

美国化学文摘社北京代表处

从SciFinder中获取科技信息

2020年10月

提纲

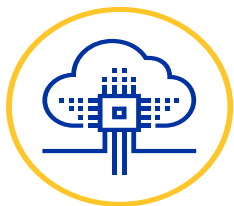
- 美国化学文摘社简介
- SciFinder简介及检索方式
 - 文献检索
 - 物质检索
 - Markush检索
 - 反应检索
 - SciPlanner
- SciFinder常见问题及解决

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
SCIENTIFIC CONTENT
独特的内容



SPECIALIZED
TECHNOLOGY
专业技术



UNMATCHED
HUMAN EXPERTISE
科学家团队

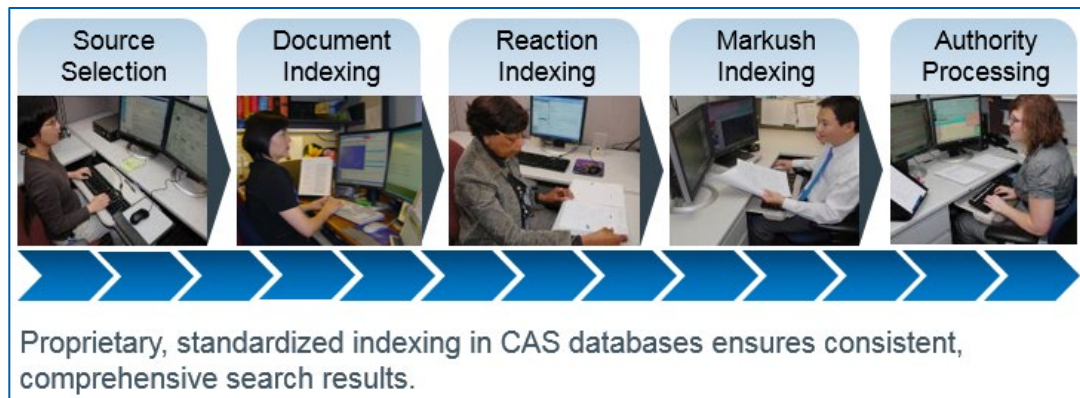


CAS
A DIVISION OF THE
AMERICAN CHEMICAL SOCIETY

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。

CAS各类科学信息研究工具

STNext

SCIFINDER
A CAS SOLUTION

PATENTPAK
A CAS SOLUTION

FORMULUS
A CAS SOLUTION

SCIFINDERⁿ
A CAS SOLUTION

CHEMZENT
A CAS SOLUTION

More
coming!

METHODSNOW
A CAS SOLUTION

NCI GLOBAL
A CAS SOLUTION



CAS最新解决方案

- CAS于2015年2月正式发布PatentPak™
- 强大的专利工作流程解决方案
- 极大节约用户在研究专利时的时间
- 快速查找定位专利中的关键化学信息
- 通过SciFinder和STN来使用

6. Preparation of substituted nucleosides, nucleotides and analogs thereof as antiviral agents

Quick View **PATENTPAK**

By Beigelman, Le...
From PCT Int. App...
Disclosed he...
phosphate, R...
methods of t...
medicament

Patent No.	Kind	Language
WO 2016100441	A1	English

Patent Family

Patent No.	Kind	Language
US 20160176911	A1	English

atkina, Natalia
Language: English, Database: CAPLUS

R⁶ is substituted purine and pyrimidine nucleobase; dashed bond between R and R⁴ is absent, then R is H, substituted
each R⁶ and R⁷ are independently
as a HCV infection with one or m...
a hepatitis C virus.

7. Process for preparation of sofosbuvir

Quick View **PATENTPAK**

By Fr...
04

ZOOM +

DOWNLOAD PDF

Search in SciFinder | View Detail

Analyst Markup Locations (1)

page 130

8. Q. By Fr...

(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(19) World Intellectual Property Organization

(43) International Publication Date
23 June 2016 (23.06.2016)

WIPO | PCT

(51) International Patent Classification:

C07H 19/10 (2006.01)	C07H 19/173 (2006.01)
C07H 19/20 (2006.01)	A61K 31/7072 (2006.01)
C07H 19/31 (2006.01)	A61K 31/7076 (2006.01)
C07H 19/215 (2006.01)	A61K 31/708 (2006.01)
C07H 19/067 (2006.01)	A61P 31/14 (2006.01)
C07H 19/073 (2006.01)	

(21) International Application Number:
PCT/US2015/065981

(22) International Filing Date:
16 December 2015 (16.12.2015)

(25) Filing Language:
English

(81) Designated States (kind of national protection):
AO, AT, AU, AZ, BA, BB, BG, BR, CA, CH, CL, CN, CO, CZ, DE, DK, EE, EG, ES, FI, FR, GB, GR, HK, HU, ID, IL, IN, JP, KE, KG, KH, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LU, LY, MA, MD, ME, MK, MN, MW, MX, MY, NG, NI, NO, NZ, OM, PA, PE, PG, PH, PL, PT, QA, RO, RS, RU, RW, SA, SC, SD, SE, SG, SK, SL, SM, ST, SV, SY, TH, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW.

(84) Designated States (unless otherwise indicated, for every kind of regional protection available): ARIPO (BW, GH, GM, KE, LU, MW, NI, SD, SN, TZ, ZM, ZW); Eurasian (AM, AZ, BY, KG, KZ, RU, TJ, TM); European (AL, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LT, LU, LV, MA, MT, NL, NO, PL, PT, RO, SE, SI, SK, TR); African and Asian (AO, AU, BB, BN, BR, BY, CA, CH, CL, CN, CO, KR, KP, KZ, LA, LC, LK, LR, LY, MA, MD, ME, MK, MN, MW, MX, MY, NG, NI, NO, NZ, OM, PA, PE, PG, PH, PL, PT, QA, RO, RS, RU, RW, SA, SC, SD, SE, SG, SK, SL, SM, ST, SV, SY, TH, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW).

Chemical Reaction Scheme:

WO 2016/100441 **PCT/US2015/065981**

EXAMPLE 1 COMPOUND 1

Reaction scheme showing the synthesis of Example 1 Compound 1. The scheme includes starting materials, reagents (dichloromethane, pyridinium dichromate, acetic anhydride, tert-butanol), and intermediates (1-1, 1-2, 1-3, 1-4, 1-5, 1-4a).

CAS RN 1206126-39-7

Search in SciFinder | View Detail

Analyst Markup Locations (1)

page 130

CAS RN 1206126-41-1



CAS最新解决方案

- CAS于2016年2月正式发布MethodsNow™
- 全球最大的方法信息合集
- 来自重要的全文信息资源：CAS高质量标引、全新的、增值的方法
- 满足合成和分析研究工作者的需求
- 合成方法通过SciFinder来使用，分析方法通过www.methodsnow.com获取

MethodsNow

A Cycloisomerization/Friedel-Crafts Alkylation Strategy for the Synthesis of Pyrano[3,4-b]indoles

By Medeiros, Matthew R.; Schaus, Scott E.; Porco, John A., Jr.
From Organic Letters, 13(15), 4012-4015; 2011
Published by American Chemical Society

35%

18%

嵌在SciFinder中的合成模块

Products	D-erythro-Hex-2-enitol, 1,5-anhydro-2,3-dideoxy-4-O-(1H-indol-2-ylmethyl)-6-O-methyl-1-C-phenyl-, (1S), 35%, CAS RN: 1314595-76-0 D-erythro-Hex-2-enitol, 1,5-anhydro-2,3-dideoxy-6-O-methyl-1-C-phenyl-, (1S), 18%, CAS RN: 1314595-77-1
Reactants	D-erythro-Hex-2-enitol, 4-O-[3-(2-aminophenyl)-2-propenyl-1-yl]-1,5-anhydro-2,3-dideoxy-6-O-methyl-1-C-phenyl-, (1S), CAS RN: 1314595-75-9
Catalysts	Platinum chloride (PtCl ₂), CAS RN: 10025-65-7
Solvents	Nitromethane, CAS RN: 75-52-5
Procedure	1. Cool a solution of 2-(3-((2R,3S,6S)-2-(methoxymethyl)-6-phenyl-3,6-dihydro-2H-pyran-3-yl)oxy)prop-1-en-1-yl)aniline (99.0 mg, 0.283 mmol) in CH ₂ Cl ₂ (2.8 mL) to 0 °C. 2. Add PtCl ₂ (15.0 mg, 0.566 mmol) to the reaction mixture. 3. Stir the reaction mixture for 20 minutes at 0 °C. 4. Remove the reaction mixture from the ice bath when TLC analysis shows no reaction. 5. Stir the reaction mixture at room temperature.

Print/Export Close

CAS Solutions

METHODSNOW™

atorvastatin

Results (528)

Sort Relevance

Return to Home

Analyte

- Atorvastatin (227)
- Atorvastatin calcium (211)
- Ezetimibe (80)
- Amlodipine besylate (56)
- Fenofibrate (46)

View All

Matrix

- Pharmaceutical tablets (293)
- Blood plasma (60)
- Tablets (49)
- Pharmaceutical capsules (34)
- Garcinia atroviridis (20)

View All

Method Category

Technique

- Reversed-phase HPLC (152)
- Spectrophotometry (101)
- UV-visible spectroscopy (71)
- HPLC (57)
- Liquid chromatographic UV detectors (43)

View All

Analysis of Atorvastatin in Blood plasma by High-performance thin layer chromatography

CAS MN: 1-101-CAS-1389

View Details & Instructions

Add to Compare

Analyte: Atorvastatin

Matrix: Blood plasma

Other Materials: Material: 60 F₂₅₄ silica gel HPLC plates

Method Category: Active Pharmaceutical Ingredient and Metabolite Analysis

Technique: High-performance thin layer chromatography

Equipment Used: Automatic TLC Sampler 3

Source: HPLC determination of atorvastatin in plasma

Jamshidi, A.; Nateghi, A. R.
Chromatographia (2007), 65 (11/12), 763-766. Vieweg Verlag/GWV Fachverlage GmbH

Document Sources

Abstract

单独的分析界面

LIMITLESS POSSIBILITIES 无限可能

定制服务应对挑战.



CONTENT SERVICES 内容服务

- 定制数据集合
Content licensing
- 数据结构
Data structure
- 数据平台
Data platforms



TECHNOLOGY SERVICES 技术服务

- 数据架构
Data architecture
- 平台整合
Platform integration
- 检索引擎
Search engines
- 定制解决方案
Custom solutions



KNOWLEDGE SERVICES 知识服务

- 外包IP检索
Outsourced IP search
- 数据分析
Analytics
- 机会分析
Opportunity exploration
- 技术评估
Technical Assessment



