

利用CAS SciFinderⁿ 获取科技信息

2021.11



ACS
International



A division of the
American Chemical Society

大纲

- CAS及CAS SciFinderⁿ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
- 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



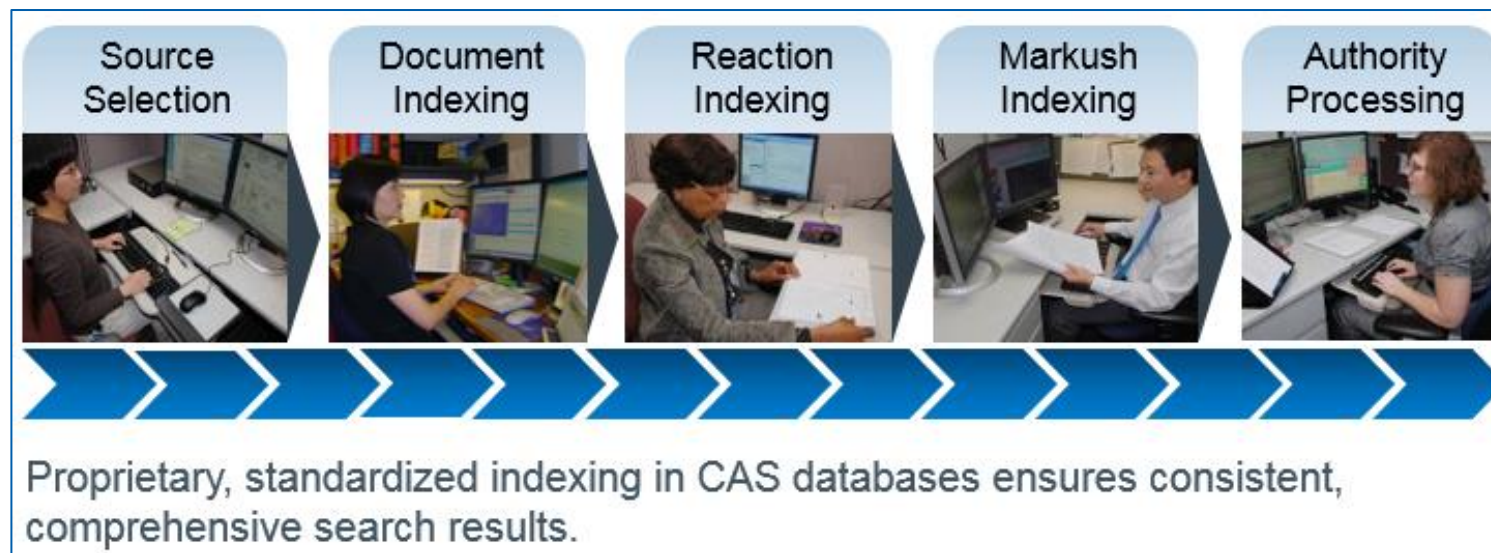
Over
50K
scientific journals
and documents

Over
250
million
substances

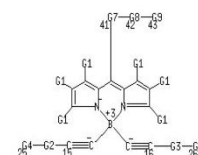
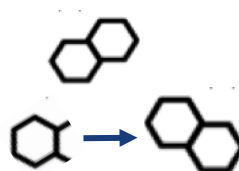
Over
50
languages
translated

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-, (17β)-

CAS科学家利用人类智慧对公开内容进行揭示，使相关信息更容易被挖掘

CAS内容合集--CAS SciFinderⁿ



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 ServicesSM

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

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




Log In to SciFinderⁿ

Username or Email Address

Next

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



Log In to SciFinderⁿ

Welcome, 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 SciFinderⁿ主界面

The screenshot shows the CAS SciFinderⁿ main interface with several key features highlighted by Chinese text and arrows:

- 检索历史 账户信息** (Search History Account Information): Located at the top right, pointing to the 'History' and 'Account' buttons.
- 已保存的结果集及信息更新的结果集** (Saved result sets and updated result sets): Located at the top center, pointing to the 'Saved' button.
- 灵活的检索选项** (Flexible search options): Located on the left side, pointing to the 'Searching for...' sidebar with options like 'All', 'Substances', 'Reactions', 'References', 'Suppliers', 'Biosequences', and 'Retrosynthesis'.
- 近期检索历史** (Recent search history): Located on the bottom left, pointing to the 'Recent Search History' section.
- 便捷地合并文本与结构检索** (Conveniently merge text and structure search): Located in the center, pointing to the search input field containing 'Heat treatment of materials' and the chemical structure drawing below it.
- 重新运行检索** (Rerun search): Located at the bottom right, pointing to the 'Rerun Search' button.
- 修改检索式** (Modify search query): Located at the bottom right, pointing to the 'Edit Search' button.

The interface includes a search bar with the text 'Heat treatment of materials', a search button, and a chemical structure drawing. Below the search bar is a 'References' section with a search prompt: 'Search by Keyword, Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. Learn More'. At the bottom, there is a 'Recent Search History' table with the following data:

Recent Search History	
November 11, 2021	
3:30 PM	
Substances	qinghaosu (1)

一站检索：一次检索，获得所有信息

The screenshot displays the CAS SciFinder interface for the search term 'qinghaosu'. The left sidebar shows navigation options: 'Return to Home', 'Show only' (Substances (1), Reactions (2,949), References (7,828), Suppliers (98)), 'All Answer Types', 'Substances (1)', and 'Reactions (2,949)'. The main content area is divided into four sections:

- Substances (1):** Shows the chemical structure of Qinghaosu (Artemisinin) with its absolute stereochemistry. The molecular formula is $C_{15}H_{22}O_5$. It includes statistics: 7,714 References, 2,949 Reactions, and 98 Suppliers.
- Reactions (2,949):** Displays a reaction scheme (Scheme 1) with 55 reactions and a 100% yield. It shows the conversion of the starting material to the product, both with absolute stereochemistry shown. There are 98 suppliers for the starting material and 86 for the product.
- References (7,828):** Lists two references:
 - Qinghaosu (Artemisinin): The Price of Success** by White, N. J. (Science, 2008, 320(5874), 330-334). A review discussing the development and use of Artemisinin and its derivatives in antimalarial treatment.
 - Qinghaosu (artemisinin): an antimalarial drug from China** by Klayman, Daniel L. (Science, 1985, 228(4703), 1049-55). A review with 94 references on the pharmacology of Artemisinin.
- Suppliers (98):** A table listing suppliers for the substance.

Supplier	Substance	Purity	Purchasing Details	Availability
1				
AK Scientific AK Scientific Product Catalog United States	63968-64-9 Artemisinin	≥99%	Order From Supplier 1g, USD 54 5g, USD 159 Bulk Screening	Maintained in stock Ships within 1 week
2				
AK Scientific AK Scientific Product Catalog United States	63968-64-9 Artemisinin	95-98%	Order From Supplier 1g, USD 14 5g, USD 21 25g, USD 54 100g, USD 147 500g, USD 507 Bulk Screening	Maintained in stock Ships within 1 week

Search in All: 无需逐步在不同信息中检索，提高检索效率

大纲

- CAS及CAS SciFinderⁿ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
- 常见问题及解决

大纲

- CAS SciFinderⁿ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



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 image shows two screenshots of a search interface. The left screenshot shows a search for "TLR or 'toll like receptor'" with a search bar containing the text and a search button. The right screenshot shows a search for "toll like receptor" with a search bar containing the text and a search button. Below the search bar in the right screenshot, a list of search results is displayed, including "Toll like receptor (Chlamys farreri gene TLR)" and several "Toll like receptor 4" entries from different mouse strains.

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

CAS SciFinder[®] Saved History Account

Searching for...

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

References

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

"G-protein coupled receptor" Draw

AND journal of medici

Journal of Medicinal Chemistry

- Journal of medical virology
- Journal of medical entomology
- Journal of medical education
- Journal of medical Internet research
- Journal of medical genetics
- Journal of medical case reports
- Journal of medical ethics
- Journal of medical microbiology
- Journal of medical systems

Volume (Optional)

Starting Page (Optional)

+ Add Advanced Search Field

AND

OR

NOT

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

Learn more about SciFinder[®] 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

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

Substances Reactions Citing

Relevance
Times Cited
Publication Date: Newest
Publication Date: Oldest



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: CAPLUS 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 effects...

[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: 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 discuss...

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文献类型

文献语言

文献结果集

研究发展趋势



CAS标引的
技术术语

- Available at My Institution
- Author
- Organization
- Publication Name

CAS学科
研究方向

- Concept
 - Homo sapiens (4,956)
 - Human (4,956)
 - Animals (4,261)
 - Humans (3,732)
 - Toll-like receptor 4 (3,128)
- View All

制剂/分析
方法信息

- CA Section
 - CAS Solutions
 - Formulus (1,184)
 - Analytical Methods (5)

二次检索

- 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.

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

3

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

Oncolmunology (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 cancer therapy.

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

4

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: CAPlus and MEDLINE

TLR-Conjugates

- Antigens**
Self-advjuvating vaccines
- Adjuvants**
Multi-valent immunostimulants
- Polymers**
Improved pharmacokinetics
- Fluorophores**
Tracking tools

Immune System Adjuvantation

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...

View More ▾

Full Text ▾ Substances (0) Reactions (0) Citing (42) Citation Map

5

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; Fucikova, Galon, Jerome; Spisek, Radek; Zitvogel, Laurence; et al

Oncolmunology (2016), 5(3), e1088631/1-e1088631/11 | Language: English, Database: CAPlus 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...

View More ▾

Full Text ▾ Substances (0) Reactions (0) Citing (48) Citation Map

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

<input type="checkbox"/> Homo sapiens (4,956)	<input type="checkbox"/> Dendritic Cells (943)	<input type="checkbox"/> Cell differentiation (606)
<input type="checkbox"/> Human (4,956)	<input type="checkbox"/> Antigens (925)	<input type="checkbox"/> Interleukin 2 (599)
<input type="checkbox"/> Animals (4,261)	<input type="checkbox"/> Cell proliferation (908)	<input type="checkbox"/> CD86 antigens (598)
<input type="checkbox"/> Humans (3,732)	<input type="checkbox"/> CD4-positive T cell (857)	<input type="checkbox"/> Interferon β (598)
<input checked="" type="checkbox"/> Toll-like receptor 4 (3,128)	<input type="checkbox"/> CD8-positive T cell (850)	<input type="checkbox"/> Protein phosphorylation (595)
<input type="checkbox"/> Mice (2,892)	<input type="checkbox"/> Antibodies and Immunoglobulins (841)	<input type="checkbox"/> Immunoglobulin G (593)
<input type="checkbox"/> Signal transduction (2,867)	<input type="checkbox"/> Adjuvants, Immunologic (831)	<input type="checkbox"/> Interleukin 4 (590)
<input checked="" type="checkbox"/> Toll-like receptors (2,608)	<input type="checkbox"/> Monocyte (828)	<input type="checkbox"/> Toll-like receptor 1 (590)
<input checked="" type="checkbox"/> Toll-like receptor 2 (2,224)	<input type="checkbox"/> Tumor necrosis factors (826)	<input type="checkbox"/> Mice, Inbred BALB C (589)
<input type="checkbox"/> Interleukin 6 (2,176)	<input type="checkbox"/> Interferon α (815)	<input type="checkbox"/> NF-kappa B (584)
<input type="checkbox"/> Toll-like receptor 7 (2,041)	<input type="checkbox"/> Interleukin 8 (810)	<input type="checkbox"/> Animal gene (560)
<input type="checkbox"/> Cytokines (1,926)	<input type="checkbox"/> Immunotherapy (804)	<input type="checkbox"/> Toll-like receptor agonists (557)
<input checked="" type="checkbox"/> Toll-like receptor 9 (1,812)	<input type="checkbox"/> T cell (771)	<input type="checkbox"/> Adult (544)
<input type="checkbox"/> Soluble tumor necrosis factors (1,799)	<input type="checkbox"/> Immunity, Innate (764)	<input type="checkbox"/> Disease Models, Animal (535)
<input type="checkbox"/> Type II interferons (1,775)	<input type="checkbox"/> Innate immunity (746)	<input type="checkbox"/> Toll-like receptor 6 (529)
<input type="checkbox"/> Female (1,759)	<input type="checkbox"/> Mice, Knockout (720)	<input type="checkbox"/> Immunostimulants (526)
<input type="checkbox"/> Lipopolysaccharides (1,640)	<input type="checkbox"/> Combination chemotherapy (715)	<input type="checkbox"/> Gene Expression Regulation (520)
<input type="checkbox"/> Inflammation (1,608)	<input checked="" type="checkbox"/> Toll-like receptor 5 (705)	<input type="checkbox"/> Melanoma (517)
<input type="checkbox"/> Dendritic cell (1,549)	<input type="checkbox"/> Macrophages (695)	<input type="checkbox"/> CXC chemokine CXCL10 (513)
<input checked="" type="checkbox"/> Toll-like receptor 3 (1,506)	<input type="checkbox"/> Immunity (684)	<input type="checkbox"/> CD80 antigens (495)
<input type="checkbox"/> Mice, Inbred C57BL (1,463)	<input type="checkbox"/> Cell activation (681)	<input type="checkbox"/> Mononuclear leukocyte (490)

Apply Cancel

Concept

Top Count Alphanumeric Search

Concept Name

T cell Search

8 Selected

<input type="checkbox"/> Killer T cell (4)	<input type="checkbox"/> Suppressor T cell (7)	<input type="checkbox"/> T cell receptor therapy (4)
<input type="checkbox"/> Linker for activation of T-cells LA2 (2)	<input checked="" type="checkbox"/> T cell (771)	<input type="checkbox"/> T-cell receptor Vdelta2, human (1)
<input type="checkbox"/> Lymphoma, T-Cell (6)	<input type="checkbox"/> T-cell activation Rho GTPase-activating proteins (1)	<input type="checkbox"/> T-cell receptor Vgamma9, human (1)
<input type="checkbox"/> Lymphoma, T-Cell, Cutaneous (9)	<input type="checkbox"/> T-Cell Antigen Receptor Specificity (4)	<input type="checkbox"/> T Follicular Helper Cells (1)
<input type="checkbox"/> Memory cytotoxic T cell (6)	<input type="checkbox"/> T cell disease (4)	<input type="checkbox"/> Tissue-resident T-cell transcription regulator protein ZNF683 (2)
<input type="checkbox"/> Memory T cell (88)	<input type="checkbox"/> T-cell immune regulator TCIRG1 (1)	<input type="checkbox"/> V-domain Ig suppressor of T-cell activation proteins (73)
<input type="checkbox"/> Mucosal-associated invariant T cell (5)	<input type="checkbox"/> T cell immunoglobulin and mucin domain-containing protein 2 (1)	
	<input type="checkbox"/> T cell immunoglobulin and mucin domain-containing protein 4 (9)	
	<input type="checkbox"/> T cell immunoglobulin and mucin domain-containing proteins (8)	
	<input type="checkbox"/> T-cell leukemia (14)	
	<input type="checkbox"/> T-cell lymphoma (50)	

Apply Cancel

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

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

通过CA Section快速
锁定学科研究方向



ACS
International



文献结果集--聚类筛选CAS Solutions

查看勾选的
Concept

The screenshot displays a search results page with a left-hand filter sidebar and a main content area for references. The filter sidebar includes sections for 'Filter Behavior', 'Document Type', 'Language', 'Publication Year' (with a bar chart), 'Available at My Institution', 'Author', 'Organization', 'Publication Name', 'Concept', 'CA Section', 'CAS Solutions' (with checkboxes for 'Formulus (861)' and 'Analytical Methods (2)'), 'Formulation Purpose', 'Database', and 'Search Within Results'. The 'CAS Solutions' section is highlighted with a blue arrow. The main content area shows a list of references, with the first one selected. A dropdown menu is open over the first reference, showing a list of selected concepts: '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', and 'Toll-like receptor 5'. The references listed include 'The pharmacokinetics of Toll-like receptor agonists and the impact on the immune system', 'Antiviral applications of Toll-like receptor agonists', and 'Trial Watch: Toll-like receptor agonists in cancer immunotherapy'. The interface also shows options for 'Full Text', 'Substances', 'Reactions', 'Citing', and 'Citation Map' for each reference.

