

程小燕

xcheng@acs-i.org

美国化学文摘社北京代表处

SciFinder在材料科学中的应用

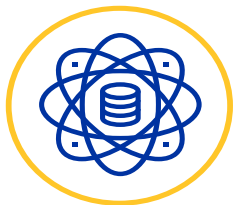
2021年3月

提纲

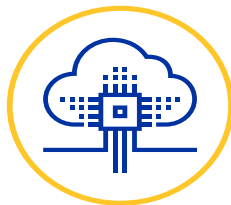
- 美国化学文摘社简介
- SciFinder简介及检索方式
 - 文献检索 (PatentPak及MethodsNow-ANA的应用)
 - 物质检索
 - Markush检索
 - 反应检索 (MethodsNow-SYN的应用)
 - SciPlanner
- SciFinder常见问题及解决

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- 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



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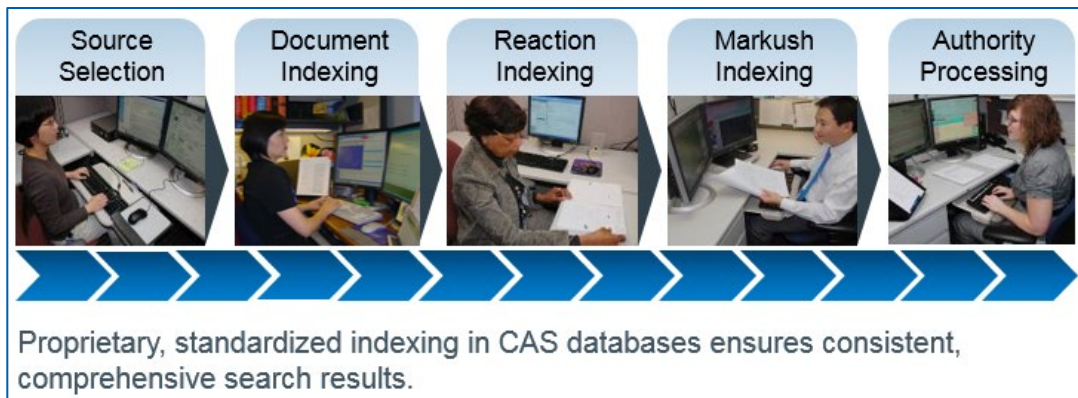
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- 检索词的同义词拓展：解决不同科研人员由于教育背景、语言、表达习惯不同导致的对同一个技术术语描述的差异。
- 用名称、分子式等检索化合物，会导致检索不全、不准的问题。CAS RN很好地解决了该问题，帮助检索人员实现精准定位化合物的目标。
- 利用SciFinder中的标引信息（Index Term, CAS RN, CAS Role），提高效率，启发思路。

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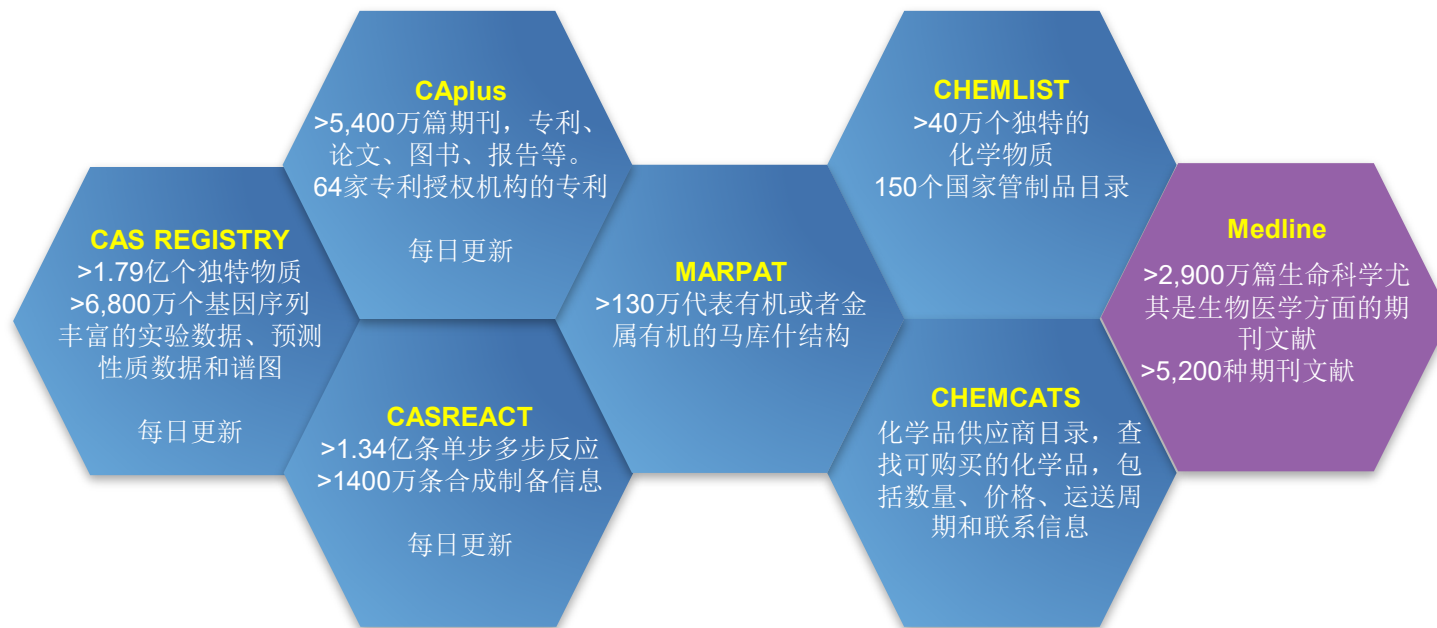
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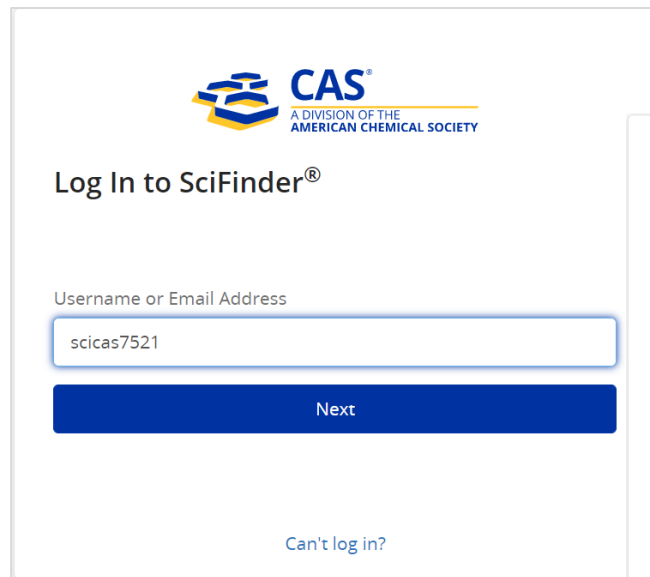
SciFinder覆盖的数据库



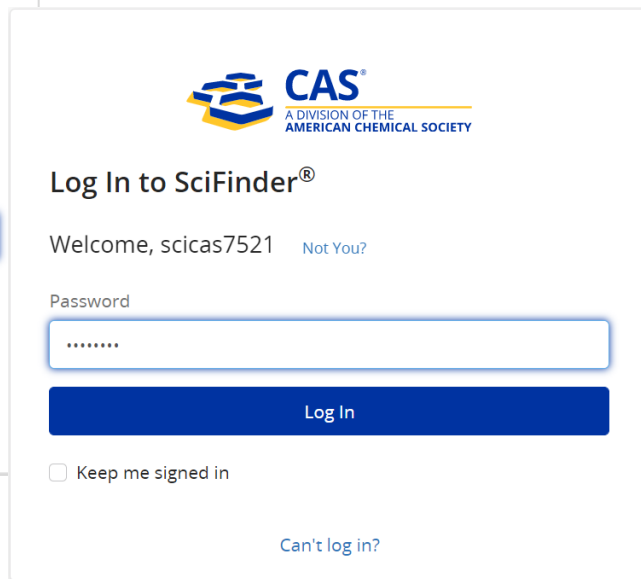
SciFinder是提供经CAS科学家人工标引内容的工具型数据库。

Sources: <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 password 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®". The page displays "Welcome, scicas7521" followed by a link "Not You?". There is a text input field labeled "Password" containing six dots. Below the input field is a blue button labeled "Log In". At the bottom of the page is a checkbox labeled "Keep me signed in" and 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 callouts 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 lists saved answer sets like 'CSF1R', 'jmc', 'EP 19870107847', etc., and a 'KEEP ME POSTED' section.

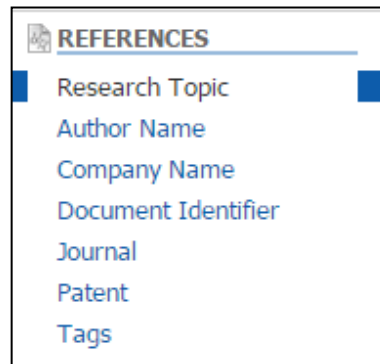
SciFinder Web检索——文献检索

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 displays the SciFinder search interface. At the top, there are navigation tabs: 'Explore', 'Saved Searches', and 'SciPlanner'. On the left side, there is a sidebar menu with three main categories: 'REFERENCES', 'SUBSTANCES', and 'REACTIONS'. Under 'REFERENCES', the following options are listed: Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, and Tags. Under 'SUBSTANCES', the options are: Chemical Structure, Markush, Molecular Formula, Property, and Substance Identifier. Under 'REACTIONS', the option 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 two example search results: 'The effect of antibiotic residues on dairy products' and 'Photocyanation of aromatic compounds'. A blue 'Search' button is positioned below the examples, and a link for 'Advanced Search' is located at the bottom of the search area.