PROFESSIONAL SERVICES 专业服务

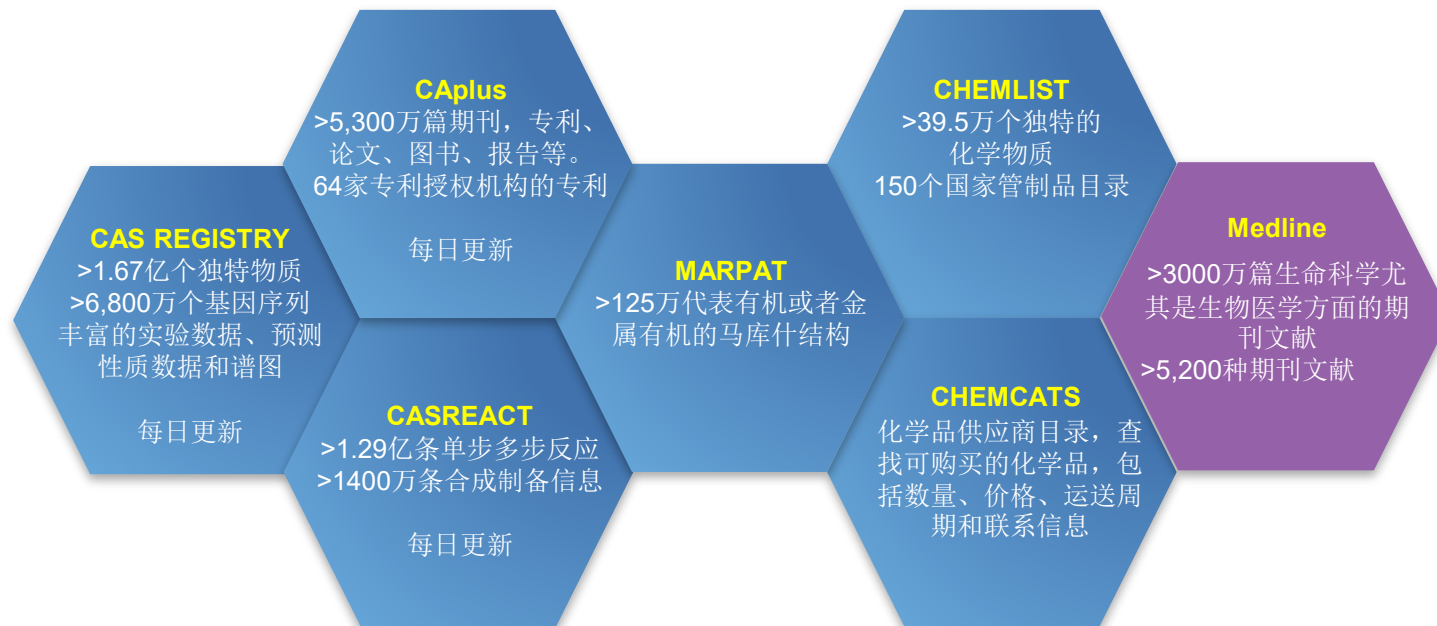
- 人员派遣
Talent augmentation
- 咨询
Consulting
- Technical writing
科技写作
- Scientific analysis
科研分析



提纲

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

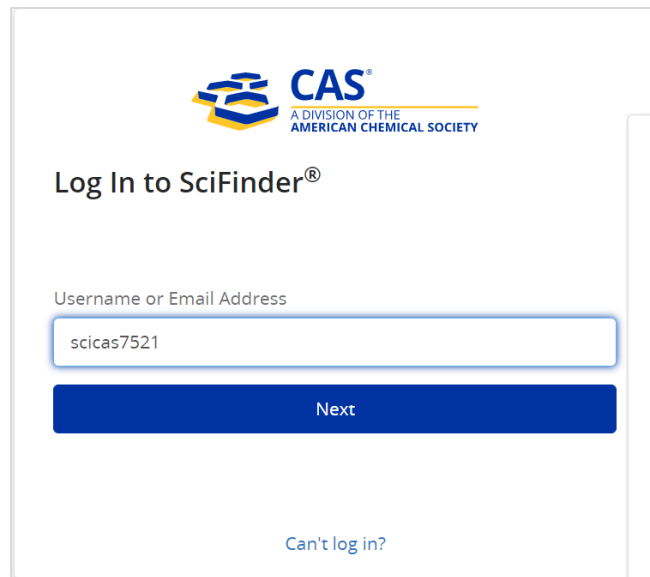
SciFinder覆盖的数据库



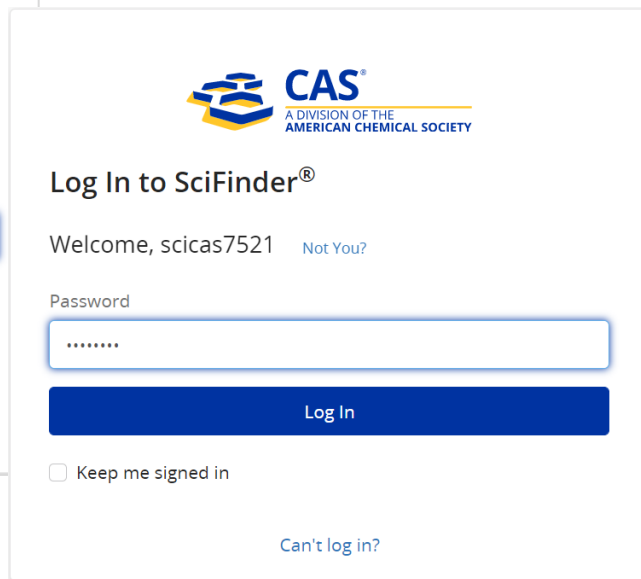
SciFinder是提供经CAS科学家人工智力标引内容的工具型数据库。

Source: <https://www.cas.org/about/cas-content>

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



The screenshot shows the SciFinder login page. At the top is the CAS logo with the text "CAS 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 "scicas7521". Below the input field is a blue button labeled "Next". At the bottom of the page is a link that says "Can't log in?".



The screenshot shows the SciFinder login page after the user has entered their username. At the top is the CAS logo with the text "CAS A DIVISION OF THE AMERICAN CHEMICAL SOCIETY". Below the logo is the heading "Log In to SciFinder®". The text "Welcome, scicas7521" is displayed, followed by a link "Not You?". There is a text input field labeled "Password" containing several dots. Below the input field is a blue button labeled "Log In". Below the button is a checkbox labeled "Keep me signed in". At the bottom of the page is a link that says "Can't log in?".

每个用户必须注册后才能使用

SciFinder Web主界面

The screenshot shows the SciFinder web interface with several callout boxes in Chinese:

- 工具栏** (Toolbar): Points to the top navigation bar containing 'Explore', 'Saved Searches', and 'SciPlanner'.
- 检索完, 请点击退出** (After search, please click exit): Points to the 'Sign Out' button in the top right corner.
- 检索入口** (Search entry): Points to the search input field in the center of the page.
- 已保存的结果集** (Saved result sets): Points to the 'SAVED ANSWER SETS' panel on the right side.
- 定题追踪** (Topic tracking): Points to the 'KEEP ME POSTED' section at the bottom of the right panel.

The interface includes a left sidebar with 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). The main search area has a search box with examples and a 'Search' button. The right panel shows a list of saved answer sets and a 'KEEP ME POSTED' section.

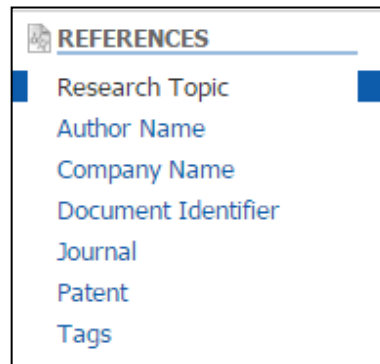
SciFinder Web检索——文献检索

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： 纳米技术在癌症免疫疗法中的应用

检索式： nano with Immunotherapy of cancer

The screenshot shows the SciPlanner search interface. At the top, there are tabs for 'Explore', 'Saved Searches', and 'SciPlanner'. On the left, there is a navigation menu with three main sections: 'REFERENCES', 'SUBSTANCES', and 'REACTIONS'. Under 'REFERENCES', there are sub-items: Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, and Tags. Under 'SUBSTANCES', there are: Chemical Structure, Markush, Molecular Formula, Property, and Substance Identifier. Under 'REACTIONS', there is: Reaction Structure. The main search area is titled 'REFERENCES: RESEARCH TOPIC'. It features a search input field containing the text 'nano with Immunotherapy of cancer'. Below the input field, there are 'Examples:' listed as 'The effect of antibiotic residues on dairy products' and 'Photocyanation of aromatic compounds'. A blue 'Search' button is positioned below the examples. At the bottom of the search area, there is a link for 'Advanced Search'.

关键词之间用介词连接：
in, with, of...



主题检索的候选项

Explore ▾ Saved Searches ▾ SciPlanner

Research Topic "nano with Immunotherapy of can..."

REFERENCES ⓘ

Select All Deselect All

1 of 12 Research Topic Candidates Selected References

<input type="checkbox"/>	3 references were found containing "nano with Immunotherapy of cancer" as entered.	3
<input checked="" type="checkbox"/>	1985 references were found containing all of the concepts "nano", "Immunotherapy" and "cancer" closely associated with one another.	1985
<input type="checkbox"/>	5974 references were found where all of the concepts "nano", "Immunotherapy" and "cancer" were present anywhere in the reference.	5974
<input type="checkbox"/>	3825 references were found containing the two concepts "nano" and "Immunotherapy" closely associated with one another.	3825
<input type="checkbox"/>	8275 references were found where the two concepts "nano" and "Immunotherapy" were present anywhere in the reference.	8275
<input type="checkbox"/>	98018 references were found containing the two concepts "nano" and "cancer" closely associated with one another.	98018
<input type="checkbox"/>	166507 references were found where the two concepts "nano" and "cancer" were present anywhere in the reference.	166507
<input type="checkbox"/>	74209 references were found containing the two concepts "Immunotherapy" and "cancer" closely associated with one another.	74209
<input type="checkbox"/>	137453 references were found where the two concepts "Immunotherapy" and "cancer" were present anywhere in the reference.	137453
<input type="checkbox"/>	3041954 references were found containing the concept "nano".	3041954
<input type="checkbox"/>	244746 references were found containing the concept "Immunotherapy".	244746
<input type="checkbox"/>	5571062 references were found containing the concept "cancer".	5571062

[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

按被引次数排序——Citing References

Explore ▾ Saved Searches ▾ SciPlanner Save Print Export

Research Topic "nano with Immunotherapy of can..." > references (1547)

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

Analyze Refine Categorize

Sort by: Citing References Accession Number Author Name Citing References Publication Year Title Sources

Analyze by: Author Name

Lu Xiaoling 22

Wang Chao 22

Liu Zhuang 21

Huang Leaf 19

Lin Wenbin 18

Steinmetz Nicole F 17

Zhao Yongxiang 17

Moon James J 16

Kong Deling 15

Li Yaping 15

Show More

1. **Photothermal Cancer Therapy: Impending Clinical Impact**
By Lal, Surbhi; Clare, Susan E.; Halas, Naomi J.
From Accounts of Chemical Research (2008), 41(12), 1842-1851. | Language: English, Database: CAPLUS
A review. Much of the current excitement surrounding **nanoscience** is directly connected to the promise of new **nanoscale** applications in **cancer** diagnostics and therapy. Because of their strongly resonant light-absorbing and light-scattering properties that depend on shape, noble metal **nanoparticles** provide a new and powerful tool for innovative light-based approaches. **Nanoshells**-spherical, dielec. core, gold shell **nanoparticles**-have been central to the development of photothermal **cancer** therapy and diagnostics for the past several years. By manipulating **nanoparticle** shape, researchers can tu...

2. **Immuno Gold Nanocages with Tailored Optical Properties for Targeted Photothermal Destruction of Cancer Cells**
By Chen, Jingyi; Wang, Danling; Xi, Jiefeng; Au, Leslie; Siekkinen, Andy; Warsen, Addie; Li, Zhi-Yuan; Zhang, Hui; Xia, Younan; Li, Xingde
From Nano Letters (2007), 7(5), 1318-1322. | Language: English, Database: CAPLUS


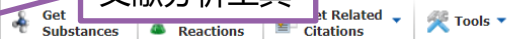

Gold **nanocages** with a relatively small size (e.g., ~45 nm in edge length) have been developed, and the structure of these **nanocages** was tailored to achieve strong absorption in the near-IR (NIR) region for photothermal **cancer** treatment. Numerical calcs. show that the **nanocage** has a large absorption cross section of 3.48×10^{-14} m², facilitating conversion of NIR irradiation into heat. The gold **nanocages** were conjugated with monoclonal antibodies (anti-HER2) to target epidermal growth factor receptors (EGFR) that are overexpressed on the surface of breast **cancer** cells (SK-BR-3). Our preliminary p...

