

利用CAS SciFinderⁿ 获取科技信息

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ACS
International



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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
 - 分析方法的获取 (Analytical Methods)
- 常见问题及解决

CAS致力于提高创新效率

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



HINDSIGHT

Connecting past discoveries
to build a better future

连接前人的发现，建设更美好的未来

INSIGHT

Revealing unseen relationships that spark ideas and speed
discovery

揭示能激发想法和加速发现的，未预见的联系

FORESIGHT

Identifying trends and emerging opportunities to accelerate
growth

确定加速增长的趋势和新机遇

CAS具有最全面的学科连接内容合集



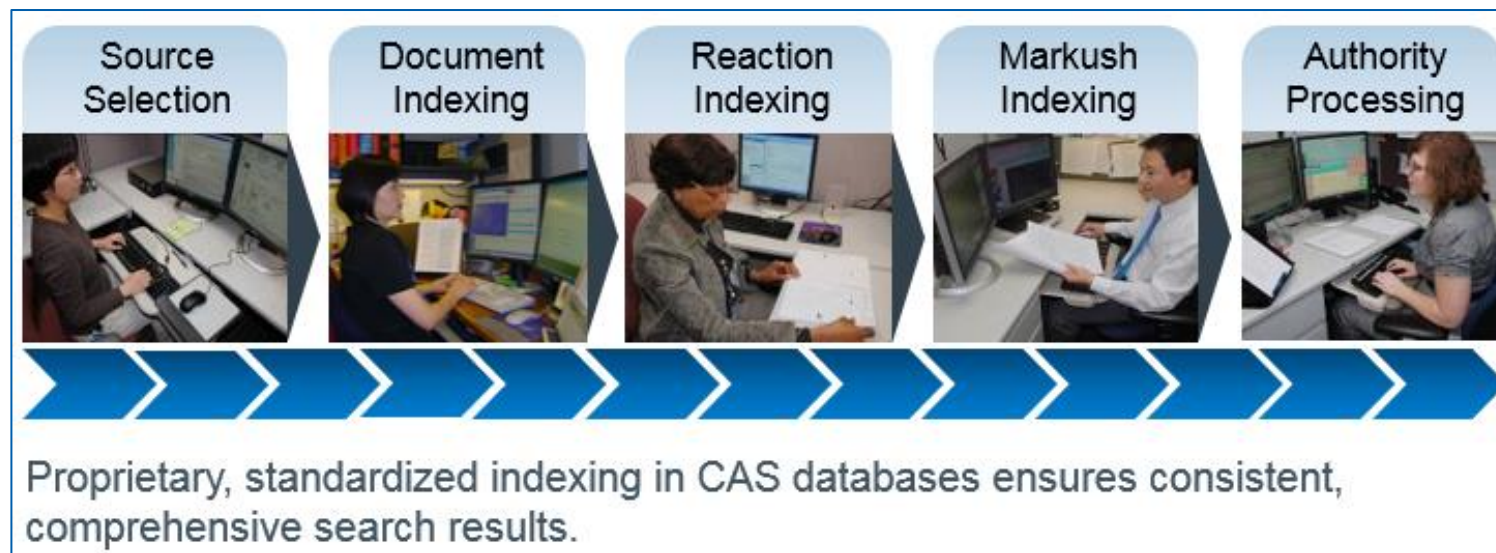
Over
50K
scientific journals
and documents

Over
250
million
substances

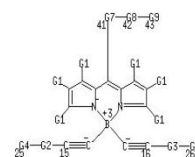
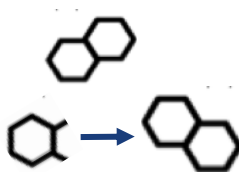
Over
50
languages
translated

64
patent offices
worldwide

CAS科学家的智力标引



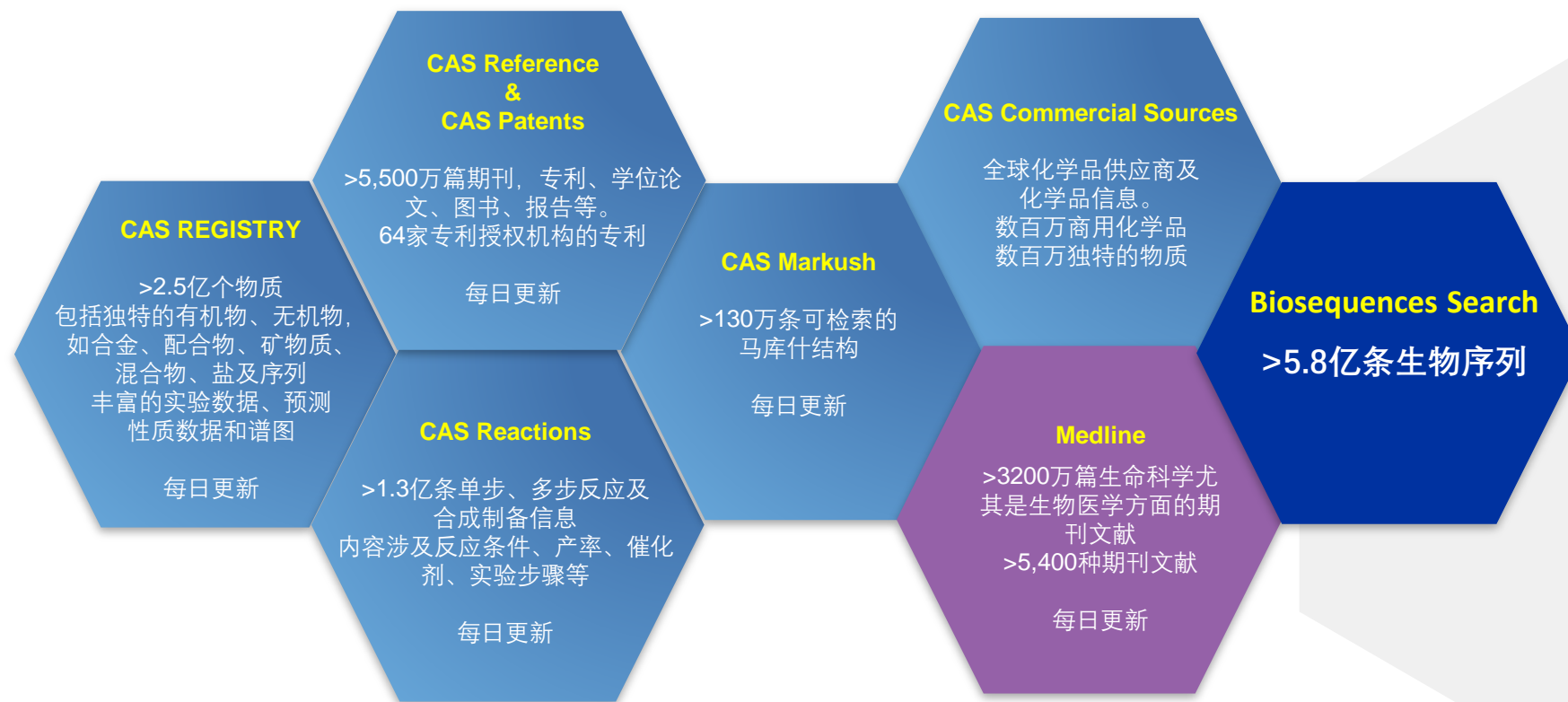
1990
Smith, M.
anthracene



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




CAS
SciFinderⁿ

Log In to SciFinderⁿ

Username or Email Address

Next

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



CAS
SciFinderⁿ

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

检索历史 账户信息

已保存的结果集及
信息更新的结果集

灵活的
检索选项

近期检
索历史

便捷地合并文
本与结构检索

重新运行检索

修改检索式

The screenshot shows the CAS SciFinderⁿ main interface. At the top, there is a navigation bar with the CAS SciFinderⁿ logo on the left and three buttons: 'Saved' (with a star icon), 'History' (with a clock icon), and 'Account' (with a person icon). Below the navigation bar, the main content area is divided into two columns. The left column is titled 'Searching for...' and contains a list of search options: 'All', 'Substances', 'Reactions', 'References' (which is highlighted with a blue bar), 'Suppliers', 'Biosequences', and 'Retrosynthesis'. The right column is titled 'References' and contains a search bar with the text 'Heat treatment of materials'. Below the search bar is a button '+ Add Advanced Search Field'. To the right of the search bar is a button 'Edit' with a pencil icon and a search button 'Q' with a magnifying glass icon. Below the search bar is a chemical structure diagram of a biphenyl derivative. Below the chemical structure diagram are two buttons: 'Edit Drawing' and 'Remove'. Below the search bar and chemical structure diagram is a section titled 'Recent Search History' which contains a table with the following data: 'November 11, 2021', '3:30 PM', 'Substances', and 'qinghaosu (1)'. At the bottom right of the interface are two buttons: 'Rerun Search' and 'Edit Search'. The interface also features the ACS International and CAS logos at the bottom right.

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大纲

- CAS及CAS SciFinderⁿ简介
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- 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

视频链接:

https://american-chemical-society.zoom.us/rec/share/9PrTtd4gKFB245SuJax26so0a4WAHC9MMsgB74Bt3mPRK9TgcwZI753ROg4eHHseL.I_K0dQtNjGzGJK5y



文献检索

— 文献检索方法

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

— 检索策略推荐

- 关注某特定领域的文献：主题检索
- 关注物质有关的文献：先获得物质，再获得文献或文本+结构联合检索
- 关注某科研人员的文献：作者名检索
- 关注某机构科研进展：机构名检索

文献检索--主题词检索

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

The screenshot displays the CAS database 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 search area is titled 'References' and includes a search bar with the text 'TLR or "toll like receptor"'. Below the search bar, there is a button labeled '+ Add Advanced Search Field'. To the right of the search bar, there are buttons for 'x', 'Draw', and a magnifying glass icon. The search results are displayed in a table with the following entries:

Search Results
Toll like receptor (Chlamys farreri gene TLR)
Toll like receptor 4 (Mus caroli strain C0423 gene Tlr4)
Toll like receptor 4 (Mus caroli strain L0014 gene Tlr4)
Toll like receptor 4 (Mus caroli strain L0211 gene Tlr4)
Toll like receptor 4 (Mus caroli strain L0275 gene Tlr4)
Toll like receptor 4 (Mus cookii strain L0103 gene Tlr4)
Toll like receptor 4 (Mus cookii strain L0178 gene Tlr4)
Toll like receptor 4 (Mus cookii strain R4106 gene Tlr4)

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 Name journal of medic ✕

Volume (Optional)

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

Starting Page (Optional)

Learn more about SciFinder[®] Advanced Search.

+ 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

可单独使用，也可联用下面的检索方法：

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

文献结果集

排序：
更快查找相关信息

获得更多文献

文献类型

文献语言

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

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

Document Type

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

[View All](#)

Language

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

[View All](#)

References (9,495)

Sort: Relevance View: Partial Abstract

☐ Substances ☐ Reactions ☐ Citing

Relevance
Times Cited
Publication Date: Newest
Publication Date: Oldest

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

1

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

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

[View More](#)

文献结果集

研究发展趋势

CAS标引的
技术术语

CAS学科
研究方向

制剂/分析
方法信息

二次检索

The screenshot displays the CAS database search results interface. On the left, a sidebar contains various filters: 'Publication Year' (2000 to 2022), 'Available at My Institution', 'Author', 'Organization', 'Publication Name', 'Concept' (Homo sapiens, Human, Animals, Humans, Toll-like receptor 4), 'CA Section', 'CAS Solutions' (Formulus, Analytical Methods), 'Formulation Purpose', 'Database', and 'Search Within Results'. The main area shows three search results, each with a title, author, journal, and abstract. The first result is 'Trial Watch: Toll-like receptor agonists in cancer immunotherapy'. The second is 'Toll-like Receptor Agonist Conjugation: A Chemical Perspective'. The third is 'Trial Watch: Immunostimulation with Toll-like receptor agonists in cancer therapy'. Each result has a 'Full Text' button and a 'Citing' button.

Publication Year

2000 to 2022

No Min to No Max Apply

View Larger

Available at My Institution

Author

Organization

Publication Name

Concept

☐ Homo sapiens (4,956)

☐ Human (4,956)

☐ Animals (4,261)

☐ Humans (3,732)

☐ Toll-like receptor 4 (3,128)

View All

CA Section

CAS Solutions

☐ Formulus (1,184)

☐ Analytical Methods (5)

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

Oncolimmunology (2018), 7(12), e1526250/1-e1526250/15 | Language: English, Database: CAPus 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: CAPus and MEDLINE

TLR-Conjugates

Antigens

Self-adjuvant vaccines

Adjuvants

Multi-valent immunostimulants

Polymers

Improved pharmacokinetics

Fluorophores

Tracking tools

Immune System

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

Oncolimmunology (2016), 5(3), e1088631/1-e1088631/11 | Language: English, Database: CAPus 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



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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)		

Apply Cancel

通过CA Section快速
锁定学科研究方向

文献结果集--聚类筛选CAS Solutions

查看勾选的
Concept

The screenshot displays the CAS Solutions interface. On the left, the 'Filter Behavior' panel is active, showing a 'Filter by' button and a list of filters. The 'Publication Year' filter is expanded, showing a bar chart from 2000 to 2022. Below the chart, there are 'No Min' and 'No Max' options, and an 'Apply' button. The 'Available at My Institution' filter is also expanded. The 'CAS Solutions' filter is expanded, showing 'Formulus (861)' and 'Analytical Methods (2)'. The 'Formulation Purpose' filter is expanded. The 'Database' filter is expanded. The 'Search Within Results' section is at the bottom of the filter panel, with a search bar and a 'Search' button. The 'Filter Content Report' section is at the bottom of the filter panel, with a 'Download filter data from this result set' button.

The main panel shows the 'References' section with 7,597 results. The 'Filtering' section shows 'Concept: 8 Selected'. A dropdown menu is open, showing the following 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
- ☒ Toll-like receptor 5

The first reference is titled 'The pharmacology of Toll-like receptor agonists and the impact on the immune system'. The second reference is titled 'Antiviral applications of Toll-like receptor agonists'. The third reference is titled 'Trial Watch: Toll-like receptor agonists in cancer immunotherapy'.

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

Formulation Purpose

Database

Search Within Results

Enter a query...

References (7,597)

Sort: Relevance View: Partial Abstract

Substances Reactions Citing

Filtering: Concept: 8 Selected X 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: 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...

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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...

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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: 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...

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Substance (1) Reactions (0) **Citing (42)** Citation Map Download Email Save

JOURNAL

Source
Journal of Antimicrobial Chemotherapy
Volume: 67
Issue: 4
Pages: 789-801
Journal: General Review; Article; Review
2012
DOI: [10.1093/jac/dkr588](https://doi.org/10.1093/jac/dkr588)
CODEN: JACHDX
E-ISSN: 1460-2091
ISSN-L: 0305-7453

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AN: 2012:423823
CAN: 156:387108
PubMed ID: 22258929
CASP and MEDLINE

Company/Organization
Pfizer Global R & D
Sandwich, Kent CT13 9NJ
United Kingdom

Email
nhorscro@gmail.com

Publisher
Oxford University Press

Language
English

Antiviral applications of Toll-like receptor agonists
By: Horscroft, Nigel J.; Pryde, David C.; Bright, Helen

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

Keywords: review Toll like receptor agonist antiviral

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(含Caspus、Medline的关键词)
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^ Concepts	
Antiviral agents	Toll-like receptors
Receptor agonists	Role: Biological Study, Unclassified
	Viral infection

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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

