

# CAS SciFinder

# 全程助力医药科学研究

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ACS  
International



A division of the  
American Chemical Society

# 大纲

- **CAS及CAS SciFinder介绍**
- **文献相关信息的获取策略**
  - 文献检索方法
  - 文献结果排序、筛选和详情
  - 如何高效阅读专利文献详情(CAS PatentPak)
- **物质相关信息的获取策略**
  - 常见的物质检索方法
  - 物质结果排序、筛选和详情
- **反应相关信息的获取策略**
  - 反应的获取方法
  - 反应结果排序、筛选和详情
  - 如何高效获取反应详情 (Synthetic Methods)
- **分析相关信息的获取 (CAS Analytical Methods)**



# 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

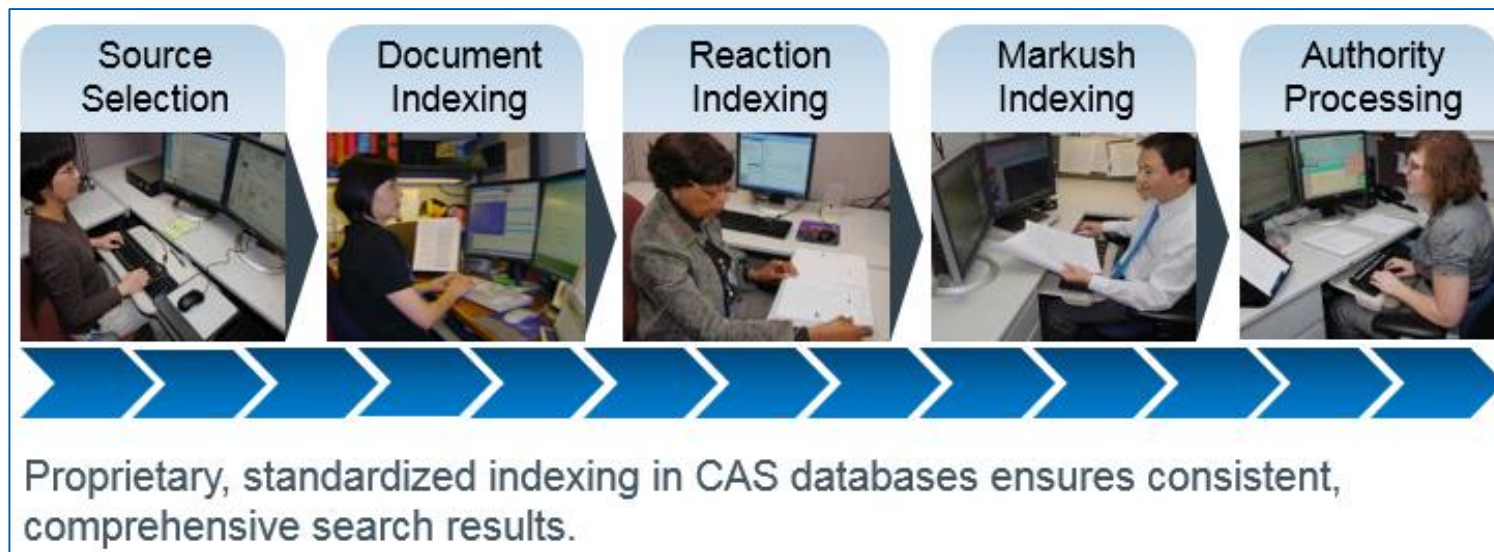
**64**  
patent offices  
worldwide



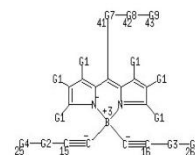
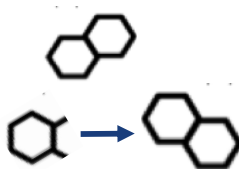
# CAS SciFinder覆盖的学科

- 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



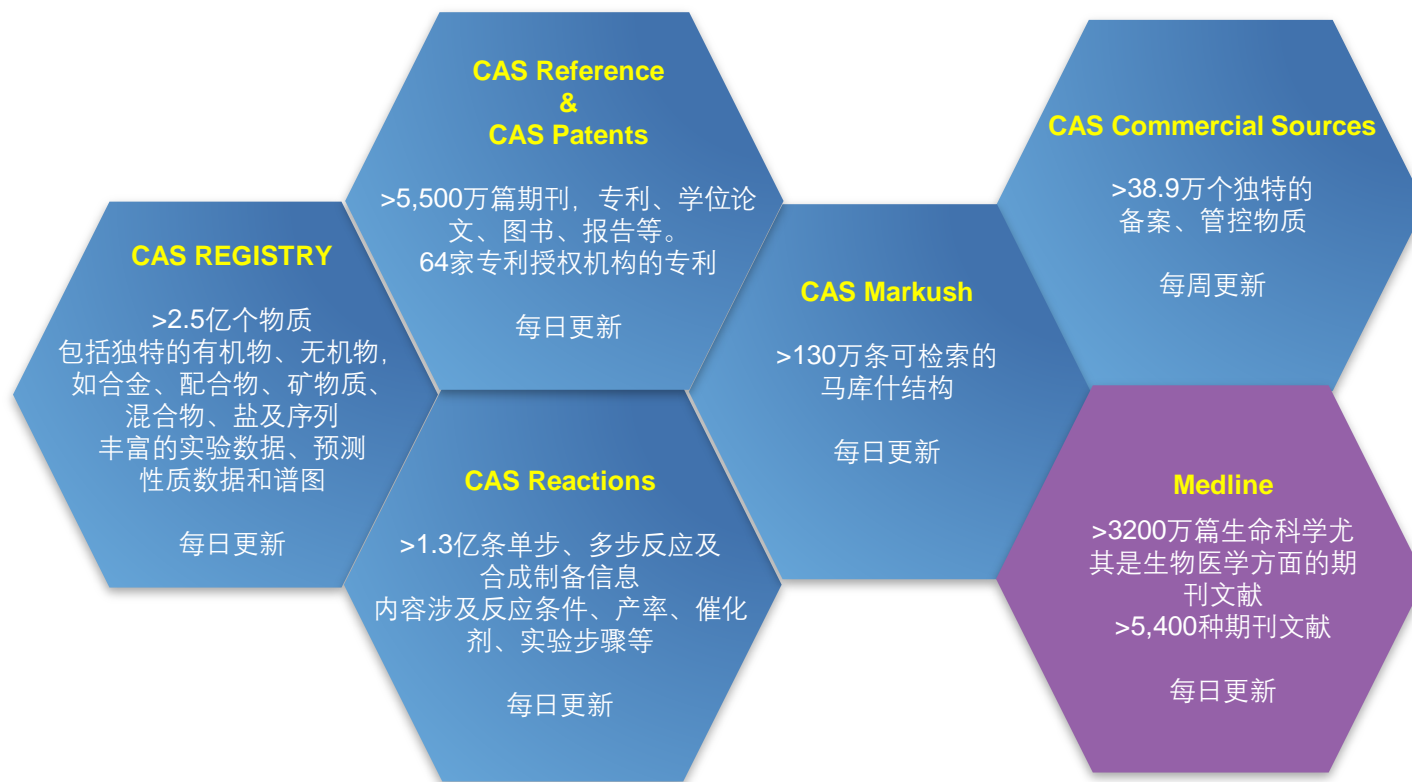
1990  
Smith, M.  
anthracene



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 SciFinder



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

# CAS解决方案与服务

DISCOVERY



## CAS SciFinder Discovery Platform™

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

INTELLECTUAL  
PROPERTY



## STN IP Protection Suite™

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

CUSTOM  
SOLUTIONS



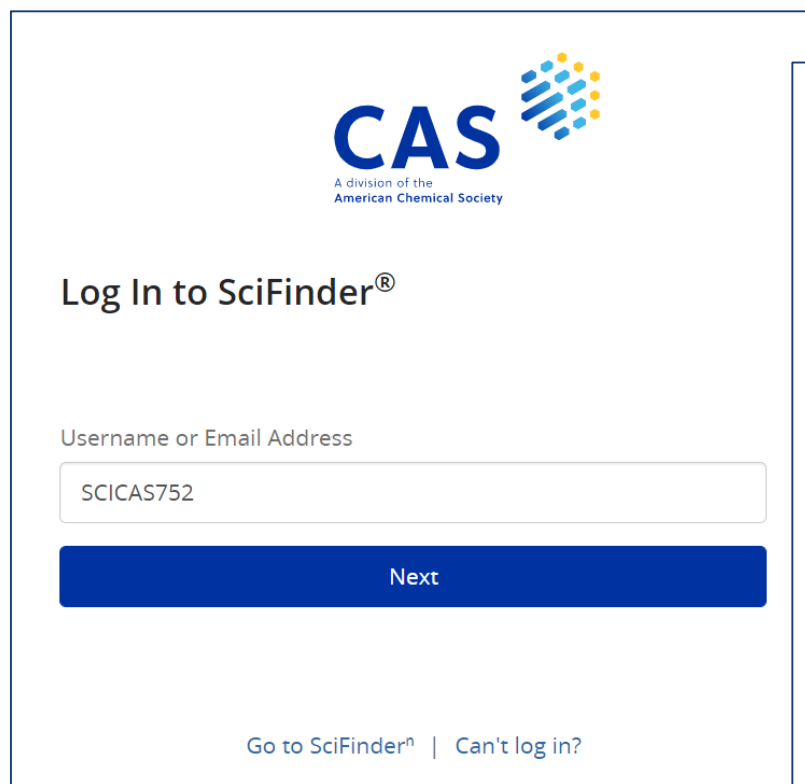
## CAS Custom Services<sup>SM</sup>

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

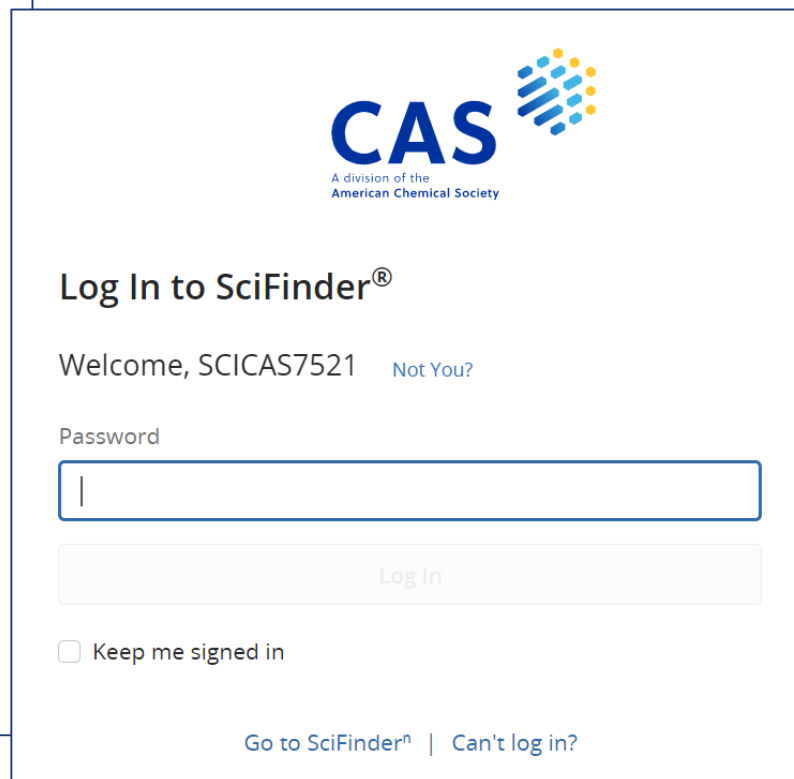


# CAS SciFinder登录网址

<https://SciFinder.cas.org>



The screenshot shows the initial login page for CAS SciFinder. At the top left is the CAS logo with the text "A division of the American Chemical Society". Below the logo is the heading "Log In to SciFinder®". There is a text input field labeled "Username or Email Address" containing the text "SCICAS752". Below the input field is a blue button labeled "Next". At the bottom of the page, there are two links: "Go to SciFinder<sup>n</sup>" and "Can't log in?".



The screenshot shows the next step of the login process. The CAS logo and heading "Log In to SciFinder®" are at the top. Below the heading, it says "Welcome, SCICAS7521" followed by a link "Not You?". There is a text input field labeled "Password" which is currently empty. Below the password field is a grey button labeled "Log In". At the bottom left, there is a checkbox labeled "Keep me signed in". At the bottom center, there are two links: "Go to SciFinder<sup>n</sup>" and "Can't log in?".

每个用户必须注册后才能使用

# CAS SciFinder主界面

The screenshot shows the CAS SciFinder main interface. At the top, there is a navigation bar with the SciFinder logo, a '工具栏' (Toolbar) annotation, and user options like 'Preferences', 'SciFinder Help', and 'Sign Out'. Below this is a secondary navigation bar with 'Explore', 'Saved Searches', and 'SciPlanner'. The main content area is titled 'REFERENCES: RESEARCH TOPIC' and features a search input field with examples like 'The effect of antibiotic residues on dairy products' and a 'Search' button. On the left, a sidebar lists search categories: 'REFERENCES' (Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, Tags), 'SUBSTANCES' (Chemical Structure, Markush, Molecular Formula, Property, Substance Identifier), and 'REACTIONS' (Reaction Structure). Annotations on the left point to these categories: '文献检索' (Literature Search) for REFERENCES, '物质检索' (Substance Search) for SUBSTANCES, and '反应检索' (Reaction Search) for REACTIONS. On the right, a 'SAVED ANSWER SETS' panel lists various saved search results, with an annotation '已保存的结果集' (Saved Results Set) pointing to it. Below that is a 'KEEP ME POSTED' section with an annotation '定题追踪' (Topic Tracking).

# 大纲

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  - 文献检索方法
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- 物质相关信息的获取策略
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  - 反应的获取方法
  - 反应结果排序、筛选和详情
  - 如何高效获取反应详情 (Synthetic Methods)
- 分析相关信息的获取 (CAS Analytical Methods)



# CAS SciFinder检索--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

主题检索：老药新用治疗COVID-19

检索式：drug repurposing in COVID-19

The screenshot displays the SciFinder search interface. At the top, there is a navigation bar with 'CAS Solutions' and the SciFinder logo. Below this is a yellow banner with the text 'SciFinder<sup>n</sup> is here! Learn more about the power of n. Par'. The main navigation area includes 'Explore', 'Saved Searches', and 'SciPlanner'. The search topic is 'Research Topic "drug repurposing in COVID-19"'. On the left, there is a sidebar with 'REFERENCES' and 'SUBSTANCES' sections. The 'REFERENCES' section lists various search criteria: Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, and Tags. The main search area shows the search term 'drug repurposing in COVID-19' in a text box, with 'Examples:' and 'The effect of antibiotic residues on dairy products' and 'Photocyanati' listed below. A blue 'Search' button is at the bottom. A callout box highlights the search term with the text '关键词之间用介词连接：in, with, of...'.

关键词之间用介词连接：in, with, of...

# 主题检索的候选项

Select All Deselect All

0 of 9 Research Topic Candidates Selected

	References
<input type="checkbox"/> 80 references were found containing "drug repurposing in COVID-19" as entered.	80
<input type="checkbox"/> 955 references were found containing the two concepts "drug repurposing" and "COVID 19" closely associated with one another.	955
<input type="checkbox"/> 1633 references were found where the two concepts "drug repurposing" and "COVID 19" were present anywhere in the reference.	1633
<input type="checkbox"/> 25118 references were found containing at least two of the concepts "drug", "repurposing", "COVID" or "19" closely associated with one another.	25118
<input type="checkbox"/> 282603 references were found where at least two of the concepts "drug", "repurposing", "COVID" or "19" were present anywhere in the reference.	282603
<input type="checkbox"/> 8049 references were found containing the concept "drug repurposing".	8049
<input type="checkbox"/> 9339226 references were found containing either the concept "drug" or the concept "repurposing".	9339226
<input type="checkbox"/> 116406 references were found containing the concept "COVID 19".	116406
<input type="checkbox"/> 1980199 references were found containing either the concept "COVID" or the concept "19".	1980199

Get References

“Concepts”表示对主题词做了同义词的扩展；

“Closely associated with one another”表示同时出现在一个句子中；

“were present anywhere in the reference”表示同时出现在一篇文献中；

# 文献结果集的排序--Citing Reference

Explore Saved Searches SciPlanner Save Print Export

Research Topic "drug repurposing in COVID-19" 文献筛选工具

REFERENCES Get Substances Reactions Citations Tools

Create Keep Me Posted Alert Send to SciPlanner

Analyze Refine Categorize

Analyze by: Author Name

Zheng Wei	20
Shen Min	18
Chen Catherine Z	17
Shinn Paul	17
Xu Miao	14
Guo Hui	12
Cheng Feixiong	11
Hall Matthew D	11
Itkin Zina	11

Sort by: Citing References

1. **Epidemiology and clinical therapies on coronavirus disease 2019 (COVID-19) outbreak - an update on the status**  
By Guo Yan-Rong; Tan Yuan-Yang; Chen Shou-Deng; Jin Hong-Jun; Yan Yan; Cao Qing-Dong; Hong Zhong-Si; Tan Kai-Sen; Wang De-Yun; Yan Yan  
From Military Medical Research (2020), 7(1), 11. | Language: English, Database: MEDLINE  
An acute respiratory disease, caused by a novel coronavirus (previously known as 2019-nCoV), the coronavirus disease 2019 (COVID-19) has spread throughout China and received worldwide attention. On 30 January 2020, World Health Organization declared COVID-19 epidemic as a public health emergency of international concern. The emergence of SARS-CoV-2, since the severe acute respiratory syndrome coronavirus (SARS-CoV) in 2002, marked the third introduction of a highly pathogenic and large-scale ...