Citing Reference: 帮助找到最重要的文献

文献结果集

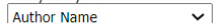
Explore ▾ Saved Searches ▾ SciPlanner Save Print Export

Research Topic "nano with Immunotherapy of

REFERENCES   

Sort by: Accession Number ▾

0 of 1547 References Selected



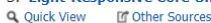
Analyze by: 

Lu Xiaoling	22
Wang Chao	22
Liu Zhuang	21
Huang Leaf	19
Lin Wenbin	18
Steinmetz Nicole F	17
Zhao Yongxiang	17
Moon James J	16
Kong Deling	15
Li Yaping	15

[Show More](#)

文献分析工具

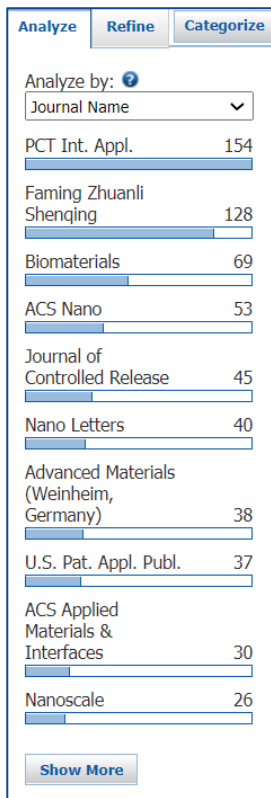
获取原文

- 1. Improving STING Agonist Delivery for Cancer Immunotherapy Using Biodegradable Mesoporous Silica Nanoparticles**

By Park, Kyung Soo; Xu, Cheng; Sun, Xiaoj; Louttit, Cameron; Moon, James J.
From Advanced Therapeutics (Weinheim, Germany) (2020), 3(10), 2000130. | Language: English, Database: CAPLUS
Stimulator of interferon genes (STING) activation by intratumoral STING agonist treatment has been recently shown to eradicate tumors in preclin. models of **cancer immunotherapy**, generating intense research interest and leading to multiple clin. trials. However, there are many challenges assoc. with STING agonist-based **cancer immunotherapy**, including low cellular uptake of STING agonists. Here, biodegradable mesoporous silica **nanoparticles** (bMSN) are developed for efficient cellular delivery of STING agonists. STING agonists delivered via bMSN potently activate inn...
- 2. Engineered Ovalbumin Nanoparticles for Cancer Immunotherapy**

By Habibi, Nahal; Christau, Stephanie; Ochyl, Lukasz J.; Fan, Zixing; Hassani Najafabadi, Alireza; Kuehnhammer, Matthias; Zhang, Mengwen; Helgeson, Matthew; von Kitzing, Regine; Moon, James J.; et al
From Advanced Therapeutics (Weinheim, Germany) (2020), 3(10), 2000100. | Language: English, Database: CAPLUS
Ovalbumin (OVA) is a protein antigen that is widely used for eliciting cellular and humoral immune responses in **cancer immunotherapy**. As an alternative to solute OVA, engineering approach is developed herein towards protein **nanoparticles** (pNPs) based on reactive electrospraying. The resulting pNPs are comprised of polymd. OVA, where individual OVA mols. are chem. linked via poly(ethylene glycol) (PEG) units. Controlling the PEG/OVA ratio allows for fine-tuning of crit. phys. properties, such as particle size, elasticity, and, at the mol. level, mesh size. As the PEG/OVA ratio decreased, OV...
- 3. Light-Responsive Core-Shell Nanoplatfor for Bimodal Imaging-Guided Photothermal Therapy-Primed Cancer Immunotherapy**

By Zhang, Wei; Zhang, Cun-cheng; Wang, Xing-Yue; Li, Lin; Chen, Qiao-Qi; Liu, Wei-Wei; Cao, Yang; Ran, Hai-Tao
From ACS Applied Materials & Interfaces (2020), Ahead of Print. | Language: English, Database: CAPLUS
Photothermal therapy (PTT) as a noninvasive and effective thermal **therapeutic** approach has attracted tremendously increasing interest because it can effectively eliminate the primary tumor and generate tumor-assoc. antigens, which could elicit antitumor immune responses. Herein, we report on the rational design and fabrication of copper sulfide (CuS)-based **nanoplatfor** for **cancer photothermal immunotherapy**. The as-prepd. core-shell CuS@mSiO₂-PPF-PEG (CPPs) **nanocomposites** possess high biocompatibility, photoacoustic (PA)/ultrasound (US) imaging, and strong PTT effect upon 808 nm laser irradi...

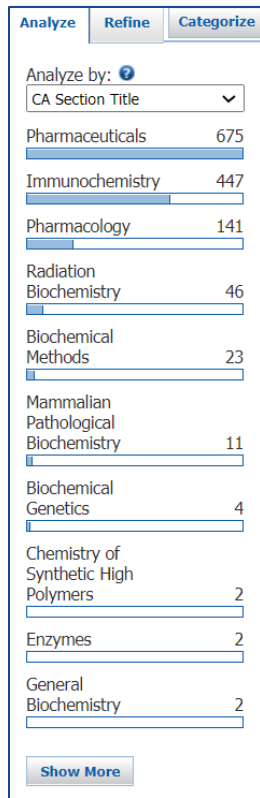
SciFinder提供强大的文献处理工具，帮助处理文献

分析文献结果集——Analyze

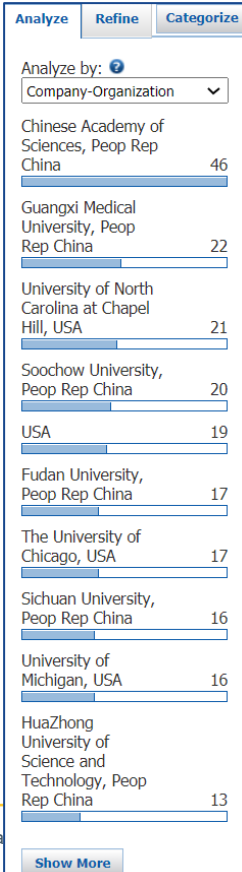
期刊



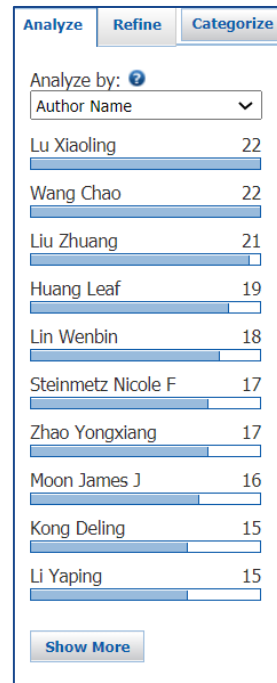
涉及学科领域



本领域研究机构、
合作伙伴、竞争对手



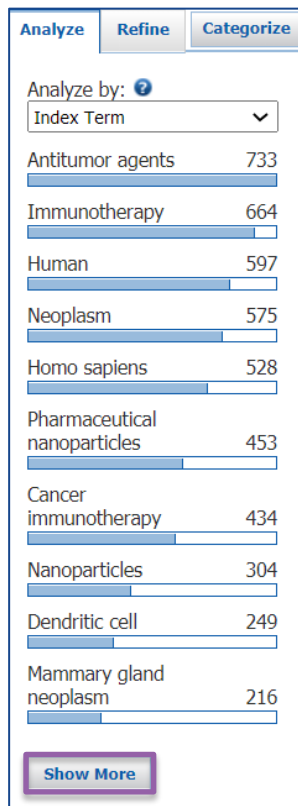
本领域研究人员



CAS[®]

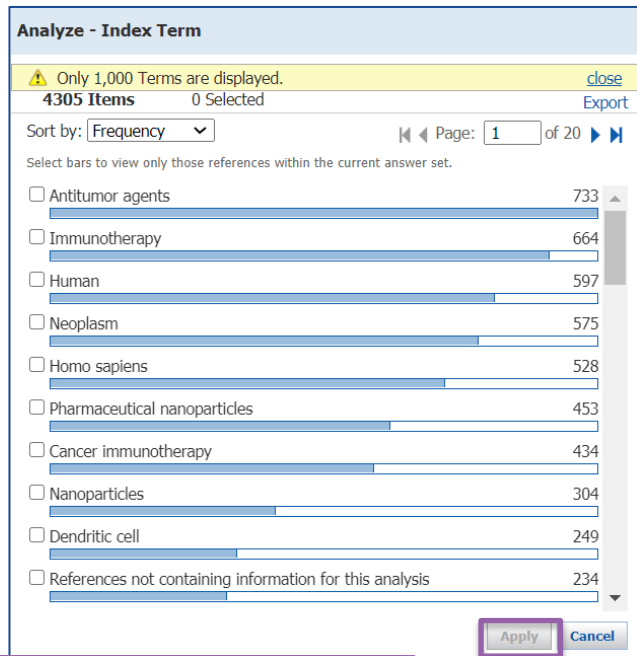
A DIVISION OF THE
AMERICAN CHEMICAL SOCIETY

分析文献结果集——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



CAS
A DIVISION OF THE
AMERICAN CHEMICAL SOCIETY

筛选文献结果集——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 347 References Selected

Page: 1 of 18

1. **Applications of inorganic nanomaterials in photothermal therapy based on combinational cancer treatment**
By Wang, Ji; Wu, Xia; Shen, Peng; Wang, Jun; Shen, Yidan; Shen, Yan; Webster, Thomas J.; Deng, Junjie
From International Journal of Nanomedicine (2020), 15, 1903-1914. | Language: English, Database: CAPLUS
A review. **Cancer** is one of the major causes of death and is difficult to cure using existing clin. therapies. Clin. **cancer** treatments [such as surgery, chemotherapy (CHT), radiotherapy (RT) and **immunotherapy** (IT)] are widely used but they have limited **therapeutic** effects and unavoidable side effects. Recently, the development of novel **nanomaterials** offers a platform for combinational therapy (meaning a combination of two or more **therapeutic** agents) which is a promising approach for **cancer** therapy. Recent studies have demonstrated several types of **nanomaterials** suitable for photothermal the...

2. **Exploiting nanoscale cooperativity for precision medicine**
By Wilhelm, Jonathan; Wang, Zhaohui; Sumer, Baran D.; Gao, Jiming
From Advanced Drug Delivery Reviews (2020), Ahead of Print. | Language: English, Database: CAPLUS
A review. Precise spatiotemporal control of mol. transport is vital to functional physiol. systems. Nature evolved to apply macromol. cooperativity to achieve precision over systemic delivery of important mol. In drug delivery, conventional **nanocarriers** employ inert materials and rely on passive accumulation for tissue targeting and diffusion for drug release. Early clin. studies show these **nanodrugs** have not delivered the anticipated impact on therapy. Inspired by nature, we propose a design principle that incorporates **nanoscale** cooperativity and phase transition to sense and amplify ph...

3. **Modulation of tumor microenvironment for immunotherapy: focus on nanomaterial-based strategies**
By Liu, Yun; Guo, Jianfeng; Huang, Leaf
From Theranostics (2020), 10(7), 3099-3117. | Language: English, Database: CAPLUS
A review. Recent advances in the field of **immunotherapy** have profoundly opened up the potential for improved **cancer** therapy and reduced side effects. However, the tumor microenvironment (TME) is highly immunosuppressive, therefore, clin. outcomes of currently available **cancer immunotherapy** are still poor. Recently, **nanomaterial**-based strategies have been developed to modulate the TME for robust **immunotherapeutic** responses. In this review, the immunoregulatory cell types (cells relating to the regulation of immune responses) inside the TME in terms of stimulatory and suppressive roles are d...

4. **pH-responsive nanoparticles for cancer immunotherapy: a brief review**
By Yan, Yunfeng; Ding, Hangwei
From Nanomaterials (2020), 10(8), 1613. | Language: English, Database: CAPLUS
A review. **Immunotherapy** has recently become a promising strategy for the treatment of a wide range of **cancers**. However, the broad implementation of **cancer immunotherapy** suffers from inadequate efficacy and toxic side effects. Integrating pH-responsive **nanoparticles** into **immunotherapy** is a powerful approach to tackle these challenges because they are able to target the tumor tissues and organelles of antigen-presenting cells (APCs) which have a characteristic acidic microenvironment. The spatiotemporal control of **immunotherapeutic** drugs using pH-responsive **nanoparticles** endows **cancer immuno...**

Refine: 帮助用户迅速获得需要的文献

分类文献结果集——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.