直接获得有制
剂方法的文献

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
Available at My Institution
Author
Organization
Publication Name
Concept
CA Section
CAS Solutions
Formulus (861)
Analytical Methods (2)
Formulation Purpose
Database
Search Within Results
Enter a query...

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

Substances Reactions Citing

Filtering: Concept: 8 Selected Clear All Filters

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 effects is important for the development of TLR agonists.
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 how this may be used to improve antiviral therapy.
View More

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

3
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
Oncoimmunology (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 immunotherapy.
View More

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

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
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Include: Task History Abstract Concepts Substances Formulations Analytical Methods Citations
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Download: 可保存成ris、PDF、rtf、Excel格式

点击文献标题查看文献详情

文献详情

被引文献

引文地图

The screenshot shows a CAS Reference Detail page for the article "Antiviral applications of Toll-like receptor agonists" by Horscroft, Nigel J.; Pryde, David C.; Bright, Helen. The page includes a left sidebar with journal information (Journal of Antimicrobial Chemotherapy, Volume 67, Issue 4, 2012) and database information (AN: 2012:423823, CAN: 156:387108, PubMed ID: 22258929). The main content area features the article title, authors, abstract, and keywords. A navigation bar at the top includes "Citing (42)" and "Citation Map" buttons. A "Full Text" dropdown menu is highlighted with a blue box and labeled "获取原文". Below the article text, there are expandable sections for "Concepts", "MEDLINE® Medical Subject Headings", "Substances", and "Cited Documents", each with a blue arrow pointing to it from the right. The "Cited Documents" section is specifically labeled "参考文献".

文献详情界面包括:

- 标题
- 摘要
- 文献中重要的技术术语 (含Capius、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:
CAS科学家提供的标准技术术语，
能更全面、更精准地检索。

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

^ 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:
从不同的专业角度将文献研究
核心点标出，更全面了解文献

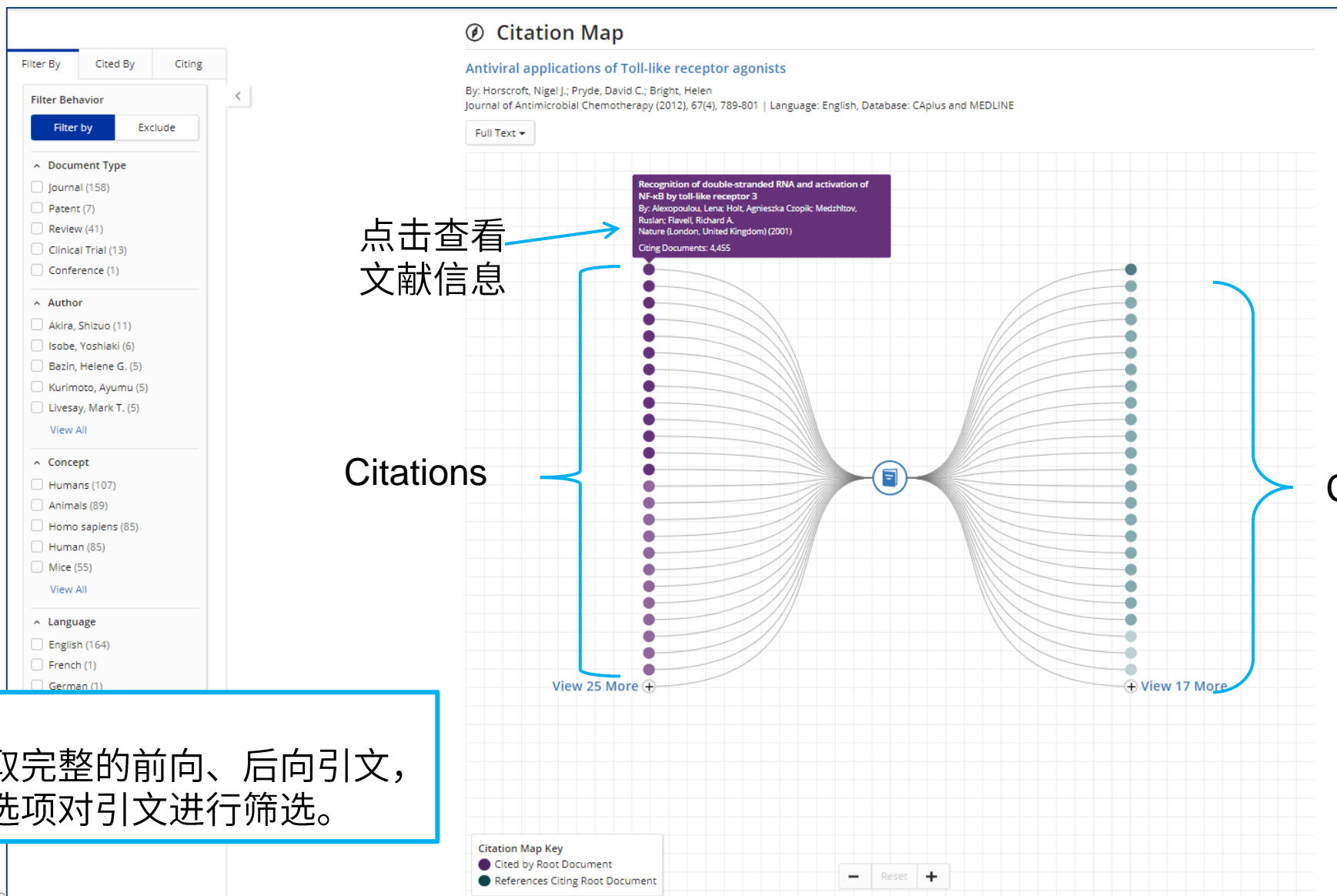
^ Substances	
☰ Substance (1)	
9008-11-1	Image Not Available
Unspecified Interferons	
Role: Unspecified	

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。



点击查看
文献信息

Citations

Cited By

文献检索--主题词+结构联合检索

Searching for...

All
Substances
Reactions

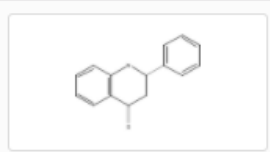
References

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

Antitumor

+ Add Advanced Search Field

Learn more about Sci



Edit Drawing Remove

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)
[View All](#)

Language
 English (67)
 Czech (4)
 Chinese (3)
 Korean (1)

Publication Year


No Min to No Max Apply
[View Larger](#)

Available at My Institution

References (75)

Sort: Relevance View: Partial Abstract

Substances Reactions Citing Save

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: CPlus 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 ED₅₀ values in the nanomolar or subnanomolar range in almost all.

Full Text Substances (41) Reactions (26) Citing (256) Citation Map

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, Pabbaraja; Reddy, Chada Raji; Janaki Ramaiah, M.; Bhadra, Utpal
Bioorganic & Medicinal Chemistry Letters (2012), 22(1), 645-648 | Language: English, Database: CPlus 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.

Full Text Substances (18) Reactions (7) Citing (32) Citation Map

3

Relationship between structure and antiproliferative activity of 1-azaflavonones
By: Kawaii, Satoru; Endo, Kotaro; Tokiwano, Tetsuo; Yoshizawa, Yuko
Anticancer Research (2012), 32(7), 2819-2826 | Language: English, Database: CPlus
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-azaflavonones.

Full Text Substances (40) Reactions (22) Citing (9) Citation Map

主题词+结构联合检索
大大提高检索的效率

文献检索小结

1. 使用布尔逻辑算符and、or、not连接主题词
2. 通过聚类筛选工具快速获得目标文献
3. 用CAS Solutions选项快速获取信息
4. 从引文地图拓展检索，获得更多灵感
5. 用PatentPak提高专利阅读效率
6. 主题词+结构联合检索快速获得文献



大纲

- CAS SciFinderⁿ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



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

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...

Molecular Formula

Draw

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

Learn more about SciFinder® Advanced Search.

+ Add Advanced Search Field

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

1 50-56-6

Absolute stereochemistry shown

$C_{43}H_{66}N_{12}O_{12}S_2$
Oxytocin
Protein/Peptide Sequence
Sequence Length: 9

31K References 390 Reactions 66 Suppliers

2 1190307-88-0

Absolute stereochemistry shown

$C_{22}H_{29}FN_3O_9P$
Sofosbuvir

3,695 References 720 Reactions 66 Suppliers

3 1809249-37-3

Absolute stereochemistry shown

$C_{27}H_{35}N_6O_8P$
GS 5734

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 image displays two screenshots of the CAS SciFinder search interface. The left screenshot shows a search for 'flavone*' resulting in 4,467 substances. The right screenshot shows a search for 'flavone?' resulting in 20 substances. A text box at the bottom center states: '物质名称中使用通配符可以检索多个物质' (Using wildcards in substance names can retrieve multiple substances).

Left Screenshot (Search: flavone*)

- Substances: 4,467
- Sort: Relevance
- View: Partial
- Filter Behavior: Filter by (selected), Exclude
- Commercial Availability: Available (1,873), Not Available (2,594)
- Reaction Role: Product (1,934), Reactant (729), Reagent (15), Catalyst (12), Solvent (1)
- Reference Role: Preparation (3,950), Synthetic Preparation (2,005), Biological Study (1,445), Properties (1,219), Biological Study, Unclassified (1,127)
- Stereochemistry: View All
- Number of Components: View All
- Substance Class: View All
- Isotopes: View All
- Metals: View All
- Molecular Weight: View All

Right Screenshot (Search: flavone?)

- Substances: 20
- Sort: Relevance
- View: Partial
- Filter Behavior: Filter by (selected), Exclude
- Commercial Availability: Available (1), Not Available (19)
- Reference Role: Biological Study (18), Uses (17), Therapeutic Use (12), Biological Study, Unclassified (8), Pharmacological Activity (8)
- Number of Components: View All
- Substance Class: View All
- Isotopes: View All
- Metals: View All
- Experimental Property: View All
- Bioactivity Indicator: View All

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

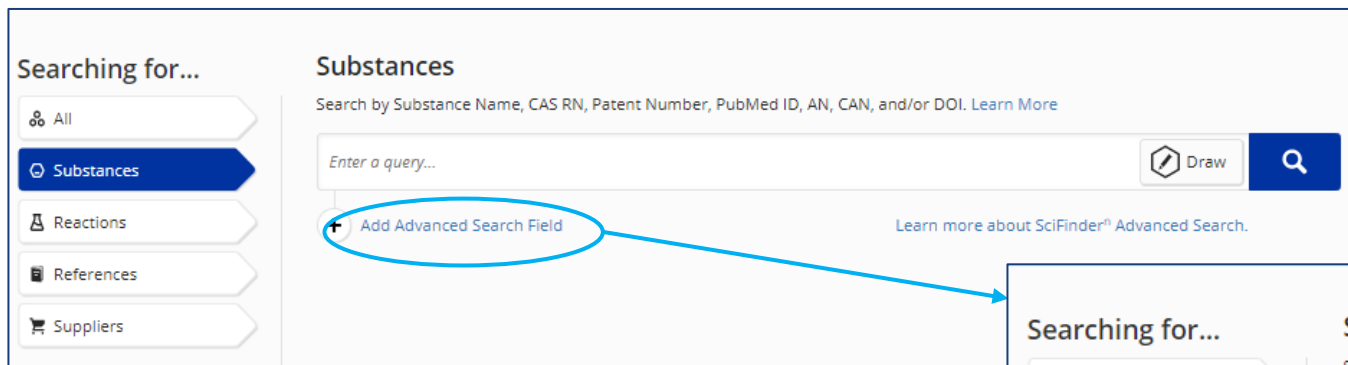
The screenshot displays the CAS SciFinder search results page for the patent number WO2011123645. The interface includes a search bar at the top with the patent number entered. Below the search bar, there are navigation options like 'Return to Home' and 'Substances (129)'. A filter sidebar on the left allows users to refine results by 'Commercial Availability', 'Reaction Role', 'Reference Role', 'Stereochemistry', 'Number of Components', 'Substance Class', 'Isotopes', 'Metals', 'Molecular Weight', 'Experimental Property', 'Experimental Spectrum', 'Regulatory Data by Country', 'Regulatory Data by List', 'Bioactivity Indicator', and 'Target Indicator'. The main content area shows a grid of 9 substance cards, each with a chemical structure, name, and associated data (References, Reactions, Suppliers).