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

Substances:
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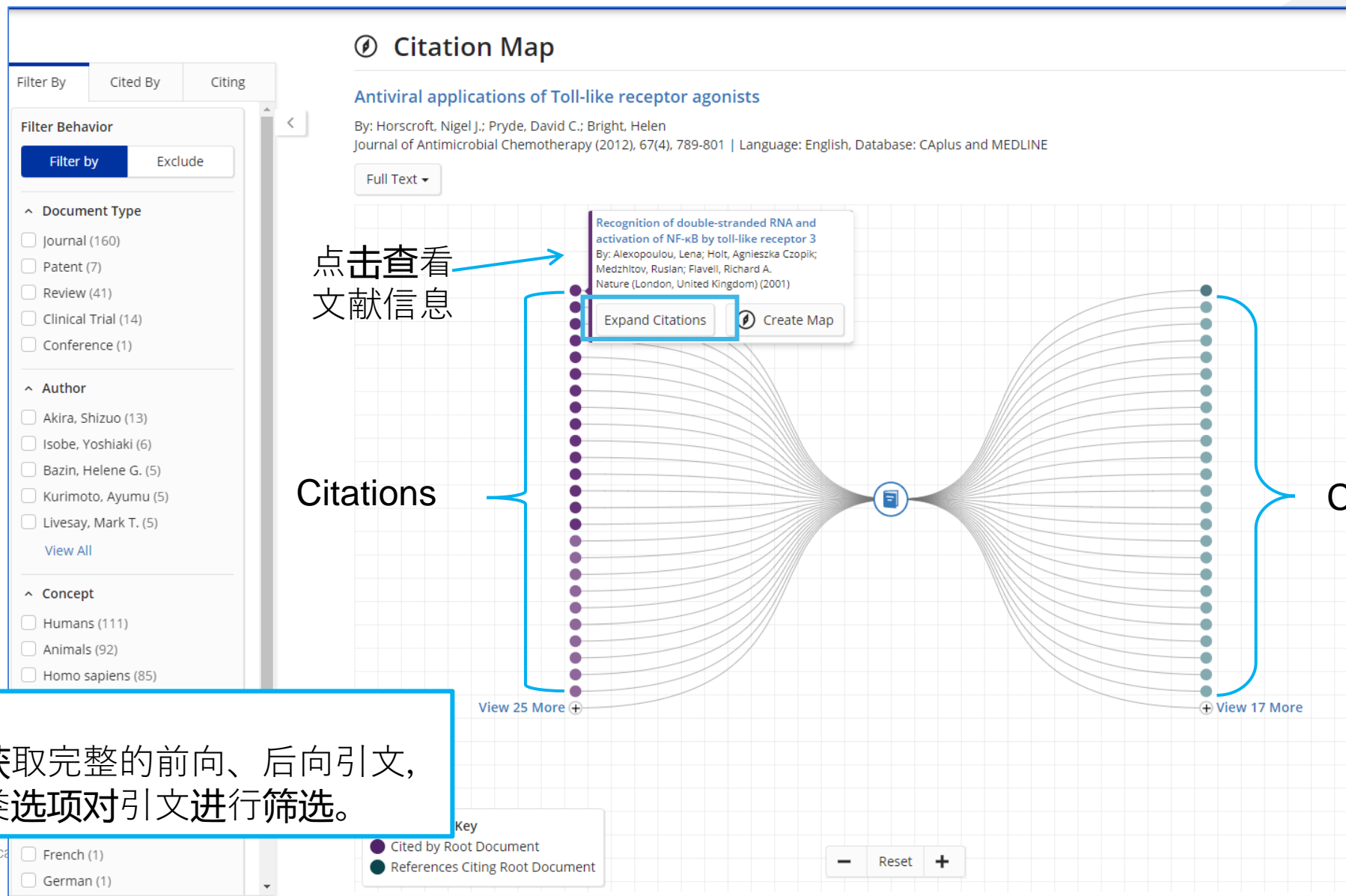
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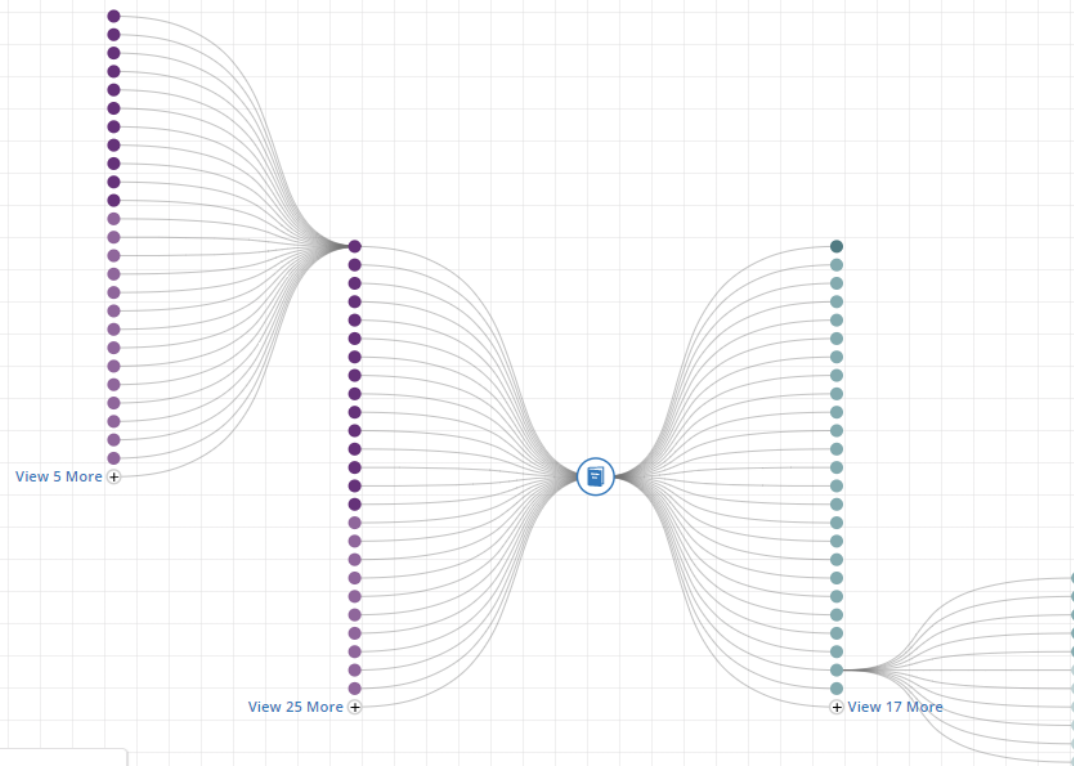
Citation Map

Antiviral applications of Toll-like receptor agonists

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

Journal of Antimicrobial Chemotherapy (2012), 67(4), 789-801 | Language: English, Database: CAPus and MEDLINE

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☐ 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)

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Substances

Reactions

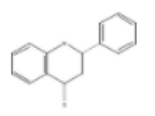
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References (75)

Sort: Relevance View: Partial Abstract

☐ Substances ☐ Reactions ☐ Citing

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

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: CAlus 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 t...

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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; Vijender, Kandi; Srihari, Pabbaraja; Reddy, Chada Raji; Janaki Ramaiah, M.; Bhadra, Utpal

Bioorganic & Medicinal Chemistry Letters (2012), 22(1), 645-648 | Language: English, Database: CAlus 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: CAlus

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

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- 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

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通过物质名称、CAS RN，文献标识符检索物质

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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

C43H66N12O12S2

Oxytocin

Protein/Peptide Sequence

Sequence Length: 9

31K References 390 Reactions 66 Suppliers

2

1190307-88-0

Absolute stereochemistry shown

C22H29FN3O9P

Sofosbuvir

3,695 References 720 Reactions 66 Suppliers

3

1809249-37-3

Absolute stereochemistry shown

C27H35N6O8P

GS 5734

2,264 References 504 Reactions 47 Suppliers

sofosbuvir
50-56-6
"GS 5734"

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Substances (4,467) Sort: Relevance View: Partial

Filter Behavior: Filter by 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) View All

Stereochemistry: Number of Components: Substance Class: Isotopes: Metals: Molecular Weight

Results (6 shown):

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

CAS SciFinder® Substances Draw Search

Substances (20) Sort: Relevance View: Partial

Filter Behavior: Filter by 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) View All

Number of Components: Substance Class: Isotopes: Metals: Experimental Property: Bioactivity Indicator

Results (6 shown):

- 11075-56-2: Notes: A flavone C₁₅H₁₀O₇ Junipin
- 1415244-57-3: Notes: A flavone C-glucoside Unspecified Vicinin II
- 887129-31-9: Notes: Described as a flavone deriv. Unspecified Griseon I
- 2095202-76-7: Notes: A flavone from Dysosma versipellis C₂₆H₂₈O₇ Dysosmaflavone G
- 125521-97-3: Notes: A flavone deodorant (Daiwa Chem. Co.) Unspecified Asutenchi P 110
- 209861-32-5: Notes: A flavone deriv. (Rilis Kagaku Kogyo K.K.) Unspecified Pancil FG 50

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物质检索--文献标识符

CAS SciFinder® Substances WO2011123645

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Commercial Availability

- Available (77)
- Not Available (52)

Reaction Role

- Product (128)
- Reactant (106)
- Reagent (27)
- Catalyst (20)
- Solvent (17)

Reference Role

- Preparation (127)
- Synthetic Preparation (125)
- Reactant (109)
- Reactant or Reagent (109)
- Uses (72)
- View All

Stereochemistry

Number of Components

Substance Class

Isotopes

Metals

Molecular Weight

Experimental Property

Experimental Spectrum

Regulatory Data by Country

Regulatory Data by List

Bioactivity Indicator

Target Indicator

Search Within Results

Substances (129)

Sort: Relevance View: Partial

References Reactions Suppliers

1 108-95-2 Oc1ccccc1 Phenol
215K References 91K Reactions 188 Suppliers

2 108-24-7 CC(=O)OC(C)=O Acetic anhydride
153K References 375K Reactions 80 Suppliers

3 100-46-9 NCCc1ccccc1 Benzylamine
57K References 93K Reactions 82 Suppliers

4 18162-48-6 CC(C)(C)Si(C)(C)Cl tert-Butyldimethylsilyl chloride
36K References 64K Reactions 127 Suppliers

5 10025-87-3 ClP(=O)(Cl)Cl Phosphorus oxychloride
25K References 214K Reactions 46 Suppliers

6 58-96-8 O=C1NC=CC2=C1N=CN2[C@@H]3O[C@H](CO)[C@@H](O)[C@H]3O Uridine
24K References 3,429 Reactions 106 Suppliers

7 149-30-4 C1=CC2=C(C=C1)SC(=S)N2 2-Mercaptobenzothiazole
18K References 6,303 Reactions 120 Suppliers

8 501-53-1 ClCOC(=O)c1ccccc1 Benzyl chloroformate
17K References 28K Reactions 75 Suppliers

9 616-47-7 CN1C=NC=C1 1-Methylimidazole
16K References 34K Reactions 112 Suppliers

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

生物（生物富集因子、LD50）

化学（Koc, LogD, LogP、溶解度、分子量、pKa、蒸汽压）

密度属性（密度、摩尔体积）

电学（电导/电导率、电阻/电阻率）

Lipinski（自由旋转键、H受体/供体）

磁（磁力矩）

机械属性（拉伸强度）

光散射（旋光性、折射率）

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Molecular Formula

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

AND

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Molecular Formula

CAS Registry Number

Chemical Name

Document Identifier

Patent Identifier

Experimental Spectra

Biological

Chemical Properties

Density

Electrical

Lipinski

Magnetic

Mechanical

Optical and Scattering

Structure Related

Thermal

物质检索--分子式

Na₂SO₄: H₂O₄S.2Na

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Molecular Formula: H₂SO₄.2Na

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

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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)

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Number of Components

Substance Class

Isotopes

Metals

Molecular Weight


Experimental Property


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
Regulatory Data by Country


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
References Reactions Suppliers


1 7757-82-6  • 2 Na
H₂O₄S.2Na
Components: 2
Component RN: 7664-93-9
Sodium sulfate
103K References 51K Reactions 178 Suppliers

2 13759-07-4  • 2 Na
H₂O₄S.2Na
Components: 2
Component RN: 7664-93-9
Thenardite (Na₂(SO₄))
906 References 0 Reactions 1 Supplier

3 14262-80-7  • 2 Na
H₂O₄S.2Na
Components: 2
Component RN: 13770-01-9
Sulfuric-³⁵S acid, disodium salt
73 References 1 Reaction 4 Suppliers

4 225640-22-2  • 2 Na
H₂O₄S.2Na
Components: 2
Component RN: 778561-01-6
Sulfuric-³⁴S acid, disodium salt
8 References 1 Reaction 1 Supplier

5 20581-68-4  • 2 Na
H₂O₄S.2Na
Components: 2
Component RN: 7664-93-9
Metathenardite (Na₂(SO₄))
3 References 0 Reactions 0 Suppliers

6 911392-46-6  • 2 Na
H₂O₄S.2Na
Components: 2
Component RN: 911422-29-2
Sulfuric-³³S acid, disodium salt
1 Reference 0 Reactions 1 Supplier

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...

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.

Molecular Weight <200

Predicted values only.

+ Add Advanced Search Field

AND

References

Suppliers

Biosequences

Retrosynthesis

多参数检索，提高检索效率

Substances (6)

Sort: Relevance View: Partial

References Reactions Suppliers

139-13-9

OC(=O)CNC(C(=O)O)C(=O)O

C₆H₉NO₆
Nitrilotriacetic acid

13K References 713 Reactions 91 Suppliers

7631-86-9

O=Si=O

O₂Si
Silica

1.1M References 90K Reactions 407 Suppliers

593-88-4

C[As](C)C

C₃H₉As
Trimethylarsine

34560-16-2

CCOC(C(=O)O)C(=O)O

C₆H₁₃NO₄
1,1-Diethoxy-2-nitroethane

25 References 42 Reactions 50 Suppliers

79-02-7

ClC(Cl)C=O

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



ACS
International

CAS
A division of the
American Chemical Society



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

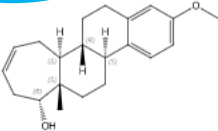
References

Reactions

Suppliers

1

1354644-05-5



Absolute stereochemistry shown, Rotation (+)

$C_{21}H_{28}O_2$
(4bS,6aS,7R,11aS,11bR)-4b,6,6a,7,8,11,11a,11b,12,13-Decahydro-2-methoxy-6a-methy...

2

References

4

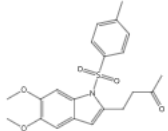
Reactions

1

Supplier

2

921073-43-0



$C_{21}H_{23}NO_5S$
4-[5,6-Dimethoxy-1-[(4-methylphenyl)sulfonyl]-1H-indol-2-yl]-2-butanone

1

Reference

6

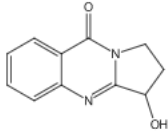
Reactions

0

Suppliers

3

35387-16-7



$C_{11}H_{10}N_2O_2$
2,3-Dihydro-3-hydroxypyrrolo[2,1-b]quinazolin-9(1H)-one

51

References

37

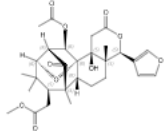
Reactions

10

Suppliers

4

879288-35-4



Absolute stereochemistry shown, Rotation (-)

$C_{29}H_{36}O_{10}$
Methyl (4S,4aS,6aR,7S,8S,10R,11R,12R,12aR,12bS)-12-(acetyloxy)-4-(3-furanyl)dode...

2

References

0

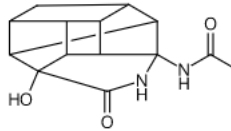
Reactions

0

Suppliers

5

693235-19-7



$C_{14}H_{16}N_2O_3$
Acetamide, N-(decahydro-3-hydroxy-2-oxo-3,7,4,6-ethanediylidene-7aH-pentaleno[1,...

2

References

2

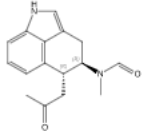
Reactions

0

Suppliers

6

1245281-17-7



Absolute stereochemistry shown

$C_{16}H_{18}N_2O_2$
N-Methyl-N-[(4R,5R)-1,3,4,5-tetrahydro-5-(2-oxopropyl)benz[cd]indol-4-yl]formami...

1

Reference


0

Reactions


0

Suppliers

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物质详情

Substance Detail (1 of 1,143)

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

← Prev Next →

Download Email Save

CAS Registry Number
1354644-05-5

Absolute stereochemistry shown, Rotation (+)

C₂₁H₂₈O₂
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

View Carbon-13 NMR Spectrum

(1) ACD

Sources

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

Predicted Properties

Predicted Spectra

Bioactivity Indicators

Carbo

1354644-05

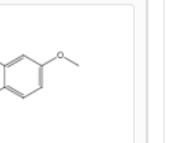


Absolute stereochemistry

C₂₇H₄₆O₅

Carbon-13 NMR Spectrum Detail (1 of 1)

1354644-05-5



Absolute stereochemistry shown, Rotation (+)

$C_{21}H_{28}O_2$

CAS Name
(4b5,6a5,7R,11a5,11bR)-4b,6,6a,7,8,11,11a,11b,12,13-Decahydro-2-methoxy-6a-methyl-5H-cyclohepta[σ]phenan thren-7-ol

Conditions

Working Frequency
150 MHz

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

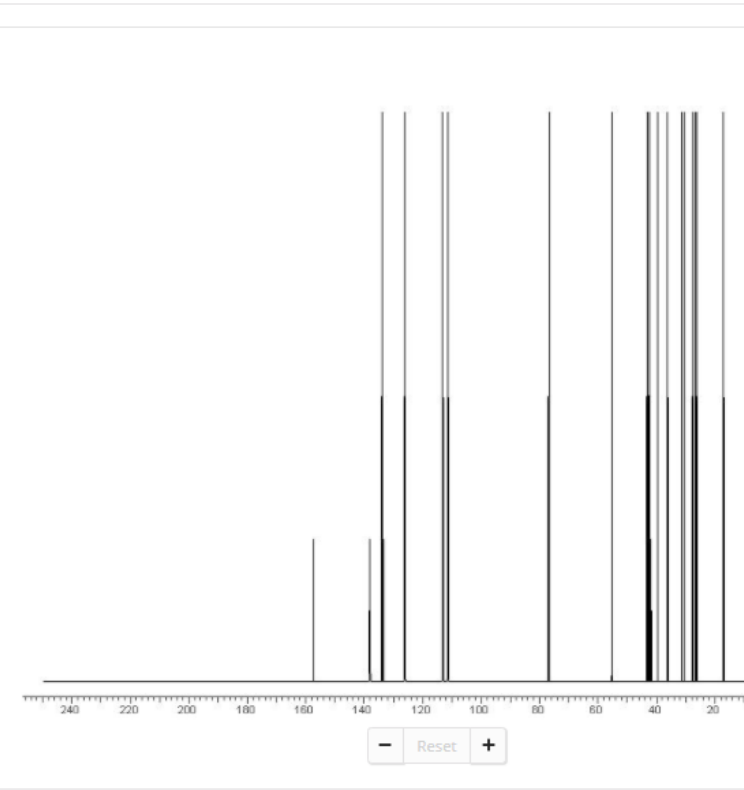
Temperature
25 °C

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.



