

朱传娴

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SciFINDERⁿ

A CAS SOLUTION

江南大学

2020.11

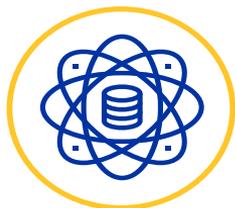


提纲

- 为什么需要美国化学文摘社
- SciFinder-n简介及检索方式
 - 文献检索
 - 物质检索
 - Markush检索
 - 反应检索
- 常见问题及解决

美国化学文摘社 (CAS) 隶属美国化学会 (ACS)，致力于追踪、收录、标引科学信息

- 拥有超过110年的经验；创立权威化学索引《化学文摘》(CA)
- 密切追踪、标引和提炼着全球化学相关的文献（包括专利）
- 提供各种科学信息和相关技术产品与服务
- 协助创新和保护创新, 助力于解决科研方面的难题与挑战



UNPARALLELED
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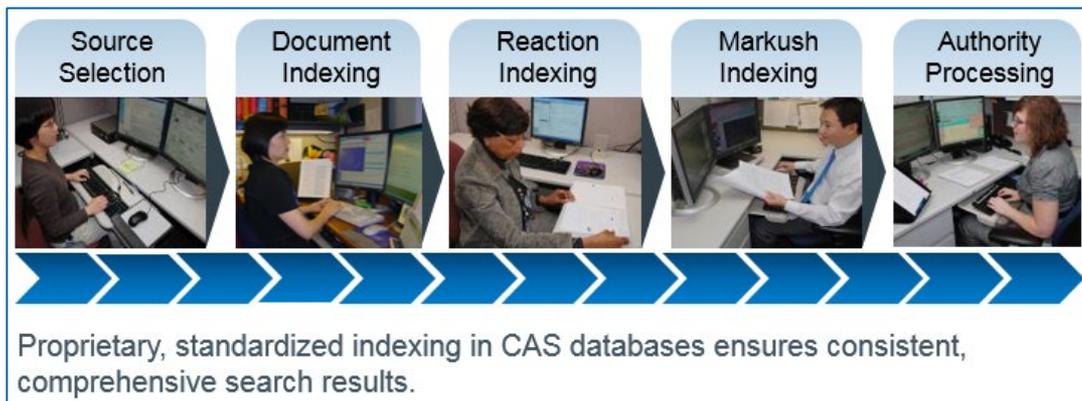
CAS[®]

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CAS数据覆盖学科

- 生物化学：
 - 农化产品管控信息、生化遗传学、发酵、免疫化学、药理学
- 有机化学各领域：
 - 氨基酸、生物分子、碳水化合物、有机金属化合物、类固醇
- 大分子化学各领域：
 - 纤维素、木质素、造纸；涂料、墨水
 - 染料、有机颜料；合成橡胶；纺织品、纤维
- 应用化学各领域：
 - 大气污染、陶瓷、精油、化妆品、化石燃料、黑色金属、合金
- 物理、无机、分析化学各领域：
 - 表面化学、催化剂、相平衡、核现象、电化学

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



- 检索词的同义词拓展：解决不同科研人员由于教育背景、语言、表达习惯不同导致的对同一个技术术语描述的差异。
- 用名称、分子式等检索化合物，会导致检索不全、不准的问题。CAS RN很好地解决了该问题，帮助检索人员实现精准定位化合物的目标。
- 利用SciFinder中的标引信息（Index Term, CAS RN, CAS Role），提高效率，启发思路。

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提纲

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 - 反应检索
- 常见问题及解决

SciFinder-n覆盖的数据库



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



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Next

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使用SciFinder账号登录

SciFinder-n主界面

The screenshot shows the SciFinder-n main interface with several callouts highlighting key features:

- 已保存的结果集** (Saved Results): Points to the "Saved" button in the top right navigation bar.
- 全部检索历史** (All Search History): Points to the "History" button in the top right navigation bar.
- 账户信息** (Account Information): Points to the "Account" button in the top right navigation bar.
- 灵活的检索选项** (Flexible Search Options): Points to the left sidebar menu containing "All", "Substances", "Reactions", "References", and "Suppliers".
- 便捷地合并文本与结构检索** (Conveniently merge text and structure search): Points to the search input field containing "phosphorescent material and OLED" and a chemical structure drawing below it.
- 检索历史** (Search History): Points to the "Recent Search History" section at the bottom, which shows a search for "phosphorescent material and OLED (7,577)" on March 24, 2020.

Additional callouts at the bottom right point to the "Rerun Search" and "Edit Search" buttons, labeled as:

- 重新运行检索** (Rerun Search)
- 修改检索式** (Modify Search Query)

一站检索：一次检索，获得所有信息

The screenshot shows the SciFinder interface with search results for 'Qinghaosu'. A purple box highlights the left-hand navigation menu, which includes 'Return to Home', 'Show only', 'Substances (1)', 'Reactions (2,742)', 'References (7,344)', and 'Suppliers (105)'. The main content area is divided into sections: 'All Answer Types' (top two answers by relevance), 'Substances (1)' (showing the chemical structure of Qinghaosu, C₁₅H₂₂O₅, with 7,231 references, 2,742 reactions, and 105 suppliers), and 'Reactions (2,742)' (showing a reaction scheme for the synthesis of Qinghaosu with 105 suppliers on the left and 99 on the right).

The screenshot shows the 'References (7,344)' section. It lists two references:

- Qinghaosu.**
By: Hien, T T; White, N J
Lancet (London, England) (1993), 341(8845), 603-8 | Language: English, Database: MEDLINE
There is no abstract available for this document.
Full Text | Substance (1) | Reactions (0) | Cited By (338) | Citation Map
- Qinghaosu (Artemisinin): The Price of Success**
By: White, N.J.
Science (Washington, DC, United States) (2008), 320(5874), 330-334 | Language: English, Database: CAPIus and MEDLINE
A review. Artemisinin and its derivatives have become essential components of antimalarial treatment. These plant-derived peroxides are unique among antimalarial drugs in killing the young intraerythrocytic malaria parasites, thereby preventing their development to more pathol. mature stages. This results in rapid clin. and parasitol. responses to treatment and life-saving benefit in severe malaria. Artemisinin combination treatments (ACTs) are now first-line drugs for uncomplicated falciparum malaria, but access to ACTs is still limited in most malaria endemic countries. Improved agricultural
View More | Full Text | Substance (1) | Reactions (0) | Cited By (579) | Citation Map

Below the references is a 'Suppliers (105)' table:

Supplier	Substance	Purity	Purchasing Details	Availability
1 Wurck KGaA Bismark, Germany Aldrich Partner Products - USA United States	63968-64-9 (5aS,6R,9R,12S,12aR)-3,6,9-trimethyloctahydro-12H-3,12-epoxy[1,2]dioxepino[4,3- <i>l</i>]isochromen-10(3H)-one	95-98%	Order From Supplier 100 mg 10 g 1 g 2 g 250 mg View all	Typically in stock Ships within 1 week
2	63968-64-9 Artemisinin	95-98%	Order From Supplier 1mg, GBP 29.00 View	Typically in stock

Search in All: 无需逐步在不同信息中检索，提高检索效率

提纲

- 美国化学文摘社简介
- SciFinder-n简介及检索方式
 - 文献检索
 - 物质检索
 - Markush检索
 - 反应检索
- 常见问题及解决

文献检索

■ 文献检索方法

- 主题检索
- 作者名检索
- 机构名检索
- 文献标识符检索
- 期刊名称和专利信息（公开号，申请号等）
- 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
- 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

主题检索： 中药治疗新冠肺炎

检索式： Chinese Medicine **and** COVID-19

The screenshot shows the CAS search interface. On the left, there is a sidebar with navigation options: All, Substances, Reactions, References (highlighted), and Suppliers. The main search area is titled 'References' and includes a search bar with the text 'Chinese Medicine and COVID-19'. Below the search bar, a list of suggestions is displayed, including 'Chinese Medicine and COVID-19', 'Chinese Medicine and COVID-19 virus', 'Chinese Medicine and COVID-19 vaccine', 'Chinese Medicine and COVID-19-related', 'Chinese Medicine and COVID-19 vaccines', 'Chinese Medicine and COVID-19-positive', and 'Chinese Medicine and COVID-19-associated'. A callout box points to the search bar with the text '关键词之间用布尔运算符连接'. Another callout box points to the list of suggestions with the text '利用CAS科学家编制的叙词表, 创建高质量的检索式'.

可用关键词、物质名称、CAS RN、入库号、PubMed编号、DOI号、专利号、专利申请号进行检索；

打开Advanced Search, 可做作者名、机构名、期刊名检索

文献检索——布尔运算符：and, or, not

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References Chinese Medicine and COVID-19

Return to Home

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](#)

References (3,977) Sort: Relevance View: Partial Abstract

Substances Reactions Cited By Save

Formulus, the comprehensive formulations database and workflow solution, is now available for all SciFinder[®] users. Use the CAS Solutions: Formulus filter to view available content. [Learn more about Formulus.](#)

Filter by

Document Type

- Journal (2,186)
- Patent (178)
- Review (901)
- Biography (2)
- Clinical Trial (12)

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Language

- English (2,532)
- Chinese (1,402)
- German (18)
- Spanish (12)
- Italian (4)

[View All](#)

Publication Year

1

Traditional Chinese medicine for COVID-19 treatment
By: Ren, Jun-ling; Zhang, Ai-Hua; Wang, Xi-Jun
Pharmacological Research (2020), 155, 104743 | Language: English, Database: CAPlus and MEDLINE
A review discussing the use of **traditional Chinese medicine** for the treatment of **COVID-19**.

Full Text Substances (0) Reactions (0) Cited By (79) Citation Map

2

Can Chinese Medicine Be Used for Prevention of Corona Virus Disease 2019 (COVID-19)? A Review of Historical Classics, Research Evidence and Current Prevention
By: Luo, Hui; Tang, Qiao-ling; Shang, Ya-xi; Llang, Shi-bing; Yang, Ming; Robinson, Nicola; Liu, Jian
Chinese Journal of Integrative Medicine (2020), 26(4), 243-250 | Language: English, Database: CA
A review. Since Dec. 2019, an outbreak of **corona virus** disease 2019 (**COVID-19**) occurred in W all parts of China. This was followed by prevention programs recommending **Chinese medicine** provide evidence for CM recommendations, we reviewed ancient classics and human studies. H treatment of infections in CM classics, clin. evidence of CM on the prevention of severe acute res influenza, and CM prevention programs issued by health authorities in China since the

View More Full Text Substances (0) Reactions (0) Cited By (92) Citation Map

Chinese Medicine and COVID-19

“and”表示文献中包含所有关键词

“or”表示文献中包含其中一个关键词即可

“not”表示文献包含一个关键词而没有另一个关键词

文献检索——检索式修饰符：括号 ()

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References Chinese Medicine and (COVID-19 or pneumonia) Draw

Return to Home

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

References (8,208) Sort: Relevance View: Partial Abstract

Substances Reactions Cited By Save

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1

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By: Ren, Jun-ling; Zhang, Ai-Hua; Wang, Xi-Jun
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A review discussing the use of **traditional Chinese medicine** for the treatment of **COVID-19**.
Full Text Substances (0) Reactions (0) Cited By (79) Citation Map

2

Traditional Chinese medicine in the treatment of patients infected with 2019-new coronavirus (SARS-CoV-2): a review and perspective
By: Yang, Yang; Islam, Sahidul Md; Wang, Jin; Li, Yuan; Chen, Xin
International Journal of Biological Sciences (2020), 16(10), 1708-1717 | Language: English, Database: CAplus and MEDLINE
A review. Currently, Severe Acute Respiratory Syndrome Coronavirus 2 (SARS-CoV-2, formerly known as 2019-nCoV, the causative pathogen of Coronavirus Disease 2019 (**COVID-19**)) has rapidly spread across China and around the world, causing an outbreak of acute infectious **pneumonia**. No specific anti-virus **drugs** or vaccines are available for the treatment of this sudden and lethal disease. The supportive care and non-specific treatment to ameliorate the symptoms of the patient are the only options currently. At the top of these conventional therapies, greater than 85% of SARS-CoV-2 infected patients.
View More
Full Text Substances (0) Reactions (0) Cited By (106) Citation Map

Filter by

Document Type

- Journal (4,640)
- Patent (1,930)
- Review (1,214)
- Biography (5)
- Book (1)

View All

Language

- English (4,620)
- Chinese (3,371)
- German (54)
- Japanese (45)
- Russian (40)

View All

Publication Year

Chinese Medicine and
(COVID-19 or pneumonia)

括号中的检索式被当做
是一个关键词参与检索

文献检索——检索式修饰符：引号“ ”

The screenshot shows the SciFinder interface with a search query "total synthesis" and taxol. The results are displayed in a list format. The first result is titled "Two-Phase Synthesis of Taxol" and includes a chemical structure of Taxol. The second result is titled "Total synthesis of taxol" and includes a chemical reaction scheme. The interface includes a search bar, navigation buttons, and filters for document type, language, and publication year.