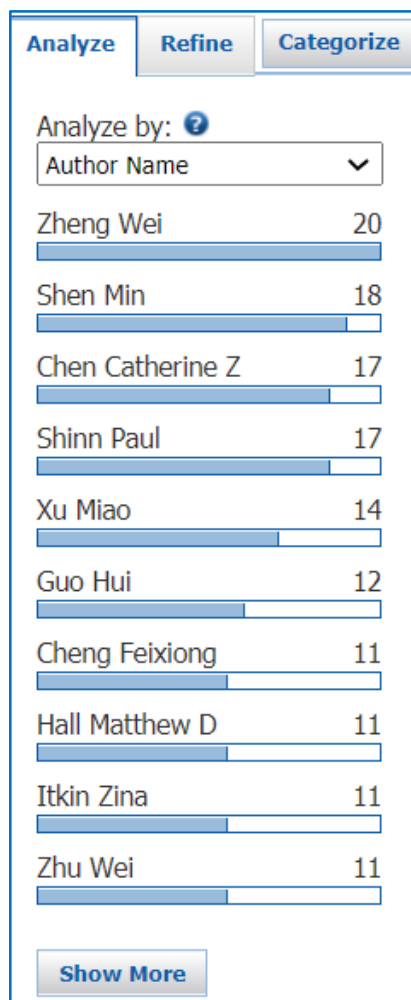
2. **Clinical and biochemical indexes from 2019-nCoV infected patients linked to viral loads and lung injury**  
By Liu Yingxia; Yang Yang; Wang Fuxiang; Yuan Jing; Wang Zhaoqin; Li Jinxiu; Li Jianming; Feng Cheng; Zhang Zheng; Wang Lifei; et al  
From Science China. Life sciences (2020), 63(3), 364-374. | Language: English, Database: MEDLINE  
The outbreak of the 2019-nCoV infection began in December 2019 in Wuhan, Hubei province, and rapidly spread to many provinces in China as well as other countries. Here we report the epidemiological, clinical, laboratory, and radiological characteristics, as well as potential biomarkers for predicting disease severity in 2019-nCoV-infected patients in Shenzhen, China. All 12 cases of the 2019-nCoV-infected patients developed pneumonia and half of them developed acute respiratory distress syndrome (ARDS). The most common laboratory abnormalities were hypoalbuminemia, lymphopenia, decreased pe...

3. **A SARS-CoV-2 protein interaction map reveals targets for drug repurposing**  
By Gordon David E; Jang Gwendolyn M; Bouhaddou Mehdi; Xu Jiewei; Obernier Kirsten; Guo Jeffrey Z; Swaney Danielle L; Tummino Tia A; Huttenhain Ruth; Kaake Robyn M; et al

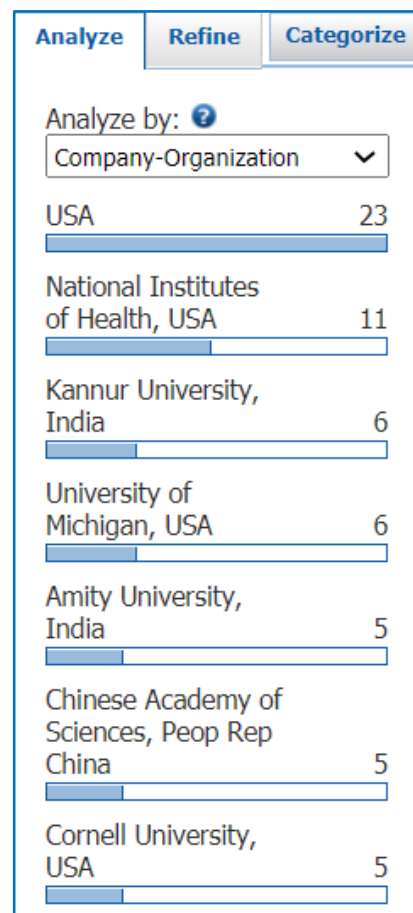
Citing Reference: 帮助找到最重要的文献

# 文献结果集的筛选--Analyze

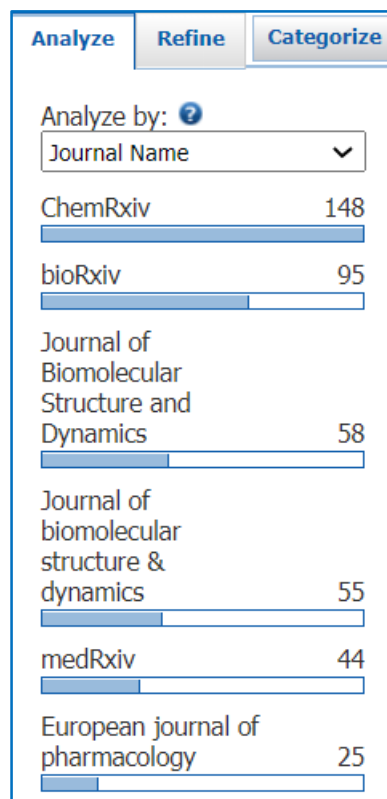
本领域研究人员



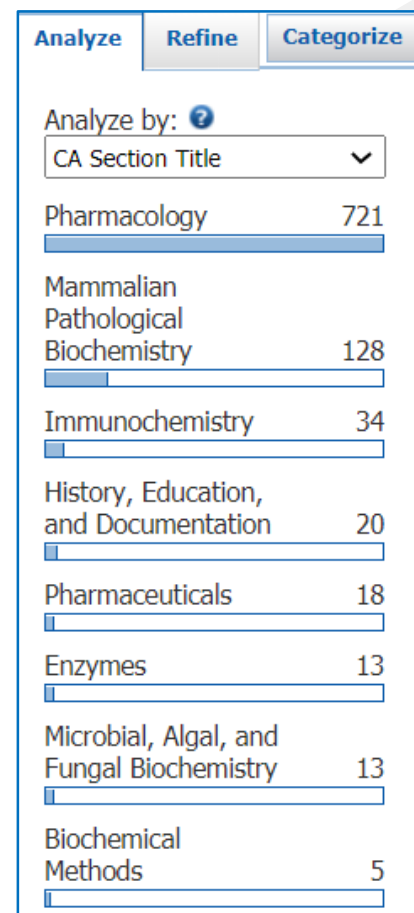
本领域研究机构、  
合作伙伴、竞争对手



期刊

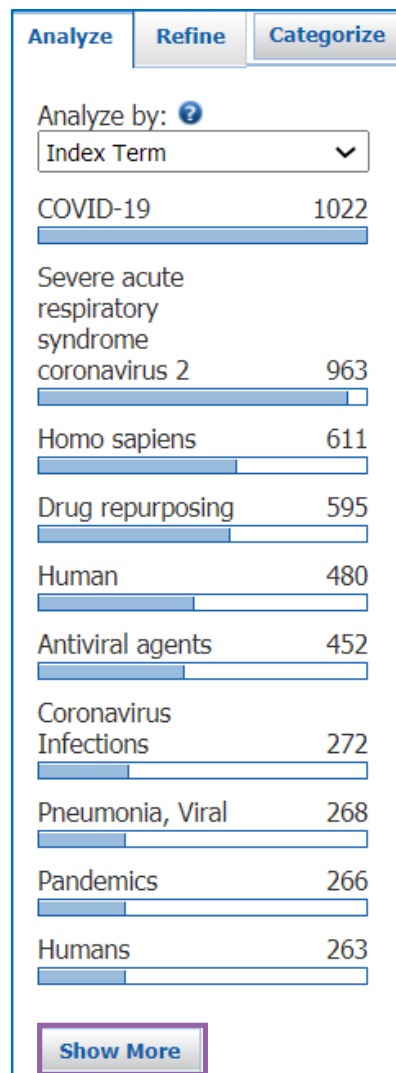


涉及学科领域



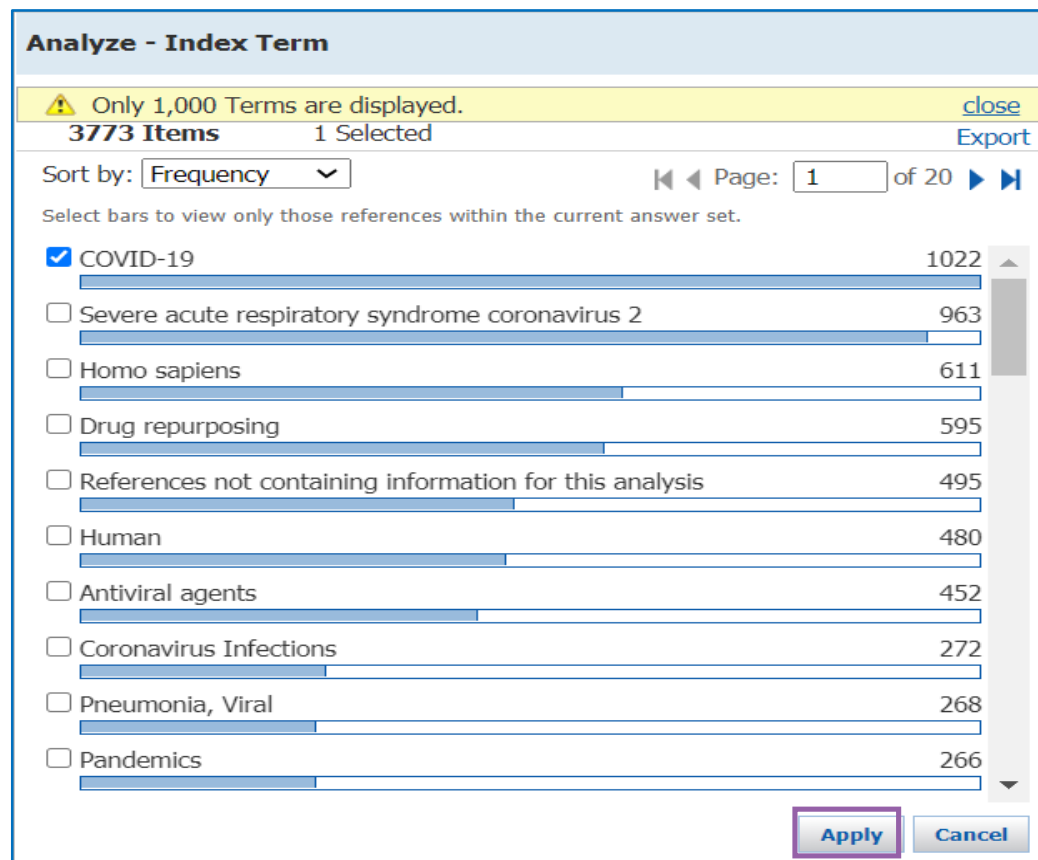


# 文献结果集的筛选--Analyze



Index Term:

帮助用户了解涉及到的重要技术术语，并修正检索词



选择感兴趣的内容，点击Apply

# 文献结果集的筛选--Refine

Analyze Refine Categorize

Refine by: ?

- Research Topic
- Author
- Company Name
- Document Type
- Publication Year
- Language
- Database

Document Type(s)

- Biography
- Book
- Clinical Trial
- Commentary
- Conference
- Dissertation
- Editorial
- Historical
- Journal
- Letter
- Patent
- Preprint
- Report
- Review

Refine

Get Substances Get Reactions Get Related Citations Tools

Sort by: Accession Number

0 of 481 References Selected

1. **Therapeutic strategies in an outbreak scenario to treat the novel coronavirus originating in Wuhan, China [version 2; peer review: 2 approved]**  
Quick View Other Sources  
By Kruse, Robert L.  
From F1000Research (2020), 9, 72. | Language: English, Database: CAPLUS  
A review. A novel coronavirus (2019-nCoV) originating in Wuhan, China presents a potential respiratory viral pandemic to the world population. Current efforts are focused on containment individuals. Ultimately, the outbreak could be controlled with a protective vaccine to prevent 2019-nCoV infection. While vaccine research should be pursued intensely, there exists today no t upon infection, despite an urgent need to find options to help these patients and preclude potential death. Herein, I review the potential options to treat 2019-nCoV...
2. **ACE2 as a potential therapeutic target for pandemic COVID-19**  
Quick View Other Sources  
By Chatterjee, Bhaswati; Thakur, Suman S.  
From RSC Advances (2020), 10(65), 39808-39813. | Language: English, Database: CAPLUS  
A review. SARS-CoV-2 virus invades the host through angiotensin-converting enzyme 2 (ACE2) receptors by decreasing the ACE2 expression of the host. This disturbs the dynamic equil. betw axis and ACE2/Ang (1-7)/Mas receptor axis. Therefore, the clin. approved **drugs** belonging to (i) angiotensin converting enzyme (ACE) inhibitors such as captopril, and enalaprilat, (ii) ang (ARBs) such as losartan, candesartan, olmesartan, azilsartan, irbesartan, and telmisartan and (iii) the combination of ACE inhibitors and ARBs such as losartan with lisinopri...
3. **Tutankhamun's Antimalarial Drug for Covid-19**  
Quick View Other Sources  
By Sommer, Andrei P.; Forsterling, Horst-Dieter; Sommer, Katlin E.  
From Drug Research (Stuttgart, Germany) (2020), Ahead of Print. | Language: English, Database: CAPLUS  
A review. **Drug** repositioning is a strategy that identifies new uses of approved **drugs** to treat conditions different from their original purpose. Current efforts to treat **Covid-19** are based **drugs** used in patients infected with SARS-CoV-2 were antimalarial **drugs**. It is their mechanism of action, i.e., rise in endosomal pH, which recommends them against the new coronaviru effects, the study of their antiviral activity provides valuable hints for the choice and design of **drugs** against SARS-CoV-2. One prominent **drug** candidate is thymoquinone...
4. **COVID-19 antibody therapeutics tracker: a global online database of antibody therapeutics for the prevention and treatment of COVID-19**  
Quick View Other Sources

Refine: 帮助用户迅速获得需要的文献

# 文献结果集的筛选--Categorize

学科领域  
主分类

学科领域  
副分类

Index Term

选中的Index Term

**Categorize** ?

1. Select a heading and category.      2. Select index terms of interest.

Category Heading	Category	Index Terms	Selected Terms
All	<b>Substances in medicine (2530)</b>	Page: 1 of 26 Select All   Deselect All	Click 'x' to remove the category from 'Selected Terms'
General chemistry	Medicine (976)	<input checked="" type="checkbox"/> Hydroxychloroquine 152	<input checked="" type="checkbox"/> Biotechnology > Substances in medicine (13 Terms)
<b>Biotechnology</b>	Agriculture (66)	<input checked="" type="checkbox"/> Chloroquine 124	<input checked="" type="checkbox"/> 羟氯喹
Biology	Substances in adverse effects (118)	<input checked="" type="checkbox"/> Remdesivir 109	<input checked="" type="checkbox"/> 氯喹
Genetics & protein chemistry	Toxicology & forensics (27)	<input checked="" type="checkbox"/> Lopinavir 99	<input checked="" type="checkbox"/> 瑞德西韦
Physical chemistry	Food (30)	<input checked="" type="checkbox"/> Ritonavir 83	<input checked="" type="checkbox"/> 洛匹那韦
Polymer chemistry	Substances in biological uses (13)	<input checked="" type="checkbox"/> Favipiravir 54	<input checked="" type="checkbox"/> 利托那韦
Technology		<input checked="" type="checkbox"/> Saquinavir 45	<input checked="" type="checkbox"/> 法匹那韦
Analytical chemistry		<input checked="" type="checkbox"/> Nelfinavir 42	<input checked="" type="checkbox"/> 沙喹那韦
Synthetic chemistry		<input checked="" type="checkbox"/> Indinavir 38	<input checked="" type="checkbox"/> 奈非那韦
Environmental chemistry		<input checked="" type="checkbox"/> Darunavir 36	
Catalysis		<input checked="" type="checkbox"/> Ivermectin 36	
		<input checked="" type="checkbox"/> Ribavirin 34	
		<input type="checkbox"/> Azithromycin 33	
		<input type="checkbox"/> Tocilizumab 33	
		<input type="checkbox"/> Simeprevir 28	
		<input type="checkbox"/> Lopinavir/ritonavir 27	

Biotechnology > Substances in medicine > 13 Index Term(s) Selected

OK   Cancel

Categorize学科分类功能，基于Index Term，根据大学科方向对文献进行自动分类。

# 药剂学文献信息检索策略

- Step 1: 由结构信息获取文献
- Step 2: 通过Catagorize系统分类功能筛选药剂学文献

**Categorize** ?

1. Select a heading and category.      2. Select index terms of interest.

Category Heading	Category	Index Terms	Selected Terms
All	Substances in medicine (16665)	Page: 1 of 26 Select All   Deselect All	Click 'X' to remove the category from 'Selected Terms'
General chemistry			
<b>Biotechnology</b>	<b>Medicine (2522)</b>	<input checked="" type="checkbox"/> Pharmaceutical tablets 223	<input checked="" type="checkbox"/> Biotechnology > Medicine (3 Terms)
Physical chemistry	Substances in adverse effects (3264)	<input type="checkbox"/> Anticoagulants 173	
Biology	Agriculture (249)	<input type="checkbox"/> Combination chemotherapy	
Genetics & protein chemistry	Food (107)	<input checked="" type="checkbox"/> Drug delivery systems 108	
Synthetic chemistry	Substances in biological uses (342)	<input type="checkbox"/> Polyethylene glycol 103	
Analytical chemistry	Toxicology & forensics (59)	<input type="checkbox"/> Hydroxypropyl cellulose 101	
Technology	Substances in food chemistry (40)	<input type="checkbox"/> D-Mannitol 91	
Polymer chemistry	Substances in agriculture (20)	<input type="checkbox"/> Ethanol 80	
Environmental chemistry		<input type="checkbox"/> Simvastatin 79	
Catalysis		<input type="checkbox"/> Ticlopidine 79	
		<input type="checkbox"/> Cardiovascular agents 77	
		<input type="checkbox"/> Oral drug delivery systems 76	
		<input checked="" type="checkbox"/> Pharmaceutical capsules 76	

