

朱传娴

客户顾问

hzhu@acs-i.org

如何使用SciFinder获取科技信息

江南大学

2018.11.26



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—Chemical Abstracts Service

- ACS的分支机构
- 创建于1907年，简称“CAS”
- 最早创立了《化学文摘》
- 密切关注，索引和提炼着全球化学相关的文献和专利
- 总部座落于俄亥俄州的哥伦布市



CAS——构建最高质量的化学数据库



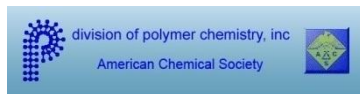
arXiv.org

Aldrichimica ACTA

ACS
chemical
biology



 BEILSTEIN JOURNAL
OF ORGANIC CHEMISTRY



J | A | C | S
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

ACS Chemical
Neuroscience



THE JOURNAL OF
PHYSICAL CHEMISTRY
Letters

 **SCIFINDER**
A CAS SOLUTION

CAS——构建最高质量的化学数据库



CAS数据库——源于化学，超越化学

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数据库最具价值的内容——人工索引

4. Process for preparation of novel sofosbuvir crystal

By: Zhou, Haohui; Lin, Guoliang; Wu, Yao; Zou, Wenjuan; Chan, Yunxia
Assignee: Beijing Winsunny Pharmaceutical Co., Ltd., Peop. Rep. China

The invention relates to a novel sofosbuvir crystal having high stability and soly. The novel sofosbuvir crystal is prepd. through crystg. sofosbuvir in pos. solvent and neg. solvent. The method has high repeatability, easy control, high yield, and high product purity.

Patent Information

Patent No.	Kind	Language	Date	Application No.	Date
CN 105732751 PATENTPAK	A		Jul 6, 2016	CN 2014-10742897	Dec 9, 2014

Priority Application

CN 2014-10742897	Dec 9, 2014
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Indexing

Carbohydrates (Section33-9)

Section cross-reference(s): 34, 63

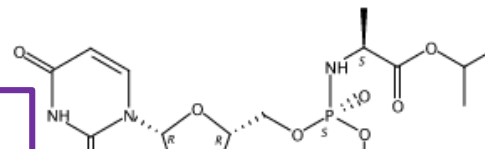
Concepts

Crystallization	Drug bioavailability
Hepatitis C	Hepatitis C virus
Homo sapiens	Human
Pharmaceutical coated tablets	

Substances

1190307-88-0P Sofosbuvir Q
Absolute stereochemistry.

Page 2 in **PATENTPAK**



Tips:

1. 98%以上的文献，都经过人工索引
2. 用Index Term标引文献中的重要技术术语
3. 用CAS RN标引出文献中的重要物质
4. 用CAS Role标引文献中重要物质的研究领域

CAS人工标引解决的问题

- 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很好的解决了该问题，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。

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登录网址: <https://scifinder.cas.org/>



Sign In

Username

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Remember me
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[Learn more about gaining access to SciFinder.](#)

What is SciFinder?
SciFinder® is a research discovery application that provides integrated access to the world's most comprehensive and authoritative source of references, substances and reactions in chemistry and related sciences.

News & Updates

Welcome to SciFinder

Did you notice our new look?
Our new branding will also be phased into training and other support materials in the coming months. If you are a Key Contact and have questions, or need assistance updating logos on any of your organization's websites, please contact the [CAS Customer Center](#).

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New Commercial Source Logos



输入SciFinder帐号和密码

SciFinder主界面

检索完，请点击退出

工具栏

The screenshot shows the SciFinder web interface. At the top left is the SciFinder logo with the text 'CAS Solutions' and 'A CAS SOLUTION'. To the right of the logo is a navigation bar with 'Explore', 'Saved Searches', and 'SciPlanner' buttons. Further right are links for 'Preferences', 'SciFinder Help', and a 'Sign Out' button. Below the navigation bar is a search area with a text input field, a 'Search' button, and an 'Advanced Search' link. On the left side, there is a sidebar menu with categories: 'REFERENCES' (including Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, Tags), 'SUBSTANCES' (including Chemical Structure, Markush, Molecular Formula, Property, Substance Identifier), and 'REACTIONS' (including Reaction Structure). On the right side, there is a 'SAVED ANSWER SETS' section listing various saved sets like 'CSF1R', 'jmc', 'EP 19870107847', etc. Below that is a 'KEEP ME POSTED' section with a message: 'You have no proxies. Learn how to: Create Keep Me Posted'. Callouts in Chinese point to these specific features: '工具栏' points to the navigation bar; '检索入口' points to the search input field; '已保存的结果集' points to the 'SAVED ANSWER SETS' list; and '定题追踪' points to the 'KEEP ME POSTED' section.