References (227) Sort: Relevance View: Partial Abstract

Substances Reactions Cited By Save

1

Two-Phase Synthesis of Taxol

By: Kanda, Yuzuru; Nakamura, Hugh; Umeyama, Shigenobu; Puthukanoori, Ravi Kumar; Murthy Appala, Venkata Ramana; Gaddamanugu, Gopi Krishna; Paraselli, Bheema Rao; Baran, Phil S.
Journal of the American Chemical Society (2020), 142(23), 10526-10533 | Language: English, Database: CPlus and MEDLINE

Taxol is widely regarded as amongst the most famed natural isolates ever discovered, and has been the subject of innumerable studies in both basic and applied science. Its documented success as an anticancer agent, coupled with early concerns over supply, stimulated a furious worldwide effort from chemists to provide a solution for its preparation through total synthesis. Those pioneering studies proved the feasibility of retrosynthetically-guided access to synthetic Taxol, albeit in minute quantities and with enormous effort. In practice, all medicinal chem. efforts and eventual commercializa.

View More

Full Text Substances (50) Reactions (1,307) Cited By (7) Citation Map

2

Total synthesis of taxol

By: Nicolaou, K. C.; Yang, Z.; Liu, J.; Ueno, H.; Nantermet, P. G.; Guy, R. K.; Claiborne, C. F.; Renaud, J.; Couladouros, E. A.
Nature (London, United Kingdom) (1994), 367(6464), 630-4 | Language: English, Database: CPlus and MEDLINE

The total synthesis of taxol (I) from the benzofuranone II by a convergent strategy, which opens a chem. pathway for the production of both I and a variety of designed taxoids is reported.

View More

Full Text Substances (26) Reactions (23) Cited By (718) Citation Map

“total synthesis” and taxol

引号中的关键词仅
扩展检索其单复数

文献检索——检索式通配符：* 与？

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References ▾ org* comp* and toxicity test and model* × Draw 🔍 ★ ⌚ 👤

← Return to Home

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 by

- Document Type
 - Journal (179K)
 - Patent (7,831)
 - Review (12K)
 - Biography (10)
 - Book (38)
 - View All
- Substance Role
 - Adverse Effect (3,886)
 - Analytical Study (1,879)
 - Biological Study (18K)
 - Combinatorial Study (10)
 - Formation (775)
 - View All
- Language
 - English (180K)
 - Chinese (8,488)
 - Japanese (2,436)

References (196,958) Sort: Relevance ▾ View: Partial Abstract ▾

Substances ▾ Reactions ▾ Cited By ▾

1

Quantitative Structure-Activity Relationship Modeling of Rat Acute Toxicity by Oral Exposure
By: Zhu, Hao; Martin, Todd M.; Ye, Lin; Sedykh, Alexander; Young, Douglas M.; Tropsha, Alexander
Chemical Research in Toxicology (2009), 22(12), 1913-1921 | Language: English, Database: CPlus and MEDLINE

Few quant. structure-activity relationship (QSAR) studies have successfully modeled large, diverse rodent toxicity end points. In this study, a comprehensive data set of compounds with their most conservative LD (LD₅₀) values has been compiled. A combinatorial QSAR approach has been employed to develop robust and predictive models of acute toxicity in rats caused by oral exposure to chemicals. To enable fair comparison between the predictive power of models generated in this study vs. a commercial predictor, TOPKAT (Toxicity Prediction by Komputer Assisted Technology), a model of...

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Full Text ▾ Substances (11) Reactions (0) Cited By (97)

2

Prediction of the Acute Toxicity (96-h LC₅₀) of Organic Compounds to the Fathead Minnow (*Pimephales promelas*) Using a Group Contribution Method
By: Martin, Todd M.; Young, Douglas M.
Chemical Research in Toxicology (2001), 14(10), 1378-1385 | Language: English, Database: CPlus and MEDLINE

A group contribution method has been developed to correlate the acute toxicity (96-h LC₅₀) to the fathead minnow (*Pimephales promelas*) for 397 organic chemicals. Multilinear regression and computational neural networks (CNNs) were used for model building. The models were able to achieve a fairly good correlation of the data ($r^2 > 0.9$). The linear model, which included specific interaction terms, provided a rapid means of predicting the toxicity of a compound. The CNN model was able to yield virtually the same predictions with or without the four interaction terms that were included in the model.

View More ▾

org* comp* and toxicity test
and model*

通配符星号(*)代表0或多个字符

通配符问号(?)代表0或1个字符

通配符可用于词中间或词尾，不可用于词首

一个检索词中至少包含3个非通配符的字符

一个检索词中只用一个通配符

一个检索式中不可超过五个通配符

文献结果集

References (3,977)

Sort: Relevance

- Relevance
- Times Cited
- Publication Date: Newest
- Publication Date: Oldest

Load More Results

Filter by

Document Type

- Journal (2,186)
- Patent (178)
- Review (901)
- Biography (2)
- Clinical Trial (12)
- View All

Language

- English (2,532)
- Chinese (1,402)
- German (18)
- Spanish (12)
- Italian (4)
- View All

1

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Pharmacological Research (2020), 155, 104743 | Language: English, Database: CAPplus and MEDLINE

A review discussing the use of **traditional Chinese medicine** for the treatment of **COVID-19**.

Full Text

Substances (0) Reactions (0) Cited By (79) Citation Map

2

Can Chinese Medicine Be Used for Prevention of Corona Virus Disease 2019 (COVID-19)? A Review of Historical Classics, Research Evidence and Current Prevention Programs

By: Luo, Hui; Tang, Qiao-ling; Shang, Ya-xi; Liang, Shi-bing; Yang, Ming; Robinson, Nicola; Liu, Jian-ping
Chinese Journal of Integrative Medicine (2020), 26(4), 243-250 | Language: English, Database: CAPplus and MEDLINE

A review. Since Dec. 2019, an outbreak of **corona virus** disease 2019 (**COVID-19**) occurred in Wuhan, and rapidly spread to almost all parts of China. This was followed by prevention programs recommending **Chinese medicine** (CM) for the prevention. In order to provide evidence for CM recommendations, we reviewed ancient classics and human studies. Historical records on prevention and treatment of infections in CM classics, clin. evidence of CM on the prevention of severe acute respiratory syndrome (SARS) and H1N1 influenza, and CM prevention programs issued by health authorities in China since the

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研究发展趋势

CAS标引的技术术语

制剂用途

二次检索

聚类筛选项因结果集而异

The screenshot displays a search results interface with several filter panels on the left and search results on the right. The filter panels include:

- Publication Year:** A range selector from 1992 to 2021.
- Available at My Institution:** A toggle switch.
- Author:** A search field.
- Organization:** A search field.
- Publication Name:** A search field.
- Concept:** A list of concepts with counts: COVID-19 (3,546), Homo sapiens (2,629), Severe acute respiratory syndrome coronavirus 2 (2,427), Coronavirus Infections (1,311), and Humans (1,311). A "View All" link is present.
- CAS Solutions:** A section with sub-filters:
 - Formulation Purpose:** A list of purposes with counts: Anticoronaviral agents (2), Antiviral agents (2), Antibacterial agents (1), Antidiarrheals (1), and Anti-infective agents (1). A "View All" link is present.
- Database:** A section with a "Search Within Results" field and a "Find" button.

The search results on the right show three entries:

- Entry 3:** "Traditional Chinese medicine in the treatment of patients infected with 2019-new coronavirus (SARS-CoV-2): a review and perspective". By: Yang, Yang; Islam, Sahidul Md; Wang, Jin; Li, Yuan; Chen, Xin. International Journal of Biological Sciences (2020), 16(10), 1708-1717 | Language: English, Database: CAPlus and MEDLINE. A review. Currently, **Severe Acute Respiratory Syndrome Coronavirus 2 (SARS-CoV-2)**, formerly known as **2019-nCoV**, the causative pathogen of **Coronavirus Disease 2019 (COVID-19)** has rapidly spread across China and around the world, causing an outbreak of acute infectious pneumonia. No specific anti-virus **drugs** or vaccines are available for the treatment of this sudden and lethal disease. The supportive care and non-specific treatment to ameliorate the symptoms of the patient are the only options currently. At the top of these conventional therapies, greater than 85% of **SARS-CoV-2** infected patients.
- Entry 4:** "Efficacy and Safety of Integrated Traditional Chinese and Western Medicine for Corona Virus Disease 2019 (COVID-19): a systematic review and meta-analysis". By: Liu, Ming; Gao, Ya; Yuan, Yuan; Yang, Kelu; Shi, Shuzhen; Zhang, Junhua; Tian, Jinhui. Pharmacological Research (2020), 158, 104896 | Language: English, Database: CAPlus and MEDLINE. A review. **Corona virus** disease (**COVID-19**) has now spread to all parts of the world and almost all countries are battling against it. This study aimed to assess the efficacy and safety of Integrated Traditional **Chinese** and Western **Medicine** (Hereinafter referred to as "**Integrated Medicine**") to **COVID-19**. We searched six major **Chinese** and English databases to identify randomized controlled trials (RCTs) and case-control studies (CCSs) of **Integrated Medicine** on **COVID-19**. Two reviewers independently screened, identified studies, and extracted data. Cochrane Risk of Bias tool and the Newcastle-Ottawa
- Entry 5:** "COVID-19: An Update on the Epidemiological, Clinical, Preventive and Therapeutic Evidence and Guidelines of Integrative Chinese-Western Medicine for the Management of 2019 Novel Coronavirus Disease". By: Chan, Kam Wa; Wong, Vivian Taam; Tang, Sydney Chi Wai. American Journal of Chinese Medicine (2020), 48(3), 737-762 | Language: English, Database: CAPlus and MEDLINE. A review. As of 22 Feb. 2020, more than 77662 cases of confirmed **COVID-19** have been documented globally with over 2360 deaths. Common presentations of confirmed cases include fever, fatigue, dry cough, upper airway congestion, sputum production.

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

文献结果集—聚类筛选 Formulation Purpose

- Formulation Purpose
- Anticoronaviral agents (2)
- Antiviral agents (2)
- Antibacterial agents (1)
- Antidiarrheals (1)
- Anti-infective agents (1)
- Antitumor agents (1)
- Pharmaceutical formulations (1)
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Reference Detail (1 of 2)

Substance (1) Reactions (0) Cited By (4) Citation Map

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Therapeutic efficacy of Pudilan Xiaoyan Oral Liquid (PDL) for COVID-19 in vitro and in vivo

By: Deng, Wei; Xu, Yanfeng; Kong, Qi; Xue, Jing; Yu, Pin; Liu, Jiangning; Lv, Qi; Li, Fengdi; Wei, Qiang; Bao, Linlin

Pudilan Xiaoyan Oral Liquid (PDL) is a **traditional Chinese medicine** preparation composed of Indigofera Root (*Isatis indigotica*), Bunge Corydalis (*Corydalis bungeana*), Mongolian Dandelion (*Taraxacum mongolicum*), Scutellaria Amoena (*Scutellaria baicalensis*). PDL with a half-maximal effective concentration (EC50)=1.078 mg/mL, half-cytotoxic concentration (CC50)= 8.914mg/mL, selectivity index = 8.27 could effectively suppress SARS-CoV-2 viral replication in Vero cells. In SARS-CoV-2-infected, human ACE2-transgenic mice, PDL lowered viral RNA and inflammation in the lung and improved body weight. Thus, PDL exhibited anti-SARS-CoV-2 activity both in vitro and in vivo.