The figure displays a Carbon-13 NMR spectrum with the x-axis representing chemical shift in ppm, ranging from 240 to -20. The spectrum shows several sharp peaks. A cluster of peaks is visible between 120 and 160 ppm, and another cluster is visible between 20 and 80 ppm. The peaks are labeled with their corresponding chemical shift values in ppm.

Chemical Shift (ppm)
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

物质检索--结构检索

Searching for...

Substances

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

Enter a query...

Draw

Molecular Formula

Examples: C6H6 | (C8H8)x | C22H26CuN2O5 C2H3N

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

+ Add Advanced Search Field

CAS Draw

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

Draw or change atoms or bonds.

Molecular Formula:

C

Zoom: 100%

OK Cancel



选择可变基团



自定义R基团



重复片段工具

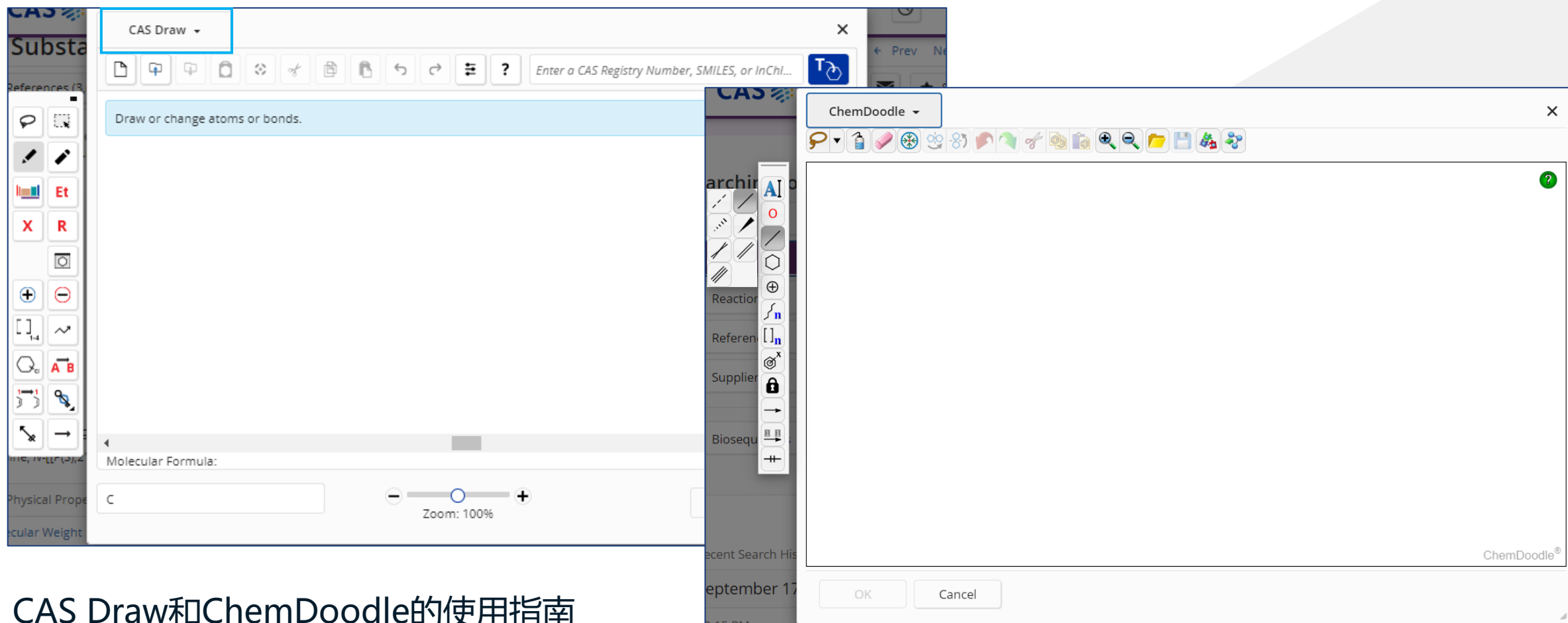


取代位点可变



锁工具

物质检索--结构绘图板



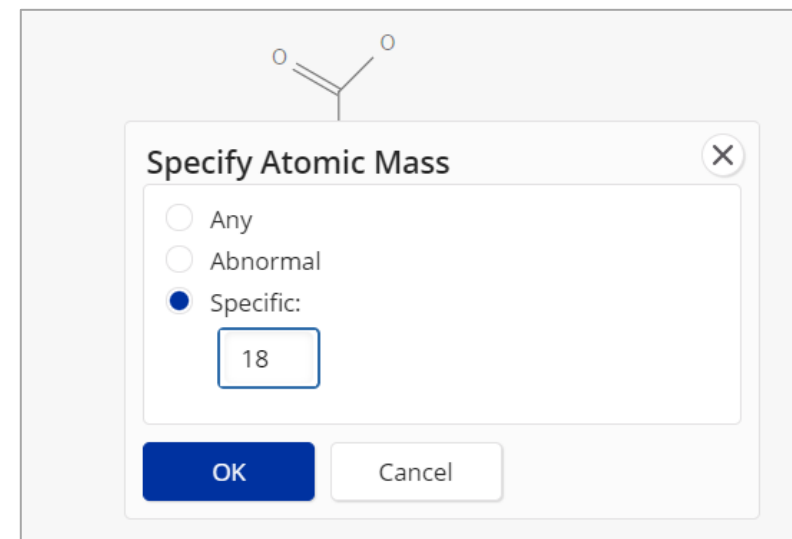
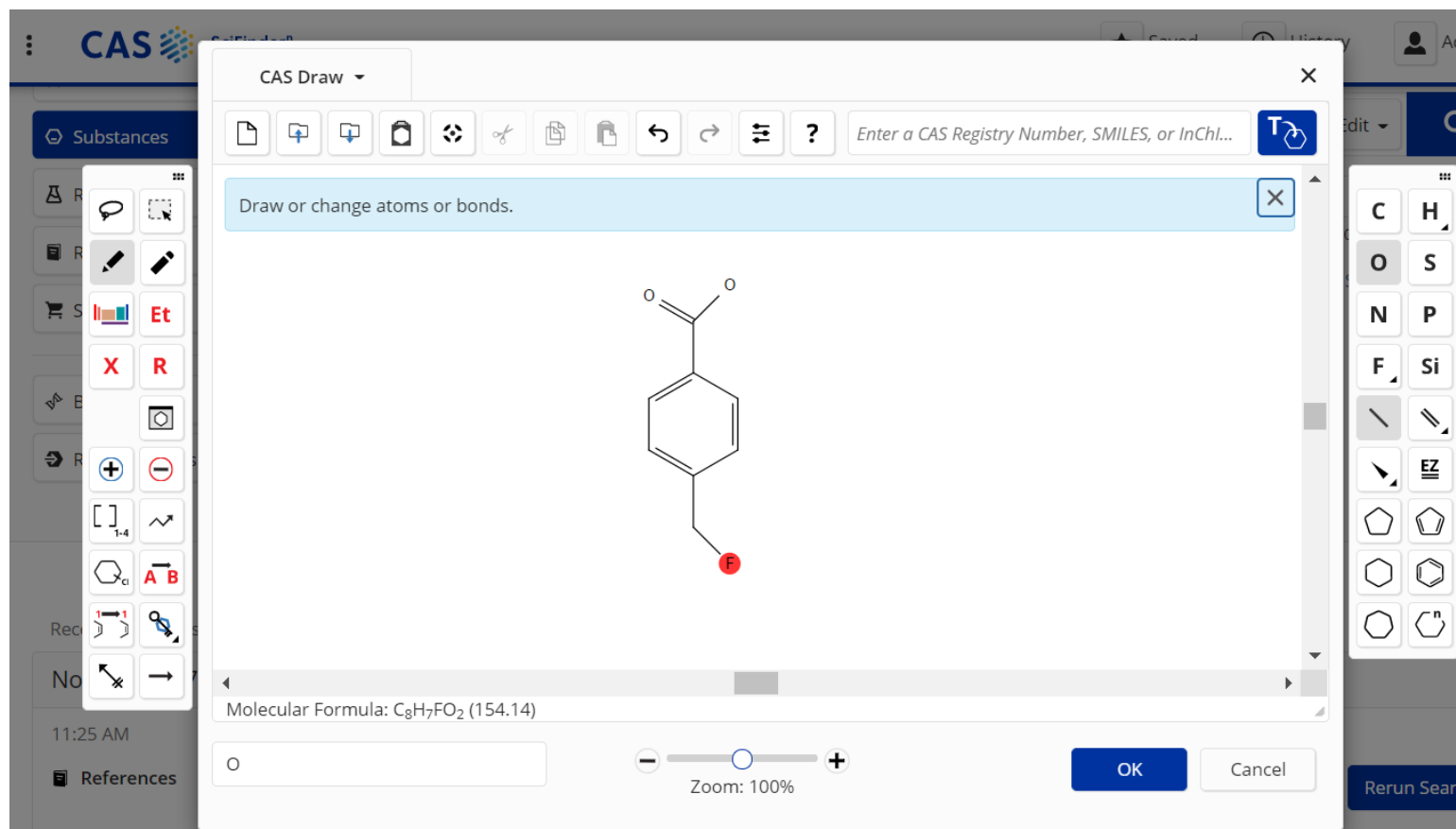
CAS Draw和ChemDoodle的使用指南

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

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

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

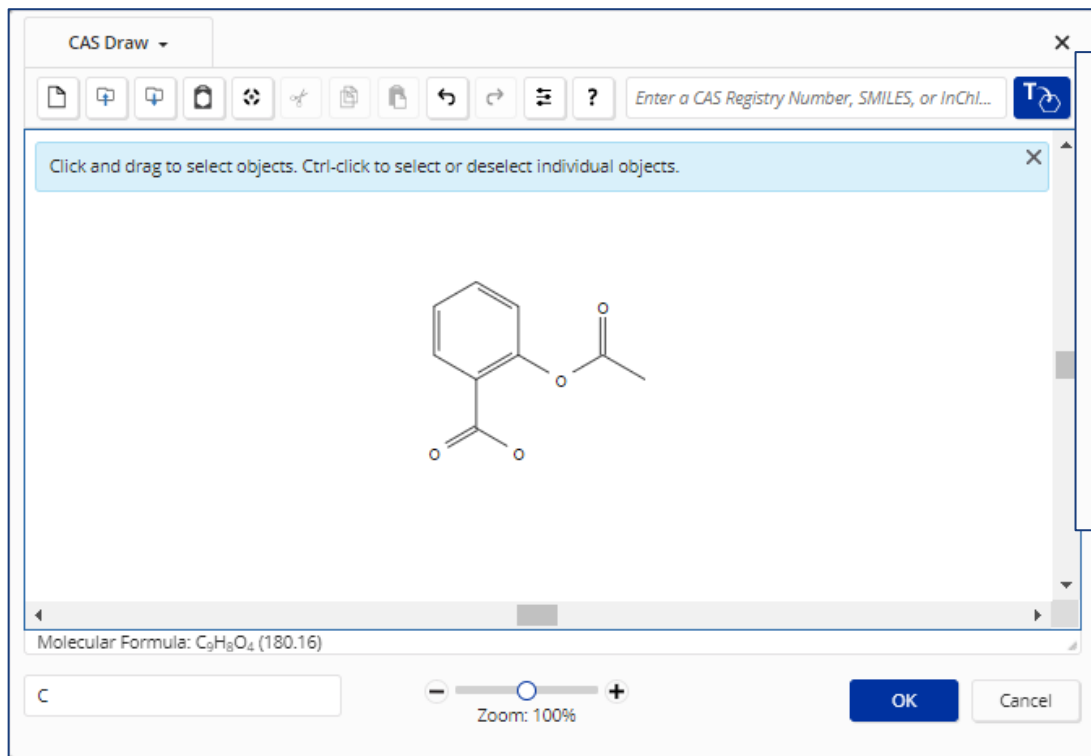
结构绘图工具的使用--同位素原子的绘制



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

物质检索--结构检索

CAS RN: 50-78-2



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: C_6H_6 | $(C_8H_8)_x$ | $CC(=O)O$

[Add Advanced Search Field](#)

[Learn more about SciFinder](#)

Edit Drawing Remove

☐ 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

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

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

1 50-78-2

CC(=O)Oc1ccccc1C(=O)O

C₉H₈O₄
Aspirin

84K References 1,997 Reactions 108 Suppliers

2 5054-56-8

CC(=O)Oc1ccccc1C(=O)O

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

19 References 0 Reactions 2 Suppliers

4 97781-16-3

CC(=O)Oc1cc2c(c(c1)O)C(=O)OC2=O

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

8 References 5 Reactions 24 Suppliers

5 921943-73-9

CC(=O)Oc1ccccc1C(=O)O

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

5 References 0 Reactions 18 Suppliers

6 59096-15-0

CC(=O)Oc1ccccc1C(=O)O

C₉H₈O₄
Benzoic acid, 2-(acetyl-1-¹⁴C-oxy)-

5 References 1 Reaction 1 Supplier

7 59096-14-9

CC(=O)Oc1ccccc1C(=O)O

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

5 References 0 Reactions 3 Suppliers

8 215935-30-1

CC(=O)Oc1ccccc1C(=O)O

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

4 References 0 Reactions 0 Suppliers

9 229030-56-2

CC(=O)Oc1ccccc1C(=O)O

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

3 References 0 Reactions 1 Supplier

物质检索--结构检索

结构检索类别:

As Drawn

亚结构

相似结构

结构精准度筛选

Chemscape分析

物质筛选类别:

反应角色

文献角色

立体化学

物质类别

同位素

金属包含

实验物性数据

二次检索……

Structure Match

As Drawn (927)

Substructure (20K)

Similarity (79K)

Analyze Structure Precision

Chemscape Analysis

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

Create Chemscape Analysis

Filter Behavior

Filter by Exclude

Commercial Availability

Available (3,959)

Not Available (16K)

Reaction Role

Product (9,393)

Reactant (2,119)

Reagent (11)

Catalyst (20)

Solvent (3)

Reference Role

Preparation (13K)

Synthetic Preparation (10K)

Uses (7,065)

Biological Study (6,643)

Therapeutic Use (3,703)

View All

Stereochemistry

Number of Components

Substance Class

Isotopes

Metals

Molecular Weight

Substances (20,611)

Sort: Relevance View: Partial

References Reactions Suppliers

1 50-78-2 CC(=O)Oc1ccccc1C(=O)O C9H8O4 Aspirin 84K References 1,997 Reactions 108 Suppliers

2 5054-56-8 CC(=O)Oc1ccccc1C(=O)O C9H7O4 Benzoic acid, 2-(acetyloxy)-, ion(1-) 19 References 0 Reactions 2 Suppliers

3 89655-56-1 CC(=O)Oc1ccccc1C(=O)O (C9H8O4)x 2-Acetylsalicylic acid homopolymer 16 References 0 Reactions 0 Suppliers

4 97781-16-3 CC(=O)Oc1ccccc1C(=O)O C9H4D4O4 Benzoic-2,3,4,5-d₄ acid, 6-(acetyloxy)- 8 References 5 Reactions 24 Suppliers

5 921943-73-9 CC(=O)Oc1ccccc1C(=O)O C9H5D3O4 2-(Acetyl-2,2,2-d₃-oxy)benzoic acid 5 References 0 Reactions 18 Suppliers

6 59096-15-0 CC(=O)Oc1ccccc1C(=O)O C9H8O4 Benzoic acid, 2-(acetyl-1-¹⁴C-oxy)- 5 References 1 Reaction 1 Supplier

7 59096-14-9 CC(=O)Oc1ccccc1C(=O)O C9H8O4 Benzoic-carboxy-¹⁴C acid, 2-(acetyloxy)- 5 References 0 Reactions 3 Suppliers

8 215935-30-1 CC(=O)Oc1ccccc1C(=O)O C9H7DO4 2-(Acetyl-2-d-oxy)benzoic acid 4 References 0 Reactions 0 Suppliers

9 229030-56-2 CC(=O)Oc1ccccc1C(=O)O C9H8O4 Benzoic acid, 2-(acetyl-1-¹³C-oxy)- 3 References 0 Reactions 1 Supplier

10 225243-55-0 CC(=O)Oc1ccccc1C(=O)O

Filter by选择感兴趣的结果
，或Exclude排除不需要的结

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

Structure Match

As Drawn (927)