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

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- “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

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

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Sort by: Citing References Accession Number Author Name Citing References Publication Year Title Quick View Other Sources Display Options

Analyze by: Author Name

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

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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 $3.48 \times 10^{-14} \text{ m}^2$, 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...

3. **Photothermal therapy with immune-adjuvant nanoparticles together with checkpoint blockade for effective cancer immunotherapy**
By Chen, Qian; Xu, Ligeng; Liang, Chao; Wang, Chao; Peng, Rui; Liu, Zhuang
From Nature Communications (2016), 7, 13193. | Language: English, Database: CAPLUS
A **therapeutic** strategy that can eliminate primary tumors, inhibit metastases, and prevent tumor relapses is developed herein by combining adjuvant **nanoparticle**-based photothermal therapy with checkpoint-blockade **immunotherapy**. Indocyanine green (ICG), a photothermal agent, and imiquimod (R837), a Toll-like-receptor-7 agonist, are co-encapsulated by poly(lactic-co-glycolic acid) (PLGA). The formed PLGA-ICG-R837 **nanoparticles** composed purely by three clin. approved components can be used for near-IR laser-triggered photothermal ablation of primary tumors, generating tumor-assoc. antigens, whi...

Citing Reference: 帮助找到最重要的文献

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Research Topic "nano with Immunotherapy of

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Huang Leaf	19
Lin Wenbin	18
Steinmetz Nicole F	17
Zhao Yongxiang	17
Moon James J	16
Kong Deling	15
Li Yaping	15

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1. **Improving STING Agonist Delivery for Cancer Immunotherapy Using Biodegradable Mesoporous Silica Nanoparticles**
Quick View Other Sources
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**
Quick View Other Sources
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...

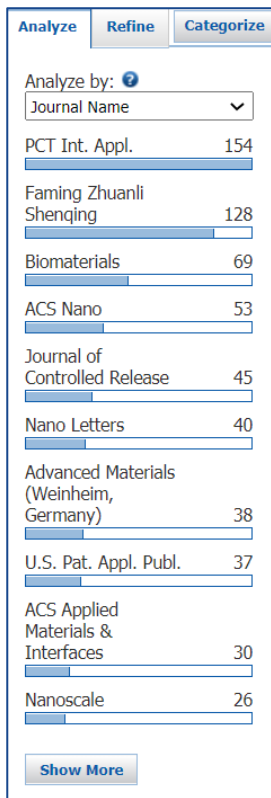
3. **Light-Responsive Core-Shell Nanoplatfor for Bimodal Imaging-Guided Photothermal Therapy-Primed Cancer Immunotherapy**
Quick View Other Sources
By Zhang, Wei; Zhang, Cun-cheng; Wang, Xing-Yue; Li, Lin; Chen, Qiao-Qi; Liu, Wei-Wei; Cao, Yang; Ran, Hai-Tao
From ACS Applied Materials & Interfaces (2020), 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...

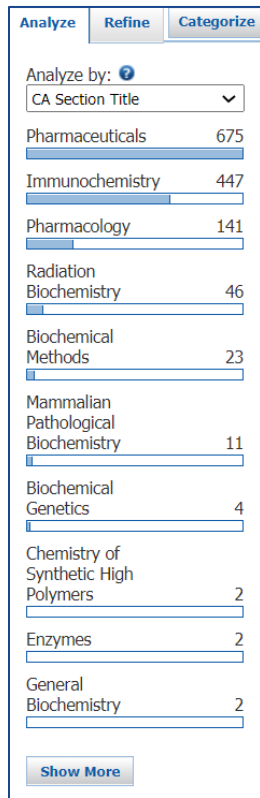
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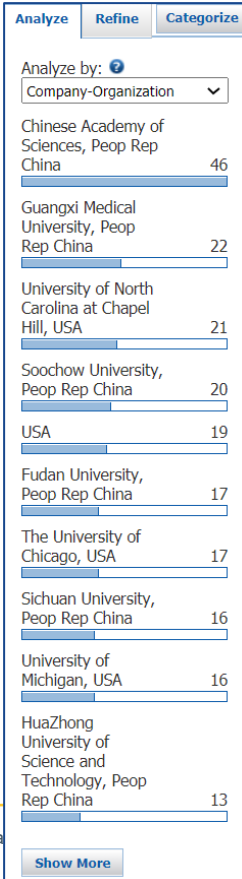
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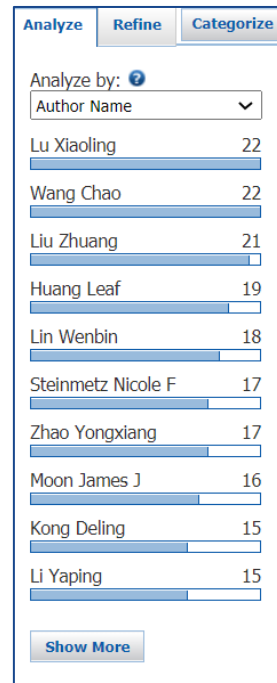
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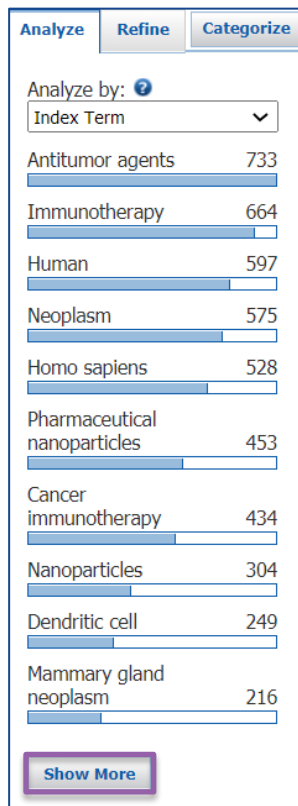
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本领域研究人员

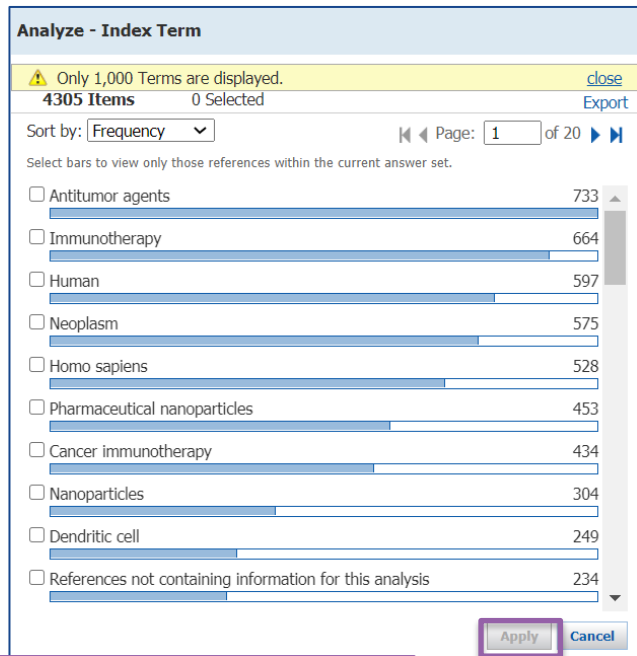


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- Author
- Company Name
- Document Type
- Publication Year
- Language
- Database

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

Refine

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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...**

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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	Count
<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

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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. Gold 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@GOK@Mn,Cu-CDs) were fabricated by integrating the ...

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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	Immunotherapy
Nanocarriers	Nanoparticles
Nanorods	Nanospheres
Photothermal therapy	Surface treatment
Therapy	

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

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

Supplementary Terms

gold nanoparticle anticancer therapy surface decoration review

Citations

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Akiyama, Y; J Controlled Release 2009, 139, 81
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Almeida, J; Small 2015, 11, 1453

文献详情界面包括:

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- 摘要
- 文献中重要的技术术语
- 文献中重要的物质
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Nanoscale
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2020
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ISSN: 2040-3372
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PatentPak——专利工作流程解决方案

By Orhan, Ilkay Erdogan; Kartal, Murat
From Turkish Journal of Pharmaceutical Sciences (2015), 12(3), 279-286. | Language: English, Database: CAPLUS

Hypericum perforation L. (St. John's Wort) is a reputed plant with a long service to humankind. In the current study, antioxidant activity of the methanol ext. of the aerial parts of if H. perforatum growing in Turkey along with hyperoside and hyperforin was evaluated by 2,2-diphenyl-1-picrylhydrazyl (DPPH) radical scavenging, metal-chelation, and ferric-reducing antioxidant power (FRAP) assays. The major components including chlorogenic acid, the flavonoid derivs.; rutin, hyperoside, quercitrin, quercetin, and biapigenin, the naphthodianthrone; pseudohypericin and hypericin, and the phlor...