Card #	Patent #	Chemical Name	Formula	References	Reactions	Suppliers
1	108-95-2	Phenol	C ₆ H ₆ O	215K	91K	188
2	108-24-7	Acetic anhydride	C ₄ H ₆ O ₃	153K	375K	80
3	100-46-9	Benzylamine	C ₇ H ₉ N	57K	93K	82
4	18162-48-6	tert-Butyldimethylsilyl chloride	C ₆ H ₁₅ ClSi	36K	64K	127
5	10025-87-3	Phosphorus oxychloride	Cl ₃ OP	25K	214K	46
6	58-96-8	Uridine	C ₉ H ₁₂ N ₂ O ₆	24K	3,429	106
7	149-30-4	2-Mercaptobenzothiazole	C ₇ H ₅ NS ₂	18K	6,303	120
8	501-53-1	Benzyl chloroformate	C ₈ H ₇ ClO ₂	17K	28K	75
9	616-47-7	1-Methylimidazole	C ₄ H ₆ N ₂	16K	34K	112

专利号
WO2011123645

帮助用户迅速获得关
注文献中的所有物质

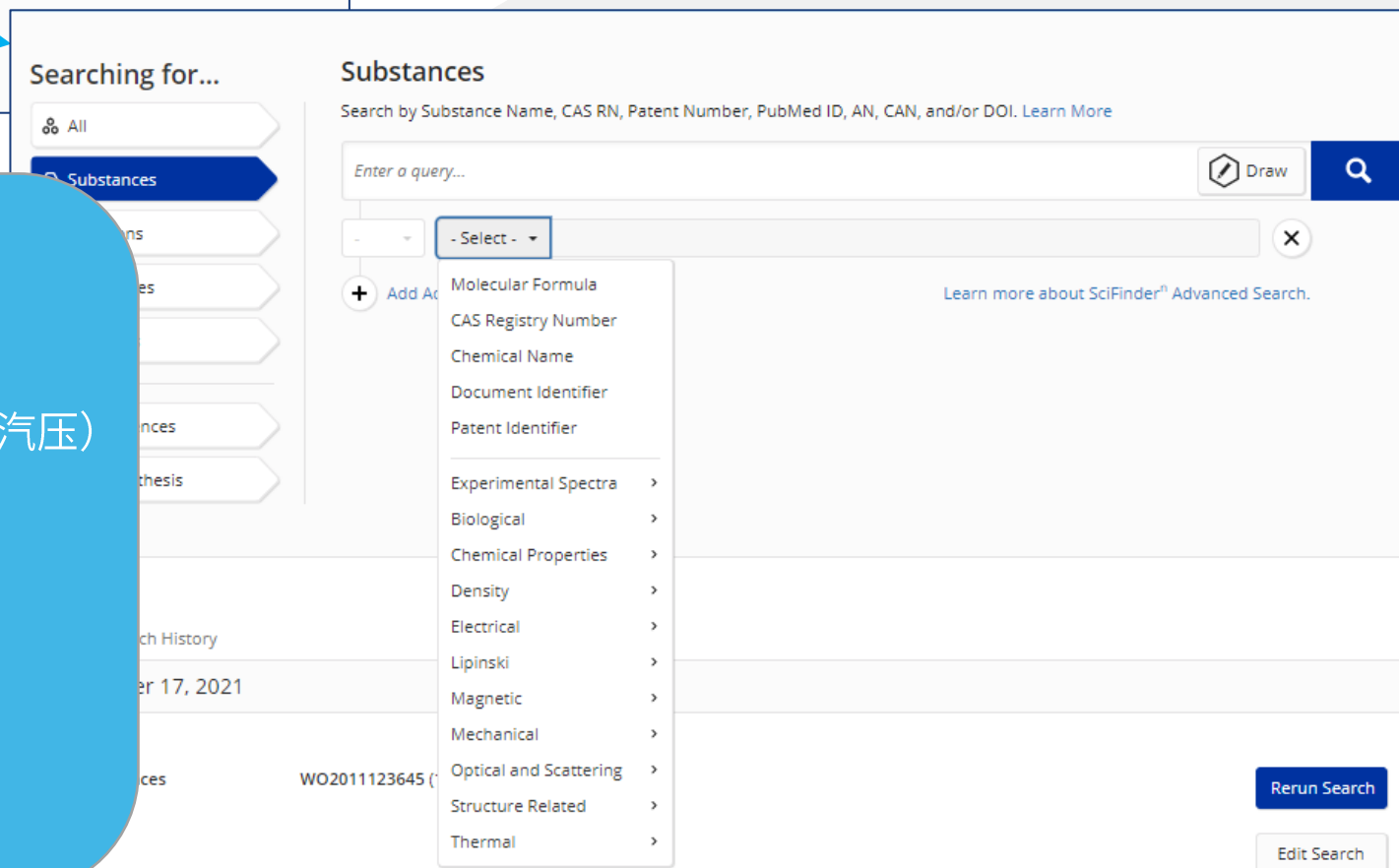
物质检索--Advanced Search



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)



物质检索--分子式

Na₂SO₄: H₂O₄S.2Na

Searching for...

Substances

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

Enter a query...

Molecular Formula H₂SO₄.2Na

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

+ 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)
- Number of Components
- Substance Class
- Isotopes
- Metals
- Molecular Weight
- Experimental Property
- Experimental Spectrum
- Regulatory Data by Country

Substances (9)

Sort: Relevance View: Partial

References Reactions Suppliers

<p>1</p> <p>7757-82-6</p>  <p>• 2 Na</p> <p>H₂O₄S.2Na</p> <p>Components: 2</p> <p>Component RN: 7664-93-9</p> <p>Sodium sulfate</p> <p>103K References 51K Reactions 178 Suppliers</p>	<p>2</p> <p>13759-07-4</p>  <p>• 2 Na</p> <p>H₂O₄S.2Na</p> <p>Components: 2</p> <p>Component RN: 7664-93-9</p> <p>Thenardite (Na₂(SO₄))</p> <p>906 References 0 Reactions 1 Supplier</p>	<p>3</p> <p>14262-80-7</p>  <p>• 2 Na</p> <p>H₂O₄S.2Na</p> <p>Components: 2</p> <p>Component RN: 13770-01-9</p> <p>Sulfuric-³⁵S acid, disodium salt</p> <p>73 References 1 Reaction 4 Suppliers</p>
<p>4</p> <p>225640-22-2</p>  <p>• 2 Na</p> <p>H₂O₄S.2Na</p> <p>Components: 2</p> <p>Component RN: 778561-01-6</p> <p>Sulfuric-³⁴S acid, disodium salt</p> <p>8 References 1 Reaction 1 Supplier</p>	<p>5</p> <p>20581-68-4</p>  <p>• 2 Na</p> <p>H₂O₄S.2Na</p> <p>Components: 2</p> <p>Component RN: 7664-93-9</p> <p>Metathenardite (Na₂(SO₄))</p> <p>3 References 0 Reactions 0 Suppliers</p>	<p>6</p> <p>911392-46-6</p>  <p>• 2 Na</p> <p>H₂O₄S.2Na</p> <p>Components: 2</p> <p>Component RN: 911422-29-2</p> <p>Sulfuric-³³S acid, disodium salt</p> <p>1 Reference 0 Reactions 1 Supplier</p>

金属盐：金属离子和阴离子间用点 (.) 分开
不同组份之间用点 (.) 分开

物质检索--物性参数

密度>150g/cm³
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](#)

Enter a query...

Density (g/cm³) >150

Include predicted values. [Examples: 1.15](#)

AND Molecular Weight <200

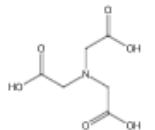
Predicted values only. [Error](#)


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

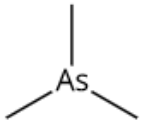
多参数检索，提高检索效率

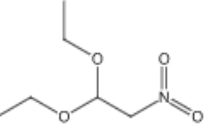
Substances (6) Sort: Relevance View: Partial

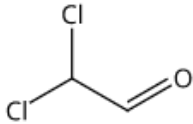
References Reactions Suppliers

1 139-13-9

C₆H₉NO₆
Nitrilotriacetic acid
13K References 713 Reactions 91 Suppliers

2 7631-86-9

O₂Si
Silica
1.1M References 90K Reactions 407 Suppliers

3 593-88-4

C₃H₉As
Trimethylarsine

4 34560-16-2

C₆H₁₃NO₄
1,1-Diethoxy-2-nitroethane
25 References 42 Reactions 50 Suppliers

5 79-02-7

C₂H₂Cl₂O
Dichloroacetaldehyde
671 References 122 Reactions 16 Suppliers

CAS RN 139-13-9
CAS Name Nitrilotriacetic acid

Substance Detail
Reactions (713)
Synthesize (48)
Create Retrosynthesis Plan
References (13K)
Suppliers (91)

Edit Structure - Reset +

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 ± 0.2 ppm. Examples: 8.03, 7.2, 2

AND Carbon-13 NMR 44.5 to 45
Allowance of ± 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

1 1354644-05-5
Absolute stereochemistry shown, Rotation (+)
C21H28O2
(4bS,6aS,7R,11aS,11bR)-4b,6,6a,7,8,11,11a,11b,12,13-Decahydro-2-methoxy-6a-methy...

2 921073-43-0
C21H23NO5S
4-[5,6-Dimethoxy-1-[(4-methylphenyl)sulfonyl]-1H-indol-2-yl]-2-butanone

3 35387-16-7
C11H10N2O2
2,3-Dihydro-3-hydroxypyrrrolo[2,1-b]quinazolin-9(1H)-one

4 879288-35-4
Absolute stereochemistry shown, Rotation (-)
C29H36O10
Methyl (4S,4aS,6aR,7S,8S,10R,11R,12R,12aR,12bS)-12-(acetyloxy)-4-(3-furanyl)dode...

5 693235-19-7
C14H16N2O3
Acetamide, N-(decahydro-3-hydroxy-2-oxo-3,7,4,6-ethanediyldene-7aH-pentaleno[1,...

6 1245281-17-7
Absolute stereochemistry shown
C16H18N2O2
N-Methyl-N-[(4R,5R)-1,3,4,5-tetrahydro-5-(2-oxopropyl)benz[cd]indol-4-yl]formami...

物质详情

Substance Detail (1 of 1,143)

← Prev Next →

References (2) Reactions (4) Supplier (1) Download Email 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-decahydro-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 ³	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

¹H NMR **¹³C NMR**

	Source
View Carbon-13 NMR Spectrum	(1) ACD

Sources

(1) Saloranta, Tiina; Steroids, (2012), 77(1-2), 110-117, CPlus

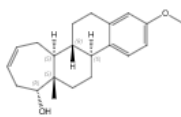
Predicted Properties

Predicted Spectra

Bioactivity Indicators

Carbon-13 NMR Spectrum Detail (1 of 1)

1354644-05-5



Absolute stereochemistry shown. Rotation (+)

C₂₁H₂₈O₂

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

Conditions

Working Frequency
150 MHz

Solvent
[Chloroform-d \(865-49-6\)](#)

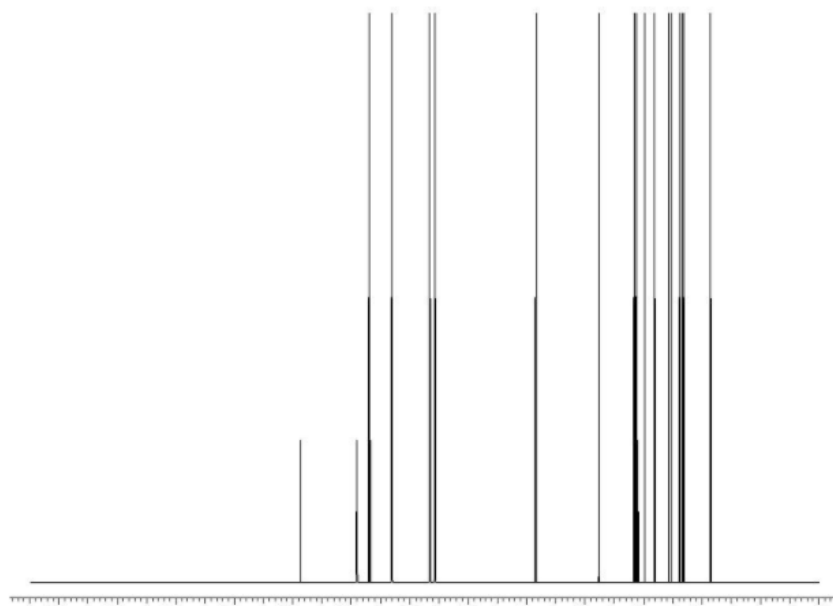
Temperature
25 °C

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.



240 220 200 180 160 140 120 100 80 60 40 20 0 -20

- Reset +

物质检索--结构检索

Searching for...

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

Substances

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

Enter a query...

Draw

Molecular Formula

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

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

CAS Draw

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

Draw or change atoms or bonds.

Molecular Formula:

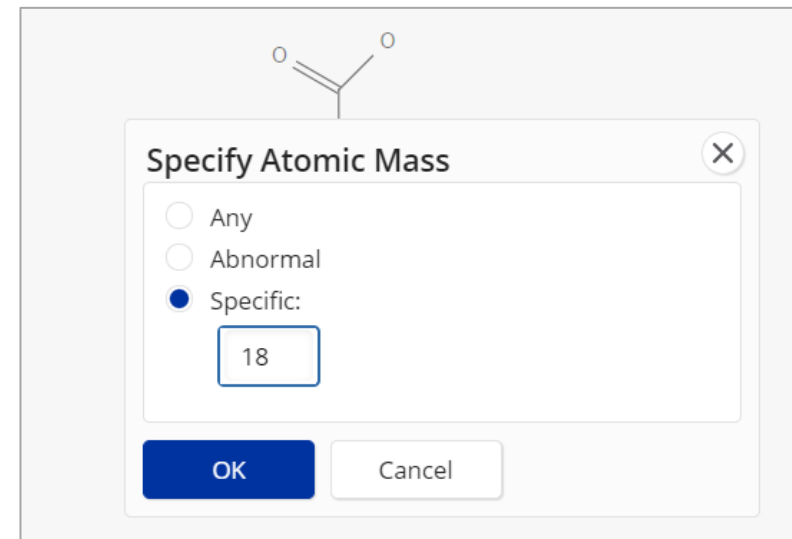
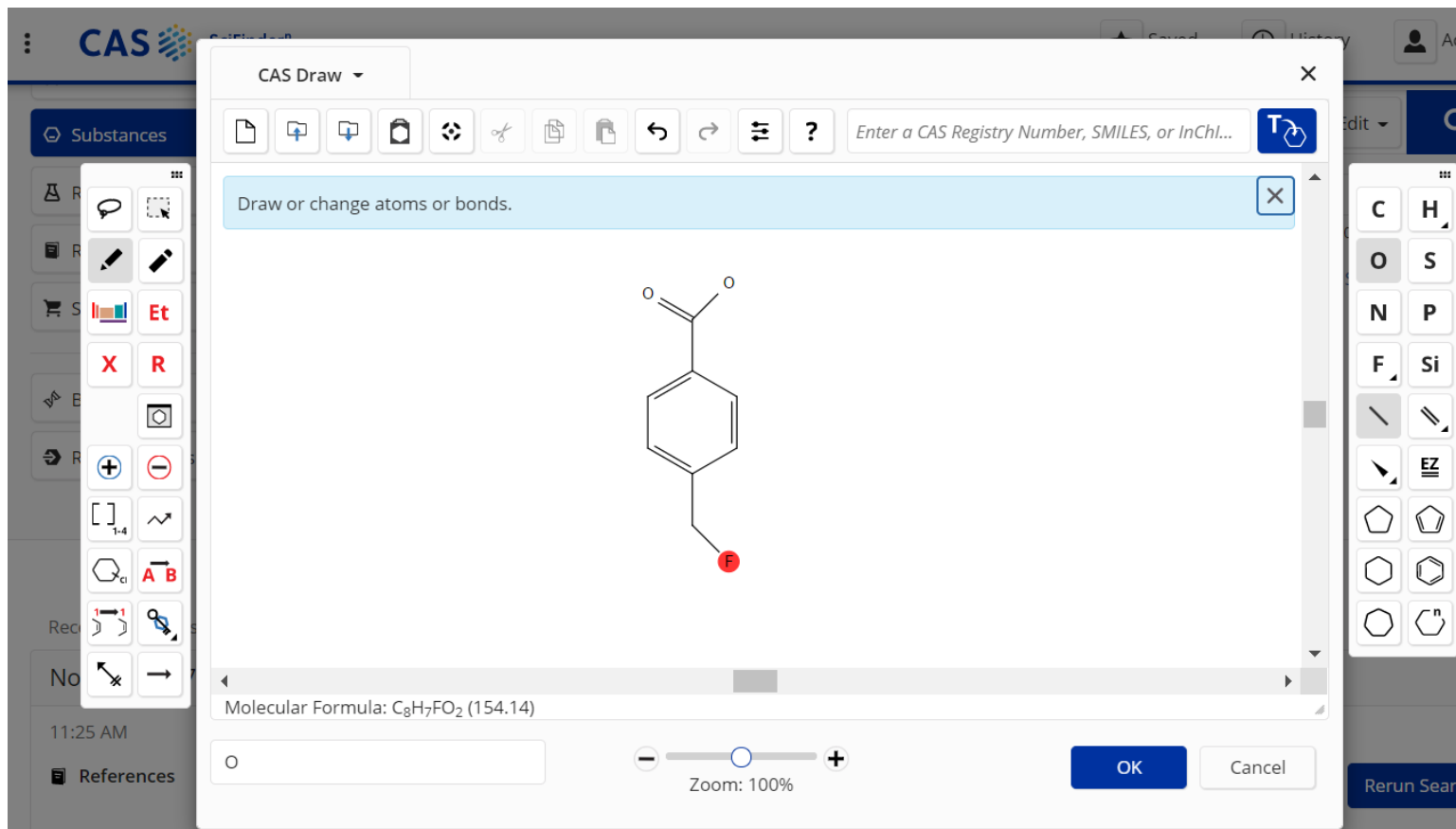
C

