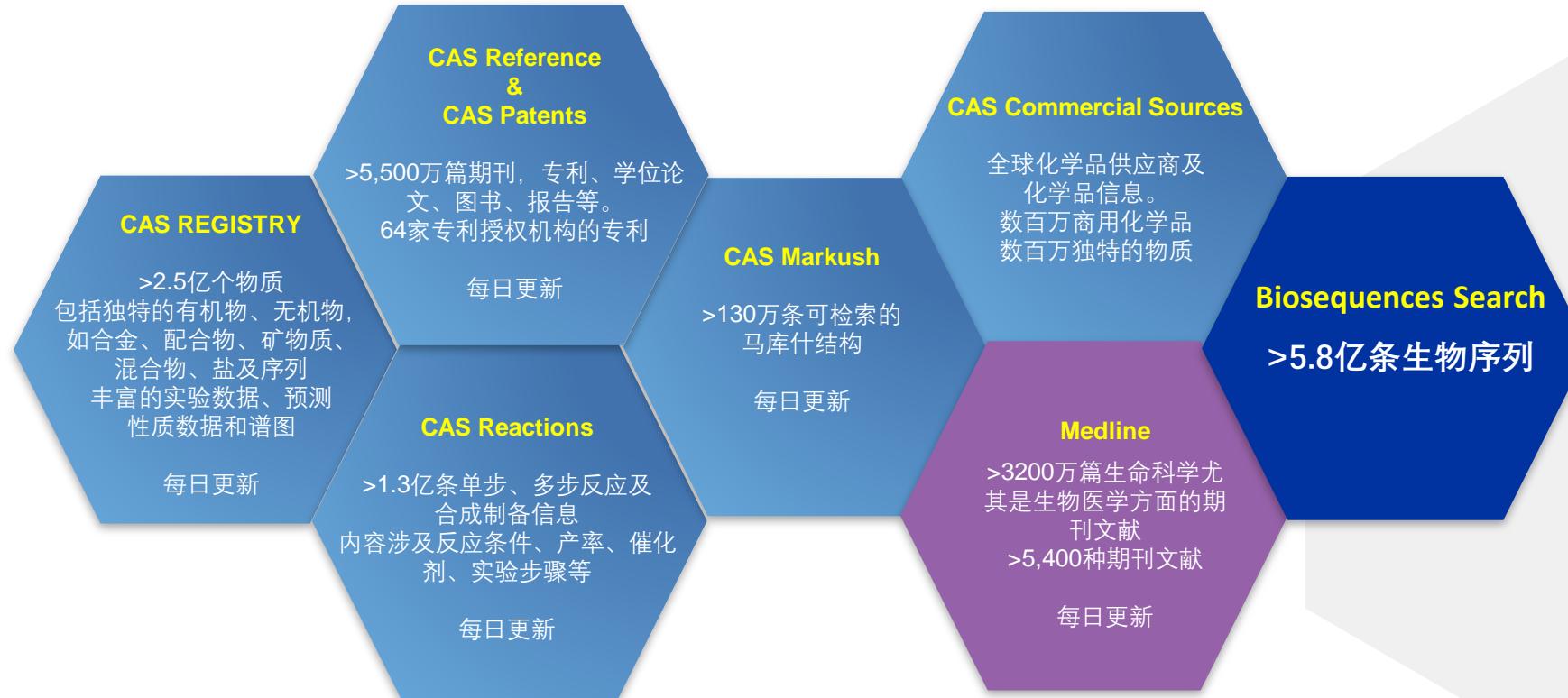
1990  
Smith, M.  
anthracene



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内容合集--CAS SciFinder<sup>n</sup>



CAS SciFinder是提供经CAS科学家人工标引内容的工具型解决方案。



# 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

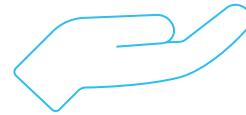
## INTELLECTUAL PROPERTY



### **STN IP Protection Suite™**

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

## CUSTOM SOLUTIONS



### **CAS Custom Services<sup>SM</sup>**

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

# CAS SciFinder<sup>n</sup>登录网址:

# <https://SciFinder-n.cas.org>

The screenshot shows the initial step of the login process. At the top, the CAS SciFinder logo is displayed. Below it, the text "Log In to SciFinder<sup>n</sup>" is centered. A text input field is labeled "Username or Email Address" and contains the text "scicas752". A large blue "Next" button is positioned below the input field. At the bottom of the screen, there are links for "Create an account." and "Can't log in?".

Log In to SciFinder<sup>n</sup>

Username or Email Address

scicas752

Next

Create an account. | Can't log in?

The screenshot shows the second step of the login process. The top half of the screen is identical to the first step, featuring the CAS SciFinder logo and the "Log In to SciFinder<sup>n</sup>" text. Below this, the user's name "Welcome, Helen Zhu" is displayed, followed by a link "Not You?". A text input field for "Password" is present, along with a "Log In" button. Below the password field is a checkbox labeled "Keep me signed in". At the bottom of the screen, there are links for "Create an account." and "Can't log in?".

Log In to SciFinder<sup>n</sup>

Welcome, Helen Zhu [Not You?](#)

Password

Log In

Keep me signed in

Create an account. | Can't log in?

使用CAS SciFinder账号登录

# CAS SciFinder<sup>n</sup>主界面

已保存的结果集及  
信息更新的结果集

灵活的检索选项

近期检索历史

便捷地合并文  
本与结构检索

重新运行检索

修改检索式

Saved History Account

Recent Search History

November 11, 2021

3:30 PM

Substances qinghaosu (1)

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

Heat treatment of materials

Add Advanced Search Field

Learn more about Sci

Edit Drawing Remove

Rerun Search Edit Search

# 大纲

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- 常见检索方式
  - 文献检索
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  - 分析方法的获取 (Analytical Methods)
- 常见问题及解决

# 大纲

## — CAS SciFinder<sup>n</sup>中的文献检索

- 主题词检索及布尔逻辑算符的运用
- 文献检索结果集的筛选
- 通过引文地图发现相关研究方向
- 文献结果集的导出和检索历史管理
- 快速锁定专利原文中披露的重要信息

视频链接：

[https://american-chemical-society.zoom.us/rec/share/9PrTtd4gKFB245SuJax26so0a4WAHC9MsgB74Bt3mPRK9TgcwZI753ROg4eHHseL.I\\_K0dQtNjGzGJK5y](https://american-chemical-society.zoom.us/rec/share/9PrTtd4gKFB245SuJax26so0a4WAHC9MsgB74Bt3mPRK9TgcwZI753ROg4eHHseL.I_K0dQtNjGzGJK5y)



# 文献检索

- 文献检索方法
  - 主题词、物质名称、CAS登记号、专利号、PubMed ID、文献号、DOI
  - 各种字段：作者名、期刊名、机构名、题目、摘要、概念词、物质标识符、出版商
  - 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

# 文献检索--主题词检索

主题词检索：TLR or “toll like receptor” 或 (TLR or “toll like receptor”) and agonist

The screenshot shows the CAS SciFinder search interface. On the left, a sidebar lists search categories: All, Substances, Reactions, References (which is selected and highlighted in blue), Suppliers, Biosequences, and Retrosynthesis. The main search area has a header "References" and a search bar containing "TLR or \"toll like receptor\"". Below the search bar are buttons for "Add Advanced Search Field", "Draw", and a magnifying glass icon. The search results list several entries related to toll-like receptors. On the right, another search panel is shown with a header "References" and a search bar containing "toll like receptor". The results list various toll-like receptor genes from different species.

Search Term	Results
TLR or "toll like receptor"	Toll like receptor (Chlamys farreri gene TLR) Toll like receptor 4 (Mus caroli strain C0423 gene Tlr4) Toll like receptor 4 (Mus caroli strain L0014 gene Tlr4) Toll like receptor 4 (Mus caroli strain L0211 gene Tlr4) Toll like receptor 4 (Mus caroli strain L0275 gene Tlr4) Toll like receptor 4 (Mus cookii strain L0103 gene Tlr4) Toll like receptor 4 (Mus cookii strain L0178 gene Tlr4) Toll like receptor 4 (Mus cookii strain R4106 gene Tlr4)
toll like receptor	(Same results as above)

基于科学家创建的叙词表，充分利用自动提示检索词，启发检索思路

支持布尔逻辑运算符(and, or, not)，默认运算顺序or > and > not

() 优先运算

“ ”不允许词形变化，但可出现单数或复数

支持通配符\*或？ (\*代表0或多个字符； ?代表0或1个字符)

# 高级检索--高效实现多项自定义组合检索

The screenshot shows the SciFinder search interface. On the left, a sidebar lists search categories: All, Substances, Reactions, References (which is selected and highlighted in blue), Suppliers, Biosequences, and Retrosynthesis. Below these are logical operators: AND, OR, and NOT. The main search area has a search bar containing "G-protein coupled receptor". Below it, a dropdown menu shows "AND" and "Journal Name" selected. A search term "journal of medi" is entered into the "Journal Name" field, which is highlighted with a red box. A dropdown menu for "Journal Name" lists several medical journals. To the right, there's a "Saved" button, a "History" button, and an "Account" button.

Searching for...

References

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

"G-protein coupled receptor"

AND Journal Name journal of medi

Volume (Optional)

+ Add Advanced Search Fields

Author Name  
Journal Name  
Organization Name  
Title  
Abstract/Keywords  
Concept  
Substances  
Publication Year  
Document Identifier  
Patent Identifier  
Publisher

Starting Page (Optional)

Learn more about SciFinder<sup>n</sup> Advanced Search.

可单独使用，也可联用下面的检索方法：

- **关键词、物质名称、CAS RN、文献号；**
- **高级检索（刊物名、Concepts、物质等）；**
- **结构检索**

# 文献结果集

排序：  
更快查找相关信息

获得更多文献

文献类型

文献语言

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](#)

- Journal (7,240)
- Patent (2,068)
- Review (890)
- Biography (1)
- Clinical Trial (187)

[View All](#)

[Language](#)

- English (9,047)
- Chinese (266)
- Japanese (63)
- Korean (51)
- German (18)

[View All](#)

## References (9,495)

Sort: Relevance ▾ View: Partial Abstract ▾

Relevance  
Times Cited  
Publication Date: Newest  
Publication Date: Oldest

[Substances](#) ▾ [Reactions](#) ▾ [Citing](#) ▾

[Download](#) [Email](#) [Save](#)

1

**The pharmacokinetics of Toll-like receptor agonists and the impact on the immune system**

By: Engel, Abbi L.; Holt, Gregory E.; Lu, Hailing  
Expert Review of Clinical Pharmacology (2011), 4(2), 275-289 | Language: English, Database: CPlus and MEDLINE

A review. Toll-like receptor (TLR) ligation activates both the innate and adaptive immune systems, and plays an important role in antiviral and anti-tumor immunity. Therefore, a significant amount of effort has been devoted to exploit the therapeutic potential of TLR agonists. Depending on the therapeutic purpose, either as adjuvants to vaccine, chemotherapy or standalone therapy, TLR agonists have been administered via different routes. Both preclin. and clin. studies have suggested that the route of administration has significant effects on pharmacokinetics, and that understanding these effe...  
[View More](#)

[Full Text](#) ▾ [Substances \(0\)](#) [Reactions \(0\)](#) [Citing \(103\)](#) [Citation Map](#)

2

**Antiviral applications of Toll-like receptor agonists**

By: Horscroft, Nigel J.; Pryde, David C.; Bright, Helen  
Journal of Antimicrobial Chemotherapy (2012), 67(4), 789-801 | Language: English, Database: CPlus and MEDLINE

A review. In the past, antiviral research has focused mainly on viral targets. As the search for effective and differentiated antiviral therapies continues, cellular targets are becoming more common, bringing with them a variety of challenges and concerns. Toll-like receptors (TLRs) provide a unique mechanism to induce an antiviral state in the host. In this review we introduce TLRs as targets for the pharmaceutical industry, including how they signal and thereby induce an antiviral state through the production of type I interferons. We examine how TLRs are being therapeutically targeted and d...  
[View More](#)

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# 文献结果集

研究发展趋势

CAS标引的技术术语

CAS学科研究方向

制剂/分析方法信息

二次检索

The screenshot displays the CAS Literature Results interface. On the left, a sidebar contains various search filters:

- Publication Year:** A bar chart from 2000 to 2022, with a 'View Larger' button.
- Available at My Institution:** A dropdown menu.
- Author:** A dropdown menu.
- Organization:** A dropdown menu.
- Publication Name:** A dropdown menu.
- Concept:** A list including Homo sapiens (4,956), Human (4,956), Animals (4,261), Humans (3,732), and Toll-like receptor 4 (3,128). A 'View All' button is present.
- CA Section:** A dropdown menu.
- CAS Solutions:** A list including Formulus (1,184) and Analytical Methods (5).
- Formulation Purpose:** A dropdown menu.
- Database:** A dropdown menu.
- Search Within Results:** An input field for up to 3 text strings and a 'Search' button.

The main area shows three search results for 'Toll-like receptor agonists':

- Trial Watch: Toll-like receptor agonists in cancer immunotherapy**  
By: Smith, Melody; Garcia-Martinez, Elena; Pittier, Michael R.; Fucikova, Jitka; Spisek, Radek; Zitvogel, Laurence; Kroemer, Guido; Galluzzi, Lorenzo  
Oncolimmunology (2018), 7(12), e1526250/1-e1526250/15 | Language: English, Database: CPlus and MEDLINE  
A review. Toll-like receptor (TLR) agonists demonstrate therapeutic promise as immunol. adjuvants for anticancer immunotherapy. To date, three TLR agonists have been approved by US regulatory agencies for use in cancer patients. Addnl., the potential of hitherto exptl. TLR ligands to mediate clin. useful immunostimulatory effects has been extensively investigated over the past few years. Here, we summarize recent preclin. and clin. advances in the development of TLR agonists for cancer therapy.
- Toll-like Receptor Agonist Conjugation: A Chemical Perspective**  
By: Ignacio, Bob J.; Albin, Tyler J.; Esser-Kahn, Aaron P.; Verdoes, Martijn  
Bioconjugate Chemistry (2018), 29(3), 587-603 | Language: English, Database: CPlus and MEDLINE  
A review. Toll-like receptors (TLRs) are vital elements of the mammalian immune system that function by recognizing pathogen-associated mol. patterns (PAMPs), bridging innate and adaptive immunity. They have become a prominent therapeutic target for the treatment of infectious diseases, cancer, and allergies, with many TLR agonists currently in clin. trials or approved as immunostimulants. Numerous studies have shown that conjugation of TLR agonists to other mols. can beneficially influence their potency, toxicity, pharmacokinetics, or function. The functional properties of TLR agonist conjuga...
- Trial Watch: Immunostimulation with Toll-like receptor agonists in cancer therapy**  
By: Iribarren, Kristina; Bloy, Norma; Buque, Aitziber; Cremer, Isabelle; Eggermont, Alexander; Fridman, Wolf Herve; Fuci Galon, Jerome; Spisek, Radek; Zitvogel, Laurence; et al  
Oncolimmunology (2016), 5(3), e1088631/1-e1088631/11 | Language: English, Database: CPlus and MEDLINE  
A review. Accumulating preclin. evidence indicates that Toll-like receptor (TLR) agonists efficiently boost tumor-targeting immune responses (re)initiated by most, if not all, paradigms of anticancer immunotherapy. Moreover, TLR agonists have been successfully employed to ameliorate the efficacy of various chemotherapeutics and targeted anticancer agents, at least in rodent tumor models. So far, only three TLR agonists have been approved by regulatory agencies for use in cancer patients. Moreover, over the past decade, the interest of scientists and clinicians in these immunostimulatory agents...

聚类筛选项节省时间，一目了然。  
无需逐步二次检索和限定，直接勾选即可定位所需信息

# 文献结果集--聚类筛选Concept

Concept

Top Count Alphanumeric Search

7 Selected

- Homo sapiens (4,956)
- Human (4,956)
- Animals (4,261)
- Humans (3,732)
- Toll-like receptor 4 (3,128)
- Mice (2,892)
- Signal transduction (2,867)
- Toll-like receptors (2,608)
- Toll-like receptor 2 (2,224)
- Interleukin 6 (2,176)
- Toll-like receptor 7 (2,041)
- Cytokines (1,926)
- Toll-like receptor 9 (1,812)
- Soluble tumor necrosis factors (1,799)
- Type II interferons (1,775)
- Female (1,759)
- Lipopolysaccharides (1,640)
- Inflammation (1,608)
- Dendritic cell (1,549)
- Toll-like receptor 3 (1,506)
- Mice, Inbred C57BL (1,463)

Concept

Top Count Alphanumeric Search

Concept Name

T cell

Search

8 Selected

PROTEIN

- Killer T cell (4)
- Linker for activation of T-cells LA2 (2)
- Lymphoma, T-Cell (6)
- Lymphoma, T-Cell, Cutaneous (9)
- Memory cytotoxic T cell (6)
- Memory T cell (88)
- Mucosal-associated invariant T cell (5)
- T cell (771)
- T-cell activation Rho GTPase-activating proteins (1)
- T-Cell Antigen Receptor Specificity (4)
- T cell disease (4)
- T-cell immune regulator TCIRG1 (1)
- T cell immunoglobulin and mucin domain-containing protein 2 (1)
- T cell immunoglobulin and mucin domain-containing protein 4 (9)
- T cell immunoglobulin and mucin domain-containing proteins (8)
- T-cell leukemia (14)
- T-cell lymphoma (50)

通过Concept纵览并精准  
定位感兴趣的核心研究点

# 文献结果集--聚类筛选CA Section

CA Section

By Count Alphanumeric

0 Selected

- Immunochemistry (4,645)
- Pharmacology (1,354)
- Pharmaceuticals (446)
- Mammalian Pathological Biochemistry (348)
- Unavailable (257)
- Heterocyclic Compounds (More Than One Hetero Atom) (81)
- Mammalian Hormones (70)
- Biochemical Genetics (61)
- Mammalian Biochemistry (51)
- Toxicology (51)
- Radiation Biochemistry (36)
- Heterocyclic Compounds (One Hetero Atom) (31)
- Amino Acids, Peptides, and Proteins (29)
- Biochemical Methods (28)
- Microbial, Algal, and Fungal Biochemistry (22)
- General Biochemistry (20)
- Animal Nutrition (15)
- Carbohydrates (12)
- Biomolecules and Their Synthetic Analogs (9)
- Fermentation and Bioindustrial Chemistry (6)
- Benzene, Its Derivatives, and Condensed Benzenoid Compounds (4)
- Chemistry of Synthetic High Polymers (3)
- Enzymes (3)
- Essential Oils and Cosmetics (2)
- Nonmammalian Biochemistry (2)
- Pharmaceutical Analysis (2)
- Agrochemical Bioregulators (1)
- Alicyclic Compounds (1)
- Food and Feed Chemistry (1)
- General Organic Chemistry (1)
- History, Education, and Documentation (1)
- Industrial Organic Chemicals, Leather, Fats, and Waxes (1)
- Organic Analytical Chemistry (1)
- Organometallic and Organometalloidal Compounds (1)
- Physical Organic Chemistry (2)

Apply Cancel

通过CA Section快速  
锁定学科研究方向



# 文献结果集--聚类筛选CAS Solutions

查看勾选的  
Concept

Filter Behavior

Filter by Exclude

Document Type

Language

Publication Year

2000 to 2022

No Min to No Max Apply

View Larger

Available at My Institution

Author

Organization

Publication Name

Concept

CA Section

CAS Solutions

Formulus (861)

Analytical Methods (2)

Formulation Purpose

Database

Search Within Results

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

Enter a query... Search

Filter Content Report

Download filter data from this result set.

References (7,597) Sort: Relevance View: Partial Abstract

Substances Reactions Citing

Clear All Filters

Filtering: Concept: 8 Selected

Toll-like receptor 4  
Toll-like receptors  
Toll-like receptor 2  
Toll-like receptor 9  
Toll-like receptor 3  
Toll-like receptor 8  
T cell  
TLR agonist  
Toll-like receptor 5

The phase of TLR agonists and the impact on the immune system

By: Engle, Daniel A.; Horscroft, Nigel J.; Pryde, David C.; Bright, Helen  
Expert Review  
A review. TLR agonists have been administered via different routes. Both preclin. and clin. studies have suggested that the route of administration has significant effects on pharmacokinetics, and that understanding these effects is crucial for therapeutic success.

Activates both the innate and adaptive immune systems, and plays an important role in the development of the adaptive immune response. A significant amount of effort has been devoted to exploit the therapeutic potential of TLR agonists, either as adjuvants to vaccine, chemotherapy or standalone therapy. TLR agonists have been administered via different routes. Both preclin. and clin. studies have suggested that the route of administration has significant effects on pharmacokinetics, and that understanding these effects is crucial for therapeutic success.

View More

Full Text Substances (0) Reactions (0) Citing (103) Citation Map

Antiviral applications of Toll-like receptor agonists

By: Horscroft, Nigel J.; Pryde, David C.; Bright, Helen  
Journal of Antimicrobial Chemotherapy (2012), 67(4), 789-801 | Language: English, Database: CPlus and MEDLINE

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View More

Full Text Substance (1) Reactions (0) Citing (42) Citation Map

Trial Watch: Toll-like receptor agonists in cancer immunotherapy

By: Smith, Melody; Garcia-Martinez, Elena; Pitter, Michael R.; Fucikova, Jitka; Spisek, Radek; Zitvogel, Laurence; Kroemer, Guido; Galluzzi, Lorenzo  
Oncolimmunology (2018), 7(12), e1526250/1-e1526250/15 | Language: English, Database: CPlus and MEDLINE

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Full Text Substances (0) Reactions (0) Citing (76) Citation Map

# 文献结果集--保存及查看详情

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

Load More Results

Filter Behavior

Filter by Exclude

Document Type

Language

Publication Year

2000 2022  
No Min to No Max Apply View Larger

Available at My Institution

Author

Organization

Publication Name

Concept

CA Section

CAS Solutions

Formulus (861)

Analytical Methods (2)

Formulation Purpose

Database

Search Within Results

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

Enter a query...

References (7,597) Sort: Relevance View: Partial Abstract

Substances Reactions Citing

Filtering: Concept: 8 Selected

Clear All Filters

Save

Save Search

Name

No Alerts As Available Weekly Monthly

Tags (optional)

No tags defined

New Tag (optional)

Save Cancel

Download Reference Results

File Type PDF Select Quantity

All Results Selected Results Range (ex. 2 to 20)

Display Result Summary Result Details

File Name Reference\_20211117\_2233

Only the first 500 references will be downloaded.

Include

Task History Abstract Formulations

Abstract Concepts Analytical Methods

Substances Citations

Download Cancel Learn more about downloads.