Substructure (20K)

Similarity (79K)

Analyze Structure Precision

Chemscape Analysis

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Create Chemscape Analysis

Filter Behavior

Filter by Exclude

Commercial Availability

Available (3)

Not Available (17)

Reaction Role

Product (9,393)

Reactant (2,119)

Reagent (11)

☒ Catalyst (20)

Solvent (3)

Reference Role

Catalyst Use (18)

Preparation (18)

Uses (18)

Synthetic Preparation (17)

Properties (6)

Isotopes

Metals

Molecular Weight

Substances (20)

Sort: Relevance View: Partial

References Reactions Suppliers

Filtering: Reaction Role: Catalyst X Clear All Filters

1 50-78-2 Aspirin CC(=O)Oc1ccccc1C(=O)O 84K References 1,997 Reactions 108 Suppliers

2 1803201-02-6 Benzeneacetic acid, 2-[(2-methylpropoxy)carbonyl]phenyl ester CC(C)OC(=O)c1ccccc1CC(=O)O 1 Reference 1 Reaction 0 Suppliers

3 875584-96-6 2-Methylpropyl 2-(benzoyloxy)benzoate CC(C)OC(=O)c1ccccc1C(=O)OC(=O)c2ccccc2 4 References 4 Reactions 2 Suppliers

4 2093113-55-2 Benzoic acid, 2-(2,2-dimethyl-1-oxopropoxy)-3-methyl-, 2-methylpropyl ester CC(C)OC(=O)c1ccccc1C(=O)OC(=O)C(C)C 2 References 2 Reactions 0 Suppliers

5 2093113-56-3 Benzoic acid, 2-(benzoyloxy)-3-methyl-, 2-methylpropyl ester CC(C)OC(=O)c1ccccc1C(=O)OC(=O)c2ccccc2 2 References 2 Reactions 0 Suppliers

6 2093113-57-4 Benzoic acid, 2-(benzoyloxy)-3,5-bis(1-methylethyl)-, 2-methylpropyl ester CC(C)OC(=O)c1ccccc1C(=O)OC(=O)c2ccccc2C(C)C 2 References 3 Reactions 0 Suppliers

7 1416949-86-4 1'-[1,4-Butanediylbis(oxyethylidene)]bis[2-(acetyloxy)benzoate] CC(=O)OC(=O)c1ccccc1C(=O)OC(=O)C(C)C 1 Reference 2 Reactions 0 Suppliers

8 2093113-58-5 Benzoic acid, 2-(benzoyloxy)-3,5-bis(1,1-dimethylethyl)-, 2-methylpropyl ester CC(C)OC(=O)c1ccccc1C(=O)OC(=O)c2ccccc2C(C)C 2 References 2 Reactions 0 Suppliers

9 948830-92-0 Methyl 1-(acetyloxy)-3-hydroxy-7-methoxy-6-[2-(trimethylsilyl)ethynyl]-2-naphtha... CC(=O)OC(=O)c1ccccc1C(=O)OC(=O)C(C)C 1 Reference 12 Reactions 0 Suppliers

利用物质反应角色
筛选物质

利用物质在反应中的角色精准定位相应的物质

物质检索--检索结果集筛选：Reference Role

Reference Role

By Count | Alphanumeric

1 Selected

<input type="checkbox"/> Preparation (13K)	<input type="checkbox"/> Cosmetic Use (372)	<input type="checkbox"/> Analytical Role, Unclassified (36)
<input type="checkbox"/> Synthetic Preparation (10K)	<input type="checkbox"/> Polymer in Formulation (314)	<input type="checkbox"/> Analytical Reagent Use (27)
<input type="checkbox"/> Uses (7,065)	<input type="checkbox"/> Food or Feed Use (248)	<input type="checkbox"/> Reagent (26)
<input type="checkbox"/> Biological Study (6,643)	<input type="checkbox"/> Analytical Study (237)	<input type="checkbox"/> Pollutant (22)
<input type="checkbox"/> Therapeutic Use (3,703)	<input type="checkbox"/> Pharmacokinetics (229)	<input type="checkbox"/> Nanoscale (21)
<input type="checkbox"/> Reactant or Reagent (3,377)	<input type="checkbox"/> Adverse Effect (189)	<input type="checkbox"/> Byproduct (17)
<input type="checkbox"/> Reactant (3,374)	<input type="checkbox"/> Modifier or Additive Use (189)	<input type="checkbox"/> Biosynthetic Preparation (14)
<input type="checkbox"/> Biological Study, Unclassified (3,079)	<input type="checkbox"/> Analyte (167)	<input type="checkbox"/> Diagnostic Use (10)
<input type="checkbox"/> Properties (2,940)	<input type="checkbox"/> Catalyst Use (102)	<input type="checkbox"/> Occurrence, Unclassified (8)
<input type="checkbox"/> Prophetic Synthesis or Use (2,778)	<input type="checkbox"/> Purification or Recovery (85)	<input type="checkbox"/> Bioindustrial Manufacture (7)
<input type="checkbox"/> Pharmacological Activity (2,628)	<input type="checkbox"/> Formation, Non-preparative (85)	<input type="checkbox"/> Combinatorial Study (6)
<input type="checkbox"/> Technical or Engineered Material Use (2,184)	<input type="checkbox"/> Biological Use, Unclassified (82)	<input type="checkbox"/> Miscellaneous (6)
<input type="checkbox"/> Industrial Manufacture (1,589)	<input type="checkbox"/> Formation, Unclassified (67)	<input type="checkbox"/> Biochemical Process (4)
<input type="checkbox"/> Agricultural Use (1,151)	<input type="checkbox"/> Occurrence (61)	<input type="checkbox"/> Removal or Disposal (4)
<input type="checkbox"/> Process (496)	<input type="checkbox"/> Other Use, Unclassified (59)	<input type="checkbox"/> Geological or Astronomical Occurrence (1)
<input type="checkbox"/> Physical, Engineering, or Chemical Process (452)	<input checked="" type="checkbox"/> Natural Product Occurrence (39)	<input type="checkbox"/> Geological or Astronomical Process (1)
	<input type="checkbox"/> Analytical Matrix (36)	

Apply Cancel

利用Reference Role（物质的研究方向）精准定位相应的物质

Structure Match

As Drawn (927)

Substructure (20K)

Similarity (79K)

Analyze Structure Precision

Chemscape Analysis

Visually explore structure similarity with a powerful new tool.

Learn more about Chemscape.

Create Chemscape Analysis

Filter Behavior

Filter by Exclude

Commercial Availability

Available (13)

Not Available (26)

Reaction Role

Product (14)

Reactant (7)

Reagent (1)

Catalyst (1)

Solvent (1)

Reference Role

Preparation (13K)

Synthetic Preparation (10K)

Uses (7,065)

Biological Study (6,643)

Therapeutic Use (3,703)

Natural Product Occurrence (39)

View All

Substances (39)

Sort: Relevance View: Partial

References Reactions Suppliers

Filtering: Reference Role: Natural Product Occurrence

Clear All Filters

1 50-78-2 C ₉ H ₈ O ₄ Aspirin 84K References 1,997 Reactions 108 Suppliers	2 1247764-46-0 C ₉ H ₈ O ₄ , Unspecified Components: 2 Benzoic acid, 2-(acetyloxy)-, mixt. with Tetrahop 1 Reference 0 Reactions 0 Suppliers	3 1247764-40-4 C ₉ H ₈ O ₄ , Unspecified Components: 2 Benzoic acid, 2-(acetyloxy)-, mixt. with redihop 1 Reference 0 Reactions 0 Suppliers
4 51-01-4 C ₁₁ H ₁₀ O ₆ 2,4-Bis(acetyloxy)benzoic acid 75 References 171 Reactions 9 Suppliers	5 756455-72-8 C ₂₃ H ₃₆ O ₄ 2-[(1-Oxoheptadecyloxy)benzoic acid 8 References 4 Reactions 0 Suppliers	6 36081-01-3 C ₁₄ H ₁₀ O ₇ 2,4-Dihydroxy-6-[(4-hydroxybenzoyloxy)benzoic acid 3 References 8 Reactions 1 Supplier
7 2724988-28-5 	8 55045-01-7 	9 1350977-80-8

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: C_9H_8 (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 X Clear All Filters

<p>1</p> <p>218453-29-3</p> <p></p> <p>$C_{28}H_{32}O_5S$ Ethyl 2-(2,2-dimethyl-1-oxopropoxy)-5-[(5-(methylthio)-2-propyl-1H-inden-1-ylidene)oxy]benzoate</p> <p>1 Reference 1 Reaction 0 Suppliers</p>	<p>2</p> <p>218453-26-0</p> <p></p> <p>$C_{28}H_{32}O_6S$ Ethyl 2-(2,2-dimethyl-1-oxopropoxy)-5-[(5-(methylsulfonyl)-2-propyl-1H-inden-1-ylidene)oxy]benzoate</p> <p>1 Reference 1 Reaction 0 Suppliers</p>	<p>3</p> <p>218453-25-9</p> <p></p> <p>$C_{28}H_{32}O_6S$ Ethyl 2-(2,2-dimethyl-1-oxopropoxy)-5-[(5-(methylsulfonyl)-2-propyl-1H-inden-1-ylidene)oxy]benzoate</p> <p>1 Reference 1 Reaction 0 Suppliers</p>
<p>4</p> <p>1962179-79-8</p> <p></p> <p>$C_{27}H_{30}O_7$ Benzoic acid, 2-(2,3-dihydro-1-oxo-1H-inden-2-yl)-3,6-bis(2,2-dimethyl-1-oxopropoxy)-</p> <p>1 Reference 3 Reactions 0 Suppliers</p>	<p>5</p> <p>1168965-99-8</p> <p></p> <p>$C_{24}H_{17}N_2O_4$ 1H-Indene-2-carboxylic acid, 3-methyl-1-[(E)-(2-amino-1-cyano-2-oxoethylidene)oxy]-</p> <p>1 Reference 0 Reactions 0 Suppliers</p>	<p>6</p> <p>1962178-79-5</p> <p></p> <p>$C_{30}H_{32}O_8$ Benzoic acid, 2-(2,3-dihydro-7-methoxy-1-oxo-1H-inden-2-yl)-3,6-bis(2,2-dimethyl-1-oxopropoxy)-</p> <p>1 Reference 4 Reactions 0 Suppliers</p>
<p>7</p> <p>1962179-44-7</p> <p></p> <p>$C_{30}H_{32}O_8$ Benzoic acid, 3,6-bis(2,2-dimethyl-1-oxopropoxy)-2-(7-methoxy-1-oxo-1H-inden-2-yl)-</p> <p>1 Reference 5 Reactions 0 Suppliers</p>	<p>8</p> <p>1168964-47-3</p> <p></p> <p>$C_{26}H_{21}BrN_2O_4$ 2-Carboxyphenyl (6Z)-7-bromo-9-methyl-2-[(3-methyl-1H-inden-2-yl)carbonyloxy]-</p> <p>1 Reference 0 Reactions 0 Suppliers</p>	<p>9</p> <p>1168960-42-6</p> <p></p> <p>$C_{26}H_{21}ClN_2O_4$ 2-Carboxyphenyl (6Z)-7-chloro-9-methyl-2-[(3-methyl-1H-inden-2-yl)carbonyloxy]-</p> <p>1 Reference 0 Reactions 0 Suppliers</p>
<p>10</p> <p>1169002-06-5</p> <p></p> <p>$C_{26}H_{21}BrN_2O_4$ 2-Carboxyphenyl (6Z)-7-bromo-9-methyl-2-[(3-methyl-1H-inden-2-yl)carbonyloxy]-</p> <p>1 Reference 0 Reactions 0 Suppliers</p>	<p>11</p> <p>1168974-14-8</p> <p></p> <p>$C_{26}H_{21}BrN_2O_4$ 2-Carboxyphenyl (6Z)-7-bromo-9-methyl-2-[(3-methyl-1H-inden-2-yl)carbonyloxy]-</p> <p>1 Reference 0 Reactions 0 Suppliers</p>	<p>12</p> <p>1499112-44-5</p> <p></p> <p>$C_{26}H_{21}BrN_2O_4$ 2-Carboxyphenyl (6Z)-7-bromo-9-methyl-2-[(3-methyl-1H-inden-2-yl)carbonyloxy]-</p> <p>1 Reference 0 Reactions 0 Suppliers</p>

物质检索-检索结果集可视化分析：ChemScape Analysis



通过ChemScape
Analysis了解物质的专利

Structure Match

As Drawn (927)

Substructure (20K)

Similarity (79K)

Analyze Structure Precision

ChemScape Analysis

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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

C₉H₈O₄
Aspirin
84K References 1,997 Reactions 108 Suppliers

2 5054-56-8
C₉H₇O₄
Benzoic acid, 2-(acetyloxy)-, ion(1-)
19 References 0 Reactions 2 Suppliers

3 89655-56-1

(C₉H₈O₄)_x
2-Acetylsalicylic acid homopolymer
16 References 0 Reactions 0 Suppliers

4 97781-16-3
C₉H₄D₄O₄
Benzoic-2,3,4,5-d₄ acid, 6-(acetyloxy)-
8 References 5 Reactions 24 Suppliers

5 921943-73-9

C₉H₅D₃O₄
2-(Acetyl-2,2,2-d₃-oxy)benzoic acid
5 References 0 Reactions 18 Suppliers

6 59096-15-0
C₉H₈O₄
Benzoic acid, 2-(acetyl-1-¹⁴C-oxy)-
5 References 1 Reaction 1 Supplier

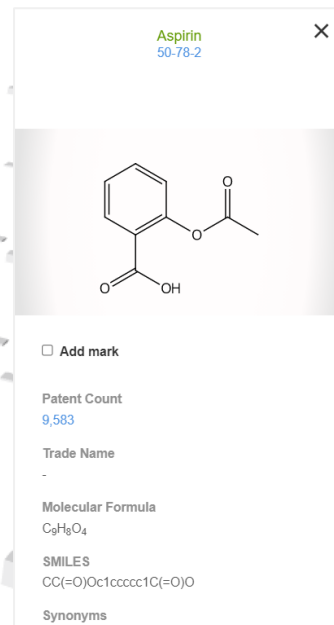
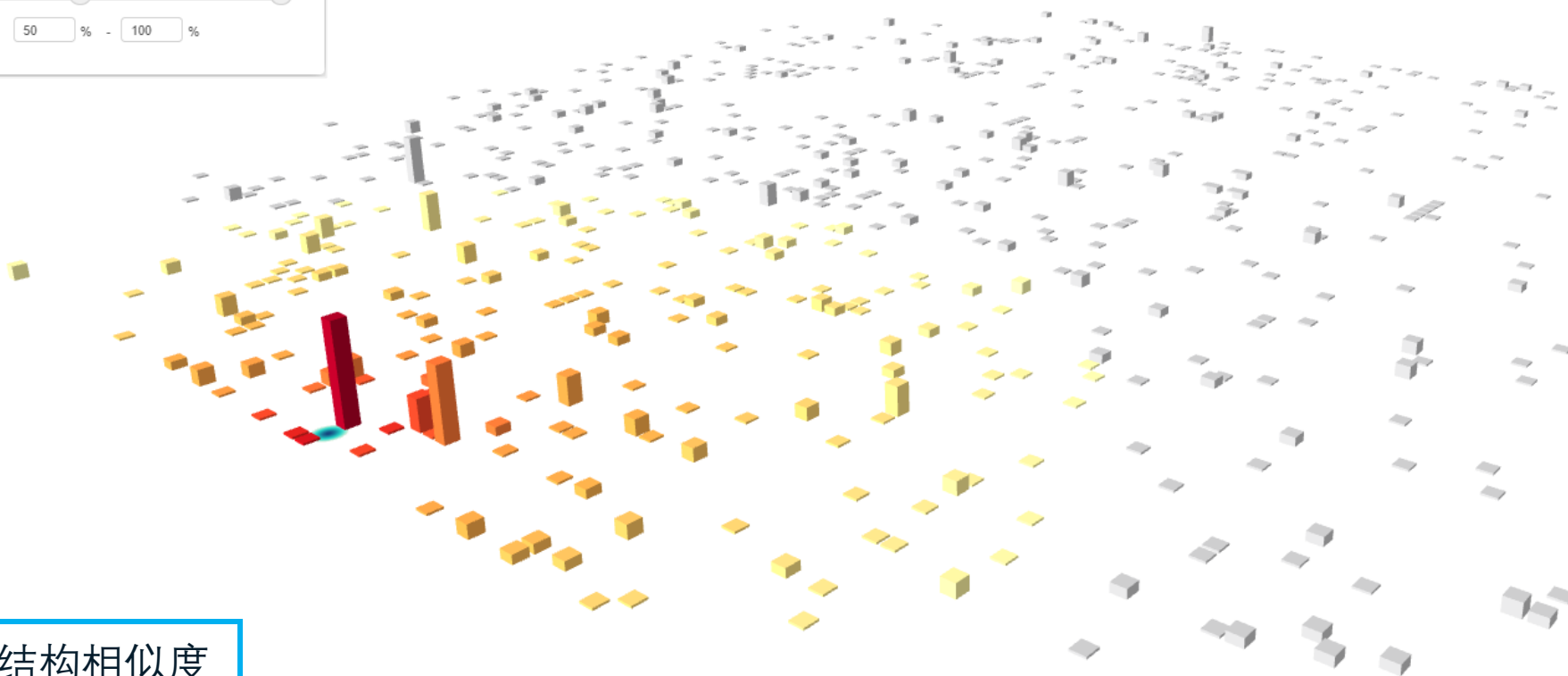
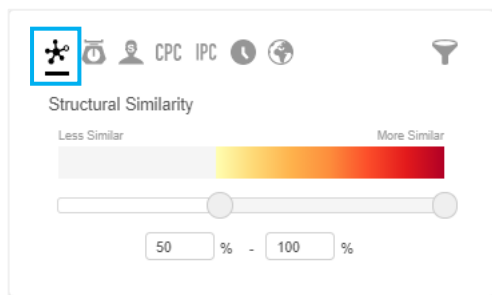
7 59096-14-9
C₉H₈O₄
Benzoic-carboxy-¹⁴C acid, 2-(acetyloxy)-
5 References 0 Reactions 3 Suppliers