28. **Flavaspidic acid BB of phloroglucinol derivatives of Dryopteris fragrans and antibacterial application**
PATENTPAK
Quick View

Patent No.	PatentPak Options	Kind	Language
CN 107837247	PDF PDF+ Viewer	A	Chinese

By Shen, Zhibin
From Faming Zhuanli (2017), 13(1), 1-4. | Language: Chinese, Database: CAPLUS

The invention discloses a flavaspidic acid BB derivative, which is shown as structure I. Flavaspidic acid BB has good antibacterial applications, can effectively inhibit the growth of drug-resistant bacteria, provides the antibacterial solution to drug-resistant bacteria. Exptl. result shows that the compd. has relatively strong antibacterial effect, esp. has good curative effect against the drug-resistant bacteria.

29. **Electrochemical properties of carbon aerogels with freeze-drying**
Quick View | Other Sources

By Xu, Yuelong; Yan, Meifang; Liu, Zhenfa
From IOP Conference Series: Materials Science and Engineering (2017), 231(2017 2nd International Seminar on Advances in Materials Science and Engineering), 012093/1-012093/5. | Language: English, Database: CAPLUS

Carbon aerogels (CAs) were prepd. via a sol-gel process by polymn. of phloroglucinol, resorcinol and formaldehyde using 2,4-dihydroxybenzoic acid as catalyst with freeze-drying. The electrochem. properties were characterized using cyclic voltammetry, galvanostatic charge-discharge measurements and electrochem. impedance spectroscopy (EIS). The specific capacitance of corresponding CAs was up to 131 F g⁻¹ and 105 F g⁻¹ at the d. of 0.5 A g⁻¹ and 1.0 A g⁻¹, resp.

30. **Organic acid catalyzed carbon aerogels with freeze-drying**
Quick View | Other Sources

By Xu, Yuelong; Yan, Meifang; Liu, Zhenfa
From IOP Conference Series: Materials Science and Engineering (2017), 231(2017 2nd International Seminar on Advances in Materials Science and Engineering), 012113/1-012113/5. | Language: English, Database: CAPLUS

Carbon aerogels (CAs) were synthesized via a sol-gel process by condensation-polymn. of phloroglucinol, resorcinol and formaldehyde using 2,4-dihydroxybenzoic acid as catalyst with freeze-drying. The effects of the freeze-drying method on the texture and pore structure were studied. Meanwhile the structure of carbon aerogels was characterized by X-ray diffraction (XRD), SEM (SEM) and a surface-area analyzer. The results show that the freeze-drying method and acid catalyst were good for the sp. surface area of carbon aerogel, up to 765m² g⁻¹, and pore size distribution.

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By Orman, İskay Erogan; Kartal, Murat
From Turkish Journal of Pharmaceutical Sciences (2015), 12(2): 279-286. | Language: English, Database: CAPLUS

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Key Substances in Patent

CAS RN 25953-19-9
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Analyst Markup Locations (1)
page 2

CAS RN 1404-90-6
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5. 根据权利要求4所述香鳞毛蕨间苯三酚类化合物黄绵马酸BB的应用,其特征在在于,所述耐药性的革兰氏阳性致病菌是对头孢唑啉、万古霉素和/或达托霉素产生耐药性的革兰氏阳性致病菌。

6. 根据权利要求4或5所述香鳞毛蕨间苯三酚类化合物黄绵马酸BB的应用,其特征在在于,所述耐药性革兰氏阳性致病菌为耐药的金黄色葡萄球菌和/或表皮葡萄球菌。

7. 权利要求1至6所述香鳞毛蕨间苯三酚类化合物黄绵马酸BB的化学合成方法,其特征在在于,包括以下步骤:

- S1. 合成2',4',6'-三羟基-3'-丁酰基苯丁酮;
- S2. 合成4,4-二甲基-3,5-二羟基-2,6-二丁酰基-2,5-环己二烯酮;
- S3. 合成4,4-二甲基-3,5-二羟基-2-丁酰基-2,5-环己二烯酮;
- S4. 合成2,4,6-三甲氧基苯甲醚;
- S5. 合成2-甲基,3,5-二甲氧基苯甲醚;
- S6. 合成3'-甲基-2',4',6'-三甲氧基苯丁酮;
- S7. 合成3'-甲基-2',4',6'-三羟基苯丁酮;
- S8. 合成4,4-二甲基-3,5-二羟基-2-丁酰基-6-(5-甲基-2,4,6-三羟基-3-丁酰基苯基)-2,5-环己二烯酮。

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- S1. 合成2',4',6'-三羟基-3'-丁酰基苯丁酮;

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28. Flavaspidic acid BB of phloroglucinol derivatives of Dryopteris fragrans and antibacterial application

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CAS RN 2216756-37-3

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CAS RN 108-73-6

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- page 8

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- S3. 合成4,4-二甲基-3,5-二羟基-2-丁酰基-2,5-环己二烯酮;
- S4. 合成2,4,6-三甲氧基苯甲醛;
- S5. 合成2-甲基,3,5-二甲氧基苯甲醛;
- S6. 合成3'-甲基-2',4',6'-三甲氧基苯丁酮;
- S7. 合成3'-甲基-2',4',6'-三羟基苯丁酮;
- S8. 合成4,4-二甲基-3,5-二羟基-2-丁酰基-6-(5-甲基-2,4,6-三羟基-3-丁酰基苯基)-2,5-环己二烯酮。

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- S1. 合成2',4',6'-三羟基-3'-丁酰基苯丁酮;

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S2. 合成4,4-二甲基-3,5-二羟基-2,6-二丁酰基-2,5-环己二烯酮;

S3. 合成4,4-二甲基-3,5-二羟基-2-丁酰基-2,5-环己二烯酮;

S4. 合成2,4,6-三甲氧基苯甲醛;

S5. 合成2-甲基,3,5-二甲氧基苯甲醛;

S6. 合成3'-甲基-2',4',6'-三甲氧基苯丁酮;

S7. 合成3'-甲基-2',4',6'-三羟基苯丁酮;

S8. 合成4,4-二甲基-3,5-二羟基-2-丁酰基-6-(5-甲基-2,4,6-三羟基-3-丁酰基苯基)-2,5-环己二烯酮。

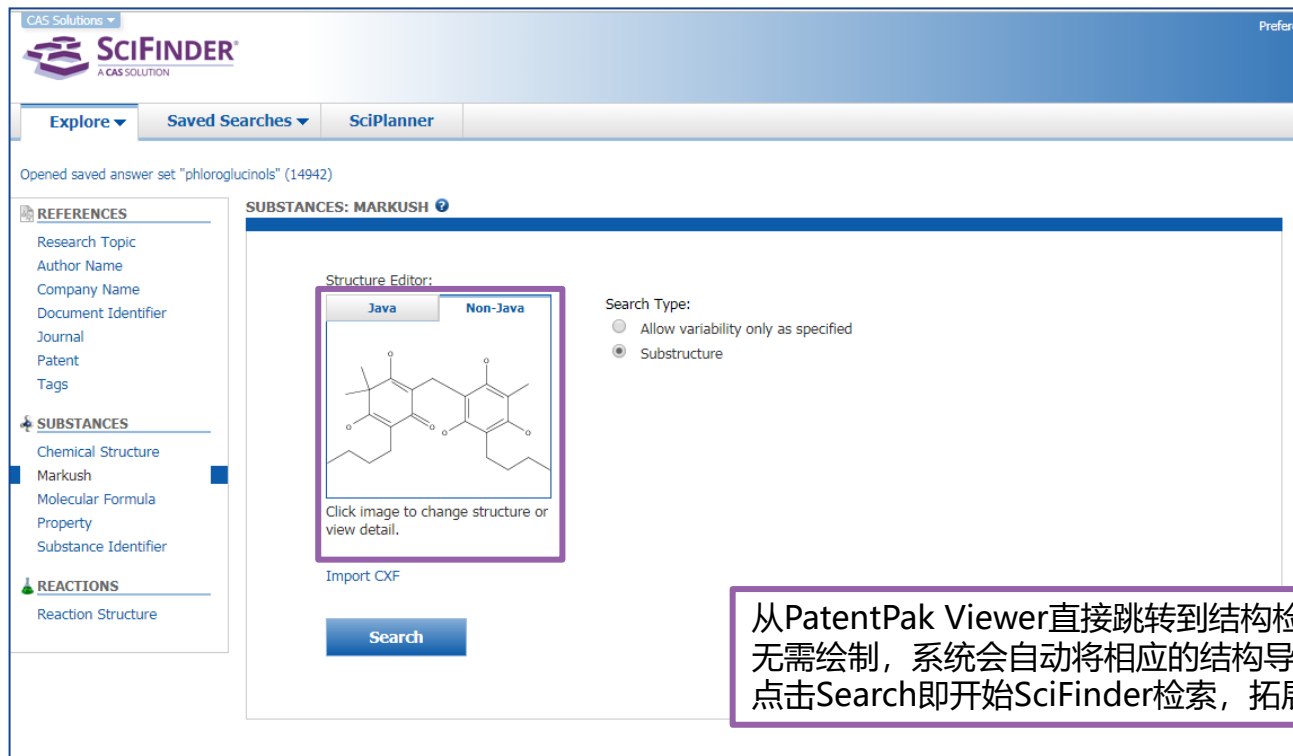
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S9. 合成2',4',6'-三羟基-3'-丁酰基苯丁酮;