Zoom: 100%

OK Cancel

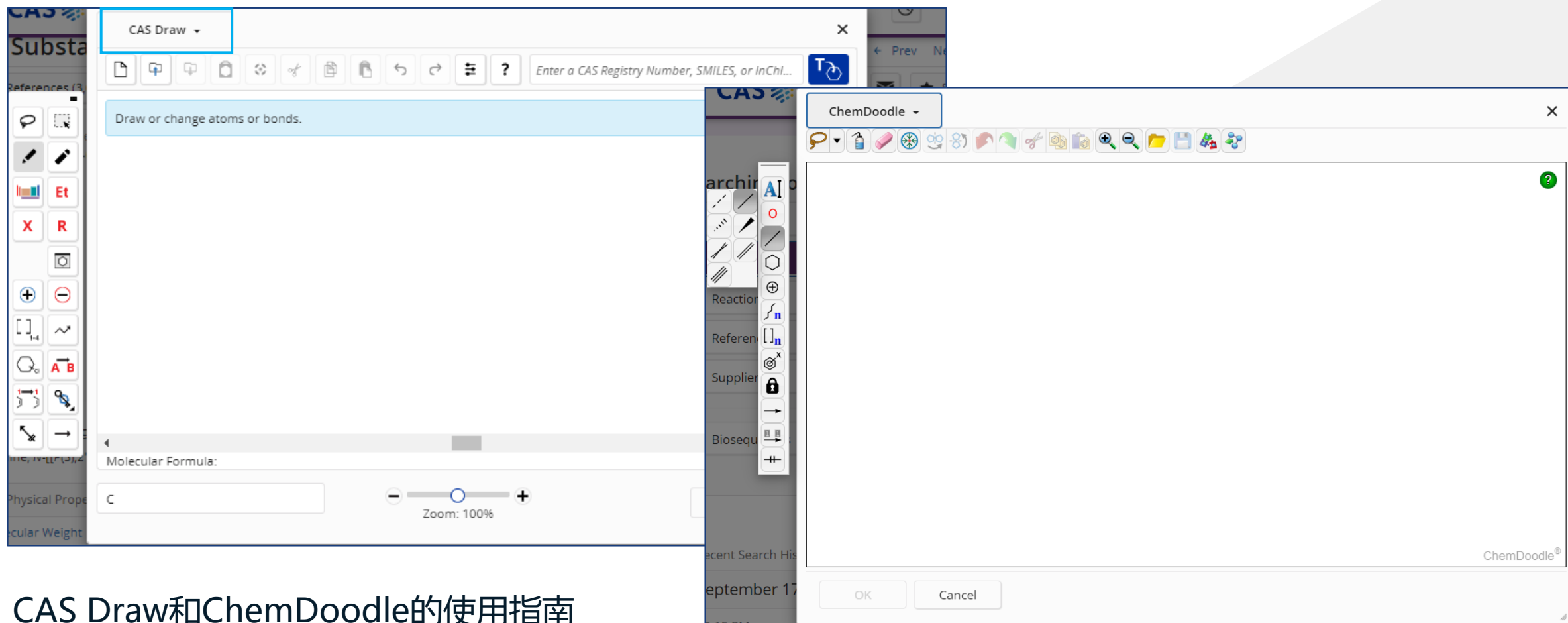
- X 选择可变基团
- R 自定义R基团
- 重复片段工具
- 取代位点可变
- 锁工具

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

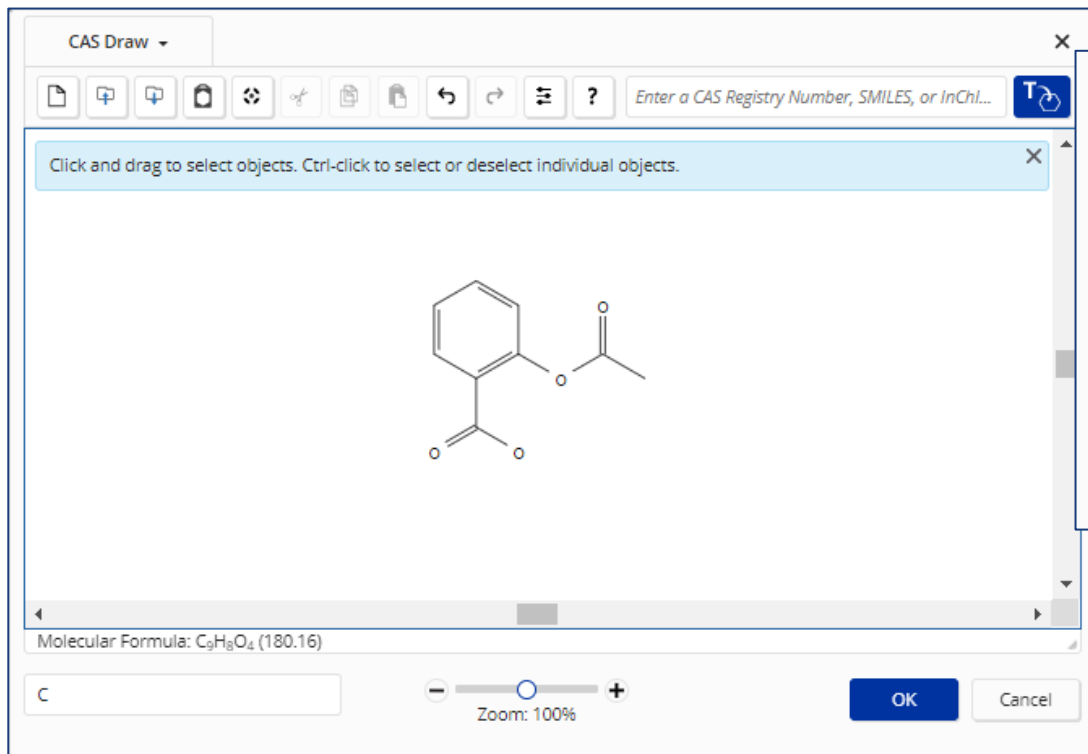
https://scifinder-n.cas.org/help/#t=Drawing_Search_Queries%2FDrawing_Structure_Queries.htm

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

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

物质检索--结构检索

CAS RN: 50-78-2



Substances

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

Enter a query...

AND Molecular Formula

Examples: C₆H₆ | (C₈H₈)_x | C₁₀H₈

Learn more about Sci

Search Patent Markush

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

Filter by选择感兴趣的结果,
或Exclude排除不需要的结果

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

References Reactions Suppliers

1 50-78-2

CC(=O)OC1=CC=CC=C1C(=O)O

C₉H₈O₄
Aspirin

84K References 1,997 Reactions 108 Suppliers

2 5054-56-8

CC(=O)OC1=CC=CC=C1C(=O)O

C₉H₇O₄
Benzoic acid, 2-(acetyloxy)-, (1S)-

19 References 0 Reactions 2 Suppliers

3 59096-15-0

CC(=O)OC1=CC=CC=C1C(=O)O

C₉H₈O₄
2-Acetylsalicylic acid homopolymer

16 References 0 Reactions 0 Suppliers

4 97781-16-3

CC(=O)OC1=CC=C(C(=O)O)C=C1

C₉H₄D₄O₄
Benzoic-2,3,4,5-d₄ acid, 6-(acetyloxy)-

8 References 5 Reactions 24 Suppliers

5 921943-73-9

CC(=O)OC1=CC=C(C(=O)O)C=C1

C₉H₅D₃O₄
2-(Acetyl-2,2,2-d₃-oxy)benzoic acid

5 References 0 Reactions 18 Suppliers

6 59096-14-9

CC(=O)OC1=CC=C(C(=O)O)C=C1

C₉H₈O₄
Benzoic-carboxy-¹⁴C acid, 2-(acetyloxy)-

5 References 0 Reactions 3 Suppliers

7 215935-30-1

CC(=O)OC1=CC=C(C(=O)O)C=C1

C₉H₇DO₄
2-(Acetyl-2-d-oxy)benzoic acid

4 References 0 Reactions 0 Suppliers

8 229030-56-2

CC(=O)OC1=CC=C(C(=O)O)C=C1

C₉H₈O₄
Benzoic acid, 2-(acetyl-1-¹³C-oxy)-

3 References 0 Reactions 1 Supplier

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

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……

The screenshot displays a search interface for chemical substances. On the left, a sidebar contains filters for 'Structure Match' (As Drawn: 927, Substructure: 20K, Similarity: 79K), 'Chemscape Analysis' (visually explore structure similarity), and 'Filter Behavior' (Filter by, Exclude). Below these are expandable sections for '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), 'Stereochemistry', 'Number of Components', 'Substance Class', 'Isotopes', 'Metals', and 'Molecular Weight'. The main area shows a grid of 12 substance cards, each with a chemical structure, name, formula, and counts for references, reactions, and suppliers. The substances listed include Aspirin, Benzoic acid, 2-(acetyloxy)-, ion(1-), 2-Acetylsalicylic acid homopolymer, Benzoic-2,3,4,5-d₄ acid, 6-(acetyloxy)-, 2-(Acetyl-2,2,2-d₃-oxy)benzoic acid, Benzoic acid, 2-(acetyl-1-¹⁴C-oxy)-, Benzoic-carboxy-¹⁴C acid, 2-(acetyloxy)-, 2-(Acetyl-2-d₂-oxy)benzoic acid, Benzoic acid, 2-(acetyl-1-¹³C-oxy)-, and 2566849-38-3.



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

利用物质反应角色获得
做过催化剂研究的物质

利用物质在反应中的角色精准定位相应的物质

The screenshot displays a search interface for chemical substances. On the left, a sidebar contains various filters, with 'Reaction Role' expanded to show 'Catalyst (20)' selected. The main area shows a grid of 9 substance cards, each with a chemical structure, name, formula, and counts for references, reactions, and suppliers. The substances are filtered by 'Reaction Role: Catalyst'.

ID	Chemical Name	Formula	References	Reactions	Suppliers
50-78-2	Aspirin	C ₉ H ₈ O ₄	84K	1,997	108
1803201-02-6	Benzenecetic acid, 2-[(2-methylpropoxy)carbonyl]phenyl ester	C ₁₉ H ₂₀ O ₄	1	1	0
875584-96-6	2-Methylpropyl 2-(benzoyloxy)benzoate	C ₁₈ H ₁₈ O ₄	4	4	2
2093113-55-2	Benzoic acid, 2-(2,2-dimethyl-1-oxopropoxy)-3-methyl-, 2-methylpropyl ester	C ₁₇ H ₂₄ O ₄	2	2	0
2093113-56-3	Benzoic acid, 2-(benzoyloxy)-3-methyl-, 2-methylpropyl ester	C ₁₉ H ₂₀ O ₄	2	2	0
2093113-57-4	Benzoic acid, 2-(benzoyloxy)-3,5-bis(1-methylethyl)-, 2-methylpropyl ester	C ₂₄ H ₃₀ O ₄	2	3	0
1416949-86-4	1'-[1,4-Butanediylbis(oxyethylidene)]bis[2-(acetyloxy)benzoate]	C ₁₆ H ₃₀ O ₁₀	1	2	0
2093113-58-5	Benzoic acid, 2-(benzoyloxy)-3,5-bis(1,1-dimethylethyl)-, 2-methylpropyl ester	C ₂₆ H ₃₄ O ₄	2	2	0
948830-92-0	Methyl 1-(acetyloxy)-3-hydroxy-7-methoxy-6-[2-(trimethylsilyl)ethynyl]-2-naphtha...	C ₂₀ H ₂₂ O ₆ Si	1	12	0

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)
- Cosmetic Use (372)
- Polymer in Formulation (314)
- Food or Feed Use (248)
- Analytical Study (237)
- Pharmacokinetics (229)
- Adverse Effect (189)
- Modifier or Additive Use (189)
- Analyte (167)
- Catalyst Use (102)
- Purification or Recovery (85)
- Biological Use, Unclassified (82)
- Formation, Unclassified (67)
- Occurrence (61)
- Natural Product Occurrence (39)
- Analytical Matrix (36)
- Analytical Role, Unclassified (36)
- Analytical Reagent Use (27)
- Reagent (26)
- Pollutant (22)
- Nanoscale (21)
- Byproduct (17)
- Biosynthetic Preparation (14)
- Diagnostic Use (10)
- Occurrence, Unclassified (8)
- Bioindustrial Manufacture (7)
- Combinatorial Study (6)
- Miscellaneous (6)
- Biochemical Process (4)
- Removal or Disposal (4)
- Geological or Astronomical Occurrence (1)
- Geological or Astronomical Process (1)

Apply | Cancel

Substances (39)

Sort: Relevance | View: Partial

Filtering: Reference Role: Natural Product Occurrence (39)