Keywords: anticoronavirus activity Pudilan Xiaoyan Oral Liquid COVID19; SARS CoV2 anticoronavirus Liquid

Full Text

- Concepts
- MEDLINE® Medical Subject Headings
- Supplementary Concepts
- Substances
- Formulations
- Citations

Journal: Signal Transduction and Targeted Therapy
Volume: 5
Issue: 1
Pages: 66
Journal: Letter; Research Support, Non-U.S. Gov't
2020
DOI: 10.1038/s41392-020-0176-0

Database Information
AN: 2020:903866
CAN: 172:510653
PubMed ID: 32385228
CAlplus and MEDLINE

Company/Organization
NHC Key Laboratory of Human Disease Comparative Medicine, Beijing Key Laboratory for Animal Models of Emerging and Remerging Infectious Diseases, Institute of Laboratory Animal Science, Chinese Academy of Medical Sciences and Comparative Medicine Center
Peking Union Medical College
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Email
blmsl@aliyun.com

Publisher

Formulations

Pudilan Xiaoyan Oral Liquid: Anti-Coronaviral Agents

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Location: Article Page 1
Purpose: Anticoronaviral agents
Target: CoVID-19, mumps, pharyngitis, respiratory diseases, human

Component	Function	Amount Reported
Isatis tinctoria	-	-
bunge Corydalis	-	-
Taraxacum mongolicum	-	-
Scutellaria amoena	-	-

查看配方/制剂信息，包括配方在原文中的页码，配方成份、含量、作用等



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文献结果集—聚类筛选 Concept

Concept ×

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1 Selected

<input type="checkbox"/> COVID-19 (3,546)	<input type="checkbox"/> Aged (144)	<input type="checkbox"/> COVID-19 diagnostic testing (71)
<input type="checkbox"/> Homo sapiens (2,629)	<input type="checkbox"/> Medicine, Chinese Traditional (141)	<input type="checkbox"/> Infection Control (71)
<input type="checkbox"/> Severe acute respiratory syndrome coronavirus 2 (2,427)	<input type="checkbox"/> Fever and Hyperthermia (129)	<input type="checkbox"/> Databases (70)
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<input type="checkbox"/> Public health (368)	<input type="checkbox"/> Interleukin 6 (99)	<input type="checkbox"/> Comorbidity (58)
<input type="checkbox"/> Diagnosis (336)	<input type="checkbox"/> Signal transduction (98)	<input type="checkbox"/> Depression (56)
<input type="checkbox"/> Female (332)	<input type="checkbox"/> Tomography (98)	<input type="checkbox"/> Aged, 80 and over (54)

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- Publication Name
- Concept
 - COVID-19 (3,546)
 - Homo sapiens (2,629)
 - Severe acute respiratory

References (378) Sort: Relevance View: Partial Abstract

Substances Reactions Cited By

1

[Traditional Chinese medicine in the treatment of patients infected with 2019-new coronavirus \(SARS-CoV-2\): a review and perspective](#)
By: Yang, Yang; Islam, Sahidul Md; Wang, Jin; Li, Yuan; Chen, Xin
International Journal of Biological Sciences (2020), 16(10), 1708-1717 | Language: English, Database: CAPlus and MEDLINE

A review. Currently, **Severe Acute Respiratory Syndrome Coronavirus 2 (SARS-CoV-2)**, formerly known as **2019-nCoV**, the causative pathogen of **Coronavirus Disease 2019 (COVID-19)** has rapidly spread across China and around the world, causing an outbreak of acute infectious pneumonia. No specific anti-virus **drugs** or vaccines are available for the treatment of this sudden and lethal disease. The supportive care and non-specific treatment to ameliorate the symptoms of the patient are the only options currently. At the top of these conventional therapies, greater than 95% of **SARS-CoV-2** infected patients.

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2

[Clinical observation and management of COVID-19 patients](#)
By: Li, Taisheng; Lu, Hongzhou; Zhang, Wenhong
Emerging Microbes & Infections (2020), 9(1), 687-690 | Language: English, Database: CAPlus and MEDLINE

A review with commentary. Three leading infectious disease experts in China were invited to share their bedside observations in the management of **COVID-19** patients. Professor Taisheng Li was sent to Wuhan to provide frontline medical care. He depicts the clinical course of **SARS-CoV-2** infection. Furthermore, he observes the significant abnormality of coagulation function and proposes that the early **Low molecular weight heparin** anticoagulation therapy are very important. Professor Hongzhou Lu, a leader in China to try various **antibacterial** **drugs**, expresses concern on the quality of the evidence.

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3

[COVID-19 infection and rheumatoid arthritis: Faraway, so close!](#)
By: Favalli, Ennio Giulio; Ingegnoli, Francesca; De Lucia, Orazio; Cincinelli, Gilberto; Cimaz, Rolando; Caporali, Roberto
Autoimmunity Reviews (2020), 19(5), 102523 | Language: English, Database: CAPlus and MEDLINE

A review. The outbreak of the new **coronavirus infections COVID-19** in Dec. 2019 in China has quickly become a global health emergency. Given the lack of specific anti-viral therapies, the current management of severe acute respiratory syndrome coronaviruses (**SARS-CoV-2**) is mainly supportive, even though several compounds are now under investigation for the treatment of this life-threatening disease. **COVID-19** pandemic is certainly conditioning the treatment strategy of a complex disorder as rheumatoid arthritis (RA), whose infectious risk is increased compared to the general population because of...

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Journal

Source
Journal of Medical Virology
Volume: 92
Issue: 7
Pages: 797-806
Journal: Article; Research Support, Non-U.S. Gov't
2020
DOI:
10.1002/jmv.25783

Database Information
AN: 2020:741973
CAN: 173:29845
PubMed ID: 32198776
CAPlus and MEDLINE

Company/Organization
Pharmaceutical Department of Chongqing Three Gorges Central Hospital
Chongqing University Three Gorges Hospital
Chongqing
China

Publisher
Wiley-Blackwell

Language
English

Clinical features and treatment of **COVID-19** patients in northeast Chongqing

By: Wan, Suxin; Xiang, Yi; Fang, Wei; Zheng, Yu; Li, Boqun; Hu, Yanjun; Lang, Chunhui; Huang, Daoqiu; Sun, Qiuyan; Xiong, Yan; et al
View All

The outbreak of the **novel coronavirus** in China (**SARS-CoV-2**) that began in Dec. 2019 presents a significant and urgent threat to global health. This study was conducted to provide the international community with a deeper understanding of this new infectious disease. Epidemiol., clin. features, laboratory findings, radiol. characteristics, treatment, and clin. outcomes of 135 patients in northeast Chongqing were collected and analyzed in this study. A total of 135 hospitalized patients with **COVID-19** were enrolled. The median age was 47 years (interquartile range, 36-55), and there was no significant gender difference (53.3% men). The majority of patients had contact with people from the Wuhan area. Forty-three (31.9%) patients had underlying disease, primarily hypertension (13 [9.6%]), diabetes (12 [8.9%]), cardiovascular disease (7 [5.2%]), and malignancy (4 [3.0%]). Common symptoms included fever (120 [88.9%]), cough (102 [76.5%]), and fatigue (44 [32.5%]). Chest computed tomog. scans showed bilateral patchy shadows or ground glass opacity in the lungs of all the patients. All patients received antiviral therapy (135 [100%]) (Kaletra and interferon were both used), antibacterial therapy (59 [43.7%]), and corticosteroids (36 [26.7%]). In addition, many patients received **traditional Chinese medicine** (TCM) (124 [91.8%]). It is suggested that patients should receive Kaletra early and should be treated by a combination of Western and **Chinese medicines**. Compared to the mild cases, the severe ones had lower lymphocyte counts and higher plasma levels of Pt. APTT, d-dimer, lactate dehydrogenase, PCT, ALB, C-reactive protein, and aspartate aminotransferase. This study demonstrates the clinic features and therapies of 135 **COVID-19** patients. Kaletra and TCM played an important role in the treatment of the viral pneumonia. Further studies are required to explore the role of Kaletra and TCM in the treatment of **COVID-19**.

Keywords: **COVID19** disease Kaletra antiviral **Chinese medicine** Chongqing China; **COVID-19**; clinical features; cognition; northeast Chongqing; treatment

Full Text

Concepts

MEDLINE® Medical Subject Headings

Supplementary Concepts

Substances

Citations

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文献详情

Concepts	
Adult respiratory distress syndrome	Diastolic blood pressure
Albumins Role: Biological Study, Unclassified	Fatigue, biological
Antibacterial agents	Fever and Hyperthermia
Antibiotics	Fibrin fragment D-dimer Role: Biological Study, Unclassified
Antiviral agents	Hemoglobins Role: Biological Study, Unclassified
Appetite Modifier: loss	Hemoptysis
B cell	Homo sapiens
Blood platelet	Hypertension
Breathing disorders	Interferons Role: Pharmacological Activity, Therapeutic Use
C-reactive protein Role: Biological Study, Unclassified	Kidney injury
Cardiac injury	Leukocyte
Cardiovascular disease	Morbidity rate
CD4-positive T cell	Natural killer cell
CD8-positive T cell	Neoplasm
Chinese medicine	Neutrophil
Common cold	Prognosis
Corticosteroids Role: Pharmacological Activity, Therapeutic Use	Severe acute respiratory syndrome coronavirus 2
Cough	Shock (circulatory collapse)
COVID-19	
Diabetes mellitus	
Diarrhea	

Supplementary Concepts

loglinavir-ritonavir drug combination

COVID-19

COVID-19 diag

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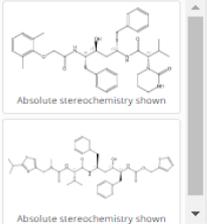
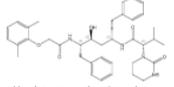
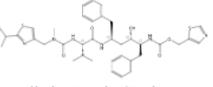
MEDLINE® Medical Subject Headings	
Adolescent	Drug Combinations
Adrenal Cortex Hormones Qualifier: therapeutic use	Drugs, Chinese Herbal Qualifier: therapeutic use
Adult	Fatigue Qualifier: diagnosis; physiopathology; virology
Aged	Female
Anti-Bacterial Agents Qualifier: therapeutic use	Fever Qualifier: diagnosis; physiopathology; virology
Antiviral Agents Qualifier: therapeutic use	Humans
Betacoronavirus Qualifier: isolation & purification; pathogenicity	Interferons Qualifier: therapeutic use
Biomarkers Qualifier: blood	Loglinavir Qualifier: therapeutic use
Cardiovascular Diseases Qualifier: complications; diagnosis; drug therapy; pathology	Male
China Qualifier: Geographic	Middle Aged
Clinical Laboratory Techniques Qualifier: methods	Neoplasms Qualifier: complications; diagnosis; drug therapy; pathology
Coronavirus Infections Qualifier: complications; diagnosis; drug therapy; pathology	Pandemics
Cough Qualifier: diagnosis; physiopathology; virology	Pneumonia, Viral Qualifier: complications; diagnosis; drug therapy; pathology
Diabetes Complications Qualifier: blood; drug therapy	Retrospective Studies
Diabetes Mellitus Qualifier: diagnosis; drug therapy; pathology	Ritonavir Qualifier: therapeutic use
	Severity of Illness Index
	Tomography, X-Ray Computed

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文献详情

Substances

Substances (16)

<p>369372-47-4</p>  <p>Absolute stereochemistry shown</p> <p>$C_{37}H_{48}N_6O_5S_2 \cdot C_{37}H_{48}N_4O_5$ Lopinavir-ritonavir mixt.</p> <p>Role: Pharmacological Activity, Therapeutic Use, Biological Study, Uses</p>	<p>192725-17-0</p>  <p>Absolute stereochemistry shown</p> <p>$C_{37}H_{48}N_6O_5$ Lopinavir</p> <p>Role: Unspecified</p>	<p>155213-67-5</p>  <p>Absolute stereochemistry shown</p> <p>$C_{37}H_{48}N_6O_5S_2$ Ritonavir</p> <p>Role: Unspecified</p>
<p>72162-96-0</p> <p>Image Not Available</p> <p>Unspecified Prothrombinase</p> <p>Role: Biological Study, Unclassified, Biological Study</p>	<p>56645-65-9</p> <p>Image Not Available</p> <p>Unspecified Procalcitonin</p> <p>Role: Biological Study, Unclassified, Biological Study</p>	<p>9008-11-1</p> <p>Image Not Available</p> <p>Unspecified Interferons</p> <p>Role: Unspecified</p>
<p>9001-60-9</p> <p>Image Not Available</p> <p>Unspecified L-Lactate dehydrogenase</p> <p>Role: Biological Study, Unclassified, Biological Study</p>	<p>9001-26-7</p> <p>Image Not Available</p> <p>Unspecified Prothrombin</p> <p>Role: Biological Study, Unclassified, Biological Study</p>	<p>9001-15-4</p> <p>Image Not Available</p> <p>Unspecified Creatine kinase</p> <p>Role: Biological Study, Unclassified, Biological Study</p>