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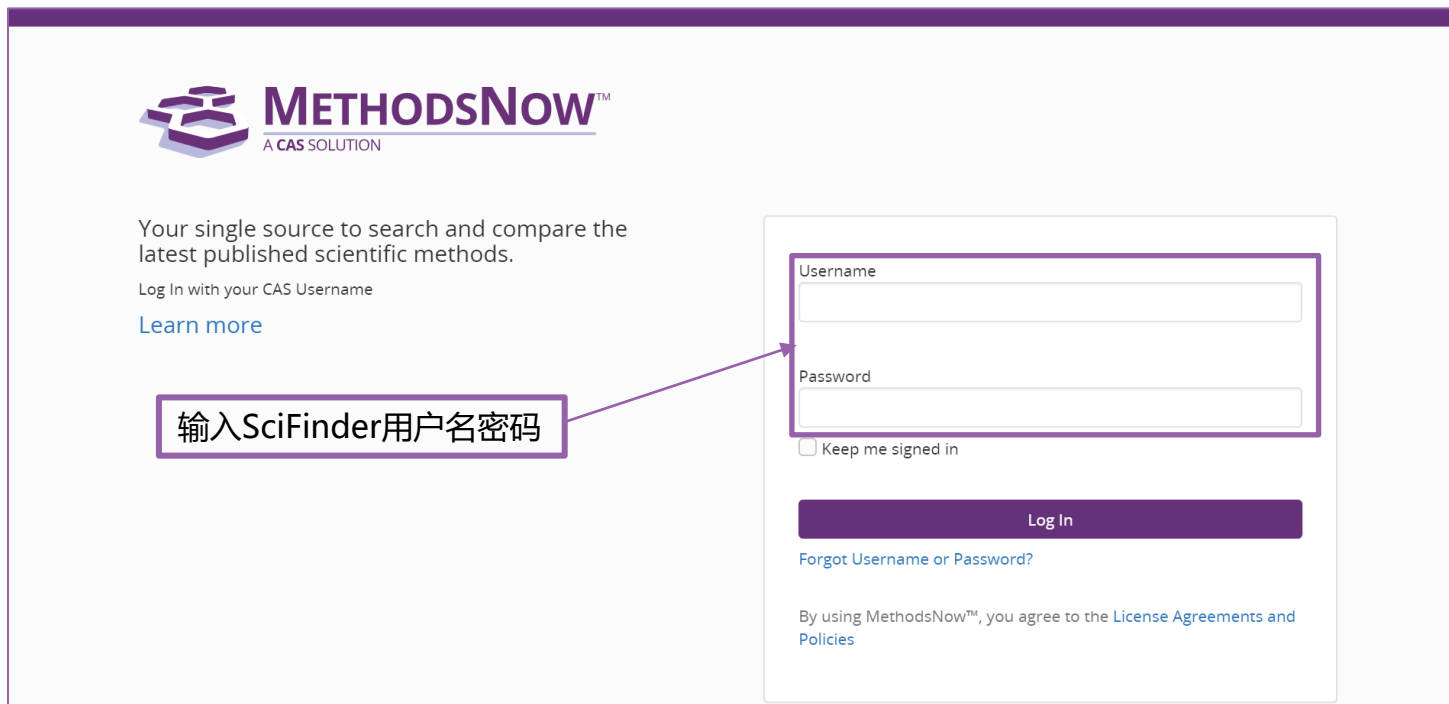
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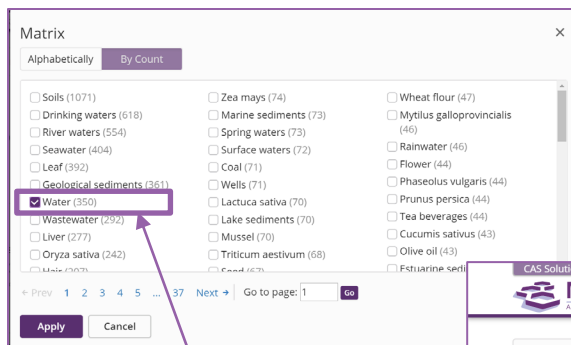
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 - River waters (554)
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 - Leaf (392)
- View All
- Method Category
- Technique

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- Analyte: Cadmium
- Matrix: Brown rice
- Other Materials: Reagent: Tris(hydroxymethyl)aminomethane hydrochloride; Ethylenediaminetetraacetic acid; Nitric acid; Hydrochloric acid
- Material: Anti-Cd-EDTA antibody; Cd assay kit; Cd isolation column
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- Technique: Immunoaffinity chromatography; Extraction

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- Drinking waters (618)
- River waters (554)
- Seawater (404)
- Water (350)

Method Category

Technique

Analyte: Cadmium

Matrix: Water; Geological sediments; Corbicula fluminea

Other Materials: Reagent: Nitric acid; Material: Plastic tank; Mixed cellulose filters (25 mm diameter, 0.45 µm thick); Resin gel

Method Category: Element Detection; Water / Wastewater / Sludge Analysis

Technique: Inductively coupled plasma mass spectrometry

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

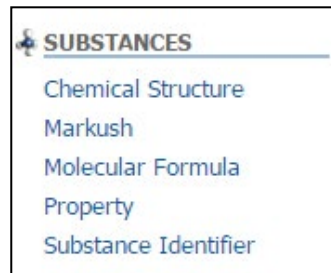
提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
 - 文献检索 (PatentPak及MethodsNow-ANA的应用)
 - 物质检索
 - Markush检索
 - 反应检索 (MethodsNow-SYN的应用)
 - 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

The screenshot displays the SciFinder interface for a specific chemical substance. At the top left, a search bar contains the CAS Registry Number "63968-64-9". Below the search bar, the chemical structure of the substance is shown in a 3D perspective view, with stereochemistry indicated by wedged and dashed bonds. The structure is a complex polycyclic molecule with multiple oxygen atoms and methyl groups. Below the structure, the text "Absolute stereochemistry." is displayed. To the right of the structure, a dropdown menu is open, listing various actions that can be performed on the substance, such as "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", and "Send to SciPlanner".

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

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

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

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

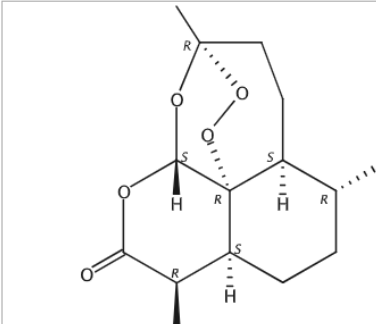
Melting Point (Experimental)
Value: 156-157 °C

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[®]

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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

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

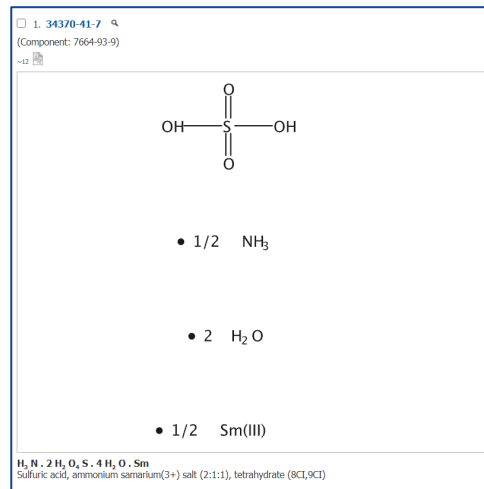
物质检索——分子式

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

The screenshot shows the CAS SciPlanner interface. At the top, there are tabs for 'Explore', 'Saved Searches', and 'SciPlanner'. Below the tabs, the breadcrumb path is 'Property "Experimental - Electric Conduc..." > substances (51)'. On the left, there are two main sections: 'REFERENCES' and 'SUBSTANCES'. Under 'REFERENCES', there are links for Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, and Tags. Under 'SUBSTANCES', there are links for Chemical Structure, Markush, Molecular Formula (which is highlighted), Property, and Substance Identifier. The main area is titled 'SUBSTANCES: MOLECULAR FORMULA'. It contains a search input field with the text 'H3 N . 2 H2 O4 S . 4 H2 O . Sm'. Below the input field, there are 'Examples:' listed as 'H4SiO4' and '(C3H6O.C2H4O)x'. A blue 'Search' button is positioned below the examples.

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



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** section includes radio buttons for **Exact Structure**, **Substructure** (selected), and **Similarity**, along with a **Show precision analysis** checkbox. A **ChemDraw** logo is visible with the text "Launch a SciFinder substance or r". A blue **Search** button is positioned below the structure editor. At the bottom, there are links for **Advanced Search** and a checked **Always Show** option.