Category Heading	Category
All	(54)
Biotechnology	Gas, liquid, & solid phenomena (112)
Genetics & protein chemistry	Subatomics (72)
Physical chemistry	Mechanics (44)
Biology	Electric & magnetic phenomena (33)
Synthetic chemistry	Substances in processes (189)
General chemistry	Thermodynamics (24)
Technology	Spectra & spectroscopy (45)
Polymer chemistry	Surface phenomena (37)
Analytical chemistry	Quantum mechanics (4)
Environmental chemistry	Atomic & molecular phenomena (1)
Catalysis	

2. Select index terms of interest.

Index Terms	
Select All	Deselect All
<input type="checkbox"/>	Hydrophobicity 14
<input checked="" type="checkbox"/>	Pore size 9
<input type="checkbox"/>	Hydrophilicity 7
<input checked="" type="checkbox"/>	Surface treatment 7
<input type="checkbox"/>	Surfactants 7
<input type="checkbox"/>	Coating process 6
<input type="checkbox"/>	Permeability 6
<input type="checkbox"/>	Surface electric charge 6
<input type="checkbox"/>	Surface 5
<input type="checkbox"/>	Surface area 5
<input type="checkbox"/>	Porosity 4
<input type="checkbox"/>	Surface functionalization 4
<input type="checkbox"/>	Pressure 3
<input type="checkbox"/>	Detergents 2
<input type="checkbox"/>	Lipophilicity 2
<input type="checkbox"/>	Nanoscale surface 2

Selected Terms

Click 'X' to remove the category from 'Selected Terms'

Physical chemistry > Surface phenomena (2 Terms)

Physical chemistry > Surface phenomena > 2 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。

文献结果集的保存——Save, Print, Export

Searches: SciPlanner Save Print Export

ally removed.

therapy of can... > references (1547) > refine by categories

Get Substances Get Reactions Get Related Citations Tools

Create Keep Me Posted Alert Send to SciPlanner

Sort by: Accession Number

0 of 16 References Selected

1. Post translational modification-assisted cancer immunotherapy for effective breast cancer treatment

Quick View Other Sources

By Theivendran, Shevanuja; Tang, Jie; Lei, Chang; Yang, Yannan; Song, Hao; Gu, Zhengying; Wang, Yue; Yang, Yang; Jin, Lei; Yu, Chengzhong

From Chemical Science (2020), 11(38), 10421-10430. | Language: English, Database: CAPLUS

Post translational modifications (PTM) such as phosphorylation are often correlated with tumorigenesis and malignancy in breast cancer. Herein, we report a PTM-assisted strategy as a simplified version of a personalized cancer vaccine for enhanced cancer immunotherapy. Titanium modified dendritic mesoporous silica nanoparticles (TIDMSN) are applied to assist the specific enrichment of phosphorylated tumor antigens released upon immunogenic cell death. This strategy significantly improved the tumor inhibition efficacy in a bilateral breast cancer model and the...

2. Cold nanospheres and nanorods for anti-cancer therapy: comparative studies of fabrication, surface-decoration, and anti-cancer treatments

Quick View Other Sources

By Mao, Wei; Son, Young Ju; Yoo, Hyuk Sang

From Nanoscale (2020), 12(28), 14996-15020. | Language: English, Database: CAPLUS

A review. Various gold nanoparticles have been explored as cancer therapeutics because they can be widely engineered for use as efficient drug carriers and diagnostic agents, and in photo-irradn. therapy. In the current review, we focused on shape-dependent biomedical applications of gold nanoparticles including gold nanospheres and nanorods. Fabrication and functionalization strategies of two different gold nanoparticles for anti-cancer therapy are introduced and the distinguishing performance depending on the shape is discussed to suggest the best carrier shape for specific applications. ...

3. Biodegradable Poly(γ -glutamic acid)@glucose oxidase@carbon dot nanoparticles for simultaneous multimodal imaging and synergetic cancer therapy

Quick View Other Sources

By Zhang, Ming; Wang, Wentao; Wu, Fan; Zheng, Tao; Ashley, Jon; Mohammadniaei, Mohsen; Zhang, Qicheng; Wang, Mingqian; Li, Li; Shen, Jian; et al

From Biomaterials (2020), 252, 120106. | Language: English, Database: CAPLUS

It is known that tumor antigens could induce obvious anti-tumor immune responses for efficient cancer immunotherapy when combined with checkpoint blockade. However, it is limited due to the suppressive tumor microenvironment (TME). Here, a new type of nanomaterial was developed to improve tumor treatment by the combined action of starving the /photothermal therapy (PTT) and checkpoint-blockade immunotherapy. In detail, the Immunoadjuvant nanoagents (y-PGA@GOx@Mn,Cu-CDs) were fabricated by integrating the...

Save: 保存在服务器上, 方便以后登陆查看, 每次可存2万条记录。

Export: 导出至本地电脑。

Print: 打印成PDF格式

Export

Export: All Selected Range

Example: 2-20

For: Citation Manager Quoted Format (*.txt) Tagged Format (*.txt)

Offline review: Portable Document Format (*.pdf) Rich Text Format (*.rtf) Answer Keys (*.txt)

Saving locally: Answer Key eXchange (*.aex)

Details: * Required

File Name: Reference_06_19_2012_100848

Format: Summary without abstracts Summary with partial abstracts Summary with full abstracts Detail (full record)

Include: Task History Tags Comments

Export Cancel

Citation manager: 保存成RIS等格式, 可导入EndNote 等文献管理工具

Offline Review: 保存成PDF, RTF等格式, 用于脱机浏览

文献信息——题录、摘要、索引

2. Gold nanospheres and nanorods for anti-cancer therapy: comparative studies of fabrication, surface-decoration, and anti-cancer treatments

By: Mao, Wei; Son, Young Ju; Yoo, Hyuk Sang

A review. Various gold nanoparticles have been explored as cancer therapeutics because they can be widely engineered for use as efficient drug carriers and diagnostic agents, and in photo-irrad. therapy. In the current review, we focused on shape-dependent biomedical applications of gold nanoparticles including gold nanospheres and nanorods. Fabrication and functionalization strategies of two different gold nanoparticles for anti-cancer therapy are introduced and the distinguishing performance depending on the shape is discussed to suggest the best carrier shape for specific applications. Moreover, recent advances in anti-cancer immunotherapy using gold nano-carriers are discussed. Thus, this comparative review can be helpful in deciding on suitable shapes and surface-modification strategies for prep. various gold nanoparticle-based therapeutics in anti-cancer therapy.

Indexing

Pharmacology (Section 1.0)

Concepts

重要概念

Diagnosis
Nanocarriers
Nanorods
Photothermal therapy
Therapy

Immunotherapy
Nanoparticles
Nanospheres
Surface treatment

comparative studies of fabrication, surface-decoration, and anti-cancer treatments of gold nanospheres and nanorods

Supplementary Terms

gold nanoparticle anticancer therapy surface decoration review

Citations

Ahn, S; Adv Healthcare Mater 2014, 3, 1194
Ajnai, G; J Exp Clin Med 2014, 6, 172
Akiyama, Y; J Controlled Release 2009, 139, 81
Alexandridis, P; Chem Eng Technol 2011, 34, 15
Alhasan, A; Anal Chem 2012, 84, 4153
Ali, M; Biomaterials 2016, 102, 1
Ali, M; J Phys Chem C 2019, 123, 15375
Allen, J; J Colloid Interface Sci 2017, 505, 1172
Almeida, J; Nanomedicine 2014, 10, 503
Almeida, J; Small 2015, 11, 1453

Substances

重要物质

7440-57-5 Gold

comparative studies of fabrication, surface-decoration, and anti-cancer treatments of gold nanospheres and nanorods

Technical or engineered material use; Therapeutic use; Biological study; Uses

文献详情界面包括:

- 标题
- 摘要
- 文献中重要的技术术语
- 文献中重要的物质
- 书目信息
- 获得文献中的物质、反应
- 参考文献
- 链接原文

QUICK LINKS

0 Tags, 0 Comments

SOURCE

Nanoscale
Volume12
Issue28
Pages14996-15020
Journal; General Review;
Online Computer File
2020
CODEN:NANOHL
ISSN:2040-3372
DOI:10.1039/d0nr01690j

COMPANY/ORGANIZATION

Department of Biomedical
Materials Engineering
Kangwon National University
Chuncheon, S. Korea 24341

ACCESSION NUMBER

2020:1210714
CAPLUS

PUBLISHER

Royal Society of Chemistry

LANGUAGE

English



CAS

A DIVISION OF THE
AMERICAN CHEMICAL SOCIETY

文献检索小结

- 主题检索时，使用介词 **in, with, of** 等作为连接词
- 跟据检索要求选择合适的候选项
- 通过**SciFinder** 的**Analyze/Refine**功能来缩小检索的范围
- 尝试将不同的**Analyze/Refine**功能组合起来用，会有更多的收益
- 使用**Categorize**可以让系统来实现自动分类

文献检索上机练习

检索关于有机硅化合物在光电材料领域的研究文献，具体有哪些细分研究方向？主要的研究者，研究机构有哪些？研究发展趋势如何？

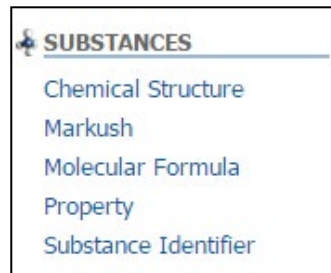
提纲

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

SciFinder检索选项——物质检索

■ 物质检索方法

- 结构式检索
- 分子式检索
- 理化性质检索
- 物质标识符检索：化学名称，CAS RN



■ 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——标识符检索

Explore ▾ Saved Searches ▾ SciPlanner

Research Topic "nano with Immunotherapy of can..." > references (1547) > refine by categories > Gold nanospheres and nanorods ...

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: SUBSTANCE IDENTIFIER ⓘ

qinghaosu

Enter one per line.
Examples:
50-00-0
999815
Acetaminophen

Search

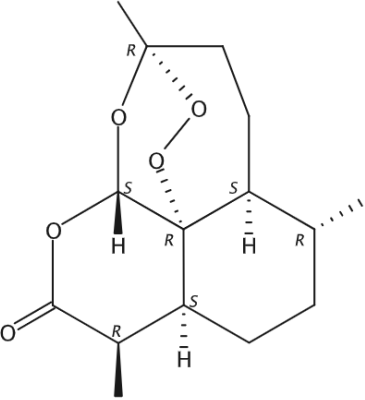
提示:
• 一次最多可输入25个物质。
• 每行一个物质标识符。

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。

SciFinder中的物质记录

点击CAS RN 获得物质详细信息

63968-64-9



Absolute stereochemistry.