8 215935-30-1

C₉H₇DO₄
2-(Acetyl-2-d-oxy)benzoic acid
4 References 0 Reactions 0 Suppliers

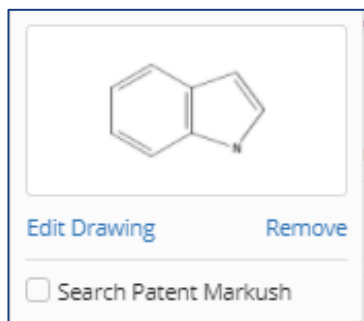
9 229030-56-2
C₉H₈O₄
Benzoic acid, 2-(acetyl-1-¹³C-oxy)-
3 References 0 Reactions 1 Supplier

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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Create Chemscape Analysis

Filter Behavior

Filter by Exclude

Commercial Availability

☐ Available (3)

☐ Not Available (17)

Reaction Role

☐ Product (1)

☐ Reactant (1)

Reference Role

☐ Properties (15)

☐ Formation, Non-preparative (7)

☐ Formation, Unclassified (7)

☐ Uses (7)

☐ Reactant (4)

[View All](#)

Number of Components

Substance Class

Isotopes

Metals

Substances (20)

Sort: Relevance View: Partial

References Reactions Suppliers

1 271-26-1 C8H7N 3H-Indole

2 1001205-42-0 C8H7N 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

The screenshot displays the CAS search results interface. On the left, there is a sidebar with various filters and options, including 'Structure Match', 'Substructure (3.7M)', 'Similarity (10K)', 'Structure Precision', 'Chemical Analysis', 'Filter Behavior', 'Commercial Availability', 'Reaction Role', 'Reference Role', and 'Number of Components'. The main area shows a grid of search results, each containing a chemical structure, a name, and associated data. The results are sorted by 'Relevance' and viewed in 'Partial' view. The grid includes items like 271-26-1, 1001205-42-0, 22493-45-4, 1426415-91-9, 107715-56-0, 111632-87-2, 2609928-58-5, 578731-99-4, and 271-23-8. Each item has a 'References' button, a 'Reactions' button, and a 'Suppliers' button. The 'References' button is highlighted with a blue box and an arrow pointing to the '获得相关文献' label. The 'Reactions' button is highlighted with a blue box and an arrow pointing to the '获得相关反应' label. The 'Suppliers' button is highlighted with a blue box and an arrow pointing to the '获得商品信息' label. The 'Save' button is highlighted with a blue box and an arrow pointing to the 'Save Search' dialog box. The 'Download' button is highlighted with a blue box and an arrow pointing to the 'Download Substance Results' dialog box.

Save Search

Name

No Alerts As Available Weekly Monthly

Tags (optional)

No tags defined

New Tag (optional)

Save Cancel

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 Substance Results

File Type

PDF

Select Quantity

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

Display

Result Summary Result Details

File Name

Substance_20211117_2357

Include


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

Download Cancel Learn more about downloads.

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

(10) 申请公布号 CN 104945470 A

(43) 申请公布日 2015.09.30

(21) 申请号 201410122313.4

(22) 申请日 2014.03.30

(71) 申请人 浙江大学

地址 310027 浙江省杭州市西湖区浙大路38号

申请人 中国科学院上海药物研究所

(72) 发明人 胡永洲 李佳 刘滔 张建康 周宇波 杨波 何倩军 许磊 胡小蓓

(74) 专利代理机构 杭州求是专利事务所有限公司 33200

代理人 张法高 赵杭丽

(51) Int. Cl.

C07K 5/087(2006.01)

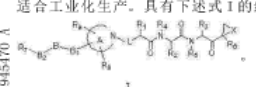
C07K 5/083(2006.01)

(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体抑制剂。本发明化合物具有极强的蛋白酶体抑制活性及细胞增殖抑制活性,是有前景的蛋白酶体抑制剂,为癌症治疗药物的研究提供了新的思路。本发明化合物的合成所需原料易得,路线设计合理,反应条件温和,各步产率高,操作简便,适合工业化生产。具有下述式I的结构通式:



CN 104945470 A



具体实施方式

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

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

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

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

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

具体物质[Specific Substance]:

以具体化学结构陈述的特定物质, 会被分配CAS RN

CAS Markush检索

预测性物质[Prophetic Substance]:

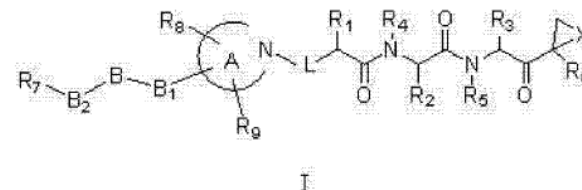
- 使用Markush结构陈述的预测物质，一个Markush可以陈述上百或上千个化学物质
- 被Markush结构包含，但未被实施或呈现在表格、权利要求书或说明书中的结构，不会被CAS分配CAS Registry Number
- Markush检索，能检索到通过结构检索检不到的专利

CN 104945470 A

权 利 要 求 书

1/3 页

1. 一种杂环构建的三肽环氧酮类化合物，具有下述结构通式 I：



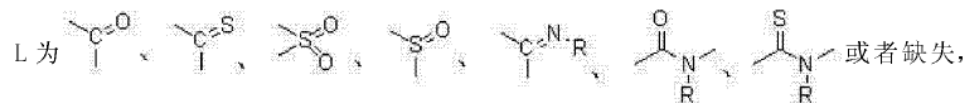
其中：

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_0) (R_0) 或缺失， R_0, R_0 各自独立选自 H、OH、 C_{1-6} 烷基、卤代的 C_{1-6} 烷基或 N 末端保护基；

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

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

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

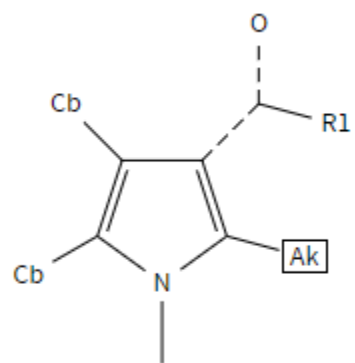


其中 R 选自 H、 C_{1-6} 烷基或卤代的 C_{1-6} 烷基；

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

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

CAS Markush检索



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

CAS SciFinder®

Substances Enter a query...

Patent Markush Match

As Drawn (34)

Substructure (305)

Filter Behavior

Filter by Exclude

Patent Office

☐ World Intellectual Property Organization (16)

☐ Japan (5)

☐ European Patent Organization (4)

☐ China (3)

☐ Germany (3)

View All

CA Section

☐ Heterocyclic Compounds (More Than One Hetero Atom) (10)

☐ Heterocyclic Compounds (One Hetero Atom) (8)

☐ Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes (3)

☐ Industrial Organic Chemicals, Leather, Fats, and Waxes (2)

☐ Pharmacology (2)

View All

Filter Content Report

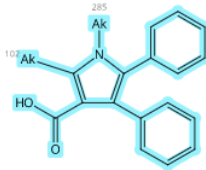
Download filter data from this result set.

Patent Markush (34)

References

1

JP2000086713



Radiation-curable method for forming a polymer from them and

By: Shiono, Teruo; Arishima, Shinji; Tanaka, Hiroaki
Japan, JP2000086713 A 2000-03-28 | Language: Japanese, Database: CAplus
Assignee: Toyo Ink Mfg. Co., Ltd.

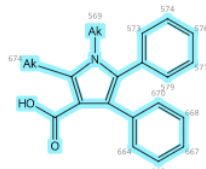
Patent claim 2

PatentPak Full Text

102: alkyl <containing 1-17 C>
285: alkyl <containing 1-17 C>

2

EP732325



Process and catalysts for the preparation of 5- or 6-membered, nitrogen-containing heterocyclic aldehydes by the hydrogenation of the corresponding heterocyclic carboxylic acid or ester

By: Schnurr, Werner; Fischer, Rolf; Wulff-Doering, Joachim; Hesse, Michael; Goetz, Norbert; Maywald, Volker
European Patent Organization, EP732325 A1 1996-09-18 | Language: German, Database: CAplus
Assignee: BASF A.-G.

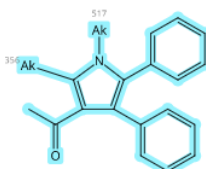
Patent claim 1

PatentPak Full Text

569: alkyl <containing 1-8 C>
573,574,576,577,579: substd. by alkyl

3

WO2016184429



Pyrazoline sensitizer and preparation method and use thereof

By: Qian, Xiaochun
World Intellectual Property Organization, WO2016184429 A1 2016-11-24 | Language: Chinese, Database: CAplus
Assignees: Changzhou Tronly Advanced Electronic Materials Co., Ltd., Changzhou Tronly New Electronic Materials Co., Ltd.

Patent claim 14

PatentPak Full Text

356: alkyl <containing 1-10 C>
517: alkyl <containing 1-10 C>

直观呈现检索结构与专利原文中Markush匹配部分的结构
标引其在专利中出现的位置

物质检索小结

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

视频链接:

https://american-chemical-society.zoom.us/rec/share/JPoebb74K7-dbzGw2Aj8vRqqeddGB5zzBnQTV8MYcW2E2QQqq2rkYWoBtkHy_tt2.ag1fUmL880MKBne3?startTime=1647943207000

Biosequences Search™--Blast检索

The screenshot shows the CAS SciFinder Biosequences Search page. At the top, there's a navigation bar with the CAS SciFinder logo, a 'Saved' button, a 'History' button, and an 'Account' button. Below this is a banner for Retrosynthesis plans. The main section is titled 'Biosequences' and includes a search bar with a placeholder 'Enter a query or upload a file...'. To the left of the search bar is a sidebar with navigation options: 'All', 'Substances', 'Reactions', 'References', 'Suppliers', 'Biosequences' (highlighted), and 'Retrosynthesis'. Above the search bar are tabs for 'BLAST', 'CDR', and 'Motif', with 'BLAST' selected. To the right of the search bar are buttons for 'Upload Sequence' and 'Clear Search'. Below the search bar is a dropdown for 'Advanced Biosequence Search'. On the right side of the search bar, there are settings for 'Sequence Type' (Nucleotide or Protein, with 'Protein' selected), 'Search Within' (Nucleotides or Proteins, with 'Proteins' selected), a checkbox for 'Include NCBI Sequences' (checked), and a dropdown for 'Limit Total Sequence Results to' (set to 1000). At the bottom right is a 'Start Biosequence Search' button.

CAS SciFinder[®]

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



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American Chemical Society



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

AACAACAACATATCAAATCCTACTGGTGGCACAACCTTGA

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%	AACAACAACATATCAAATCCTACTGGTGGCACAACCTTGA	<div>View Results</div> <div>Edit Search</div> <div>Complete</div>
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

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

Apply Reset Filters

Biosequences (63)

Sort: Alignment Identity View: Collapsed

References

Query Details AACAACAACATATCAAACTCTACTGGTGSCAACTTGA 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: 1.06695-11

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

1

Query 1 39

Subject 1 592

Matches: 39 Mismatches: 0

Alignment Identity: 100%

View Less

Alignment Subject References

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

Sequence

1 ACACACAACA CCAAGTACCA GTCATCACA TCCATCTCAT TCTACTACTG CCTCAGAGAC CAAAGTCTGT CAACCGGAGA
81 AGGAGATCTA CTCTACTCTT CAGAGCACTG TGCATTGGGA CATGGAACCC GTCTGGGAG ACCTCATGGC GACCGAGCTG
161 AGGCTTGGCC TGCCGGGAC CAGTGGACGAC TGCAGCCAGC ACCAGCAGCA GACCCAGCTG AAGGTGGCCG CGCCGCCGTC
241 CAACCTCTACT AGGGGCAAGA AGCGCCCGC CGGTGCTGCA CTCACGCTGC TGCCTGCCG CTACCTCTCT CTGCTGCTGC
321 CAGAGCTGTC CCAAGTCTGT TCTAGTGGC TGTCTCACTG TGTCTCACTG TGTCTCACTG TGTCTCACTG TGTCTCACTG

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

source

1..592
/organism="Zea mays"
/mol_type="mRNA"
/db_xref="taxon:4577"
/clone="423468"
122..346
/codon_start=1
/product="hypothetical protein"
/protein_id="ACG45998.1"
/translation="METVVGDLHATELRLLGLPGTVDDCSQHQQQTQLKVAAPPSNPTR GKKRPAGAALTVLLAGYLLLPVLPSPSF"

CDS

ORIGIN

1 acacacaaca ccagtcacca gtcctacaca tccatctcat tctactactg cctcagagac ccaagctgctg
61 caagctgctg caacgggaga agggagatcta ctctactctt cagagcactg tgcattggga
121 catgaaacac gtcgtgggag acctcatggc gaccgagctg aggcctggcc tgcggggcac
181 cgtggagcac tgcagccagc accagcagca gaccgagctg aaggtggcgc cgcgcgccgc
241 caaccctact aggggcaaga agcgcgccgc cggctgctga ctacaggtgc tgcctgccgc
301 ctacctcttc ctgctgctgc cagagctgtc gcctagctgc ttctagacc tctgtcaagt
361 ttgtgccaca gttagatttg atatgttgtt gttctttcta gtacgtgac tgacagacaa
421 ttgtgctgtg gtgtccttgt tttgttagta gttgcactgc gtgttcttgt tatgctatgg
481 gtacgagatg ttaggccatg gtttaagcta agctaaggcg atgggggatc agtaccttac
541 ctctcatctc tggctgctga tctcttttgt 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 CGTGCCCCG

81

AGCGGAGGGA GCTTGACAGG GCCAACGCAC ACATAACACA AGCTCGTCGT CGATGGCGCG GTGGGCTGCG GTGCTGGCGC

161

TGGCCGCGGC CACGGCCATC GCCGTGGCGT CCGTGCGGGG CGGCGACATG AACGCGGACA AGACGGAGTG CGCGGACCAG

241

CTGGTGGGCC TGGGCCCGTG CCTGCAGTAC GTGCAGGGG AGGCCCGCGC GCCCGCGCC GACTGTGCG GCGGCTCGC

321

CCAGGTGCTG GGAAGAGCC CCAAGTGCT GTGCGTGCTC GTCAAGGACA AGGACGACCC CAACCTGGGC ATCAAGATCA

401

ACGCCACCTC CGCGCTCGCG CTCCTCAACG CCGCGGCGC CACCCGCGCC AACGTCTCCC ACTGCGCTCA GTCCTGCAT

481

ATTCCTCCCG GCTCCAAAGA CGCCGCGCTC TTCAGTCCCG GCAGCGACAA GGGCTCCACT GCCGTCCAG CCAAGGACAA

561

CTGCACGGCG ACGACCGACT CCCGCGCGCT GCAGGCGACC ACCGAGCGCG GCGTGTCTCT CTCGCGGCG ACCGCCGGTG

641

CTGCACTCAC GGTGCTGCTC GCCGGCTACC TCCTCTGCT CGTGCCAGAG CTGTGCGCTA GCTCGTTCTA GACCTCTGT

721

CAAGTTGTC CACCAAGAG ATTGATAG 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	ctcgggccc	gccgggagct	cgcaactact	cactcacaag
51	tcacacagcc	acacttgaac	cgctgcccgc	agcggaggga	gcttgacagg
101	gccaacgcac	acataacaca	agctcgtcgt	cgatggcgcg	gtgggctgcg
151	gtgctggcg	tggccgccc	cacggccatc	gccgtggcgt	ccgtggcggg
201	cggcgacatg	aacgcggaca	agacggagtg	cgcgaccag	ctggtaggcc
251	tggcgccgtg	cctgcagtac	gtcagggg	agccccgcgc	gcgcgcgcc
301	gactgctg	gcggcctg	ccaggtgctg	gggaagagcc	ccaagtgcct
351	gtgctgctc	gtcaaggaca	aggacgaccc	caacctgggc	atcaagatca
401	acgccacct	cgcgctcg	ctcccaacg	ctgcccgc	caccgcgcc
451	aacgtctccc	actgcgtca	gctcctcat	attccccgg	gctccaaaga
501	cgccgctgc	ttcagtcgg	gcagcgacaa	gggctccact	gcgctccag
551	ccaaggacaa	ctcgagggcg	acgaccgact	cccgcgct	gcaggcgacc
601	accggagcgc	gcgtgtcctc	ctcgcggg	accgctggtg	ctgcactcac

Patent Annotations

Source: Zea mays

Reference: US20040214272. SEQID 16999: claimed

Feature	Location	Description
misc_feature		Clone ID: MRT4577_1154C.1

BioScape Analysis

[illegible]

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

序列详情及相关的专利文献结果

Filter Behavior

Filter by

Exclude

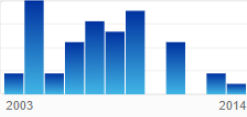
Document Type

☐ Patent (47)

Language

☐ English (47)

Publication Year



No Min to No Max Apply

Author

Organization

Publication Name

Concept

CA Section

Database

Search Within Results

References (47)

Sort: Relevance View: Partial Abstract

☐ Substances

☐ Reactions

☐ Citing

Download

Email

Save

☐ 1

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

By: La Rosa, Thomas J.; Zhou, Yihua; Kovalic, David K.; Cao, Yongwei; Cheikh, Nor...