物质检索——结构

The image shows a screenshot of the 'Structure Editor' software interface. The interface is annotated with numerous Chinese labels pointing to specific tools and features. On the left side, a vertical toolbar contains icons for drawing and editing, with labels such as '橡皮' (Eraser), '铅笔' (Pencil), '元素周期表' (Periodic Table), '可变基团' (Variable Group), '重复基团工具' (Repeat Group Tool), '碳链工具' (Carbon Chain Tool), '选择工具' (Select Tool), '环锁定工具' (Ring Lock Tool), '旋转工具' (Rotate Tool), '正电子' (Positron), and '负电子' (Negatron). The main workspace shows a chemical structure being edited, with labels for '常用基团' (Common Group), 'R基团定义工具' (R-Group Definition Tool), '可变位置连接工具' (Variable Position Connection Tool), '模版工具' (Template Tool), '索套选择工具' (Loop Selection Tool), '原子锁定工具' (Atom Lock Tool), and '镜面旋转工具' (Mirror Rotate Tool). On the right side, there is a 'Drawing Editor' panel with options for 'Structure', 'Reaction', and 'Markush', and a search panel with options for 'Exact search', 'Substructure search', and 'Similarity search'. At the bottom, there is a 'Structure检索选择' (Structure Search Selection) label pointing to the search options, and a '常见环, 多元环工具' (Common Ring, Polycyclic Tool) label pointing to a set of ring icons. The bottom status bar shows the chemical formula 'C H O S N F Cl Br F I Si' and a '(query)' field.

橡皮

结构和反应切换功能

铅笔

元素周期表

可变基团

重复基团工具

碳链工具

选择工具

环锁定工具

旋转工具

正电子

C原子和单键恢复工具

常用基团

R基团定义工具

可变位置连接工具

模版工具

索套选择工具

原子锁定工具

镜面旋转工具

结构检索选择

负电子

单双键, RS构型, 不确定键定义工具

常见环, 多元环工具

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: CAS Registry Number ↑ Display Options

0 of 5 Substances Selected **倒序排列**

1. **34370-41-7**

(Component: 7664-93-9)

~12

- 1/2 NH₄⁺
- 2 H₂O
- 1/2 Sm(OH)₂

H₂N · 2 H₂O₂ S · 4 H₂O · Sm
Sulfuric acid, ammonium samarium(3+) salt (2:1:1), tetrahydrate (8CI,9CI)

2. **40148-71-8**

(Component: 7664-93-9)

~1

- NH₄⁺
- 1/3 H₂O
- 1/3 Sm(OH)₂

H₂N · H₂O₂ S · 1/3 H₂O · 1/3 Sm
Sulfuric acid, ammonium samarium(3+) salt (3:3:1), monohydrate (9CI)

3. **40148-74-1**

(Component: 7664-93-9)

~1

- 1/2 NH₄⁺
- H₂O
- 1/2 Sm(OH)₂

H₂N · 2 H₂O₂ S · 2 H₂O · Sm
Sulfuric acid, ammonium samarium(3+) salt (2:1:1), dihydrate (9CI)

4. **42949-48-4**

~1

49856-58-8 (Component: 736080-59-4)
H₆ O₁₁ S₂ Sm · H₄ N · H₂O

- NH₄⁺
- H₂O

(H₆O₁₁S₂Sm · H₄N · H₂O)_x
Samarate(1-), triaquabis[sulfato(2-)-O,O']-, ammonium, monohydrate, homopolymer (9CI)

5. **49856-58-8**

(Component: 736080-59-4)

~0

- NH₄⁺
- H₂O

H₆O₁₁S₂Sm · H₄N · H₂O
Samarate(1-), triaquabis[sulfato(2-)-O,O']-, ammonium, monohydrate (9CI)



CAS[®]

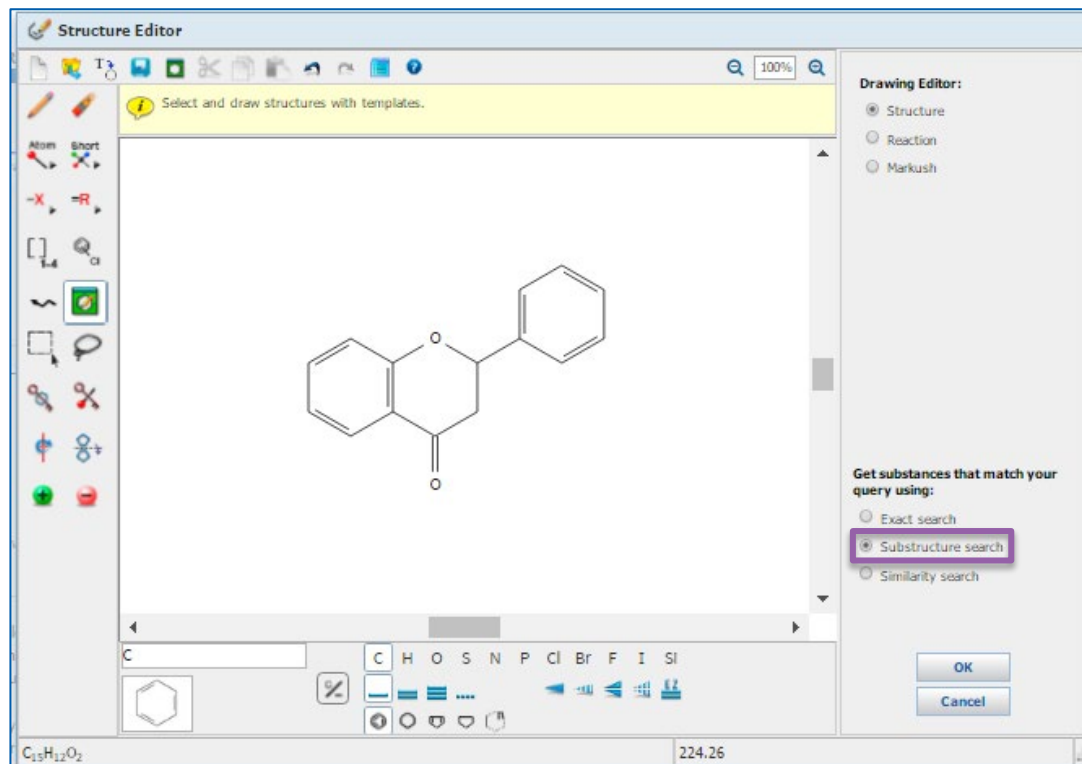
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AMERICAN CHEMICAL SOCIETY

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

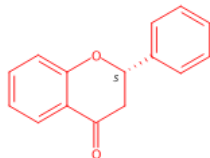
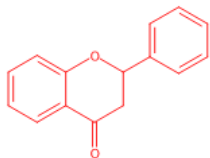


物质检索——亚结构检索

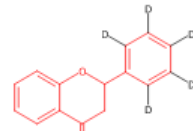
0 of 23824 Substances Selected

1. 487-26-3

2. 17002-31-2



10. 146196-91-0



同位素

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

Key Physical Properties
Regulatory Information
Spectra
Experimental Properties

281. 123251-10-5



取代物

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

Key Physical Properties
Experimental Properties

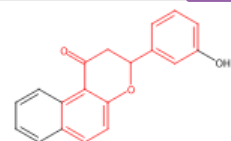
295. 780723-19-5



离子

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

284. 136116-23-9



稠环物质

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

Key Physical Properties



CAS®

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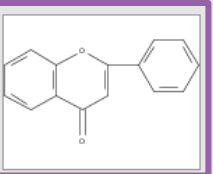
亚结构检索结果的限定

Analysis Refine

Refine by:

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

Chemical Structure:



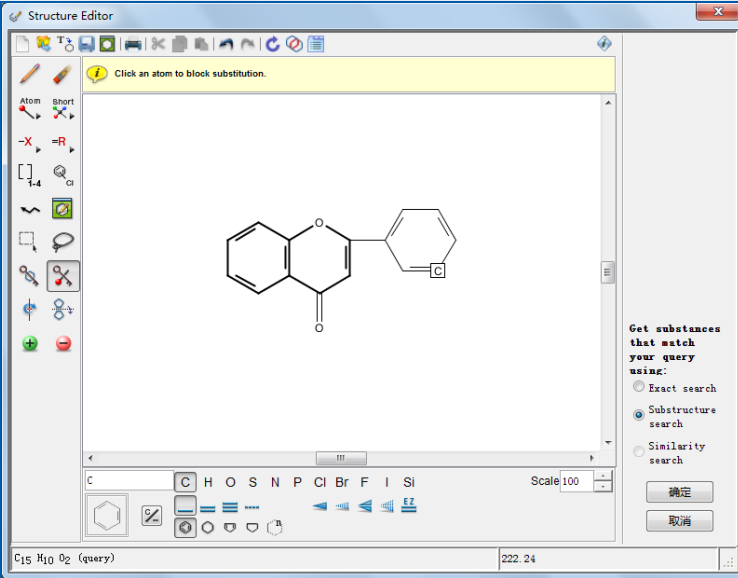
Click image to change structure or view detail

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

C₁₆ H₁₀ O₂ (query) 222.24



环锁定



原子锁定



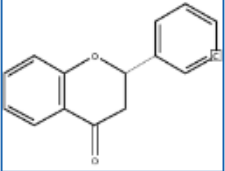
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亚结构检索结果的限定