The pharmacokinetics of Toll-like receptor agonists and the impact on the immune system  
By: Engel, Abbi L.; Holt, Gregory E.; Lu, Hailing  
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View More

Full Text Substances (0) Reactions (0) Citing (103) Citation Map

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By: Horscroft, Nigel J.; Pryde, David C.; Bright, Helen  
Journal of Antimicrobial Chemotherapy (2012), 67(4), 789-801 | Language: English, Database: CAplus and MEDLINE  
A review. In the past, antiviral research has focused mainly on viral targets. As the search for effective and differentiated antiviral therapies continues, cellular targets are becoming more common, bringing with them a variety of challenges and concerns. Toll-like receptors (TLRs) provide a unique mechanism to induce an antiviral state in the host. In this review we introduce TLRs as targets for the pharmaceutical industry, including how they signal and thereby induce an antiviral state through the production of type I Interferons. We examine how TLRs are being therapeutically targeted and...  
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Full Text Substance (1) Reactions (0) Citing (42) Citation Map

Trial Watch: Toll-like receptor agonists in cancer immunotherapy  
By: Smith, Melody; Garcia-Martinez, Elena; Pitter, Michael R.; Fucikova, Jitka; Spisek, Radek; Zitvogel, Laurence; Kroemer, Guido; Galluzzi, Lorenzo  
OncolImmunology (2018), 7(12), e1526250/1-e1526250/15 | Language: English, Database: CAplus and MEDLINE  
A review. Toll-like receptor (TLR) agonists demonstrate therapeutic promise as immunol. adjuvants for anticancer immunotherapy. To date, three TLR agonists have been approved by US regulatory agencies for use in cancer patients. Addnl., the potential of hitherto exptl. TLR ligands to mediate clin. useful immunostimulatory effects has been extensively investigated over the past few years. Here, we summarize recent preclin. and clin. advances in the development of TLR agonists for...  
Full Text Substances (0) Reactions (0) Citing (76) Citation Map

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# 文献详情

被引文献

引文地图

Reference Detail (1 of 12)

Substance (1) Reactions (0) Citing (42) Citation Map

Antiviral applications of Toll-like receptor agonists

By: Horscroft, Nigel J.; Pryde, David C.; Bright, Helen

A review. In the past, antiviral research has focused mainly on viral targets. As the search for effective and differentiated antiviral therapies continues, cellular targets are becoming more common, bringing with them a variety of challenges and concerns. Toll-like receptors (TLRs) provide a unique mechanism to induce an antiviral state in the host. In this review we introduce TLRs as targets for the pharmaceutical industry, including how they signal and thereby induce an antiviral state through the production of type I interferons. We examine how TLRs are being therapeutically targeted and discuss several clin. precedented agents for which efficacy and safety data are available. We describe some of the chemistries that have been applied to both small mol. and large mol. leads to tune agonist potency, and offer a differentiated safety profile through targeting certain compartments such as the gut or the lung, thereby limiting systemic drug exposure and affecting systemic cytokine levels. The application of low-dose agonists of TLRs as vaccine adjuvants or immunoprotective agents is also presented. Some of the challenges presented by this approach are then discussed, including viral evasion strategies and mechanism-linked inflammatory cytokine induction.

Keywords: review Toll like receptor agonist antiviral

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Concepts MEDLINE® Medical Subject Headings Substances Cited Documents

文献详情界面对包括：

- 标题
- 摘要
- 文献中重要的技术术语  
(含Caplus、Medline的关键词)
- 文献中重要的物质
- 书目信息
- 获得文献中的物质、反应
- 参考文献
- 链接原文
- 引文地图

CAS科学家增值标引的信息

参考文献



# 文献详情

Concepts

Antiviral agents	Toll-like receptors Role: Biological Study, Unclassified
Receptor agonists	Viral infection

Concepts:  
CAS科学家提供的标准技术术语，  
能更全面、更精准地检索。

MEDLINE® Medical Subject Headings

Antiviral Agents Qualifier: administration & dosage; chemistry; pharmacology	Interferons Qualifier: immunology; metabolism
Humans	Toll-Like Receptors Qualifier: agonists
Immunologic Factors Qualifier: administration & dosage; chemistry; pharmacology	Virus Diseases Qualifier: drug therapy; immunology

Medline Subject Headings：  
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核心点标出，更全面了解文献

Substances

Substance (1)

9008-11-1  
Image Not Available

Unspecified  
Interferons

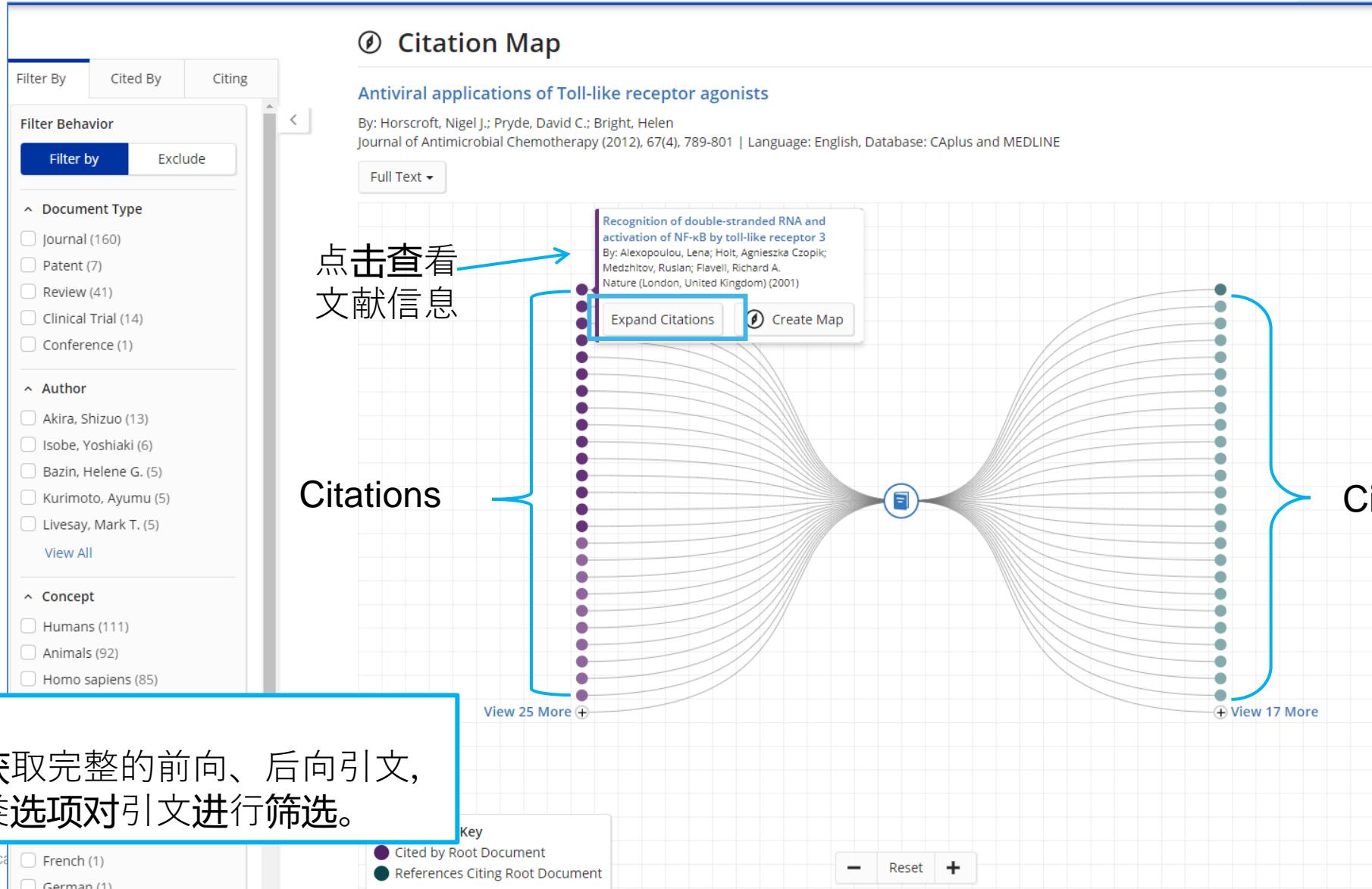
Role: Unspecified

Substances：  
对原文中重点研究的物质信息一目了然；  
由Role了解文献对物质研究的学科方向

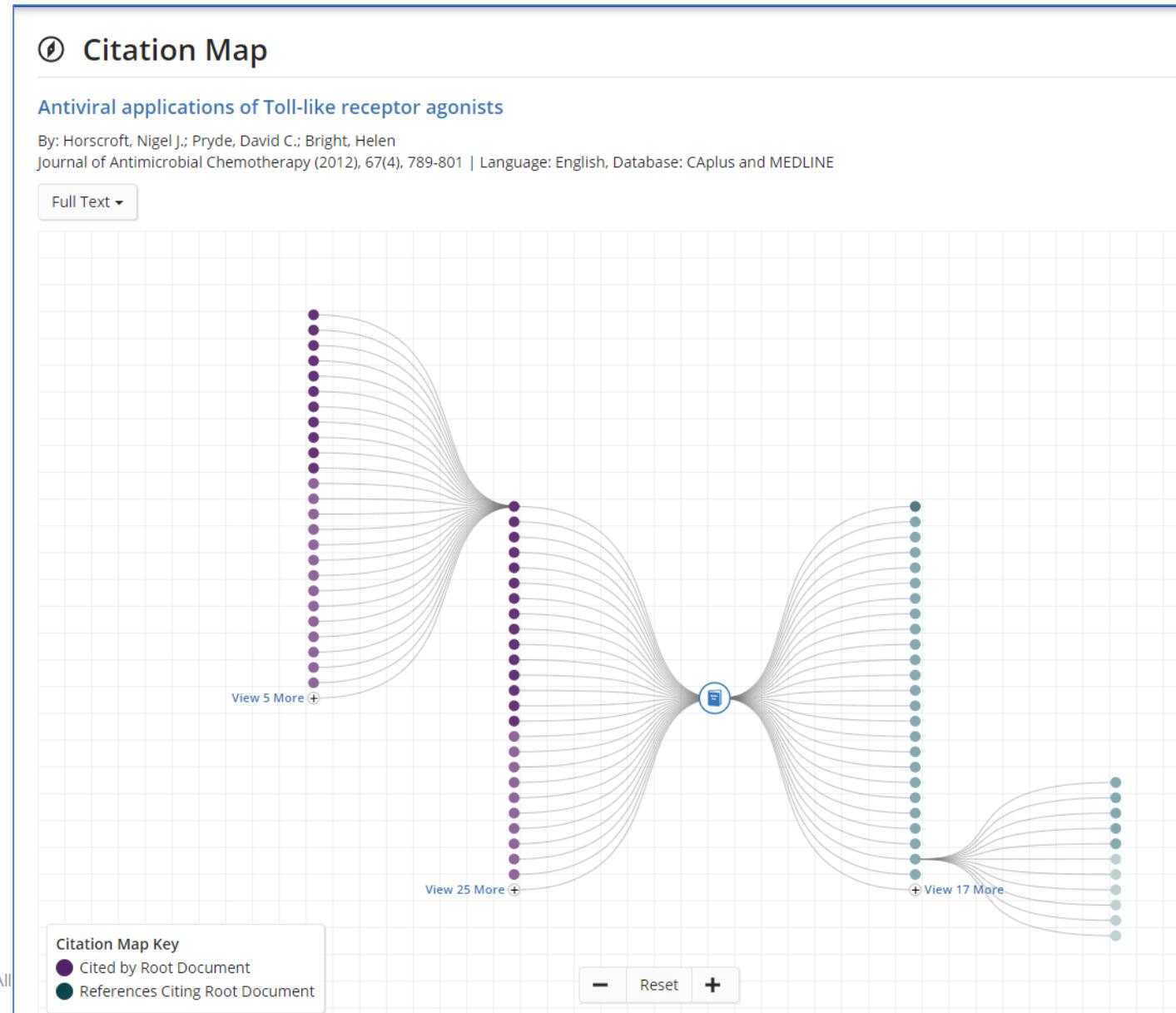
# 引文地图

对引文  
做筛选

引文地图：  
在一个页面获取完整的前向、后向引文，  
并有多个聚类选项对引文进行筛选。



# 引文地图



# 专利文献

PATENT	
Patent Number	WO2015011254
Publication Date	2015-01-29
Application Number	WO2014-EP66007
Application Date	2014-07-25

Kind Code  
A1  
  
Assignee  
INSERM (Institut National de la Sante et de la Recherche Medicale), France  
  
Universite de Droit et de la Sante de Lille 2, France  
  
Centre National de la Recherche Scientifique (CNRS), France  
  
Institut Pasteur de Lille, France  
  
Universite de Lille 1 Sciences et Technologies, France  
  
ETH Zurich, France

## 专利族信息

Source  
World Intellectual Property Organization  
CODEN: PIXXD2

Database Information  
AN: 2015:167126  
CAN: 162:266207  
CAplus

Language  
English

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Methods using toll-like receptor (TLR) agonists in combination with antibiotics for the bacterial infections

By: Hardt, Wolf-Dietrich; Kaiser, Patrick; Sirard, Jean-Claude; Carnoy, Christophe; Fougeron, Delphine; Chabalgoity, Munoz, Natalia

The invention relates to methods and pharmaceutical compositions for the treatment of bacterial infections. In particular, the invention relates to a toll-like receptor (TLR) agonist (e.g. flagellin polypeptide, biomols, peptides, antibodies, nucleic acids) for the treatment of a bacterial infection in a subject in need thereof wherein the TLR agonist is administered to the subject in combination with at least one antibiotic. In another aspect of the invention the antibiotic is selected from the group of aminoglycosides, beta-lactams, quinolones or fluoroquinolones, macrolides, sulfonamides, sulfamethoxazoles, tetracyclines, streptogramins, oxazolidinones, rifamycins, glycopeptides, polymixins, and lipo-peptide antibiotics.

Keywords: antibacterial toll like receptor TLR agonist bacterial infection treatment; antibiotic TLR agonist antibiotic therapy bacterial infection

[PatentPak Viewer](#) [Full Text](#)

## Patent Family

Patent	Language	Kind Code	PatentPak Options	Publication Date	Application Number
WO2015011254	English	A1	<a href="#">PDF</a>   <a href="#">PDF+</a>   <a href="#">Viewer</a>	2015-01-29	WO2014-EP66007
					EP2013-306086
EP3024476	English	A1		2016-06-01	EP2014-749736
EP3632458	English	A1	<a href="#">PDF</a>	2020-04-08	EP2019-207885
US20160151453	English	A1	<a href="#">PDF</a>	2016-06-02	US2016-14906747
US9919029	English	B2		2018-03-20	US2016-14906747

## IPC Data

Patent	Class	Patent Family Classification Codes
WO2015011254	IPCI	A61K 0038/16; A61K 0045/06; A61K 0031/43; A61K 0031/505; A61K 0031/635; A61K 0031/635; A61K 0031/635
EP3024476	IPCI	A61K 0038/16; A61K 0045/06; A61K 0031/43; A61K 0031/505; A61K 0031/635; A61K 0031/635; A61K 0031/635
EP3632458	IPCI	A61K 0038/16; A61K 0045/06; A61K 0031/43; A61K 0031/505; A61K 0031/635; A61K 0031/635
US20160151453	IPCI	A61K 0038/16; A61K 0031/505; A61K 0031/42; A61K 0031/43; A61K 0045/06; A61K 0031/635
US9919029	IPCI	A61K 0038/16; A61K 0031/505; A61K 0031/42; A61K 0031/43; A61K 0045/06; A61K 0031/635

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PCT/EP2014/066007

WO 2015/011254

sulfonamides, sulfamethoxazoles, tetracyclines, streptogramins, oxazolidinones, rifamycins, glycopeptides, polymixins, and lipo-peptide antibiotics.

18. The method of claim 1 wherein the antibiotic is a tetracycline selected from the group consisting of chlortetracycline, demeclocycline, doxycycline, minocycline, oxytetracycline, chlortetracycline, methacycline, meccocycline, tigecycline, limecycline, and tetracycline.

19. The method of claim 1 wherein the antibiotic is an aminoglycoside selected from the group consisting of amikacin (Amikin®), gentamicin (Garamycin®), kanamycin (Kantrex®), neomycin (Mycifradin®), netilmicin (Netromycin®), paromomycin (Humatin®), streptomycin, and tobramycin (TOBI Solution®, TobraDex®).

20. The method of claim 1 wherein the antibiotic is a macrolide selected from the group consisting of azithromycin (Zithromax®), clarithromycin (Biaxin®), dirithromycin (Dynabac®), erythromycin, clindamycin, josamycin, roxithromycin and lincomycin.

21. The method of claim 1 wherein the antibiotic is a fluoroquinolone selected from the group consisting of nalidixic acid, cinoxacin, oxolinic acid, flumequine, pipemidic acid, rosroxacin, norfloxacin, lomefloxacin, ofloxacin, enrofloxacin, ciprofloxacin, enoxacin, amifloxacin, fleroxacin, gatifloxacin, gemifloxacin, clinafloxacin, sitafloxacin, pefloxacin, rufloxacin, sparfloxacin, temafloxacin, tosufloxacin, grepafloxacin, levofloxacin, moxifloxacin.

22. The method of claim 1 wherein the antibiotic is selected from the group consisting of mafenide, phtalylsulfadiazine, sulfadoxine, sulfametopirazine, sulfametoxypp sulfamylon, sulfanilamide, su

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# 文献检索--主题词+结构联合检 索

Searching for...

All

Substances

Reactions

Structure Match

As Drawn (10)

**Substructure (75)**

Filter Behavior

Filter by

Exclude

Document Type

Journal (43)

Patent (32)

Review (2)

Substance Role

Preparation (59)

Reactant or Reagent (41)

Biological Study (37)

Uses (32)

Properties (17)

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Language

English (67)

Czech (4)

Chinese (3)

Korean (1)

Publication Year



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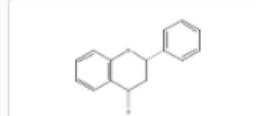
References

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Antitumor

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**References (75)**

Sort: Relevance View: Partial Abstract

1 **Antitumor Agents. 181. Synthesis and Biological Evaluation of 6,7,2',3',4'-Substituted-1,2,3,4-tetrahydro-2-phenyl-4-quinolones as a New Class of Antimitotic Antitumor Agents**

By: Xia, Yi; Yang, Zheng-Yu; Xia, Peng; Bastow, Kenneth F.; Tachibana, Yoko; Kuo, Sheng-Chu; Hamel, Ernest; Hackl, Torben; Lee, Kuo-Hsiung

Journal of Medicinal Chemistry (1998), 41(7), 1155-1162 | Language: English, Database: CAPIUS and MEDLINE

A novel series of 6,7,2',3',4'-substituted-1,2,3,4-tetrahydro-2-phenyl-4-quinolones were synthesized and evaluated for interactions with tubulin and for cytotoxic activity against a panel of human tumor cell lines, including ileocecal carcinoma (HCT-8), breast cancer (MCF-7), lung carcinoma (A-549), epidermoid carcinoma of the nasopharynx (KB), renal cancer (CAKI-1), and melanoma cancer (SKMEL-2). Most compounds showed potent cytotoxic and antitubulin effects. The most active compounds demonstrated strong cytotoxic effects with ED<sub>50</sub> values in the nanomolar or subnanomolar range in almost all t.

[View More](#)

2 **aza-Flavanones as potent cross-species microRNA inhibitors that arrest cell cycle**

By: Chandrasekhar, Srivari; Pushpavalli, Sreerangam N. C. V. L.; Chatla, Srinivas; Mukhopadhyay, Debasmita; Ganganna, Bogonda; Vijeender, Kandi; Srihari, Pabbareja; Reddy, Chada Raji; Janaki Ramaiah, M.; Bhadra, Utpal

Biorganic & Medicinal Chemistry Letters (2012), 22(1), 645-648 | Language: English, Database: CAPIUS and MEDLINE

Aza-Flavanones have been identified as a new class of selective microRNA inhibitors. These compounds were found to arrest cell cycle via a novel cross species microRNA-dependent regulatory pathway interpreting an unexpected link between cell cycle arrest and microRNA mediated control in cancer.

3 **Relationship between structure and antiproliferative activity of 1-azaflavavones**

By: Kawai, Satoru; Endo, Kotaro; Tokiwano, Tetsuo; Yoshizawa, Yuko

Cancer Research (2012), 52(7), 2819-2826 | Language: English, Database: CAPIUS

The synthesis of 19 derivatives of 2-phenyl-3,4-dihydroquinolin-4(1H)-one, as aza analogs of flavanones, was carried out and these compounds were further screened for their antiproliferative activity toward HL60 promyelocytic leukemia cells. In comparison with flavanone the replacement of C-ring ether oxygen atom with a nitrogen atom potentiated activity by more than 100-fold. It was suggested that the aromaticity of the B-ring contributes greatly to the activity of 1-azaflavavones.

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# 文献检索小结

1. 使用布尔逻辑算符and、or、not连接主题词
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# 大纲

## - CAS SciFinder<sup>n</sup>中的物质检索

- 检索物质的常用方法
- 物质详情的解读
- 结构绘图板的应用
- 物质结果集的分析及筛选
- 物质结果集的可视化分析

视频链接：

<https://american-chemical-society.zoom.us/rec/share/C8gGlyhcc1N22z3JdJ3yrRdFXdEfb9qMXz9vo2tjyiGLdd-6Qke9taq5Y1LL5SM.daLElpuwQKEepf-S?startTime=1646733603000>

# 物质检索

- 物质检索方法
  - 物质标识符：化学名称, CAS RN
  - 文献标识符：专利号、文献号、PubMed ID、DOI
  - 分子式
  - 物性参数
  - 谱图数据
  - 结构式
- 物质检索策略推荐
  - 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

通过物质名称、CAS RN, 文献标识符检索物质

The screenshot shows the SciFinder search interface. On the left, a sidebar lists categories: All, Substances (highlighted in blue), Reactions, References, Suppliers, Biosequences, and Retrosynthesis. The main area is titled "Substances" and contains a search bar with the placeholder "Enter a query...". Below the search bar are dropdown menus for "Search by Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. Learn More" and "Molecular Formula". To the right of the search bar is a "Draw" button with a pencil icon and a search icon. A blue arrow points from the text "通过物质名称、CAS RN, 文献标识符检索物质" to the search bar. Another blue arrow points from the text "打开结构绘制面板进行结构检索" to the "Draw" button.

通过分子式、物性参数、谱图数据检索物质

打开结构绘制面板进行结构检索

# 物质检索--物质名称、CAS RN、代码

Filter Behavior

Filter by Exclude

Commercial Availability

Available (3)

Reaction Role

Product (3)

Reactant (3)

Catalyst (1)

Reference Role

Adverse Effect (3)

Analyte (3)

Analytical Role, Unclassified (3)

Analytical Study (3)

Biochemical Process (3)

## Substances (3)

Sort: Relevance View: Partial

References Reactions Suppliers

Save

Rank	CAS RN	Chemical Structure	Description	References	Reactions	Suppliers
1	50-56-6		Absolute stereochemistry shown C <sub>43</sub> H <sub>66</sub> N <sub>12</sub> O <sub>12</sub> S <sub>2</sub> Oxytocin Protein/Peptide Sequence Sequence Length: 9	31K References	390 Reactions	66 Suppliers
2	1190307-88-0		Absolute stereochemistry shown C <sub>22</sub> H <sub>29</sub> FN <sub>3</sub> O <sub>9</sub> P <b>Sofosbuvir</b>	3,695 References	720 Reactions	66 Suppliers
3	1809249-37-3		Absolute stereochemistry shown C <sub>27</sub> H <sub>35</sub> N <sub>6</sub> O <sub>8</sub> P <b>GS 5734</b>	2,264 References	504 Reactions	47 Suppliers

sofosbuvir  
50-56-6  
"GS 5734"

多个物质同时检索，  
中间用空格隔开

# 物质检索--物质名称中间或词尾使用通配符\*或?

The screenshot shows two separate SciFinder search results for the query "flavone\*".

**Left Panel (Search for "flavone"):**

- Filter Behavior: Filter by
- Substances (4,467)
- Sort: Relevance
- View: Partial

**Right Panel (Search for "flavone?"):**

- Filter Behavior: Filter by
- Substances (20)
- Sort: Relevance
- View: Partial

**Common Results (Both Panels):**

- 1. 28625-66-3: Flavone, 6,8-bis[(dimethylamino)methyl]-3,4',5,7-pentahydroxy-, 3-[6-O-(6-deo...]
- 2. 18423-37-5: Flavone, 6-[β-D-mannopyranosylamino]-
- 3. 18423-35-3: Flavone, 6-(D-glucopyranosylamino)-
- 4. 30137-81-6: Flavone, 3-hydroxy-3',4',5,7-tetramethoxy-, 3-hexopyranoside
- 5. 10481-54-6: Flavone, 4',7-bis(benzyloxy)-3-[[6-O-(6-deoxy-α-L-mannopyranosyl)-β-D-glucopyranosy...]
- 6. 6758-49-2: Junipin

**Text Box:** 物质名称中使用通配符可以检索多个物质

# 物质检索--文献标识符

The screenshot shows the SciFinder interface with a search bar at the top containing the identifier "WO2011123645". The main area displays a grid of substance cards, each showing a chemical structure, CAS number, name, and reference statistics (e.g., 215K References, 91K Reactions, 188 Suppliers). The sidebar on the left contains various filtering options such as Commercial Availability, Reaction Role, Reference Role, Stereochemistry, and Number of Components.