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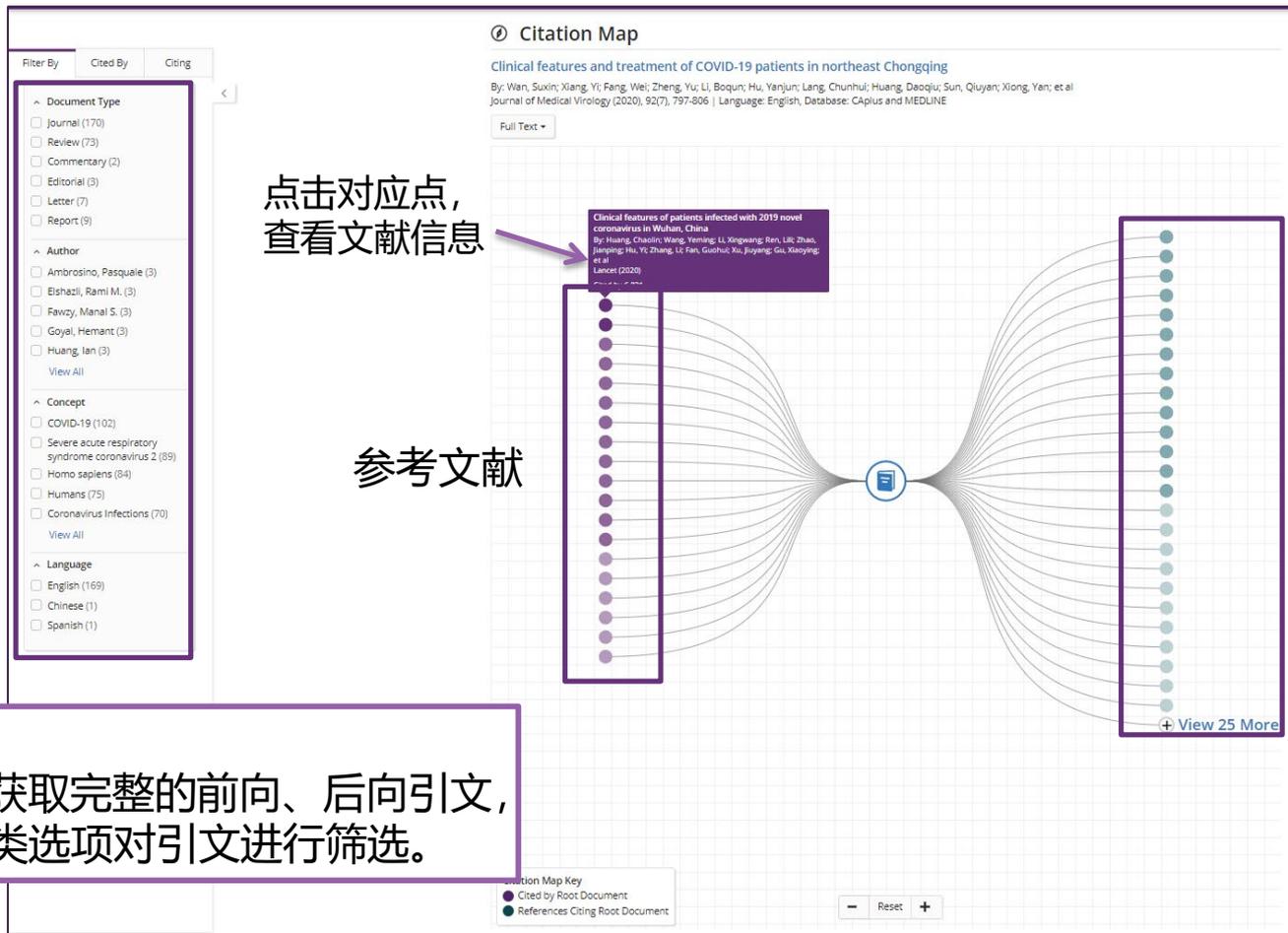
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Substances (56) Reactions (278) Cited By (1) Citation Map

Patent

Patent Information

Patent Number
WO9929704

Publication Date
1999-06-17

Application Number
WO1998-US26472

Application Date
1998-12-11

Kind Code
A1

Assignee
The Trustees of Columbia University in the City of New York, United States

Source
World Intellectual Property Organization

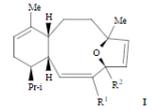
Database Information
AN: 1999-390407
CAN: 131-45046
CPlus

Language
English

Total synthesis of eleutherobin and its analogs as carcinoma inhibitors

By: Danishefsky, Samuel J.; Chen, Xiao-Tao; Gutteridge, Clare E.; Bhattacharya, Samit K.; Zhou, Bishan

This invention provides a process for the **preparation** of a eleutherobin I wherein R¹ is a hydrogen, ester, nitrile or CH₂-R² (I), wherein R¹ is a carbohydrate, an alc, an amine, an amide, an alkyne; or R² is a linear or branched alkyl moiety; R² is an ester, an amide, a carbamate, an acetal compound, an ether or a urethane; R² is a hydrogen or CH₃. Addnl., this experiment provides a method for inhibiting growth of cancerous cells comprising contracting an amount of Eleutherobin derivative effective to inhibit the growth of said cells. Further provided is a method for treating cancer in a subject which comprises administering to the subject a therapeutically effective amount of the eleutherobin derivative. Thus, I (R¹ = H, R² = OMe, R² = N(CH₃)-methyluronic acid ester) was prepared and tested for its antitumor activity for lung carcinoma (resistant, IC₅₀ = 4000 nM) and for ovarian carcinoma (resistant, IC₅₀ = 1350 nM).



Keywords: uronic acid **synthesis** carcinoma inhibitor; carcinoma inhibitor eleutherobin **synthesis** cytotoxicity; structure activity eleutherobin **synthesis** antitumor cytotoxicity

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Patent Family

Patent	Language	Kind Code	PatentPak Options	Publication Date	Application Number	Application Date
WO9929704	English	A1	PDF PDF+ Viewer	1999-06-17	WO1998-US26472	1998-12-11
		P			US1997-69248P	1997-12-11
AU9919122	Undetermined	A		1999-06-28	AU1999-19122	1998-12-11
US6172205	Undetermined	B1		2001-01-09	US1998-210290	1998-12-11

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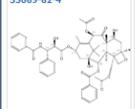
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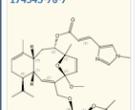
Key Substances in Patent

CAS RN 33069-62-4



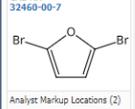
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Page 72

CAS RN 174545-76-7



Analyst Markup Locations (1)
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CAS RN 32460-00-7



Analyst Markup Locations (2)
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CAS RN 4221-98-1



Analyst Markup Locations (1)
Page 63

CAS RN 27490-33-1



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WO 99/29704 PCT/US98/26472

-54-

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46. Nicolaou, K. C., J.-Y. Xu, S. Kim, T. Ohshima, S. Hosokawa, and J. Pfefferkorn. Synthesis of the Tricyclic Core of Eleutherobin and Sarcodictyins and Total Synthesis of Sarcodictyin A. *J. Am. Chem. Soc.* 1997, 119, 11351-11354.

47. Nicolaou, K. C., et al., Total Synthesis of Eleutherobin. *Angew. Chem. Int. Ed. Engl.* 1997, 36:22.

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49. Long, Byron H., et al. Eleutherobin, A Novel Cytotoxic Agent That Induces Tubulin Polymerization Is Similar to Paclitaxel (Taxol). *Cancer Res.* 1997, 53.

50. Nicolaou, K. C., Solid and Solution Phase Synthesis and Biological Evaluation of Combinatorial Sarcodictyin Libraries. *J. Am. Chem. Soc.* 1998, 120,

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 - Reaction Role:** Product (55), Reactant (48), Reagent (15), Catalyst (12), Solvent (9).
 - Reference Role:** Adverse Effect (12), Analytical Study (15), Biological Study (20), Combinatorial Study (9), Formation (13).
 - Stereochemistry:** Number of Components, Substance Class, Isotopes, Metals.
 - Molecular Weight:** Experimental Property, Experimental Spectrum, Regulatory Information, Bioactivity Indicator, Target Indicator, Search Within Results.
- Substance Grid (9 items):**

ID	Chemical Name	Formula	References	Reactions	Suppliers
67-56-1	Methanol	<chem>CH4O</chem>	580K	3.1M	398
108-24-7	Acetic anhydride	<chem>C4H6O3</chem>	148K	359K	84
74-88-4	Methyl iodide	<chem>CH3I</chem>	113K	244K	83
33069-62-4	Paclitaxel	<chem>C27H42NO14</chem>	61K	3,827	146
124-63-0	Methanesulfonyl chloride	<chem>CH3ClO2S</chem>	40K	148K	46
151-50-8	Potassium cyanide	<chem>CKN</chem>	19K	33K	57
917-54-4	Methylithium	<chem>CH3Li</chem>	14K	38K	35
3282-30-2	Fivallyl chloride	<chem>C6H9ClO</chem>	13K	28K	49
58479-61-1	tert-Buylidiphenylsilyl chloride	<chem>C16H19ClSi</chem>	10K	15K	94



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- 理化性质检索

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- 谱图数据检索

- 物质检索策略推荐

- 有机化合物，天然产物：结构检索

- 无机物，合金：分子式检索

- 高分子化合物：分子式检索和结构检索



物质检索

Searching for...

- All
- Substances
- Reactions
- References
- Suppliers

Substances

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

Enter a query...

Use [Advanced Search](#) for Molecular Formula, Substance Property, or Experimental Spectra

Draw

通过物质名称、CAS RN，文献标识符检索物质

打开结构绘制面板进行结构检索

物质检索—物质名称、CAS RN、代码

The screenshot shows the SciFinder search results for the query "sofosbuvir 50-56-6 carbon dioxide GS 5734". The interface includes a search bar, a filter sidebar on the left, and a main results area displaying four entries:

- Entry 1:** 50-56-6. Chemical structure of Sofosbuvir. CAS: $C_{43}H_{66}N_{12}O_{12}S_2$. Name: Oxytocin. Protein/Peptide Sequence Length: 9. 38K References, 354 Reactions, 72 Suppliers.
- Entry 2:** 1190307-88-0. Chemical structure of Sofosbuvir. CAS: $C_{22}H_{29}FN_2O_9P$. Name: Sofosbuvir. 3,231 References, 583 Reactions, 73 Suppliers.
- Entry 3:** 124-38-9. Chemical structure of Carbon dioxide. CAS: CO_2 . Name: Carbon dioxide. 634K References, 83K Reactions, 23 Suppliers.
- Entry 4:** 1809249-37-3. Chemical structure of GS 5734. CAS: $C_{27}H_{35}N_6O_8P$. Name: GS 5734. 21 References, 295 Reactions, 17 Suppliers.

The left sidebar contains filter options such as Commercial Availability, Reaction Role, Reference Role, Stereochemistry, Number of Components, Substance Class, Isotopes, Metals, Molecular Weight, Experimental Property, and Experimental Spectrum.

sofosbuvir
50-56-6
"carbon dioxide"
"GS 5734"

多个物质同时检索,
中间用空格隔开

物质检索—文献标识符

SCIFINDERⁿ
A CAS SOLUTION

Substances WO2011123645

Draw

Return to Home

Filter by

- Commercial Availability
- Reaction Role
 - Product (119)
 - Reactant (95)
 - Reagent (24)
 - Catalyst (20)
 - Solvent (16)
- Reference Role
 - Adverse Effect (32)
 - Analytical Study (40)
 - Biological Study (67)
 - Combinatorial Study (19)
 - Formation (22)
- Stereochemistry
- Number of Components
- Substance Class
- Isotopes

Substances (122) Sort: Relevance View Partial

References Reactions Suppliers Save

Patent No.	Chemical Structure	References	Reactions	Suppliers
108-95-2	<chem>Oc1ccccc1</chem>	196K	74K	153
108-24-7	<chem>CC(=O)OC(=O)C</chem>	140K	326K	60
100-46-9	<chem>NCC1=CC=CC=C1</chem>	51K	79K	84
18162-48-6	<chem>ClSi(C)(C)C</chem>	32K	54K	119
58-96-8	<chem>C1=CN2C(=O)N(C2)C1O</chem>	24K	3,236	128
10025-87-3	<chem>ClP(=O)(Cl)Cl</chem>	23K	176K	44

专利号
WO2011123645

帮助用户迅速获得关
注文献中的所有物质



物质检索

Search

All Substances Reactions References Suppliers

Search by Substance Name, CAS RN, Patent Number, etc.

Enter a query...

Use **Advanced Search** for Molecular Formula, Substance Property, or Experimental Spectra

通过分子式、物性参数、谱图数据进行检索

+ Return to Home Page

Substances References

Advanced Substance Search

Molecular Formula
Enter one Molecular Formula.

Ex: C6H6
(C8H8)
C22H26CuN2O5.C2H3N

Add Another Molecular Formula

— AND —

Substance Property
Select Property Enter Value

- Select One -

Add Another Property

AND

Experimental Spectra
Select Spectrum Enter Value

Carbon-13 NMR 152.3, 127.6, 155.02 to 207.59

(Search includes allowance of ± 2 ppm)
Example: 152.3, 127.6, 133.1
155.02 to 207.59
187

Add Another Spectra

Clear All



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物质检索—分子式

Na₂SO₄: H₂O₄S.2Na

Molecular Formula

Enter one Molecular Formula.

H₂O₄S.2Na

Ex: C₆H₆
(C₈H₈)_x
C₂₂H₂₆Cu₂N₂O₅.C₂H₃N

Add Another Molecular Formula

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

The screenshot shows the CAS search results for the molecular formula H₂O₄S.2Na. The interface includes a filter sidebar on the left with categories like Commercial Availability, Reaction Role, Reference Role, Number of Components, Substance Class, Isotopes, Metals, Experimental Property, Experimental Spectrum, Regulatory Information, and Search Within Results. The main area displays 9 search results in a grid. Each result card shows a chemical structure (sulfuric acid), the molecular formula H₂O₄S.2Na, the number of components (2), and the component RN (e.g., 7664-93-9 for sodium sulfate). It also provides counts for references, reactions, and suppliers.



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物质检索—物性参数

密度 $>150\text{g/cm}^3$
分子量 <200

Substance Property

Select Property Enter Value

Include results with predicted properties.