<p>50-78-2</p> <p><chem>CC(=O)Oc1ccc(O)cc1</chem></p> <p>C₉H₈O₄ Aspirin</p> <p>84K References 1,997 Reactions 108 Suppliers</p>	<p>1247764-46-0</p> <p>1150656-00-0 Image Not Available</p> <p><chem>CC(=O)Oc1ccc(O)cc1</chem></p> <p>C₉H₈O₄, Unspecified Components: 2 Benzoic acid, 2-(acetyloxy)-, mixt. with Tetrahop</p> <p>1 Reference 0 Reactions 0 Suppliers</p>	<p>1247764-40-4</p> <p>664979-08-2 Image Not Available</p> <p><chem>CC(=O)Oc1ccc(O)cc1</chem></p> <p>C₉H₈O₄, Unspecified Components: 2 Benzoic acid, 2-(acetyloxy)-, mixt. with redihop</p> <p>1 Reference 0 Reactions 0 Suppliers</p>
<p>51-01-4</p> <p><chem>CC(=O)Oc1ccc(O)cc1</chem></p> <p>C₁₁H₁₀O₆ 2,4-Bis(acetyloxy)benzoic acid</p> <p>75 References 171 Reactions 9 Suppliers</p>	<p>756455-72-8</p> <p><chem>CCCCCCCCCCCCCCCC(=O)Oc1ccc(O)cc1</chem></p> <p>C₂₃H₃₀O₄ 2-[(1-Oxohexadecyl)oxy]benzoic acid</p> <p>8 References 4 Reactions 0 Suppliers</p>	<p>36081-01-3</p> <p><chem>O=C(O)c1ccc(O)c(O)c1</chem></p> <p>C₁₄H₁₀O₇ 2,4-Dihydroxy-6-[(4-hydroxybenzoyl)oxy]benzoic acid</p> <p>3 References 8 Reactions 1 Supplier</p>
<p>2724988-28-5</p> <p><chem>CC(=O)Oc1ccc(O)cc1</chem></p> <p>View All</p>	<p>55045-01-7</p> <p><chem>CC(=O)Oc1ccc(O)cc1</chem></p> <p>View All</p>	<p>1350977-80-8</p> <p><chem>CC(=O)Oc1ccc(O)cc1</chem></p> <p>View All</p>

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

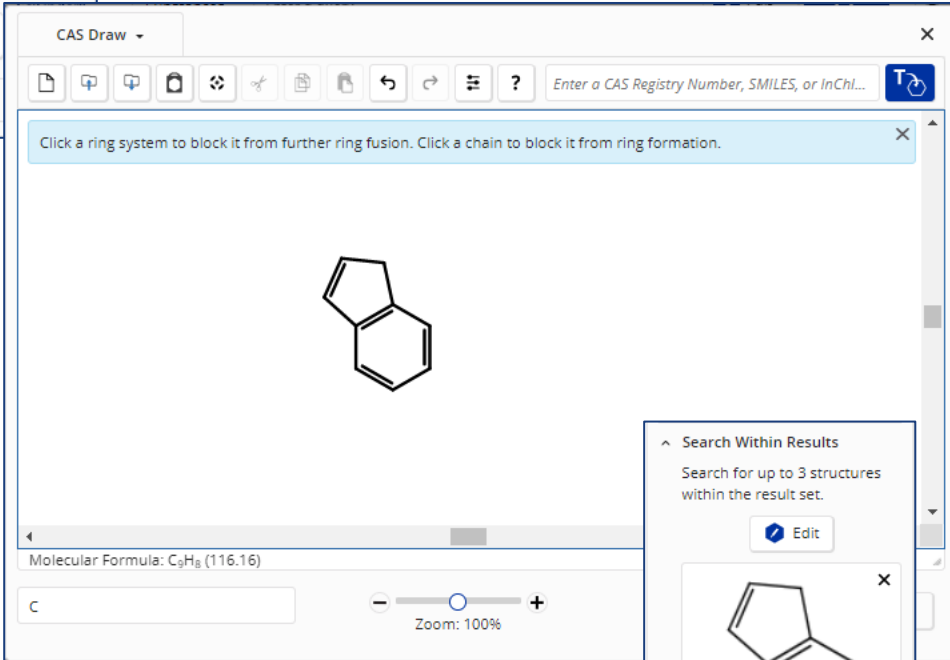
Search Within Results
Search for up to 3 structures within the result set.

Draw

CAS Draw

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

Click a ring system to block it from further ring fusion. Click a chain to block it from ring formation.



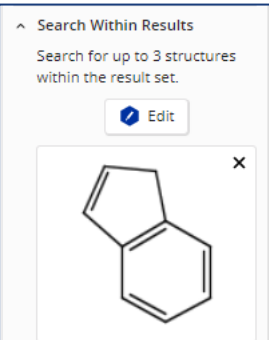
Molecular Formula: C₉H₈ (116.16)

c

Zoom: 100%

Search Within Results
Search for up to 3 structures within the result set.

Edit



As Drawn
 Substructure

Search

利用物质筛选工具
快速锁定目标物质

Substances (13)

Sort: Relevance View: Partial

References Reactions Suppliers

Filtering: Search Within Results: Drawn Structure Clear All Filters

1 218453-29-3 C ₂₈ H ₃₂ O ₅ Ethyl 2-(2,2-dimethyl-1-oxopropoxy)-5-[[5-(methylthio)-2-propyl-1H-inden-1-ylidene... 1 Reference 1 Reaction 0 Suppliers	2 218453-26-0 C ₂₈ H ₃₂ O ₅ Ethyl 2-(2,2-dimethyl-1-oxopropoxy)-5-[[E]-5-(methylsulfonyl)-2-propyl-1H-inden... 1 Reference 1 Reaction 0 Suppliers	3 218453-25-9 C ₂₈ H ₃₂ O ₅ Ethyl 2-(2,2-dimethyl-1-oxopropoxy)-5-[[Z]-5-(methylsulfonyl)-2-propyl-1H-inden... 1 Reference 1 Reaction 0 Suppliers
4 1962179-79-8 C ₂₇ H ₃₀ O ₇ Benzoic acid, 2-(2,3-dihydro-1-oxo-1H-inden-2-yl)-3,6-bis(2,2-dimethyl-1-oxoprop... 1 Reference 3 Reactions 0 Suppliers	5 1168965-99-8 C ₂₈ H ₃₂ N ₂ O ₈ 1H-Indene-2-carboxylic acid, 3-methyl-1-[[[E]-2-amino-1-cyano-2-oxoethylidene... 1 Reference 0 Reactions 0 Suppliers	6 1962178-79-5 C ₂₈ H ₃₂ O ₈ Benzoic acid, 2-(2,3-dihydro-7-methoxy-1-oxo-1H-inden-2-yl)-3,6-bis(2,2-dimethyl... 1 Reference 4 Reactions 0 Suppliers
7 1962179-44-7 C ₂₈ H ₃₂ O ₈ Benzoic acid, 3,6-bis(2,2-dimethyl-1-oxopropoxy)-2-(7-methoxy-1-oxo-1H-inden-2-y... 1 Reference 5 Reactions 0 Suppliers	8 1168964-47-3 C ₂₈ H ₃₂ BrN ₂ O ₈ 2-Carboxyphenyl (6Z)-7-bromo-9-methyl-2-[[[3-methyl-1H-inden-2-yl] carbonyloxy]... 1 Reference 0 Reactions 0 Suppliers	9 1168960-42-6 C ₂₈ H ₃₂ ClN ₂ O ₈ 2-Carboxyphenyl (6Z)-7-chloro-9-methyl-2-[[[3-methyl-1H-inden-2-yl] carbonyloxy]... 1 Reference 0 Reactions 0 Suppliers
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

References Reactions Suppliers

1 50-78-2 CC(=O)OC1=CC=CC=C1C(=O)O
C₉H₈O₄
Aspirin
84K References 1,997 Reactions 108 Suppliers

2 5054-56-8 CC(=O)OC1=CC=CC=C1C(=O)O
C₉H₇O₄
Benzoic acid, 2-(acetyloxy)-, ion(1-)
19 References 0 Reactions 2 Suppliers

3 89655-56-1 CC(=O)OC1=CC=CC=C1C(=O)O
(C₉H₈O₄)_x
2-Acetylsalicylic acid homopolymer
16 References 0 Reactions 0 Suppliers

4 97781-16-3 CC(=O)OC1=CC=C(C=C1)C(=O)OC2=CC=CC=C2C(=O)O
C₉H₄D₄O₄
Benzoic-2,3,4,5-*d*₄ acid, 6-(acetyloxy)-
8 References 5 Reactions 24 Suppliers

5 921943-73-9 CC(=O)OC1=CC=C(C=C1)C(=O)OC2=CC=CC=C2C(=O)O
C₉H₅D₃O₄
2-(Acetyl-2,2,2-*d*₃-oxy)benzoic acid
5 References 0 Reactions 18 Suppliers

6 59096-15-0 CC(=O)OC1=CC=C(C=C1)C(=O)OC2=CC=CC=C2C(=O)O
C₉H₈O₄
Benzoic acid, 2-(acetyl-1-¹⁴C-oxy)-
5 References 1 Reaction 1 Supplier

7 59096-14-9 CC(=O)OC1=CC=C(C=C1)C(=O)OC2=CC=CC=C2C(=O)O
C₉H₈O₄
Benzoic-carboxy-¹⁴C acid, 2-(acetyloxy)-
5 References 0 Reactions 3 Suppliers

8 215935-30-1 CC(=O)OC1=CC=C(C=C1)C(=O)OC2=CC=CC=C2C(=O)O
C₉H₇DO₄
2-(Acetyl-2-*d*-oxy)benzoic acid
4 References 0 Reactions 0 Suppliers

9 229030-56-2 CC(=O)OC1=CC=C(C=C1)C(=O)OC2=CC=CC=C2C(=O)O
C₉H₈O₄
Benzoic acid, 2-(acetyl-1-¹³C-oxy)-
3 References 0 Reactions 1 Supplier

通过ChemScape Analysis
了解物质的专利布局

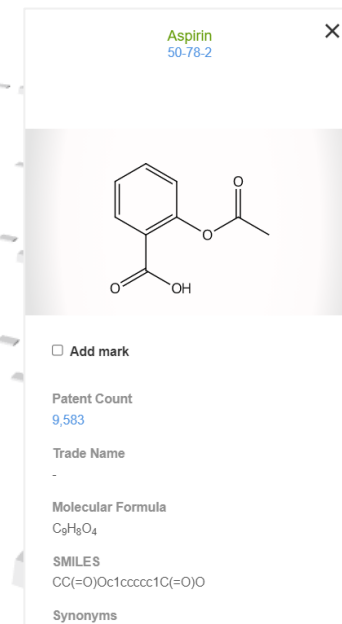
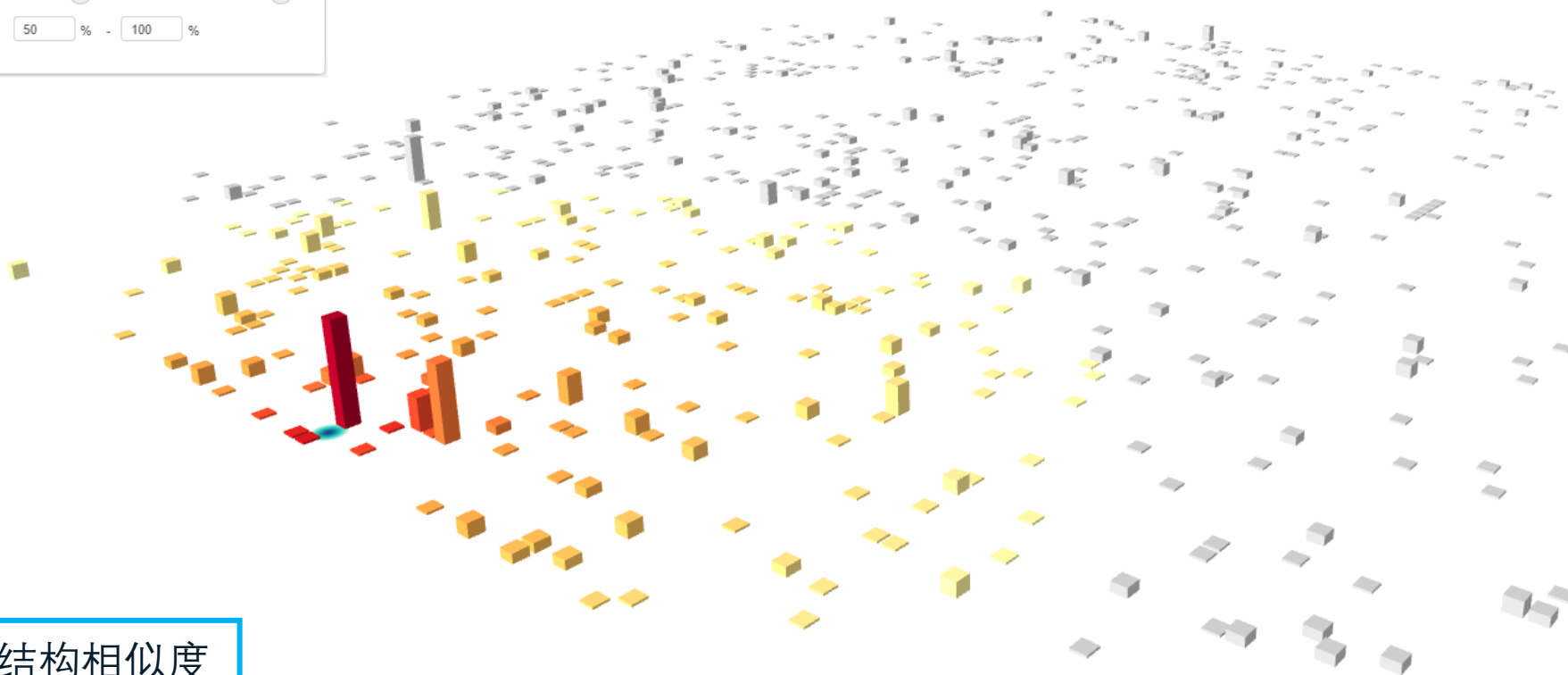
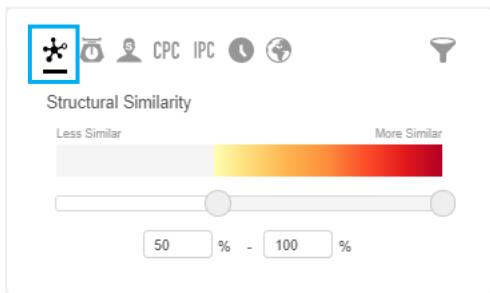


ACS
International

CAS
A division of the
American Chemical Society

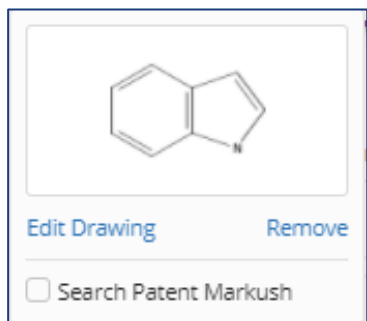


物质检索-检索结果集可视化分析: ChemScape Analysis



分析结构相似度

物质检索--Structure Precision



Structure Match

As Drawn (524)

Substructure (3.7M)

Similarity (10K)

Structure Precision

Conventional Results (504)

Tautomers and Zwitterions (20)

Chemscape Analysis

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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

Substances (20)

Sort: Relevance View: Partial

References Reactions Suppliers

1 271-26-1 C8H7N 3H-Indole

2 1001205-42-0 C8H6N 3H-Indol-2-yl

3 22493-45-4 C8H7N.H Components: 2
Component RN: 271-26-1
3H-Indole, conjugate acid (1:1)

4 1426415-91-9 C8H7N.D Components: 2
Component RN: 271-26-1
3H-Indole, conjugate acid-d (1:1)

5 107715-56-0 C8H7N.BF4.H Components: 3
3H-Indole, tetrafluoroborate(1-)

6 111632-87-2 C8H7N.F6P.H Components: 3
Phosphate(1-), hexafluoro-, hydrogen, compd. with 3H-indole (1:1)

7 2609928-58-5

8 578731-99-4

9 271-23-8 C8H7N

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

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

Download: 可存成 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



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38号

A61P 35/00(2006.01)

A61P 35/02(2006.01)

申请人 中国科学院上海药物研究所

A61P 25/28(2006.01)

A61P 37/02(2006.01)

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周宇波 杨波 何倩军 许磊
胡小蓓

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33200

代理人 张法高 赵机丽

(51) Int. Cl.