C₁₅H₂₂O₅
3,12-Epoxy-12H-pyrano[4,3-f]-1,2-benzodioxepin-10(3H)-one, octahydro-3,6,9-trimethyl-, (3R,5a,S,6R,8a,S,9R,12,S,12a,R)-

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

CAS Registry Number: 63968-64-9

- » View Substance Detail
- » Explore by Structure
- Synthesize this...
- Get Reactions where Substance is a
- Get Commercial Sources
- Get Regulatory Information
- Get References
- Export as Image
- Export as molfile
- Send to SciPlanner

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

SciFinder中的物质记录

物质详情

SUBSTANCE DETAIL

[Get References](#) [Get Reactions](#) [Get Commercial Sources](#)

[Return](#)

CAS Registry Number 63968-64-9

~6,028 ~132

C₁₅H₂₂O₅
3,12-Epoxy-12*H*-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*)-

Molecular Weight
282.33

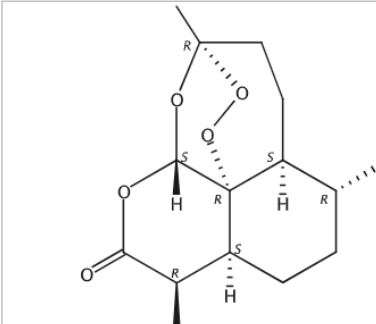
Melting Point (Experimental)
Value: 156-157 °C

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

Density (Experimental)
Value: 1.300 g/cm³

Other Names
3,12-Epoxy-12*H*-pyrano[4,3-*f*]-1,2-benzodioxepin-10(3*H*)-one,
octahydro-3,6,9-trimethyl-, [3*R*-(3*o*,5*a*β,6β,8*a*β,9*o*,12β,12*a**R*^{*})]-
(3*R*,5*a*,5,6*R*,8*a*,5,9*R*,12*S*,12*a**R*)-Octahydro-3,6,9-trimethyl-3,12-epoxy-
12*H*-pyrano[4,3-*f*]-1,2-benzodioxepin-10(3*H*)-one
(+)-Arteannuin
(+)-Artemisinin
(+)-Qinghaosu
[View more...](#)

由物质获得文献, 反应, 供应商等信息



Absolute stereochemistry.



CAS[®]

A DIVISION OF THE
AMERICAN CHEMICAL SOCIETY

SciFinder中的物质记录

EXPERIMENTAL PROPERTIES

EXPERIMENTAL SPECTRA

实验数据与实验谱图

¹H NMR ¹³C NMR Hetero NMR IR Mass Raman UV and Visible Additional Spectra

¹³ 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		

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

PREDICTED SPECTRA

预测数据与预测谱图

REGULATORY INFORMATION

BIOACTIVITY INDICATORS

TARGET INDICATORS

CAS REFERENCE ROLES

ADDITIONAL DETAILS

Carbon-13 NMR Spectrum

SPECTRUM ID
7MED36_38.C

CAS REGISTRY NUMBER
63968-64-9

FORMULA
C₁₅ H₂₂ O₃

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

NUCLEUS
13C

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

C[C@H]1[C@@H](OC2=CC=CC=C2O1)C[C@H](C)C[C@H](C)C

物质检索——Property explore

Explore ▾ Saved Searches ▾ SciPlanner

Substance Identifier "qinghaosu" > substances (1) > 63968-64-9

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: PROPERTY

Experimental

Electric Conductivity (S/cm) ▾ 50-80
Examples: 44, 25-35, >125

Predicted

Select Property... ▾
Examples: 44, 25-35, >125

Search

寻找导电率在50-80的含铜元素的物质

物质结果集的筛选

Explore ▾ Saved Searches ▾ SciPlanner Save Print Export

Property "Experimental - Electric Conduc..." > substances (51)

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 51 Substances Selected Display Options Page: 1 of 4

Analyze by: Elements

C	32
H	31
O	23
S	19
N	13
Cl	7
La	5
Sr	5
Cd	4
Cu	4

[Show More](#)

1. 1311475-58-7

2. 1189417-05-7

Component	Component Ratio
O	3
Co	0 - 1
Ba	0 - 1
Sr	0 - 1
Fe	0 - 1

Ba . Co . Fe . O . Sr
Barium cobalt iron strontium oxide ((Ba,Sr)(Co,Fe)O₂)
[Experimental Properties](#)

82428-14-6
C₁₀H₆S₈ · 1/2 Br₂ Cd
C₁₀H₆S₆

筛选出含铜元素的物质

物质检索——分子式

检索(N H4) Sm (S O4)2 (H2 O)4, Ammonium Samarium Bis(sulfate(VI)) Tetrahydrate

Property "Experimental - Electric Conduc..." > substances (51)

REFERENCES

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

SUBSTANCES

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

SUBSTANCES: MOLECULAR FORMULA

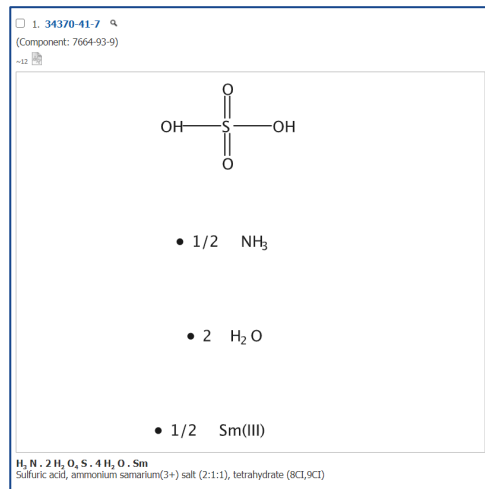
H3 N . 2 H2 O4 S . 4 H2 O . Sm

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

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



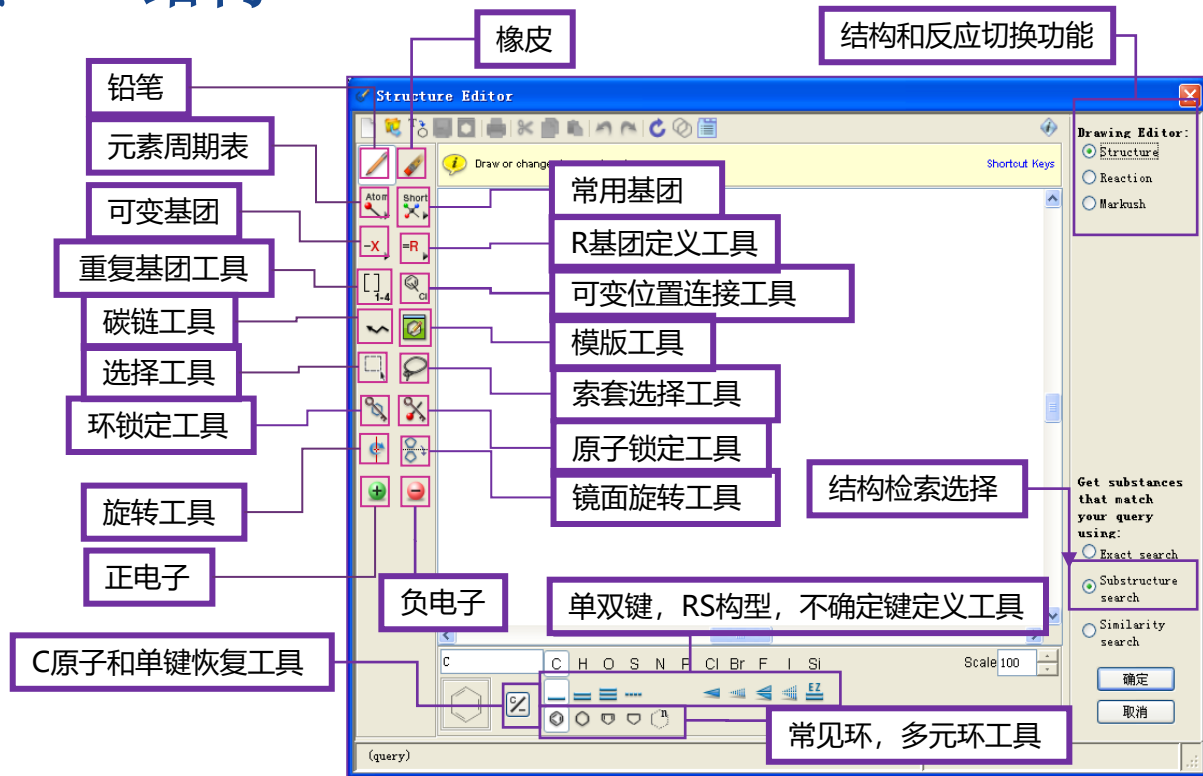
CAS[®]

A DIVISION OF THE
AMERICAN CHEMICAL SOCIETY

物质检索——结构

The screenshot displays the CAS Substance Search interface. On the left, a navigation menu is organized into three sections: **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). The **Chemical Structure** option is highlighted with a purple box. The main content area is titled **SUBSTANCES: CHEMICAL STRUCTURE** and features a **Structure Editor** window with **Java** and **Non-Java** tabs, a **Click to Edit** prompt, and an **Import CXF** button. To the right, the **Search Type** options are **Exact Structure**, **Substructure** (selected), and **Similarity**, along with a **Show precision analysis** checkbox. A **ChemDraw** logo and a button to **Launch a SciFinder substance or reaction** are also visible. At the bottom, there is a blue **Search** button, an **Advanced Search** link, and a checked **Always Show** checkbox.

物质检索——结构



CAS[®]
A DIVISION OF THE
AMERICAN CHEMICAL SOCIETY

物质检索——精确结构检索

The screenshot displays the 'Structure Editor' window. The main canvas shows three chemical structures: ammonia (NH₃), sulfur dioxide (SO₂), and water (H₂O). The interface includes a toolbar on the left with various drawing tools, a top menu bar, and a right-hand panel. The right-hand panel contains the 'Drawing Editor' section with radio buttons for 'Structure', 'Reaction', and 'Markush'. Below this is the 'Get substances that match your query using:' section, where 'Exact search' is selected and highlighted with a purple box. Other options are 'Substructure search' and 'Similarity search'. At the bottom of the right panel are 'OK' and 'Cancel' buttons. The status bar at the bottom of the window shows the chemical formula 'Sm . H₄N . H₂O₂S . H₂O' and a numerical string '150.36 . 18.04 . 98.08 . 18.02'.

- Characteristics
- Single component
 - Commercially available
 - Included in references
- Classes
- Alloys
 - Coordination compounds
 - Incompletely defined
 - Mixtures
 - Polymers
 - Organics, and others not listed
- Studies
- Analytical
 - Biological
 - Preparation
 - Reactant or reagent

精确结构检索

精确结构检索结果集

Sort by Display Options

0 of 5 Substances Selected

<p><input type="checkbox"/> 1. 34370-41-7 </p> <p>(Component: 7664-93-9)</p> <p>~12 </p> <div style="text-align: center;"><p>• 1/2 NH₃ • 2 H₂O • 1/2 Sm(OH)₃</p></div> <p>H₂N · 2 H₂O₂ S · 4 H₂O · Sm Sulfuric acid, ammonium samarium(3+) salt (2:1:1), tetrahydrate (8CI,9CI)</p>	<p><input type="checkbox"/> 2. 40148-71-8 </p> <p>(Component: 7664-93-9)</p> <p>~1 </p> <div style="text-align: center;"><p>• NH₃ • 1/3 H₂O • 1/3 Sm(OH)₃</p></div> <p>H₂N · H₂O₂ S · 1/3 H₂O · 1/3 Sm Sulfuric acid, ammonium samarium(3+) salt (3:3:1), monohydrate (9CI)</p>	<p><input type="checkbox"/> 3. 40148-74-1 </p> <p>(Component: 7664-93-9)</p> <p>~1 </p> <div style="text-align: center;"><p>• 1/2 NH₃ • H₂O • 1/2 Sm(OH)₃</p></div> <p>H₂N · 2 H₂O₂ S · 2 H₂O · Sm Sulfuric acid, ammonium samarium(3+) salt (2:1:1), dihydrate (9CI)</p>	<p><input type="checkbox"/> 4. 42949-48-4 </p> <p>~1 </p> <div style="text-align: center;"><p>49856-58-8 (Component: 736080-59-4) H₆ O₁₁ S₂ Sm · H₄ N · H₂O</p><p>• NH₄⁺ • H₂O</p></div> <p>(H₆O₁₁S₂Sm · H₄N · H₂O)_x Samarate(1-), triaquabis[sulfato(2-)-O,O']-, ammonium, monohydrate, homopolymer (9CI)</p>
<p><input type="checkbox"/> 5. 49856-58-8 </p> <p>(Component: 736080-59-4)</p> <p>~0 </p> <div style="text-align: center;"><p>• NH₄⁺ • H₂O</p></div> <p>H₆O₁₁S₂Sm · H₄N · H₂O Samarate(1-), triaquabis[sulfato(2-)-O,O']-, ammonium, monohydrate (9CI)</p>			