Biotechnology > Medicine > 3 Index Term(s) Selected

OK   Cancel



# 药代动力学文献信息检索策略

- Step 1: 由结构信息获取文献
- Step 2: 通过Catagorize系统分类功能筛选药代动力学文献

**Categorize** ⓘ

1. Select a heading and category.      2. Select index terms of interest.

Category Heading	Category	Index Terms	Selected Terms
All	Substances in biology (5344)	◀ Page: 1 of 2 ▶ Select All   Deselect All	Click 'x' to remove the category from 'Selected Terms'
General chemistry	Substances in adverse effects (3410)	<input type="checkbox"/> Platelet aggregation 127	✘ Biology > Processes & systems (2 Terms)
Biotechnology	Animal pathology (864)	<input type="checkbox"/> Genetic polymorphism 37	
Physical chemistry	Immunology (332)	<input checked="" type="checkbox"/> Drug bioavailability 35	
<b>Biology</b>	Anatomy (241)	<input type="checkbox"/> Aging, animal 26	
Genetics & protein chemistry	Endocrinology (257)	<input checked="" type="checkbox"/> Drug metabolism 23	
Synthetic chemistry	<b>Processes &amp; systems (179)</b>	<input type="checkbox"/> Blood coagulation 20	
Analytical chemistry		<input type="checkbox"/> Drug targets 16	
Technology		<input type="checkbox"/> Aging, animal, elderly 14	
Polymer chemistry		<input type="checkbox"/> Drug resistance 13	
Environmental chemistry		<input type="checkbox"/> Signal transduction 13	
Catalysis		<input type="checkbox"/> Platelet activation 12	
		<input type="checkbox"/> Single nucleotide polymorphism 12	
		<input type="checkbox"/> Circulation 11	
		<input type="checkbox"/> Death 10	
		<input type="checkbox"/> Angiogenesis 9	

Biology > Processes & systems > 2 Index Term(s) Selected

OK   Cancel

# 药理学文献信息检索策略

Step 1: 由结构信息获取文献

Step 2: 选择analyze, CA section title, Pharmacology, 点击keep analysis

The screenshot displays the SciFinder search results page. At the top, there are navigation tabs: 'Explore', 'Saved Searches', and 'SciPlanner'. On the right, there are buttons for 'Save', 'Print', and 'Export'. A yellow banner indicates '380 references with the CA Section Title Pharmacology are displayed'. Below this, there are buttons for 'Keep Analysis' and 'Clear Analysis'. The main content area shows the search path: 'Substance Identifier "plavix" > substances (1) > get references (1099) > keep analysis "CA Section Title" (380)'. There are buttons for 'REFERENCES', 'Get Substances', 'Get Reactions', 'Get Related Citations', and 'Tools'. On the left, there are tabs for 'Analyze', 'Refine', and 'Categorize'. The 'Analyze by:' dropdown is set to 'CA Section Title'. A list of categories is shown, with 'Pharmacology' selected and highlighted in yellow, showing 380 references. The main results area shows a list of references, with the first one selected. The first reference is: '1. Clinical trial of clopidogrel bisulfate tablets combined with aspirin on the protection of myocardium after percutaneous coronary intervention'. The second reference is: '3. Clinical efficacy of antiplatelet combined with anticoagulation therapy for restenosis prophylaxis after stent placement in diabetic patients with leg atherosclerosis obliterans'.

# 药理学文献信息检索策略

获得体外实验文献的检索方法

Step 3: 选择refine, research topic, 输入vitro

The screenshot shows a search interface with three tabs: 'Analyze', 'Refine', and 'Categorize'. The 'Refine' tab is active. On the left, under 'Refine by:', 'Research Topic' is selected. Below it, the 'Research Topic' filter is set to 'vitro'. A 'Refine' button is at the bottom of this section. The main area shows '0 of 380 References Selected' and a list of three results:

- 1. Clinical trial of clopidogrel bisulfate tablets combined with aspirin on the protection of myocardium after percutaneous coronary intervention**  
By Sun, Xue-mei  
From Zhongguo Linchuang Yaolixue Zazhi (2016), 32(13), 1158-1161. | Language: Chinese, Database: CAPLUS  
Objective To explore the clin. effects of combined clopidogrel bisulfate tablets with aspirin on the protection of myocardium after percutaneous coron...  
Methods Ninety-eight cases with coronary heart disease were randomly divided into control group 49 cases and expt. group 49 cases, the patients in conventional treatment and symptomatic treatment. Then the control group received aspirin 150 mg, 1 times a day, the expt. group combined with 75 r... tablets, 1 times a day, 7days of continuous use. Two groups of patients were underw...
- 2. Clinical efficacy of antiplatelet combined with anticoagulation therapy for restenosis prophylaxis after stent placement in diabetic patients with leg athe...**  
By Sun, Jinhong; Wang, Jian; Zhang, Jie  
From Zhongguo Yaoshi (Wuhan, China) (2016), 19(5), 935-938. | Language: Chinese, Database: CAPLUS  
Objective: To investigate the clin. efficacy and safety of antiplatelet combined with anticoagulation therapy for restenosis prophylaxis after stent placement leg atherosclerosis obliterans (LASO). Methods: 83 diabetic LASO patients with stent placement were collected and randomly divided into the treatment gr... control group (41 cases) with 49 sick limbs in each. The control group was treated with clopidogrel (75 mg, for 1 yr) plus bayaspirin (100 mg), while th... treated with low mol. heparin (withdrawal when INR = 2.0-3.0) pl...
- 3. Clinical efficacy of enoxaparin sodium combined with clopidogrel hydrogen sulfate on treatment of 64 cases of patients with unstable angina pectoris**

# 文献结果集的保存

Searches ▾ SciPlanner Save Print Export

g in COVID-19" > references (1633) > refine by categories > Potential Therapeutic Options ...

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Sort by: Accession Number ↓ Display Options

0 of 34 References Selected Page: 1 of 2

1. COSMO-RS-based descriptors for the machine learning-enabled screening of nucleotide analogue drugs against SARS-CoV-2  
By Gusarov, Sergey; Stoyanov, Stanislav R.  
From Journal of Physical Chemistry Letters (2020), 11(21), 9408-9414. | Language: English, Database: CAPLUS

Chem. similarity-based approaches employed to repurpose or develop new treatments for emerging diseases, such as COVID-19, correlates mol. structure-based descriptors of drugs with those of a physiol. counterpart or clin. phenotype. We propose novel descriptors based on a COSMO-RS (short for conductor-like screening model for real solvents)  $\sigma$ -profiles for enhanced drug screening enabled by machine learning (ML). The descriptors' performance is hereby illustrated for nucleotide analog drugs that inhibit the RNA-dependent RNA polymerase, key to viral transcription and genome replication. The ...

查看文献详情

2. Potential Therapeutic Options for COVID-19  
By Zheng, Xiaojin; Li, Lanjuan  
From Infectious Microbes & Diseases (2020), 2(3), 89-95. | Language: English, Database: CAPLUS

Save: 保存在服务器上，方便以后登陆查看，每次可存1万条记录。

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# 文献结果详情--题录、摘要、索引

## 2. Potential Therapeutic Options for COVID-19

By: Zheng, Xiaoqin; Li, Lanjuan

A review. The recently emerged coronavirus disease 2019 (COVID-19) has rapidly evolved into a pandemic with over 10 million infections and over 500 thousand deaths. There are currently no effective therapies or vaccines available to protect against this coronavirus infection. In this review, we discuss potential therapeutic options for COVID-19 based on the available information from previous research on severe acute respiratory syndrome (SARS) and Middle East respiratory syndrome (MERS). Substantial efforts are underway to discover new therapeutic agents for COVID-19, including the repurposing of existing agents and the development of novel agents that specifically target SARS-coronavirus 2 (SARS-CoV-2) or host factors. Through the screening of compd. libraries, various classes of drugs, such as ribavirin, remdesivir, lopinavir/ritonavir, and hydroxychloroquine have been identified as potential therapeutic candidates against COVID-19. Novel antiviral drugs for SARS-coronavirus 2 are being developed to target viral enzymes or functional proteins, as well as host factors or cell signaling pathways.

### Indexing

Pharmacology (Section1-0)

Section cross-reference(s): 14

### Concepts

重要概念

Anticoronaviral agents	Antiviral agents
COVID-19	Drug repurposing
Drug screening	Middle East respiratory syndrome
Severe acute respiratory syndrome	Severe acute respiratory syndrome coronavirus 2

potential therapeutic options for COVID-19

### Supplementary Terms

review SARS CoV2 coronavirus COVID19 antiviral agent

### Substances

重要物质

118-42-3 Hydroxychloroquine
36791-04-5 Ribavirin
369372-47-4 Lopinavir/ritonavir
1809249-37-3 Remdesivir

potential therapeutic options for COVID-19

Therapeutic use; Biological study; Uses

### QUICK LINKS

0 Tags, 0 Comments

### SOURCE

*Infectious Microbes & Diseases*  
Volume2  
Issue3  
Pages89-95  
Journal; General Review;  
Online Computer File  
2020  
CODEN:IMDNQ  
ISSN:2641-5917  
DOI:10.1097/IM9.0000000000000033

### COMPANY/ORGANIZATION

State Key Laboratory for  
Diagnosis and Treatment of  
Infectious Diseases, National  
Research Center for  
Emerging Infectious Diseases, National  
Center for Infectious  
Disease Control and  
Laboratory  
Center for  
Diagnosis and Treatment of  
Infectious Diseases, The First  
Hospital of  
University School of

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1. 标题
2. 摘要
3. 文献中重要的技术术语
4. 文献中重要的物质
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7. 参考文献
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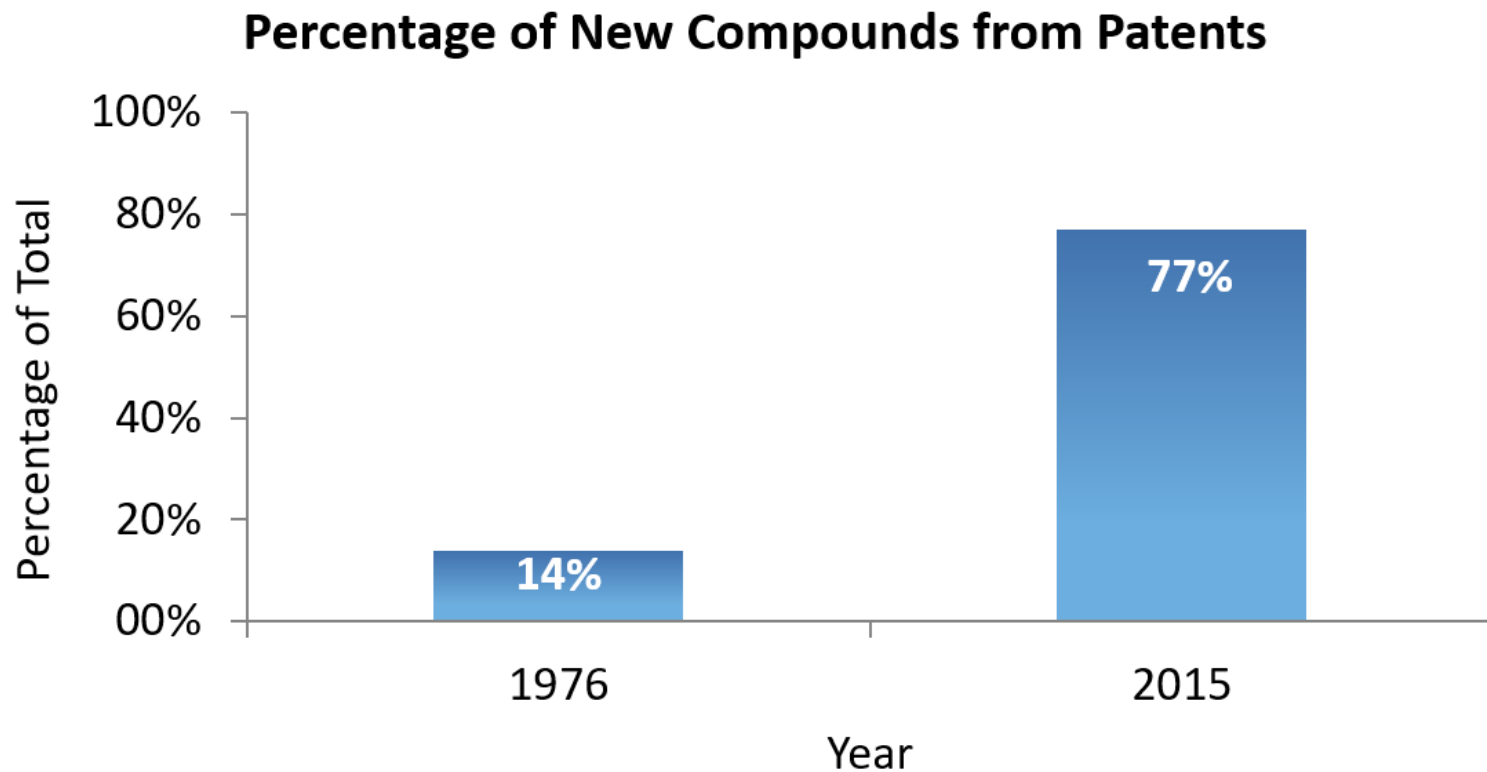


# PatentPak™

专利工作流程解决方案



# 越来越多的新化合物倾向于首先通过专利公布



# CAS PatentPak

## ——专利工作流程解决方案：

8. A process for the preparation of N-[[P(S),2'R]-2'-deoxy-2'-fluoro-2'-methyl-P-phenyl-5'-uridylyl]-L-alanine 1-methylethyl ester

Quick View PATENTPAK

By Ross, Bruce S. From Can. (2020)

The invention to obtain I; c a mixt. of dia

9. Preparation Quick View By Guzel, Mustafa From PCT Int. App The patent a discloses ex naphthylami

10. Method of

Patent No. CA 2988217

Patent Family CA 2988217 CA 2819700 CA 2915187 CA 2915187 EP 2610264 EP 2610264 CN 104292256 EP 2910562 EP 2913337 EP 2913337

PatentPak Options PDF | PDF+ | Viewer

Kind C

Language English

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Zhang, Hai Ren; Chun, Byoung Kwon; Wang, Peiyuan

compd. II [LG = p-nitrophenoxy, p-chlorophenoxy, o-chlorophenoxy, 2,4-dinitrophenoxy, or pentafluorophenoxy] with a basic reagent and a compd. III [Z = H] (group), and deprotecting to obtain I. Thus, reacting H-L-Ala-OPR-i.bul.HCl with 4-nitrophenyl phosphorodichloridate in the presence of PhOH/TEA in DCM gave ing to room temp. and stirring for 1 h, seeding wi...

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Patent Information

Patent No.	PatentPak Options	Kind	Language	Date	Application No.	Date
CA 2988217	PDF   PDF+   Viewer	C		Jun 23, 2020	CA 2010-2988217	May 20, 2010
CA 2988217	PDF	A1	English	Nov 25, 2010		
CA 2819700	PDF	A1	English	Nov 25, 2010	CA 2010-2819700	May 20, 2010
CA 2819700	PDF	C	English	Mar 22, 2016		
CA 2915187	PDF	A1	English	Nov 25, 2010	CA 2010-2915187	May 20, 2010
CA 2915187	PDF	C	English	Jan 23, 2018		
CA 3077960	PDF	A1	English	Nov 25, 2010	CA 2010-3077960	May 20, 2010
EP 2610264	PDF	A2	English	Jul 3, 2013	EP 2013-159903	May 20, 2010
EP 2610264	PDF	A3	English	Jan 22, 2014		
CN 104292256	PDF	A	Chinese	Jan 21, 2015	CN 2014-10487915	May 20, 2010
EP 2910562	PDF	A1	English	Aug 26, 2015	EP 2015-152204	May 20, 2010
EP 2913337	PDF	A1	English	Sep 2, 2015	EP 2015-152203	May 20, 2010
EP 2913337	PDF	B1	English	Sep 6, 2017		
NZ 623602	PDF	A	English	Oct 30, 2015	NZ 2010-623602	May 20, 2010
CN 105085592	PDF	A	Chinese	Nov 25, 2015	CN 2015-10552266	May 20, 2010
CN 105198949	PDF	A	Chinese	Dec 30, 2015	CN 2015-10552267	May 20, 2010
NZ 709926	PDF	A	English	Nov 25, 2016	NZ 2010-709926	May 20, 2010
EP 3321275	PDF	A1	English	May 16, 2018	EP 2017-189286	May 20, 2010
US 20110257121	PDF	A1	English	Oct 20, 2011	US 2011-13076718	Mar 31, 2011
US 8563530	PDF	B2	English	Oct 22, 2013		
EP 2752422	PDF	A1	English	Jul 9, 2014	EP 2014-163247	Mar 31, 2011
EP 2752422	PDF	B1	English	Aug 16, 2017		
ZA 2011008749	PDF	A	English	May 29, 2013	ZA 2011-8749	Nov 29, 2011
ZA 2013001620	PDF	A	English	Oct 30, 2013	ZA 2013-1620	Mar 4, 2013
JP 2015028060	PDF	A	Japanese	Feb 12, 2015	JP 2014-197788	Sep 29, 2014
JP 5909535	PDF	B2	Japanese	Apr 26, 2016		
AU 2014274548	PDF	A1	English	Jan 22, 2015	AU 2014-274548	Dec 10, 2014
AU 2014274548	PDF	B2	English	Feb 4, 2016		
JP 2016053045	PDF	A	Japanese	Apr 14, 2016	JP 2015-203614	Oct 15, 2015
JP 6355605	PDF	B2	Japanese	Jul 11, 2018		

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the description (n)substituted

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## ——专利工作流程解决方案

The screenshot displays the PatentPak viewer interface. On the left, there is a sidebar with 'Key Substances in Patent' listing two CAS RNs: 863329-66-2 and 817204-32-3, each with a chemical structure and search options. The main area shows a patent document page (page 41 of 117) with a 'Method of Preparation' section. A callout box points to a lightbulb icon under the first substance, with the text: '在PatentPak Viewer中点击物质下面的灯泡, 快速定位到PDF文件中的物质信息'. Another callout box points to the 'DOWNLOAD PDF' button, with the text: '下载PDF文件'. A third callout box points to the 'DOWNLOAD PDF' button in the top navigation bar, with the text: '下载包含物质位置等信息的专利PDF文件'. A fourth callout box points to the main document content, with the text: '专利PDF文件'. The interface also includes a 'PatentPak浏览器' label in the top right corner.