序号	CAS号	名称	分子式	描述
1	108-95-2	Phenol	C <sub>6</sub> H <sub>5</sub> O	酚类，215K References, 91K Reactions, 188 Suppliers
2	108-24-7	Acetic anhydride	C <sub>4</sub> H <sub>6</sub> O <sub>3</sub>	羧酸酐，153K References, 375K Reactions, 80 Suppliers
3	100-46-9	Benzylamine	C <sub>7</sub> H <sub>9</sub> N	胺类，57K References, 93K Reactions, 82 Suppliers
4	18162-48-6	tert-Butyldimethylsilyl chloride	C <sub>6</sub> H <sub>15</sub> ClSi	硅烷衍生物，36K References, 64K Reactions, 127 Suppliers
5	10025-87-3	Phosphorus oxychloride	Cl <sub>3</sub> OP	磷酰氯，25K References, 214K Reactions, 46 Suppliers
6	58-96-8	Uridine	C <sub>9</sub> H <sub>12</sub> N <sub>2</sub> O <sub>6</sub>	核苷类，24K References, 3,429 Reactions, 106 Suppliers
7	149-30-4	2-Mercaptobenzothiazole	C <sub>7</sub> H <sub>5</sub> NS <sub>2</sub>	杂环类，18K References, 6,303 Reactions, 120 Suppliers
8	501-53-1	Benzyl chloroformate	C <sub>8</sub> H <sub>7</sub> ClO <sub>2</sub>	有机氯化物，17K References, 28K Reactions, 75 Suppliers
9	616-47-7	1-Methylimidazole	C <sub>4</sub> H <sub>6</sub> N <sub>2</sub>	杂环类，16K References, 34K Reactions, 112 Suppliers

专利号  
WO2011123645

帮助用户迅速获得关注文献中的所有物质



# 物质检索--Advanced Search

Searching for...  
Substances  
Reactions  
References  
Suppliers

Enter a query...  
Draw Search

+ Add Advanced Search Field

通过分子式、物性参数、  
谱图数据等进行检索

高级检索字段：  
CAS RN (物质、组份)、物质名、分子式、文献号、专利号  
实验谱图 (1H, 13C, 15N, 19F, 31P NMR)  
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)

Searching for...  
Substances  
Reactions  
References  
Suppliers  
Biosequences  
Retrosynthesis

Enter a query...  
Molecular Formula Search

- Select - Molecular Formula

AND Select

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

Recent Search History  
April 12, 2022  
References 11:56 PM TLR or "toll like rec"  
March 30, 2022

Rerun Search Edit Search

# 物质检索--分子式

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

Searching for...

All

**Substances**

Reactions

References

Suppliers

Substances

Enter a query...

Molecular Formula

Examples: C<sub>6</sub>H<sub>6</sub> | (C<sub>6</sub>H<sub>5</sub>)<sub>2</sub>C | C<sub>22</sub>H<sub>26</sub>CuN<sub>2</sub>O<sub>5</sub>.C<sub>2</sub>H<sub>3</sub>N

Add Advanced Search Field

Learn more about SciFinder® Advanced Search.

Filter Behavior

Filter by Exclude

Commercial Availability

Available (5)

Not Available (4)

Reaction Role

Product (2)

Reagent (2)

Catalyst (1)

Reference Role

Uses (6)

Biological Study (5)

Process (5)

Analytical Study (4)

Biological Study, Unclassified (4)

View All

Number of Components

Substance Class

Isotopes

Metals

Molecular Weight

Experimental Property

Experimental Spectrum

Regulatory Data by Country

Substances (9)

Sort: Relevance View: Partial

1 7757-82-6  • 2 Na H<sub>2</sub>O<sub>4</sub>S.2Na Components: 2 Component RN: 7664-93-9 Sodium sulfate 103K References 51K Reactions 178 Suppliers

2 13759-07-4  • 2 Na H<sub>2</sub>O<sub>4</sub>S.2Na Components: 2 Component RN: 7664-93-9 Thenardite (Na<sub>2</sub>(SO<sub>4</sub>)) 906 References 0 Reactions 1 Supplier

3 14262-80-7  • 2 Na H<sub>2</sub>O<sub>4</sub>S.2Na Components: 2 Component RN: 13770-01-9 Sulfuric-<sup>35</sup>S acid, disodium salt 73 References 1 Reaction 4 Suppliers

4 225640-22-2  • 2 Na H<sub>2</sub>O<sub>4</sub>S.2Na Components: 2 Component RN: 778561-01-6 Sulfuric-<sup>34</sup>S acid, disodium salt 8 References 1 Reaction 1 Supplier

5 20581-68-4  • 2 Na H<sub>2</sub>O<sub>4</sub>S.2Na Components: 2 Component RN: 7664-93-9 Metathenardite (Na<sub>2</sub>(SO<sub>4</sub>)) 3 References 0 Reactions 0 Suppliers

6 911392-46-6  • 2 Na H<sub>2</sub>O<sub>4</sub>S.2Na Components: 2 Component RN: 911422-29-2 Sulfuric-<sup>33</sup>S acid, disodium salt 1 Reference 0 Reactions 1 Supplier

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# 物质检索--物性参数

密度>150g/cm<sup>3</sup>  
分子量<200

Searching for...

All

Substances

Reactions

References

Suppliers

Biosequences

Retrosynthesis

Substances

Search by Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. Learn more about these fields.

Enter a query...

Density (g/cm<sup>3</sup>) > 150

Include predicted values.

Molecular Weight < 200

Predicted values only.

Add Advanced Search Field

多参数检索，提高检索效率

Substances (6)

Sort: Relevance View: Partial

1 139-13-9

C<sub>6</sub>H<sub>9</sub>NO<sub>6</sub> Nitrilotriacetic acid

2 7631-86-9

O=Si=O

3 593-88-4

C<sub>3</sub>H<sub>9</sub>As Trimethylarsine

4 34560-16-2

C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub> 1,1-Diethoxy-2-nitroethane

5 79-02-7

C<sub>2</sub>H<sub>2</sub>Cl<sub>2</sub>O Dichloroacetaldehyde

Substance Detail

Reactions (713)

Synthesize (48)

Create Retrosynthesis Plan

References (13K)

Suppliers (91)

Edit Structure Reset

13K References 713 Reactions 91 Suppliers

1.1M References 90K Reactions 407 Suppliers

25 References 42 Reactions 50 Suppliers

671 References 122 Reactions 16 Suppliers

Learn more about these fields.

单击结构打开物质菜单链接至物质相关信息

# 物质检索--谱图数据

H谱特征峰保留时间： 7 to 8, 2.2, 3 to 4

C谱特征峰保留时间： 44.5 to 45

Searching for...

All

**Substances**

Reactions

References

Suppliers

Biosequences

Retrosynthesis

Substances

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

Enter a query...

Proton NMR ▾ 7 to 8, 2.2, 3 to 4  
Allowance of  $\pm 0.2$  ppm. Examples: 8.03, 7.2, 2.2

AND Carbon-13 NMR ▾ 44.5 to 45  
Allowance of  $\pm 2$  ppm. Examples: 152.3, 127.6, 133.1

Add Advanced Search Field

Learn more about Search

通过谱图数据进行检索

Substances (1,143)

Sort: Relevance View: Partial

References Reactions Suppliers

Download Email Save

1 1354644-05-5

Absolute stereochemistry shown, Rotation (+)

C<sub>21</sub>H<sub>28</sub>O<sub>2</sub>  
(4bS,6aS,7R,11aS,11bR)-4b,6,6a,7,8,11,  
11a,11b,12,13-Decahydro-2-methoxy-6a-methy...

2 References 4 Reactions 1 Supplier

2 921073-43-0

C<sub>21</sub>H<sub>23</sub>NO<sub>5</sub>S  
4-[5,6-Dimethoxy-1-[(4-methylphenyl)sulfonyl]-1H-indol-2-yl]-2-butanone

1 Reference 6 Reactions 0 Suppliers

3 353387-16-7

C<sub>11</sub>H<sub>10</sub>N<sub>2</sub>O<sub>2</sub>  
2,3-Dihydro-3-hydroxypyrido[2,1-*b*]quinazolin-9(1*H*)-one

51 References 37 Reactions 10 Suppliers

4 879288-35-4

Absolute stereochemistry shown, Rotation (-)

C<sub>29</sub>H<sub>36</sub>O<sub>10</sub>  
Methyl (4S,4aS,6aR,7S,8S,10R,11R,12R,  
12aR,12bS)-12-(acetoxy)-4-(3-furanyl)dode...

2 References 0 Reactions 0 Suppliers

5 693235-19-7

C<sub>14</sub>H<sub>16</sub>N<sub>2</sub>O<sub>3</sub>  
Acetamide, *N*-(decahydro-3-hydroxy-2-oxo-3,7,4,6-ethanediylidene-7a*H*-pentalenol[1,...]

2 References 2 Reactions 0 Suppliers

6 1245281-17-7

Absolute stereochemistry shown

C<sub>16</sub>H<sub>18</sub>N<sub>2</sub>O<sub>2</sub>  
*N*-Methyl-*N*-(4*R*,5*R*)-1,3,4,5-tetrahydro-5-(2-oxopropyl)benz[cd]indol-4-yl)formami...

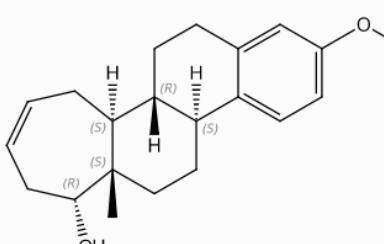
1 References 0 Reactions 0 Suppliers

# 物质详情

Substance Detail (1 of 1,143)

References (2) Reactions (4) Supplier (1) Save

CAS Registry Number  
1354644-05-5



Absolute stereochemistry shown, Rotation (+)

$C_{21}H_{28}O_2$

5H-Cyclohepta[a]phenanthren-7-ol, 4b,6,6a,7,8,11,11a,11b,12,13-dehydro-2-methoxy-6a-methyl-, (4bS,6aS,7R,11aS,11bR)- (ACI)

Key Physical Properties	Value	Condition
Molecular Weight	312.45	-
Boiling Point (Predicted)	458.5±45.0 °C	Press: 760 Torr
Density (Predicted)	1.088±0.06 g/cm <sup>3</sup>	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	14.81±0.40	Most Acidic Temp: 25 °C

Spectra

- ▼ Other Names and Identifiers
- ▼ Experimental Spectra
- ▼ Predicted Properties
- ▼ Predicted Spectra
- ▼ Bioactivity Indicators
- ▼ Additional Details

折叠菜单显示物质各类信息



# 物质详情

- Other Names and Identifiers
- Experimental Spectra
  - <sup>1</sup>H NMR
  - <sup>13</sup>C NMR
- Sources
  - (1) Saloranta, Tiina; Steroids, (2012), 77(1-2), 110-117, CPlus
- Predicted Properties
- Predicted Spectra
- Bioactivity Indicators

**Carbon-13 NMR Spectrum Detail (1 of 1)**

[View Carbon-13 NMR Spectrum](#)

Source: (1) ACD

**1354644-05-5**

Absolute stereochemistry shown, Rotation (+)

**C<sub>21</sub>H<sub>28</sub>O<sub>2</sub>**

**CAS Name:** (4bS,6aS,7R,11aS,11bR)-4b,6,6a,7,8,11,11a,11b,12,13-Decahydro-2-methoxy-6a-methyl-5H-cyclohepta[a]phenanthren-7-ol

**Conditions:**

- Working Frequency: 150 MHz
- Solvent: Chloroform-d (865-49-6)
- Temperature: 25 °C

**Spectrum Summary:**

Spectrum ID: 04phy12n1\_131.C

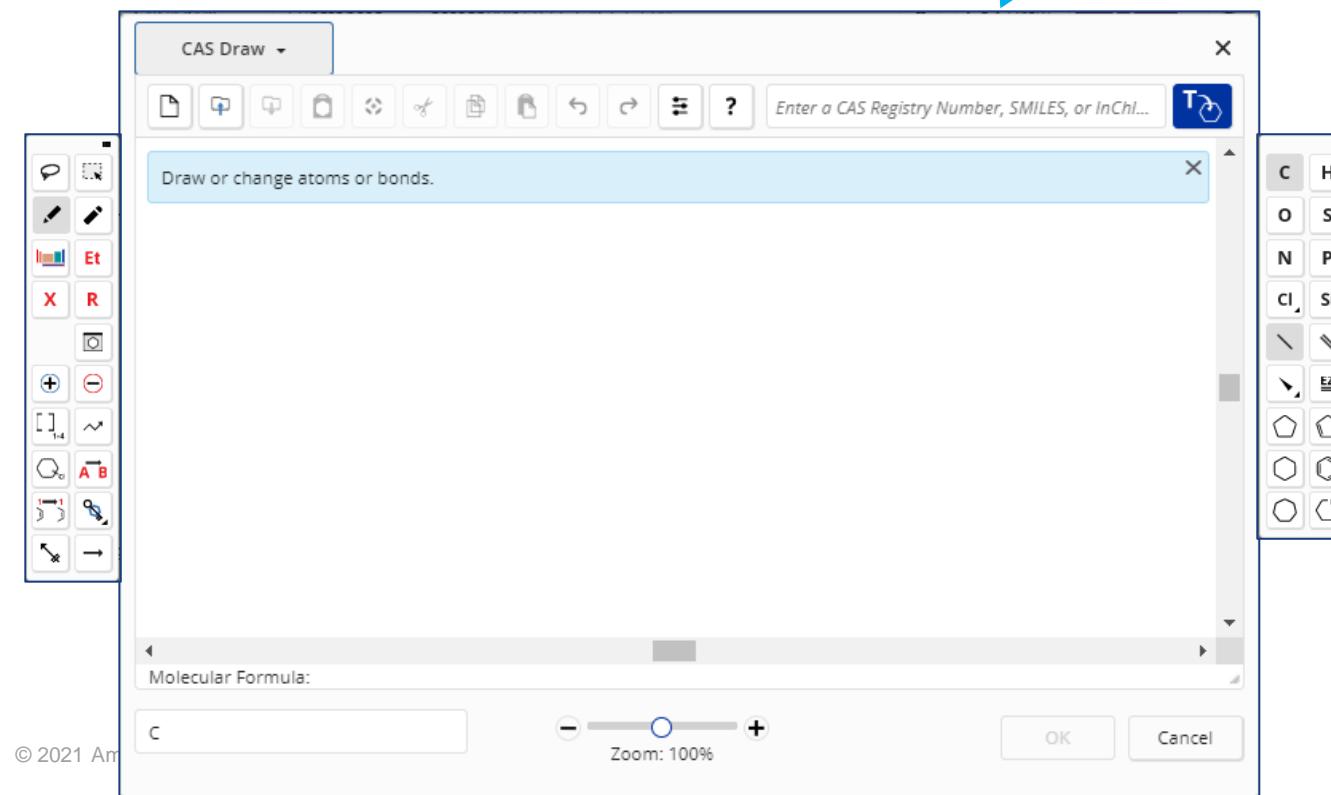
**Peak Data:**

157.5, 138.1, 133.9, 133.4, 126.1, 126.0, 113.2, 111.4, 76.9, 55.2, 43.2, 42.5, 41.9, 39.5, 36.2, 31.4, 30.3, 27.6, 26.6, 26.2, 17.1 ppm

**Source:** Spectral data were obtained from Advanced Chemistry Development, Inc.

# 物质检索--结构检索

The screenshot shows the SciFinder search interface. On the left, a sidebar lists categories: All, Substances (highlighted in blue), Reactions, References, and Suppliers. The main area is titled 'Substances' and contains a search bar with placeholder 'Enter a query...', a 'Draw' button, and a 'Search' button. Below the search bar is a 'Molecular Formula' dropdown menu. A blue arrow points from the 'Draw' button on the main page down to the 'Draw' tool window.



X 选择可变基团

R 自定义R基团

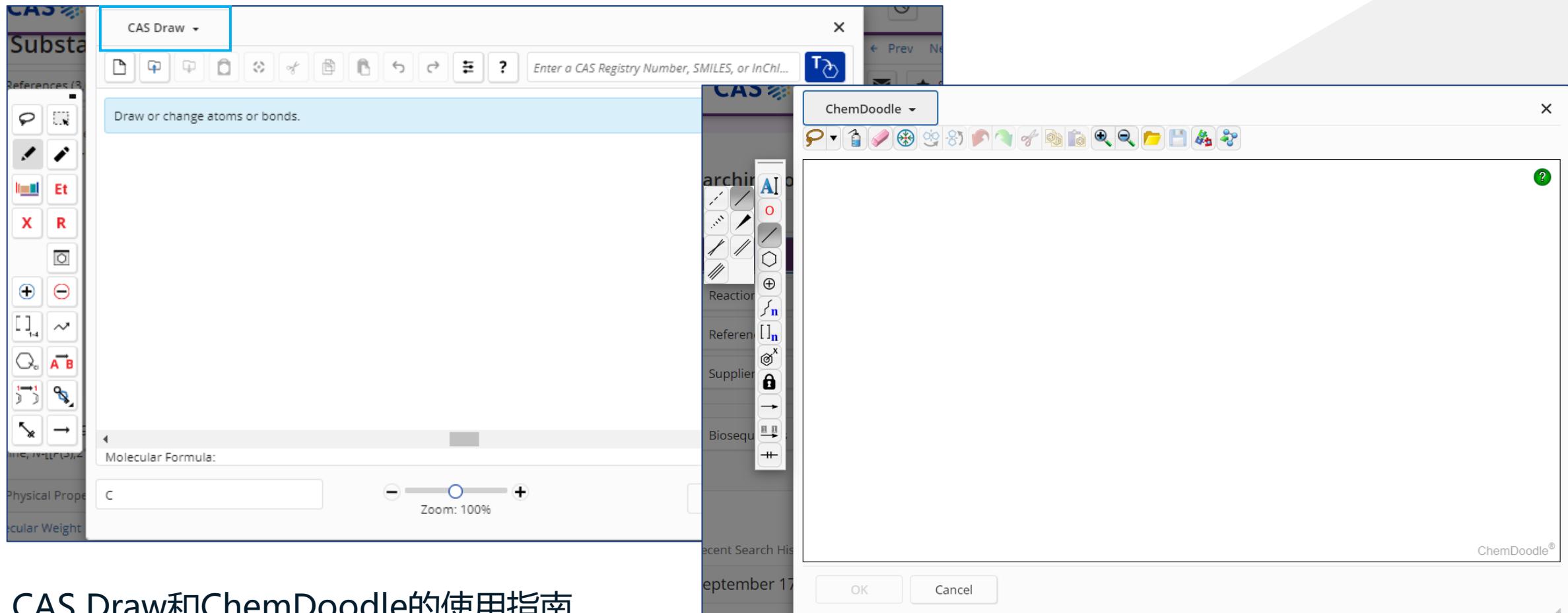
□ 重复片段工具

Q 取代位点可变

锁工具



# 物质检索--结构绘图板



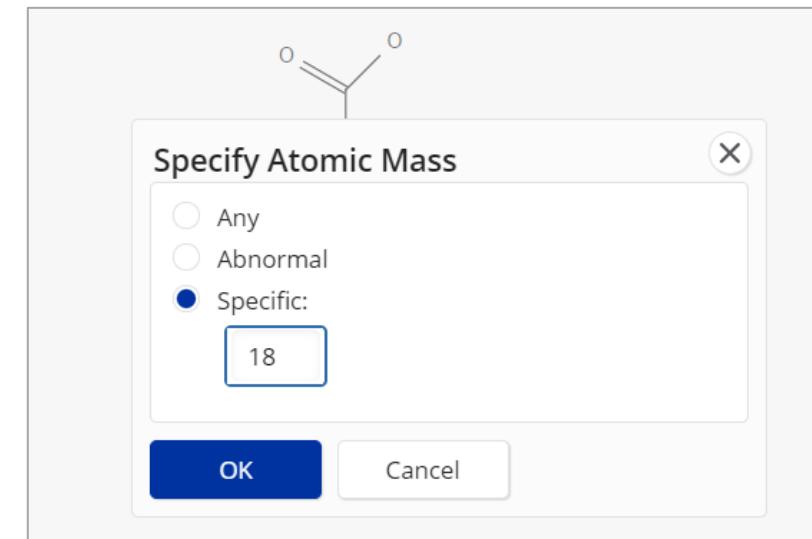
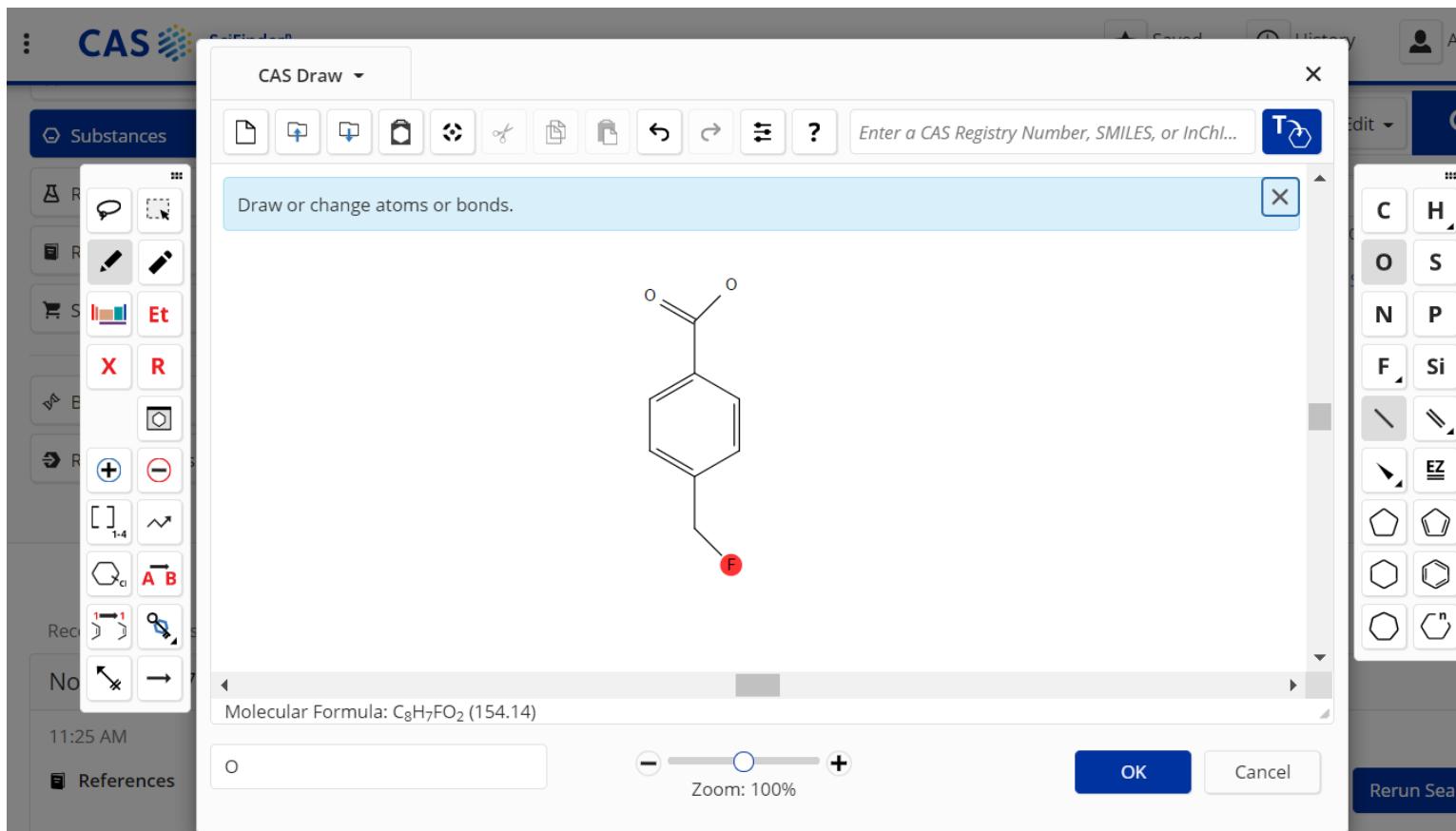
## CAS Draw和ChemDoodle的使用指南

[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>

# 结构绘图工具的使用--同位素原子的绘制



鼠标右键点击某原子，选中Abnormal  
获取其各种同位素的化合物，选择  
Specific可以精准输入具体的同位素

# 物质检索--结构检索

CAS RN: 50-78-2

The screenshot shows the CAS Draw software interface on the left and the Substances search results page on the right.