C07K 5/087(2006.01)

C07K 5/083(2006.01)

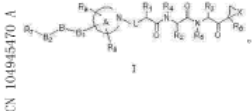
权利要求书3页 说明书24页 附图4页

(54) 发明名称

杂环构建的三肽环氧酮类化合物及制备和应用

(57) 摘要

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



具体实施方式

[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-基氨基酰基)哌啶-1-甲酸叔丁酯(1a,1b)

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

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

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

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]:

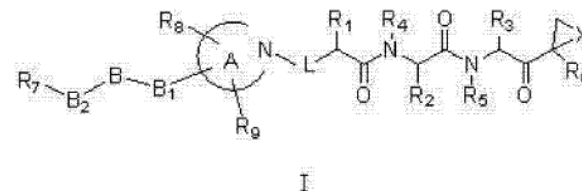
- 使用Markush结构陈述的预测物质，一个Markush可以陈述上百或上千个化学物质
- 被Markush结构包含，但未被实施或呈现在表格、权利要求书或说明书中的结构，不会被CAS分配CAS Registry Number
- Markush检索，能检索到通过结构检索检不到的专利

CN 104945470 A

权利要求书

1/3 页

1. 一种杂环构建的三肽环氧化物类化合物，具有下述结构通式 I：



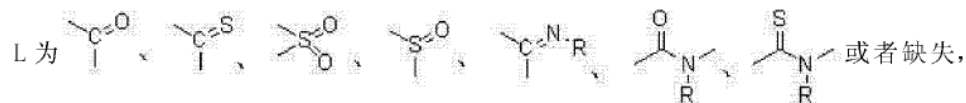
其中：

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

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

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

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

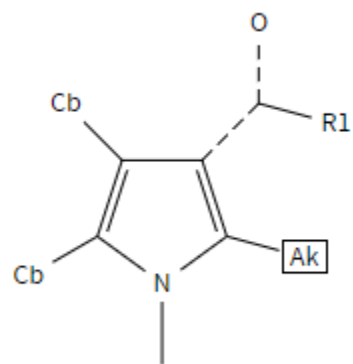


其中 R 选自 H、 C_{1-6} 烷基或卤代的 C_{1-6} 烷基；

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

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

CAS Markush检索



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

References Reactions Suppliers

1 113859-96-4

$C_{20}H_{19}NO$
1-(1,2-Dimethyl-4,5-diphenyl-1H-pyrrol-3-yl)ethanone

1 Reference 1 Reaction 1 Supplier

2 117712-13-7

$C_{19}H_{17}NO_2$
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

The screenshot displays the CAS SciFinder interface for a Markush search. The search results are sorted by relevance and show three entries:

- Entry 1:** JP2000086713. Title: Radiation-curable... method for formation...
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>
- Entry 2:** EP732325. Title: 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, Roif; 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
- Entry 3:** WO2016184429. Title: 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
详细的结构取代信息描述

物质检索小结

1. 利用结构绘制工具合理扩大结构检索范围：R基团、可变基团、可变位置取代等
2. 利用结构绘制工具适当限定检索结构：环锁工具、原子锁工具、EZ构型限定等
3. 正确理解As Drawn、Substructure、Similarity检索结果集的意义和范围
4. 充分利用物质筛选项准确定位目标物质：Reaction Role、Reference Role等
5. 利用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 SciFinderⁿ中的生物序列检索
 - BLAST
 - CDR
 - Motif



Biosequences Search™--Blast检索

CAS SciFinder[®] Saved History Account

Retrosynthesis plans now have a new rule-set trained on our full collection of single-step reactions, offering greater coverage of synthetic methods and added novelty. [Learn more about Retrosynthesis searching in CAS SciFinder[®].](#)

Searching for...

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

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

Enter a query or upload a file...

Sequence Type:
 Nucleotide Protein

Search Within:
 Nucleotides Proteins

Include NCBI Sequences

Limit Total Sequence Results to:
1000

Start Biosequence Search

Advanced Biosequence Search ▾

四种检索选择:

Protein-Protein

Protein-Nucleotides

Nucleotide-Nucleotides

Nucleotide-Proteins

CAS SciFinder-n Help:

https://scifinder-n.cas.org/help/#t=Searching_in_SciFinder-n%2FBiosequence_Search%2FBiosequence_Search.htm&rhsearch=biosequence&rhhlterm=biosequence&rhsyns=%20

高级检索： 设置相关参数

Searching for...

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

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

AACAACAACATATCAAATCCTACTGGTGGCACAACTTGA

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

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

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%

View Results Edit Search Complete

View All

BLAST检索结果

序列结果排序

导出Excel格式
的序列检索结果

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

BLAST Search Details

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

Bioscope Analysis

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Filter by

E-Value

0 to 10⁶

Query Coverage %

0 to 100

Apply Reset Filters

Biosequences (63)

Sort: Alignment Identity View: Collapsed

References

Query Details AACACAACATATCAAACTCTACTGGTGCACAACCTTGA View More

1

Query 1 39

Subject 1 595

Matches: 39
Mismatches: 0

Alignment Identity: 100%

View Less

Alignment Subject References

Alignment Data

BLAST Score: 78
E-Value: 1.06695e-11

Q 1 AACACAACA TATCAATCC TACTGGTGC ACAACTTGA 39
S 393 AACACAACA TATCAATCC TACTGGTGC ACAACTTGA 431

Alignment Identity: 100%

Query 1 39

Subject 1 592

Matches: 39
Mismatches: 0

View Less

Alignment Subject References

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

Sequence

1 ACACACAACA CCAAGTCACCA GTCATCACA TCCATCTCAT TCTACTACTG CCTCAGAGAC CAAGCTGCTG CAACCGGAGA
81 AGGAGATCTA CTCTACTCTT CAGAGCACTG TGCATTGGGA CATGAAACC GTCGTGGGAG ACCTCATGCG GACCCGAGCTG
161 AGGCTTGGCC TGCCGGGAC CAGTGGACGAC TGCAGCCAGC ACCAGCAGCA GACCCAGCTG AAGGTGGCCG CCCCAGCTC
241 CAACCCCTACT AGGGCAAGA AGGCCCCCG CGGTGCTGCA CTCACAGGTGC TGTCCGCGG CTACTCCCTC CTGCTGTGC
321 CAGAGCTGTC CCGGATGTC TGTGAGGCG TGTGCACTG TGTGAGGCA CAGGATGTC AAGGTTGCTC CTGTTGCTC

Zea mays clone 423468 hypothetical protein mRNA, complete cds

GenBank: EU973880.1
FASTA Graphics

Go to: [v]

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;
Zea.
REFERENCE 1 (bases 1 to 592)
AUTHORS Alexandrov,N.N., Brover,V.V., Freidin,S., Troukhan,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.,
Tatarinova,T.V., Zhang,H., Swaller,T.J., Lu,Y.-P., Bouck,J.,
Flavell,R.B. and Feldmann,K.A.
TITLE Direct Submission
JOURNAL Submitted (04-AUG-2008) Ceres, Inc., 1535 Rancho Conejo Blvd.,
Thousand Oaks, CA 91320, USA
FEATURES
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CDS
ORIGIN
1 acacacaaca ccagtcacca gtcatcaca tccatctcat tctactactg cctcagagac caagctgctg caacccggaga
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121 catggaaac gtcgtggag acctcatggc gaccgactg aggcttggc tgcgggac
181 cgtggagcag tgcagccagc accagcagca gaccgactg aaggctgctg cggcggcctc
241 caaccctact agggcaaga agcggcccg cggtgctgca CTCACAGGTGC TGTCCGCGG CTACTCCCTC CTGCTGTGC
301 ctacctctc ctgctgctg cagagctgct gcctagctgc ttctagacc tctgtcaagt
361 tgtgccacca gtagatttg atatgttgtt gttctttcta gtagctgag tgacagacaa
421 ttgtgctgct gttgcttctg ttgttagtga gttgcactgc gtttctctgt tatgctatgg
481 gtacagagat ttaggcatg gtttaagcta agctaaggcg atgggggatc gatcactttac
541 ctctcatctc tggctgctga tcctttttgt tcttgacaaa aaaaaaaaaa aa

BLAST检索结果

6 Alignment Identity: 100%

Query 1 39

Subject 1 1,060

Matches: 39
Mismatches: 0

View Less ▾

Alignment Subject References

CAS Registry Number: [785872-37-9](#)
Length: 1,060 nt

Sequence

```
1 CATTGGGTAC CTCGAGGCCG GCCGGGAGCT CGCACTCACT CACTCACAAG TCACACAGCC ACACTTGAAC CGTGCCCGC
81 AGCCGAGGGA GCTTGACCG GCCAACGCAC ACATAACACA AGCTCGTCGT CGATGGCGCG GTGGGCTGCG GTGCTGGCG
161 TGGCCGCGC CACGGCCATC GCCGTGGCGT CCGTGGCGGG CGGCGACATG AACCGGACA AGACGGAGTG CGCGACCAAG
241 CTGTGGGCC TGGCCCGTG CCTGCACTAC GTGCAGGGC AGGCCCGCG GCCCGCGCC GACTGTGCG GCGCCCTGCG
321 CCAGGTGCTG GGAAGAGCC CCAAGTGCCT GTGCGTCTC GTCAAGGACA AGGACGACCC CAACCTGGG ATCAAGATCA
401 ACGCCACCCT CGCGTCTCG CTCCCAACG CTGCGGCGC CACCGCGCC AACGTCTCC ACTGCGTCA GCTCCTGAT
481 ATTCCCCCG GCTCAAAGA CGCCGCGTC TTCAGTCCG GCAGCGACAA GGGTCCACT GCCGCTCAG CCAAGGACAA
561 CTCGACGGC ACGACCGACT CCCGCGCGT GCAGGCGACC ACCGAGCGC GCGTGTCTC CTCGGCGCG ACCGCCGGT
641 CTGACTCAC GGTGCTGCT GCCGGTACC TCCTCTGCT CGTGCCAGAG CTGTCGCTA GCTCGTTCTA GACCCTCTG
721 CAAGTGTGC CACCACTAGG ATTGATATG TTGTTGTTCT TTCTAGTAGG TGAGGTGACA GACAATTTC TGCTGGTGC
```

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 this Substance
1999: PN: US200

Sequence Details

Sequence: DNA: linear

```
1 cattgggtac ctcgagccg gccgggagct cgcactcact cactcacaag
51 tcacacagcc acaactgaac cgctgccgc agcggaggga gcttgacgg
101 gccaacgca acataacaca agctctcgt cgatggcgc gtbggctgc
151 gtgctggcg tggccggcg cagccatc gccgtggct cggcgccgg
201 cggcgacatg aacgcgaca agacggagt cgcgaccag ctgggggcc
251 tggcgccgtg cctgacgtac gtcaaggcc agccccgc gcccgccc
301 gactgctgc gccgctgc caggtgctg ggaagagcc ccaagtgcct
351 gtgctgctc gtcaaggaca aggacgacc caacctggc atcaagatca
401 agccaccct cgcctcgc ctcccaagc cctgcccgc caccgccc
451 aacgtctcc actgctca gctcctcat attccccgg gctccaaaga
501 cgcgccgtc ttactccc gcagcgaca gggctcact gccgtccag
551 ccaaggacaa ctgagggcg acgaccgact cccgcgct gcaggcacc
601 accggagcg gctgtctc ctggcgcg acccgctg ctgactcac
```

Patent Annotations
Source: Zea mays
Reference: US20040214272. SEQID 16999: claimed

Feature	Location	Description
misc_feature		Clone ID: MRT4577_1154C.1

序列详情及相关的专利文献结果

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

References (47) Sort: Relevance View: Partial Abstract

Substances Reactions Citing

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, Noureddine; United States, US20130326723 A1 2013-12-05 | Language: English, Database: CA

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

PatentPak Full Text Substances (0)

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: CA

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, is used to provide a classification tool for polypeptides find use in production of transgenic plants to produce plants having improved traits.

PatentPak Full Text Substances (0)

Substance Detail

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

CAS Registry Number
661510-85-6

Image Not Available

Sequence Details

Sequence: DNA; linear

1	cacaagtac	acagccacac	ttgaaccgca	gcccgcagcg	gaggagcctt
51	gcacgggcca	acgcacacat	aacacaagct	ctgctcgat	ggcgcggtgg
101	gctgcggtgc	tggcgtggc	cgcgccaag	gccatcgccg	tggcgtccgt
151	ggcggcgcc	gacatgaacg	cggacaagac	ggagtgcccg	gaccagctgg
201	tggccctggc	gccgtgcctg	cagtacgtgc	agggcgagbc	ccgcgcgccg
251	ccgccgact	gctgcggcgg	cctgcgccag	gtgctgggga	agagcccaaa
301	gtcctctg	gtgctgtca	aggacaagga	cgacccaac	ctgggcatca
351	agatcaacgc	caccctcg	ctcgcgctcc	ccaacgctg	cgcgccacc
401	cgcgccaacg	tctccactg	cgctcagctc	ctgcatattc	ccccgggctc
451	caaagagccc	gccgttcca	gtcccgcag	cgacaaggcc	tccactgccg
501	ctccagccaa	ggacaactcg	acggcgacga	ccgactccc	cgcgctcgag
551	gcgaccaccg	gacgcggcgt	gtcctcctcg	gcggcgaccg	ccggtcgtgc
601	actcacggtg	ctgctcgccg	gctacctcct	cctgctctgtg	ccagagctgt

Other Names and Identifiers

1 Other Name for this Substance

1627: PN: US20040034888 SEQID: 25627 claimed DNA

Patent Annotations

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

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

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

CDR1	<input type="text" value="VFPLAPSSKS"/>	<input type="button" value="x"/>
CDR2	<input type="text" value="TSGGTAALGC"/>	<input type="button" value="x"/>
CDR3	<input type="text" value="LVKDYFPEPV"/>	<input type="button" value="x"/>

Include NCBI Sequences

Limit Total Sequence Results to:

CAS SciFinder-n Help:

https://scifinder-n.cas.org/help/#t=Searching_in_SciFinder-n%2FBiosequence_Search%2FBiosequence_Search_-_CDR.htm&rhsearch=CDR&rhhlterm=CDR&rhsyns=%20

CDR检索结果

- 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。

Query Coverage % = coverage/query
Subject Coverage % = coverage/subject
Alignment Identity % = matches/query

CDR Segments

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

CDR1 CDR2 CDR3

7 0 0
31 8,048 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 10⁶

Query Coverage %
0 to 100

Subject Coverage %
0 to 100

Alignment Identity %
0 to 100

Biosequences (10,000) Sort: Alignment Identity View: Collapsed

References

Query Details View Less

> CDR1
VFPLAPSSKS

> CDR2
TSGGTAALGC

> CDR3
LVKDYFPEPV

1 Alignment Identity: 100%

Subject 1 466

CDR3
1 10

Matches: 10
Mismatches: 0

References

Alignment Data
BLAST Score: 79
E-Value: 0.00262316

CDR3	1	LVKDYFPEPV	10
S	167	LVKDYFPEPV	176

View Less

2 Alignment Identity: 100%

Subject 1 440

CDR3
1 10

Matches: 10
Mismatches: 0

View More

下载Excel格式文件

获取CAS SciFinder-n
中披露该序列的文献

CDR检索结果

查看query中三个CDR区都被包含的8048个序列结果

The screenshot displays the 'Biosequences' search results page for 8,048 sequences. On the left, the 'CDR Segments' section features a Venn diagram with three overlapping circles labeled CDR1, CDR2, and CDR3. The central intersection of all three circles is shaded blue and contains the number '8,048'. Below the diagram are 'Apply' and 'Reset Segments' buttons. The 'Bioscape Analysis' section includes a description and a 'Create Bioscape Analysis' button. The 'Filter by' section contains four filter controls: 'E-Value' (0 to 10⁶), 'Query Coverage %' (0 to 100), 'Subject Coverage %' (0 to 100), and 'Alignment Identity %' (0 to 100).