CAS[®]

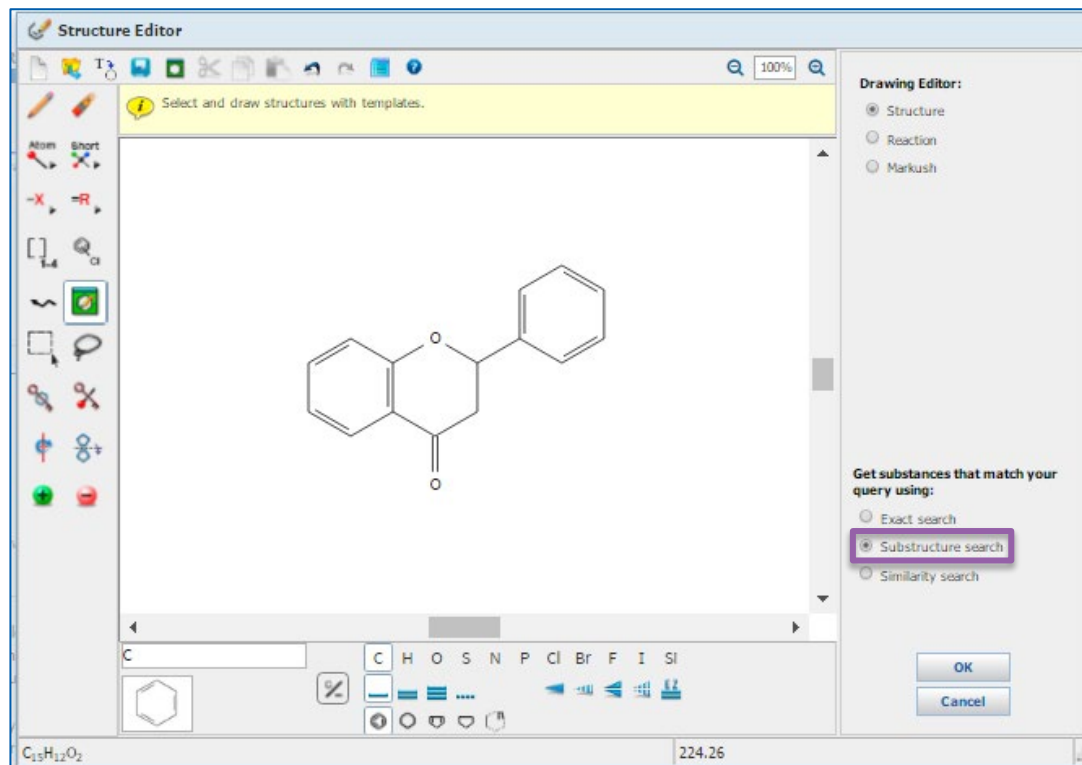
A DIVISION OF THE
AMERICAN CHEMICAL SOCIETY

物质检索——精确结构检索

- 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

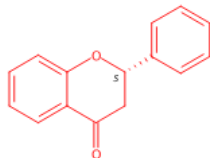
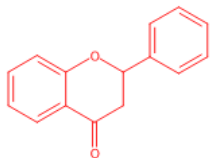


物质检索——亚结构检索

0 of 23824 Substances Selected

1. 487-26-3

2. 17002-31-2

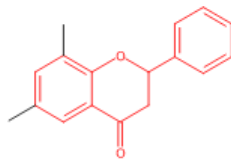


$C_{15}H_{12}O_2$
4#1-Benzopyran-4-one, 2,3-dihydro-1H-

Key Physical Properties
Regulatory Information
Spectra
Experimental Properties

取代物

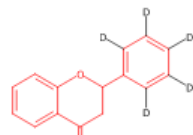
281. 123251-10-5



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

Key Physical Properties
Experimental Properties

10. 146196-91-0



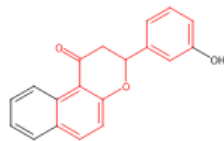
同位素

$C_{15}H_7D_6O_2$
4#1-Benzopyran-4-one, 2,3-dihydro-1H-

Spectra

稠环物质

284. 136116-23-9

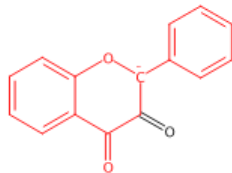


$C_{19}H_{14}O_3$
1#Naphtho[2,1-b]pyran-1-one, 2,3-dihydro-3-(3-hydroxyphenyl)-1H-

Key Physical Properties

离子

295. 780723-19-5



$C_{15}H_8O_3$
2#1-Benzopyran-3,4-dione, 2-phenyl-, ion(1-)



CAS®

A DIVISION OF THE
AMERICAN CHEMICAL SOCIETY

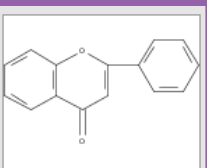
亚结构检索结果的限定

Analysis Refine

Refine by:

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

Chemical Structure:



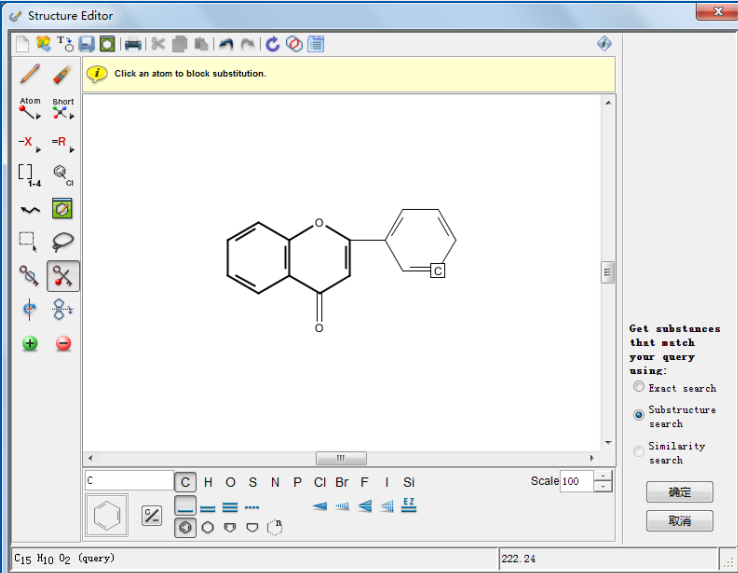
Click image to change structure or view detail

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

C₁₅ H₁₀ O₂ (query) 222.24



环锁定



原子锁定



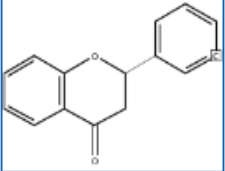
CAS[®]

A DIVISION OF THE
AMERICAN CHEMICAL SOCIETY

亚结构检索结果的限定

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

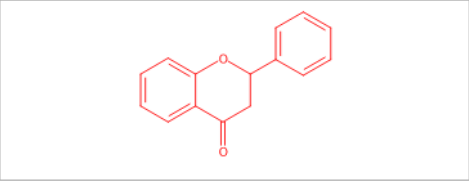
Refine

Get References Get Reactions Get Commercial Sources Tools

Sort by: Relevance

0 of 13826 Substances Selected

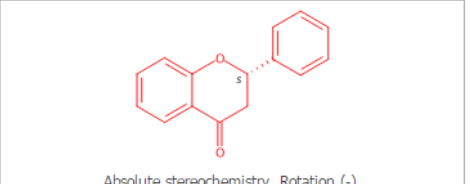
1. 487-26-3



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

Key Physical Properties
Regulatory Information
Spectra
Experimental Properties

2. 17002-31-2



Absolute stereochemistry., Rotation (-).

$C_{15}H_{12}O_2$
4*H*-1-Benzopyran-4-one, 2,3-dihydro-2-phenyl-, (2*S*)-

Key Physical Properties
Experimental Properties

4. 104550-32-5

5. 75524-43-5



CAS[®]

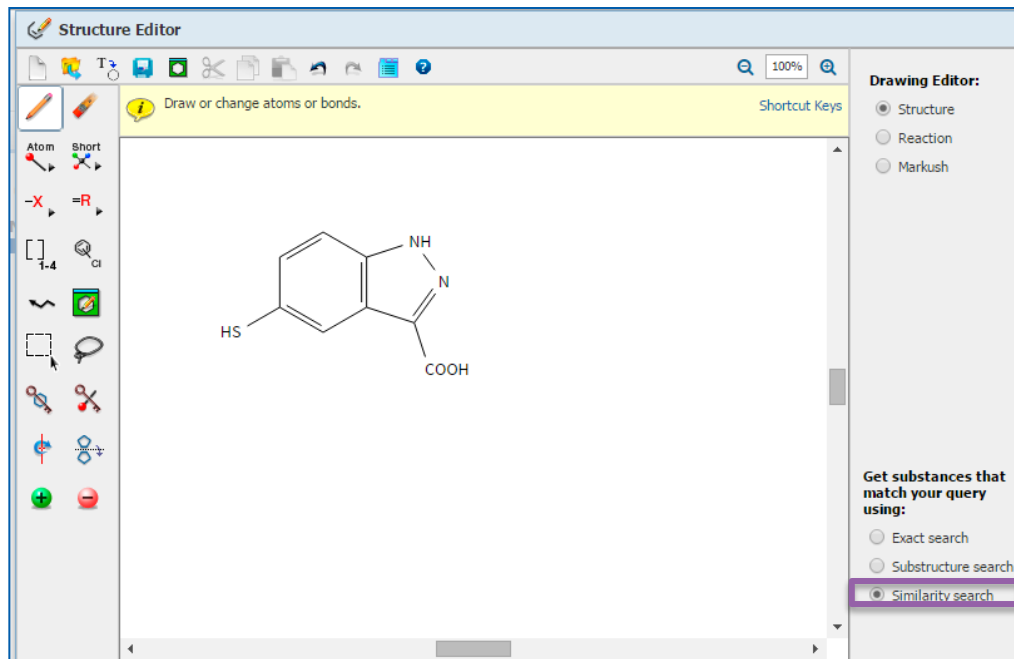
A DIVISION OF THE
AMERICAN CHEMICAL SOCIETY

物质检索——亚结构检索

- 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



相似结构检索结果

Select All Deselect All

0 of 6 Similarity Candidates Selected

	Substances
<input type="checkbox"/> ≥ 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
<input type="checkbox"/> 65-69	696
<input type="checkbox"/> 0-64 (least similar)	1818

Get Substances

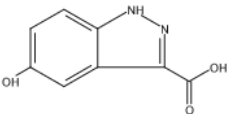
评分越高，相似度越高，结构越相似

Score: 88

1. 885518-94-5

~1 ~35

取代基变化



$C_8H_6N_2O_3$
1H-Indazole-3-carboxylic acid, 5-hydroxy-

▶ Key Physical Properties

Score: 86

5. 858227-12-0

~7 ~41

取代基位置变化



$C_9H_8N_2O_2$
1H-Indazole-3-carboxylic acid, 6-methyl-

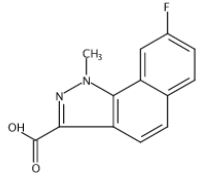
▶ Key Physical Properties

Score: 65

541. 1100422-

~1

母体结构变化



$C_{13}H_8FN_2O_2$
1H-Benz[*g*]indazole-3-carboxylic acid, 8-fluoro-1-methyl-

▶ Key Physical Properties

物质检索——相似结构检索

- 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

提纲

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

Markush检索

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_2 保护下加入25mL无水 CH_2Cl_2 ,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_2Cl_2 后缓缓滴入上述反应液,室温反应6小时。反应液加30mL饱和食盐水稀释,分出有机层,水层 CH_2Cl_2 提取(15mL \times 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 $^{\circ}C$; 1H NMR (500MHz, $CDCl_3$): 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_2), 2.81 (m, 2H, CH_2), 2.48 (m, 1H, CH), 1.93 (d, 2H, J =12.5Hz, CH_2), 1.76 (m, 2H, CH_2), 1.47 (s, 9H, CH_3) ppm; ESI-MS: m/z = 307[M+H] $^+$ 。