# CAS PatentPak

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The screenshot displays the CAS PatentPak interface. At the top, there are navigation controls: a 'PAGE' dropdown set to 49 of 117, 'ZOOM' in and out buttons, and a 'DOWNLOAD PDF' button. The main content area shows a patent document with chemical structures and text. A callout box with a purple border and a purple arrow pointing to a location marker on the text says: '也可实现PDF文件与 PatentPak Viewer 互动' (It can also achieve interaction between PDF files and PatentPak Viewer). The interface also shows a sidebar with 'Key Substances in Patent' and 'Analyst Markup Locations' for two different CAS RNs (1256490-31-9 and 1256490-49-9).

**5** O=[N+]([O-])c1ccc(O)cc1 + CC(C)C(C)C(=O)N[H+]Cl  $\xrightarrow{\text{PhOH, Et}_3\text{N, DCM, -78}^\circ\text{C}}$  CC(C)C(C)C(=O)Nc1ccc(O)cc1

To a stirred solution of 4-nitrophenyl phosphorodichloridate 12.8g, 50 mmol) in dichloromethane (100 mL) was added a solution of phenol and triethylamine (7.7 mL, 55 mmol) in dichloromethane (100 mL) at -78°C over a period of 20min. The mixture was stirred at this temperature for 30min and then transferred to another round bottom

**10** flask containing L-alanine isopropyl ester hydrochloride (8.38g, 50mmol) in dichloromethane (100 mL) at 0°C. To the mixture was added second portion of dichloromethane (14.6 mL, 105 mmol) over a period of 15min. The mixture was stirred at 0°C for 1h and then the solvent was evaporated. The residue was triturated with ethyl acetate (150 mL) and the white solid was filtered off. The filtrate was concentrated under reduced pressure to give pale yellow oil. The crude compound

**15** was chromatographed using 0-20% ethyl acetate/hexanes as gradient to give product (17g, 83 %yield) as a mixture of diastereomers in about 1:1 ratio. <sup>31</sup>P NMR (162 MHz, DMSO-d6): δ -0.31, -0.47; <sup>1</sup>H NMR (400 MHz, DMSO-d6): δ 8.31-8.27 (m, 2H), 7.51-7.37(m, 4H), 7.27-7.19(m, 3H), 6.70-6.63(m, 1H), 4.85-4.78(m, 1H), 3.97-

**20** 3.86(m, 1H), 1.21-1.19(m, 3H), 1.11-1.09 (m, 6H); MS (ESI) *m/z* 407 (M-1)<sup>+</sup>. <sup>31</sup>P NMR (162 MHz, CDCl<sub>3</sub>): δ -2.05, -2.10; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 8.22 (d, J = 9.2Hz, 2H), 7.41-7.33(m, 4H), 7.26-7.18(m, 3H), 5.05-4.96(m, 1H), 4.14-4.05(m, 1H), 3.93-3.88(m, 1H), 1.38(d, J = 6.8Hz, 3H), 1.22 (dd, J = 6.2 & 3.0Hz, 6H); MS (ESI) *m/z* 407 (M-1)<sup>+</sup>.

# CAS PatentPak

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**PATENTPAK**  
A CAS SOLUTION

PAGE 41 / 117 ZOOM DOWNLOAD PDF

Key Substances in Patent

CAS RN 863329-66-2

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Search in SciFinder View Detail

Structure Markush Reactions

CAS RN 817204-32-3

可在PatentPak Viewer中直接返回SciFinder进行结构、马库什和反应检索

Search in SciFinder View Detail

Analyst Markup Locations (1) page 41

CAS RN 863329-65-1

CAS Registry Number 863329-66-2

$\sim 256$   $\sim 120$

$C_{10}H_{13}FN_2O_5$   
Uridine, 2'-deoxy-2'-fluoro-2'-methyl-, (2'R)-

Molecular Weight 260.22

Melting Point (Experimental)  
Value: 237.3-238.0 °C

Density (Predicted)  
Value: 1.55±0.1 g/cm3 | Condition: Temp: 20 °C Press: 760 Torr

pKa (Predicted)  
Value: 9.39±0.10 | Condition: Most Acidic Temp: 25 °C

Rotation (+), Absolute stereochemistry.

3'-O-phosphoramidate-5'-C-ribidines  
(2 diastereomers)

After working up the silylation reaction, the desired product is subjected to

5 chromatography on silica gel and is eluted with a gradient of methanol in dichloromethane (1-4%). The desired 5'-monophosphoramidate 4 elutes last.

Method of Preparation

Example 1. Preparation of 2'-deoxy-2'-fluoro-2'-C-methyluridine (3)

10 In a 10 L flask, was added 3', 5'-O-dibenzyloxy-2'-deoxy-2'-fluoro-2'-C-methyl-N<sup>4</sup>-benzoylcytidine (500 g, 0.874 mol) and 70% aqueous acetic acid (7.5 L). The solution was heated to reflux (110°C) for 20 h. TLC indicated a complete reaction (R<sub>f</sub> 0.6 in 5% methanol in dichloromethane (DCM)). The mixture was cooled to ambient temperature and diluted with water (2 L). After stirring for 2 h, the resulting precipitate was collected by filtration and the solid was rinsed with water (5 L) and dried in the atmosphere at ambient temperature for 12 h to afford 360 g (88%). This dibenzyloxyuridine intermediate was used directly in the next step by adding it all to

15

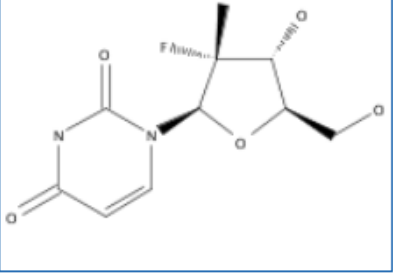
# CAS PatentPak

## ——专利工作流程解决方案

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# 大纲

- CAS及CAS SciFinder介绍
- 文献相关信息的获取策略
  - 文献检索方法
  - 文献结果排序、筛选和详情
  - 如何高效阅读专利文献详情(CAS PatentPak)
- 物质相关信息的获取策略
  - 常见的物质检索方法
  - 物质结果排序、筛选和详情
- 反应相关信息的获取策略
  - 反应的获取方法
  - 反应结果排序、筛选和详情
  - 如何高效获取反应详情 (Synthetic Methods)
- 分析相关信息的获取 (CAS Analytical Methods)



# CAS SciFinder检索--物质检索

## ■ 物质检索方法

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- 分子式检索
- 理化性质 (物质属性) 检索
- 物质标识符检索: 化学名称、CAS RN
- 从文献或反应结果获得

## ■ 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

### SUBSTANCES

Chemical Structure  
Markush  
Molecular Formula  
Property  
Substance Identifier

# 物质检索--标识符检索

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2. 每行一个物质标识符。

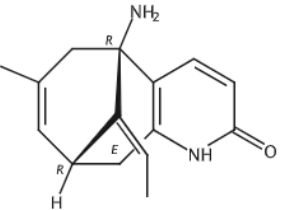
物质标识符包括CAS RN和化学名称，化学名称可以是通用名称、商品名、俗名。

# 物质结果集

点击CAS RN 获得物质详细信息

1. **102518-79-6** 🔍

~1494 📄 ~132 🧪



Double bond geometry as shown.,Rotation (-),Absolute stereochemistry.

**C<sub>15</sub>H<sub>18</sub>N<sub>2</sub>O**  
5,9-Methanocycloocta[*b*]pyridin-2(1*H*)-one, 5-amino-11-ethylidene-5,6,9,10-tetrahydro-7-methyl-, (5*R*,9*R*,11*E*)-

▶ **Key Physical Properties**  
Regulatory Information  
Spectra  
Experimental Properties

CAS Registry Number: 102518-79-6

View Substance Detail

Explore by Structure ▶

Synthesize this...

Get Reactions where Substance is a ▶ Product

Get Commercial Sources Reactant

Get Regulatory Information Reagent

Get References Reactant/Reagent

Export as Image Catalyst

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在SciFinder中，鼠标滑过物质，即可打开物质标准菜单，获得与物质相关的所有内容

# 物质结果详情

**SUBSTANCE DETAIL** [Get References](#) [Get Reactions](#) [Get Commercial Sources](#)

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**CAS Registry Number** 63968-64-9

~6,284 ~126

**C<sub>15</sub> H<sub>22</sub> O<sub>5</sub>**  
3,12-Epoxy-12H-pyrano[4,3-j]-1,2-benzodioxepin-10(3H)-one, octahydro-3,6,9-trimethyl-, (3R,5aS,6R,8aS,9R,12S,12aR)-

**Molecular Weight**  
282.33

**Melting Point (Experimental)**  
Value: 156-157 °C

**Boiling Point (Predicted)**  
Value: 389.9±42.0 °C | Condition: Press: 760 Torr

**Density (Experimental)**  
Value: 1.300 g/cm<sup>3</sup>

**Other Names**  
3,12-Epoxy-12H-pyrano[4,3-j]-1,2-benzodioxepin-10(3H)-one, octahydro-3,6,9-trimethyl-, [3R-(3α,5aβ,6β,8aβ,9α,12β,12aR\*)]-(3R,5aS,6R,8aS,9R,12S,12aR)-Octahydro-3,6,9-trimethyl-3,12-epoxy-12H-pyrano[4,3-j]-1,2-benzodioxepin-10(3H)-one  
(+)-Arteannuin  
(+)-Artemisinin  
(+)-Qinghaosu  
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**Absolute stereochemistry**

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## Get References

### Limit results to:

- |   |   |
|---|---|
| <input type="checkbox"/> Adverse Effect, including toxicity | <input checked="" type="checkbox"/> Preparation |
| <input checked="" type="checkbox"/> Analytical Study        | <input checked="" type="checkbox"/> Process     |
| <input type="checkbox"/> Biological Study                   | <input type="checkbox"/> Properties             |
| <input type="checkbox"/> Combinatorial Study                | <input type="checkbox"/> Prophetic in Patents   |
| <input checked="" type="checkbox"/> Crystal Structure       | <input type="checkbox"/> Reactant or Reagent    |
| <input type="checkbox"/> Formation, nonpreparative          | <input type="checkbox"/> Spectral Properties    |
| <input type="checkbox"/> Miscellaneous                      | <input type="checkbox"/> Uses                   |
| <input type="checkbox"/> Occurrence                         |   |

### For each sequence, retrieve:

- Additional related references, e.g., activity studies, disease studies.

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# 物质结果详情—实验数据实验谱图

EXPERIMENTAL PROPERTIES 实验数据

EXPERIMENTAL SPECTRA 实验谱图

<sup>1</sup>H NMR <sup>13</sup>C NMR Hetero NMR IR Mass Raman UV and Visible Additional Spectra

<sup>13</sup> C NMR Properties	Value	Condition	Note
Carbon-13 NMR Spectrum	See spectrum		3)ACD
Carbon-13 NMR Spectrum	See spectrum		4)ACD
Carbon-13 NMR Spectrum	See full text		5)CAS

Notes

- (3) ACD: Spectral data were obtained from Advanced Chemistry Development, Inc.
- (4) Han, Jaehong; Journal of Natural Products 2001, V64(9), P1201-1205 CAPLUS
- (5) Yadav, J. S.; Tetrahedron 2010, V66(11), P2005-2009 CAPLUS

PREDICTED PROPERTIES 预测数据

PREDICTED SPECTRA 预测谱图

REGULATORY INFORMATION 管制信息

BIOACTIVITY INDICATORS 生物活性指示剂

TARGET INDICATORS 生物靶点指示剂

CAS REFERENCE ROLES CAS文献角色

ADDITIONAL DETAILS 其他

### Carbon-13 NMR Spectrum

SPECTRUM ID: 7MED36\_38.C

CAS REGISTRY NUMBER: 63968-64-9

FORMULA: C<sub>15</sub>H<sub>22</sub>O<sub>5</sub>

CAS INDEX NAME: 3,12-Epoxy-12H-pyrano[4,3-*f*]-1,2-benzodioxepin-10(3*H*)-one, octahydro-3,6,9-trimethyl-, (3*R*,5*a*,5,6*R*,8*a*,5,9*R*,12*S*,12*a**R*)-

NUCLEUS: <sup>13</sup>C

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



# 物质结果详情—生物活性

▼BIOACTIVITY INDICATORS		
Indicators		References
Cytoprotective agents (all) > Neuroprotective agents	神经保护剂	134
Enzyme inhibitors (all) > Cholinesterase inhibitors	胆碱酯酶抑制剂	130
Natural products, pharmaceutical		140
Nervous system agents (all) > Anti-Alzheimer agents	抗阿尔茨海默病	198
Nervous system agents (all) > > Cognition enhancers	认知促进剂	97
Nervous system agents (all) > Neuroprotective agents		134

▼TARGET INDICATORS		
Indicators		References
Apoptosis-regulating proteins (all) > Bax proteins	Bax蛋白	10
Cytokines (all) > > Interleukin 1 $\beta$		12
Cytokines (all) > > Interleukin 1 $\beta$	白细胞介素-1 $\beta$	12
Cytokines (all) > Interleukin 6		10
Cytokines (all) > Interleukin 6	白细胞介素6	10
Cytokines (all) > Interleukin 6	肿瘤坏死因子- $\alpha$	10
Cytokines (all) > Tumor necrosis factor $\alpha$		15
Cytokines (all) > Tumor necrosis factor $\alpha$		15
Cytoskeletal proteins (all) > > Tau proteins		12

# 物质检索--Property Explorer

The screenshot shows the SciFinder Property Explorer interface. The browser address bar displays <https://scifinder.cas>. The SciFinder logo is visible at the top left. The interface is divided into several sections:

- Left Sidebar:** Contains navigation options under 'REFERENCES' (Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, Tags) and 'SUBSTANCES' (Chemical Structure, Markush, Molecular Formula, Property, Substance Identifier).
- Top Navigation:** Includes 'Explore' and 'Saved Searches' tabs.
- Property Selection:** A dropdown menu titled 'Select Property...' is open, listing various properties. 'Molecular Weight' is selected and highlighted in blue.
- Search Criteria:** Below the dropdown, a search range is specified as '250-400'. Examples provided are '44, 25-35, >125'.
- Search Button:** A prominent blue 'Search' button is located at the bottom center of the main content area.

寻找分子量在250-400之间的物质

# 物质结果集的筛选--Refine

Property "Predicted - Molecular Weight, ..." > substances (78557824)

SUBSTANCES

Get References Get Reactions Get Commercial Sources Tools

Create Keep Me Posted Alert Send to SciPlanner

Analyze Refine

Sort by: CAS Registry Number

0 of 78557824 Substances Selected

Display Options

Page: 1 of 1571157

Refine by:

- Chemical Structure
- Isotope-Containing
- Metal-Containing
- Commercial Availability
- Property Availability
- Property Value
- Reference Availability
- Atom Attachment

Structure Editor:

Java Non-Java

Click to Edit

Search type: **Exact Structure**

Only retrieve substances that:

- Have references
- Are commercially available
- Are a single component
- Are in specific substance classes
- Are in specific ty

<input type="checkbox"/> 1. 2640164-31-2 ~1  <b>C<sub>26</sub>H<sub>18</sub>O<sub>4</sub></b> INDEX NAME NOT YET ASSIGNED ▶ <b>Key Physical Properties</b>	<input type="checkbox"/> 2. 2640164-29-8 ~1  <b>C<sub>14</sub>H<sub>20</sub>O<sub>4</sub></b> INDEX NAME NOT YET ASSIGNED ▶ <b>Key Physical Properties</b>	<input type="checkbox"/> 3. 2640164-28-7 ~1  <b>C<sub>18</sub>H<sub>22</sub>O<sub>4</sub></b> INDEX NAME NOT YET ASSIGNED ▶ <b>Key Physical Properties</b>	<input type="checkbox"/> 4. 2640164-27-6 ~1  <b>C<sub>21</sub>H<sub>30</sub>O<sub>4</sub></b> INDEX NAME NOT YET ASSIGNED ▶ <b>Key Physical Properties</b>
<input type="checkbox"/> 5. 2640164-26-5 ~1  <b>C<sub>15</sub>H<sub>26</sub>O<sub>4</sub></b> INDEX NAME NOT YET ASSIGNED ▶ <b>Key Physical Properties</b>	<input type="checkbox"/> 6. 2640164-25-4 ~1  <b>C<sub>15</sub>H<sub>26</sub>O<sub>4</sub></b> INDEX NAME NOT YET ASSIGNED ▶ <b>Key Physical Properties</b>	<input type="checkbox"/> 7. 2640164-20-9 ~1  Relative stereochemistry. <b>C<sub>13</sub>H<sub>21</sub>N O<sub>6</sub></b> INDEX NAME NOT YET ASSIGNED ▶ <b>Key Physical Properties</b>	<input type="checkbox"/> 8. 2640164-19-6 ~1  Relative stereochemistry. <b>C<sub>13</sub>H<sub>21</sub>N O<sub>6</sub></b> INDEX NAME NOT YET ASSIGNED ▶ <b>Key Physical Properties</b>
<input type="checkbox"/> 9. 2640164-18-5 ~1 	<input type="checkbox"/> 10. 2640164-17-4 ~1 	<input type="checkbox"/> 11. 2640164-15-2 ~1 	<input type="checkbox"/> 12. 2640164-14-1 ~1 

7855万多个结构,  
如何筛选黄酮类物质?

# 物质结果集的筛选--Refine

Structure Editor

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

Get substances that match your query using:

- Exact search
- Substructure search

OK

Cancel

C<sub>15</sub>H<sub>10</sub>O<sub>2</sub>

锁环工具：避免在被锁定的环结构上出现新的环结构

Analyze Refine

Refine by: ?