**CAS Draw Interface:**

- Toolbar: Includes icons for file operations (New, Open, Save, Print, Copy, Paste, Find, Undo, Redo), zoom controls, and a search bar.
- Search Bar: "Enter a CAS Registry Number, SMILES, or InChI..."
- Message Bar: "Click and drag to select objects. Ctrl-click to select or deselect individual objects."
- Chemical Structure Input: A drawing of 4,4-dimethyl-2-methoxyacetophenone (C=C(C)C(=O)c1ccccc1OC(=O)C).
- Molecular Formula: C<sub>9</sub>H<sub>10</sub>O<sub>4</sub> (180.16)
- Zoom Control: Zoom: 100%
- Buttons: OK and Cancel.

**Substances Search Results:**

- Search Bar: "Enter a query..."
- Search Options: AND, Molecular Formula, Add Advanced Search Field.
- Search Examples: C6H6 | (C8H8)x | C2H2
- Search Buttons: Edit, Search (blue button), Learn more about SciFinder.
- Result Preview: Shows the same chemical structure as the input.
- Action Buttons: Edit Drawing, Remove, Search Patent Markush.

**Text Overlay:**

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

# 物质检索--检索结果集排序

利用物质排序快速  
查找目标物质：  
相关度  
CAS RN  
分子式  
分子量  
文献量  
供应商数量

Structure Match

As Drawn (927) **Substructure (20K)** Similarity (79K) 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

Commercial Availability Available (121) Not Available (806)

Reaction Role Product (300) Reactant (11) Reagent (1) Catalyst (1) Solvent (1)

Reference Role Biological Study (577) Uses (431) Preparation (402) Therapeutic Use (393) Synthetic Preparation (340) View All

Stereochemistry Number of Components

Substances (927) Sort: Relevance View: Partial Save

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

Rank	CAS RN	Chemical Structure	Chemical Name	References	Reactions	Suppliers
1	50-78-2		C <sub>9</sub> H <sub>8</sub> O <sub>4</sub> Aspirin	84K	1,997	108
2	5054-56-8		C <sub>9</sub> H <sub>7</sub> O <sub>4</sub> Benzoic acid, 2-(acetyloxy)-, ion(+)	19	0	2
3	97781-16-3		C <sub>9</sub> H <sub>4</sub> D <sub>4</sub> O <sub>4</sub> Benzoic-2,3,4,5-d <sub>4</sub> acid, 6-(acetyloxy)-	8	5	24
4	921943-73-9		C <sub>9</sub> H <sub>5</sub> D <sub>3</sub> O <sub>4</sub> 2-(Acetyl-2,2-d <sub>3</sub> -oxy)benzoic acid	5	0	18
5	59096-15-0		C <sub>9</sub> H <sub>8</sub> O <sub>4</sub> Benzoic acid, 2-(acetyl-1- <sup>14</sup> C-oxy)-	5	1	1
6	59096-14-9		C <sub>9</sub> H <sub>8</sub> O <sub>4</sub> Benzoic-carboxy- <sup>14</sup> C acid, 2-(acetyloxy)-	5	0	3
7	215935-30-1		C <sub>9</sub> H <sub>7</sub> DO <sub>4</sub> 2-(Acetyl-2-d-oxy)benzoic acid	4	0	0
8	229030-56-2		C <sub>9</sub> H <sub>8</sub> O <sub>4</sub> Benzoic acid, 2-(acetyl-1- <sup>13</sup> C-oxy)-	3	0	1

# 物质检索--结构检索

结构检索类别:

As Drawn

亚结构

相似结构

结构精准度筛选

Chemscape分析

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.....

Structure Match

As Drawn (927)

**Substructure (20K)**

Similarity (79K)

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

Commercial Availability

Available (3,959)

Not Available (16K)

Reaction Role

Product (9,393)

Reactant (2,119)

Reagent (11)

Catalyst (20)

Solvent (3)

Reference Role

Preparation (13K)

Synthetic Preparation (10K)

Uses (7,065)

Biological Study (6,643)

Therapeutic Use (3,703)

View All

Stereochemistry

Number of Components

Substance Class

Isotopes

Metals

Molecular Weight

Substances (20,611)

Sort: Relevance View: Partial

References Reactions Suppliers

1 50-78-2 C<sub>9</sub>H<sub>8</sub>O<sub>4</sub> Aspirin 84K References 1,997 Reactions 108 Suppliers

2 5054-56-8 C<sub>9</sub>H<sub>7</sub>O<sub>4</sub> Benzoic acid, 2-(acetoxy)-, ion(1-) 19 References 0 Reactions 2 Suppliers

3 89655-56-1 (C<sub>9</sub>H<sub>8</sub>O<sub>4</sub>)<sub>x</sub> 2-Acetylsalicylic acid homopolymer 16 References 0 Reactions 0 Suppliers

4 97781-16-3 C<sub>9</sub>H<sub>4</sub>D<sub>4</sub>O<sub>4</sub> Benzoic-2,3,4,5-d<sub>4</sub> acid, 6-(acetoxy)- 8 References 5 Reactions 24 Suppliers

5 921943-73-9 C<sub>9</sub>H<sub>5</sub>D<sub>3</sub>O<sub>4</sub> 2-(Acetyl-2,2,2-d<sub>3</sub>-oxy)benzoic acid 5 References 0 Reactions 18 Suppliers

6 59096-15-0 C<sub>9</sub>H<sub>8</sub>O<sub>4</sub> Benzoic acid, 2-(acetyl-1-<sup>14</sup>C-oxy)- 5 References 1 Reaction 1 Supplier

7 59096-14-9 C<sub>9</sub>H<sub>8</sub>O<sub>4</sub> Benzoic-carboxy-<sup>14</sup>C acid, 2-(acetoxy)- 5 References 0 Reactions 3 Suppliers

8 215935-30-1 C<sub>9</sub>H<sub>7</sub>DO<sub>4</sub> 2-(Acetyl-2-d-oxy)benzoic acid 4 References 0 Reactions 0 Suppliers

9 229030-56-2 C<sub>9</sub>H<sub>8</sub>O<sub>4</sub> Benzoic acid, 2-(acetyl-1-<sup>13</sup>C-oxy)- 3 References 0 Reactions 1 Supplier

10 225243-55-0 C<sub>9</sub>H<sub>8</sub>O<sub>4</sub>

Filter by选择感兴趣的结果  
, 或Exclude排除不需要的结果



# 物质检索--结构检索

结构检索类别：

- As Drawn

可用可变基团X或R基团等可变工具定义，其他位点默认为原子锁定，环系默认为环锁定

- 亚结构

包括As Drawn检索结果，及被检索结构的修饰结构。位点默认为开放，环系未被环锁定

- 相似结构

获得片段或整体结构与被检索结构相似的结果，母体结构可以被取代，也可以被改变

注：如果关注相似结构检索结果，请不要绘制通式结构

# 物质检索--检索结果集筛选：Reaction Role

Substances (20)

Sort: Relevance View: Partial

Filtering: Reaction Role: Catalyst Clear All Filters

Rank	Chemical ID	Chemical Structure	Chemical Name	References	Reactions	Suppliers
1	50-78-2		C <sub>9</sub> H <sub>8</sub> O <sub>4</sub> Aspirin	84K References	1,997 Reactions	108 Suppliers
2	1803201-02-6		C <sub>19</sub> H <sub>20</sub> O <sub>4</sub> Benzeneacetic acid, 2-[(2-methylpropoxy)carbonyl]phenyl ester	1 Reference	1 Reaction	0 Suppliers
3	875584-96-6		C <sub>18</sub> H <sub>18</sub> O <sub>4</sub> 2-Methyl(propyl 2-(benzoyloxy)benzoate)	4 References	4 Reactions	2 Suppliers
4	2093113-55-2		C <sub>17</sub> H <sub>24</sub> O <sub>4</sub> Benzoic acid, 2-(2,2-dimethyl-1-oxopropoxy)-3-methyl-, 2-methylpropyl ester	2 References	2 Reactions	0 Suppliers
5	2093113-56-3		C <sub>19</sub> H <sub>20</sub> O <sub>4</sub> Benzoic acid, 2-(benzoyloxy)-3-methyl-, 2-methylpropyl ester	2 References	2 Reactions	0 Suppliers
6	2093113-57-4		C <sub>24</sub> H <sub>30</sub> O <sub>4</sub> Benzoic acid, 2-(benzoyloxy)-3,5-bis(1-methylethyl)-, 2-methylpropyl ester	2 References	3 Reactions	0 Suppliers
7	1416949-86-4		C <sub>18</sub> H <sub>30</sub> O <sub>10</sub> 1'-(1,4-Butanediylbis(oxyethylidene))bis[2-(acetoxy)benzoate]	1 Reference	2 Reactions	0 Suppliers
8	2093113-58-5		C <sub>26</sub> H <sub>34</sub> O <sub>4</sub> Benzoic acid, 2-(benzoyloxy)-3,5-bis(1,1-dimethylethyl)-, 2-methylpropyl ester	2 References	2 Reactions	0 Suppliers
9	948830-92-0		C <sub>20</sub> H <sub>22</sub> O <sub>5</sub> Si Methyl 1-(acetoxy)-3-hydroxy-7-methoxy-6-[2(trimethylsilyl)ethynyl]-2-naphtha...	1 Reference	12 Reactions	0 Suppliers

利用物质反应角色  
筛选物质

利用物质在反应中的角色精准定位相应的物质

# 物质检索--检索结果集筛选：Reference Role

Reference Role

By Count Alphanumeric

1 Selected

- Preparation (13K)
- Synthetic Preparation (10K)
- Uses (7,065)
- Biological Study (6,643)
- Therapeutic Use (3,703)
- Reactant or Reagent (3,377)
- Reactant (3,374)
- Biological Study, Unclassified (3,079)
- Properties (2,940)
- Prophetic Synthesis or Use (2,778)
- Pharmacological Activity (2,628)
- Technical or Engineered Material Use (2,184)
- Industrial Manufacture (1,589)
- Agricultural Use (1,151)
- Process (496)
- Physical, Engineering, or Chemical Process (452)
- Natural Product Occurrence (39)
- Analytical Matrix (36)

Apply Cancel

Structure Match

As Drawn (927) Substructure (20K) Similarity (79K) 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

Commercial Availability Available (13) Not Available (26)

Reaction Role Product (14) Reactant (7) Reagent (1) Catalyst (1) Solvent (1)

Reference Role Preparation (13K) Synthetic Preparation (10K) Uses (7,065) Biological Study (6,643) Therapeutic Use (3,703) Natural Product Occurrence (39)

View All

Substances (39) Sort: Relevance View: Partial

Filtering: Reference Role: Natural Product Occurrence... Clear All Filters

1 50-78-2 C<sub>9</sub>H<sub>8</sub>O<sub>4</sub> Aspirin 84K References 1,997 Reactions 108 Suppliers

2 1247764-46-0 C<sub>9</sub>H<sub>8</sub>O<sub>4</sub>.Unspecified Components: 2 Benzolic acid, 2-(acetoxy)-, mixt. with Tetrahop 1 Reference 0 Reactions 0 Suppliers

3 1247764-40-4 C<sub>9</sub>H<sub>8</sub>O<sub>4</sub>.Unspecified Components: 2 Benzolic acid, 2-(acetoxy)-, mixt. with redihop 1 Reference 0 Reactions 0 Suppliers

4 51-01-4 C<sub>11</sub>H<sub>10</sub>O<sub>6</sub> 2,4-Bis(acetoxy)benzoic acid 75 References 171 Reactions 9 Suppliers

5 756455-72-8 C<sub>23</sub>H<sub>36</sub>O<sub>4</sub> 2-[1-Oxohexadecyloxy]benzoic acid 8 References 4 Reactions 0 Suppliers

6 36081-01-3 C<sub>14</sub>H<sub>10</sub>O<sub>7</sub> 2,4-Dihydroxy-6-[(4-hydroxybenzoyl)oxy]benzoic acid 3 References 8 Reactions 1 Supplier

7 2724988-28-5 8 References 4 Reactions 0 Suppliers

8 55045-01-7 8 References 4 Reactions 0 Suppliers

9 1350977-80-8 8 References 4 Reactions 0 Suppliers

利用Reference Role (物质的研究方向) 精准定位相应的物质

# 物质检索--检索结果集筛选：结构

利用物质筛选工具  
快速锁定目标物质

The screenshot shows the CAS Draw interface. A search bar at the top right contains the text "Search Within Results". Below it is a "Draw" button and a "Search" button. The main workspace displays a chemical structure of naphthalene. A tooltip above the structure says: "Click a ring system to block it from further ring fusion. Click a chain to block it from ring formation." At the bottom left, a status bar shows "Molecular Formula: C<sub>10</sub>H<sub>8</sub> (116.16)". On the right, there is a zoom slider set to 100% and a "Search Within Results" panel. This panel includes a "Search" button and two radio button options: "As Drawn" (unchecked) and "Substructure" (checked). The "Search" button is highlighted in blue.

The screenshot shows the "Substances" search results page. The search term "Search Within Results: Drawn Structure" is visible. The results are displayed in a grid of 12 cards, each representing a different substance. The first card is for 218453-29-3, which is naphthalene. Subsequent cards show various naphthalene derivatives with additional substituents like methyl, ethyl, and propyl groups. Each card includes the substance's name, its chemical structure, and basic metadata such as "Reference", "Reactions", and "Suppliers".

Index	Substance ID	Chemical Name	Structure
1	218453-29-3	naphthalene	
2	218453-26-0	Ethyl 2-(2,2-dimethyl-1-oxopropoxy)-5-[(E)-5-(methylsulfonyl)-2-propyl]-1H-inden-1-ylidene...	
3	218453-25-9	Ethyl 2-(2,2-dimethyl-1-oxopropoxy)-5-[(Z)-5-(methylsulfonyl)-2-propyl]-1H-inden-1-ylidene...	
4	1962179-79-8	Benzoic acid, 2-(2,3-dihydro-1-oxo-1H-inden-2-yl)-3,6-bis(2,2-dimethyl-1-oxoprop...	
5	1168965-99-8	1H-Indene-2-carboxylic acid, 3-methyl-, 1-[[[[(E)-(2-amino-1-cyano-2-oxyethyl...	
6	1962178-79-5	Benzoic acid, 2-(2,3-dihydro-7-methoxy-1-oxo-1H-inden-2-yl)-3,6-bis(2,2-dimethyl...	
7	1962179-44-7	Benzaldehyde, 3,6-bis(2,2-dimethyl-1-oxopropoxy)-2-(7-methoxy-1-oxo-1H-inden-2-yl...	
8	1168964-47-3	2-Carboxyphenyl (6Z)-7-bromo-9-methyl-2-[(3-methyl-1H-inden-2-yl)carbonyl]oxy-...	
9	1168960-42-6	2-Chlorophenyl (6Z)-7-chloro-9-methyl-2-[(3-methyl-1H-inden-2-yl)carbonyl]oxy-...	
10	1169002-06-5		
11	1168974-14-8		
12	1499112-44-5		

# 物质检索—检索结果集可视化分析：ChemScape Analysis

Structure Match

- As Drawn (927)
- Substructure (20K)**
- Similarity (79K)
- 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

Commercial Availability

- Available (3,959)
- Not Available (16K)

Reaction Role

- Product (9,393)
- Reactant (2,119)
- Reagent (11)
- Catalyst (20)
- Solvent (3)

Reference Role

- Preparation (13K)
- Synthetic Preparation (10K)
- Uses (7,065)
- Biological Study (6,643)
- Therapeutic Use (3,703)

View All

Stereochemistry

Number of Components

Substances (20,611)

Sort: Relevance View: Partial

1 50-78-2 Aspirin C<sub>9</sub>H<sub>8</sub>O<sub>4</sub> 84K References 1,997 Reactions 108 Suppliers

2 5054-56-8 Benzoic acid, 2-(acetoxy)-, ion(1-) C<sub>9</sub>H<sub>7</sub>O<sub>4</sub> 19 References 0 Reactions 2 Suppliers

3 89655-56-1 (C<sub>9</sub>H<sub>8</sub>O<sub>4</sub>)<sub>x</sub> 2-Acetylsalicylic acid homopolymer C<sub>9</sub>H<sub>8</sub>O<sub>4</sub> 16 References 0 Reactions 0 Suppliers

4 97781-16-3 Benzoic-2,3,4,5-d<sub>4</sub> acid, 6-(acetoxy)- C<sub>9</sub>H<sub>4</sub>D<sub>4</sub>O<sub>4</sub> 8 References 5 Reactions 24 Suppliers

5 921943-73-9 2-(Acetyl-1,2,2-d<sub>3</sub>-oxy)benzoic acid C<sub>9</sub>H<sub>5</sub>D<sub>3</sub>O<sub>4</sub> 5 References 0 Reactions 18 Suppliers

6 59096-15-0 Benzoic acid, 2-(acetyl-1-<sup>14</sup>C-oxy)- C<sub>9</sub>H<sub>8</sub>O<sub>4</sub> 5 References 1 Reaction 1 Supplier

7 59096-14-9 Benzoic-carboxy-<sup>14</sup>C acid, 2-(acetoxy)- C<sub>9</sub>H<sub>8</sub>O<sub>4</sub> 5 References 0 Reactions 3 Suppliers

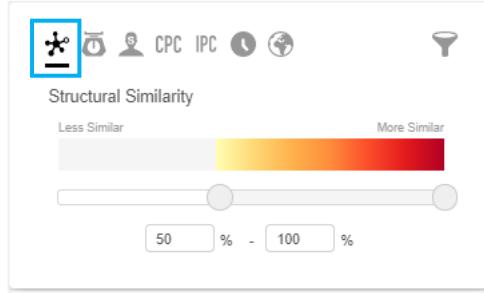
8 215935-30-1 2-(Acetyl-1-d-oxy)benzoic acid C<sub>9</sub>H<sub>7</sub>DO<sub>4</sub> 4 References 0 Reactions 0 Suppliers

9 229030-56-2 Benzoic acid, 2-(acetyl-1-<sup>13</sup>C-oxy)- C<sub>9</sub>H<sub>8</sub>O<sub>4</sub> 3 References 0 Reactions 1 Supplier



通过Chemscape  
Analysis了解物质的专利

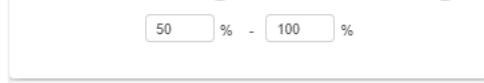
# 物质检索—检索结果集可视化分析：ChemScape Analysis



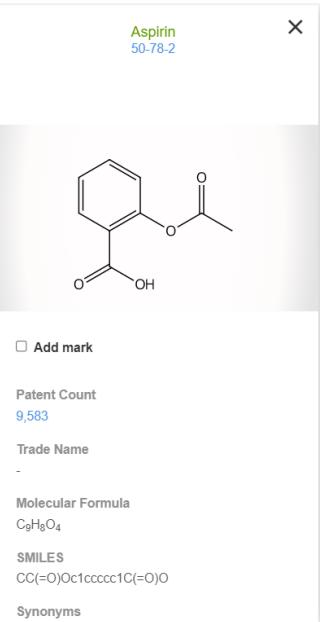
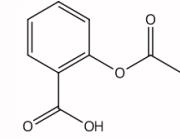
50 % - 100 %

Structural Similarity

More Similar



Aspirin  
50-78-2



Add mark

Patent Count  
9,583

Trade Name

Molecular Formula  
C<sub>9</sub>H<sub>8</sub>O<sub>4</sub>

SMILES  
CC(=O)Oc1ccccc1C(=O)O

Synonyms

分析结构相似度

# 物质检索--Structure Precision

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Substance Search Results for 3H-Indole

Structure Match

- As Drawn (524)
- Substructure (3.7M)
- Similarity (10K)

Structure Precision

- Conventional Results (504)
- Tautomers and Zwitterions (20)

Chemscape Analysis

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

Create Chemscape Analysis

Filter Behavior

Filter by

Exclude

- Commercial Availability
  - Available (3)
  - Not Available (17)
- Reaction Role
  - Product (1)
  - Reactant (1)
- Reference Role
  - Properties (15)
  - Formation, Non-preparative (7)
  - Formation, Unclassified (7)
  - Uses (7)
  - Reactant (4)
- View All
- Number of Components
- Substance Class
- Isotopes
- Metals

Sort: Relevance View: Partial

Substances (20)

Rank	Chemical ID	Chemical Structure	Chemical Name	Components	References	Reactions	Suppliers
1	271-26-1		C <sub>8</sub> H <sub>7</sub> N 3H-Indole	2	188	23	4
2	1001205-42-0		C <sub>8</sub> H <sub>6</sub> N 3H-Indol-2-yl	1	1	0	0
3	22493-45-4		C <sub>8</sub> H <sub>7</sub> .H Components: 2 Component RN: 271-26-1 3H-Indole, conjugate acid (1:1)	10	0	0	0
4	1426415-91-9		C <sub>8</sub> H <sub>7</sub> N.D Components: 2 Component RN: 271-26-1 3H-Indole, conjugate acid-d (1:1)	1	0	0	0
5	107715-56-0		C <sub>8</sub> H <sub>7</sub> N.BF <sub>4</sub> .H Components: 3 3H-Indole, tetrafluoroborate(1-)	1	0	0	0
6	111632-87-2		C <sub>8</sub> H <sub>7</sub> N.F <sub>6</sub> P.H Components: 3 Phosphate(1-), hexafluoro-, hydrogen, compd. with 3H-indole (1:1)	1	0	0	0
7	2609928-58-5		271-23-8	1	0	0	0
8	578731-99-4			1	0	0	0

Structure Precision  
筛选互变异构体/内盐



# 物质检索--检索结果集的保存及获得其他信息

获得商品信息

获得相关文献

获得相关反应

The screenshot shows the Chematico Substance search results page. At the top left, there's a sidebar for 'Structure Match' with options like 'As Drawn (524)', 'Substructure (3.7M)', and 'Similarity (10K)'. Below that are sections for 'Structure Precision' (checkboxes for 'Conventional Results (104)' and 'Tautomers and Zwitterions (20)'), 'Chemscape Analysis' (button 'Create Chemscape Analysis'), and 'Filter Behavior' (checkboxes for 'Commercial Availability' and 'Reaction Role'). The main area displays a grid of substance cards. Each card includes a chemical structure, the substance name, its components (e.g., C<sub>8</sub>H<sub>7</sub>N), and its conjugate acid form. Below each card are buttons for 'References' (188), 'Reactions' (23), and 'Suppliers' (4). The cards are numbered 1 through 10.

This dialog box allows users to save their search results. It includes fields for 'Name', 'Alerts' (checkboxes for 'No Alerts', 'As Available', 'Weekly', 'Monthly'), 'Tags (optional)', 'New Tag (optional)', and a color palette for tags. Buttons for 'Save' and 'Cancel' are at the bottom.

Save: 保存成结果集，并可同时设置定题提醒或添加标签（包括文献，物质，反应结果集）

This dialog box is for downloading substance results. It lets users choose a 'File Type' (PDF, RTF, or Excel), 'Select Quantity' (checkboxes for 'All Results', 'Selected Results', or 'Range (ex. 2 to 20)'), 'Display' (checkboxes for 'Result Summary' or 'Result Details'), 'File Name' (text input 'Substance\_20211117\_2357'), and 'Include' (checkboxes for 'Task History', 'Experimental Properties', 'Predicted Properties', 'Experimental Spectra', 'Predicted Spectra', 'Bioactivity Indicators', 'Regulatory Information'). A 'Download' button and a 'Learn more about downloads' link are at the bottom.