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

吡嗪-2-羧酸(1.5g,12mmol)置于50ml反应瓶中,加入35mL无水 CH_2Cl_2 溶解,随即加入1-羟基苯并三氮唑(1.6g,12mmol)和N-(3-二甲氨基丙基)-N'-乙基碳二亚胺盐酸盐(3.5g,18mmol),室温反应半小时。随后,哌啶-1-甲酸叔丁酯(1.9g,10mmol)加入反应液中,室温反应3小时。反应液加入30mL饱和碳酸氢钠水溶液稀释,分出有机层,饱和食盐

具体物质[Specific Substance]:

以具体化学结构陈述的特定物质, 会被分配CAS RN

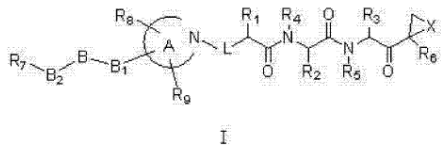
Markush检索

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:



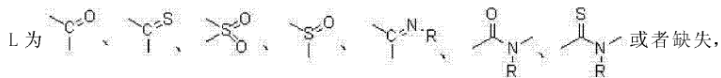
其中:

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_0) (R_0) 或缺失, R_0, R_6 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;

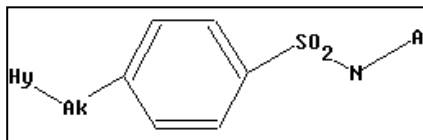
R_8, R_9 分别独立选自 H、OH、 C_{1-6} 烷基、 C_{1-6} 烷氧基、 C_{1-6} 羟基烷基、 C_{1-6} 巯基烷基、 C_{1-6} 烷基 -D、芳基、杂环芳基、环烷基和杂环基,这些基团可以被卤素、硝基、氨基、CN、 C_{1-6} 烷基、卤代的 C_{1-6} 烷基、 C_{1-6} 烷氧基或卤代的 C_{1-6} 烷氧基取代,每个基团可与一个或多个芳基或杂环

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

— 专利中所陈述的预测物质, 不会被分配CAS RN

— Markush检索, 能检索到通过结构检索检不到的专利



可用SciFinder中的Markush检索
查看专利中化合物结构保护范围

Structure Editor

Draw or change atoms or bonds. Shortcut Keys

100%

Atom Short

-X =R

1-4

Get Markush patents where the structure(s) are:

- Variable only at the specified positions
- Substructures of more complex structures

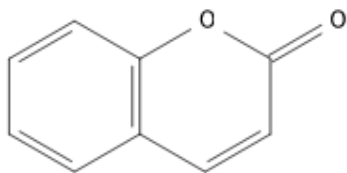
OK

Cancel

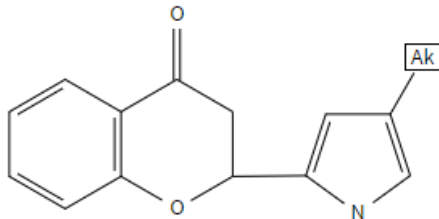
A C H O S N P Cl Br F I Si

物质及Markush检索练习

1. 检索分子量在400-600之间，且包含如下母体结构的物质



2. 检索包含有如下结构的物质是否有公开文献报告？



提纲

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

SciFinder检索选项——反应检索

- 反应检索方法

结构式



REACTIONS

Reaction Structure

- 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

Get reactions where
the structure(s)
are:

Variable only at the
specified positions

Substructures of
more complex structures



CAS[®]

A DIVISION OF THE
AMERICAN CHEMICAL SOCIETY

反应绘制工具

The screenshot shows the Structure Editor software interface. The main window is titled "Structure Editor" and contains a toolbar with various drawing tools. Three specific tools are highlighted with purple boxes and Chinese labels:

- 反应箭头** (Reaction Arrow): Points to the reaction arrow tool in the toolbar.
- 反应原子标记工具** (Reaction Atom Marking Tool): Points to the tool used for marking atoms in a reaction.
- 反应位置标记工具** (Reaction Position Marking Tool): Points to the tool used for marking positions in a reaction.

Other visible elements include the "Drawing Editor" panel on the right with radio buttons for "Structure", "Reaction", and "Markush", and a status bar at the bottom showing "CH₄" and "16.04".

SciFinder反应检索——原子和环被锁定

Structure Editor

Draw or change atoms or bonds. Shortcut Keys

Atom Short

-X =R

1-4 Cl

reactant

product

NO₂

NH₂

Get reactions where the structure(s) are:

- Variable only at the specified positions
- Substructures of more complex structures

OK

Cancel

C₇H₇NO₂ - C₇H₉N

137.14 . 107.16

原子和环被锁定

反应检索结果

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

1. [View Reaction Detail](#) [Similar Reactions](#) 获取相似反应

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

Cc1ccc([N+](=O)[O-])cc1 → Cc1ccc(N)cc1 100%

~102 ~122

Overview

Steps/Stages

1.1 R:NaBH₄, C:1832616-28-0, C:Ru, S:H₂O, 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

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

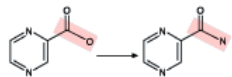
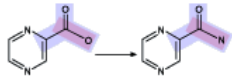
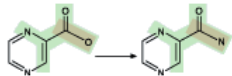
Narrow: 反应中心及扩展的原子和键

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

$$\text{Ar-NO}_2 \longrightarrow \begin{array}{c} \text{Ar} \quad \text{Ar} \\ \quad \backslash \quad / \\ \quad \text{N}=\text{N} \\ \quad / \quad \backslash \\ \text{Ar} \end{array}$$

3. Reduction of Nitro to Azoxy Compounds
11 Reactions

$$\text{Ar-NO}_2 \longrightarrow \begin{array}{c} \text{O}^- \\ | \\ \text{Ar} \quad \text{N}^+ = \text{N} \quad \text{Ar} \\ | \\ \text{Ar} \end{array}$$

更精确的查找需要的反应



反应检索结果的筛选

获得特定物质做还原剂的反应

The screenshot displays a search interface for chemical reactions. On the left, a 'Reagent' filter is active, showing a list of reagents with their respective counts. A purple box highlights 'NaBH₄' with a count of 51. An arrow points from this box to the main reaction area. The main area shows a reaction scheme: 4-nitrotoluene (with a nitro group, O₂N) is reduced to 4-aminotoluene (with an amino group, NH₂). The reaction is labeled '100%' and has a small icon below it. Below the reaction scheme, there is an 'Overview' section with 'Steps/Stages' and 'Notes'. The 'Steps/Stages' section lists: 1.1 R:NaBH₄, C:1832616-28-0, C:Ru, S:H₂O, S:THF, 45 min, 25°C. The 'Notes' section contains text about a solid-supported catalyst and reagents. The 'References' section lists a publication: 'Fabrication of Ruthenium Nanoparticles in Porous Organic Polymers: Towards Advanced Heterogeneous Catalytic Nanoreactors'.

Reagent	Count
H ₂	198
NaBH ₄	51
N ₂ H ₄ ·H ₂ O	43
KOH	17
CO	16
HCO ₂ H	16
NH ₄ ⁺ + HCO ₂ ⁻	16
H ₂ O	14
N ₂ H ₄	14
NaOH	14

Overview

Steps/Stages

1.1 R:NaBH₄, C:1832616-28-0, C:Ru, S:H₂O, 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

SciFinder囊括全球最大的反应实验过程合集

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



~102  ~122 

100%

▼ **Overview**

Steps/Stages

1.1 R:H₂, R:Cs₂CO₃, 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 H₂ to a mixture of nitroarene (0.3 mmol), Cs₂CO₃ (0.3 mmol), anisole as internal standard (0.3 mmol), and NHC-Pd-rGO (6 × 10⁻³ mmol, based on metal) in toluene (5 mL). The system was then evacuated and backfilled with H₂ 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

亚结构反应检索

通过C-H活化对苯并噁唑或者恶唑进行烷基化

The screenshot displays the ChemDraw Structure Editor interface. The main window shows a benzimidazole derivative with an R1 group at the 2-position. A purple arrow points from the R1 group in the structure to the R-group definition panel on the right. The R-group definition panel is titled "R-group Definitions" and shows a list of R1 through R10. The R1 group is defined as "O, S". Below this, a periodic table is shown with the "Atoms" section expanded, highlighting the elements O and S. The "Variables" and "Shortcuts" sections are also visible but collapsed. The bottom status bar indicates "Formula is not available".

亚结构反应检索

The screenshot displays the Structure Editor interface. The main workspace shows a chemical reaction: a benzimidazole derivative with an R1 group and a hydrogen atom at the 2-position (labeled 'reactant') reacts to form the same derivative with an 'Ak' group at the 2-position (labeled 'product'). A purple arrow points from the 'Ak' variable in the product to the 'Variables' dialog box.

Structure Editor

Draw or change atoms or bonds. Shortcut Keys

Drawing Editor:

- Structure
- Reaction
- Markush

Variables

X	Any halogen
M	Any metal
A	Any atom except H
Q	Any atom except C or H
Ak	Any carbon chain
Cy	Any cycle
Cb	Any carbocycle
Hy	Any heterocycle

Get reactions where the structure(s) are:

- Variable only at the specified positions
- Substructures of more complex structures

Formula is not available

亚结构反应检索

The screenshot displays the 'Structure Editor' window. The main workspace shows a chemical reaction: a benzimidazole derivative with an R1 group and a hydrogen atom at the 2-position (labeled 'reactant') reacts to form a benzimidazole derivative with an R1 group and an 'Ak' group at the 2-position (labeled 'product').

On the right side, the 'Drawing Editor' panel has three radio buttons: 'Structure', 'Reaction' (which is selected), and 'Markush'. Below this, the section 'Get reactions where the structure(s) are:' contains two radio buttons: 'Variable only at the specified positions' and 'Substructures of more complex structures' (which is selected and highlighted with a purple box).

At the bottom of the window, there is a search bar containing 'Ak', a list of elements (C, H, O, S, N, P, Cl, Br, F, I, Si), and a 'Formula is not available' message at the very bottom.

通过后处理工具筛选反应

通过催化剂筛选反应

The screenshot displays a web interface for a chemical reaction database. On the left, a 'Refine' panel lists various catalysts with their respective counts. A purple box highlights the 'Catalyst' dropdown menu, with an arrow pointing to a callout box above it that says '通过催化剂筛选反应'. The main area shows a reaction detail for a specific reaction (1. View Reaction Detail). The reaction scheme shows the synthesis of a fluorinated benzothiazole derivative from a long-chain alkyl iodide and a benzothiazole derivative, yielding an 83% product. Below the reaction scheme, an 'Overview' section lists the steps/stages: 1.1 R: LiO-Bu-t, C: 1905414-33-6, S: Dioxane, 16 h, 100°C; 1.2 S: H2O, rt; 1.3 R: HCl, S: H2O, neutralized. A 'Notes' section mentions 'catalyst prepared and used, screw cap tube used, Reactants: 2, Reagents: 2, Catalysts: 1, Solvents: one step: 3'. The 'References' section is also visible.