- Chemical Structure
- Isotope-Containing
- Metal-Containing
- Commercial Availability
- Property Availability
- Property Value
- Reference Availability
- Atom Attachment

Structure Editor:

Java Non-Java

Click image to change structure or view detail.

Search type: **Substructure**

Only retrieve substances that:

- Have references
- Are commercially available
- Are a single component
- Are in specific substance classes
- Are in specific types of studies

Refine

# 物质结果集的筛选--Refine

Substances interface showing a refined list of 19,423 substances. The interface includes a left sidebar with filters, a top navigation bar, and a main grid of 12 compound cards. A blue box highlights the '19423 Substances Selected' count.

Sort by: Relevance

0 of 19423 Substances Selected

Page: 1 of 389

1. 1373355-19-1  
C17H14O2  
4*H*-1-Benzopyran-4-one, 2-(3,5-dimethylphenyl)-  
▶ Key Physical Properties

2. 912915-64-1  
C15H10O4  
4*H*-1-Benzopyran-4-one, 2-(3,5-dihydroxyphenyl)-  
▶ Key Physical Properties

3. 1174710-12-3  
C17H14O2  
4*H*-1-Benzopyran-4-one, 2-(4-ethylphenyl)-  
▶ Key Physical Properties

4. 6665-68-5  
C15H10O4  
4*H*-1-Benzopyran-4-one, 5-hydroxy-2-(3-hydroxyphenyl)-  
▶ Key Physical Properties  
Spectra  
Experimental Properties

5. 22395-22-8  
C16H12O3  
4*H*-1-Benzopyran-4-one, 7-methoxy-2-phenyl-  
▶ Key Physical Properties  
Regulatory Information  
Spectra  
Experimental Properties

6. 108238-40-0  
C15H10O4  
4*H*-1-Benzopyran-4-one, 7-hydroxy-2-(3-hydroxyphenyl)-  
▶ Key Physical Properties  
Spectra  
Experimental Properties

7. 58996-67-1  
C16H14O3  
Benzaldehyde, 4-(4-oxo-4*H*-1-benzopyran-2-yl)-  
▶ Key Physical Properties  
Experimental Properties

8. 40052-90-2  
C15H12O3  
4*H*-1-Benzopyran-4-one, 7-(hydroxymethyl)-2-phenyl-  
▶ Key Physical Properties

9. 700843-44-3  
C17H14O2

10. 480-40-0  
C15H10O4

11. 4143-74-2  
C17H14O2

12. 53906-83-5  
C15H10O4

从7855万多个结构中  
筛选出19423个黄酮类物质

# 物质检索--分子式检索

**REFERENCES**

- Research Topic
- Author Name
- Company Name
- Document Identifier
- Journal
- Patent
- Tags

**SUBSTANCES**

- Chemical Structure
- Markush
- Molecular Formula**
- Property
- Substance Identifier

**REACTIONS**

- Reaction Structure

**SUBSTANCES: MOLECULAR FORMULA**

Examples:  
H4SiO4  
(C3H6O.C2H4O)x

**Search**

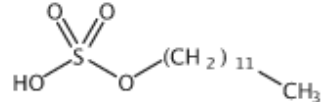
分子式输入需要遵守Hill排序规则:不含碳化合物,按元素符号的字母顺序排列;分子式为含碳化合物时,则“C”在前;如有氢则紧随其后,其它元素符号按字母顺序排在氢的后面

无机金属盐: 金属离子和阴离子间用点 (.) 分开

40. **151-21-3** 🔍

(Component: 151-41-7)

~79363 📄 ~283 🧪



• Na

**C<sub>12</sub> H<sub>26</sub> O<sub>4</sub> S . Na**  
Sulfuric acid monododecyl ester sodium salt (1:1)

▶ **Key Physical Properties**

- Regulatory Information
- Spectra
- Experimental Properties

# 物质检索--结构式检索

**REFERENCES**

- Research Topic
- Author Name
- Company Name
- Document Identifier
- Journal
- Patent
- Tags

**SUBSTANCES**

- Chemical Structure
- Markush
- Molecular Formula
- Property
- Substance Identifier

**REACTIONS**

- Reaction Structure

**SUBSTANCES: CHEMICAL STRUCTURE**

Structure Editor:

Java Non-Java

Click to Edit

Import CXF

Search

Advanced Search  Always Show

Search Type:

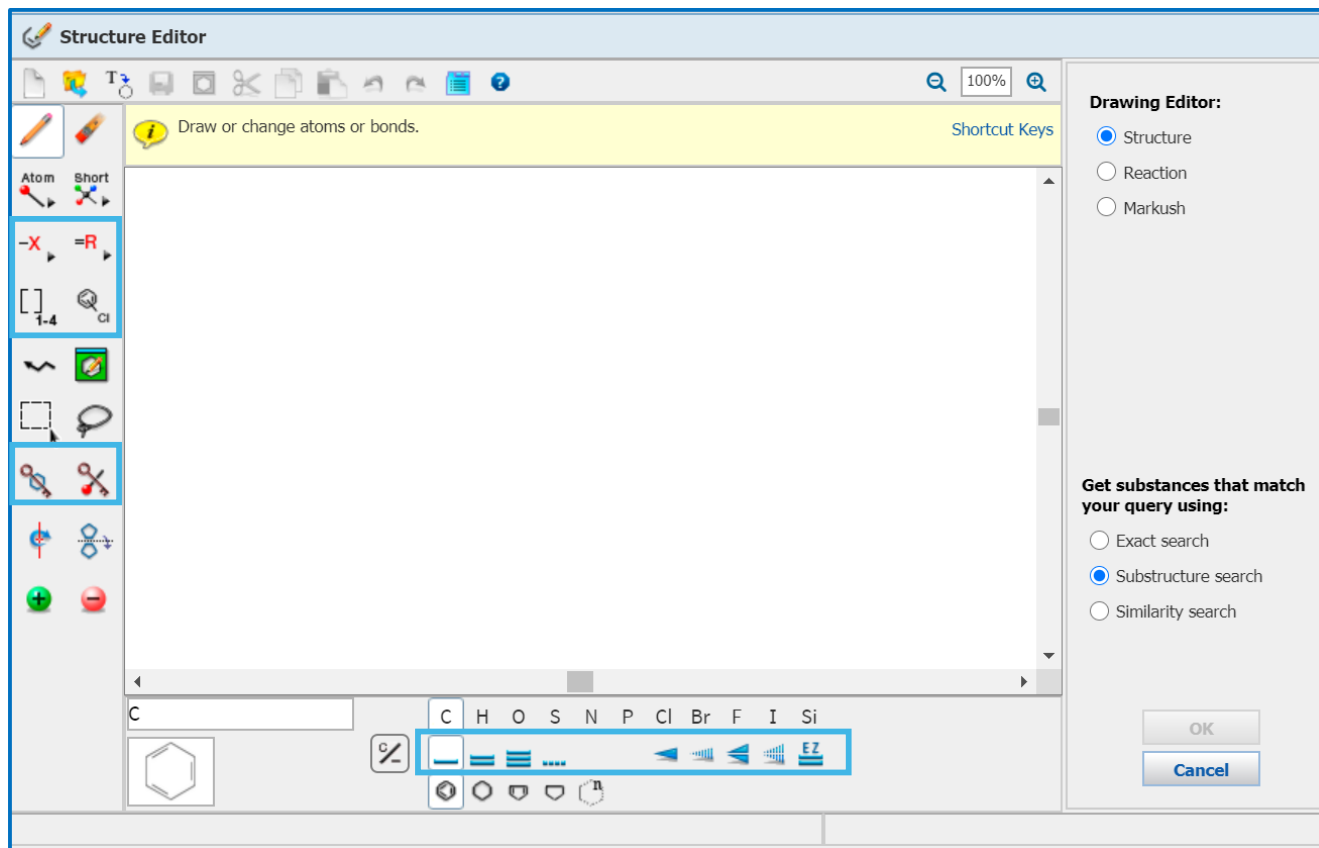
- Exact Structure
- Substructure
- Similarity

Show precision analysis


**ChemDraw**  
Launch a SciFinder substance or re...

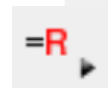


# 物质检索--结构编辑器




## 重要绘制工具注释

 选择可变基团

 自定义R基团

 重复工具

 取代位置可变

 锁环工具

 锁原子工具

# 物质检索--精确结构检索

The screenshot displays the 'Structure Editor' window. At the top, a toolbar contains various icons, with the 'Import' icon (a blue square with a white 'I') highlighted by a blue box. A callout bubble points to this icon, containing the text: '通过CAS RN转换结构: CAS RN: 50-36-2'. The main workspace shows a chemical structure of a bicyclic amine with a benzoyl group and a methoxy group. On the right side, the 'Drawing Editor' panel has 'Structure' selected. Below it, the 'Get substances that match your query using:' section has 'Exact search' selected, also highlighted by a blue box. At the bottom of the window, the molecular formula  $C_{17}H_{21}NO_4$  and the molecular weight 303.36 are displayed.

精确结构检索

# 物质检索--精确结构检索

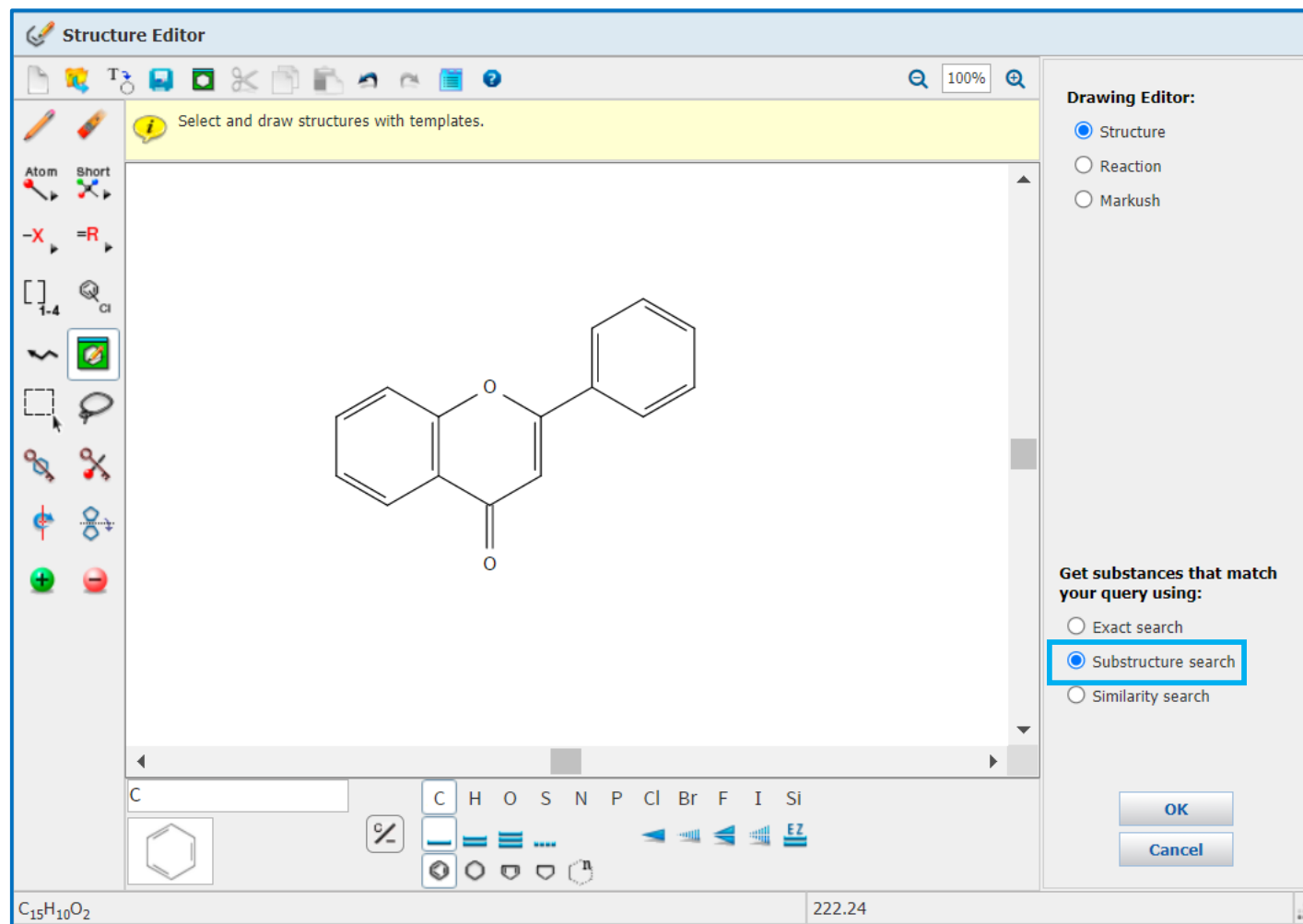
The screenshot displays a search interface with three results:

- Result 1:** 668-19-9. Structure of cocaine. **可卡因** (Cocaine) label.
- Result 2:** 114599-38-1. Labeled **可卡因组合物** (Cocaine combination). It shows two sub-entries:
  - 668-19-9,  $C_{17}H_{21}NO_4$ . Structure of cocaine. Absolute stereochemistry.
  - 88-89-1,  $C_6H_3N_3O_7$ . Structure of picric acid. Absolute stereochemistry.Below these is the formula  $C_{17}H_{21}NO_4 \cdot C_6H_3N_3O_7$  and the name "Alcocaine, picrate (6Cl)".
- Result 3:** 109496-04-0. Labeled **盐酸可卡因** (Cocaine hydrochloride). It shows the cocaine structure and the formula  $C_{17}H_{21}NO_4 \cdot ClH$  and name "Alcocaine, hydrochloride (6Cl)".

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

# 物质检索--亚结构检索

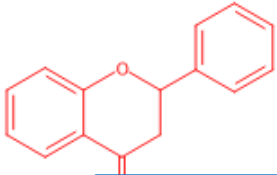


# 物质检索--亚结构检索结果集

0 of 23824 Substances Selected

1. 487-26-3

~2093

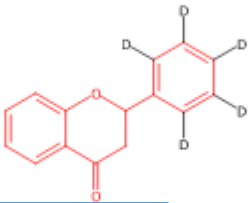


$C_{15}H_{12}O_2$   
4H-1-Benzopyran-4-one, 2,3-dihydro-

Key Physical Properties  
Regulatory Information  
Spectra  
Experimental Properties

10. 146196-91-0

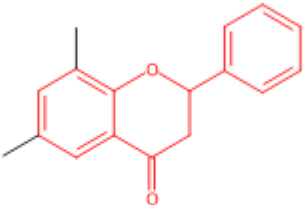
~1 ~5



同位素

281. 123251-10-5

~3 ~1



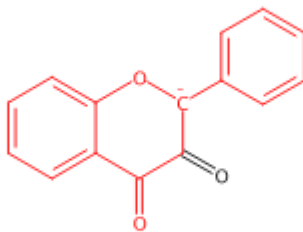
取代物

$C_{17}H_{16}O_2$   
4H-1-Benzopyran-4-one, 2,3-dihydro-6,8-dimethyl-

Key Physical Properties  
Experimental Properties

295. 780723-19-5

~0

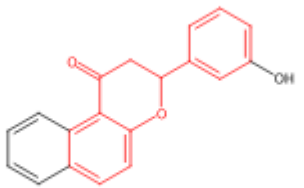


离子

$C_{15}H_9O_3$   
2H-1-Benzopyran-3,4-dione, 2-phenyl-, ion(1-)

284. 136116-23-9

~2



稠环物质

$C_{19}H_{14}O_3$   
1H-Naphtho[2,1-b]pyran-1-one, 2,3-dihydro-3-(3-hydroxyphenyl)-

Key Physical Properties

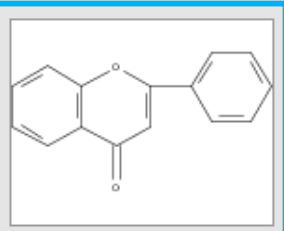
# 物质检索--亚结构检索结果集的限定

Analysis Refine

Refine by:

- Chemical Structure
- Isotope-Containing
- Metal-Containing
- Commercial Availability
- Property Availability
- Property Value
- Reference Availability
- Atom Attachment

Chemical Structure:



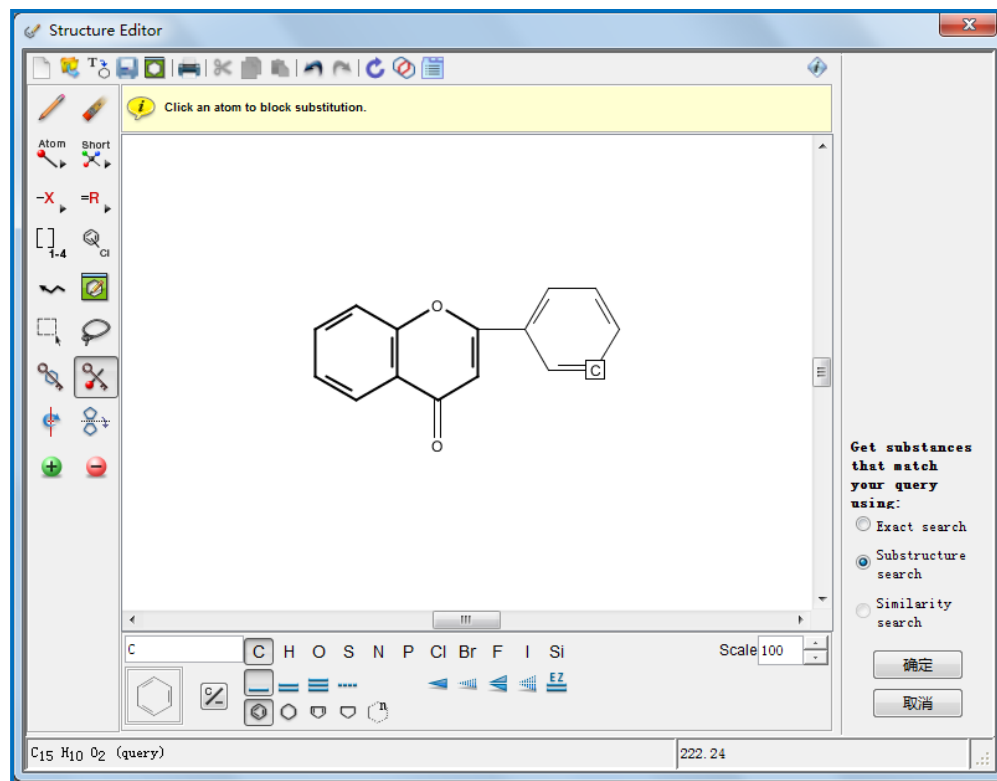
Click image to change structure or view detail

Search type: **Substructure**

化学结构的再次限定

Structure Editor

Click an atom to block substitution.