已保存的结果集

检索入口

定题追踪



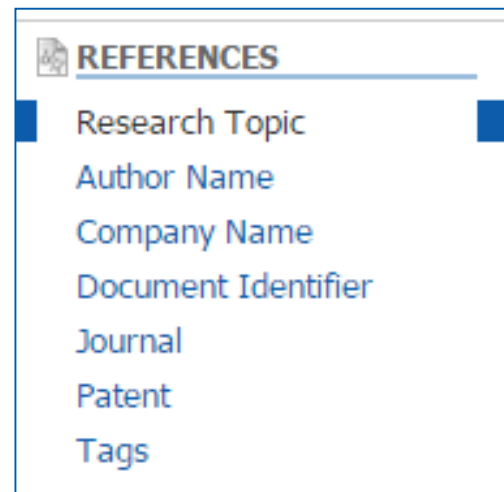
SciFinder检索——文献检索

■ 文献检索方法

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

■ 检索策略推荐

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



文献检索——主题

主题检索：生物传感器在酶检测中的应用

检索式：detection of enzyme

The screenshot displays the SciFinder web interface. At the top, there is a navigation bar with 'Explore', 'Saved Searches', and 'SciPlanner' tabs. Below this, a breadcrumb trail reads: 'Opened saved answer set "detection of enzyme with biose..." (5293) > Electrochemical biosensor base...'. On the left side, there is a sidebar menu with two main sections: 'REFERENCES' and 'SUBSTANCES'. Under 'REFERENCES', options include 'Research Topic', 'Author Name', 'Company Name', 'Document Identifier', 'Journal', 'Patent', and 'Tags'. Under 'SUBSTANCES', options include 'Chemical Structure', 'Markush', 'Molecular Formula', and 'Property'. The main content area is titled 'REFERENCES: RESEARCH TOPIC' and features a search input field containing the text 'detection of enzyme'. 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, 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

CAS Solutions

Preferences | SciFinder Help | Sign Out

WELCOME SCIFINDER[®]
A CAS SOLUTION

Welcome Helen Zhu

Explore ▾ Saved Searches ▾ SciPlanner

Research Topic "detection of enzyme"

REFERENCES ?

Select All Deselect All

1 of 5 Research Topic Candidates Selected

	References
<input type="checkbox"/> 1915 references were found containing "detection of enzyme" as entered.	1915
<input checked="" type="checkbox"/> 101716 references were found containing the two concepts "detection" and "enzyme" closely associated with one another.	101716
<input type="checkbox"/> 361177 references were found where the two concepts "detection" and "enzyme" were present anywhere in the reference.	361177
<input type="checkbox"/> 5970034 references were found containing the concept "detection".	5970034
<input type="checkbox"/> 2444659 references were found containing the concept "enzyme".	2444659

Get References

“Concepts”表示对主题词做了同义词的扩展；

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

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

文献检索结果的Refine

Explore ▾ Saved Searches ▾ SciPlanner Save Print Export

⚠ Duplicates not removed. Answer set exceeds 10,000 reference limit.

Research Topic "detection of enzyme" > references (101716)

REFERENCES ⓘ

Get Substances Get Reactions Get Related Citations View Only CHEMZENT Tools ▾ Create Keep Me Posted Alert Send to SciPlanner

Analyze Refine Categorize

Sort by: Accession Number ▾ ↓ Display Options

0 of 101716 References Selected

Refine by: ⓘ

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

Research Topic biosensor

Examples:

The effect of antibiotic residues on dairy products

Photocyanation of aromatic compounds

Refine

- 1. The detection of level of free light chains of immunoglobulins using enzyme-linked immunosorbent assay techniques for diagnostic of monoclonal gammopathy**
Quick View Other Sources
By Dubina, I. A.; Pervakova, M. Yu.; Lapin, S. V.; Emanuel, V. L.; Totolian, A. A.; Surkova, E. A.; Gryazeva, I. V.; Samoilovitch, M. P.; Klimovitch, V. B.
From *Klinicheskaya Laboratornaya Diagnostika* (2016), 61(11), 781-786. | Language: Russian, Database: CAPLUS
The content of free light chains of Igs kappa and lambda and also ratio of their concns. in blood serum are important diagnostic and prognostic markers in case of monoclonal gammopathy. The technique FreelightTM based on nephelometric **detection** of free light chains using polyclonal antibodies is one of common modes of **detection** of free light chains. The actual study was carried out with purpose of validating of national test-system for **detection** of level of free light chains in blood serum using technique of ELISA. The samples of blood serum were taken from 89 healthy donors and 165 patient...
- 2. Estimating the survival advantage based on telomere length and serum biomarkers of aging**
Quick View Other Sources
By Zhao, Yilin; Li, Shijun; Liu, Hui
From *Journal of Translational Medicine* (2017), 15, 166/1-166/7. | Language: English, Database: CAPLUS
Background: This study aimed to establish a model that ests. the survival advantage at the mol. level based on telomere length and serum biomarkers of aging, to explore clin. significance. Methods: The study consisted of 100 healthy subjects and 40 type 2 diabetes mellitus patients, 20-90 years of age. Saliva telomere relative length (LnTL) was measured by the quant. real-time polymerase chain reaction and the serum biochem. parameters, including albumin (ALB), total proteins, total cholesterol, triglycerides, and some **enzyme** parameters were **detected** by a biochem. analyzer. The Z values wer...
- 3. The effect of various inducers and their combinations with copper on laccase production of Trametes versicolor pellets in a repeated-batch process**
Quick View Other Sources
By Birhanli, Emre; Yesilada, Ozfer
From *Turkish Journal of Biology* (2017), 41(4), 587-599. | Language: English, Database: CAPLUS
The aim of this study was to increase laccase prodn. in Trametes versicolor ATCC 200801 pellets by using various inducers and their combinations under repeated...