1.15
<7.53
>150
9.3 to 15
8.9e-2

— AND —

Select Property Enter Value

Results based on predicted properties only.

46.07
125 to 350
>300

可多参数检索，提高检索效率

Substances (6) Sort: Relevance View: Partial

References Reactions Suppliers

1 139-13-9
CC(=O)N(CC(=O)O)CC(=O)O
C₆H₉NO₆
Nitrilotriacetic acid
13K References 713 Reactions 91 Suppliers

2 7631-86-9
O=[Si]=O
O₂Si
Silica
1.1M References 90K Reactions 407 Suppliers

3 593-88-4
C[As](C)C
C₃H₉As
Trimethylarsine

4 34560-16-2
CCOC(C)C(=O)OCC
C₆H₁₃NO₄
1,1-Diethoxy-2-nitroethane
25 References 42 Reactions 50 Suppliers

5 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 +

双击结构打开物质菜单

物质检索—谱图数据检索

碳谱特征峰保留时间：
152.3, 127.6, 155.02 to 207.59

Experimental Spectra

Select Spectrum: Carbon-13 NMR

Enter Value: 152.3, 127.6, 155.02 to 207.59

(Search includes allowance of ± 2 ppm)

Example: 152.3, 127.6, 133.1
155.02 to 207.59
187

Add Another Spectra

通过谱图数据进行检索

Filter by

- Commercial Availability
 - Available (3,236)
 - Not Available (5,335)
- Reaction Role
 - Product (6,738)
 - Reactant (2,855)
 - Reagent (115)
 - Catalyst (72)
 - Solvent (27)
- Reference Role
 - Adverse Effect (454)
 - Analytical Study (860)
 - Biological Study (3,310)
 - Combinatorial Study (125)
 - Formation (387)
 - View All
- Stereochemistry
- Number of Components
- Substance Class

Substances (8,571)

Sort: Relevance View Partial

References Reactions Suppliers

50-02-2
View Detail

C22H29FO5
Dexamethasone

97K References 276 Reactions 141 Suppliers

50-78-2
View Detail

C9H8O4
Aspirin

87K References 1,754 Reactions 110 Suppliers

51-21-8
View Detail

C4H3FN2O2
5-Fluorouracil

80K References 1,854 Reactions 156 Suppliers

56-75-7
View Detail

C11H12Cl2N2O5
(-)-Chloramphenicol

56-75-7
View Detail

C8H8O3
Vanillin

121-33-5
View Detail

98-92-0
View Detail

C6H6N2O
Nicotinamide

物质详情

Substance Detail (1 of 1)

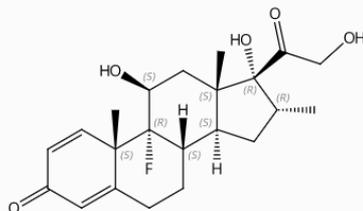
References (82K)

Reactions (412)

Suppliers (144)

CAS Registry Number

50-02-2



$C_{22}H_{29}FO_5$

Pregna-1,4-diene-3,20-dione, 9-fluoro-11,17,21-trihydroxy-16-methyl-, (11 β ,16 α)

Key Physical Properties	Value	Condition
Molecular Weight	392.46	-
Melting Point (Experimental)	262-264 °C	-
Boiling Point (Predicted)	568.2±50.0 °C	Press: 760 Torr
Density (Predicted)	1.32±0.1 g/cm ³	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	12.13±0.70	Most Acidic Temp: 25 °C

Experimental Properties | Spectra

Other Names and Identifiers

Experimental Properties

Experimental Spectra

Predicted Properties

Predicted Spectra

Bioactivity Indicators

Target Indicators

Regulatory Information

Additional Details

折叠菜单显示物质各类信息



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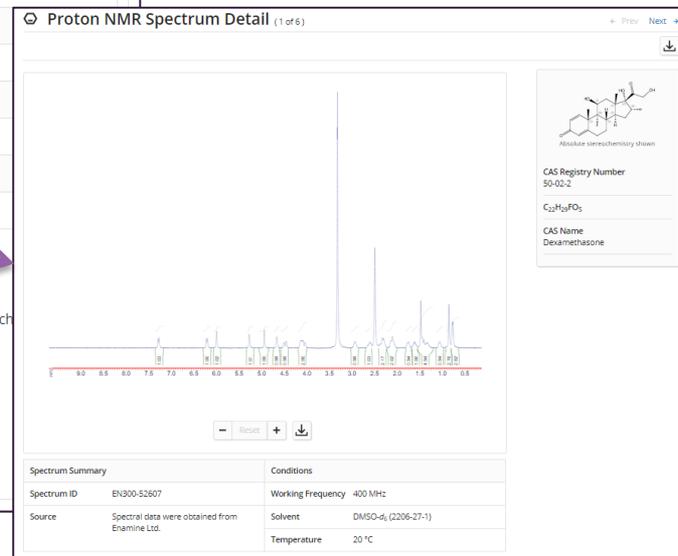
物质详情

Experimental Spectra

¹ H NMR	¹³ C NMR	Hetero NMR	IR	Mass	Raman	UV and Visible
Source						
View Proton NMR Spectrum	(1) ENAMINE					
View Proton NMR Spectrum	(1) ENAMINE					
View Proton NMR Spectrum	(2) AIST					
View Proton NMR Spectrum	(2) AIST					
View Proton NMR Spectrum	(3) ACD-A					
View Proton NMR Spectrum	(4) ACD					
Proton NMR Spectrum - 3 Sources	(5-7) CAS					

Sources

- (1) Spectral data were obtained from Enamine Ltd.
- (2) "Integrated Spectral Data Base System of Organic Compounds" data were obtained from the National Institute of Advanced Industrial Science and Tech
- (3) Sigma-Aldrich (Spectral data were obtained from Advanced Chemistry Development, Inc.)
- (4) Edmonds, John S.; Steroids, (2006), 71(1), 34-41, CAplus
- (5) Zhai, Ying Lei; Chinese Science Bulletin, (2009), 54(17), 2918-2924, CAplus
- (6) Zhang, Zheng; Journal of Controlled Release, (2006), 111(3), 263-270, CAplus
- (7) Zaccigna, M.; Journal of Drug Delivery Science and Technology, (2008), 18(3), 155-159, CAplus



物质检索—结构检索

Searching for...

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

Substances

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

Enter a query... Draw

Use [Advanced Search](#) for Molecular Formula, Substance Property, or Experimental Spectra

CAS Draw

Enter a CAS RN, SMILES or InChI

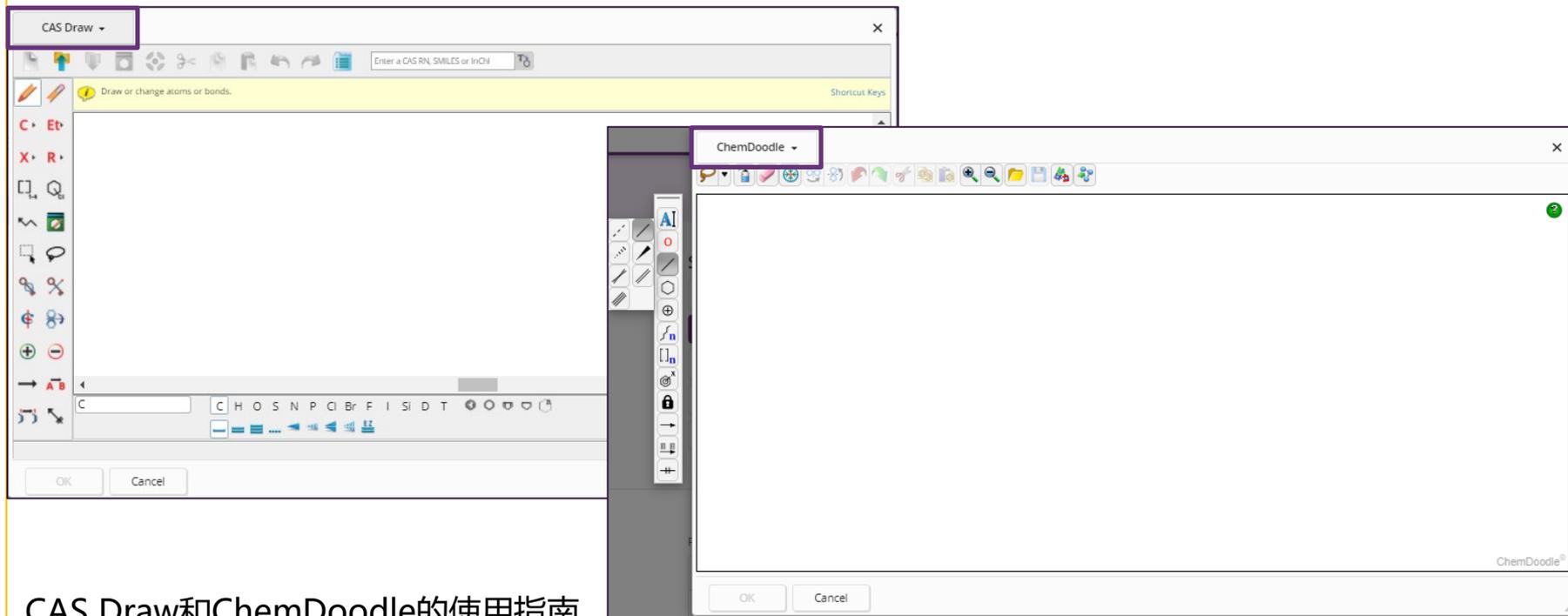
Draw or change atoms or bonds. Shortcut Keys

C • Et
X • R

C H O S N P Cl Br F I Si D T

OK Cancel

物质检索—结构检索



CAS Draw和ChemDoodle的使用指南

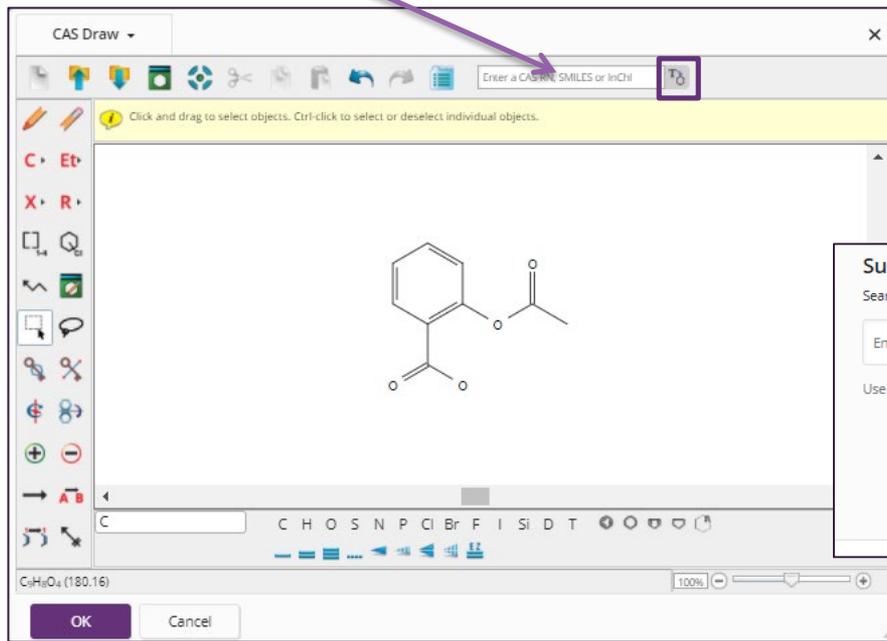
https://scifinder-n.cas.org/help/#t=Drawing_Search_Queries%2FDrawing_Structure_Queries.htm

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

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

物质检索—结构检索

CAS RN: 50-78-2



Substances

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

Enter a query...

Edit

Use [Advanced Search](#) for Molecular Formula, Substance Property, or Experimental Spectra

Edit Drawing Remove

Search Patent Markush

物质检索—结构检索

结构检索类别:

精确结构检索

亚结构检索

相似结构检索

物质筛选类别:

反应角色

立体化学

同位素

金属包含

实验物性数据

结构

.....