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

The present invention provides 285,684 nucleic acid (cDNA) and protein sequen...

transforming plants such as soy, corn, cotton, wheat, with the nucleic acids in o...

thereby improving plant traits.

PatentPak

Full Text

Substances (0)

Reactions (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 provid...

hierarchical classification tool, termed FunCAT, for Functional Categories Annota...

polypeptides find use in production of transgenic plants to produce plants havin...

PatentPak

Full Text

Substances (0)

Reactions (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	gagggagctt
51	gcacgggcca	acgcacacat	aacacaagct	cgctcgtgat	ggcgcggtgg
101	gctgcggtgc	tggcgctggc	cgcgccacg	gccatgccg	tgggtcctgt
151	ggcggggggc	gacatgaacg	cggacaagac	ggagtgccg	gaccagctgg
201	tgggcctggc	gccgtgcctg	cagtacgtgc	aggggcaggc	ccgcgcgccg
251	ccgcccgact	gctgcggcgg	cctgcgccag	gtgctgggga	agagcccca
301	gtgctctgct	gtgctcgtca	aggacaagga	cgacccaac	ctgggcatca
351	agatcaacgc	caccctcgcg	ctcgcgctcc	ccaacgcctg	cggcgccacc
401	cgcgccaacg	tctccactg	cgctcagctc	ctgatattc	ccccgggctc
451	caaagacgcc	gccgtcttca	gtcccggcag	cgacaagggc	tccactgccg
501	ctccagccaa	ggacaactcg	acggcgacga	ccgactccc	cgcgctgcag
551	gcgaccaccg	gacgcggcgt	gtcctcctcg	gcggcgaccg	ccgggtcgtc
601	actcacgttg	ctgctcgccg	gctacctcct	cctgctcgtg	ccagagctgt

Patent Annotations

Source: Zea mays

Reference: US20040034888, SEQID 25627: claimed

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

Unspecified

DNA (corn clone LIB3957-004-F11_FLI protein fragment-specifying cDNA) (9)

Nucleic Acid Sequence

Sequence Length: 929

154 a, 310 c, 281 g, 184 t

Other Names and Identifiers

1 Other Name for this Substance

1627: PN: US20040034888 SEQID: 25627 claimed DNA

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Biosequences Search™--CDR检索

Searching for...

All

Substances

Reactions

References

Suppliers

Biosequences

Retrosynthesis

Biosequences

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

BLAST

CDR

Motif

Upload Sequence

Clear Search

CDR1

VFPLAPSSKS

×

CDR2

TSGGTAALGC

×

CDR3

LVKDYFPEPV

×

☒ Include NCBI Sequences

Limit Total Sequence Results to:

10000

Start Biosequence Search

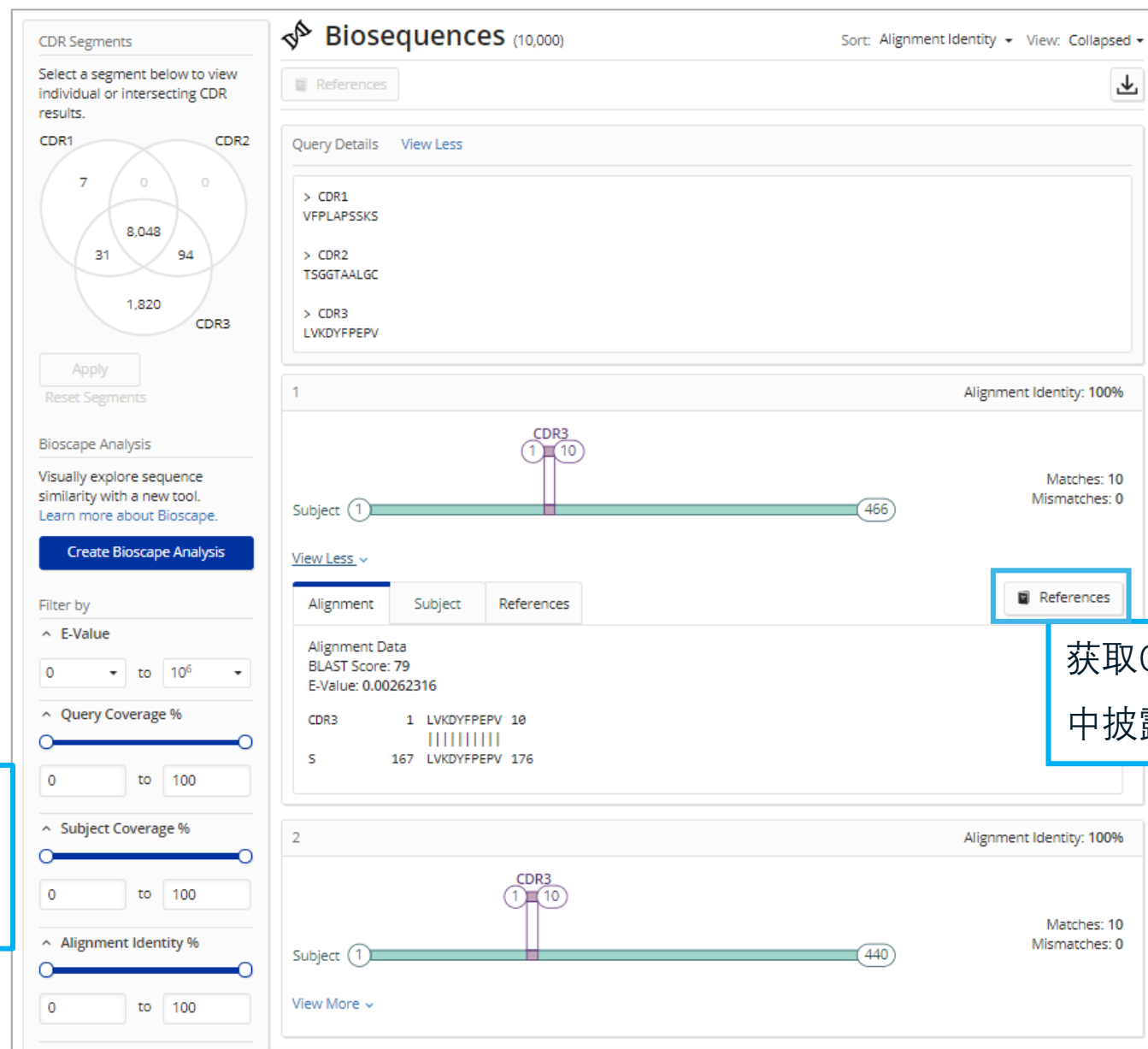
CAS SciFinder-n Help:

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

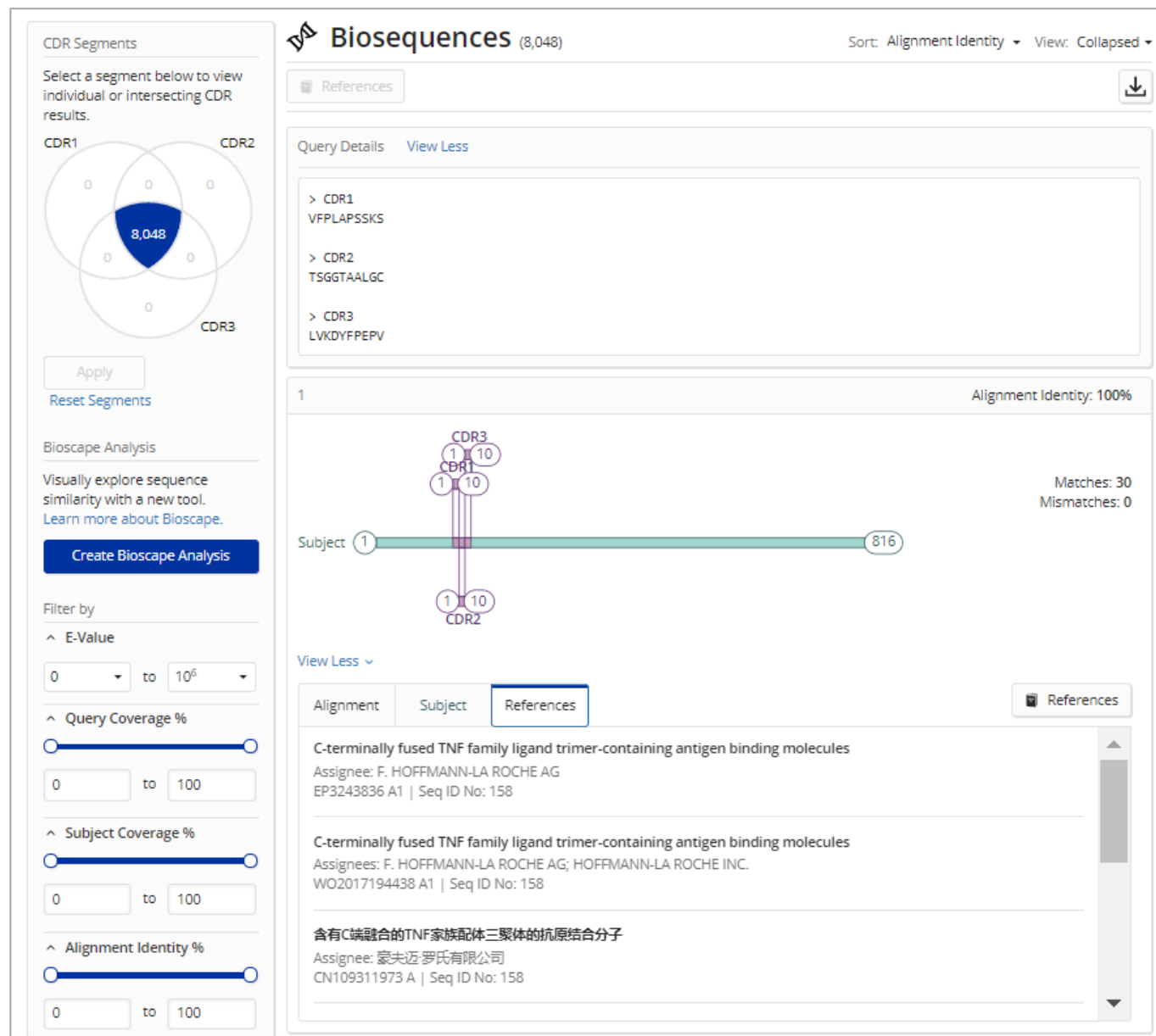


下载Excel格式文件

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



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 % ?

90

E-Value ?

10

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

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 ACS
International

 CAS
A division of the
American Chemical Society



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 10^6

^ Query Coverage %

0 to 100

^ Subject Coverage %

0 to 100

^ Alignment Identity %

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 MLLRLFLFI IATKPVQASG FSESTTVVG CSEMLVRLFL LFIATKPAQ AGGFSEVSL RFVGEEAQR MKPYGYGLIK
81 VDDQYGMTTL EEVAKPIPK PQLTVDEQNR AETQNRALVD IIVKFYQLRD GYLAQHAGD FIQTLKYGF 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

视频链接:

https://american-chemical-society.zoom.us/rec/share/eheXjH8iLM3q7tT2flBtPm-c-_IMCDEF8qCgXmSngeTk7DtcuLPYx1IZZn83BYc.cAuZdpJTknUmPvaK?startTime=1647338414000



反应检索

— 反应检索方法

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

— 常用获取方法推荐

- 已知物质：由物质获取反应
- 已知文献：从文献中获取反应
- 精确结构反应检索
- 亚结构反应检索

反应检索

Searching for...

All

Substances

Reactions

References


Suppliers


Reactions

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

Qinghaosu

×

 Draw



通过物质标识符、文献标识符进行检索

反应检索--标识符

Reactions (2,949) Group: By Scheme View: Expanded

Filter Behavior: Filter by Exclude

Substance Role

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

Yield

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

[View All](#)

Number of Steps

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

[View All](#)

Non-Participating Functional Groups

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

[View All](#)

Experimental Protocols

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


Reaction Type

Stereochemistry

Reagent

Catalyst

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


Absolute stereochemistry shown

[Suppliers \(98\)](#) [Suppliers \(86\)](#)

Reaction Summary Steps: 1 Yield: 100% [Method for preparing dihydroartemisinin bulk antimalarial drug by single process](#)

1.1 Reagents: [Sodium borohydride](#)
Catalysts: [Benzyltriethylammonium chloride](#)
Solvents: [Water](#); -10 °C; < 0 °C; 5 h, < 0 °C

1.2 Reagents: [Acetic acid](#)
Solvents: [Water](#); pH 7, 0 - 5 °C

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

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

[View Reaction Detail](#)

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

1.1 Reagents: [Sodium borohydride](#)
Solvents: [Methanol](#); 3 h, 0 °C

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

[Full Text](#)

[View Reaction Detail](#)

Reaction Summary Steps: 1 Yield: 100% [An efficient synthesis of deoxoqinghaosu from dihydroqinghaosu](#)

1.1 Reagents: [Sodium borohydride](#)

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


[Full Text](#)

[View Reaction Detail](#)

[View All Reaction Summaries](#)

[Collapse Scheme](#)

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


Absolute stereochemistry shown, Rotation (-)

一步由物质标识符或文献标识符获得反应信息

反应检索

通过结构式进行检索


Searching for...

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

Reactions

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

Enter a query...

Draw 

CAS Draw

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

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

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

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(u-acetato-κ^Oκ^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. Esmail; 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%

Suppliers (131)

Suppliers (62)

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

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

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

Full Text View 3 Related Reactions

Suppliers (131)

Suppliers (62)

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

Structure Match

As Drawn (7,236)

Substructure (4.3M)

Similarity (222K)

Filter Behavior

Filter by Exclude

Yield

Number of Steps

Non-Participating Functional Groups

Experimental Protocols

Reaction Type

Stereochemistry

Reagent

Catalyst

Solvent

Commercial Availability

Reaction Notes

Search Within Results

Source Reference

Document Type

Language

Publication Year

Publication Name

CA Section

Filter Content Report

Download filter data from this result set.