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

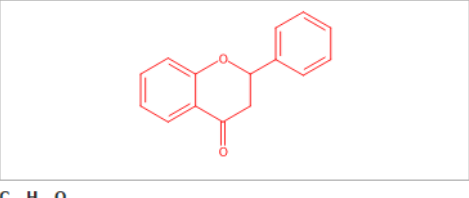
Refine

Get References Get Reactions Get Commercial Sources Tools

Sort by: Relevance

0 of 13826 Substances Selected

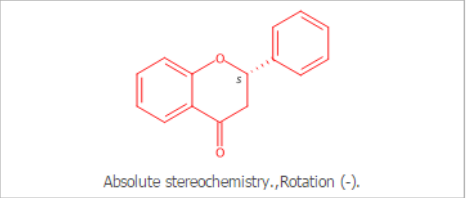
1. 487-26-3



$C_{15}H_{12}O_2$
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

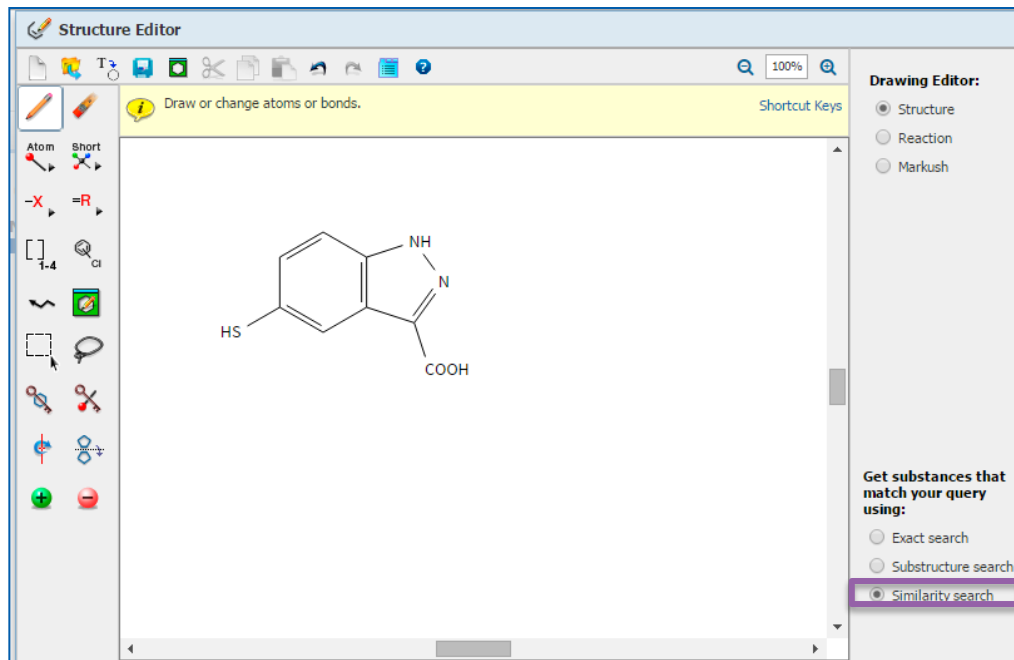
5. 75524-43-5

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

取代基变化

O=C(O)c1n[nH]c2ccc(O)cc12

$C_8 H_6 N_2 O_3$
1H-Indazole-3-carboxylic acid, 5-hydroxy-

▶ Key Physical Properties

Score: 86

5. 858227-12-0

取代基位置变化

Cc1ccc2c(c1)[nH]n2C(=O)O

$C_9 H_8 N_2 O_2$
1H-Indazole-3-carboxylic acid, 6-methyl-

▶ Key Physical Properties

Score: 65

541. 1100422-

母体结构变化

Cn1c2ccc(F)cc2[nH]1C(=O)O

$C_{13} H_8 F N_2 O_2$
1H-Benz[γ]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 (PatentPak及MethodsNow-ANA的应用)
 - 物质检索
 - Markush检索
 - 反应检索 (MethodsNow-SYN的应用)
 - 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, N₂保护下加入25mL无水CH₂Cl₂,然后缓缓滴入吡啶(2.5mL,30mmol)和二氯亚砷(1.1mL,14mmol),该反应液置于室温反应半小时。随后,2-氨基吡嗪(0.95g,10mmol)和三乙胺(5.7mL,40mmol)溶于15mL CH₂Cl₂后缓缓滴入上述反应液,室温反应6小时。反应液加30mL饱和食盐水稀释,分出有机层,水层CH₂Cl₂提取(15mL×3),合并有机层,无水硫酸钠干燥后减压除去溶剂,柱层析分离得白色固体2.3g,收率74%。m.p.: 134-136°C; ¹H NMR (500MHz, CDCl₃): δ = 9.55 (s, 1H, pyrazine-H), 8.35 (d, 1H, J=2.0Hz, pyrazine-H), 8.23 (s, 1H, pyrazine-H), 7.97 (s, 1H, NH), 4.20 (m, 2H, CH₂), 2.81 (m, 2H, CH₂), 2.48 (m, 1H, CH), 1.93 (d, 2H, J=12.5Hz, CH₂), 1.76 (m, 2H, CH₂), 1.47 (s, 9H, CH₃) ppm; ESI-MS: m/z = 307[M+H]⁺。

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

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

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

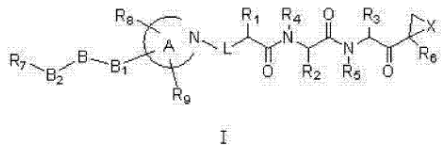
Markush检索

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:



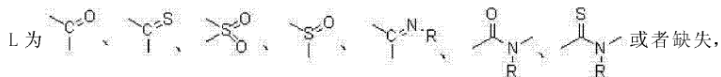
其中:

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

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

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

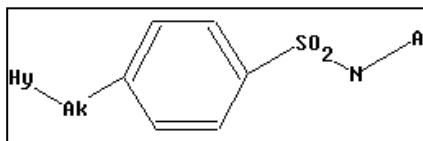
R_8, R_9 分别独立选自 H、OH、 C_{1-6} 烷基、 C_{1-6} 烷氧基、 C_{1-6} 羟基烷基、 C_{1-6} 巯基烷基、 C_{1-6} 烷基 -D、芳基、杂芳基、环烷基和杂环基,这些基团可以被卤素、硝基、氨基、CN、 C_{1-6} 烷基、卤代的 C_{1-6} 烷基、 C_{1-6} 烷氧基或卤代的 C_{1-6} 烷氧基取代,每个基团可与一个或多个芳基或杂环

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 interface showing the chemical structure from the previous image. The interface includes a toolbar with various drawing tools, a central canvas displaying the structure, and a right-hand panel with options for Drawing Editor (Structure, Reaction, Markush) and Get Markush patents where the structure(s) are (Variable only at the specified positions, Substructures of more complex structures). The bottom of the interface shows a list of elements (A, C, H, O, S, N, P, Cl, Br, F, I, Si) and a search bar.

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 - Markush检索
 - 反应检索 (MethodsNow-SYN的应用)
 - 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

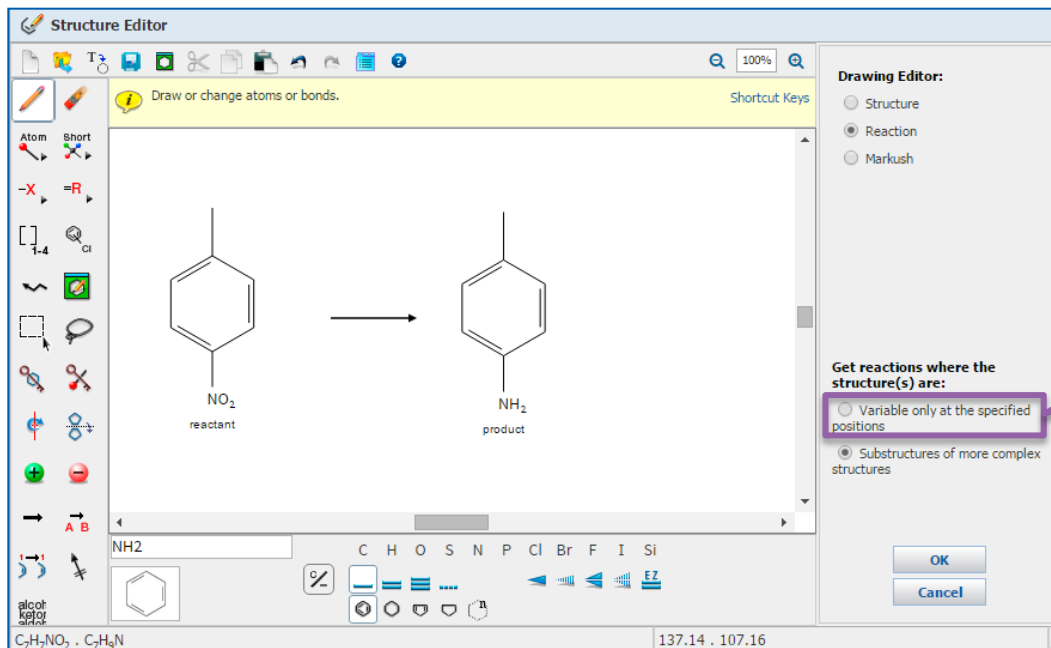
The screenshot shows the Structure Editor software interface. The main window is titled "Structure Editor" and contains a toolbar with various drawing tools. A yellow banner at the top of the main workspace says "Draw or change atoms or bonds." On the right side, there is a "Drawing Editor" panel with radio buttons for "Structure", "Reaction", and "Markush", with "Reaction" selected. Below this panel, there are options for "Get reactions where the structure(s) are:" with radio buttons for "Variable only at the specified positions" and "Substructures of more complex structures". At the bottom right, there are "OK" and "Cancel" buttons. The bottom status bar shows "16.04".