Download: 可生成 PDF、rtf、Excel 格式

# CAS Markush检索

(19) 中华人民共和国国家知识产权局

(12) 发明专利申请

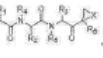


(10) 申请公布号 CN 104945470 A  
(43) 申请公布日 2015.09.30

(21) 申请号 201410122313.4  
(22) 申请日 2014.03.30  
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(74) 专利代理机构 杭州求是专利事务所有限公司 33200  
代理人 张法高 赵杭丽  
(51) Int. Cl.  
C07K 5/087(2006.01)  
C07K 5/083(2006.01)

权利要求书3页 说明书24页 附图4页

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



CN 104945470 A

## 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)哌啶-1-甲酸叔丁酯 (1c, 1d)

吡嗪-2-羧酸 (1.5g, 12mmol) 置于 50mL 反应瓶中，加入 35mL 无水  $CH_2Cl_2$  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，哌啶-1-甲酸叔丁酯 (1.9g, 10mmol) 加入反应液中，室温反应 3 小时。反应液加入 30mL 饱和碳酸氢钠水溶液稀释，分出有机层，饱和食盐

## 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



# CAS Markush检索

预测性物质[Prophetic Substance]:

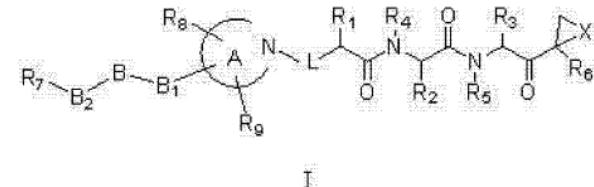
- 使用Markush结构陈述的预测物质，一个Markush可以陈述上百或上千个化学物质
- 被Markush结构包含，但未被实施或呈现在表格、权利要求书或说明书中的结构，不会被CAS分配CAS Registry Number
- Markush检索，能检索到通过结构检索检不到的专利

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：



I

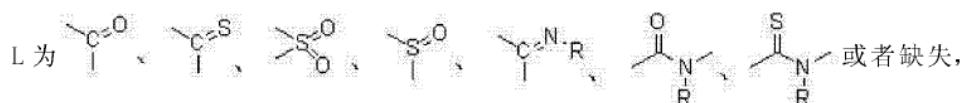
其中：

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> 硫基烷基、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；

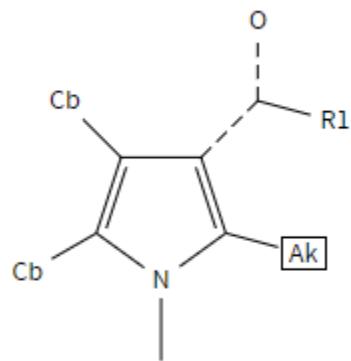


其中 R 选自 H、C<sub>1-6</sub> 烷基或卤代的 C<sub>1-6</sub> 烷基；

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> 硫基烷基, 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



Structure Match

- As Drawn (2)
- Substructure (300)
- Similarity (401)

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

## Substances (2)

Sort: Relevance ▾ View: Partial ▾

1 113859-96-4

C<sub>20</sub>H<sub>19</sub>NO  
1-(1,2-Dimethyl-4,5-diphenyl-1H-pyrrol-3-yl)ethanone

1 Reference 1 Reaction 1 Supplier

2 117712-13-7

C<sub>19</sub>H<sub>17</sub>NO<sub>2</sub>  
1,2-Dimethyl-4,5-diphenyl-1H-pyrrole-3-carboxylic acid

1 Reference 7 Reactions 1 Supplier

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

# CAS Markush检索

Screenshot of the CAS SciFinder® Patent Markush Match search interface. The search results page displays three patent documents (JP2000086713, EP732325, and WO2016184429) showing Markush structures with atom labels (e.g., Ak) and their corresponding patent claims.

**JP2000086713:** Radiation-curab [REDACTED] from them and method for formulating [REDACTED].  
By: Shiono, Teruo; Arishima, Shinji; Tanaka, Hiroaki  
Japan, JP2000086713 A 2000-03-28 | Language: Japanese, Database: CAplus  
Assignee: Toyo Ink Mfg. Co., Ltd.  
Patent claim 2:  
102: alkyl <containing 1-17 C>  
285: alkyl <containing 1-17 C>

**EP732325:** Process and catalysts for the preparation of 5- or 6-membered, nitrogen-containing heterocyclic aldehydes by the hydrogenation of the corresponding heterocyclic carboxylic acid or ester.  
By: Schnurr, Werner; Fischer, Rolf; Wulff-Doering, Joachim; Hesse, Michael; Goetz, Norbert; Maywald, Volker  
European Patent Organization, EP732325 A1 1996-09-18 | Language: German, Database: CAplus  
Assignee: BASF A.-G.  
Patent claim 1:  
569: alkyl <containing 1-8 C>  
573,574,576,577,579: subst. by alkyl

**WO2016184429:** Pyrazoline sensitizer and preparation method and use thereof  
By: Qian, Xiaochun  
World Intellectual Property Organization, WO2016184429 A1 2016-11-24 | Language: Chinese, Database: CAplus  
Assignees: Changzhou Tronly Advanced Electronic Materials Co., Ltd., Changzhou Tronly New Electronic Materials Co., Ltd.  
Patent claim 14:  
356: alkyl <containing 1-10 C>  
517: alkyl <containing 1-10 C>

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

# 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Structure Precision快速查找互变异构体/内盐
6. ChemScape Analysis帮助了解物质的专利布局
7. 利用CAS Markush检索尽可能全面的获得结构的公开信息

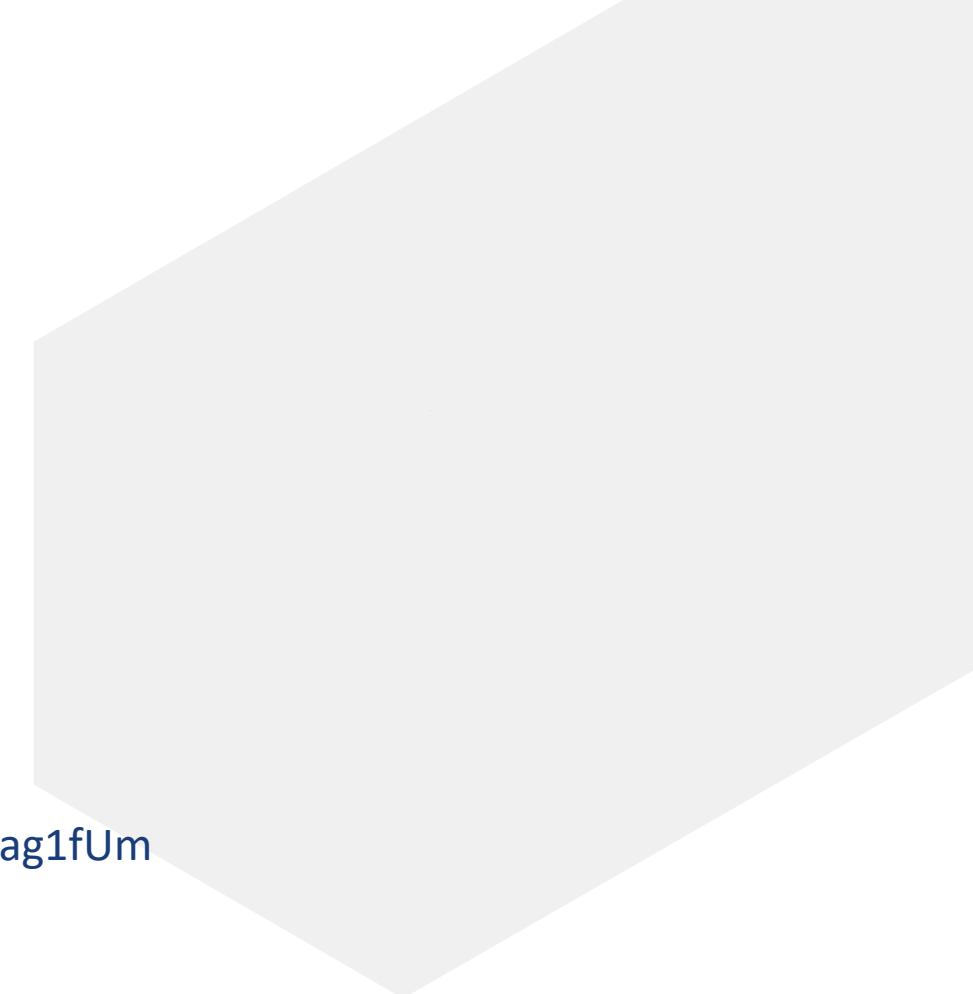
# 大纲

## — CAS SciFinder<sup>n</sup>中的生物序列检索

- 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)



# Biosequences Search™--Blast检索

The screenshot shows the CAS SciFinder Biosequences Search interface. On the left, a sidebar lists navigation options: All, Substances, Reactions, References, Suppliers, Biosequences (which is selected and highlighted in blue), and Retrosynthesis. The main search area is titled "Biosequences" and contains a search bar with placeholder text "Enter a query or upload a file...". Below the search bar are three tabs: BLAST (selected), CDR, and Motif. To the right of the search bar are buttons for "Upload Sequence" and "Clear Search". On the far right of the search area are search parameters: "Sequence Type" (Protein is selected), "Search Within" (Proteins is selected), and "Include NCBI Sequences" (checked). A dropdown menu "Limit Total Sequence Results to" is set to 1000, and a "Start Biosequence Search" button is at the bottom.

CAS SciFinder-n Help:

[https://scifinder-n.cas.org/help/#t=Searching\\_in\\_SciFinder-n%2FBiosequence\\_Search%2FBiosequence\\_Search.htm&rhsearch=biosequence&rhlterm=biosequence&rhsyns=%20](https://scifinder-n.cas.org/help/#t=Searching_in_SciFinder-n%2FBiosequence_Search%2FBiosequence_Search.htm&rhsearch=biosequence&rhlterm=biosequence&rhsyns=%20)

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



# 高级检索：设置相关参数

Searching for...

Biosequences

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

BLAST CDR Motif Upload Sequence Clear Search

AACAAACATATCAAATCCTACTGGTGGCACAACTTGA

Sequence Type: Nucleotide Protein

Search Within: Nucleotides Proteins  
 Include NCBI Sequences

Limit Total Sequence Results to: 1000

Start Biosequence Search

Advanced Biosequence Search ▾ Adjust Parameters for Short Sequences | Reset All

Alignment Identity % 80 Match with Gaps?  Yes  No Gap Costs Existence 5 Extension 2

Query Coverage % 90 Word Size 11 Reward for Match Penalty for Mismatch 2, -3

BLAST Algorithm BLASTn E-Value 10 Exclude Low Complexity Regions  Yes  No

Recent Search History November 17, 2021 9:11 AM

Biosequences Sequence Type: Nucleotide Search Within: Nucleotides NCBI Included: Yes BLAST Algorithm: BLASTn Alignment Identity: 80% Query Coverage: 90%

AACAAACATATCAAATCCTACTGGTGGCACAACTTGA

[View Results](#) [Edit Search](#) [Complete](#)

Query coverage = coverage/query  
Sequence identity= matches/coverage  
(Coverage = matches + mismatches)

# BLAST检索结果

## 序列结果排序

# 可视化地图 结果筛选

## 序列一致性详情

目标序列

## 披露序列的专利文献

The screenshot shows the Biosequences search results page. On the left, there are search details and a Bioscape Analysis section. The main area displays two sequence alignments between a Query (1) and a Subject (1). Each alignment has a purple box indicating the aligned region. Below each alignment is a detailed view with tabs for Alignment, Subject, and References. The first alignment's Subject view shows a sequence from position 393 to 431. The second alignment's Subject view shows a sequence from position 393 to 592. The top right corner shows summary statistics: Alignment Identity: 100%, E-Value: 1.0669e-11, Query Coverage: 90%, Subject Coverage: 592 nt, Matches: 39, and Mismatches: 0.

BLAST Search Details

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

Bioscape Analysis

Visually explore sequence similarity with a new tool.  
Learn more about Bioscape.

Create Bioscape Analysis

Filter by

^ E-Value

0 to  $10^6$

^ Query Coverage %

0 to 100

^ Identity %

0 to 100

文献

Sort: Alignment Identity ▾ View: Collapse

Sort: Alignment Identity ▾

Alignment Identity  
E-Value  
Query Coverage  
Subject Coverage

Alignment Data

BLAST Score: 78  
E-Value: 1.0669e-11

Q 1 AACACAAACA TATCAAATCC TACTGGTGGC ACAACTTGA 39  
S 393 AACACAAACA TATCAAATCC TACTGGTGGC ACAACTTGA 431

Alignment Identity: 100%

Query 1 39

Subject 1 595

View Less ▾

Alignment Subject References

Alignment Data

BLAST Score: 78  
E-Value: 1.0669e-11

Q 1 AACACAAACA TATCAAATCC TACTGGTGGC ACAACTTGA 39  
S 393 AACACAAACA TATCAAATCC TACTGGTGGC ACAACTTGA 431

Alignment Identity: 100%

Query 1 39

Subject 1 592

View Less ▾

Alignment Subject References

CAS Registry Number: -  
NCBI Identifier: EU973880.1  
Length: 592 nt

Sequence

1 ACACACAAACA CCAGTCACCA GCTCATCACCA TCCATCTCAT TCTTACTACTG CCTCAGAGAC CAAGCTGTG CAACCGGAGA  
81 AGGAGATCTA CTCTACTCTT CAGAGCATCG TGCTATTGGGA CATGGAAACC GTCTGGGGAG ACCTCATGGC GACCGAGCTG  
161 AGGCTTGCCG TGCCCCGGCAC CGTGGACGAC TGCAAGCCAGC ACCAGCAAGCA GACCCAGCTG AAGGGTGGCG CGCCGCCGTC  
241 CAAACCTACT AGGGGCAAGA AGGGCCCCCG CGGTGCTGCA CTACAGGTGC TGCTCCCGG CTACCTCTC CTGCTCGTC  
321 CAGGCTCTT CCTCTACTCG TTCTAGACCC TCTCTCTGCT TGTGGCAAGA GTGAGATTC ATATGCTGTG CTGCTCTGCA

## 导出Excel格式 的序列检索结果

Zea mays clone 423468 hypothetical protein mRNA, complete cds

GenBank: EU973880.1

[FASTA](#) [Graphics](#)

Go to: ▾  
LOCUS EU973880 592 bp mRNA linear PLN 10-DEC-2008  
DEFINITION Zea mays clone 423468 hypothetical protein mRNA, complete cds.

ACCESSION EU973880  
VERSION EU973880.1  
KEYWORDS FLI\_CDNA.  
SOURCE Zea mays  
ORGANISM Zea mays  
Eukaryota; Viridiplantae; Streptophyta; Embryophyta; Tracheophyta;  
Spermatophyta; Magnoliopsida; Liliopsida; Poales; Poaceae; PACMAD  
clade; Panicoideae; Andropogonodae; Andropogoneae; Tripsacinae;

**REFERENCE** Zea.  
**AUTHORS** 1 (bases 1 to 592)  
 Alexandrov,N.N., Brover,V.V., Freidin,S., Trouhan,M.E.,  
 Tatarinova,T.V., Zhang,H., Swaller,T.J., Lu,Y.P., Bouck,J.,  
 Flavell,R.B. and Feldmann,K.A.  
**TITLE** Insights into corn genes derived from large-scale cDNA sequencing  
**JOURNAL** Plant Mol. Biol. 69 (1-2), 179-194 (2009)

PUBMED [18937034](#)  
REFERENCE 2 (bases 1 to 592)  
AUTHORS Alexandrov,N.N., Brover,V.V., Freidin,S., Troukhan,M.E., Tikhonova,T.Ya., Zhuravlev,S.I., Tikhonov,Y.P., Pashkov,I.

Tatarinova,T.V., Zhang,J., Swaller,T.J., Lu,Y.-F., Bouck,J., Flavell,R.B. and Feldmann,K.A.  
TITLE Direct Submission  
JOURNAL Submitted (04-AUG-2008) Ceres, Inc., 1535 Rancho Conejo Blvd.,

FEATURES      Thousand Oaks, CA 91320, USA  
                  Location/Qualifiers

```
source          1..592
/organism="Zea mays"
/mol_type="mRNA"
/db_xref="taxon:4577"
/clone="423468"
/label="Zea mays ssp. mays L."
```

```
CDS          122..346
/codon_start=1
/product="hypothetical protein"
/protein_id="ACG45998_1"
/transl_table="11"
//translation="METVVGDLMATETRLGLPLGTWDDCSQHQQQTQLKVAAPPSNPTR
GKKRPAGAAI TVL IAGY LLI VPFELSPSSSE"
```

# BLAST检索结果

6 Alignment Identity: 100%

Query (1) [1] 39 Subject (1) [1] 1,060 Matches: 39 Mismatches: 0

View Less ▾

Alignment Subject References

CAS Registry Number: 785872-37-9  
Length: 1,060 nt

Sequence

```
1 CATTGGGTAC CTCGAGGCCG GCCGGGAGCT CGCACTCACT CACTCACAAG TCACACAGCC ACACTTGAAC CGCTGCCGC
 81 AGCGGAGGGA GCTTGACCGG GCCAACGCAC ACATAACACA AGCTCGTGT CGATGGCGCG GTGGGCTCGG GTGCTGGCG
 161 TGGCGCGGC CACGGCCATC GCGTGGCGT CGTGGCGGG CGGGACATG AACGGGACA AGACGGAGTG CGCGGACAG
 241 CTGGTGGGCC TGGCGCGTGT CCTGCAGTAC GTGCAAGGGC AGGGCCGCGC GCCGCGGCC GACTGCTCGG GCGGCCGCG
 321 CCAGGTGCTG GGGAAAGAGCC CAAAGTGCCT GTGCGTGTCT GTCAGGACA AGGACGACCC CAACCTGGC ATCAAGATCA
 401 ACGCCACCT CGCGCTCGG CTCCCGAAC CCTCGGGCGC CACCGCGCC AACGCTCTCC ACTGCGCTCA GCTCCTGCTA
 481 ATTCCCCCG GCTCCAAAGA CGCCGCCGTC TTCAGTCCC GCAGCGACAA GGGCTCCACT GCCGCTCCAG CCAAGGACAA
 561 CTCGACGGCG ACGACCGACT CCCGCGCGT GCAGGGACCC ACCGGACCG GCGTGTCTC CTCGGCGGCC ACCGGCGGTG
 641 CTGCACTCAC GGTGCTGCTC GCGGCTTAC TCCCTCTGCT CGTGCAGAG CTGCGCTTA GCTCGTTCA GACCCCTGTG
 721 CAAGTTGTCG CACCAAGTAGG ATTGATATG TTGTTGTTCT TTCTAGTACG TGACGTGACA GACAATTTCG TGCTGGTGTG
```

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

### Other Names and Identifiers

1 Other Name for 1999: PN: US200

Sequence Details

Sequence: DNA; linear
1 cattgggtac ctcgaggccg gccgggagct cgcaactcaact cactcacaag
51 tcacacagcc acatctaaca acgtcggtgt cgatggcgcg gtgggtcg
101 gccaacgcac acataacaca agctcggtgt cgatggcgcg gtgggtcg
151 gtgctggcgcc tggccgcgc acggccatc gccgtggcggt ccgtggcg
201 cggccatcg aacgcggaca agacggatg cgccggaccat ctggggcc
251 tgccgcgtg ctcgtgtac gtgcagggtc agggccggcc gcccgcggcc
301 gactgtcgcc gcgccgtcg ccagggtgt ggaaagagcc ccaagtgcct
351 gtgcgtgtcg tcgtacggaca aggacgaccc caacctggc atcaagatca
401 acggccacctt cgcgtcgcc ctccccaaacg cctggccgc accccgc
451 aacgtctccc actcgctca gtccttgcgt attccccgg gctccaaaga
501 cgcgcgcgtc ttcaatcccg gcacgtacaa gggctccact gccgcgtcc
551 ccaaggacaa ctcgtacggcg acgacggact cccgcgcgtc gcaggccacc
601 accggacgcgc gctgtgtcc tcgtacggcg accggccgtg ctgcactac

Patent Annotations

Source: Zea mays  
Reference: US20040214272, SEQID 16999: claimed

Feature	Location	Description
misc_feature		Clone ID: MRT4577_11549C.1

# BioScape Analysis

BioScape Analysis: 依据相似性可视化序列，获得相应专利布局信息



# 序列详情及相关的专利文献结果

Filter Behavior

Filter by Exclude

Document Type

Patent (47)

Language

English (47)

Publication Year

No Min to No Max Apply View Larger

Author

Organization

Publication Name

Concept

CA Section

Database

Search Within Results

PatentPak Full Text Substances (0) Reactions (0) Citing (0) Sort: Relevance View: Partial Abstract

References (47)

1

Protein-coding nucleic acid mols. from soybean, and use for plant transformation and modifying protein expression levels in plants

By: La Rosa, Thomas J.; Zhou, Yihua; Kovalic, David K.; Cao, Yongwei; Cheikh, Nor United States, US20130326723 A1 2013-12-05 | Language: English, Database: C

The present invention provides 285,684 nucleic acid (cDNA) and protein sequences transforming plants such as soy, corn, cotton, wheat, with the nucleic acids in order thereby improving plant traits.

PatentPak Full Text Substances (0) Reactions (0) Citing (0) Sort: Relevance View: Partial Abstract

2

Nucleic acid molecules and other molecules associated with improvement

By: Liu, Jingdong; Zhou, Yihua; Kovalic, David K.; Screen, Steven E.; Tabaska, Jack Michael D.; Fincher, Karen L.; Hammond-Kosack, Kim; et al United States, US20110277178 A1 2011-11-10 | Language: English, Database: C

Polynucleotides useful for improvement of plants are provided. In particular, 34 sources. Polypeptides encoded by the polynucleotide sequences are also provided. A hierarchical classification tool, termed FunCAT, for Functional Categories Annotation of polypeptides find use in production of transgenic plants to produce plants having

PatentPak Full Text Substances (0) Reactions (0) Citing (0) Sort: Relevance View: Partial Abstract

## Substance Detail

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

CAS Registry Number  
661510-85-6

Image Not Available

### Unspecified

DNA (corn clone LIB3957-004-F11\_FLI protein fragment-specifying cDNA) (90%)

Nucleic Acid Sequence

Sequence Length: 929

154 a, 310 c, 281 g, 184 t

### Other Names and Identifiers

1 Other Name for this Substance

1627: PN: US20040034888 SEQID: 25627 claimed DNA

Sequence: DNA; linear

1	cacaagtac	acagccacac	ttgaaccgca	ggccgcacgc	gaggagacctt
51	gcacgggcca	acgcacacat	aacacaagct	cgtcgctgat	ggcgccgtgg
101	gctgcgggtgc	tggcgctggc	cgcggccacg	gccatcccg	tggcgtcgt
151	ggcgcggccgc	gacatcaacg	cggacaagac	ggagtgcgcg	gaccagctgg
201	tgggcttgc	gccgtgcctg	cagtaactgc	aggggcaggc	ccgcgcggcc
251	ccggcccact	gctgcggccg	cctgcgcctag	gtgctggggaa	agagccccaa
301	gtgcctctgc	gtgcgtgtca	aggacaaggaa	cgaccccaac	ctgggcataca
351	agatcaacgc	caccctcgcc	ctcgcgtctcc	ccaaacgcctc	ggcgccacc
401	cgcgccaacg	tctcccactg	cgctcagctc	ctgcataattc	ccccggctc
451	caaagacgcc	ggccgtttca	gtccggcag	cgacaaggcc	tccactggcc
501	ctccagccaa	ggacaactcg	acggcgcacg	ccgactcccg	cgcgctgcag
551	gcgaccaccg	gacgcggcgt	gtccctctcg	gcggcgaccg	ccgggtcgtc
601	actcacggtg	ctgctcgccg	gctacacct	cctgcgtctg	ccagagctgt

### Patent Annotations

Source: Zea mays  
Reference: US20040034888, SEQID 25627; claimed

Feature	Location	Description
misc_feature		Clone ID: LIB3957-004-F11_FLI

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# Biosequences Search™--CDR检索

Searching for...