The main 'Biosequences (8,048)' section shows 'Sort: Alignment Identity' and 'View: Collapsed'. A 'References' button is present. The 'Query Details' section lists three CDR regions with their respective sequences: CDR1 (VFPLAPSSKS), CDR2 (TSGGTAALGC), and CDR3 (LVKDYFPEPV).

The alignment view for 'Subject 1' shows 'Alignment Identity: 100%'. A diagram illustrates the alignment of the subject sequence (1 to 816) with the CDR regions. The CDR1 region is highlighted in purple, and the CDR2 and CDR3 regions are highlighted in green. The alignment shows 30 matches and 0 mismatches.

The 'References' section lists three entries for 'C-terminally fused TNF family ligand trimer-containing antigen binding molecules':
1. Assignee: F. HOFFMANN-LA ROCHE AG; EP3243836 A1 | Seq ID No: 158
2. Assignees: F. HOFFMANN-LA ROCHE AG; HOFFMANN-LA ROCHE INC.; WO2017194438 A1 | Seq ID No: 158
3. 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

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 ^ Reset All

Query Coverage % E-Value

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&rhhlterm=motif&rhsyns=%20

Motif检索结果

Motif Search Details

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

Bioscape Analysis

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

[Create Bioscape Analysis](#)

Filter by

^ E-Value

0 to 10⁶

^ Query Coverage %

0 to 100

^ Subject Coverage %

0 to 100

^ Alignment Identity %

0 to 100

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

Subject 1 220

Matches: 8
Mismatches: 0

View Less

Alignment Subject

References

CAS Registry Number: -
NCBI Identifier: [A0A1I7ZK68](#)
Length: 220 aa

Sequence

```
1 MLLRLLFFI IATKPVQASG FSERSTTVVG CSEMLVRLFL LFIATKPAQ AGGFSEVSGL RFVGEAAQKR MKPYGYGLIK
81 VDDQYGMTTL EEVAKPIPQK PQLTVDEQNR AETQNRALVD IIVKFYQLRD GYLAQHAGAD FIQTLISKYGF IYDSGKVKNL
161 NELTLTKTQT QVTQLDTPRS SSGIADHLRR SFLIRAKKKS NRKNKEGTSX XXXGKDGAND
```

2 Alignment Identity: 100%

大纲

- CAS SciFinderⁿ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 MethodsTM的使用
 - 关键词与反应式的联合检索



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

× Draw 🔍

通过物质标识符、文献标识符进行检索

反应检索--标识符

The screenshot displays a search interface for chemical reactions. On the left, a 'Filter Behavior' sidebar includes sections for Substance Role, Yield, Number of Steps, Non-Participating Functional Groups, Experimental Protocols, Reaction Type, Stereochemistry, Reagent, and Catalyst. The main area shows 'Reactions (2,949)' with a 'Scheme 1 (55 Reactions)' section. It features chemical structures for the reaction, 'Suppliers' buttons, and three 'Reaction Summary' entries with details on reagents, solvents, and literature references. A 'Scheme 2 (13 Reactions)' section is partially visible at the bottom.

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

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

Drag the reaction arrow to specify reaction direction.

reactant

product

Molecular Formula: C₇H₈O (108.14) . C₇H₆O (106.12)

Zoom: 100%

OK Cancel

反应检索--结果集排序

Structure Match

As Drawn (7,236)

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

References

By Scheme

By Document

Scheme 1 (5,685 Reactions) Steps: 1 Yield: 100%

Suppliers (131)

Suppliers (62)

Reaction Summary Steps: 1 Yield: 100%

1.1 Reagents: Potassium peroxymonosulfate sulfate (2KHSO₅·K₂SO₄) Catalysts: Tetrabutylammonium bromide, (OC-6-21)-Tris(2,4,5-dihydro-2-oxazolyl-κ^N)phenolato-κ^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-κ^O,κ^O)bis(pyridine)dicopper 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: [7-4]-(2-[(2-(5,7-Bis(1,1-dimethylethyl)-2-benzoxazolyl-κ^N)phenyl)amino-κ^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

View All Reaction Summaries

Collapse Scheme

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

反应排序：
按类型排序
按文献排序

Structure Match

As Drawn (7,236)

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

Reaction Summary

Steps: 1 Yield: 100%

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

View Reaction Detail

Reactions (7,236)

Group: By Document View: Expanded

References

1

Atomically dispersed Fe⁵⁺ anchored on nitrogen-rich carbon for enhancing benzyl alcohol oxidation through Mott-Schottky effect

By: Wei, Qinrong; Wang, Jiashi; Shen, Wenzhong Applied Catalysis, B: Environmental (2021), 292, 120195 | Language: English, Database: CAPUSO

Full Text View 3 Related Reactions

Suppliers (131)

Suppliers (62)

Reaction Summary

Steps: 1 Yield: 100%

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

View Reaction Detail

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 displays a search interface for chemical reactions. On the left, a sidebar contains search filters categorized into 'Structure Match' (As Drawn, Substructure, Similarity), 'Filter Behavior' (Filter by, Exclude), and various chemical parameters (Yield, Number of Steps, Non-Participating Functional Groups, Experimental Protocols, Reaction Type, Stereochemistry, Reagent, Catalyst, Solvent, Commercial Availability, Reaction Notes, Search Within Results). Below these are 'Source Reference' filters (Document Type, Language, Publication Year, Publication Name, CA Section) and a 'Filter Content Report' section with a download button.

The main area shows 'Reactions (7,236)' with a 'Scheme 1' section containing 5,685 reactions. A chemical reaction is shown: benzyl alcohol (benzene ring with a -CH₂-OH group) reacting to form benzaldehyde (benzene ring with a -CHO group). Below the reaction, there are buttons for 'Suppliers (131)' and 'Suppliers (62)'. Three reaction summaries are listed, each with a 'Full Text' button:

- Reaction Summary 1:** Steps: 1 Yield: 100%. A new and highly effective method for catalytic oxidation of alcohols to the corresponding carbonyl compounds using the tris[2-oxazoliny]phenolato]manganese(III)/Oxone/n-Bu₄NBr oxidation system. By: Bagherzadeh, Mojtaba. Tetrahedron Letters (2003), 44(50), 8943-8945.
- Reaction Summary 2:** Steps: 1 Yield: 100%. Supercritical carbon dioxide, a new medium for aerobic alcohol oxidations catalyzed by copper-TEMPO. By: Herbert, Matthew; et al. Dalton Transactions (2010), 39(3), 900-907.
- Reaction Summary 3:** Steps: 1 Yield: 100%. Synthesis, characterization and catalytic activity of copper(II) complexes containing a redox-active iminosemiquinone ligand. By: Balaghi, S. Esmael; et al. Dalton Transactions (2013), 42(19), 3333-3340.

At the bottom, there is a 'Scheme 2' section with 6 reactions.

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

References

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 (Cu₂O)
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 (Cu₂O), 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)butane
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
未发生变化的官能团


反应检索--结果集筛选: Synthetic Methods™

The screenshot displays the ACS Reactions database interface. On the left, a sidebar contains various filters: Structure Match (As Drawn, Substructure, Similarity), Filter Behavior (Filter by, Exclude), Yield, Number of Steps, Non-Participating Functional Groups (Amide, Ether, Halide, Alkene, Phenyl halide, Aldehyde), Experimental Protocols (Synthetic Methods, Experimental Procedure), Reaction Type, Stereochemistry, Reagent, Catalyst, Solvent, Commercial Availability, Reaction Notes, and Search Within Results. The main area shows a list of reactions under the heading 'Reactions (2,610)'. Two reactions are visible: Scheme 1 (2 Reactions) and Scheme 2 (3 Reactions). Each reaction entry includes a chemical scheme, a reaction summary with steps, yield, and reagents, and a 'Full Text' button. A blue box highlights the 'Experimental Protocols' section in the sidebar, and another blue box highlights the 'View Reaction Detail' and 'Experimental Protocols' buttons for a specific reaction. A third blue box highlights the reaction summary 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™



Suppliers (88) 67% Suppliers (62)

Step 1 Alternative Steps (1)

Stage	Reagents	Catalysts	Solvents	Conditions
1	-	1,10-Phenanthroline Copper oxide (Cu ₂ O) Potassium bromide	Quinoline N-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 (Cu₂O)
Potassium bromide

Solvents Quinoline
N-Methyl-2-pyrrolidone

Procedure

1. Charge an oven-dried vessel with 2-carboxybenzaldehyde (1.00 mmol), Cu₂O (10.7 mg, 0.075 mmol), phenanthroline (27.0 mg, 0.15 mmol) and potassium bromide (0.015 mmol).
2. Flush the vessel with alternating vacuum and nitrogen purge cycles.
3. Add a degassed solution of *n*-tetradecane in a mixture of NMP (1.5 mL) and quinoline (0.5 mL) to the reaction mixture *via* syringe.
4. Stir the resulting mixture at 170 °C for 6 hours.
5. Allow the reaction mixture to cool to room temperature.
6. Dilute the reaction mixture with ethyl acetate (2 mL).
7. Dissolve a sample of the reaction mixture (0.25 mL) in ethyl acetate (2 mL).
8. Wash the reaction mixture with HCl (1 N, 2 mL).
9. Dry the reaction mixture over MgSO₄/NaHCO₃.
10. Analyze the product by GC.

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 displays the ACS search interface. On the left, a sidebar titled "Searching for..." lists various search categories: All, Substances, Reactions, References (highlighted), Suppliers, Biosequences, and Retrosynthesis. The main area is titled "References" and includes a search bar with the text "suzuki". Below the search bar, there are options for "AND" and "Author Name" with a placeholder "Enter last name, first name middle name.". A blue arrow points from the text "文献检索框里输入关键词" to the search bar. To the right of the search bar, there is a "Structure Editor" window showing a chemical reaction scheme with a benzene ring and a carbonyl group. A blue arrow points from the text "结构编辑器中绘制反应" to this window. The window also contains "Edit Drawing" and "Remove" buttons.

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

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: CAplus 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 Pd(OAc)₂, K₃PO₄ and TBAB in water to give MeO-4-C₆H₄Ph 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: CAplus and MEDLINE

Pd(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 °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 Pd(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: CAplus

The coupling reaction of diverse aryl halides with phenylboronic acid under solvent-free conditions was performed using Pd(PPh₃)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: CAplus 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: CAplus and MEDLINE

联合检索提高了检索速度



ACS
International

CAS

A division of the
American Chemical Society

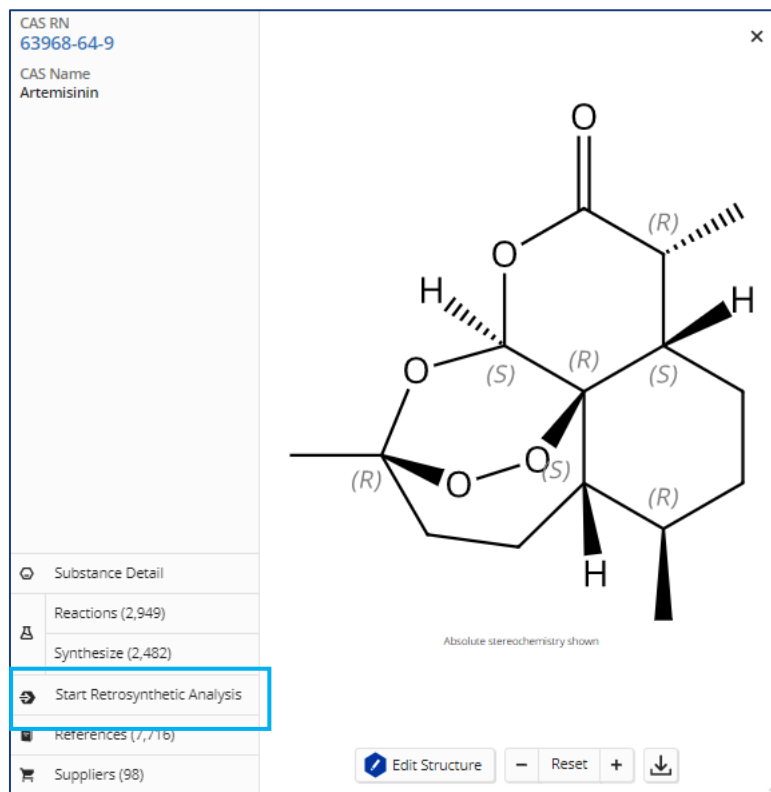
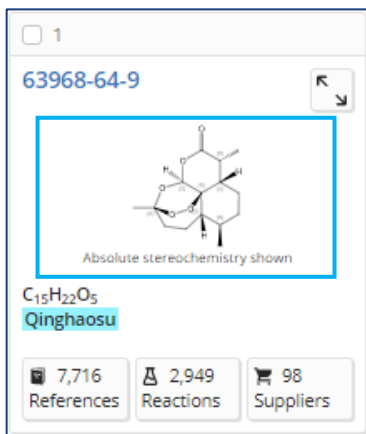


大纲

- 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.](#)

Enter a CAS Registry Numbers, SMILES...

Draw or change atoms or bonds.

Molecular Formula: C₁₉H₁₉BrN₄O₅ (463.29)

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

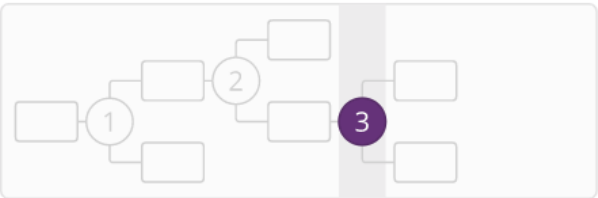
CAS Retrosynthesis Tool—预设参数

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.](#)

Email me when my plan is complete

Break and Protect Bonds

[Learn more.](#)



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—路线详情

路线概览

重设参数

Retrosynthesis

Powered by ChemPlanner®

Overview Steps Predicted Results ON

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

Powered by ChemPlanner®

Overview Steps Predicted Results ON

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

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

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

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

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

Click Evidence to view the specific synthesis conditions and literature for this step.