Four purple boxes with white text labels are overlaid on the interface, pointing to specific tools:

- 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 that allows marking atoms in a reaction.
- 官能团列表 (Functional Group List) - points to the list of functional groups at the bottom left.
- 反应位置标记工具 (Reaction Position Marking Tool) - points to the tool that allows marking reaction positions.

Other visible labels in the interface include "Structure Editor", "Drawing Editor:", "Structure", "Reaction", "Markush", "Get reactions where the structure(s) are:", "Variable only at the specified positions", "Substructures of more complex structures", "OK", "Cancel", "16.04", "C H O S N P Cl Br F I Si", and "alcohol ketone".

SciFinder反应检索——原子和环被锁定



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.*

O=[N+]([O-])c1ccc(C)cc1 → Nc1ccc(C)cc1
~102 ~122

100%

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

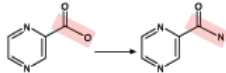
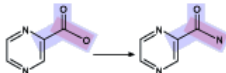
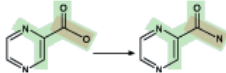
Narrow: 反应中心及扩展的原子和键

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

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

3. Reduction of Nitro to Azoxy Compounds
11 Reactions


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



更精确的查找需要的反应



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 R1 group definition in the 'R-group Definitions' panel. In this panel, the R1 group is defined as 'O.S'. Below the definition, a periodic table is shown with the 'Atoms' section expanded, highlighting the 'O.S' (Oxygen) element. 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 (reactant) reacts to form the same derivative with an R1 group and an 'Ak' variable at the 2-position (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

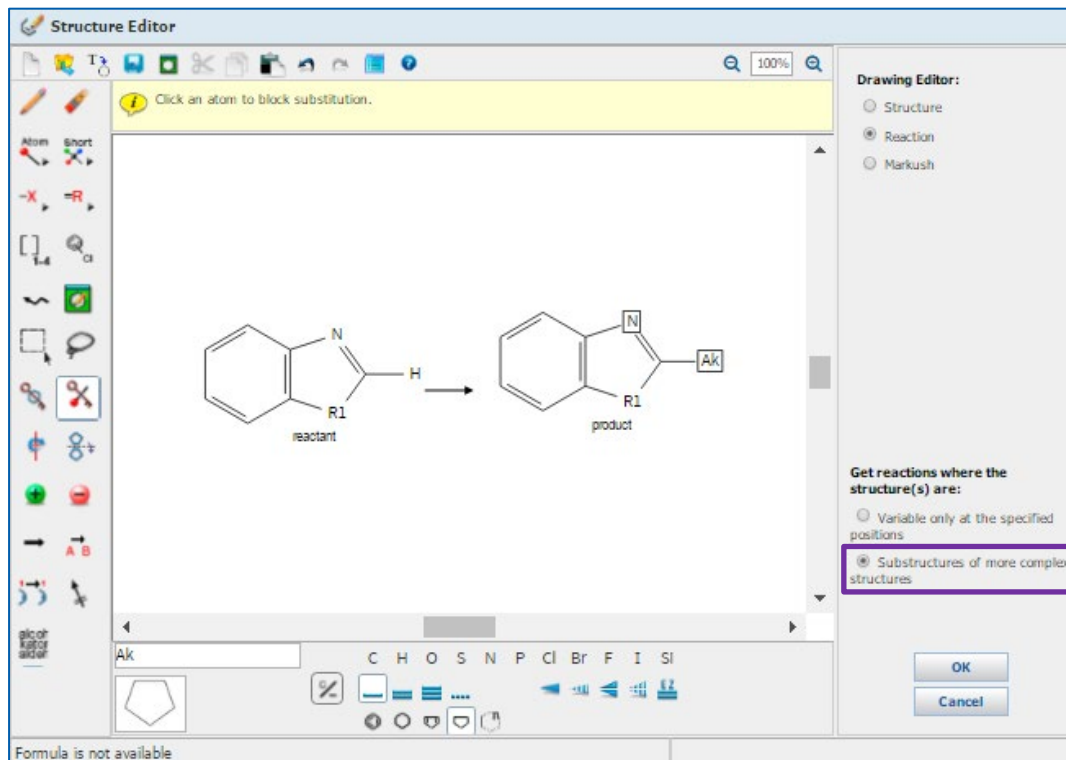
X	Any halogen
M	Any metal
A	Any atom except H
Q	Any atom except C or H
Ak	Any carbon chain
Cy	Any cycle
Cb	Any carbocycle
Hy	Any heterocycle

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



通过后处理工具筛选反应--Analyze

CAS Solutions
SCIFINDER
A CAS SOLUTION

Preferences | SciFinder Help | Sign Out

Welcome Helen Zhu

Explore | Saved Search | **筛选出有实验步骤的反应** | Save | Print | Export

Reaction Structure substructure with limiters > reactions (282)

REACTIONS

Get References | Tools

Send to SciPlanner

Analyze | Refine

Analyze by: MethodsNow

MethodsNow Available 184

MethodsNow Not Available 98

Show More

Group by: No Grouping | Sort by: Accession Number

0 of 282 Reactions Selected

1. View Reaction Detail | Link | Similar Reactions

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

C[CH-](F)(F)F.[K+].BrC1=CC=C2N=C(S1)C=C2 >> BrC1=CC=C2N=C(S1)C=C2

~76 | ~108 | 78% | ~4

Overview

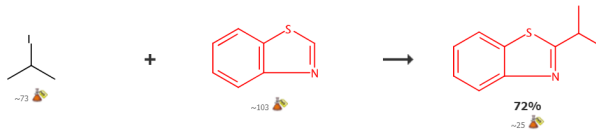
2. View Reaction Detail | Link | Similar Reactions

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

通过后处理工具筛选反应--Analyze

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

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



Overview

METHODS NOW™

Procedure

1. Add one equivalent of indole, 3 equivalents of benzothiazole to a Chemglass vial.
2. Purge the vial for 5 minutes under vacuum.

[View more...](#)

Available Experimental Data

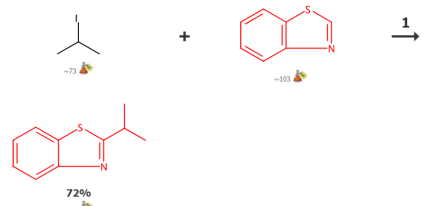
¹H NMR, ¹³C NMR, HRMS

[View with MethodsNow](#)

MethodsNow

C-H Functionalization of Heteroarenes Using Unactivated Alkyl Halides through Visible-Light Photoredox Catalysis under Basic Conditions

By Bissonnette, Noah B.; Boyd, Michael J.; May, Gregory D.; Giroux, Simon; Nuhant, Philippe
From Journal of Organic Chemistry, 83(18), 10933-10940, 2018
Published by American Chemical Society



Products	2-(1-Methylethyl)benzothiazole, 72%, CAS RN: 17626-86-7
Reactants	Isopropyl iodide, CAS RN: 75-30-9 Benzothiazole, CAS RN: 95-16-9
Reagents	2,2,6,6-Tetramethylpiperidine, CAS RN: 768-66-1
Catalysts	Iridium(III), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine-κ ^{N,N'}]-bis[2-(2-pyridinyl)-κ ^N phenyl]-hexafluorophosphate(1-)(1:1), CAS RN: 676525-77-2

Solvents	Methanol, CAS RN: 67-56-1
Procedure	<ol style="list-style-type: none"> 1. Add one equivalent of indole, 3 equivalents of benzothiazole and 2.5 mol % of [Ir(ppy)₃]/(tbbpy)]PF₆ to a vial (1 dram, ~3.7 mL), 15 × 45 mm, 13-425 thread with red pressure relief cap Chemglass vial. 2. Purge the vial for 5 minutes under vacuum. 3. Fill the vial with nitrogen gas. 4. Add MeOH (0.5 mL), 3:1 equivalents of Et₃N and 1 equivalent of indole to the reaction mixture under N₂ atmosphere. 5. Remove the nitrogen line. 6. Add 3 equivalents of benzothiazole to the reaction mixture. 7. Irradiate the vial under blue LED light. 8. Stir the reaction mixture overnight at room temperature at 1000 rpm with a small cooling fan (approximately 16 hours). 9. After the completion of the reaction, add 0.25 equivalent of 1,4-dinitrobenzene to the vial. 10. Evaporate the volatiles using a V10 Biotage system. 11. Load the crude mixture onto a 40 g gold ISCO column using hexane/ethyl acetate (100:0 to 0:100) as eluents.
Transformation	Friedel-Crafts Alkylation
¹H NMR	(400 MHz, chloroform-d) δ 7.98 (dd, <i>J</i> = 8.2, 1.2 Hz, 1H), 7.85 (dd, <i>J</i> = 8.0, 1.3 Hz, 1H), 7.45 (ddd, <i>J</i> = 8.3, 7.2, 1.3 Hz, 1H), 7.34 (ddd, <i>J</i> = 8.3, 7.3, 1.2 Hz, 1H), 3.43 (hept, <i>J</i> = 6.9 Hz, 1H), 1.48 (d, <i>J</i> = 6.9 Hz, 6H).
¹³C NMR	(101 MHz, chloroform-d) δ 178.7, 153.3, 134.8, 126.0, 124.7, 122.7, 121.7, 34.2, 23.1 (2C).
HRMS	(ESI), m/z: calcd for C ₁₀ H ₁₂ NS[M + H] ⁺ : 178.0690, found: 178.0687.
CAS Method Number	3-085-CAS-19169886