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

**Biosequences**

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

BLAST CDR Motif

Upload Sequence Clear Search

Include NCBI Sequences

Limit Total Sequence Results to:

10000

Start Biosequence Search

CDR1	VFPLAPSSKS	X
CDR2	TSGGTAAALGC	X
CDR3	LVKDYFPEPV	X

CAS SciFinder-n Help:

[https://scifinder-n.cas.org/help/#t=Searching\\_in\\_SciFinder-n%2FBiosequence\\_Search%2FBiosequence\\_Search\\_-\\_CDR.htm&rhsearch=CDR&rhhterm=CDR&rhsyns=%20](https://scifinder-n.cas.org/help/#t=Searching_in_SciFinder-n%2FBiosequence_Search%2FBiosequence_Search_-_CDR.htm&rhsearch=CDR&rhhterm=CDR&rhsyns=%20)

# CDR检索结果

下载Excel格式文件

- 左侧呈现匹配到query中某一个或者多个CDR区的subject序列的数量。
- 点击圈内的数字，再点Apply即可查看匹配的序列结果。
- 点Reset segments，可重新选择查看匹配的序列结果。

biosequences (10,000)

Sort: Alignment Identity ▾ View: Collapsed ▾

CDR Segments

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

CDR1      CDR2      CDR3

8,048  
31      94  
1,820

Apply      Reset Segments

Bioscape Analysis

Visually explore sequence similarity with a new tool. Learn more about Bioscape.

Create Bioscape Analysis

Filter by

^ E-Value  
0 to  $10^{-6}$

^ Query Coverage %  
0 to 100

^ Subject Coverage %  
0 to 100

^ Alignment Identity %  
0 to 100

1

Alignment Identity: 100%

Subject 1      466

Matches: 10      Mismatches: 0

CDR3      1 10

View Less ▾

Alignment      Subject      References

References

Alignment Data  
BLAST Score: 79  
E-Value: 0.00262316

CDR3      1 LVKDYFPEPV 10  
S      167 LVKDYFPEPV 176

2

Alignment Identity: 100%

Subject 1      440

Matches: 10      Mismatches: 0

CDR3      1 10

View More ▾

获取CAS SciFinder-n 中披露该序列的文献

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

Query Coverage % = coverage/query

Subject Coverage % = coverage/subject

Alignment Identity % = matches/query

# CDR检索结果

查看query中三个CDR区都被包含的8048个序列结果

Biosequences (8,048)

Sort: Alignment Identity ▾ View: Collapsed ▾

Query Details View Less

> CDR1  
VFPLAPSSKS

> CDR2  
TSGGTAALGC

> CDR3  
LVKDYFPEPV

1 Alignment Identity: 100%

Subject (1) 816

Matches: 30 Mismatches: 0

View Less ▾

Alignment Subject References

C-terminally fused TNF family ligand trimer-containing antigen binding molecules  
Assignee: F. HOFFMANN-LA ROCHE AG  
EP3243836 A1 | Seq ID No: 158

C-terminally fused TNF family ligand trimer-containing antigen binding molecules  
Assignees: F. HOFFMANN-LA ROCHE AG; HOFFMANN-LA ROCHE INC.  
WO2017194438 A1 | Seq ID No: 158

含有C端融合的TNF家族配体三聚体的抗原结合分子  
Assignee: 豪夫迈罗氏有限公司  
CN109311973 A | Seq ID No: 158

CDR Segments

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

CDR1 CDR2 CDR3

8,048

Apply Reset Segments

Bioscape Analysis

Visually explore sequence similarity with a new tool.  
Learn more about Bioscape.

Create Bioscape Analysis

Filter by

^ E-Value 0 to  $10^6$

^ Query Coverage % 0 to 100

^ Subject Coverage % 0 to 100

^ Alignment Identity % 0 to 100

# Biosequences Search™--Motif检索

Searching for...

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

## Biosequences

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

BLAST CDR Motif Clear Search

[SG]x{4}GK[DT]

[ ] 或  
{} 重复次数

Advanced Biosequence Search ▾

Query Coverage % ? E-Value ?

90 10

Reset All

Sequence Type:

Nucleotide  Protein

Include NCBI Sequences

Limit Total Sequence Results to:

1000

Start Biosequence Search

CAS SciFinder-n Help:

[https://scifinder-n.cas.org/help/#t=Searching\\_in\\_SciFinder-n%2FBiosequence\\_Search%2FBiosequence\\_Search\\_-\\_Motif.htm&rhsearch=motif&rhhterm=motif&rhsyns=%20](https://scifinder-n.cas.org/help/#t=Searching_in_SciFinder-n%2FBiosequence_Search%2FBiosequence_Search_-_Motif.htm&rhsearch=motif&rhhterm=motif&rhsyns=%20)

# Motif检索结果

**Biosequences (1,000)**

Sort: Alignment Identity ▾ View: Collapsed ▾

References 

Query Details View More

> Seq 1: 1 SXXXXGKD 8

1 Alignment Identity: 100%

Query 1 8 Matches: 8 Mismatches: 0

Subject 1 220

View Less ▾

Alignment Subject 

CAS Registry Number: -  
NCBI Identifier: A0A117ZK68   
Length: 220 aa

Sequence

```
1 MLLRLFLLFI IATKPVQASG FSERSTTVVG CSEMLVRLFL LFIIATKPAQ AGGFSEVSGL RFVGEEAQKR MKPYGGYGLIK
 81 VDDQYGM TTL EEVAKPIPQK PQLTVDEQNR AETQNRALVD IIVKFYQLRD GYLAQHGAGD FIQLTSKYGF IYDSGKVKNL
 161 NELTLTKTQT QVTQLDTPRS SSGIADHLRR SFLIRAKKKS NRKNKEGTSX XXXGKDGAN
```

2 Alignment Identity: 100%

Motif Search Details

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

Bioscape Analysis

Visually explore sequence similarity with a new tool.  
Learn more about Bioscape.

Create Bioscape Analysis

Filter by

^ E-Value  
0 to  $10^6$

^ Query Coverage %  
0 to 100

^ Subject Coverage %  
0 to 100

^ Alignment Identity %  
0 to 100

# 大纲

## — CAS SciFinder<sup>n</sup>中的反应检索

- 检索反应的常用方法
- 反应结果集的排序与筛选
- Synthetic Methods<sup>TM</sup>的使用
- 关键词与反应式的联合检索

视频链接：

<https://american-chemical-society.zoom.us/rec/share/eheXjH8iLM3q7tT2flBtPm-c-IMCDEF8qCgXmSngeTk7DtcuIPYx1IZZn83BYc.cAuZdpJTknUmPvaK?startTim=1647338414000>

# 反应检索

- 反应检索方法
  - 结构式
  - 关键词
  - 物质名称、登记号
  - 文献标识符：专利号、收录号、DOI
- 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

Searching for...

- All
- Substances
- Reactions
- References
- Suppliers

Reactions

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

Qinghaosu

X Draw 

通过物质标识符、文献标识符进行检索

# 反应检索--标识符

Filter Behavior

Substance Role

- Product (2,482)
- Reactant (455)
- Reagent (12)
- Catalyst (2)
- Solvent (1)

Yield

- 90-100% (61)
- 80-89% (50)
- 70-79% (45)
- 50-69% (128)
- 30-49% (74)

[View All](#)

Number of Steps

- 1 (654)
- 2 (124)
- 3 (169)
- 4 (241)
- 5 (310)

[View All](#)

Non-Participating Functional Groups

- Ether (420)
- Acetal (369)
- Cyclic ester (137)
- Alkene (35)
- Cyclic alkene (22)

[View All](#)

Experimental Protocols

- Synthetic Methods (150)
- Experimental Procedure (1,849)

Reaction Type

Stereochemistry

Reagent

Catalyst

**Reactions (2,949)**

Group: By Scheme ▾ View: Expanded ▾

References ▾

Scheme 1 (55 Reactions) Steps: 1 Yield: 100%

Absolute stereochemistry shown 

Reaction Summary Steps: 1 Yield: 100% Method for preparing dihydroartemisinin bulk antimalarial drug by single process

1.1 Reagents: Sodium borohydride  
Catalysts: Benzyltriethylammonium chloride  
Solvents: Water; -10 °C; < 0 °C; 5 h, < 0 °C  
1.2 Reagents: Acetic acid  
Solvents: Water; pH 7, 0 - 5 °C

By: Peng, Xuedong; et al  
World Intellectual Property Organization, WO2020238294 A1  
2020-12-03

[View Reaction Detail](#)

Reaction Summary Steps: 1 Yield: 100% Synthesis of novel artemisinin dimers with polyamine linkers and evaluation of their potential as anticancer agents

1.1 Reagents: Sodium borohydride  
Solvents: Methanol; 3 h, 0 °C

By: Magoulas, George E.; et al  
Bioorganic & Medicinal Chemistry (2017), 25(14), 3756-3767

[View Reaction Detail](#)

Reaction Summary Steps: 1 Yield: 100% An efficient synthesis of deoxoqinghaosu from dihydroqinghaosu

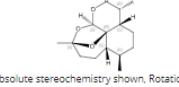
1.1 Reagents: Sodium borohydride

By: Rong, Ya Jing; et al  
Chinese Chemical Letters (1993), 4(10), 859-60

[View Reaction Detail](#)

[View All Reaction Summaries](#)

Scheme 2 (13 Reactions) Steps: 1 Yield: 94-100%

Absolute stereochemistry shown 

Absolute stereochemistry shown, Rotation (-)

一步由物质标识符或文献标识符获得反应信息



# 反应检索

通过结构式进行检索

Searching for...

- All
- Substances
- Reactions**
- References
- Suppliers

## Reactions

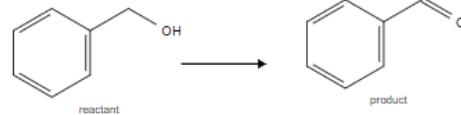
Search by Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. Learn More

Enter a query...

Draw 

CAS Draw

Drag the reaction arrow to specify reaction direction.



Molecular Formula: C<sub>7</sub>H<sub>8</sub>O (108.14), C<sub>7</sub>H<sub>6</sub>O (106.12)

OK Cancel

# 反应检索--结果集排序

Structure Match

As Drawn (7,236) **By Scheme** **By Document**

Substructure (4.3M)

Similarity (222K)

Filter Behavior

Filter by Exclude

Yield

90-100% (2,047)  
80-89% (670)  
70-79% (396)  
50-69% (549)  
30-49% (356)

View All

Number of Steps

1 (7,120)  
2 (91)  
3 (25)

Non-Participating Functional Groups

Ether (28)  
Halide (26)  
Alcohol (23)  
Acyclic ketone (20)  
Ketone (20)

View All

Experimental Protocols

Synthetic Methods (2,865)  
Experimental Procedure (1,141)

Reaction Type

Stereochemistry

Reagent

Catalyst

Solvent

Commercial Availability

## Reactions (7,236)

Group: By Scheme View: Expanded

Scheme 1 (5,685 Reactions)

By Scheme By Document

Supplier (131) Supplier (62)

Reaction Summary Steps: 1 Yield: 100%

1.1 Reagents: Potassium\_peroxymonosulfate sulfate (2KHSO<sub>5</sub>) Catalysts: Tetraethylammonium bromide, (OC<sub>2</sub>H<sub>5</sub>)<sub>4</sub>NBr; Tris[2-(4,5-dihydro-2-oxazolyl-*k*N)phenolato-*k*O] manganese Solvents: Dichloromethane, Water; 2 min, rt

By: Bagherzadeh, Mojtaba Tetrahedron Letters (2003), 44(50), 8943-8945

Full Text

View Reaction Detail

Reaction Summary Steps: 1 Yield: 100%

1.1 Reagents: Oxygen Catalysts: Tetrakis[*μ*-(acetato-*k*O<sub>2</sub>)bis(pyridine)]copper Solvents: Carbon dioxide; 1.5 bar, rt; 1.5 bar → 151.5 bar, rt → 80 °C; 12 h; 151.5 bar, 80 °C

By: Herbert, Matthew; et al Dalton Transactions (2010), 39(3), 900-907

Full Text

View Reaction Detail

Reaction Summary Steps: 1 Yield: 100%

1.1 Reagents: Cesium carbonate, Oxygen Catalysts: [T4b][2-[2-[5,7-Bis(1,1-dimethylethyl)-2-benzoxazolyl-*k*N]phenyl]amino-*k*N]-4,6...

Solvents: Toluene; 4 h, 333 K

By: Balaghi, S. Esmael; et al Dalton Transactions (2013), 42(19), 6829-6839

Full Text

View Reaction Detail | Experimental Protocols

View All Reaction Summaries

Collapse Scheme ▾

Scheme 2 (6 Reactions) Steps: 1 Yield: 100%

Supplier (131) Supplier (62)

Chemical reaction scheme showing the oxidation of benzyl alcohol to benzaldehyde.

反应排序：  
按类型排序  
按文献排序

Structure Match

As Drawn (7,236) **By Document** View: Expanded

Substructure (4.3M)

Similarity (222K)

Filter Behavior

Filter by Exclude

Yield

90-100% (2,047)  
80-89% (670)  
70-79% (396)  
50-69% (549)  
30-49% (356)

View All

Number of Steps

1 (7,120)  
2 (91)  
3 (25)

Non-Participating Functional Groups

## Reactions (7,236)

Group: By Document View: Expanded

1

Atomically dispersed Feδ<sup>+</sup> anchored on nitrogen-rich carbon for enhancing benzyl alcohol oxidation through Mott-Schottky effect

By: Wei, Qinhong; Wang, Jia Shi; Shen, Wen Zhong Applied Catalysis, B: Environmental (2021), 292, 120195 | Language: English, Database: Cplus

Full Text View 3 Related Reactions

Supplier (131) Supplier (62)

Reaction Summary Steps: 1 Yield: 100%

1.1 Catalysts: Iron, Carbon Solvents: Water; 24 h, 1 MPa, 800 °C

View Reaction Detail

Chemical reaction scheme showing the oxidation of benzyl alcohol to benzaldehyde using atomically dispersed Feδ<sup>+</sup> anchored on nitrogen-rich carbon.

按文献分类：来自同一篇文献的反应收在一条记录里

# 反应检索--结果集筛选

精确反应检索

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

商业来源……

文献筛选类别：

文献类型、语言

出版年份、刊物名

The screenshot shows the Reaxys search interface. On the left, there is a sidebar with filtering options under 'Structure Match' (As Drawn, Substructure, Similarity), 'Filter Behavior' (Filter by, Exclude), and various reaction parameters like Yield, Number of Steps, Non-Participating Functional Groups, etc. Below this is a 'Source Reference' section and a 'Filter Content Report'. The main area displays 'Reactions (7,236)' grouped by Scheme. Scheme 1 (5,685 Reactions) shows a reaction from phenol to benzaldehyde. Scheme 2 (6 Reactions) shows a reaction involving cesium carbonate and oxygen. At the bottom, there are buttons for 'View All Reaction Summaries' and 'Collapse Scheme'.

折叠菜单显示：

相同反应类型的反应放在一个菜单里，方便阅读和筛选

# 反应检索--结果集筛选：不参与反应官能团

Structure Match  
As Drawn (7,236)

**Substructure (4.3M)**

Similarity (222K)

Filter Behavior  
**Filter by** Exclude

Yield

Number of Steps

Non-Participating Functional Groups

- Amide (718K)
- Halide (639K)
- Ether (540K)
- Phenyl halide (419K)
- Alkene (399K)
- Aldehyde (9,333)**

[View All](#)

Experimental Protocols

Synthetic Methods (2,610)

Experimental Procedure (2,532)

Reaction Type

Stereochemistry

Reagent

Catalyst

Solvent

Commercial Availability

Reaction Notes

Search Within Results

Source Reference

Document Type

Language

Publication Year

Publication Name

CA Section

## Reactions (9,333)

Group: By Scheme View: Expanded

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

Scheme 1 (2 Reactions) Steps: 1 Yield: 67-91%



[Suppliers \(88\)](#) [Suppliers \(62\)](#)

Reaction Summary Steps: 1 Yield: 91% Copper-catalyzed protodecarboxylation of aromatic carboxylic acids

1.1 Catalysts: [1,10-Phenanthroline](#), [Copper oxide \(Cu<sub>2</sub>O\)](#)  
Solvents: [Quinoline](#), [N-Methyl-2-pyrrolidone](#); 12 h, 170 °C

1.2 Reagents: [Hydrochloric acid](#)  
Solvents: [Water](#)

By: Goossen, Lukas J.; et al Advanced Synthesis & Catalysis (2007), 349(14+15), 2241-2246

[Full Text ▾](#)

View Reaction Detail | Experimental Protocols

Reaction Summary Steps: 1 Yield: 67% Biaryl Synthesis via Pd-Catalyzed Decarboxylative Coupling of Aromatic Carboxylates with Aryl Halides

1.1 Catalysts: [1,10-Phenanthroline](#), [Copper oxide \(Cu<sub>2</sub>O\)](#), [Potassium bromide](#)  
Solvents: [Quinoline](#), [N-Methyl-2-pyrrolidone](#); 6 h, 170 °C

By: Goossen, Lukas J.; et al Journal of the American Chemical Society (2007), 129(15), 4824-4833

[Full Text ▾](#)

[View Reaction Detail](#) | [Experimental Protocols](#)

[Collapse Scheme ▾](#)

Scheme 2 (3 Reactions) Steps: 1 Yield: 77-90%



[Suppliers \(94\)](#) [Suppliers \(62\)](#)

Reaction Summary Steps: 1 Yield: 90% Highly-chemoselective step-down reduction of carboxylic acids to aromatic hydrocarbons via palladium catalysis

1.1 Reagents: [Triethylsilane](#), [Pivalic anhydride](#)  
Catalysts: [Palladium diacetate](#), [1,4-Bis\(diphenylphosphino\)biphenyl](#)  
Solvents: [Toluene](#); 15 h, 160 °C

By: Liu, Chengwei; et al Chemical Science (2019), 10(22), 5736-5742

[Full Text ▾](#)

[View Reaction Detail](#) | [Experimental Protocols](#)

不参与反应官能团：  
出现在反应前后，但

# 反应检索--结果集筛选： Synthetic Methods™

Structure Match

As Drawn (7,236)

**Substructure (4.3M)**

Similarity (222K)

Filter Behavior

Filter by Exclude

Yield

Number of Steps

Non-Participating Functional Groups

- Amide (132K)
- Ether (100K)
- Halide (99K)
- Alkene (65K)
- Phenyl halide (65K)
- Aldehyde (2,610)**

View All

Experimental Protocols

- Synthetic Methods (2,610)**
- Experimental Procedure (2,532)

Reaction Type

Stereochemistry

Reagent

Catalyst

Solvent

Commercial Availability

Reaction Notes

Search Within Results

Source Reference

Document Type

Language

Publication Year

Publication Name

CA Section

**Reactions (2,610)**

Group: By Scheme View: Expanded

References

Non-Participating Functional Groups: Aldehyde

Experimental Protocols: Synthetic Methods

Scheme 1 (2 Reactions)

Steps: 1 Yield: 67-91%



Suppliers (88) Suppliers (62)

Reaction Summary Steps: 1 Yield: 91% Copper-catalyzed protodecarboxylation of aromatic carboxylic acids

1.1 Catalysts: 1,10-Phenanthroline, Copper oxide ( $\text{Cu}_2\text{O}$ ) Solvents: Quinoline, N-Methyl-2-pyrrolidone; 12 h, 170 °C

1.2 Reagents: Hydrochloric acid Solvents: Water

By: Goossen, Lukas J.; et al Advanced Synthesis & Catalysis (2007), 349(14+15), 2241-2246

View Reaction Detail | Experimental Protocols

Full Text ▾

Scheme 2 (3 Reactions)

Steps: 1 Yield: 67%



Suppliers (94) Suppliers (62)

Reaction Summary Steps: 1 Yield: 67% Biaryl Synthesis via Pd-Catalyzed Decarboxylative Coupling of Aromatic Carboxylates with Aryl Halides

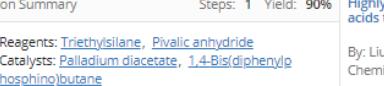
1.1 Catalysts: 1,10-Phenanthroline, Copper oxide ( $\text{Cu}_2\text{O}$ ), Potassium bromide Solvents: Quinoline, N-Methyl-2-pyrrolidone; 6 h, 170 °C

By: Goossen, Lukas J.; et al Journal of the American Chemical Society (2007), 129(15), 4824-4833

View Reaction Detail | Experimental Protocols

Full Text ▾

Steps: 1 Yield: 77-90%



Suppliers (94) Suppliers (62)

Reaction Summary Steps: 1 Yield: 90% Highly-chemoselective step-down reduction of carboxylic acids to aromatic hydrocarbons via palladium catalysis

1.1 Reagents: Triethylsilane, Pivalic anhydride Catalysts: Palladium diacetate, 1,4-Bis(diphenylphosphino)butane Solvents: Toluene; 15 h, 160 °C

By: Liu, Chengwei; et al Chemical Science (2019), 10(22), 5736-5742

View Reaction Detail | Experimental Protocols

Full Text ▾

**查看反应详情**

**Synthetic Methods™ :**  
经过标引和编辑的完整的反应操作信息

# 反应检索--结果集筛选： Synthetic Methods™

Chemical reaction scheme: 2-Carboxybenzaldehyde → Benzaldehyde (67% yield)

Suppliers (88)      Suppliers (62)

Step 1      Alternative Steps (1)

Stage	Reagents	Catalysts	Solvents	Conditions
1	-	1,10-Phenanthroline Copper oxide ( $\text{Cu}_2\text{O}$ ) Potassium bromide	Quinoline <i>N</i> -Methyl-2-pyrrolidone	6 h, 170 °C

CAS Reaction Number: 31-109-CAS-15004422

Experimental Protocols

Synthetic Methods	Experimental Procedure
Products	Benzaldehyde, Yield: 67%
Reactants	2-Carboxybenzaldehyde
Catalysts	1,10-Phenanthroline Copper oxide ( $\text{Cu}_2\text{O}$ ) Potassium bromide
Solvents	Quinoline <i>N</i> -Methyl-2-pyrrolidone
Procedure	<ol style="list-style-type: none"><li>Charge an oven-dried vessel with 2-carboxybenzaldehyde (1.00 mmol), <math>\text{Cu}_2\text{O}</math> (0.7 mg, 0.075 mmol), phenanthroline (27.0 mg, 0.15 mmol) and potassium bromide (0.015 mmol).</li><li>Flush the vessel with alternating vacuum and nitrogen purge cycles.</li><li>Add a degassed solution of <i>n</i>-tetradecane in a mixture of NMP (1.5 mL) and quinoline (0.5 mL) to the reaction mixture <i>via</i> syringe.</li><li>Stir the resulting mixture at 170 °C for 6 hours.</li><li>Allow the reaction mixture to cool to room temperature.</li><li>Dilute the reaction mixture with ethyl acetate (2 mL).</li><li>Dissolve a sample of the reaction mixture (0.25 mL) in ethyl acetate (2 mL).</li><li>Wash the reaction mixture with HCl (1 N, 2 mL).</li><li>Dry the reaction mixture over <math>\text{MgSO}_4/\text{NaHCO}_3</math>.</li><li>Analyze the product by GC.</li></ol>
Transformation	Decarboxylation of Aromatic Acids
Scale	milligram

CAS Method Number 3-109-CAS-15004422

Synthetic Methods™：  
分类显示详尽信息，方便操作

# 联合检索--反应式与关键词

The screenshot shows a search interface with a sidebar on the left and a main search area on the right.

**Sidebar:**

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

**Main Search Area:**

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

Search term: suzuki

Search filters: AND (dropdown), Author Name (dropdown), Enter last name, first name middle name.

Add Advanced Search Field

Learn more about Sci

**Reaction Drawing:** A chemical reaction scheme is shown with a blue arrow pointing to it. The reaction shows a Suzuki coupling between a benzene ring and a halide.

Edit Drawing Remove

文献检索框里  
输入关键词

结构编辑器  
中绘制反应

# 联合检索--反应式与关键词

Structure Match

As Drawn (2,771) Substructure (13K)

Filter Behavior

Filter by Exclude

Document Type

Journal (2,633) Patent (133) Review (3) Conference (4) Preprint (1)

Language

English (2,614) Chinese (123) Japanese (12) Korean (6) French (5) View All

Publication Year

1998 2021

No Min to No Max Apply View Larger

Available at My Institution

Author

Organization

Publication Name

Concept

CA Section

CAS Solutions

Database

Search Within Results

Filter Content Report

Download filter data from this result set.