Structure Match

As Drawn (911)

Substructure (20K)

Similarity (15K)

Analyze Structure Precision

Filter by

Commercial Availability

Available (3,957)

Not Available (16K)

Reaction Role

Product (9,020)

Reactant (2,036)

Reagent (10)

Catalyst (20)

Solvent (3)

Reference Role

Adverse Effect (188)

Analytical Study (204)

Biological Study (6,491)

Combinatorial Study (6)

Formation (85)

View All

Stereochemistry

Number of Components

Substance Class

Isotopes

Metals

Molecular Weight

Experimental Property

Experimental Spectrum

Regulatory Information

Bioactivity Indicator

Target Indicator

Search Within Results

Substances (20,064)

Sort: Relevance View: Partial

References Reactions Suppliers

1 50-78-2 CC(=O)Oc1ccc(O)cc1
C₉H₈O₄
Aspirin
80K References 1,888 Reactions 113 Suppliers

2 5054-56-8 CC(=O)Oc1ccc(O)cc1
C₉H₈O₄
Benzoic acid, 2-(acetyloxy), ion(1-)
19 References 0 Reactions 3 Suppliers

3 89655-56-1 CC(=O)Oc1ccc(O)cc1
(C₉H₈O₄)
2-Acetylsalicylic acid homopolymer
16 References 0 Reactions 0 Suppliers

4 97781-16-3 CC(=O)Oc1ccc(O)cc1
C₉H₈D₄O₄
Benzoic-2,3,4,5-d₄ acid, 6-(acetyloxy)-
7 References 2 Reactions 23 Suppliers

5 59096-15-0 CC(=O)Oc1ccc(O)cc1
C₉H₈O₄
Benzoic acid, 2-(acetyl-1-¹⁴C-oxy)-
5 References 1 Reaction 1 Supplier

6 59096-14-9 CC(=O)Oc1ccc(O)cc1
C₉H₈O₄
Benzoic-carboxy-¹⁴C acid, 2-(acetyloxy)-
5 References 0 Reactions 3 Suppliers

7 921943-73-9 CC(=O)Oc1ccc(O)cc1
C₉H₈D₂O₄
2-(Acetyl-2,2-d₂-oxy)benzoic acid
4 References 0 Reactions 16 Suppliers

8 215935-30-1 CC(=O)Oc1ccc(O)cc1
C₉H₈D₂O₄
2-(Acetyl-2-d-oxy)benzoic acid
4 References 0 Reactions 0 Suppliers

9 229030-56-2 CC(=O)Oc1ccc(O)cc1
C₉H₈O₄
Benzoic acid, 2-(acetyl-1-¹³C-oxy)-
3 References 0 Reactions 1 Supplier

10 225243-55-0 CC(=O)Oc1ccc(O)cc1
C₉H₈O₄
Benzoic-carboxy-¹¹C acid, 2-(acetyloxy)-
4 References 0 Reactions 16 Suppliers

11 2357155-75-8 CC(=O)Oc1ccc(O)cc1
C₉H₈O₄
Benzoic acid, 2-(acetyl-2-¹³C-oxy)-
4 References 0 Reactions 1 Supplier

12 1350310-06-3 CC(=O)Oc1ccc(O)cc1
C₉H₈O₄
Benzoic acid, 2-(acetyl-2-¹³C-oxy)-
3 References 0 Reactions 1 Supplier

物质检索—结构检索

结构检索类别：

- 精确结构检索

获得被检索结构的盐、混合物、配合物、聚合物等，被检结构不能被取代

- 亚结构检索

包括精确结构检索结果，及被检索结构的修饰结构

- 相似结构检索

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

物质检索—物质筛选：结构

Search Within Results

Draw

Draw using cur

CAS Draw

Enter a CAS RN, SMILES or InChI

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

C1=CC=CC=C1

Search Within Results

Edit Drawing Remove

As Drawn

Substructure

Find

利用物质筛选工具
快速锁定目标物质

Substances (7)

Sort: Relevance View: Partial

References Reactions Suppliers

1 1257527-68-6

CC(=O)OCC1=CC=CC=C1

$C_{11}H_{10}O_4$
Benzoic acid, 2-(acetyloxy)-, 2-(1,3-cyclopentadien-1-yl)ethyl ester

1 Reference 3 Reactions 1 Supplier

2 1257527-69-7

CC(=O)OCC1=CC=CC=C1

$C_{17}H_{14}O_4$
Benzoic acid, 2-(acetyloxy)-, 3-(1,3-cyclopentadien-1-yl)propyl ester

1 Reference 3 Reactions 1 Supplier

3 1257527-70-0

CC(=O)OCC1=CC=CC=C1

$C_{18}H_{16}O_4$
Benzoic acid, 2-(acetyloxy)-, 4-(1,3-cyclopentadien-1-yl)butyl ester

1 Reference 3 Reactions 1 Supplier

4 226718-24-7

O=C1C=CC(O)=C1

Absolute stereochemistry shown, Rotation (-)

$C_{13}H_{10}O_6 \cdot 1/2 C_7H_6O_2$
Components: 2
6H, 12H, 18H-Tribenzo[*b,f*][1,5,9]trioxacyclododecin-6,12,18-trione, 1,7,13-trime...

1 Reference 1 Reaction 0 Suppliers

5 226718-12-3

O=C1C=CC(O)=C1

Absolute stereochemistry shown, Rotation (+)

$C_{13}H_{10}O_6 \cdot 1/2 C_7H_6O_2$
Components: 2
6H, 12H, 18H-Tribenzo[*b,f*][1,5,9]trioxacyclododecin-6,12,18-trione, 1,7,13-trime...

1 Reference 1 Reaction 0 Suppliers

6 226423-37-6

O=C1C=CC(Cl)=C1

$C_{33}H_{30}O_6 \cdot 1/2 C_7H_6O_2$
Components: 2
6H, 12H, 18H-Tribenzo[*b,f*][1,5,9]trioxacyclododecin-6,12,18-trione, 1,7,13-trime...

1 Reference 1 Reaction 0 Suppliers

7 2413763-69-4

C1=CC=CC=C1

$C_{27}H_{28}NO_7$

1 Reference 1 Reaction 0 Suppliers

物质检索—物质筛选: Substance Role

物质的反应角色

物质的文献角色

利用物质角色精准
获得相应的物质

Structure Match

- As Drawn (911)
- Substructure (20K)**
- Similarity (15K)

Analyze Structure Precision

Filter by

- Commercial Availability
- Reaction Role**
 - Product (9,020)
 - Reactant (2,036)
 - Reagent (10)
 - Catalyst (20)
 - Solvent (3)
- Reference Role
 - Adverse Effect (188)
 - Analytical Study (204)
 - Biological Study (6,491)
 - Combinatorial Study (6)
 - Formation (85)
 - [View All](#)
- Stereochemistry
- Number of Components

Substances (20,064) Sort: Relevance View: Partial

References Reactions Suppliers

1 50-78-2 CC(=O)Oc1ccc(O)cc1
 $C_9H_8O_4$
Aspirin
80K References 1,888 Reactions 113 Suppliers

2 5054-56-8 CC(=O)Oc1ccc(O)cc1
 $C_9H_7O_4$
Benzoic acid, 2-(acetyloxy)-, ion(1-)
19 References 0 Reactions 3 Suppliers

3 89655-56-1 CC(=O)Oc1ccc(O)cc1
 $(C_9H_8O_4)_x$
2-Acetylsalicylic acid homopolymer
16 References 0 Reactions 0 Suppliers

4 97781-16-3 CC(=O)Oc1ccc(O)c2c(O)c(O)c(O)c12
 $C_9H_4D_4O_4$
Benzoic-2,3,4,5-*d_4* acid, 6-(acetyloxy)-
7 References 2 Reactions 23 Suppliers

5 59096-15-0 CC(=O)Oc1ccc(O)c1
 $C_9H_8O_4$
Benzoic acid, 2-(acetyl-1-¹⁴C-oxy)-
5 References 1 Reaction 1 Supplier

6 59096-14-9 CC(=O)Oc1ccc(O)c1
 $C_9H_8O_4$
Benzoic-carboxy-¹⁴C acid, 2-(acetyloxy)-
5 References 0 Reactions 3 Suppliers

物质检索—物质筛选: Substance Role

利用物质反应角色获得
做过催化剂研究的物质

The screenshot displays a search results page for 'Substances' with 20 results. The left sidebar shows filters, with 'Catalyst (20)' selected under 'Filter by'. The main area shows a grid of substance cards, each with a chemical structure, name, formula, and statistics for references, reactions, and suppliers.

Substance ID	Chemical Name	Formula	References	Reactions	Suppliers
50-78-2	Aspirin	C ₉ H ₈ O ₄	80K	1,888	113
875584-96-6	2-Methylpropyl 2-(benzoyloxy)benzoate	C ₁₈ H ₁₄ O ₄	4	4	2
2093113-55-2	Benzoic acid, 2-(2,2-dimethyl-1-oxopropoxy)-3-methyl-, 2-methylpropyl ester	C ₁₇ H ₂₄ O ₄	2	2	0
1803201-02-6	Benzoic acid, 2-[(2-methylpropoxy)carbonyl]phenyl ester	C ₁₆ H ₁₈ O ₄	1	1	0
2093113-56-3	Benzoic acid, 2-(benzoyloxy)-3-methyl-, 2-methylpropyl ester	C ₁₈ H ₁₆ O ₄	2	2	0
23642-01-5	Tetradakis[μ-(2-(acetoxy)benzoato-κO×O)]dicopper	C ₁₆ H ₁₆ Cu ₄ O ₁₆	91	37	3
2245149-62-4		C ₂₄ H ₁₈ O ₁₄ Rh ₂	1	3	0
1416949-86-4	Benzoic acid, 2-(acetoxy)-, 1,1'-[1,4-butanediyl]bis(oxyethylene) ester	C ₁₈ H ₂₀ O ₆	1	2	0
2093113-57-4	Benzoic acid, 2-(benzoyloxy)-3,5-bis(1-methylethyl)-, 2-methylpropyl ester	C ₂₄ H ₂₈ O ₄	2	3	0



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物质检索—物质排序

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 (911)

Substructure (20K)

Similarity (15K)

Analyze Structure Precision

Filter by

Commercial Availability

Reaction Role

Product (9,020)

Reactant (2,036)

Reagent (10)

Catalyst (20)

Solvent (3)

Reference Role

Adverse Effect (2)

Analytical Study (2)

Biological Study (4)

Combinatorial Study (1)

Formation (1)

View All

Number of Components

Substance Class

Isotopes

Substances (20)

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

C₉H₈O₄
Aspirin

80K References 1,888 Reactions 113 Suppliers

2

875584-96-6

CC(C)OC(=O)C1=CC=C(C=C1)OC(=O)C2=CC=CC=C2

C₁₈H₁₈O₄
2-Methylpropyl 2-(benzoxy)benzoate

4 References 4 Reactions 2 Suppliers

4

1803201-02-6

CC(C)OC(=O)C1=CC=C(C=C1)OC(=O)C2=CC=C(C=C2)C3=CC=CC=C3

C₁₉H₂₀O₄
Benzoic acid, 2-[[[2-methylpropoxy]carbonyl]phenyl] ester

1 Reference 1 Reaction 0 Suppliers

5

2093113-56-3

CC(C)OC(=O)C1=CC=C(C=C1)OC(=O)C2=CC=C(C=C2)C3=CC=CC=C3

C₁₉H₂₀O₄
Benzoic acid, 2-[(benzoxy)-3-methyl-, 2-methylpropyl] ester

2 References 2 Reactions 0 Suppliers

6

23642-01-5

CC(C)OC(=O)C1=CC=C(C=C1)OC(=O)C2=CC=C(C=C2)C3=CC=CC=C3

C₃₆H₂₈Cu₂O₁₆
Tetrakis[μ-[2-(acetoxy)benzoato-κO:κO]]dicopper

91 References 37 Reactions 3 Suppliers



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提纲

- 美国化学文摘社简介
- SciFinder-n简介及检索方式
 - 文献检索
 - 物质检索
 - Markush检索
 - 反应检索
- 常见问题及解决

Markush检索

(19) 中华人民共和国国家知识产权局



(12) 发明专利申请



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A61P 25/28(2006.01)
A61P 37/02(2006.01)

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(51) Int. Cl.