提纲

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 - 反应检索 (MethodsNow-SYN的应用)
 - 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

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

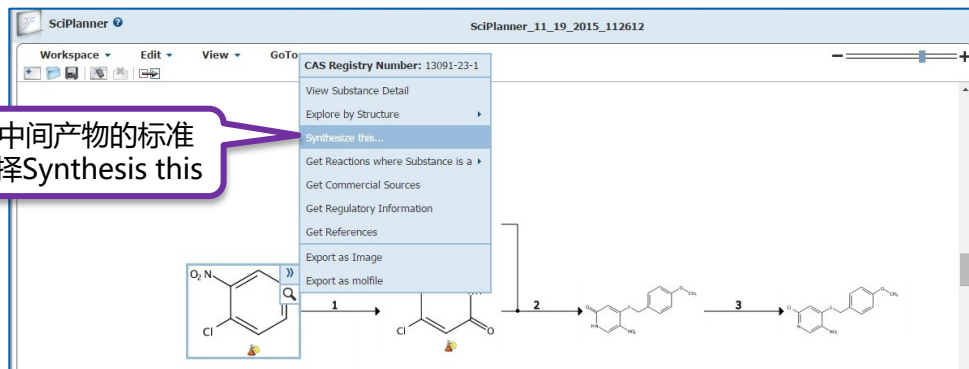
Syntheses of 4- and 6-substituted thiazolo[4,5-c]pyridines

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

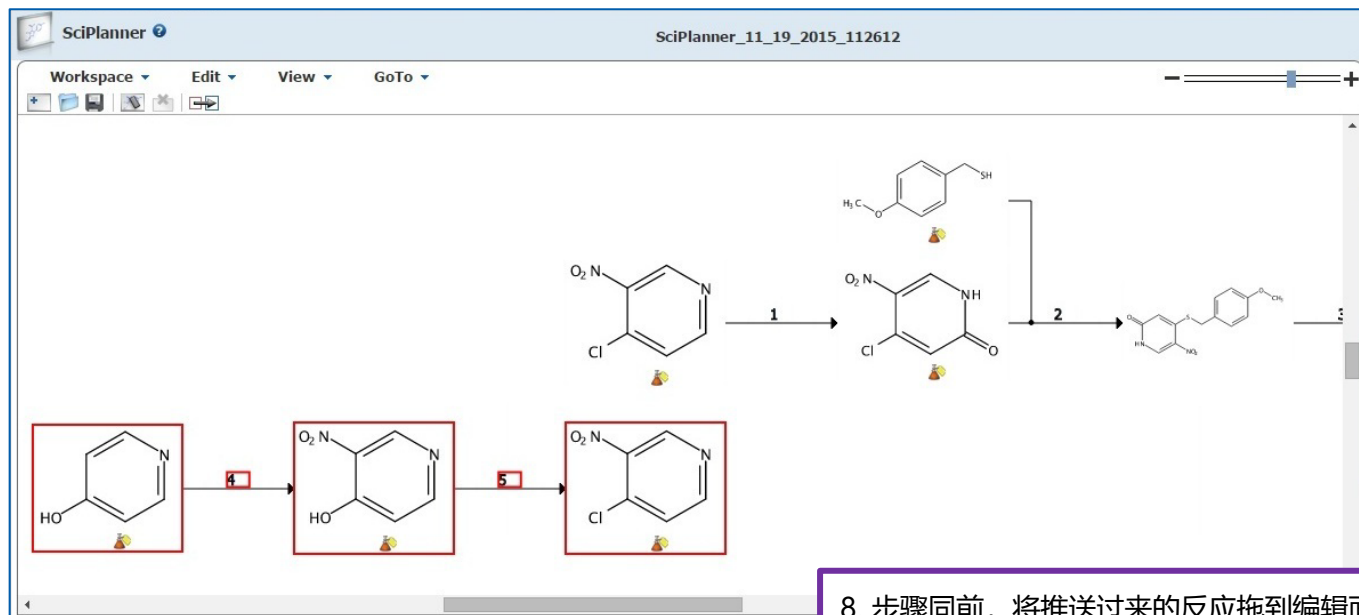
1. View Reaction Detail

2 Steps Hover over any structure for more options.

~161 ~192

7. 继续推送到SciPlanner

SciPlanner使用简介



SciPlanner使用简介

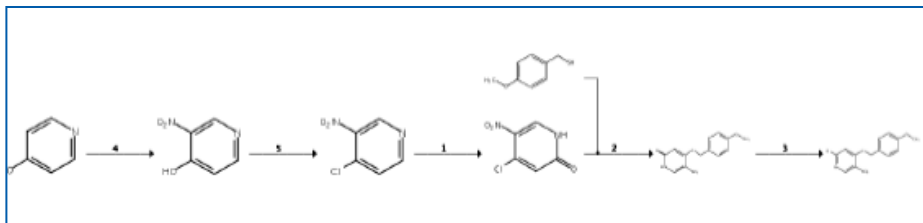
The screenshot displays the SciPlanner software interface with a chemical reaction workflow and an export dialog box. The workflow consists of four chemical structures connected by arrows labeled 4, 5, 1, and 2. Structure 1 is a pyridine ring with a nitro group (O₂N) and a hydroxyl group (HO). Structure 2 is a pyridine ring with a nitro group (O₂N) and a chlorine atom (Cl). Structure 3 is a pyridine ring with a nitro group (O₂N) and a chlorine atom (Cl), with an NH group. Structure 4 is a pyridine ring with a nitro group (O₂N) and a chlorine atom (Cl), with an NH group and a hydroxyl group (OH). The export dialog box is open, showing options for offline review and saving locally. The 'Export' button is highlighted.

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	1.1 R:POCl ₃ , S:PhMe, 0°C → rt, 16 h, rt → 110°C 1.2 R:K ₂ CO ₃ , S:H ₂ O, cooled, pH 10	Reactants: 1, Reagents: 2, Solvents: 2, Steps: 1, Stages: 2 Transformation: 1. Formation of Alkyl Halides from Alcohols	90%
References 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 By Poloek, Anurach et al From Journal of Materials Chemistry C: Materials for Optical and Electronic Devices, 2(48), 10343-10356; 2014			

Substance Information		
1228150-22-8 C ₁₂ H ₁₂ N ₂ O ₂ S 2-(1-(4-methylphenyl)methylthio)pyridine Related Info: ~ 2 References Reactions	1228150-23-9 C ₁₃ H ₁₄ ClN ₂ O ₂ S Pyridine, 2-(chloro-4-(2-(4-methoxyphenyl)methylthio)5-nitro- Related Info: ~ 2 References Reactions	13091-23-1 C ₅ H ₃ ClN ₂ O ₂ Pyridine, 4-chloro-3-nitro- Related Info: ~ 361 References Reactions ~ 100 Commercial Sources Regulatory Information
5435-54-1 C ₅ H ₄ N ₂ O ₃ 4-Pyridinol, 3-nitro- Related Info: ~ 115 References Reactions ~ 167 Commercial Sources Regulatory Information	6258-66-2 C ₇ H ₁₀ O ₂ S Benzenemethanethiol, 4-methoxy- Related Info: ~ 749 References Reactions ~ 71 Commercial Sources Regulatory Information	626-44-2 C ₅ H ₄ NO 4-Pyridinol Related Info: ~ 1551 References Reactions ~ 100 Commercial Sources Regulatory Information
850653-54-6 C ₉ H ₇ ClN ₂ O ₃ 2-(1-(4-chloro-5-nitro- Related Info: ~ 22 References Reactions ~ 136 Commercial Sources		



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提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
 - 文献检索 (PatentPak及MethodsNow-ANA的应用)
 - 物质检索
 - Markush检索
 - 反应检索 (MethodsNow-SYN的应用)
 - 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

如何获取SciFinder账号

The screenshot shows a registration form with three main sections:

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

At the bottom of the form 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. 从下拉列表中选择**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

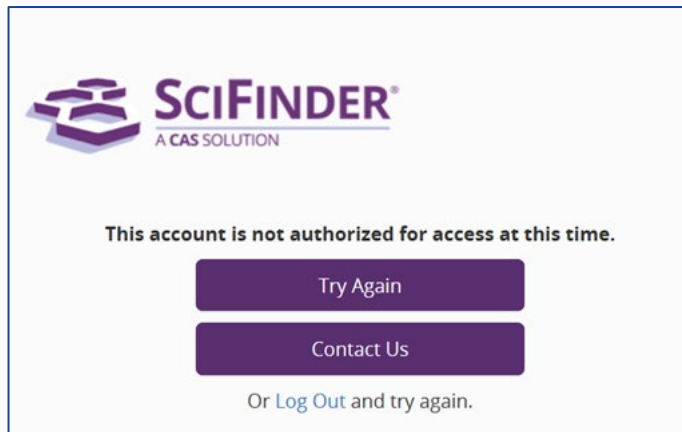
SciFinder常见问题

Unauthorized IP Address

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

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

SciFinder常见问题



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

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