References (2,771) Sort: Relevance View: Partial Abstract

Substances Reactions Citing Save

1

The Suzuki coupling of aryl chlorides in TBAB-water mixtures

By: Bedford, Robin B.; Blake, Michael E.; Butts, Craig P.; Holder, Debbie  
Chemical Communications (Cambridge, United Kingdom) (2003), (4), 466-467 | Language: English, Database: Cplus and MEDLINE

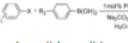
Palladium acetate in a mixture of tetrabutylammonium bromide (TBAB) and water can be used as an effective catalyst for the Suzuki coupling of deactivated aryl chloride substrates. E.g., phenylboronic acid was reacted with 4-chloroanisole using  $\text{Pd}(\text{OAc})_2$ ,  $\text{K}_3\text{PO}_4$ , and TBAB in water to give  $\text{MeO}-4-\text{C}_6\text{H}_4-\text{Ph}$  with 65.5% yield with only 3% yield of biphenyl.

Full Text Substances (11) Reactions (4) Citing (195) Citation Map

2

Phosphine-Free Palladium Acetate Catalyzed Suzuki Reaction in Water

By: Liu, Leifang; Zhang, Yuhong; Wang, Yanguang  
Journal of Organic Chemistry (2005), 70(15), 6122-6125 | Language: English, Database: Cplus and MEDLINE

  $\text{Pd}(\text{OAc})_2$  in a mixture of water and poly(ethylene glycol) (PEG) was an extremely active catalyst for the Suzuki reaction of aryl iodides and bromides. The reaction was conducted under mild conditions ( $50^\circ\text{C}$ ) without the use of a microwave or phosphine ligand in high yields. The isolation of the products was readily performed by extraction with di-Et ether, and the  $\text{Pd}(\text{OAc})_2$ -PEG can be reused without significant loss in activity.

Full Text Substances (44) Reactions (34) Citing (202) Citation Map

3

The Suzuki reaction under solvent-free conditions

By: Nielsen, Simon Feldbaek; Peters, Dan; Axelsson, Oskar  
Synthetic Communications (2000), 30(19), 3501-3509 | Language: English, Database: Cplus

The coupling reaction of diverse aryl halides with phenylboronic acid under solvent-free conditions was performed using  $\text{Pd}(\text{PPh}_3)_4$  catalyst under ball-milling conditions. Inert NaCl was added to the reaction mixtures to make them sufficiently powdery. The order of reactivity was complementary to the normal Suzuki reaction.

Full Text Substances (64) Reactions (24) Citing (86) Citation Map

4

Rapid and Amenable Suzuki Coupling Reaction in Water Using Microwave and Conventional Heating

By: Leadbeater, Nicholas E.; Marco, Maria  
Journal of Organic Chemistry (2003), 68(3), 888-892 | Language: English, Database: Cplus and MEDLINE

It is possible to prepare biaryls in good yield very rapidly (5-10 min) on small (1 mmol) and larger (10-20 mmol) scales from aryl halides and phenylboronic acid using water as solvent and palladium acetate as catalyst. The reaction can be performed equally well using microwave and conventional heating, probably showing that no nonthermal microwave effects are associated with the impressive speed of the reaction.

Full Text Substances (15) Reactions (12) Citing (233) Citation Map

5

Transition-metal-free Suzuki-type coupling reactions

By: Leadbeater, Nicholas E.; Marco, Maria  
Angewandte Chemie, International Edition (2003), 42(12), 1407-1409 | Language: English, Database: Cplus and MEDLINE

联合检索提高了检索速度



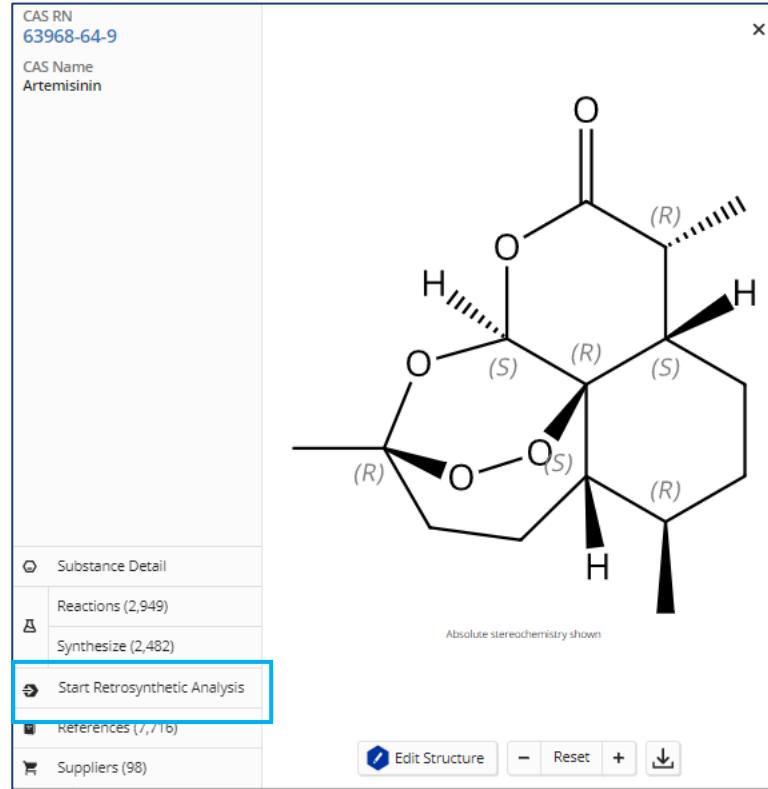
# 大纲

## — 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



从已知化合物获得逆合成路线：

点击物质结构，弹出的物质菜单中点击Create Retrosynthesis

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

Searching for...

All  
Substances  
Reactions  
References  
Suppliers  
Biosequences  
**Retrosynthesis**

Retrosynthesis

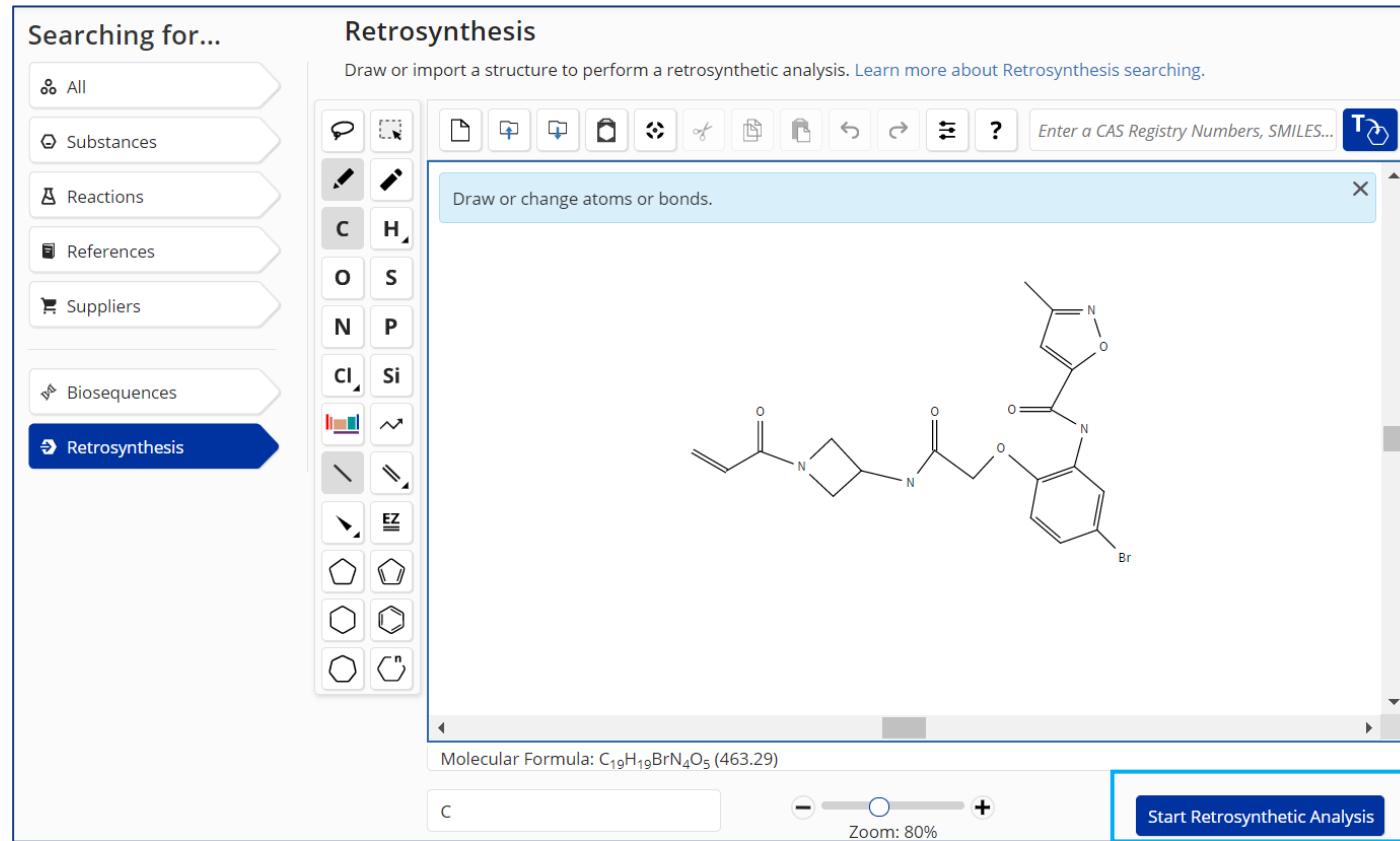
Draw or import a structure to perform a retrosynthetic analysis. Learn more about Retrosynthesis searching.

Draw or change atoms or bonds.

CC=CC1(CCN1C(=O)CCN(CC(=O)c2ccc(Br)cc2)C(=O)Oc3ccccc3)C(=O)O

Molecular Formula: C<sub>19</sub>H<sub>19</sub>BrN<sub>4</sub>O<sub>5</sub> (463.29)

C Zoom: 80% Start Retrosynthetic Analysis



绘制目标化合物：

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

# CAS Retrosynthesis Tool—预设参数

## Retrosynthesis Plan Options

Powered by ChemPlanner®

Select Synthetic Depth [Learn more.](#)

1  
 2  
 3  
 4



Set Rules Supporting Predicted Reactions [Learn more.](#)

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

Set Starting Materials Cost Limit [Learn more.](#)

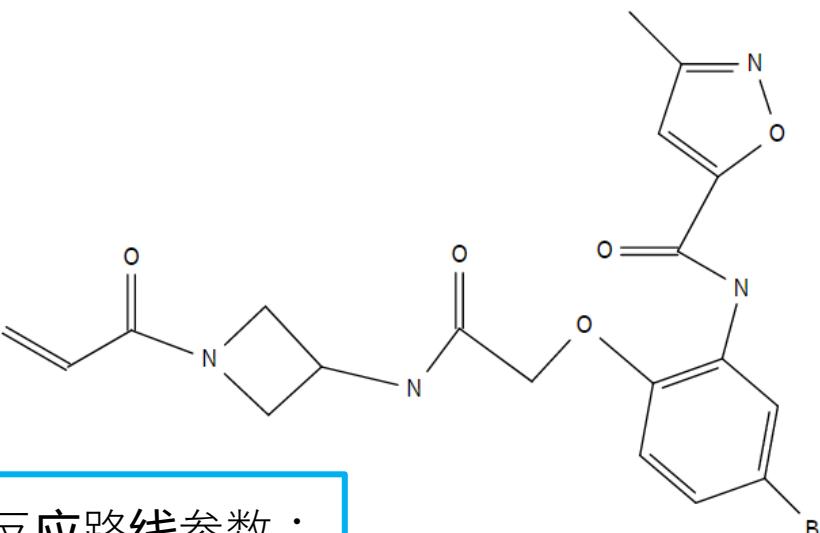
1000 [USD/mol](#) [USD/mol](#) [USD/g](#)

Email me when my plan is complete

[Create Retrosynthesis Plan](#)

Break and Protect Bonds [Learn more.](#)

[Break Bond](#) [Protect Bond](#) [Clear All Bond Selections](#)



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

# CAS Retrosynthesis Tool—路线概览

路线概览

重设参数

Retrosynthesis

Predicted Results

Powered by ChemPlanner®

Overview Steps

Plan Information  
Estimated Yield: 15%  
Overall Price: \$375.68  
(USD per 100 grams)  
Commercially Available:  
B, C, D, F, G, H, I

Plan Options  
Synthetic Depth: 3  
Predicted Rules: Common  
Break & Protect Bonds: No  
Starting Material Cost Limit: \$1,000.00/mol  
Edit Plan Options

Scoring Profiles  
Complexity Reduction  
Convergence  
Evidence  
Cost  
Yield  
Atom Efficiency

Apply Reset Scoring

Retrosynthesis Step Key  
Hover on the options below to highlight experimental and predicted steps within this plan. View Steps Menu.  
Experimental Steps  
Predicted Steps

已报道的逆合成路线  
预测的逆合成路线

Scoring Profiles : 每项有4个设置 (off, low, medium, high)

- Complexity Reduction : 可调整每一步原料结构的复杂性
- Convergence : 可调整逆合成路线中前体的数量
- Evidence : 表示预测路线支持的文献数量多少
- Cost : 表示预测路线大概的成本
- Yield : 表示每一步的产率
- Atom Efficiency : 表示每一步的原子转化效率

# CAS Retrosynthesis Tool—路线详情

Retrosynthesis

Predicted Results ON

Powered by ChemPlanner®

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

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

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

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

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

**点击Evidence查看该步具体的合成条件和文献**

Retrosynthesis Step Key  
Hover on the options below to highlight experimental and predicted steps within this plan. View Steps Menu.  
Experimental Steps  
Predicted Steps

**Reactions (1,181)**  
Scheme 1 (1 Reaction)  
Steps: 1

Reaction Summary  
Steps: 1  
1.1 Reagents: 1-Ethyl-3-(3'-dimethylaminopropyl)carbodimide, 1-Hydroxybenzotriazole, Diisopropylethylamine  
Solvents: Dichloromethane; overnight, rt  
1.2 Reagents: Zinc  
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

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

**Collage Scheme**

The screenshot shows the CAS Retrosynthesis Tool interface. On the left, a retrosynthetic tree is displayed with nodes A through I. Nodes A, B, and C are labeled 'Predicted Steps'. Node A has an average yield of 37% and 181 pieces of evidence. Node B has a maximum yield of 80%. Node C has a maximum yield of - and 15 alternative steps. Node E has a maximum yield of - and 24 alternative steps. A blue arrow points from the 'Evidence' link for node A to a callout box containing the text: '点击Evidence查看该步具体的合成条件和文献' (Click Evidence to view the specific synthesis conditions and literature for this step). To the right of the tree is a detailed reaction scheme for Scheme 1, showing reagents, solvents, and suppliers. A large blue box on the right side lists four key features of the tool: '快速获取最优的逆合成路线' (Quickly get the best retrosynthetic route), '可查看每步路线的详细条件' (Can view the detailed conditions for each step), '可自定义选择替代路线' (Can customize to choose alternative routes), and '可获取预测逆合成路线' (Can get predicted retrosynthetic routes).

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

# CAS Retrosynthesis Tool—路线详情

The screenshot shows the ChemPlanner Retrosynthesis interface. The top navigation bar includes 'Overview' and 'Steps' tabs, with 'Predicted Results' set to 'ON'. A sidebar on the left lists retrosynthetic steps:  $A \Rightarrow B + C + D$  (Average Yield: 37%, Evidence: 11,181),  $B \Rightarrow E$  (Maximum Yield: 80%, Evidence: 180,876, Alternative Steps: 20),  $C \Rightarrow F + G$  (Maximum Yield: -, Evidence: 1, Alternative Steps: 15), and  $E \Rightarrow H + I$  (Maximum Yield: -, Evidence: 1, Alternative Steps: 24). The main area displays 'Alternative Steps (85)' with a filter for 'Predicted (85)'. Two examples are shown:

**2 of 85**

Predicted Step: Evidence (1,836) | Average Yield: 55%

**3 of 85**

Predicted Step: Evidence (974,306) | Average Yield: 64%

On the right, a vertical panel shows a retrosynthetic tree starting from the target molecule, with node 24 highlighted. A shopping cart icon indicates 168 items.

点击Alternative Steps查看并选择替换路线。

## 得到自定义的合成路线

The screenshot shows a retrosynthetic analysis interface with the following components:

- Header:** "Retrosynthesis" with a back arrow, "Powered by ChemPlanner®", and a toolbar with download, email, and save icons.
- Predicted Results:** A toggle switch labeled "Predicted Results ON".
- Reaction Plan:** A sequence of retrosynthetic steps:
  - Step 1: Compound A (a complex polycyclic molecule) reacts via a predicted step (green dashed arrow) to compound C (2-bromo-4-nitrophenyl propanoate). Yield: Avg. Yield 55%.
  - Step 2: Compound C reacts via a predicted step (green dashed arrow) to compound D (2-hydroxy-4-oxo-5H-pyran-3-carboxylic acid). Yield: Avg. Yield 61%.
  - Step 3: Compound D reacts via an experimental step (blue dashed arrow) to compound G (2-bromo-4-aminobiphenyl). Yield: Max Yield 80%.
  - Step 4: Compound G reacts via a predicted step (green dashed arrow) to compound F (2-hydroxypropanoic acid). Yield: Avg. Yield 61%.
  - Step 5: Compound F reacts via a predicted step (green dashed arrow) to compound E (2-(2-acryloyl)cyclobutanemethanol). Yield: Max Yield 80%.
  - Step 6: Compound E reacts via a predicted step (green dashed arrow) to compound B (2-(2-acryloyl)-N-methylcyclobutanemethylamine). Yield: Max Yield 80%.
  - Step 7: Compound B reacts via a predicted step (green dashed arrow) to compound H (2-(2-acryloyl)-N,N-dimethylcyclobutanemethylamine).
- Inventory:** A sidebar on the left lists available reagents with their quantities:
  - A: 0
  - B: 10
  - C: 0
  - D: 103
  - E: 0
  - F: 123
  - G: 337
  - H: 168
  - I: 45
- Step Key:** A legend for experimental and predicted steps.
- Buttons:** "Experimental Steps" and "Predicted Steps" buttons at the bottom left, and a zoom control ("-", "Reset", "+") at the bottom right.

# 检索信息的管理

- 保存&导出检索结果及标签
- 设置提醒检索结果
- 合并保存的检索结果
- 历史检索记录

视频链接：

<https://casevents.webex.com/ec3300/eventcenter/enroll/register.do?siteurl=casevents&formId=307159432&confId=307159432&formType=1&loadFlag=1&eventType=1&accessType=viewRecording&internalPBRecordTicket=4832534b00000005f9f2504b4d303988091b40fd51809aeb9c8ce4f3074cbeb71e9b2937afea5257>

# 检索信息的管理--保存、下载，设置提醒和标签

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

- Journal (3,278)
- Review (542)
- Biography (1)
- Clinical Trial (9)
- Commentary (8)

[View All](#)

Language

- English (3,250)
- Chinese (21)
- Japanese (6)
- Russian (1)

Publication Year

No Min to No Max Apply View Larger

Available at My Institution

Author

Organization

Publication Name

Concept

CA Section

CAS Solutions

Formulation Purpose

Database

- CPlus (7,396)
- MEDLINE (3,278)

References (3,278) Sort: Relevance View Partial Abstract

Substances Reactions Citing

Filtering: Database: MEDLINE

Save Search

Name:

No Alerts As Available Weekly Monthly

Tags (optional): No tags defined

New Tag (optional):

Substances

Save Cancel

1 Nano-graphene in biomedicine: theranostic applications By: Yang, Kai; Feng, Liangzhu; Shi, Xiaozhe; Liu, Zhuang Chemical Society Reviews (2013), 42(2), 530-547 | Language: English A review. Owing to their unique phys. and chem. properties, g... graphene oxide (RGO) and GO-nanocomposites have attracted in recent years. With every atom exposed on its surface, single mol. loading and bioconjugation, and was widely explored as near-IR (NIR) optical absorbance, *in vivo* graphene-based ph... View More

2 Poly-cyclodextrin and poly-paclitaxel nano-assembly for anticancer therapy By: Namgung, Ran; Mi Lee, Yeong; Kim, Jihoon; Jang, Yuna; Lee, Byung-Heon; Kim, In-San; Sokkar, Pandian; Rhee, Young Min; Hoffman, Allan S.; Kim, Won Jong Nature Communications (2014), 5, 3702 | Language: English, Database: CPlus and MEDLINE Effective anticancer therapy can be achieved by designing a targeted drug-delivery system with high stability during circulation and efficient uptake by the target tumor cancer cells. We report here a novel nano-assembled drug-delivery system, formed by multivalent host-guest interactions between a polymer-cyclodextrin conjugate and a polymer-paclitaxel conjugate. The multivalent inclusion complexes confer high stability to the nano-assembly, which efficiently delivers paclitaxel into the targeted cancer cells via both passive and active targeting mechanisms. The ester linkages between pacl... View More

3 Nano-graphene oxide for cellular imaging and drug delivery By: Sun, Xiaoming; Liu, Zhuang; Welsher, Kevin; Robinson, Joshua Tucker; Goodwin, Andrew; Zaric, Sasa; Dai, Hongjie Nano Research (2008), 1(3), 203-212 | Language: English, Database: CPlus and MEDLINE Two-dimensional graphene offers interesting electronic, thermal, and mech. properties that are currently being explored for advanced electronics, membranes, and composites. Here we synthesize and explore the biol. applications of nano-graphene oxide (NGO), i.e., single-layer graphene oxide sheets down to a few nanometers in lateral width. We develop functionalization chem. in order to impart solubility and compatibility of NGO in biol. environments. We obtain size separated pegylated NGO sheets that are soluble in buffers and serum without agglomeration. The NGO sheets are found to be photolum... View More

4 Doxil - The first FDA-approved nano-drug: Lessons learned By: Barenholz, Yechezkel Journal of Controlled Release (2012), 160(2), 117-134 | Language: English, Database: CPlus and MEDLINE A review. Doxil, the first FDA-approved nano-drug (1995), is based on three unrelated principles: (i) prolonged drug circulation time

下载  
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保存

设置提醒频率：  
即时, 每周, 每月

# 检索信息的管理--导出文件格式

Download Reference Results

File Type: PDF  
Select Quantity: All Results

Display: Result Summary

File Name: Reference\_20211118\_1536

Only the first 500 references will be downloaded.

Include:  
 Task History  
 Abstract  
 Concepts  
 Substances

Formulations  
 Analytical Methods  
 Citations

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

Download Substance Results

File Type: PDF  
Select Quantity: All Results

Display: Result Summary

File Name: Substance\_20211118\_1537

Only the first 500 substances will be downloaded.

Include:  
 Task History  
 Substance Names  
 Experimental Spectra  
 Predicted Spectra  
 Regulatory Information

Experimental Properties  
 Predicted Properties  
 Bioactivity Indicators  
 Target Indicators

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

Download Reaction Results

File Type: PDF  
Select Quantity: All Results

Display: Result Summary

File Name: Reaction\_20211118\_1537

Only the first 500 reaction summaries will be downloaded.

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

# 检索信息的管理--查看保存结果，更改提醒设置

The screenshot shows the SciFinder interface with a blue header bar. The search bar contains 'Reactions' and '7782-42-5'. The top right includes icons for Draw, Search, Favorites, and Profile.