007K 5/087(2006.01)
007K 5/083(2006.01)

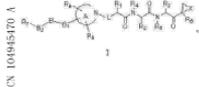
权利要求书3页 说明书24页 附图4页

(54) 发明名称

杂环构建的三肽环酰胺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酰胺类化合物,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羧酰胺、水解、在缩合剂作用下获得。本发明是小分子短肽类蛋白酶抑制剂。本发明化合物具有极强的蛋白酶抑制活性及细胞增殖抑制活性,是有前景的蛋白酶抑制剂。为癌症治疗药物的研究提供了新的思路。本发明化合物的合成所需原料易得,路线设计合理,反应条件温和,各步产率高,操作简便,适合工业化生产。具有下述式1的结构式:



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-基氨基羰基)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,在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-氨基吡啶(0.95g,10mmol)和三乙胺(5.7mL,40mmol)溶于15mL CH₂Cl₂后缓缓滴入上述反应液,室温反应6小时。反应液加30mL饱和食盐水稀释,分出有机层,水层CH₂Cl₂提取(15mL×3),合并有机层,无水硫酸钠干燥后减压除去溶剂,柱层析分离得白色固体2.3g,收率74%。m.p.: 134-136°C; ¹H NMR (500MHz, CDCl₃): δ = 9.55 (s, 1H, pyrazine-H), 8.35 (d, 1H, J=2.0Hz, pyrazine-H), 8.23 (s, 1H, pyrazine-H), 7.97 (s, 1H, NH), 4.20 (m, 2H, CH₂), 2.81 (m, 2H, CH₂), 2.48 (m, 1H, CH), 1.93 (d, 2H, J=12.5Hz, CH₂), 1.76 (m, 2H, CH₂), 1.47 (s, 9H, CH₃) ppm; ESI-MS: m/z = 307[M+H]⁺。

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

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

具体物质[Specific Substance]:

以具体化学结构陈述的特定物质, 会被分配CAS RN



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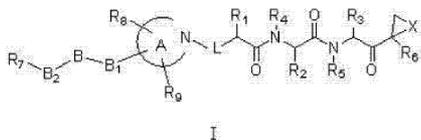
Markush检索

CN 104945470 A

权利要求书

1/3 页

1. 一种杂环构建的三肽环氧酮类化合物,具有下述结构通式 I:



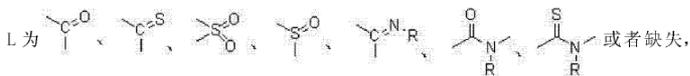
其中:

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

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)- 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

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

物质检索—检索的物质来自CAS Registry

该物质
不存在

Substances (46,805)

Structure Match

As Drawn (0)

Substructure (46K)

Similarity (21K)

Analyze Structure Precision

Filter by

Commercial Availability

- Available (206)
- Not Available (46K)

Reaction Role

- Product (19K)
- Reactant (3,721)
- Reagent (22)
- Catalyst (102)
- Solvent (1)

Reference Role

- Adverse Effect (91)
- Analytical Study (337)
- Biological Study (1,518)
- Combinatorial Study (9)

604800-58-0

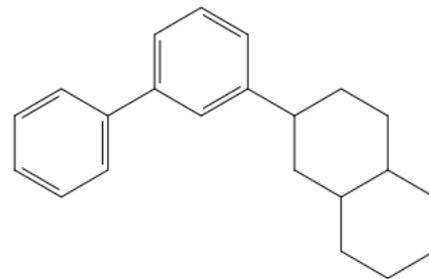
382151-38-4

79123-37-8

79123-36-7

79111-07-2

604811-78-1



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Markush检索—检索结果来自Marpat

SCI FINDERⁿ
A CAS SOLUTION

Substances ▾ Enter a query... [Edit] [Search] [Star] [Clock] [User]

Return to Home

Patent Markush Match

As Drawn (2) [Arrow]

Substructure (39) [Arrow]

Filter by

Patent Office

Germany (1)

Japan (1)

Patent Markush (2)

References ▾

Sort: Relevance ▾

[Download] [Email] [Save]

Search Patent Markush

DE102018001260

Patent claim 2

PATENTPAK ▾ Full Text ▾

236,237,239,240,242: opt. subst. by G3

2003261514

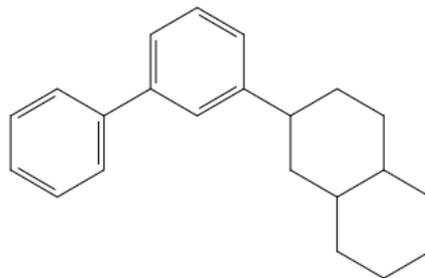
Patent claim 1

PATENTPAK ▾ Full Text ▾

831,833,835,837: opt. subst. by 1 or more G12

1015,1017,1019,1020: opt. subst. by 1 or more G12

匹配部分高亮显示，方便阅读



Markush检索：
帮助判定化合物的专利性，
避免化合物专利风险

提纲

- 美国化学文摘社简介
- SciFinder-n简介及检索方式
 - 文献检索
 - 物质检索
 - Markush检索
 - 反应检索
- 常见问题及解决

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号.....

- 常用获取方法

 - 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

一步由物质标识符或文献标识符获得反应信息

The screenshot displays the CAS Reactions database interface. On the left, a 'Filter by' sidebar includes categories such as Substance Role, Yield, Number of Steps, Non-Participating Functional Groups, Experimental Protocols, Reaction Type, Stereochemistry, Reagent, Catalyst, Solvent, Commercial Availability, Reaction Notes, and Search Within Results. The main area shows 'Reactions (2,742)' with a 'Group: By Scheme' and 'View: Expanded' dropdown. It lists three reaction schemes. Scheme 1 (51 Reactions) shows a chemical reaction with a yield of 100%. Below it are three reaction summaries with details on reagents, solvents, and authors. Scheme 2 (12 Reactions) shows another chemical reaction with a yield of 90-100%. Below it are two reaction summaries with details on reagents, solvents, and authors. The interface includes buttons for 'Suppliers', 'View Reaction Detail', 'Full Text', and 'PATENTPAK'.



反应检索

通过结构式进行检索

Search

All

Substances

Reactions

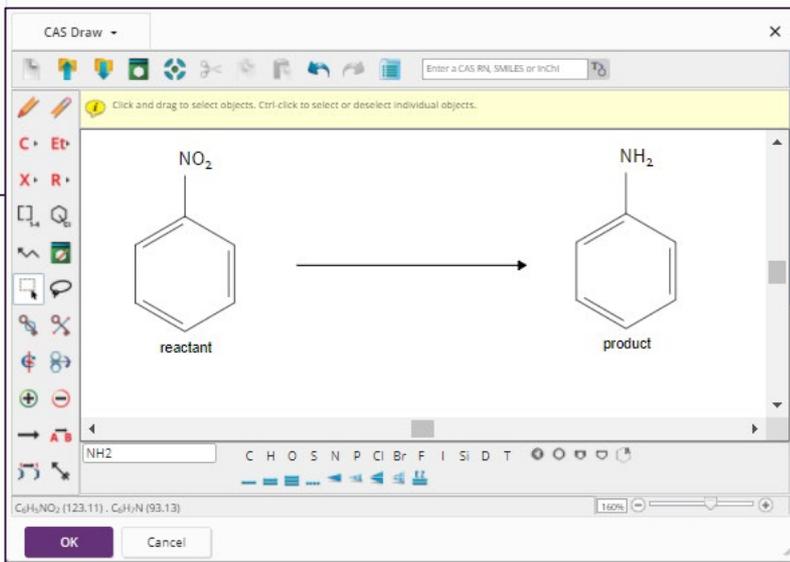
References

Suppliers

Search by Keyword, Substance Name, CAS RN, Patent Number, etc.

Enter a query...

Draw



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反应检索——结果集筛选

反应检索类别:

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

反应类型

立体化学

实验步骤

试剂、催化剂、溶剂、

.....

The screenshot displays a search interface for chemical reactions. On the left, a sidebar contains various filters: 'Structure Match' (As Drawn: 2,827, Substructure: 570K, Similarity: 191K), 'Filter by' (Yield: 90-100% (1,007), 80-89% (213), 70-79% (89), 50-69% (118), 30-49% (70)), 'Number of Steps', 'Non-Participating Functional Groups', 'Experimental Protocols' (MethodsNow: Synthesis (823), Experimental Procedure (223)), 'Reaction Type', 'Stereochemistry', 'Reagent', 'Catalyst', 'Solvent', 'Commercial Availability', 'Reaction Notes', 'Search Within Results', 'Source Reference' (Document Type, Language, Publication Year, Publication Name).

The main area shows 'Reactions (2,827)' with a 'References' dropdown and 'Save' options. It lists 'Scheme 1 (2 Reactions)' and 'Scheme 2 (2,057 Reactions)'. Each reaction entry includes a chemical structure, a 'Suppliers' button, and a 'Reaction Summary' section with details like 'Steps', 'Yield', and 'Full Text' links.

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: MethodsNow Synthesis

Carboxamidine (458)
View All

Experimental Protocols
 MethodsNow: Synthesis (6,038)
 Experimental Procedure (18K)

Reaction Type
Stereochemistry
Reagent
Catalyst
Solvent
Commercial Availability
Reaction Notes

Search Within Results

Document Type

Scheme 2 (2 Reactions)

Steps: 3

Suppliers (21) Suppliers (84) Suppliers (44)

Suppliers (94) Suppliers (83)

Reaction Summary

Reagents	Hydrazine hydrate (1:1) Potassium carbonate	Steps: 3
Catalysts	Nickel	
Solvents	1-Butanol Water Isopropanol	
Conditions	Multiple Steps - View Reaction Detail	

A Facile Total Synthesis for Large-Scale Production of Imatinib Base

By: Kompella, Amala; et al
Organic Process Research & Development (2012), 16(11), 1794-1804

Full Text

View Reaction Detail Experimental Protocols

查看反应详情

MethodsNow Synthesis:
经过标引和编辑的完整的反应操作信息

反应检索——结果集筛选: MethodsNow Synthesis

Reaction Detail (Scheme 2, Reaction 1 of 2) + Prev Next →

📄 ✉️ ★ Save

Suppliers (21) Suppliers (84) 82% Suppliers (80) Suppliers (105)

Suppliers (37) Suppliers (44) 86% Suppliers (94) Suppliers (83)

Steps: 3

Step 1 Step 2 Step 3 Alternative Steps (0)

Stage	Reagents	Catalysts	Solvents	Conditions
1	Potassium carbonate	-	Isopropanol	15 min, rt; 1.5 h, reflux

CAS Reaction Number: 31-365-CAS-5136393

Notes
commercial scale, by-products detected in ppm quantities, chloroform/solvent requires longer reaction time, optimized on base and stoichiometry, scalable, optimization study

Reference
A Facile Total Synthesis for Large-Scale Production of Imatinib Base
By: Kompella, Amala; et al
View All
Organic Process Research & Development (2012), 16(11), 1794-1804
Full Text

Company/Organization
Industrial Estate

MethodsNow Synthesis:

分类显示详尽信息, 方便操作

Experimental Protocols

MethodsNow™

Experimental Procedure

Products

o-Toluidine

Imatinib, Yield: 86%

4-Chloromethyl-N-[4-methyl-3-[[4-(pyridin-3-yl)pyrimidin-2-yl]amino]phenyl]benzamide

Reactants

Benzoyl chloride, 4-[(4-methyl-1-piperazinyl)methyl]-, hydrochloride (1:2)

6-Methyl-N-[4-(pyridin-3-yl)pyrimidin-2-yl]benzene-1,3-diamine

Reagents

Potassium carbonate

Solvents

Isopropanol

Procedure

- Charge N-(5-amino-2-methylphenyl)-4-(3-pyridinyl)-2-pyrimidineamine (37.5 kg; 135.377 mol), potassium carbonate (112.5 kg; 814.0376 mol) and isopropanol (675 L) into the reactor and stir at room temperature for 15 min.
- Charge 4-(4-methylpiperazinomethyl)benzoyl chloride dihydrochloride (65 kg, 200 mol) to the reaction mass and stir for 15 min at room temperature.
- Reflux the reaction for 1.5 hours.
- Bring the reaction mass to room temperature and filter.
- Wash the filtrate with isopropyl alcohol (37.5 L).
- Wash wet-filtered compound slurry with water (750 L).
- Dry the mixture at 55 °C to obtain 4-(4-methyl-piperazin-1-ylmethyl)-N-(4-methyl-3-[[4-(pyridin-2-ylamino]phenyl)-benzamide, o-toluidine and 4-chloromethyl-N-[4-methyl-3-(4-pyridin-3-yl-pyrimidin-2-ylamino)-phenyl]-benzamide.