Get substances that match your query using:

- Exact search
- Substructure search
- Similarity search

确定 取消

C<sub>15</sub> H<sub>10</sub> O<sub>2</sub> (query) 222.24



环锁定

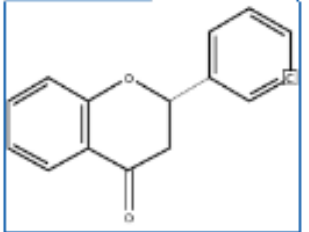


原子锁定

# 物质检索--亚结构检索结果集的限定

Structure Editor:

Java Non-Java



Click image to change structure or view detail.  
Search type: **Substructure**

Only retrieve substances that:

- Have references
- Are commercially available
- Are a single component
- Are in specific substance classes
- Are in specific types of studies

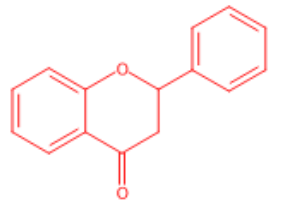
Refine

Get References Get Reactions Get Commercial Sources Tools

Sort by: Relevance

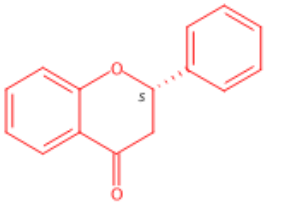
0 of 13826 Substances Selected

1. 487-26-3  
~2093 ~69



$C_{15}H_{12}O_2$   
4#-1-Benzopyran-4-one, 2,3-dihydro-2-phenyl-  
▶ Key Physical Properties  
Regulatory Information  
Spectra  
Experimental Properties

2. 17002-31-2  
~244 ~4



Absolute stereochemistry., Rotation (-).  
 $C_{15}H_{12}O_2$   
4#-1-Benzopyran-4-one, 2,3-dihydro-2-phenyl-, (2S)-  
▶ Key Physical Properties  
Experimental Properties

4. 104550-32-5  
~3

5. 75524-43-5  
~2

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



# 物质检索--相似结构检索

The screenshot displays the 'Structure Editor' software interface. The central workspace shows a chemical structure of 5-mercapto-1H-benzotriazole-4-carboxylic acid, which consists of a benzene ring fused to a triazole ring, with a thiol (-SH) group at the 5-position and a carboxylic acid (-COOH) group at the 4-position. The interface includes a top toolbar with various drawing and editing tools, a left sidebar with additional tool options, and a right sidebar with search settings. The search settings are as follows:

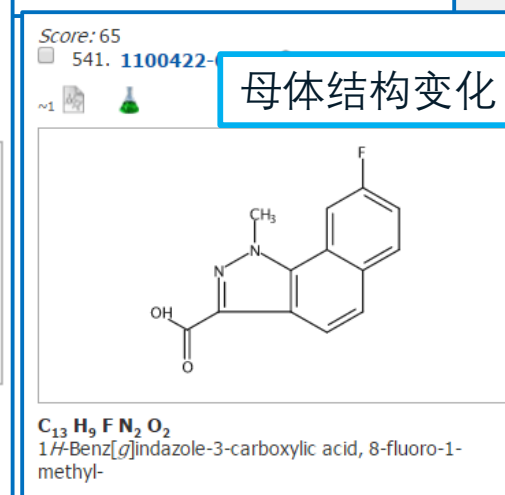
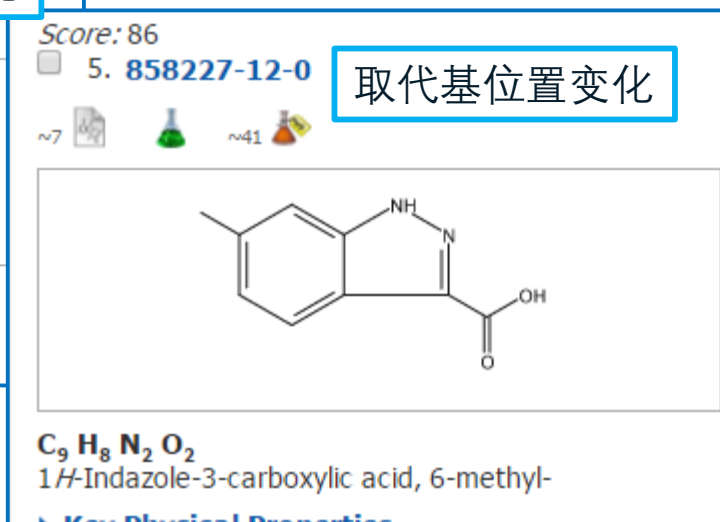
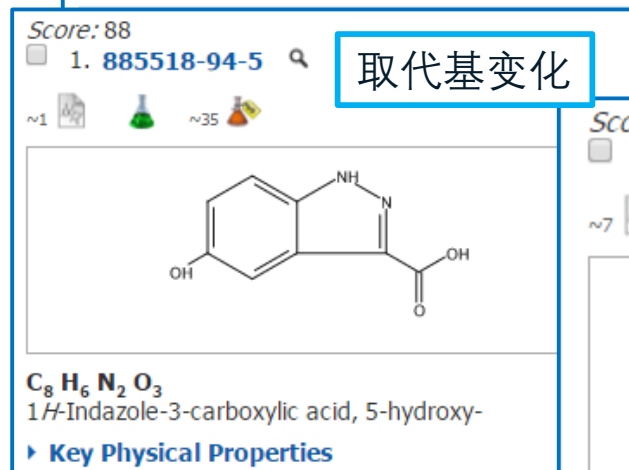
- Drawing Editor:**
  - Structure
  - Reaction
  - Markush
- Get substances that match your query using:**
  - Exact search
  - Substructure search
  - Similarity search



# 物质检索--相似结构检索结果

Select All Deselect All	
0 of 6 Similarity Candidates Selected	Substances
<input type="checkbox"/> $\geq 99$ (most similar)	0
<input type="checkbox"/> 95-98	0
<input type="checkbox"/> 90-94	0
<input type="checkbox"/> 85-89	11
<input type="checkbox"/> 80-84	34
<input type="checkbox"/> 75-79	84
<input type="checkbox"/> 70-74	267
	696
	1818

相似度越高，结构越相似




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

# 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 *C07K 1/16*(2006.01)  
(22) 申请日 2014.03.30 *C07K 1/06*(2006.01)  
*A61K 38/06*(2006.01)  
(71) 申请人 浙江大学 *A61P 35/00*(2006.01)  
地址 310027 浙江省杭州市西湖区浙大路 *A61P 35/02*(2006.01)  
38号 *A61P 25/28*(2006.01)  
申请人 中国科学院上海药物研究所 *A61P 37/02*(2006.01)

(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

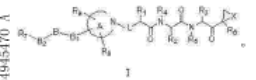
(74) 专利代理机构 杭州求是专利事务所有限公  
司 33200  
代理人 张法高 赵杭丽

(51) Int. Cl.  
*C07K 5/087*(2006.01)  
*C07K 5/083*(2006.01)

权利要求书3页 说明书24页 附图4页

(54) 发明名称  
杂环构建的三肽环氧酯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酯类化合物,以 Carfilzomib 为先导化合物,经缩合、酸性条件下脱去 Boc 保护基、碱性条件下反应得氨基酸甲酯异氰酸酯、水解、在缩合剂作用下获得。本发明是小分子短肽类蛋白酶抑制剂,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, N<sub>2</sub> 保护下加入 25mL 无水 CH<sub>2</sub>Cl<sub>2</sub>, 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 CH<sub>2</sub>Cl<sub>2</sub> 后缓缓滴入上述反应液,室温反应 6 小时。反应液加 30mL 饱和食盐水稀释,分出有机层,水层 CH<sub>2</sub>Cl<sub>2</sub> 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; <sup>1</sup>H NMR (500MHz, CDCl<sub>3</sub>): 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, CH<sub>2</sub>), 2.81 (m, 2H, CH<sub>2</sub>), 2.48 (m, 1H, CH), 1.93 (d, 2H, J=12.5Hz, CH<sub>2</sub>), 1.76 (m, 2H, CH<sub>2</sub>), 1.47 (s, 9H, CH<sub>3</sub>) ppm; ESI-MS: m/z = 307[M+H]<sup>+</sup>。

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

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

具体物质[Specific Substance]:

以具体化学结构陈述的特定物质, 会被分配CAS RN

# CAS Markush检索

预测性物质[Prophetic Substance]:

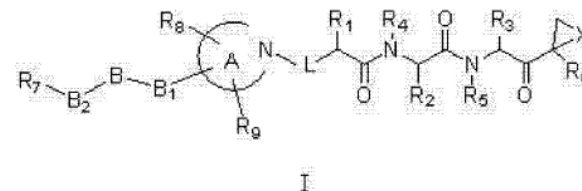
- 使用Markush结构陈述的预测物质，一个Markush可以陈述上百或上千个化学物质
- 被Markush结构包含，但未被实施或呈现在表格、权利要求书或说明书中的结构，不会被CAS分配CAS Registry Number
- Markush检索，能检索到通过结构检索检不到的专利

CN 104945470 A

权利要求书

1/3 页

1. 一种杂环构建的三肽环氧化物类化合物，具有下述结构通式 I：



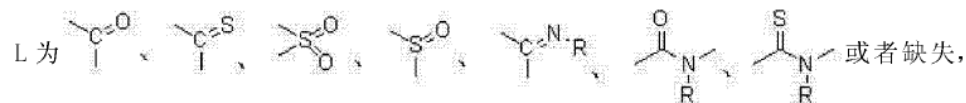
其中：

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

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

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

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

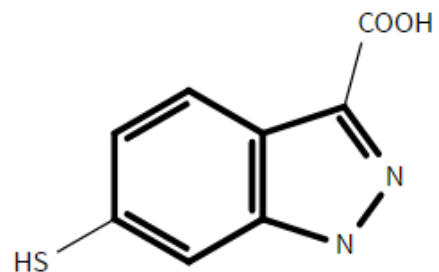


其中 R 选自 H、 $C_{1-6}$  烷基或卤代的  $C_{1-6}$  烷基；

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

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

# CAS Markush检索



<a href="#">Explore</a> ▾	<a href="#">Saved Searches</a> ▾	<a href="#">SciPlanner</a>
⚠ Explore Substances resulted in 0 substances <a href="#">Return</a>		
Chemical Structure substructure with limiters > <b>substances (0)</b>		
<b>SUBSTANCES</b>		
<a href="#">Analyze</a>	<a href="#">Refine</a>	
Analyze by: <i>No substances available</i>		

Substance检索结果为0!

# CAS Markush检索

Markush substructure > references (69)

REFERENCES Get Substances Get Reactions Get Related Citations Tools Create Keep Me Posted Alert Send to SciPlanner

Analyze Refine Categorize

Sort by: Accession Number

0 of 69 References Selected

Page: 1 of 4

Analyze by: Author Name

Boga Sobhana Babu	3
Deng Yongqi	3
Nan Yang	3
Paliwal Sunil	3
Shih Neng Yang	3
Shippis Gerald W Jr	3
Tsui Hon Chung	3
Alhassan Abdul Basit	2
Beier Norbert	2
Bulawa Christine Ellen	2

Show More

1. Preparation of ethynylheterocycles as rho-associated coiled-coil kinase (ROCK) inhibitors for the treatment of diseases

Quick View PATENTPAK

By Li, An-Hu; Sakilam, Satish Kumar; Gadhya, Satish Kumar; Lim, Dong Sung; Zong, Yao; Ponnala, Shashikanth; Zhang, Ying; Jung, Dawoon; Oehlen, Lambertus J. W. M. From PCT Int. Appl. (2021), WO 2021016256 A2 20210128. | Language: English, Database: CAPLUS

The invention relates to prepn. of ethynylheterocycles of formula (I): and pharmaceutically acceptable salts thereof, wherein Cy<sup>1</sup>, Cy<sup>2</sup>, Cy<sup>3</sup> 3 each independently represents an aryl, heteroaryl, or heterocyclic, which is optionally fused with a 3-8 membered cycloalkyl, 3-8 membered heterocycloalkyl, 6-membered aryl, or 5-6 membered heteroaryl; R<sup>1</sup>, R<sup>2</sup>, and R<sup>3</sup> each independently represents an aryl, heteroaryl, or heterocyclic, which is optionally fused with a 3-8 membered cycloalkyl, 3-8 membered heterocycloalkyl, 6-membered aryl, or 5-6 membered heteroaryl, and pharmaceutical compns. thereof, ...

2. Indazoles and azaindazoles as LRRK2 inhibitors in the treatment of CNS disorders and their preparation

Quick View PATENTPAK

By Garofalo, Albert W.; De Lombaert, Stephane; Schwarz, Jacob Bradley; Andreotti, Daniele; Sabbatini, Fabio Maria; Serra, Elena; Bernardi, Silvia; Migliore, Marco; Budassi, Federica; Beato, Claudia From PCT Int. Appl. (2021), WO 2021007477 A1 20210114. | Language: English, Database: CAPLUS



The invention relates compds. of formula I, their prepn. and their use as inhibitors of LRRK2 in the treatment of CNS disorders. Compd. I, wherein A is halo, (un)substituted C<sub>1-6</sub> alkyl, (un)substituted C<sub>2-6</sub> alkenyl, etc.; ring B is Ph and 5- to 10-membered heteroaryl wherein said 5- to 10-membered heteroaryl comprises 1, 2 and 3 ring-forming heteroatoms independently selected from N, O and S; X<sup>2</sup> is N and CR<sup>2</sup>; X<sup>3</sup> is N and CR<sup>3</sup>; X<sup>4</sup> is N and CR<sup>4</sup>; no more than two of X<sup>2</sup>, X<sup>3</sup> and X<sup>4</sup> are simultaneously N; R<sup>1</sup> is independently H, halo, C<sub>1-6</sub> alkyl, etc.; R<sup>2</sup> and R<sup>4</sup> are independently H, halo, C<sub>2-6</sub> alke...

3. Organic electroluminescent materials and devices

Quick View PATENTPAK

By Ji, Zhiqiang; Boudreaux, Pierre-Luc T.; Shih, Wei-Chun From U.S. Pat. Appl. Publ. (2020), US 20200358008 A1 20201112. | Language: English, Database: CAPLUS

Provided are organometallic compds. comprising novel ligands represented by a general chem. formula I (Y = R, OR, SR etc.; Z = O, S, NR<sup>n</sup>; X<sup>1-5</sup> = C, N; R<sup>A</sup>, R<sup>B</sup> = substitution; R, R<sup>n</sup> = alkyl, cycloalkyl heteroalkyl etc.) as OLED materials for OLED.