**Filter by:**

- Result Type:
  - Reactions (34)
  - References (48)
  - Substances (18)
- Alerts:
  - Unviewed (1)
  - No Alerts (100)

**Saved (100):**

- 1671 exclude COCl Rerun Search  
June 4, 2021, 3:57 PM  
Combined From Substance Saved Items
- include Si Rerun Search  
June 4, 2021, 3:54 PM  
Substances Advanced Search + Filters Boiling Point (°C): 80 to 100

**Alerts and Tags:**

- Alerts dropdown
- Add Tags dropdown

**Frequency:**

- No Alerts (selected)
- As Available
- Weekly
- Monthly

**Migrate Alerts & Saved Results:**

- Combine
- Migrate

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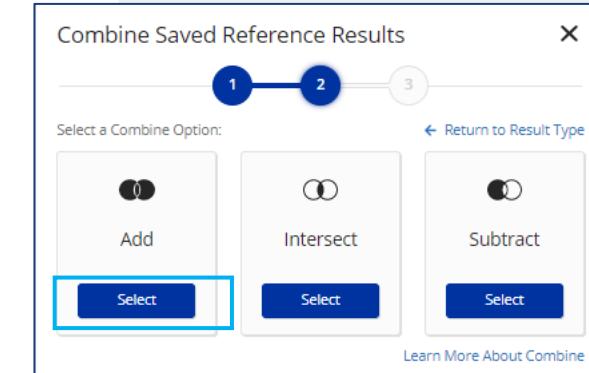
更新检索结果



# 检索信息的管理--合并保存的结果

The screenshot shows the SciFinder interface with the following elements:

- Top Bar:** CAS SciFinder, Reactions, 7782-42-5, Draw, Search, Filter, User Profile.
- Left Sidebar:** Filter by Result Type (Reactions 34, References 48, Substances 18), Alerts (Unviewed 1, No Alerts 100).
- Main Area:** ★ Saved (100) with two entries:
  - 1671 exclude COCl (Combined from Substance Saved Items)
  - include Si (Substances, Advanced Search, + Filters, Boiling Point: 80 to 100)
- Dialog Box:** Combine Saved Results (highlighted with a blue border). It shows a flowchart: 1 → 2 → 3. Options:
  - Select a Result Type:
    - Substances (Select)
    - Patent Markush (Select)
    - Reactions (Select)
    - References (Select, highlighted with a blue border)
  - Buttons: Alerts, Add Tags, Rerun Search.



在保存的结果中点击左侧Combine按钮；  
选择需要进行合并操作的结果集类型和操作类型

# 检索信息的管理--合并保存的结果

Combine Saved Reference Results: Add

1 2 3

Select Up to 5 Saved Items:

Return to Combine Option

<input checked="" type="checkbox"/> medline	Query	June 1, 2021
<input checked="" type="checkbox"/> caplus	Query	June 1, 2021
<input type="checkbox"/> Pra	Query	April 28, 2021
<input type="checkbox"/> Formulus for Pra	Query	April 28, 2021
<input type="checkbox"/> 187	Query	March 31, 2021
<input type="checkbox"/> 3	Query	March 31, 2021
<input type="checkbox"/> 2	Query	March 31, 2021
<input type="checkbox"/> 1	Query	March 31, 2021
<input type="checkbox"/> JACS	Query	March 18, 2021
<input type="checkbox"/> Nature	Query	March 18, 2021

**View Results** **Cancel** **Learn More About Combine**

Filter Behavior

Filter by Exclude

Document Type

- Journal (4,849)
- Patent (2,530)
- Review (889)
- Biography (1)
- Clinical Trial (9)

View All

Language

- English (4,929)
- Chinese (2,307)
- Korean (86)
- Japanese (70)
- German (14)

View All

Publication Year

No Min to No Max Apply View Larger

Available at My Institution

Author

Organization

Publication Name

Concept

CA Section

CAS Solutions

Formulation Purpose

Database

Search Within Results

Filter Content Report

**References** (7,452)

Sort: Publication Date: Newest ▾ View: Partial Abstract ▾

1  
Encapsulation of a cationic antimicrobial peptide into self-assembled polyion complex nano-objects enhances its antitumor properties  
By: Raileanu, Mina; Lonetti, Barbara; Serpentini, Charles-Louis; Goudouneche, Dominique; Gibot, Laure; Bacalum, Mihaela  
Journal of Molecular Structure (2022), 1249, 131482 | Language: English, Database: Cplus  
Antimicrobial peptides, a large class of mols. synthesized by various organisms as an innate defense against pathogens are more and more used for their anticancer properties as well. In order to overcome some of their limitations and to enhance their therapeutic efficiency, the use of delivery systems was taken into consideration. In this study we describe an original delivery system for antimicrobial peptides based on its physico-chem. properties, namely the self-assembled polyion complexes (PIC) based on electrostatic interactions of cationic antimicrobial peptide P6 with neg. charged double...  
View More

2  
Spectroscopic characterization of Cu(II), Ni(II), Co(II) complexes, and nano copper complex bearing a new S, O, N-donor chelating ligand. 3D modeling studies, antimicrobial, antitumor, and catalytic activities  
By: El-ghamry, Mosad A.; Shebl, Magdy; Saleh, Akila A.; Khalil, Saeid M. E.; Dawy, Magdah; Ali, Amira A. M.  
Journal of Molecular Structure (2022), 1249, 131587 | Language: English, Database: Cplus  
A new trinuclear hydrazone ligand (HL), its Co(II), Ni(II), Cu(II) complexes (in 1:1, 1:2 molar ratios of metal to ligand), and the mixed-ligand Co(II), Ni(II), Cu(II) complexes of the ligand HL, with 8-HQ in 1:1:1 (M:L:HQ) stoichiometry, in addition to a nano Cu(II) complex have been synthesized and characterized using phys., anal. and spectral methods. Octahedral geometry was assigned for all investigated complexes except Cu(II) complex 1 which exhibited square planar arrangement. The TGA results suggested the thermal stability of the current complexes. The XRD data indicated that the part...  
View More

3  
Proof of concept for dual anticancer effects by a novel nanomaterial-mediated cancer cell killing and nano-radiosensitization  
By: Duo, Yanhong; Liu, Quan; Zhu, Daoming; Zhang, Bin; Luo, Guanghong; Wang, Fu-Bing; Chen, Jinghua; Cao, Yihai  
Chemical Engineering Journal (Amsterdam, Netherlands) (2022), 429, 132328 | Language: English, Database: Cplus  
Nano-radiosensitization is an emerging concept for cancer therapy and the underlying rationale embroils enhancement of radiosensitization by nanomaterials. Here we describe a new concept of the irradiation-triggered switching of a biol. inert nanoprod to releasing an anticancer gas that executes cancer cells killing and improves radiosensitization by improving the tumor hypoxic microenvironment. This novel strategy employed chem. coordination between radiosensitive gold-coated polyethylene glycol (PEG) nanoparticles and nanoclusters (Au NCs-PEG) and sodium nitronium iside (SNi) coated by platinum...  
View More

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

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

Full Text  Substances (7)  Reactions (0)  Citing (0)  Citation Map

勾选需要合并的结果集，点击View Results，  
获得合并后的结果集

# 检索信息的管理--管理检索历史

按照检索类型或  
检索时间查找

The screenshot shows the SciFinder search history page. At the top, there is a navigation bar with the CAS SciFinder logo, a 'References' dropdown, a search input field 'Enter a query...', and several icons including 'Draw', a magnifying glass, a star, a trash can, and a user profile. A blue box highlights the trash can icon. On the left, there is a sidebar with 'Filter by' sections for 'Result Type' (All, Patent Markush, Reactions, References, Retrosynthesis, Substances) and 'Date' (a calendar showing November 2021). The main area is titled 'Search History (550)' and lists five entries from November 18, 2021:

- 3:29 PM: Retrosynthesis search for a complex molecule. Synthetic Depth: 3, Predicted Rules: Common, Break & Protect Bonds: No, Starting Material Cost Limit: \$1,000.00/mol. Status: Generating Plan.
- 3:27 PM: Retrosynthesis search for a complex molecule. Synthetic Depth: 3, Predicted Rules: Common, Break & Protect Bonds: No, Starting Material Cost Limit: \$1,000.00/mol. Status: Generating Plan.
- 3:16 PM: Substances search for 'qinghaosu'. Status: Rerun Search.
- 3:16 PM: Substances search for 'qinghaosu'. As Drawn (0), Substructure (0), Similarity (0). Status: Rerun Search.
- 3:13 PM: References search for 'suzuki'. As Drawn (2,771), Substructure (13k). Status: Rerun Search.

重新编辑检索项

# 分析方法的获取—Analytical Methods

- 介绍
- 检索方法
- 结果详情

视频链接：

[https://american-chemical-society.zoom.us/rec/play/d6Q-xA-DR\\_ODf7WaxdDaLaAYkIDyrc3K4vSquoixkuqJNL7S6dwrhwbguRgDYXekpphbY-mXLb0HlRbTU.wkg9K9htCp0Yq\\_aE](https://american-chemical-society.zoom.us/rec/play/d6Q-xA-DR_ODf7WaxdDaLaAYkIDyrc3K4vSquoixkuqJNL7S6dwrhwbguRgDYXekpphbY-mXLb0HlRbTU.wkg9K9htCp0Yq_aE)



# 分析方法的类别--13大类45小类；某些子类属多个分类

Organic Compound Analysis: 天然产物分离分析, 手性分离, 活性药物成分及代谢产物分析...

Organometallics / Inorganics: 地质分析, 无机物分析, 金属有机化合物分析

Pharmacology / Toxicology: 成瘾药物检测, 有毒物检测...

Bioassays: 生物探针, 生物标定细胞实验, 生物标定药物实验, 生物医学材料分析, 生物分子/生物组织分离测定...

Water Analysis: 阴阳离子分析, 元素测定, 痕量元素分析, 废水分析, 生物标记公共卫生分析...

Historical Analysis / Dating: 考古分析, 同位素分析

Environmental Analysis: 土壤/空气/水分分析, 农药残留分析...

Agricultural Applications / Analysis: 除草剂分析...

Food Analysis: 脂肪酸分析, 脂肪酸酯分析, 蛋白质分析...

Fuels / Geology / Biofuels: 生物燃料分析, 油气分析, 石油产品分析, 煤炭加工...

Miscellaneous: 化妆品分析, 爆炸物分析, 纳米材料分析...

Water: 阴阳离子分析、环境分析、废水分析、微量元素分析...

Polymer: 聚合物分析...



# 分析方法的获取—Analytical Methods

<https://methods.cas.org> (与SciFinder-n登录账号相同)

The screenshot shows the homepage of the CAS Analytical Methods website. At the top, there's a navigation bar with 'CAS Solutions ▾', the 'CAS Analytical Methods' logo, a 'Saved' button, and an 'Account' button. Below the header is a search bar with the placeholder 'Enter keyword, matrix, analyte, etc.' and a purple search button. To the left of the search bar is an 'Advanced Search' link. On the right, there's a 'Browse Method Categories' section showing categories like Pharmacology / Toxicology, Polymer Analysis, and Water Analysis. A callout box highlights the 'Pharmacology / Toxicology' category. Another callout box in the bottom right corner states '目前有13个大类，45个小类。' (Currently there are 13 major categories and 45 minor categories.) and '某些子类属于多种方法分类！' (Some sub-categories belong to multiple method classifications!). At the bottom left, there's a 'Recent Searches' section with two entries: 'Advanced : analyte : sofosbuvir, technique : hplc' and 'Advanced : analyte : sofosbuvir, technique : hplc, keyword : mass'. The bottom right features the ACS International logo.

CAS Solutions ▾

CAS Analytical Methods

Saved Account

Search

Enter keyword, matrix, analyte, etc.

Advanced Search

输入感兴趣的检索词进行快速检索或高级检索

Browse Method Categories

Active Pharmaceutical Ingredient and Metabolite Analysis  
Addictive Drug Assay  
Forensic Analysis

Genetic Analysis  
Nanomaterial Analysis  
Organic Compound Analysis

Toxin Assay

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

目前有13个大类，45个小类。

某些子类属于多种方法分类！

Recent Searches

Advanced : analyte : sofosbuvir, technique : hplc

Advanced : analyte : sofosbuvir, technique : hplc, keyword : mass

ACS International

CAS

# 分析方法的获取—Analytical Methods

利用运算符连接不同的检索域，快速获得更相关的结果

The screenshot shows the CAS Analytical Methods Advanced Search interface. The search bar contains the term "impurities". Below it, the search criteria are defined as follows:

- AND
- Analyte: sofosbuvir
- AND
- Technique: hplc

A dropdown menu is open over the "Technique" field, listing the following options: Keyword, Analyte, Matrix, Method Category, **Technique**, CAS Method Number, and Publication Name. The "Technique" option is highlighted with a blue selection bar.

# 分析方法的获取—Analytical Methods

The screenshot shows the CAS Analytical Methods website interface. The search term 'guaijaverin' is entered in the search bar. The results page displays 220 entries. The first result is a detailed method for 'Garcimangosone D' from 'Psidium guajava' by solvent extraction. A large blue callout box highlights the 'View Details & Instructions' button and contains the Chinese text '查看分析方法详情' (View details of the analytical method). The method details include the analyte (Garcimangosone), matrix (Psidium guajava), reagents (Methanol, Dichloromethane, Hexane, Chloroform, Ethyl acetate), material (Column 10 mm, 300-8 mm i.d.; Column 3 x 60 cm), technique (UV-visible spectroscopy, Adsorption liquid chromatography, HPLC, Solvent extraction), equipment used (HPLC system, UV detector, Column chromatography system, Fraction collector), source (A new antibacterial benzophenone glycoside from Psidium guajava (Linn.) leaves by Ukwueze, Stanley E.; Osadebe, Patience O.; Okoye, Festus B. C., Natural Product Research (2015), 29 (18), 1728-1734. Taylor & Francis Ltd.), and full text and abstract links. The second result listed is another method for 'Garcimangosone D' from 'Psidium guajava' by solvent extraction.

根据分析物、分析基质、  
方法分类、所用技术、年  
份筛选分析方法

# 分析方法详情

CAS Solutions Analytical Methods guajaverin

Method Detail (1 of 220)

### Analysis of Garcimangosone D in Psidium guajava by Solvent extraction

CAS MN: 1-131-CAS-164363

Method Category: Natural Product Isolation Analysis  
Technique: UV-visible spectroscopy; Adsorption liquid chromatography; HPLC; Solvent extraction

Materials	Role	View Structure	Chemical Name
Garcimangosone D	analyte	View Structure	356055-68-0
Guajaverin	analyte	View Structure	22255-13-6
Guajaphenone A	analyte		
Psidium guajava	matrix		
Column (10 mm, 300_8 mm i.d.)	material		
Column (3 x 60 cm)	material		
Methanol	reagent		
Dichloromethane	reagent		
Hexane	reagent		
Chloroform	reagent		
Ethyl acetate	reagent		

方法分类、技术、所用材料/物质、角色、文献来源……

Source

A new antibacterial benzophenone glycoside from *Psidium guajava* (Linn.) leaves  
Ukwueze, Stanley E.; Osadebe, Patience O.; Okoye, Festus B. C.  
Natural Product Research (2015), 29 (18), 1728 - 1734. Taylor & Francis Ltd.  
CODEN: NPRAAT | ISSN: 14786419 | DOI: 10.1080/14786419.2014.1003188

Full Text ▾

Abstract ▾

Bioactivity-guided fractionation of methanol extract from the leaves of *Psidium guajava* L. (Myrtaceae) yielded a new benzophenone glycoside, gajaphenone A (I) together with two known compounds, garcimangosone D and guajaverin. Their structures were elucidated by anal. of spectroscopic data including 1D and 2D NMR and electrospray ionisation mass spectrometry. The isolated compounds were screened against standard strains of Gram-pos. and Gram-neg. bacteria using broth dilution assay method, and the MIC values determined and compared with reference antibiotic ceftriaxone. They were found to have significant antibacterial activities against *Escherichia coli* and *Staphylococcus aureus* with all of them showing better activities against *S. aureus*, but displaying weaker activities, in comparison to ceftriaxone. However, despite reduced effect of these compounds against the organisms, this work opens the perspective to use these mols. as leads for the design of novel and selective drug candidates for some tropical infectious diseases.

Equipment Used

HPLC system, L-7100, Merck-Hitachi  
UV detector, UV-L7400, Merck-Hitachi  
Column chromatography system  
Fraction collector, Retriever II, ISCO, Germany

Conditions

Instrument  
Column: Eurospher C-18 column (10 mm, 300\_8 mm i.d.; Knauer); mobile phase: methanol and nanopure water  
Detection: 254 nm  
Column: Sephadex LH-20 column (3 x 60 cm); mobile phase: dichloromethane: methanol (1:1); flow rate: 0.2 mL/min

实验条件、实验步骤和数据有效性验证…

### Extraction of the sample

- Defat the pulverized air-dried leaves (600 g) with n-hexane.
- Extract the dried marc (450 g) with 5 L of 90% methanol for 4 days at room temperature (25 °C).
- Concentrate the extract in vacuo with rotary evaporator.
- Reconstitute the dried methanol extract (35 g, 7.7% w/w) in 20 mL of methanol.
- Dilute to 200 mL with distilled water.
- Shake for about 30 min.
- Perform liquid-liquid extraction with chloroform (3 mL x 750 mL) and ethyl acetate (3 mL x 750 mL) and PsG-WF (8.6 g; 1.9% w/w) fractions, respectively.

on of PsG-EF (4.5 g) on a Sephadex LH-20 column (3 cm x 60 cm).  
Bromethane:methanol (1:1) to obtain 10 pooled fractions PsG-EF1 to PsG-EF10.  
Preparative HPLC purification for the bioactive fraction, PsG-EF4.

### Semi-preparative HPLC analysis

- Analyze the sample using a Merck-Hitachi L-7100 pump coupled to a Merck-Hitachi UV detector.
- Perform separation with a Eurospher C-18 column (10 mm, 300\_8 mm i.d.; Knauer).
- Use methanol and nanopure water as the mobile phase.
- Set the UV detector to 254 nm.

### Validation

Concentration	3.0 mg, Garcimangosone D
	3.5 mg, Guajaphenone A
	4.5 mg, Guajaverin

# 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检索)
  - 生物序列检索
  - 反应检索
  - 逆合成反应路线设计 (CAS Retrosynthesis Tool)
  - 检索信息的管理
  - 分析方法的获取 (Analytical Methods)
- 常见问题及解决

# 浏览器选择建议

- Windows 7以上用户建议升级IE到10以上，不支持IE7、IE8
- Chrome和FireFox浏览器在所有系统上的表现都优于IE浏览器
- 不建议使用360浏览器检索SciFinder，会被自动拦截相关功能或插件

# 如何获取CAS SciFinder账号

--CONTACT INFORMATION--

First Name\*:

Last Name\*:

Email\*:

Confirm Email\*:

Phone Number:

Fax Number:

Area of Research:

Job Title:

--USERNAME AND PASSWORD--

Username\*:  Tips

Password\*:

Re-enter Password\*:

--SECURITY INFORMATION--

Security Question:

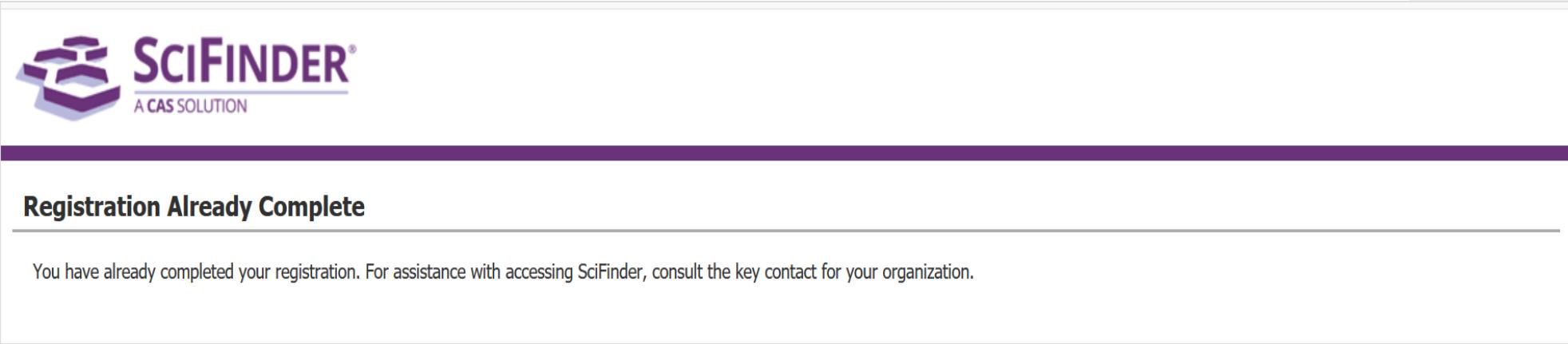
Answer\*:  Why?

请注意：

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

登录学校图书馆网站找到CAS SciFinder数据库说明页，按照提示进行注册

# 如何获取CAS SciFinder账号



The screenshot shows the SciFinder registration confirmation page. At the top left is the SciFinder logo with the text "A CAS SOLUTION". Below it, a purple header bar contains the text "Registration Already Complete". Underneath the header, a message reads: "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>即可访问。

# 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 (以电子形式存储不超过5,000条记录)
- 不得账号分享
- 不得将账号用于非学术研究

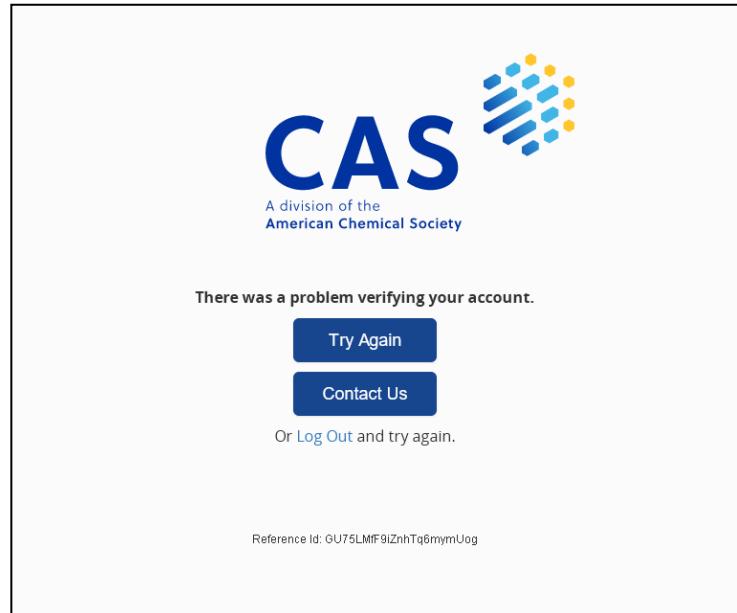
# 常见问题

## 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

# 2022年CAS SciFinder<sup>n</sup>论坛直播日程表

	日期	主题	主讲人
基础培训	3月1日	文献信息的获取	刘萌萌
	3月8日	物质信息的获取	钱欣
	3月15日	反应信息的获取	程小燕
	3月22日	生物序列的获取	刘萌萌
	3月29日	利用CAS SciFinder <sup>n</sup> 顺利开题、进行文献综述	钱欣
检索策略详解	4月25日	聚合物相关信息获取策略	程小燕
	5月24日	无机与金属有机化合物相关信息获取策略	钱欣
	6月14日	光电材料相关信息获取策略	程小燕
	7月5日	农化相关信息获取策略	钱欣
	9月13日	药物结构设计与合成	程小燕
	10月11日	天然植物化学相关信息获取策略	钱欣
	11月8日	稀土材料相关信息获取策略	程小燕
	11月29日	纳米材料相关信息获取策略	钱欣
	12月20日	催化合成信息获取策略	程小燕

直播时间：

18:00 – 19:00

关注公众号：ACS美国化学会  
随时观看回放，了解直播信息



# 2022 CAS SciFinder<sup>n</sup> 检索技能大赛

## 参赛对象：

中国大陆地区高校和科研院所的CAS SciFinder<sup>n</sup>用户

## 大赛时间：

第一阶段：2022年4月11日 - 5月8日

- 在线学习CAS SciFinder<sup>n</sup>检索技能，并参加线上考试
- 可参加幸运抽奖，成绩优秀者将获得CAS官方证书

第二阶段：2022年5月9日 - 6月7日

- 提交CAS SciFinder<sup>n</sup>检索体验PPT
- 赢取Macbook Air、投影仪、Airpods等大奖

(详情请参看ACS美国化学会微信公众号)



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## 参赛方式：

大赛将于2022年4月11日开启，请扫描二维码参加：



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

**ACS**  
International

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

# 谢谢！

关注我们



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