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)

Group: By Scheme View: Expanded

Scheme 1 (1 Reaction) Steps: 1

Reaction Summary Steps: 1

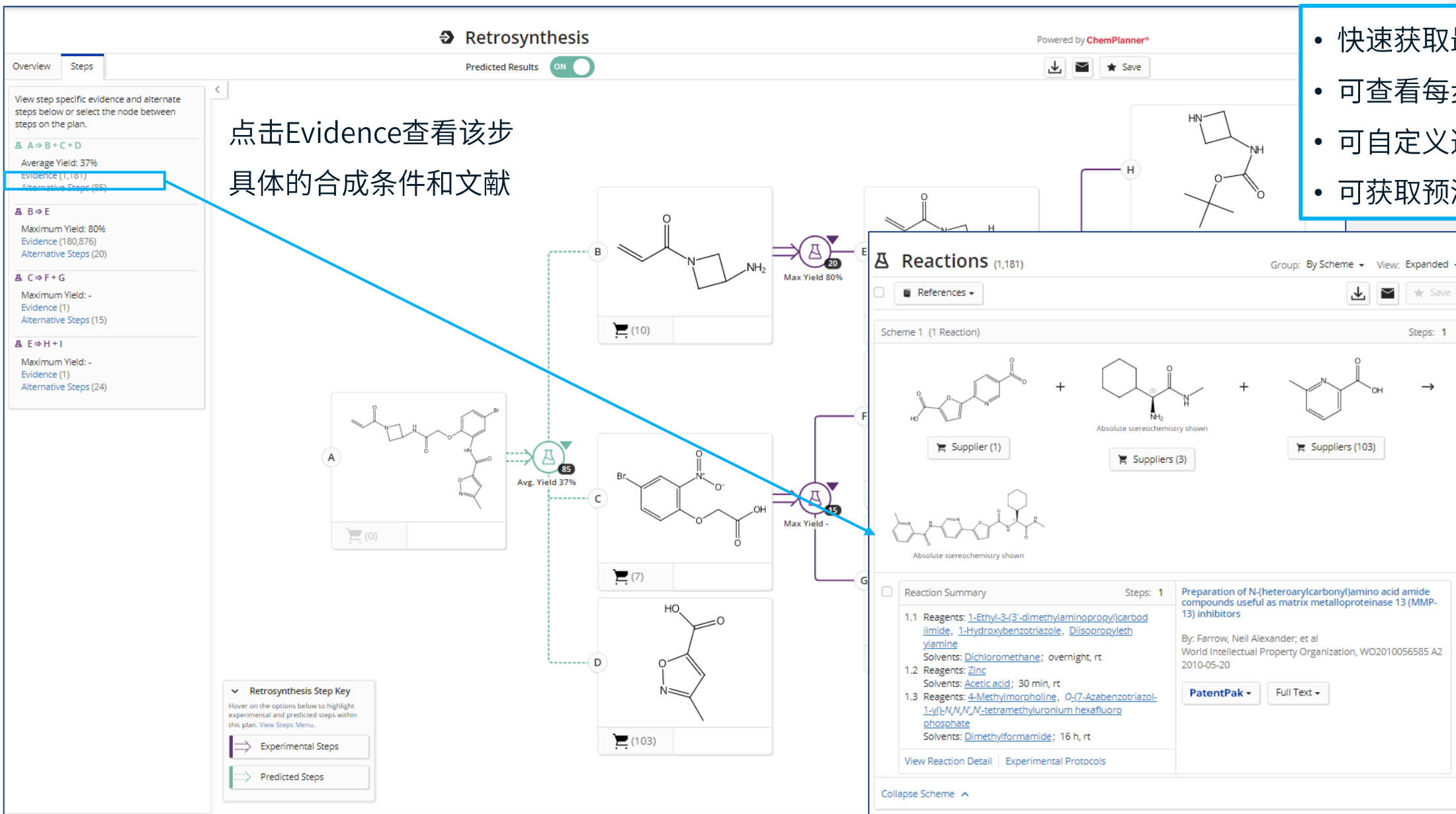
1.1 Reagents: 1-Ethyl-3-(3'-dimethylaminopropyl)carbodiimide, 1-Hydroxybenzotriazole, Diisopropylethylamine
Solvents: Dichloromethane; overnight, rt

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

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



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

CAS Retrosynthesis Tool—路线详情

Retrosynthesis
Powered by ChemPlanner®

Overview Steps

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

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

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

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

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

Alternative Steps (85)

Filter by

- Alternative Step Type
 - Predicted (85)
 - Non-Selective (85)
- Stereochemistry
 - Non-Selective (85)

2 of 85

3 of 85

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

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

Retrosynthesis
Experimental Steps
Predicted Steps

Reset

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

Retrosynthesis
Powered by ChemPlanner®

Predicted Results ON

Retrosynthesis Step Key

Hover on the options below to highlight experimental and predicted steps within this plan. View Steps Menu.

- Experimental Steps
- Predicted Steps

Retrosynthesis Step Key

Experimental Steps

Predicted Steps

Reset

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



检索信息的管理--保存、下载，设置提醒和标签

The screenshot displays a search results interface for 'References' (3,278). The main content area lists three articles:

- 1. Nano-graphene in biomedicine: theranostic applications**
By: Yang, Kai; Feng, Liangzhu; Shi, Xiaoze; Liu, Zhuang
Chemical Society Reviews (2013), 42(2), 530-547 | Language: English
- 2. Poly-cyclodextrin and poly-paclitaxel nano-assembly for anticancer therapy**
By: Namsung, 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: CAlplus and MEDLINE
- 3. Nano-graphene oxide for cellular imaging and drug delivery**
By: Sun, Xiaoming; Liu, Zhuang; Weisler, Kevin; Robinson, Joshua Tucker; Goodwin, Andrew; Zaric, Sasa; Dai, Hongjie
Nano Research (2008), 1(3), 203-212 | Language: English, Database: CAlplus and MEDLINE

A 'Save Search' dialog box is open, allowing users to name the search, set alert frequencies (No Alerts, As Available, Weekly, Monthly), and add tags. The 'Save' button is highlighted in the original image.

下载
分享链接
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, Selected Results, Range (ex. 2 to 20)

Display: Result Summary, Result Details

File Name: Reference_20211118_1536

Only the first 500 references will be downloaded.

Include: Task History, Formulations, Abstract, Analytical Methods, Concepts, Citations, Substances

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

Download Substance Results

File Type: PDF

Select Quantity: All Results, Selected Results, Range (ex. 2 to 20)

Display: Result Summary, Result Details

File Name: Substance_20211118_1537

Only the first 500 substances will be downloaded.

Include: Task History, Experimental Properties, Substance Names, Predicted Properties, Experimental Spectra, Bioactivity Indicators, Predicted Spectra, Target Indicators, Regulatory Information

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Download Reaction Results

File Type: PDF, RDFFile (.rdf)

Select Quantity: All Results, Selected Results, Range (ex. 2 to 20)

Display: Result Summary, Result Details

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 displays the CAS SciFinder web interface. At the top, the navigation bar includes the CAS SciFinder logo, a search bar with the text 'Reactions' and '7782-42-5', and icons for 'Draw', search, star, clock, and user profile. A blue box highlights the star icon in the top bar.

On the left side, there is a 'Filter by' panel with two sections: 'Result Type' (Reactions (34), References (48), Substances (18)) and 'Alerts' (Unviewed (1), No Alerts (100)). Below this are 'Combine Saved Results' and 'Migrate Alerts & Saved Results' sections.

The main content area is titled '★ Saved (100)'. It lists saved search results. The first result is '1671 exclude COCl', dated 'June 4, 2021, 3:57 PM'. It has a 'Rerun Search' button. Below the title is a dropdown menu for 'Alerts' (highlighted with a blue box) and an 'Add Tags' button. A 'Frequency' dropdown menu is open, showing options: 'No Alerts', 'As Available', 'Weekly', and 'Monthly'. Below this is a 'Rerun Search' button (pointed to by a blue arrow from the text '更新检索结果').

The second result is 'include Si', dated 'June 4, 2021, 3:54 PM', also with a 'Rerun Search' button.

Each result entry includes a 'Substances' section with 'Advanced Search + Filters' and 'Boiling Point (°C): 80 to 100'. At the bottom of each entry are 'Alerts' and 'Add Tags' buttons.

更改提醒频率或取消提醒设置

更新检索结果

检索信息的管理--合并保存的结果

The screenshot displays the CAS SciFinder web interface. At the top, the navigation bar includes the CAS logo, 'SciFinder', and search filters for 'Reactions' and '7782-42-5'. The main content area shows a list of saved search results under the heading '★ Saved (100)'. Two results are visible: '1671 exclude COCl' and 'include Si'. A 'Combine Saved Results' dialog box is open, allowing the user to select a result type (Substances, Patent Markush, Reactions, or References) and a combine option (Add, Intersect, or Subtract). The 'References' option and the 'Add' combine option are highlighted with blue boxes. The dialog box also features a progress indicator with steps 1, 2, and 3, and a 'Return to Result Type' button.

This is a close-up view of the 'Combine Saved Reference Results' dialog box. It features a progress indicator with steps 1, 2, and 3. Below the indicator, the text 'Select a Combine Option:' is followed by three buttons: 'Add', 'Intersect', and 'Subtract'. Each button has a corresponding Venn diagram icon and a 'Select' button below it. The 'Add' button and its 'Select' button are highlighted with a blue box. A 'Return to Result Type' button is located to the right of the options. At the bottom right, there is a link that says 'Learn More About Combine'.

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](#)

勾选需要合并的结果集，点击View Results，
获得合并后的结果集


References (7,452)

Sort: Publication Date: Newest | View: Partial Abstract

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:  [View Larger](#)

Available at My Institution

Author

Organization

Publication Name

Concept

CA Section

CAS Solutions

Formulation Purpose

Database

Search Within Results

Filter Content Report

1

Encapsulation of a cationic antimicrobial peptide into self-assembled polyion complex nano-objects enhances its antitumor properties

By: Raileanu, Mina; Lonetti, Barbara; Serpentine, Charles-Louis; Goudouneche, Dominique; Gibot, Laure; Bacalum, Mihaela | Journal of Molecular Structure (2022), 1249, 131482 | Language: English, Database: CAplus

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](#)

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

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, Saied M. E.; Dawy, Magdah; Ali, Amira A. M. | Journal of Molecular Structure (2022), 1249, 131587 | Language: English, Database: CAplus

A new tridentate 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:8-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](#)

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

3

Proof of concept for dual anticancer effects by a novel nanomaterial-mediated cancer cell killing and nano-radiosensitization

By: Duo, Yanhong; Liu, Qian; Zhu, Daoming; Zhang, Bin; Luo, Guanghong; Wang, Fu-Bing; Chen, Jinghua; Cao, Yihai | Chemical Engineering Journal (Amsterdam, Netherlands) (2022), 429, 132328 | Language: English, Database: CAplus

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 nano-prodrug 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 (AuNCl₂-PEG) and sodium nitroprusside (SNP) coated by plat...

[View More](#)

[Full Text](#) | [Substances \(7\)](#) | [Reactions \(0\)](#) | [Citing \(0\)](#) | [Citation Map](#)

检索信息的管理--管理检索历史

CAS SciFinder®

References Enter a query...

Draw

Filter by

Result Type

- All (57)
- Patent Markush (17)
- Reactions (48)
- References (209)
- Retrosynthesis (20)
- Substances (199)

Date

Start Date End Date

mm/dd/yyyy to mm/dd/yyyy

November, 2021

SU	MO	TU	WE	TH	FR	SA
31	1	2	3	4	5	6
7	8	9	10	11	12	13
14	15	16	17	18	19	20
21	22	23	24	25	26	27
28	29	30	+	±	3	4

Search History (550)

November 18, 2021

- 3:29 PM
Retrosynthesis
Synthetic Depth: 3
Predicted Rules: Common
Break & Protect Bonds: No
Starting Material Cost Limit: \$1,000.00/mol
Retrosynthesis Plan will expire on Feb 16, 2022.
Open Plan
Edit Search
Generating Plan
- 3:27 PM
Retrosynthesis
Synthetic Depth: 3
Predicted Rules: Common
Break & Protect Bonds: No
Starting Material Cost Limit: \$1,000.00/mol
Retrosynthesis Plan will expire on Feb 16, 2022.
Open Plan
Edit Search
Generating Plan
- 3:16 PM
Substances
qinghaosu (1)
Rerun Search
Edit Search
- 3:16 PM
Substances
qinghaosu
As Drawn (0)
Substructure (0)
Similarity (0)
Rerun Search
Edit Search
- 3:13 PM
References
suzuki
As Drawn (2,771)
Substructure (13K)
Rerun Search
Edit Search

按照检索类型或
检索时间查找

重新编辑检索项

大纲

- CAS及CAS SciFinderⁿ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
- 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



Registration Already Complete

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

点击激活链接后注册成功。

之后直接点击<https://SciFinder-n.cas.org>即可访问。

使用注意事项

- 一人注册一个帐号
- 实名注册，需提供真实姓名信息（中文名用汉语拼音全拼）
- 不得过量下载（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

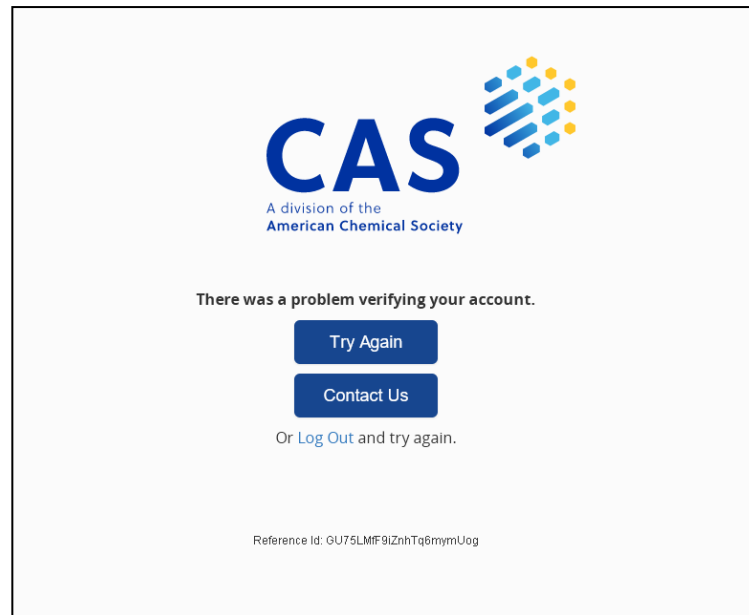
常见问题

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

谢谢!

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