Reactions (7,236)

Group: By Scheme View: Expanded

References

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·KHSO₄·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

View Reaction Detail

A new and highly effective method for catalytic oxidation of alcohols to the corresponding carbonyl compounds using the tris[2-(2-oxazolyl)phenolato]manganese(III)/Oxone/n-Bu₄NBr oxidation system

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

Full Text

Reaction Summary Steps: 1 Yield: 100%

1.1 Reagents: Oxygen Catalysts: Tetrakis[μ-(acetato-κ^Oκ^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

View Reaction Detail

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

Full Text

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

View Reaction Detail Experimental Protocols

Full Text

View All Reaction Summaries

Collapse Scheme

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

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



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反应检索--结果集筛选: Synthetic Methods™

Structure Match

As Drawn (7,236)

Substructure (4.3M)

Similarity (222K)

Filter Behavior

Filter by Exclude

Yield

Number of Steps

Non-Participating Functional Groups

Amide (132K)

Ether (100K)

Halide (99K)

Alkene (65K)

Phenyl halide (65K)

Aldehyde (2,610)

View All

Experimental Protocols

Synthetic Methods (2,610)

Experimental Procedure (2,532)

Reaction Type

Stereochemistry

Reagent

Catalyst

Solvent

Commercial Availability

Reaction Notes

Search Within Results

Source Reference

Document Type

Language

Publication Year

Publication Name

CA Section

Reactions (2,610)

Group: By Scheme View: Expanded

References

Filtering: Non-Participating Functional Groups: Aldehyde Experimental Protocols: Synthetic Methods

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

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

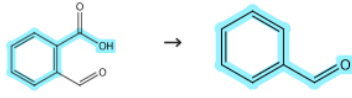
查看反应详情

Synthetic Methods™ :
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反应检索--结果集筛选: Synthetic Methods™

Synthetic Methods™ :

分类显示详尽信息, 方便操作



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

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联合检索--反应式与关键词

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- References**
- Suppliers
- Biosequences
- Retrosynthesis

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

suzuki

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

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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

1996

2021

No Min

to

No Max

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Organization

Publication Name

Concept

CA Section

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References (2,771)

Sort: Relevance

View: Partial Abstract

Substances

Reactions

Citing

Download

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

c1ccc(cc1)I.Cc1ccc(cc1)B(O)O>>c1ccc(cc1)-c2ccccc2

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: CAlplus

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: CAlplus 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: CAlplus and MEDLINE

联合检索提高了检索速度



ACS
International

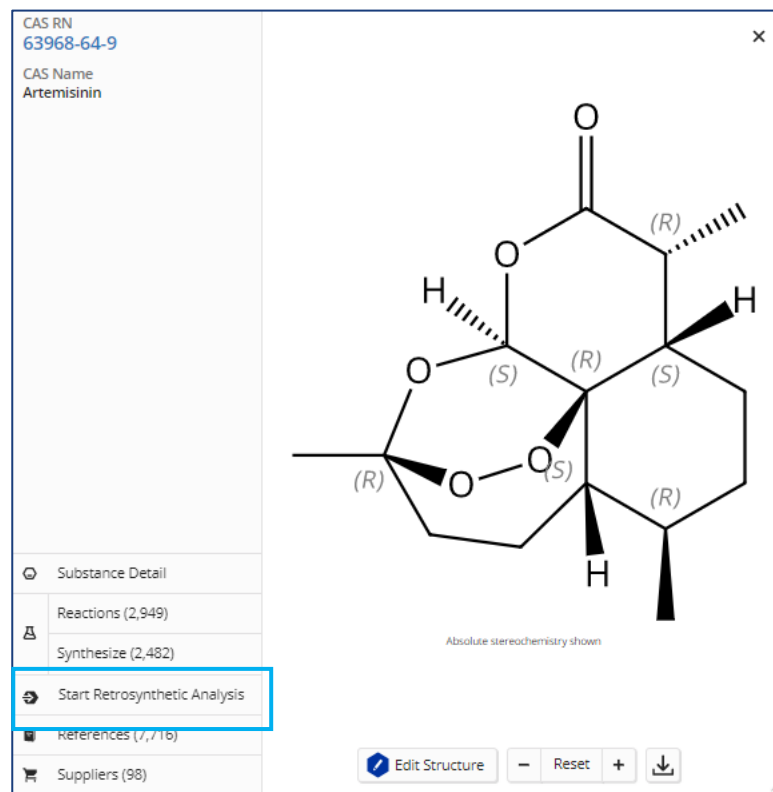
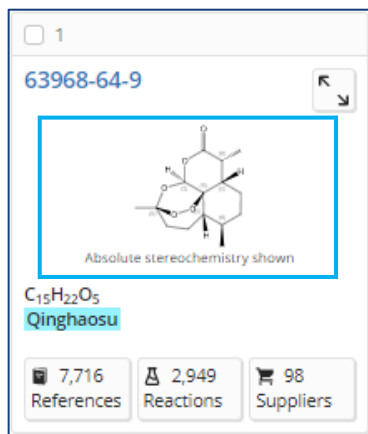


大纲

- 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

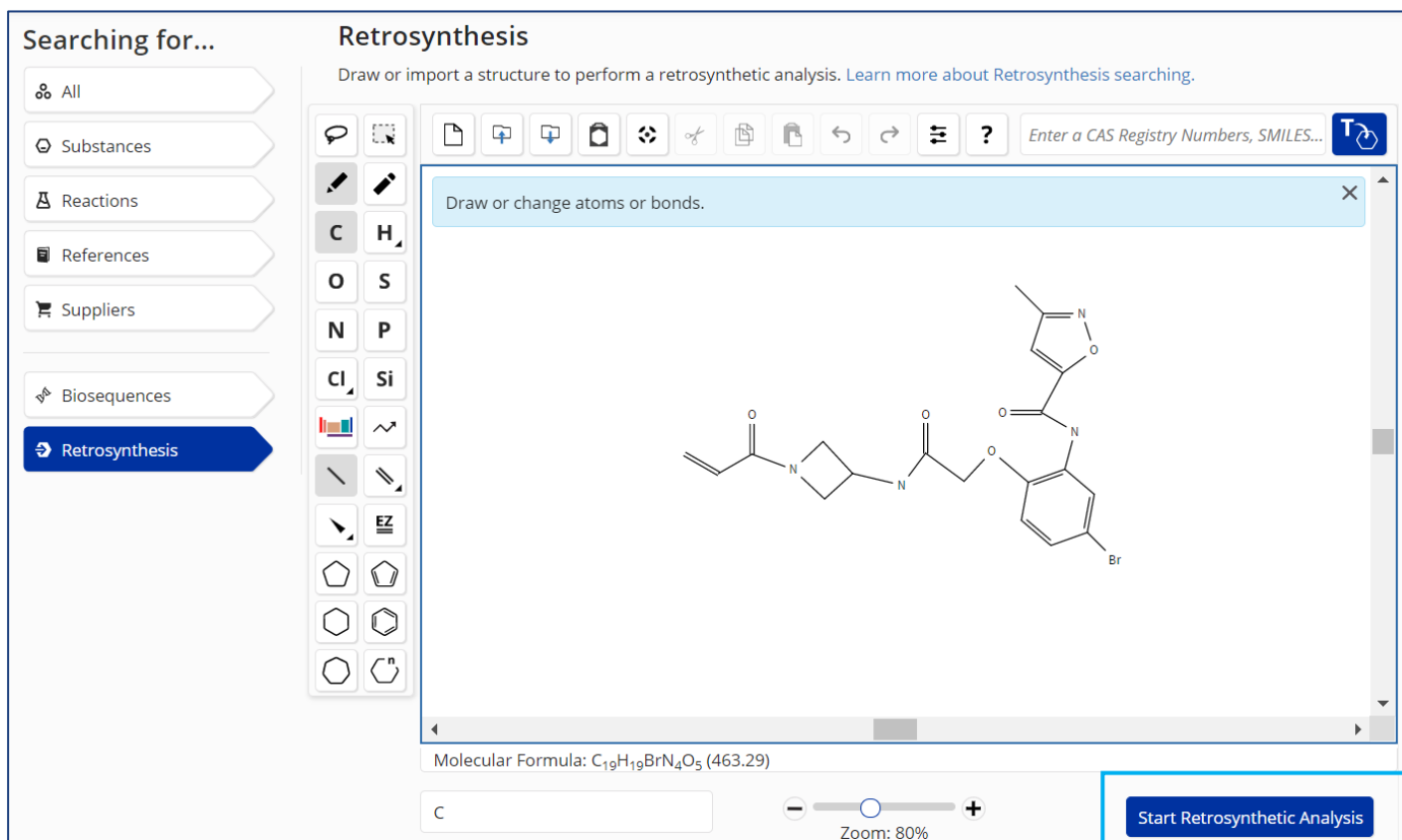


从已知化合物获得逆合成路线：

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



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

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☐ 1
☐ 2
☒ 3
☐ 4



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

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

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

USD/mol ▼
USD/mol
USD/g

☐ Email me when my plan is complete

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Break and Protect Bonds

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[Clear All Bond Selections](#)



预设反应路线参数：

反应深度

反应规则常见性

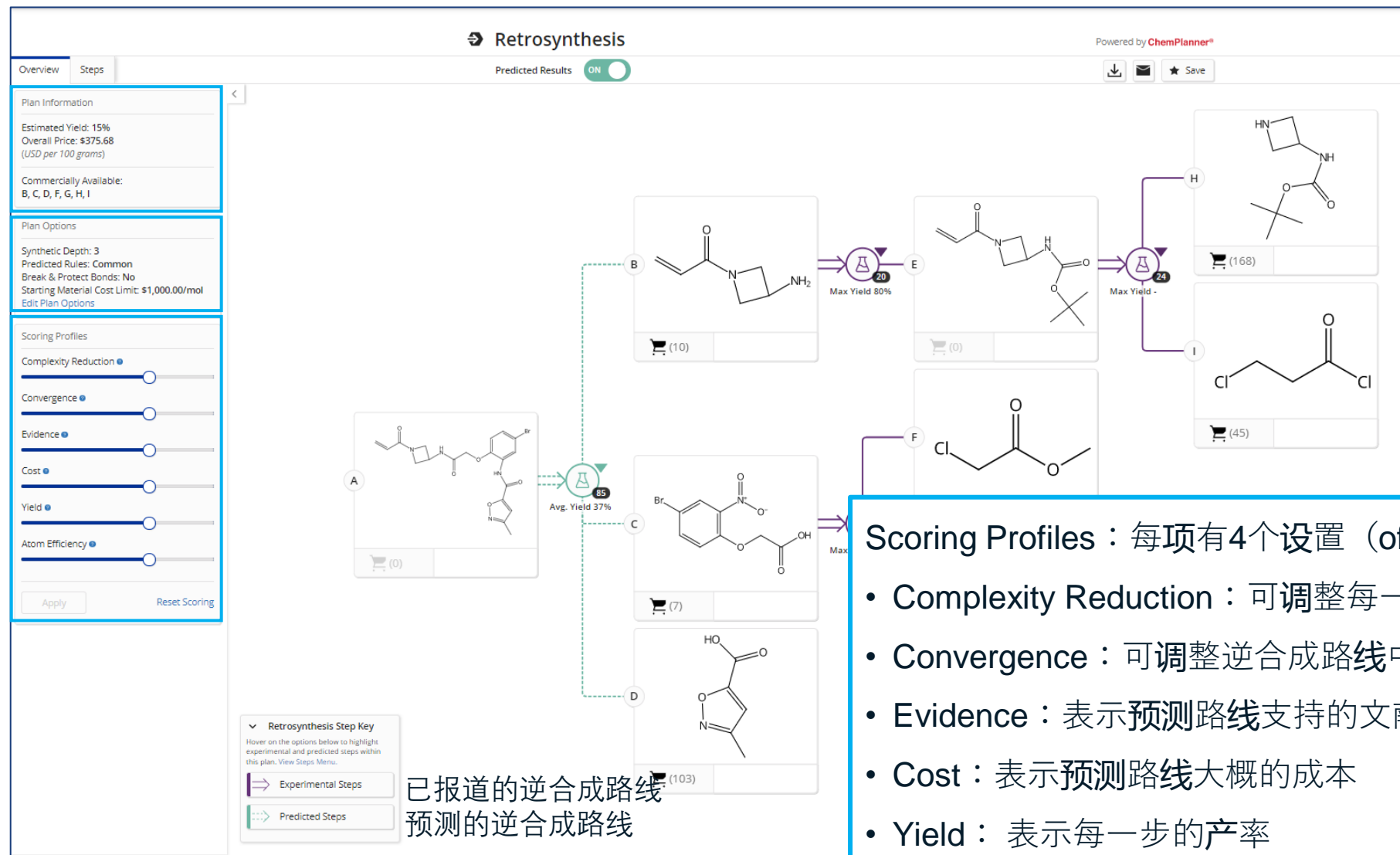
起始原料费用

设置断裂键或保护键

CAS Retrosynthesis Tool—路线概览

路线概览

重设参数



CAS Retrosynthesis Tool—路线详情

Retrosynthesis Predicted Results ON 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)

点击Evidence查看该步具体的合成条件和文献

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

View Reaction Detail | Experimental Protocols

Collapse Scheme

- 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

The screenshot displays the CAS Retrosynthesis Tool interface, powered by ChemPlanner. The main window shows a list of alternative steps (85 total) for a specific reaction. The first step is highlighted, showing a reaction scheme with a carboxylic acid and an amine. The second step is also highlighted, showing a different reaction scheme. The interface includes a sidebar with filters (Alternative Step Type, Stereochemistry) and a list of alternative steps (85 total). The main window also displays a reaction network diagram with various chemical structures and reaction steps labeled A through I. The network shows the progression from starting materials to the final product, with various reagents and conditions indicated. The interface is designed to allow users to explore different synthetic routes and select the most appropriate one for their needs.

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)

Retrosynthesis

Predicted Results ON

Alternative Steps (85)

Filter by

Alternative Step Type

☒ Predicted (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%

Experimental Steps

Predicted Steps

Reset

Retrosynthesis

Predicted Results ON

Reaction Network Diagram

Retrosynthesis Step Key

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

检索信息的管理

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

视频链接：

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



检索信息的管理--保存、下载, 设置提醒和标签

下载
分享链接
保存

设置提醒频率：
即时, 每周, 每月

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

[Load More Results](#)

Filter Behavior

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

Document Type

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

[View All](#)

Language

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

Publication Year

1994 to 2022

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

[View Larger](#)

Available at My Institution

Author

Organization

Publication Name

Concept

CA Section

CAS Solutions

Formulation Purpose

Database

- ☐ CPlus (7,396)
- ☒ MEDLINE (3,278)

References (3,278)

Sort: Relevance [View: Partial Abstract](#)

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

Filtering: Database: MEDLINE X

Save Search

Name

[No Alerts](#) [As Available](#) [Weekly](#) [Monthly](#)

Tags (optional)

No tags defined

New Tag (optional)

[Save](#) [Cancel](#)

1

[Full Text](#) [Substances](#)

Nano-graphene in biomedicine: theranostic ap

By: Yang, Kai; Feng, Liangzhu; Shi, Xiaozhe; Liu, Zhuang
Chemical Society Reviews (2013), 42(2), 530-547 | Language: E

A review. Owing to their unique phys. and chem. properties, g
graphene oxide (RGO) and GO-nanocomposites have attracte
in recent years. With every atom exposed on its surface, singl
mol. loading and bioconjugation, and was widely explored as
near-IR (NIR) optical absorbance. In vivo graphene-based pho

[View More](#)

2

[Full Text](#) [Substances \(3\)](#) [Reactions \(0\)](#) [Citing \(129\)](#) [Citation Map](#)

Poly-cyclodextrin and poly-paclitaxel nano-assembly for anticancer therapy

By: Namgung, Ran; Mi Lee, Yeong; Kim, Jihoon; Jang, Yuna; Lee, Byung-Heon; Kim, In-San; Sokkar, Pandian; Rhee, Young Min;
Hoffman, Allan S.; Kim, Won Jong
Nature Communications (2014), 5, 3702 | Language: English, Database: CPlus and MEDLINE

Effective anticancer therapy can be achieved by designing a targeted drug-delivery system with high stability during circulation and
efficient uptake by the target tumor cancer cells. We report here a novel nano-assembled drug-delivery system, formed by
multivalent host-guest interactions between a polymer-cyclodextrin conjugate and a polymer-paclitaxel conjugate. The multivalent
inclusion complexes confer high stability to the nano-assembly, which efficiently delivers paclitaxel into the targeted cancer cells via
both passive and active targeting mechanisms. The ester linkages between paclita

[View More](#)

3

[Full Text](#) [Substances \(7\)](#) [Reactions \(0\)](#) [Citing \(2,550\)](#) [Citation Map](#)

Nano-graphene oxide for cellular imaging and drug delivery

By: Sun, Xiaoming; Liu, Zhuang; Welscher, Kevin; Robinson, Joshua Tucker; Goodwin, Andrew; Zaric, Sasa; Dai, Hongjie
Nano Research (2008), 1(3), 203-212 | Language: English, Database: CPlus and MEDLINE

Two-dimensional graphene offers interesting electronic, thermal, and mech. properties that are currently being explored for
advanced electronics, membranes, and composites. Here we synthesize and explore the biol. applications of nano-graphene oxide
(NGO), i.e., single-layer graphene oxide sheets down to a few nanometers in lateral width. We develop functionalization chem. in
order to impart solubility and compatibility of NGO in biol. environments. We obtain size separated pegylated NGO sheets that are
soluble in buffers and serum without agglomeration. The NGO sheets are found to be photolum...

[View More](#)

4

[Full Text](#) [Substances \(7\)](#) [Reactions \(0\)](#) [Citing \(2,550\)](#) [Citation Map](#)

Doxil - The first FDA-approved nano-drug: Lessons learned

By: Barenholz, Yechezkel
Journal of Controlled Release (2012), 160(2), 117-134 | Language: English, Database: CPlus and MEDLINE

A review. Doxil, the first FDA-approved nano-drug (1995), is based on three unrelated principles: (i) prolonged drug circulation time



ACS
International



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
☒ Abstract
☐ Concepts
☐ Substances

☐ Formulations
☐ Analytical Methods
☐ Citations

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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
☐ Substance Names
☐ Experimental Spectra
☐ Predicted Spectra
☐ Regulatory Information

☐ Experimental Properties
☐ Predicted Properties
☐ Bioactivity Indicators
☐ Target Indicators

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Download Reaction Results

File Type

☒ PDF
☐ RDFile (.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.