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

# 物质检索小结

1. 选择合适的检索方式
2. 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
3. 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
4. 正确理解Exact、Substructure、Similarity检索结果集的意义和范围
5. 充分利用物质筛选项准确定位目标物质：Reaction Role、Reference Role等
6. 利用CAS Markush检索尽可能全面的获得结构的公开信息



# 大纲

- CAS及CAS SciFinder介绍
- 文献相关信息的获取策略
  - 文献检索方法
  - 文献结果排序、筛选和详情
  - 如何高效阅读专利文献详情(CAS PatentPak)
- 物质相关信息的获取策略
  - 常见的物质检索方法
  - 物质结果排序、筛选和详情
- 反应相关信息的获取策略
  - 反应的获取方法
  - 反应结果排序、筛选和详情
  - 如何高效获取反应详情 (Synthetic Methods)
- 分析相关信息的获取 (CAS Analytical Methods)



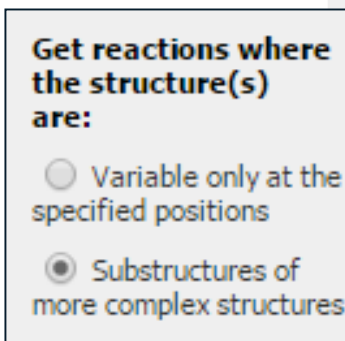
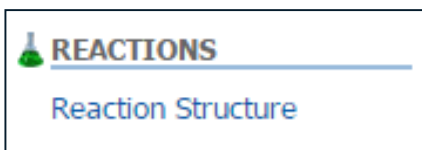
# CAS SciFinder检索--反应检索

## ■ 反应检索方法

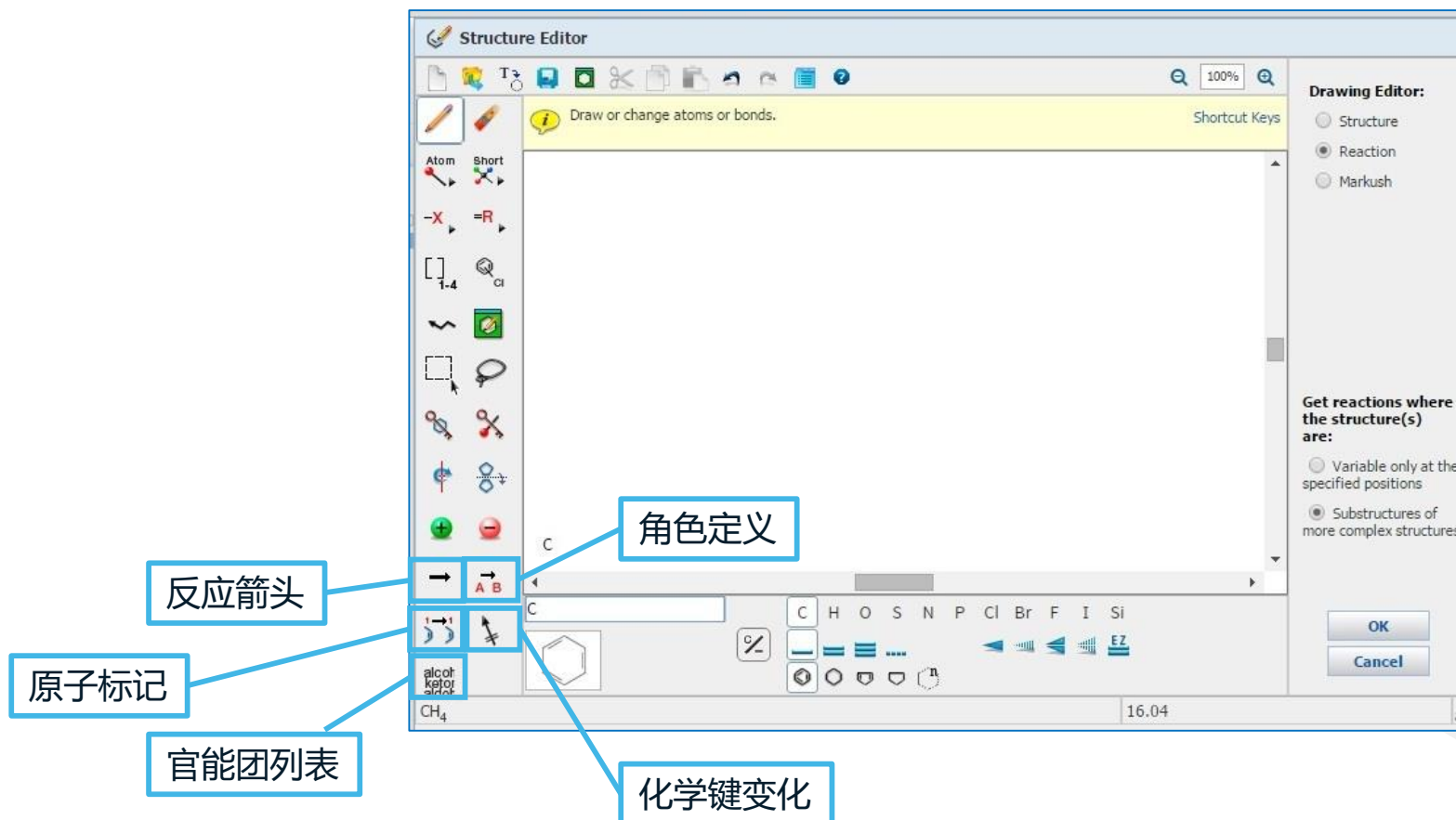
- 结构式

## ■ 常用获取方法

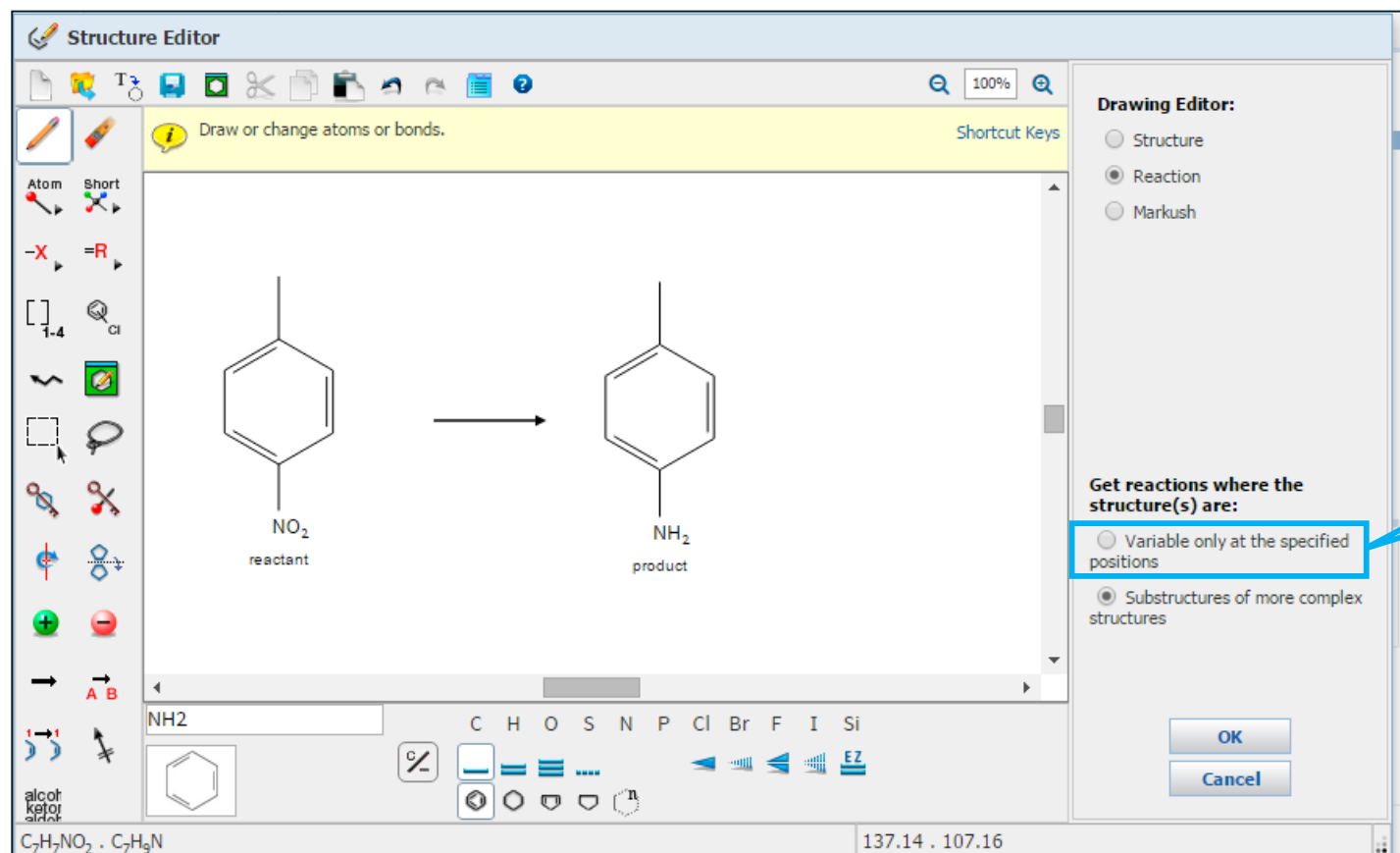
- 已知物质：由物质获取反应
- 已知文献：从文献中获取反应
- 精确结构反应检索
- 亚结构反应检索



# 结构编辑器--绘制反应工具



# 反应检索--精确反应检索



# 反应检索结果集--排序

浏览记录，发现很多反应来自同一篇文献，  
通过Group by Document合并。

The screenshot shows a web interface for viewing a chemical reaction. At the top, there are navigation options like 'Get References' and 'Tools'. A dropdown menu for 'Group by:' is open, showing 'No Grouping', 'Document', and 'Transformation', with 'Document' selected. A 'Sort by:' dropdown is set to 'Relevance'. A 'Send to SciPlanner' button is visible in the top right. Below the navigation, there are pagination controls showing 'Page: 1 of 11'. A 'Similar Reactions' button is highlighted with a callout box containing the text '获取相似反应'. The main reaction is shown as a chemical structure of 4-nitrotoluene reacting to form 4-aminotoluene, with a yield of 100%. Below the reaction, there is an 'Overview' section with 'Steps/Stages' (1.1 R:NaBH<sub>4</sub>, C:1832616-28-0, C:Ru, S:H<sub>2</sub>O, S:THF, 45 min, 25°C) and 'Notes' (solid-supported catalyst, ruthenium supported on porous organic polymer used, reusable catalyst, sealed tube used, scalable, Reactants: 1, Reagents: 1, Catalysts: 2, Solvents: 2, Steps: 1, Stages: 1, Most stages in any one step: 1). A 'References' section lists 'Fabrication of Ruthenium Nanoparticles in Porous Organic Polymers: Towards Advanced Heterogeneous Catalytic Nanoreactors'.

# 扩展反应检索--获取相似反应

选择相似反应的相似限制:

Broad: 仅反应中心相似

Medium: 反应中心及附属原子和键

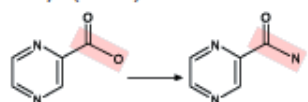
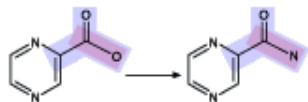
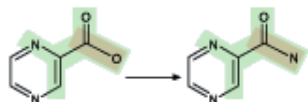
Narrow: 反应中心及扩展的原子和键

**Get Similar Reactions ?**

**Retrieve similar reactions from:**

- All reactions
- Current answer set

**Include this level of similarity:**

- Broad - Reaction centers only (2934)  

- Medium - Reaction centers plus adjacent atoms and bonds (109)  

- Narrow - Reaction centers plus extended atoms and bonds (95)  


# 按照反应类型排序

Group by: Transformation ▼ Sort by: Frequency ▼ ↓

0 of 560 Reactions Selected

1. Reduction of Nitro Compounds to Amines  
538 Reactions

$$\text{R-NO}_2 \longrightarrow \text{R-NH}_2$$

2. Reduction of Nitro to Azo Compounds  
11 Reactions

$$\text{Ar-NO}_2 \longrightarrow \text{Ar-N=N-Ar}$$

3. Reduction of Nitro to Azoxy Compounds  
11 Reactions

$$\text{Ar-NO}_2 \longrightarrow \text{Ar-N}^+\text{=N-Ar} \text{O}^-$$

更精确的查找需要的反应

# 反应检索结果集--筛选

获得特定物质做还原剂的反应

REACTIONS

Get References Tools

Send to SciPlann

Analyze Refine

Analyze by: Reagent

H <sub>2</sub>	148
NaBH <sub>4</sub>	51
N <sub>2</sub> H <sub>4</sub> ·H <sub>2</sub> O	43
KOH	17
CO	16
HCO <sub>2</sub> H	16
NH <sub>4</sub> <sup>+</sup> ·HCO <sub>2</sub> <sup>-</sup>	16
H <sub>2</sub> O	14
N <sub>2</sub> H <sub>4</sub>	14
NaOH	14

Show More

Group by: No Grouping Sort by: Relevance

0 of 512 Reactions Selected

1. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.

Cc1ccc(cc1[N+](=O)[O-]) → Cc1ccc(cc1)N

~102 100% ~122

Overview

Steps/Stages

1.1 R:NaBH<sub>4</sub>, C:1832616-28-0, C:Ru, S:H<sub>2</sub>O, S:THF, 45 min, 25°C

Notes

solid-supported catalyst, ruthenium supported on porous organic polymer used, reusable catalyst, sealed tube used, scalable, Reactants: 1, Reagents: 1, Catalysts: 2, Solvents: 2, Steps: 1, Stages: 1, Most stages in any one step: 1

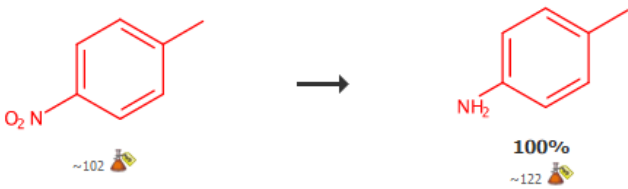
References



Fabrication of Ruthenium Nanoparticles in Porous Organic Polymers: Towards Advanced Heterogeneous Catalytic Nanoreactors



# 反应检索结果--Experimental Procedure

Single Step *Hover over any structure for more options.*



~102       100%  
~122 

▼ **Overview**


**Steps/Stages**

1.1 R:H<sub>2</sub>, R:Cs<sub>2</sub>CO<sub>3</sub>, C:1610424-70-8, C:1034343-98-0 (oxide), S:PhMe, 2 h, 100°C, 1 atm


**Notes**

solid-supported catalyst, palladium catalyst supported on graphene oxide prepared and used, reusable catalyst, Reactants: 1, Reagents: 2, Catalysts: 2, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

**References**

Catalyst Enhancement and Recyclability by Immobilization of Metal Complexes onto Graphene Surface by Noncovalent Interactions  
Quick View  Other Sources  
By Sabater, Sara et al  
From ACS Catalysis, 4(6), 2038-2047; 2014

▼ **Experimental Procedure**

 **Catalysis** General/Typical Procedure: **General Procedure for Nitroarene Reductions.** Molecular hydrogen was added with a balloon filled with 1 atm of H<sub>2</sub> to a mixture of nitroarene (0.3 mmol), Cs<sub>2</sub>CO<sub>3</sub> (0.3 mmol), anisole as internal standard (0.3 mmol), and NHC-Pd-rGO (6 × 10<sup>-3</sup> mmol, based on metal) in toluene (5 mL). The system was then evacuated and backfilled with H<sub>2</sub> in cycles for three times before putting the reaction vessel in an oil bath at 100°C for 2h. Yields were determined by GC analyses using anisole (0.3 mmol) as internal standard. Products were identified according to spectroscopic data of the commercially available compounds. Entry: 4; Yield 100%.

不用阅读全文，直接获得包含实验过程的反应记录

# 反应检索结果--MethodsNow

REACTIONS Get References Tools

Analyze Refine

Analyze by: MethodsNow

MethodsNow Not Available 1890

MethodsNow Available 1029

Show More

Group by: No Grouping Sort by: Relevance

0 of 2919 Reactions Selected

20. [View Reaction Detail](#) [Link](#) [Similar Reactions](#)

Single Step *Hover over any structure for more options.*

Overview

**METHODSNOW™**

**Procedure**

1. Place Pd@Hal-CCD catalyst (1 wt%) and nitroarene (1 mmol) in deionized water
2. Purge hydrogen (1 bar) as reducing agent into the stirring reaction mixture at r

[View more...](#)

[View with MethodsNow](#)

**MethodsNow**

**Pd stabilized on nanocomposite of halloysite and  $\beta$ -cyclodextrin derived carbon: An efficient catalyst for hydrogenation of nitroarene**

By Sadjadi, Samahe; Ghoreyshi Kahangi, Fatemeh; Heravi, Majid M.  
From Polyhedron, 175, 114210; 2020  
Published by Elsevier Ltd.

Products

Aniline, 100%, CAS RN: 62-53-3

Reactants

Nitrobenzene, CAS RN: 98-95-3

Reagents

Hydrogen, CAS RN: 1333-74-0

Catalysts

Palladium, CAS RN: 7440-05-3

Solvents

Water, CAS RN: 7732-18-5

**Procedure**

1. Place Pd@Hal-CCD catalyst (1 wt%) and nitroarene (1 mmol) in deionized water as solvent (2 mL) in the reaction vessel.
2. Purge hydrogen (1 bar) as reducing agent into the stirring reaction mixture at room temperature for 1.5 h.
3. Hold the reaction and separate Pd@Hal-CCD from the reaction mixture.
4. Isolate the aniline by evaporation of water.
5. Recycle Pd@Hal-CCD and wash the recovered catalyst with water and EtOH several times.
6. Dry in oven at 80°C for 8 h.

Transformation

Reduction of Nitro Compounds to Amines

CAS Method Number

3-522-CAS-21010612

Print/Export Close

物质信息  
名称、角色

实验过程

反应类型

MethodsNow中的实验详情不仅包含原文中描述的实验内容，还包括supporting information中涉及的实验内容

# SciPlanner--设计合成反应路线

点击打开SciPlanner工作界面

The screenshot displays the SciPlanner web interface. At the top, there are navigation tabs: 'Explore', 'Saved Searches', and 'SciPlanner'. Below this, the breadcrumb path reads 'Reaction Structure substructure > reactions (1208) > refine "Catalyzed" (535)'. The main area is titled 'REACTIONS' and includes options for 'Get References' and 'Tools'. A list of reactions is shown, with the first one selected. A callout box points to the 'Send to SciPlanner' button in the top right of the reaction list. Below the list, a chemical reaction scheme is shown, featuring a benzimidazole derivative reacting with cyclohexylamine to form a substituted benzimidazole. The reaction is labeled '1. View Reaction Detail' and 'Single Step'. A callout box points to the reaction scheme with the text '选择感兴趣的反应, 点击send to SciPlanner'.

选择感兴趣的反应, 点击send to SciPlanner

# SciPlanner--工作界面

SciPlanner\_09\_01\_2016\_172400

Workspace Edit View GoTo

Click and drag to workspace

Clear Reactions

SciPlanner\_09\_01\_2016\_172400

Workspace Edit View GoTo

Clear Reactions

# SciPlanner--工作界面

The screenshot displays the SciPlanner software interface. At the top, the title bar reads "SciPlanner" and "SciPlanner\_09\_01\_2016\_172400". Below the title bar is a menu bar with "Workspace", "Edit", "View", and "GoTo". The main workspace shows a chemical structure of cyclohexylamine with a double-headed arrow icon in its top right corner. A context menu is open over this structure, listing options: "CAS Registry Number: 85-44-9", "View Substance Detail", "Explore by Structure", "Synthesize this...", "Get Reactions where Substance is a", "Get Commercial Sources", "Get Regulatory Information", "Get References", and "Export as Image". A blue callout box points to the double-headed arrow icon with the text: "点击物质右上角的双箭头, 检索其合成方法".

Below the workspace, a panel titled "Get References" and "Tools" shows search results. It includes a "Group by" dropdown set to "No Grouping" and a "Sort by" dropdown set to "Accession Number". Below this, it indicates "1 of 382 Reactions Selected". A specific reaction is highlighted: "4. View Reaction Detail" with a "Link" icon and "Similar Reactions" link. The reaction is a "Single Step" conversion of phthalic acid to phthalic anhydride, with a yield of 97%. A "Send to SciPlanner" button is located in the top right corner of this panel, with a blue callout box pointing to it containing the text: "从结果中选择感兴趣的反应, 继续推送至SciPlanner".