Transformation

Acylation of Nitrogen Nucleophiles by Acyl/ Thioacyl/ Carbamoyl Halides and Analogs
Reduction of the C-N Bond/ Deamination

Scale

kilogram

Characterization Data

Imatinib

Proton NMR Spectrum

(AV 400 MHz, DMSO-*d*₆) δ 10.11 (s, 1H), 9.28 (s, 1H), 8.97 (s, 1H), 8.69 (d, 1H), 8.51 (d, 1H), 8.48 (d, 1H), 8.08 (s, 1H), 7.91 (d, 2H), 7.53-7.42 (m, 5H), 7.21 (d, 1H), 3.52 (s, 2H), 2.37 (bs, 8H), 2.22 (s, 3H), 2.14 (s, 3H)

Carbon-13 NMR

(AV 400 MHz, DMSO-*d*₆) δ 165.43, 161.75, 161.21 159.63, 151.49, 148.25, 142.20, 137.80, 137.17, 134.64, 133.80, 132.36, 130.22, 128.86, 127.68, 123.98, 117.18, 116.85, 107.73, 61.73, 54.74, 52.62, 45.79, 17.73 (24 signals)

IR Absorption

(KBr, cm⁻¹): 3424.22, 3280.01, 2966, 2928.44, 2795.98, 2695.71, 1647.76, 1575.16, 1451.83,

反应检索——结果集排序

Structure Match

As Drawn (2,700)

Substructure (551K)

Similarity (185K)

Filter by

- 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

Reactions (2,700)

References

Scheme 1 (2 Reactions)

1 Yield: 100%

Suppliers (6)

Supplier (1)

Group: By Scheme

- By Scheme
- By Document

View: Expanded

Save

Reaction Summary

Steps: 1 Yield: 100%

Synthesis of carbon-14-labeled flame retardants. Carbon-14-labeled-tetrabromophthalic anhydride and tetrabromo bisphenol-A

By: Susan, Alexander B.; et al
Journal of Labelled Compounds and Radiopharmaceuticals (1979), 16(4), 579-89

View Reaction Detail

Full Text

Reaction Summary

Steps: 1

Synthesis of ¹⁴C- and ³H-labeled 4-(4-nitrophenyl) aminophenylisothiocyanate (Go 9333 / CGP 4540; amoscantate)

By: Arjaneyulu, B.; et al
Journal of Labelled Compounds and Radiopharmaceuticals (1985), 22(4), 313-27

View Reaction Detail

Full Text

反应排序：
按类型排序
按文献排序

7

Pd immobilized on polymeric network containing imidazolium salt, cyclodextrin and carbon nanotubes: Efficient and recyclable catalyst for the hydrogenation of nitroarenes in aqueous media

By: Sadjadi, Samahe; Koohestani, Fatemeh
Journal of Molecular Liquids (2020), 301, 112414 | Language: English, Database: CAplus

Full Text

View 3 Related Reactions

Suppliers (76)

Suppliers (100)

Reaction Summary

Steps: 1 Yield: 100%

1.1 Reagents: Hydrogen
Catalysts: Palladium, Carbon, Silica, 2457185-07-6
Solvents: Water; 2 h, 1 bar, 60 °C

View Reaction Detail

按文献分类：来自同一篇文章的反应收在一条记录里

联合检索--反应式与关键词

The screenshot displays the CAS search interface. On the left, under 'Searching for...', there are navigation buttons for 'All', 'Substances', 'Reactions', 'References' (which is highlighted in purple), and 'Suppliers'. The main search area is titled 'References' and includes a search bar containing the text 'suzuki reaction'. Below the search bar, there is a note: 'Use Advanced Search for Author, Journal, or Organization'. To the right of the search bar, there are 'Edit' and search icons. Below the search bar, a chemical reaction drawing is shown, depicting a Suzuki-Miyaura cross-coupling reaction between a phenyl ring and a benzene ring. Below the drawing are 'Edit Drawing' and 'Remove' buttons.

文献检索框里输入关键词

结构编辑器中绘制反应

联合检索--反应式与关键词

The screenshot shows a search results page for 'Suzuki Reaction' with 4,556 references. The left sidebar includes filters for Structure Match (As Drawn: 4,556; Substructure: 86K), Document Type (Journal: 4,167; Patent: 3,43; Review: 34; Conference: 30; Dissertation: 7; Preprint: 9), Language (English: 4,098; Chinese: 2,29; Japanese: 79; Russian: 70; German: 29), and Publication Year (1939-2021). The main content area displays three search results:

- Result 1:** "Effect of Colloidal Nanocatalysis on the Metallic Nanoparticle Shape: The Suzuki Reaction" by Narayanan, Radha; El-Sayed, Mostafa A. (Langmuir 2005, 21(5), 2027-2033). Includes images of nanoparticles before and after a second cycle.
- Result 2:** "A novel Suzuki reaction system based on a supported palladium catalyst" by Mubofu, Egid B.; Clark, James H.; Macquarrie, Duncan J. (Green Chemistry 2001, 3(1), 23-25).
- Result 3:** "Ligand-Free Palladium Catalysis of the Suzuki Reaction in Water Using Microwave Heating" by Leadbeater, Nicholas E.; Marco, Maria (Organic Letters 2002, 4(17), 2978-2976).
- Result 4:** "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).

Each result includes a 'Full Text' button and filters for Substances, Reactions, Cited By, and Citation Map.

联合检索提高了检索速度



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反应检索—逆合成反应路线设计

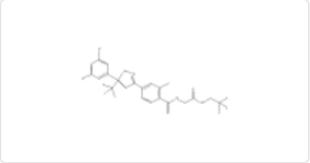
Search

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

Search by Keyword, Substance Name, CAS RN, Patent Number, etc.

Enter a query...

Edit  



Edit Drawing Remove

Create Retrosynthesis Plan

Set Plan Options

反应检索—逆合成反应路线设计

Retrosynthesis Powered by ChemPlanner®

Overview | Steps | Scoring

Step Key

- ⇒ Experimental
- ⇨ Predicted

Plan Options

Synthetic Depth: 3
Predicted Rules: Common
Break & Protect Bonds: No
[Edit Plan Options](#)

Plan Information

Estimated Yield: 76%
Overall Price: \$41,403.90
(USD per 100 grams)

Reset +

Suppliers (29) Max. Yield: 92%

Suppliers (41) Max. Yield: 91%

Suppliers (60) Max. Yield: 100%

Suppliers (8) Max. Yield: 91%

Suppliers (40)

Suppliers (58)

Suppliers (158)

Suppliers (24) Max. Yield: 85%

Suppliers (115)

Suppliers (63)

Retrosynthesis:

基于CASReact中的反应信息

路线显示每一步的底物与产物信息



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反应检索—逆合成反应路线设计

Retrosynthesis Powered by ChemPlanner®

Overview Steps Scoring

Download Email Save

A ⇒ B + C
Maximum Yield: 92%
Evidence (1)
Alternative Steps (37)

B ⇒ D
Maximum Yield: 96%
Evidence (1,990)
Alternative Steps

C ⇒ E + F
Maximum Yield: 85%
Evidence (19)
Alternative Steps (37)

D ⇒ G + H
Maximum Yield: 95%
Evidence (7,349)
Alternative Steps (27)

查看每一步反应的依据
挑选替换路线

Reset

反应检索—逆合成反应路线设计

Filter by

- Yield
- Number of Steps
- Non-Participating Functional Groups
 - Acyclic alkene (19)
 - Alkene (19)
 - Alkyl halide (19)
 - Halide (19)
 - Phenyl halide (19)
- Experimental Protocols
 - Experimental Procedure (14)
- Reaction Type
- Reagent
- Catalyst
- Solvent
- Commercial Availability
- Reaction Notes
- Search Within Results

Source Reference

- Document Type
- Language
- Publication Year
- Publication Name

Reactions (19)

Group: By Scheme View: Expanded

References

Scheme 1 (19 Reactions) Steps: 1 Yield: 80-85%

Suppliers (115) Suppliers (63) Suppliers (24)

Reaction Summary	Steps: 1 Yield: 85%	Boron-containing small molecules
1.1 Reagents: Potassium carbonate Catalysts: Dichlorobis(triphenylphosphine)palladium Solvents: Tetrahydrofuran, Water; 4 h, 70 °C		By: Akama, Tsutomu; et al United States, US20130131016 A1 2013-05-23
View Reaction Detail Experimental Protocols		PATENTPAK Full Text
Reaction Summary	Steps: 1 Yield: 83%	Preparation of isoxazoline compounds for combating invertebrate pests
1.1 Reagents: Potassium carbonate Solvents: Tetrahydrofuran, Water; rt → 0 °C 1.2 Catalysts: Dichlorobis(triphenylphosphine)palladium; 6 h, 0 °C → 90 °C		By: Koerber, Karsten; et al World Intellectual Property Organization, WO2010112545 A1 2010-10-07
View Reaction Detail Experimental Protocols		PATENTPAK Full Text
Reaction Summary	Steps: 1 Yield: 80%	Preparation of isoxazolines useful for the treatment of parasite infestation in animal
1.1 Reagents: Potassium carbonate Catalysts: Dichlorobis(triphenylphosphine)palladium Solvents: Tetrahydrofuran, Water; 6 h, 0 °C → 90 °C		By: McCooey, Seamus; et al United Kingdom, GB2523811 A 2015-09-09

反应依据



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反应检索—逆合成反应路线设计

Alternative Steps (37)

Filter by

- Alternative Step Type
 - Experimental (5)
 - Predicted (32)

1 of 37

Selected Experimental Step Evidence (19) Maximum Yield: 85%

2 of 37

Select Experimental Step Evidence (882) Maximum Yield: 56%

替换路线

反应检索—逆合成反应路线设计

Alternative Steps (37)

Filter by

- Alternative Step Type
 - Experimental (5)
 - Predicted (32)**

5 of 37

Select [Predicted Step](#) Evidence (6,431) Average Yield: 57%

6 of 37

Select [Predicted Step](#) Evidence (1,436) Average Yield: 60%

预测路线

反应检索—逆合成反应路线设计

Retrosynthesis Powered by ChemPlanner®

Overview Steps Scoring

↓ ✉ ★ Save

A ⇒ B + C
Maximum Yield: 92%
Evidence (1)
Alternative Steps (37)

B ⇒ D
Maximum Yield: 96%
Evidence (1,990)
Alternative Steps

C ⇒ E + F
Average Yield: 57%
Evidence (6,431)
Alternative Steps (37)

D ⇒ G + H
Maximum Yield: 95%
Evidence (7,349)
Alternative Steps (27)

Suppliers (29) Max. Yield: 92%

Suppliers (41) Max. Yield: 91%

Suppliers (60) Max. Yield: 100%

Suppliers (58)

Suppliers (8) Max. Yield: 91%

Suppliers (40)

Suppliers (24) Avg. Yield: 57%

Suppliers (24)

Suppliers (158)

Reset

预测路线

反应检索—新结构的逆合成反应路线设计

Searching for...

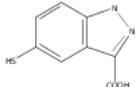
- All
- Substances
- Reactions**
- References
- Suppliers

Reactions

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

Enter a query...

Edit



Edit Drawing Remove

Create Retrosynthesis Plan

Set Plan Options

反应检索—新结构的逆合成反应路线设计

SciFinderⁿ
A CAS SOLUTION

Reactions ▾ Enter a query... Edit 🔍 ★ ⌚ 👤

⇒ Plan Options Powered by ChemPlanner[®]

Select Synthetic Depth

Synthetic depth restricts the number of steps generated in the plan. [Learn More.](#)

反应深度

1
 2
 3
 4

Break and Protect Bonds

You may select one bond to break in the first step of the plan. Any bonds you protect will not break, though their order may change. [Learn More.](#)

反应键的断裂与保护

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

Set Rules Supporting Predicted Reactions

Common rules are supported by many literature examples. Uncommon and Rare rules are supported by fewer examples, but may expose novel approaches. [Learn More.](#)

反应规则常见性

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

[Create Retrosynthesis Plan](#)

为新化合物预测合成路线设置参数

O=C(C=C1N=NC=C1)S

反应检索—新结构的逆合成反应路线设计

The screenshot displays the SciFinder Retrosynthesis interface. At the top, there is a search bar with the text "Reactions" and "Enter a query...". Below this, the "Retrosynthesis" section is active, showing a reaction pathway. The pathway starts with structure A (a complex heterocyclic molecule), which is converted to structure B (a simpler aromatic amine), and then to structure C (a substituted benzene ring with an amino group and a thiol group). Structure D is also shown as a precursor. The average yield for the pathway is 62%. On the left, a "Scoring" sidebar allows users to adjust various parameters: Complexity Reduction, Convergence, Evidence, Cost, Yield, and Atom Efficiency. Each parameter has a slider and a radio button. A "Suppliers (76)" button is visible next to structure C. The interface is powered by ChemPlanner.

调整预测合成路线参数：
原料结构相对于产物结构的复杂性；
前体数量；
预测路线支持的文献量；
产率；
原子转化经济性。

参数设置级别：
Off、Low、Medium、High

提纲

- 美国化学文摘社简介
- SciFinder-n简介及检索方式
 - 文献检索
 - 物质检索
 - Markush检索
 - 反应检索
- 常见问题及解决

SciFinder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SciFinder数据库说明页, 按照提示进行注册

如何获取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.cas.org>即可访问SciFinder数据库。

SciFinder使用注意事项

- 一人注册一个帐号，在校内完成注册
- 实名注册，需提供真实姓名信息（中文名用汉语拼音全拼）
- 严禁过量下载（以电子形式存储不超过5,000条记录）
- 严禁账号分享
- 严禁将账号用于非学术研究

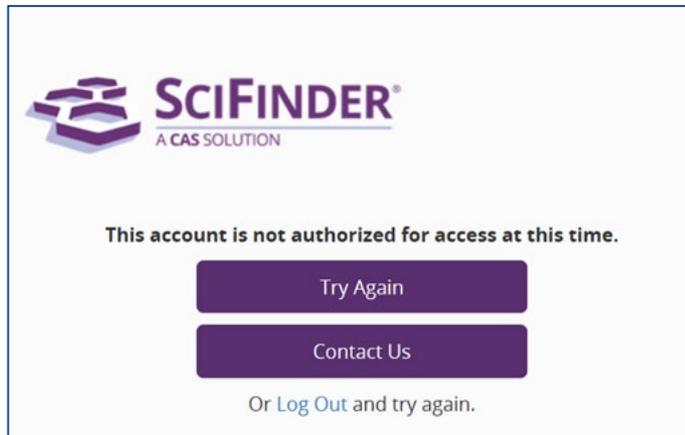
SciFinder常见问题

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，且在校园网内，请联系图书馆或china@acs-i.org

SciFinder常见问题



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

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