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检索信息的管理--查看保存结果, 更改提醒设置

Filter by

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

Combine Saved Results

Combine

Migrate Alerts & Saved Results

Migrate

★ Saved (100)

1671 exclude COCl

June 4, 2021, 3:57 PM

Combined From Substance Saved Items

Rerun Search

Alerts

Add Tags

Frequency

No Alerts As Available Weekly Monthly

Substances

Advanced Search + Filters Boiling Point (°C): 80 to 100

Rerun Search

include Si

June 4, 2021, 3:54 PM

Substances

Advanced Search + Filters Boiling Point (°C): 80 to 100

Rerun Search

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. On the left, a sidebar contains a 'Filter by' section with 'Result Type' (Reactions (34), References (48), Substances (18)) and 'Alerts' (Unviewed (1), No Alerts (100)). Below this is a 'Combine Saved Results' button, which is highlighted with a blue box. The main area shows a list of saved items. The first item, '1671 exclude COCl', is selected. A 'Combine Saved Results' dialog box is open over this item. The dialog has a progress bar with steps 1, 2, and 3. Step 1, 'Select a Result Type:', is active. It shows four options: Substances, Patent Markush, Reactions, and References. The 'References' option is highlighted with a blue box. Below the options are 'Select' buttons. The second item, 'include Si', is partially visible below the first.

This is a close-up of the 'Combine Saved Reference Results' dialog box. It features a progress bar with steps 1, 2, and 3. Step 2, 'Select a Combine Option:', is active. It presents three options: 'Add' (represented by two overlapping circles), 'Intersect' (represented by two overlapping circles with the intersection shaded), and 'Subtract' (represented by two overlapping circles with the intersection unshaded). Each option has a 'Select' button below it. The 'Add' button is highlighted with a blue box. A 'Return to Result Type' link is visible on the right. A 'Learn More About Combine' link is at the bottom right.

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

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

1994 to 2022

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

[View Larger](#)

Available at My Institution

Author

Organization

Publication Name

Concept

CA Section

CAS Solutions

Formulation Purpose

Database

Search Within Results

Filter Content Report

References (7,452)

Sort: Publication Date: Newest View: Partial Abstract

☐ Substances ☐ Reactions ☐ Citing

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

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

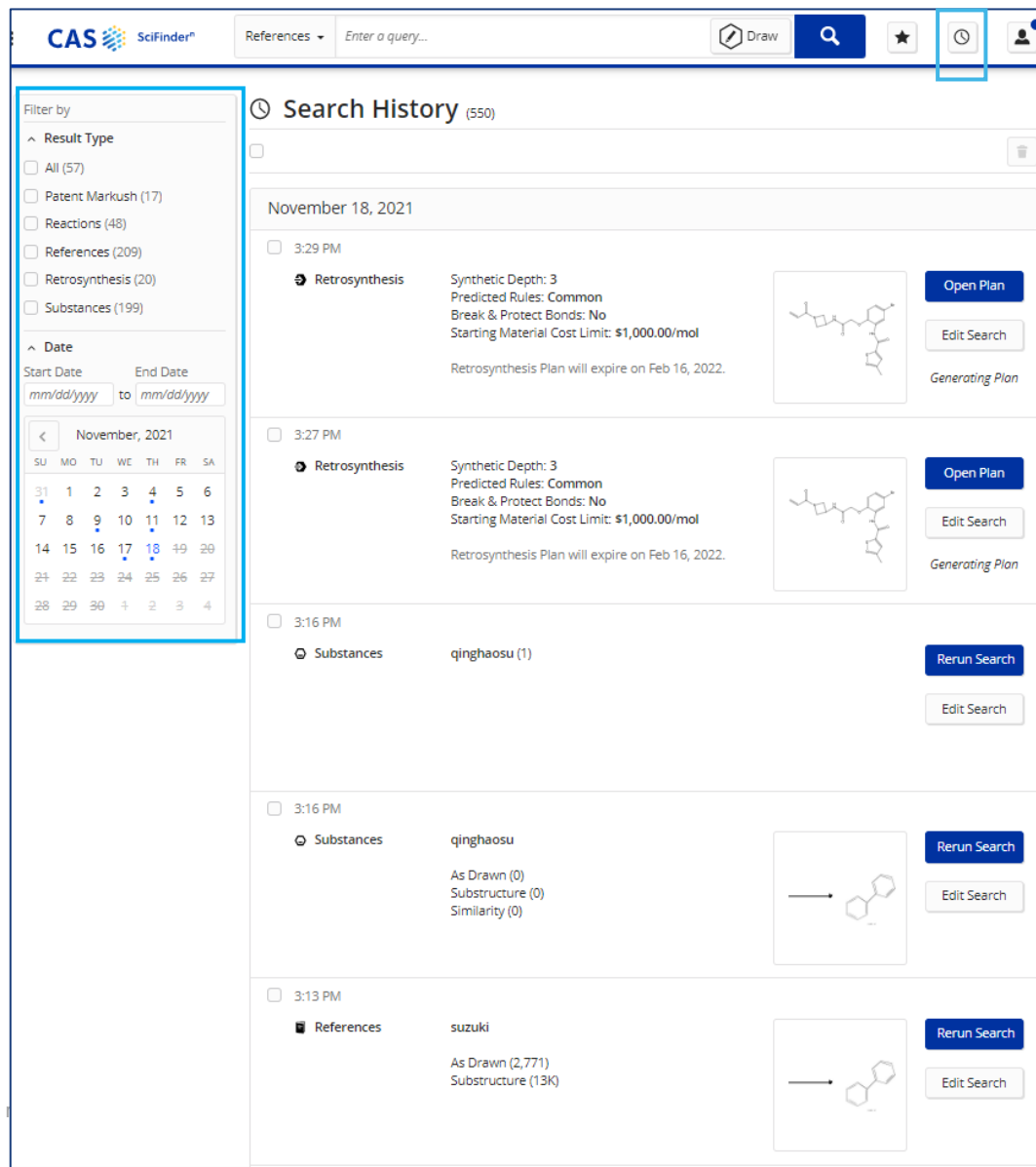
By: Duo, Yanhong; Liu, Quan; Zhu, Daoming; Zhang, Bin; Luo, Guanghong; Wang, Fu-Bing; Chen, Jinghua; Cao, Yihai
Chemical Engineering Journal (Amsterdam, Netherlands) (2022), 429, 132328 | Language: English, Database: CAPLUS

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 poly(ethylene glycol) (PEG) nanoparticles and nanoclusters (AuNCs-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	1	2	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

分析方法的获取—Analytical Methods

- 介绍
- 检索方法
- 结果详情

视频链接：

https://american-chemical-society.zoom.us/rec/play/d6Q-xA-DR_ODf7WaxdDaLaAYkIDyrc3K4vSqoixkuqJNL7S6dwrhwbguRgDYXekpphbY-mXLb0HIRbTU.wkg9K9htCp0Yq_aE

分析方法的类别--13大类45小类；某些子类属多个分类

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

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

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

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

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

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

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

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

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

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

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

Water: 阴阳离子分析、环境分析、废水分析、微量元素分析...

Polymer: 聚合物分析...

分析方法的获取—Analytical Methods

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

The screenshot shows the CAS Analytical Methods website. At the top, there's a header with 'CAS Solutions' and 'CAS Analytical Methods'. On the right, there are links for 'Saved' and 'Account'. Below the header is a 'Search' section with a text input field and a search button. A blue box with white text is overlaid on the search field, stating '输入感兴趣的检索词进行快速检索或高级检索'. Below the search field is an 'Advanced Search' link. To the left of the search field is a 'Browse Method Categories' section. A blue box with white text is overlaid on this section, stating '浏览丰富的分析方法目录, 选择查看感兴趣的方法详情'. To the right of the 'Browse Method Categories' section is a 'Browse Method Categories > Pharmacology / Toxicology' dropdown menu. A blue box with white text is overlaid on this menu, stating '目前有13个大类, 45个小类。' and '某些子类属于多种方法分类。'. Below the 'Browse Method Categories' section is a 'Recent Searches' section with two search entries. The first entry is 'Advanced : analyte : sofosbuvir, technique : hplc'. The second entry is 'Advanced : analyte : sofosbuvir, technique : hplc, keyword : mass'. The bottom of the page features logos for 'ACS International' and 'CAS A division of the American Chemical Society'.

CAS Solutions

CAS Analytical Methods

★ Saved

Account

Search

Enter keyword, matrix, analyte, etc.

输入感兴趣的检索词进行快速检索或高级检索

Advanced Search

Browse Method Categories

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

目前有13个大类, 45个小类。
某些子类属于多种方法分类。

Recent Searches

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


ACS International


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A division of the
American Chemical Society


分析方法的获取—Analytical Methods

利用运算符连接不同的检索域，快速获得更相关的结果

CAS Solutions

 Analytical Methods

 Saved

 Account

[Return to Home](#)

Advanced Search

Keyword

impurities

AND

Analyte

sofosbuvir

×


AND

Technique

hplc

×

Add Search Criteria



Keyword

Analyte

Matrix

Method Category

Technique

CAS Method Number

Publication Name

分析方法的获取—Analytical Methods

根据分析物、分析基质、
方法分类、所用技术、年
份筛选分析方法

The screenshot displays the CAS Analytical Methods database interface. The search bar at the top contains 'guajaverin'. The left sidebar shows filters for Analyte, Matrix, Method Category, Technique, and Year. The main results area shows two entries for 'Analysis of Garcimangosone D in Psidium guajava by Solvent extraction'. The first entry is highlighted with a blue box and a red callout bubble containing the text '查看分析方法详情' (View Analytical Method Details). The second entry is also visible below it.

Results (220) Sort Relevance

Analysis of Garcimangosone D in Psidium guajava by Solvent extraction
CAS MN: 1-131-CAS-164363

[View Details & Instructions](#) [Add to Compare](#)

Analyte: Garcimangosone D
Matrix: Psidium guajava
Other Materials: Reagent: Methanol; Dichloromethane; Hexane; Chloroform; Ethyl acetate
Material: Column (10 mm, 300_8 mm i.d.); Column (3 x 60 cm)
Method Category: Natural Product Isolation Analysis
Technique: UV-visible spectroscopy; Adsorption liquid chromatography; HPLC; Solvent extraction
Equipment Used: HPLC system; UV detector; Column chromatography system; Fraction collector
Source: A new antibacterial benzophenone glycoside from Psidium guajava (Linn.) leaves
Ukwueze, Stanley E.; Osadebe, Patience O.; Okoye, Festus B. C.
Natural Product Research (2015), 29 (18), 1728-1734. Taylor & Francis Ltd.
[Full Text](#)
[Abstract](#)

Analysis of Garcimangosone D in Psidium guajava by Solvent extraction
CAS MN: 2-107-CAS-55944

[View Details & Instructions](#) [Add to Compare](#)

Analyte: Guajaphenone A; Garcimangosone D; **Guajaverin**
Matrix: Psidium guajava
Other Materials: Reagent: Methanol; Dichloromethane; Chloroform; Hexane; Ethyl acetate
Material: Column (3 x 60 cm)

分析方法详情

CAS Solutions

CAS Analytical Methods

gualjaverin

1

Return to Results

Method Detail (1 of 220)

Analysis of Garcimangosone D in Psidium guajava by Solvent extraction

CAS MN: 1-131-CAS-164363

Method Category: Natural Product Isolation Analysis

Technique: UV-visible spectroscopy; Adsorption liquid chromatography; HPLC; Solvent extraction

Materials	Role	View Structure	CAS No.
Garcimangosone D	analyte	View Structure	356055-68-0
Gualjaverin	analyte	View Structure	22255-13-6
Guajaphenone A	analyte		
Psidium guajava	matrix		
Column (10 mm, 300_8 mm i.d.)	material		
Column (3 x 60 cm)	material		
Methanol	reagent		
Dichloromethane	reagent		
Hexane	reagent		
Chloroform	reagent		
Ethyl acetate	reagent		

方法分类、技术、所用材料/物质、角色、文献来源……

Source

A new antibacterial benzophenone glycoside from *Psidium guajava* (Linn.) leaves

Ukwueze, Stanley E.; Osadebe, Patience O.; Okoye, Festus B. C.

Natural Product Research (2015), 29 (18), 1728 - 1734. Taylor & Francis Ltd.

CODEN: NPRAAT | ISSN: 14786419 | DOI: 10.1080/14786419.2014.1003188

Full Text

Abstract

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

Equipment Used

HPLC system, L-7100, Merck-Hitachi

UV detector, UV-L7400, Merck-Hitachi

Column chromatography system

Fraction collector, Retriever II, ISCO, Germany

Conditions

Instrument

Column: Eurospher C-18 column (10 mm, 300_8 mm i.d.; Knauer); mobile phase: methanol and nanopure water

Detection: 254 nm

Column: Sephadex LH-20 column (3 x 60 cm); mobile phase: dichloromethane: methanol (1:1); flow rate: 0.2 mL/min

Extraction of the sample

- Defat the pulverized air-dried leaves (600 g) with n-hexane.
- Extract the dried marc (450 g) with 5 L of 90% methanol for 4 days at room temperature (25 °C).
- Concentrate the extract in vacuo with rotary evaporator.
- Reconstitute the dried methanol extract (35 g, 7.7% w/w) in 20 mL of methanol.
- Dilute to 200 mL with distilled water.
- Shake for about 30 min.
- Perform liquid-liquid extraction with chloroform (3 mL x 750 mL) and ethyl acetate (3 mL x 750 mL) to obtain 10 pooled fractions PsG-EF1 to PsG-EF10. Fractionation of PsG-EF (4.5 g) on a Sephadex LH-20 column (3 cm x 60 cm).

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

Semi-preparative HPLC analysis

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

Validation

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

实验条件、实验步骤和数据有效性验证…

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
 - 分析方法的获取 (Analytical Methods)
- 常见问题及解决

浏览器选择建议

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

如何获取CAS SciFinder账号

--CONTACT INFORMATION--

First Name:

Last Name:

Email:

Confirm Email:

Phone Number:

Fax Number:

Area of Research:

Job Title:

--USERNAME AND PASSWORD--

Username: Tips

Password:

Re-enter Password:

--SECURITY INFORMATION--

Security Question:

Answer: Why?

请注意:

1.必须输入真实姓名和**学校**邮箱。
2.用户名必须是唯一的, 且包含 5-15 个字符。它可以只包含字母或字母组合、数字和/或以下特殊字符:

- - (破折号)
- _ (下划线)
- . (句点)
- @ (表示“at”的符号)

3.密码必须包含 7-15 个字符, 并且至少包含**三种以下字符**:

- 字母
- 混合的大小写字母
- 数字
- 非字母数字的字符 (例如 @、#、%、&、*)

例: abc@123

4.从下拉列表中选择一个密码提示问题并给出答案。

单击 Register (注册)。

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

如何获取CAS SciFinder账号



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，**请**提供**真实**姓名信息（中文名用**汉语**拼音全拼）
- 不得**过量**下载（以**电子**形式存**储**不**超过**5,000条**记录**）
- 不得**账号**分享
- 不得将**账号**用于非**学术**研究

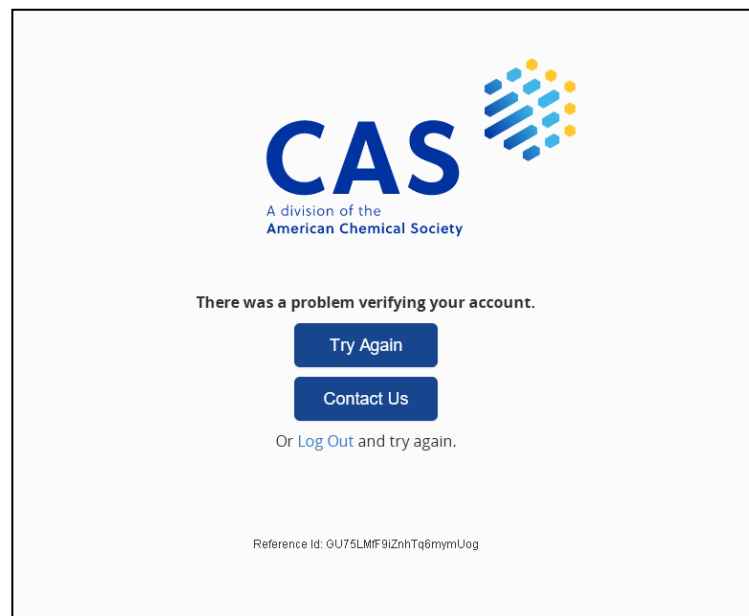
常见问题

Unauthorized IP Address

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

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

常见问题



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

2022年CAS SciFinder[®]论坛直播日程表

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

直播时间:

18:00 – 19:00

关注公众号：**ACS美国化学会**
随时观看回放，了解直播信息



2022 CAS SCIFINDERⁿ 检索技能大赛

参赛对象:

中国大陆地区高校和科研院所的CAS SciFinderⁿ用户

大赛时间:

第一阶段:2022年4月11日 - 5月8日

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

第二阶段:2022年5月9日 - 6月7日

- 提交CAS SciFinderⁿ检索体验PPT
- 赢取Macbook Air、投影仪、Airpods等大奖

(详情请查看ACS美国化学会微信公众号)

参赛方式:

大赛将于2022年4月11日开启,请扫描二维码参加:



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