# SciPlanner--工作界面

The image displays two screenshots of the SciPlanner software interface. The top screenshot shows a workspace with a chemical reaction (1) and a sidebar with another reaction (2). A blue arrow points from the sidebar to the workspace with the text "继续拽至工作区". The bottom screenshot shows the same workspace with both reactions (1) and (2) moved to the main area and highlighted with blue boxes. A blue arrow points from the top screenshot to the bottom one. Text in the bottom screenshot reads "两个反应在同一工作窗口" and "将相同的两个结构移动至重叠".

继续拽至工作区

两个反应在同一工作窗口

将相同的两个结构移动至重叠

# SciPlanner--设计拟合成的反应路线

SciPlanner 导出设计的路线

SciPlanner\_09\_01\_2016\_172400

Workspace Edit View GoTo

New  
Open  
Save  
Duplicate  
Import  
Export  
Print  
Close

合成为一的合成路线

Clear Reactions

Export

For:

Offline Review

- Portable Document Format (\*.pdf)
- Citations (\*.ris)
- Image (\*.png)

Saving Locally

- SciPlanner eXchange (\*.pkx)

Details:

File Name: \*  
SciPlanner\_09\_01\_2016\_172400

Title

Include:

- SciPlanner Image
- Reaction Details
- Substance Details
- Reference Details

Export Cancel

# 反应检索小结

1. 反应检索方法汇总与区分
2. 反应绘制工具的灵活使用
3. 反应结果排序: Group by Transformation/Document
4. 反应结果的快速纵览及筛选, 例如non-participating functional group;
5. 相似反应的获取获得更多启发
6. MethodsNow获取反应详情
7. SciPlanner工具助于自定义设计拟合成反应路线



# 大纲

- CAS及CAS SciFinder介绍
- 文献相关信息的获取策略
  - 文献检索方法
  - 文献结果排序、筛选和详情
  - 如何高效阅读专利文献详情(CAS PatentPak)
- 物质相关信息的获取策略
  - 常见的物质检索方法
  - 物质结果排序、筛选和详情
- 反应相关信息的获取策略
  - 反应的获取方法
  - 反应结果排序、筛选和详情
  - 如何高效获取反应详情 (Synthetic Methods)
- 分析相关信息的获取 (CAS Analytical Methods)



# MethodsNow – CAS Analytical Methods

## [www.methodsnow.com](http://www.methodsnow.com)

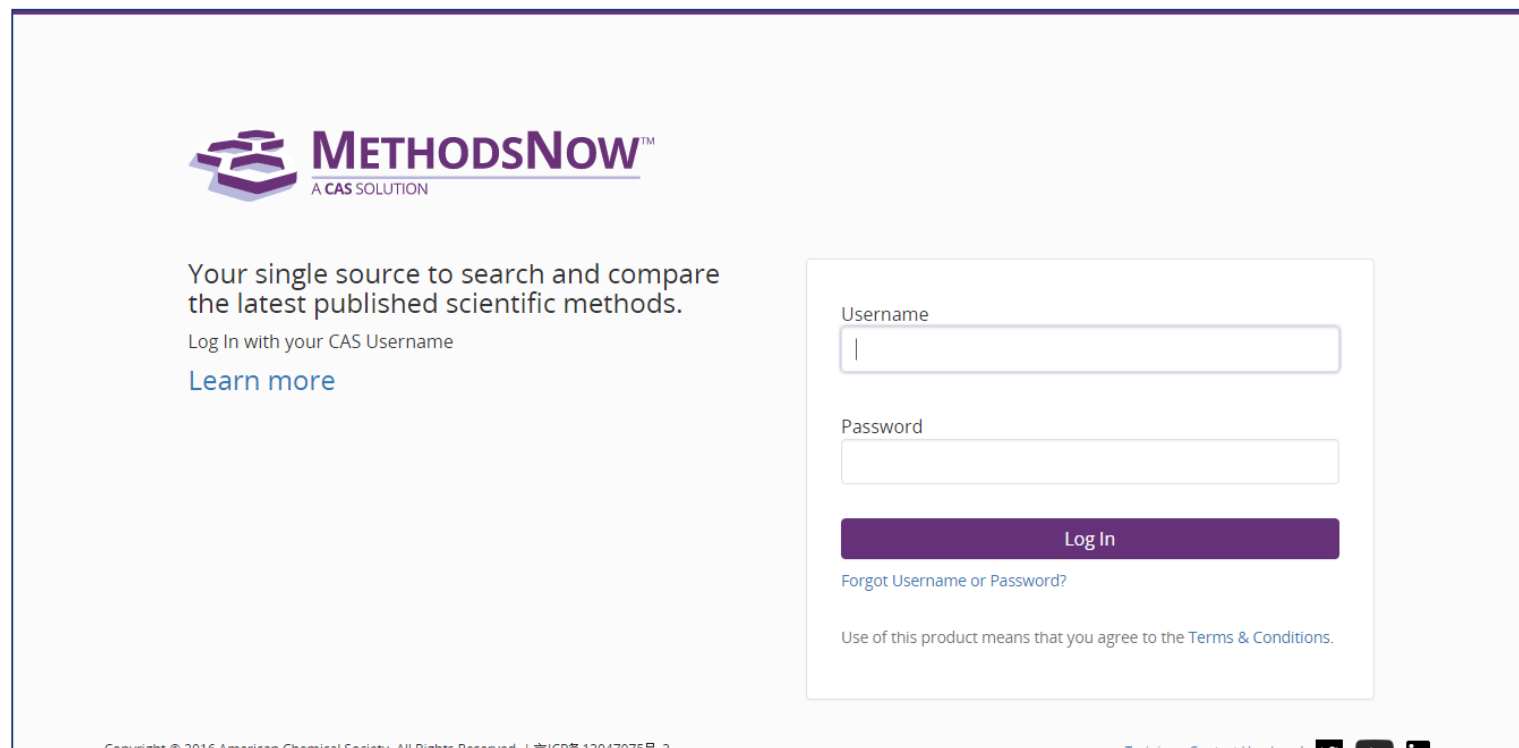
- Organic Compound Analysis: 天然产物分离分析, 手性分离, 活性药物成分及代谢产物分析...
- Organometallics / Inorganics: 地质分析, 无机物分析, 金属有机化合物分析
- Pharmacology / Toxicology: 成瘾药物检测, 有毒物检测...
- Bioassays: 生物探针, 生物标定细胞实验, 生物标定药物实验, 生物医学材料分析, 生物分子/生物组织分离测定...
- Water Analysis: 阴阳离子分析, 元素测定, 痕量元素分析, 废水分析, 生物标记公共卫生分析...
- Historical 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...


目前有13个大类, 45个小类。某些子项目属于多种方法分类



# MethodsNow – CAS Analytical Methods

([www.methodsnow.com](http://www.methodsnow.com))



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登陆[www.methodsnow.com](http://www.methodsnow.com)  
输入SciFinder的账号密码



# MethodsNow – CAS Analytical Methods

([www.methodsnow.com](http://www.methodsnow.com))

The screenshot shows the MethodsNow website interface. At the top left, there is a navigation menu with 'CAS Solutions' and the 'METHODSNOW' logo. On the top right, there are links for 'Saved' (with a star icon) and 'Account' (with a person icon). The main section is titled 'Search' and contains a search bar with the placeholder text 'Enter keyword, matrix, analyte, etc.' and a search button. Below the search bar is a link for 'Advanced Search'. The 'Browse Method Categories' section lists various categories such as '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', and 'Water Analysis'. At the bottom, there is a 'Recent Searches' section showing 'hplc lycopene analysis' with a close button (X).

检索/高级检索 →

方法分类 →

历史检索 →

保存结果集

点击一个类别浏览  
相关方法

点击历史检索重  
新运行检索

点击“X”  
删除检索历史

# MethodsNow – CAS Analytical Methods

([www.methodsnow.com](http://www.methodsnow.com))

The image shows two overlapping screenshots of the MethodsNow Advanced Search interface. The top screenshot shows the search criteria input area with annotations: '支持逻辑运算符: and, or, not' (Supports logical operators: and, or, not) pointing to the AND dropdown, and '删除检索条件' (Delete search criteria) pointing to the close button. The bottom screenshot shows the search criteria dropdown menu with an annotation: '增加检索条件' (Add search criteria) pointing to the search button. A larger annotation in the bottom screenshot lists search options: '检索选项: 关键词、分析物、基质、方法分类、技术、CAS Method Number、期刊名' (Search options: Keyword, Analyte, Matrix, Method Category, Technique, CAS Method Number, Journal Name).

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← Return to Home

Advanced Search

Keyword

AND Matrix

AND Analyte

Add Search Criteria

增加检索条件

支持逻辑运算符: and, or, not

删除检索条件

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← Return to Home

Advanced Search

Publication Name

Keyword

Analyte

Matrix

Method Category

Technique

CAS Method Number

Publication Name

检索选项: 关键词、分析物、基质、方法分类、技术、CAS Method Number、期刊名

# 案例：高效液相色谱法测定血液中罗红霉素的含量

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## Search

Enter keyword, matrix, analyte, etc.

roxithromycin

Advanced Search

### Browse Method Categories

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



# 结果显示

## Method Detail (2 of 5)

实验材料

文献信息

### Analysis of Roxithromycin in Blood plasma by HPLC

CAS MN: 1-101-CAS-67878

Method Category: Active Pharmaceutical Ingredient and Metabolite Analysis

Technique: Fluorescence; HPLC

Materials	Role
Roxithromycin	analyte
Blood plasma	matrix
Column, 125 x 4.6 mm i.d. LiChrospher RP-18e	material
SPE Bakerbond cartridges, C18	material

#### Source

Determination of roxithromycin in human plasma by HPLC with fluorescence and UV absorbance detection: Application to a pharmacokinetic study  
Glowka, Franciszek K.; Karazniewicz-Lada, Marta

Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences (2007), 852 (1-2), 669 - 673. Elsevier B.V.

CODEN: JCBAAI | ISSN: 15700232 | DOI: 10.1016/j.jchromb.2007.02.022

Document Sources

#### Abstract

A selective HPLC method with fluorescence detection for the determination of roxithromycin (ROX) in human plasma was described. After solid-phase extraction (SPE), ROX and erythromycin (internal standard, I.S.) were derivatized by treatment with 9-fluorenylmethyl chloroformate (FMOC-Cl). Optimal resolution of fluorescence derivatives of ROX and I.S. was obtained during one anal. run using reversed phase, C<sub>18</sub> column. The mobile phase was composed of potassium dihydrogenphosphate solution, pH 7.5 and acetonitrile. Fluorescence of the compounds was measured at the maximum excitation, 255 nm and emission, 313 nm, of ROX derivatives. Validation parameters of the method were also established. After SPE, differences in recoveries of ROX and erythromycin from human plasma were observed. The linear range of the standard curve of ROX in plasma was 0.5-10.0 mg/l. The validated method was successfully applied for pharmacokinetic studies of ROX after administration of a single tablet of ROX.

设备条件

### Equipment Used

HPLC system, HP 1100, Hewlett-Packard, Waldbronn, Germany

Autosampler, G1313A

### Conditions

#### Chromatographic

HPLC : mobile phase : 700 ml of acetonitrile + 300 ml of a 0.05 mol/L potassium dihydrogenphosphate solution in water, adjust to pH 7.5 with a 10% sodium hydroxide solution.  
column oven : at 40 °C, fluorescence detector excitation wavelength

### Instructions

#### Standards Preparation

1. Prepare stock solutions of roxithromycin (ROX) and erythromycin (I.S.) with 1 g each in methanol.
2. Prepare standard solutions: 5.0, 7.5, 15.0, 20.0, 50.0, 75.0 and 100.0 mg/L of ROX and I.S. in methanol.
3. Transfer the volume of 50 µL aliquots of the sample to a glass vial containing 0.5 ml blank human plasma.

#### Solid phase extraction procedure

1. Process the resulting plasma samples containing: 0.5, 0.75, 1.5, 2.0, 5.0, 7.5 and 10.0 mg/l of ROX and 20.0 mg/l of I.S. according to the SPE.
2. Add the volume of 0.5 ml of a phosphate buffer, pH 7.5 (prepared as a mixture of 85.2 ml of 1/15 M Na<sub>2</sub>HPO<sub>4</sub> and 14.8 ml 1/15 M KH<sub>2</sub>PO<sub>4</sub>).
3. Transfer the samples into C18 SPE Bakerbond cartridges (J.T. Baker Mallinckrodt Deventer, Holland).
4. Wash the absorbed analytes with water and elute with methanol.
5. Evaporate the organic liquid to dryness at 40 °C.

#### Derivatization

1. Dissolve the residue in 200 µL aliquots of acetonitrile and transfer the sample to a glass reaction vial.
2. Add a 100 µL aliquots of a 2.5 mg/L 9-fluorenylmethyl chloroformate (FMOC-Cl) in acetonitrile and 100 µL aliquots of a phosphate buffer, pH 7.5.
3. Incubate the sample at 40 °C for 40 min.
4. Inject an aliquot 100 µL after derivatization, onto the chromatographic system.

#### HPLC

1. Prepare the mobile phase by mixing 700 mL of acetonitrile with 300 ml of a 0.05 mol/L solution of potassium dihydrogenphosphate in water, adjust to pH 7.5 with a 10% sodium hydroxide solution.
2. Determine ROX and I.S. in human plasma in a chromatograph model HP 1100 (Hewlett-Packard, Waldbronn, Germany).
3. Set at a flow rate of quaternary pump at 2 mL/min, a column oven at 40 °C and a fluorescence detector model HP 1046A and G13 21 A-1100, at an excitation wavelength (Ex) of 255 nm and emission wavelength (Em) of 315 nm.
4. Inject the samples (100 µL) using autosampler model G1313A.
5. Perform the separation on a 125 x 4.6 mm i.d. LiChrospher RP-18e column packed with 5 µm particles, with a guard column (LiChrospher RP-18e), both from Merck.

实验步骤



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# 结果显示

	1	2	3
Title	Analysis of Roxithromycin in Blood plasma by HPLC-tandem mass spectrometry	Analysis of Roxithromycin in Blood plasma by HPLC	Analysis of Roxithromycin in Blood plasma by High-performance liquid chromatography-mass spectrometry
CAS Method Number	1-101-CAS-1241367	1-101-CAS-67878	1-101-CAS-10378
Method Category	Active Pharmaceutical Ingredient and Metabolite Analysis	Active Pharmaceutical Ingredient and	Active Pharmaceutical Ingredient and
Technique	HPLC-tandem mass spectrometry	Other Materials Methanol; Acetonitrile; Ammonium acetate; Heparin; C <sub>18</sub> analytical column (150 mm x 4.6 mm, 5 μm)	Column, 125 x 4.6 mm i.d. LiChrospher RP-18e; SPE Bakerbond cartridges, C18
Analyte	Roxithromycin; Ambroxol hydrochloride	Equipment Used LC-MS/MS system, Thermo Finnigan, San Jose, CA; LC pump, Surveyor, Thermo Finnigan, San Jose, CA; <a href="#">View All</a>	HPLC system, HP 1100, Hewlett-Packard, Waldbronn, Germany; Autosampler, G1313A
Matrix	Blood plasma	Conditions <b>Instrument:</b> Column: C <sub>18</sub> analytical column; column temperature: 30 °C; mobile phase: mixture of methanol <a href="#">View All</a>	<b>Instrument:</b> Detection- SIM mode. <b>Chromatographic:</b> Injection volume- 20 μL; mobile phase- (75:25, v/v) of <a href="#">View All</a>
		Source Simultaneous determination and pharmacokinetic study of roxithromycin and ambroxol <a href="#">View All</a>	Stochastic resonance is applied to quantitative analysis for weak chromatographic signal of <a href="#">View All</a>
		Preparation Collection of plasma samples	Standards Preparation Plasma samples

导出对比PDF文件



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# 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



吉林大学图书馆  
Jilin University Library

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检索

资源 | 服务 | 概况 | 帮助

首页 » 数据库 » 外文

## SciFinder美国化学文摘数据库

访问地址: <https://scifinder.cas.org>

**Access**

新用户账号注册入口

[Register Now](#)

已有账号用户访问入口

[Sign in to SciFinder](#)

SciFinder数据库最新版本使用指南: [SciFinder 使用指南.pdf](#)

### What Is SciFinder?

SciFinder由美国化学会 (American Chemical Society, ACS) 旗下的美国化学文摘社 (Chemical Abstracts Service, CAS) 出品, 是一个研发应用平台, 提供全球

# 如何获取CAS SciFinder账号

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First Name:

Last Name:

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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。

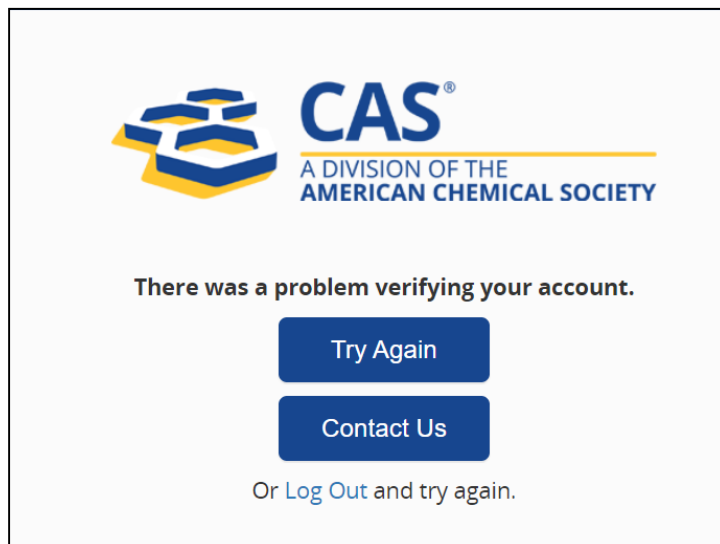
单击 Register (注册) 。

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

# 使用注意事项

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

# 常见问题



- 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](mailto:china@acs-i.org)

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