Catalyst	Count
CuI	28
312696-09-6	17
AgNO ₃	17
(MeOCH ₂ CH ₂) ₂ O	16
NaI	15
1905414-33-6	14
CoBr ₂	11
Me ₂ SiCH ₂ MgCl	10
Ph ₂ P(CH ₂) ₃ PPh ₂	10
658062-48-7	9

Reaction Detail:

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

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

Overview

Steps/Stages

- 1.1 R: LiO-Bu-t, C: 1905414-33-6, S: Dioxane, 16 h, 100°C
- 1.2 S: H₂O, rt
- 1.3 R: HCl, S: H₂O, neutralized

Notes

catalyst prepared and used, screw cap tube used, Reactants: 2, Reagents: 2, Catalysts: 1, Solvents: one step: 3

References

提纲

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

SciPlanner使用简介

3. View Reaction Detail Link

3 Steps *Hover over any structure for more options.*

1. 勾选想要的反应

2. 点击Send to SciPlanner

~192 [Step 2.1] ~72

▼ Overview

Steps/Stages

1.1 R: NH₃, R: t-BuOK, R: t-BuOOH, S: THF
2.1 R: NaH, S: THF
3.1 R: POCl₃, reflux

Notes

Reactants: 2, Reagents: 5, Solvents: 1, Steps: 3, Stages: 3, Most stages in any one step: 1

References

Syntheses of 4- and 6-substituted thiazolo[4,5-c]pyridines

3. 进入SciPlanner 新建文件

4. 将刚推送过来的反应拖至编辑面板

SciPlanner SciPlanner_11_19_201...

Workspace Edit View GoTo

New
Open
Save
Duplicate
Import
Export
Print
Close

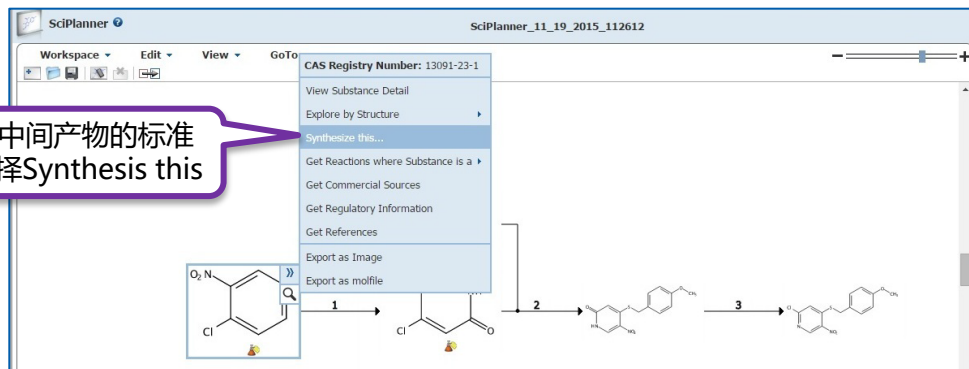
Your Workspace is empty.

Drag items from the reference, substance, and reaction libraries (on the right) to this area.

Clear Reactions

SciPlanner使用简介

5. 打开中间产物的标准菜单选择Synthesize this



6. 在检索到的反应中选择感兴趣的反应

Get References Tools

Send selected records to SciPlanner. Send to SciPlanner

Group by: No Grouping Sort by: Accession Number

1 of 34 Reactions Selected

1. View Reaction Detail

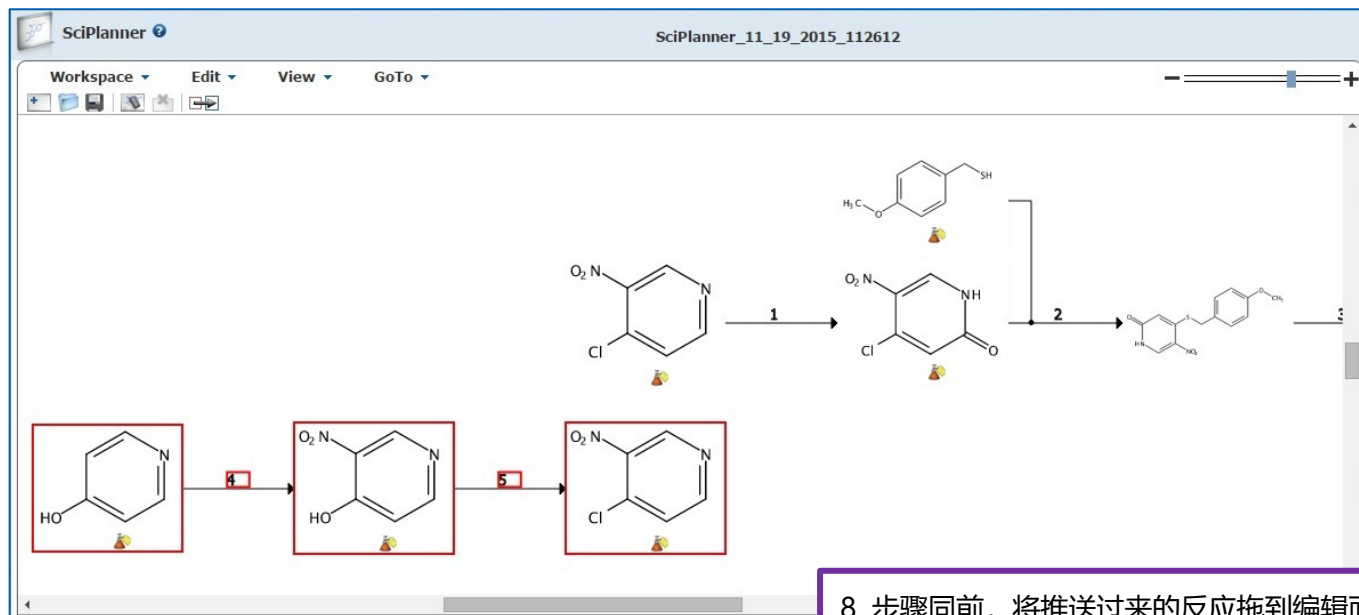
2 Steps Hover over any structure for more options.

HO C1=CC=NC=C1O \rightarrow C1=CC(=C(C=C1)N)C(=O)Cl

~161 ~192

7. 继续推送到SciPlanner

SciPlanner使用简介



SciPlanner使用简介

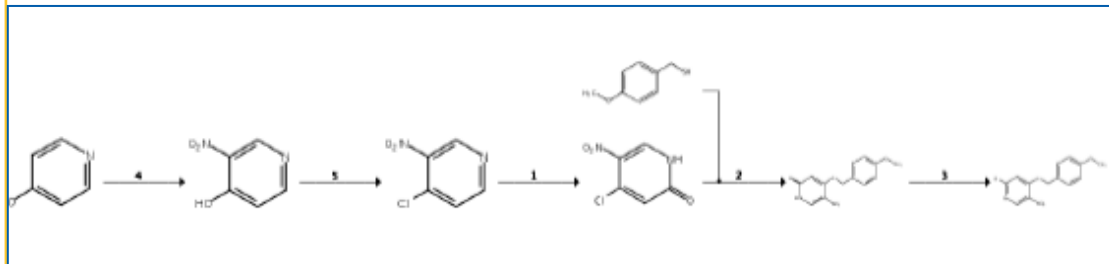
The screenshot displays the SciPlanner software interface with a chemical reaction workflow and an open 'Export' dialog box. The workflow consists of several chemical structures connected by numbered arrows (4, 5, 1, 2). The 'Export' dialog box is open on the right, showing options for 'Offline Review' and 'Saving Locally', along with a 'Details' section for file name, title, and inclusion options.

10. 点击 Workspace, 选择Export 导出结果

9. 用鼠标将两个同样的结构拖至重叠, 两条反应合并

11. 选择适当的输出格式, 输出结果

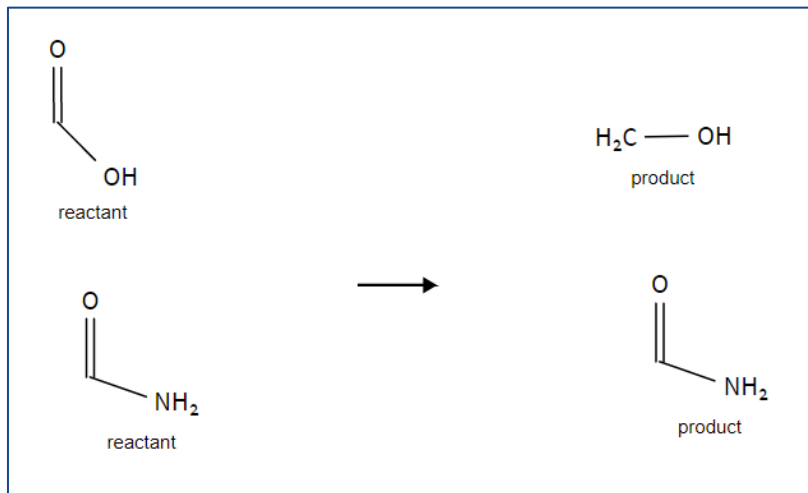
SciPlanner导出结果



Reaction	Stages	Notes	Yield
5	<p>1.1 R:POCl₃, S:PhMe, 0°C → rt; 16 h, rt → 110°C</p> <p>1.2 R:K₂CO₃, S:H₂O, cooled, pH 10</p>	<p>Reactants: 1, Reagents: 2, Solvents: 2, Steps: 1, Stages: 2</p> <p>Transformation:</p> <p>1. Formation of Alkyl Halides from Alcohols</p>	90%
<p>References</p> <p>High color rendering index and color stable hybrid white efficient OLEDs with a double emitting layer structure using a single phosphorescence dopant of heteroleptic platinum complexes</p> <p>By Poleok, Anurach et al</p> <p>From Journal of Materials Chemistry C: Materials for Optical and Electronic Devices, 2(48), 10343-10356; 2014</p>			

Substance Information		
<p>1228150-22-8</p> <p>C₁₃H₁₂N₂O₃S 2-[1-(4-methoxyphenyl)ethyl]pyridine, 4-chloro-5-nitro- Related Info: ~ 2 References Reactions</p>	<p>1228150-23-9</p> <p>C₁₃H₁₁ClN₂O₃S Pyridine, 2-chloro-4-[[1-(4-methoxyphenyl)ethyl]thio]-5-nitro- Related Info: ~ 2 References Reactions</p>	<p>13091-23-1</p> <p>C₅H₃ClN₂O₂ Pyridine, 4-chloro-3-nitro- Related Info: ~ 391 References Reactions ~ 190 Commercial Sources Regulatory Information</p>
<p>5435-54-1</p> <p>C₅H₄N₂O₃ 4-Pyridinol, 3-nitro- Related Info: ~ 113 References Reactions ~ 197 Commercial Sources Regulatory Information</p>	<p>6258-60-2</p> <p>C₈H₁₀O₂S Benzenemethanethiol, 4-methoxy- Related Info: ~ 749 References Reactions ~ 71 Commercial Sources Regulatory Information</p>	<p>626-64-2</p> <p>C₅H₅NO 4-Pyridinol Related Info: ~ 1351 References Reactions ~ 160 Commercial Sources Regulatory Information</p>
<p>850663-54-6</p> <p>C₅H₃ClN₂O₃ 2-[1-(4-chloro-5-nitrophenyl)ethyl]pyridine Related Info: ~ 22 References Reactions ~ 136 Commercial Sources</p>		

反应上机练习



检索要求:

1. 反应物中含有羧基和酰胺基团;
2. 反应物中的CO₂H被还原为产物中的CH₂-OH;
3. 反应物中的酰胺基团在反应后没有发生变化。

提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
 - 文献检索
 - 物质检索
 - Markush检索
 - 反应检索
 - SciPlanner
- SciFinder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

Source: <https://www.cas.org/products/scifinder/system-requirements-web>

如何获取SciFinder账号

The screenshot displays a registration form for SciFinder, divided into three main sections:

- CONTACT INFORMATION--**: Includes input fields for First Name, Last Name, Email, Confirm Email, Phone Number, and Fax Number. It also features dropdown menus for Area of Research and Job Title.
- USERNAME AND PASSWORD--**: Includes input fields for Username (with a 7ps character count), Password, and Re-enter Password.
- SECURITY INFORMATION--**: Includes a dropdown menu for Security Question and an input field for Answer (with a Why? character count).

At the bottom of the form, there are two buttons: "Register>>" and "Clear All".

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) 。

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

更多培训资料请访问

<https://www.cas.org/support/training/scifinder>

谢谢!



欢迎联系:

美国艾赛思国际有限公司北京代表处
ACS International Ltd Beijing Rep Office

china@acs-i.org

www.cas.org