Refine : 帮助用户迅速获得需要的文献

按被引次数排序— Citing References

CAS Solutions | Preferences | SciFinder Help | Sign Out

WELCOME Helen Zhu

Explore | Saved Searches | SciPlanner | Save | Print | Export

Research Topic "detection of enzyme" > reference (93)

文献分析工具

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

Analyze by: Author Name

Author Name	Citing References
Yuan Ruo	71
Chai Yaqin	46
Marty Jean Louis	42
Wang Joseph	40
Ju Huangxian	26
Jaffrezic Renault Nicole	25
Cosnier Serge	22
Gorton Lo	21
Liu Yue	21

1. **Carbon nanotubes as single-molecule biosensors**
By Besteman, Koen; Lee, Jeong-O.; Wiertz, Frank G. M.; Heering, Hendrik A.; Dekker, Cees
From Nano Letters (2003), 3(6), 727-730. | Language: English, Database: CAPLUS

We demonstrate the use of individual semiconducting single-wall carbon nanotubes as versatile **biosensors**. Controlled attachment of the redox **enzyme** glucose oxidase (GOx) to the nanotube sidewall is achieved through a linking mol. and is found to induce a clear change of the conductance. The **enzyme**-coated tube is found to act as a pH sensor with large and reversible changes in conductance upon changes in pH. Upon addn. of glucose, the substrate of GOx, a steplike response can be monitored in real time, indicating that our sensor is also capable of measuring enzymic activity at the level of a...

2. **Magnetic relaxation switches capable of sensing molecular interactions**
By Perez, J. Manuel; Josephson, Lee; O'Loughlin, Terrence; Hoegemann, Dagmar; Weissleder, Ralph
From Nature Biotechnology (2002), 20(8), 816-820. | Language: English, Database: CAPLUS

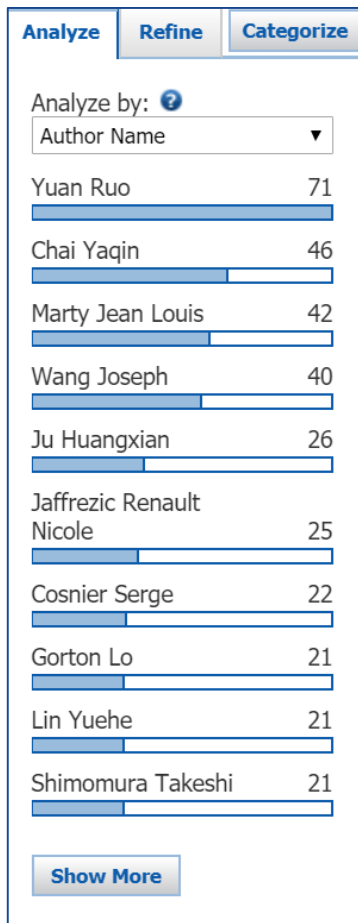
Highly sensitive, efficient, and high-throughput **biosensors** are required for genomic and proteomic data acquisition in complex biol. samples and potentially for in vivo applications. To facilitate these studies, we have developed biocompatible magnetic nanosensors that act as magnetic relaxation switches (MRS) to **detect** mol. interactions in the reversible self-assembly of disperse magnetic particles into stable nanoassemblies. Using four different types of mol. interactions (DNA-DNA, protein-protein, protein-small mol., and **enzyme** reactions) as model systems, we show that the MRS technol. ca...

3. **Carbon nanotube based electrochemical sensors for biomolecules**

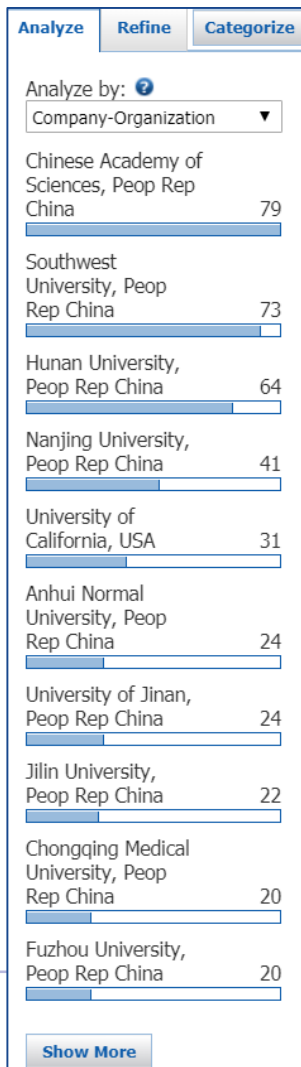
Citing Reference: 帮助找到最重要的文献

文献检索结果的Analyze

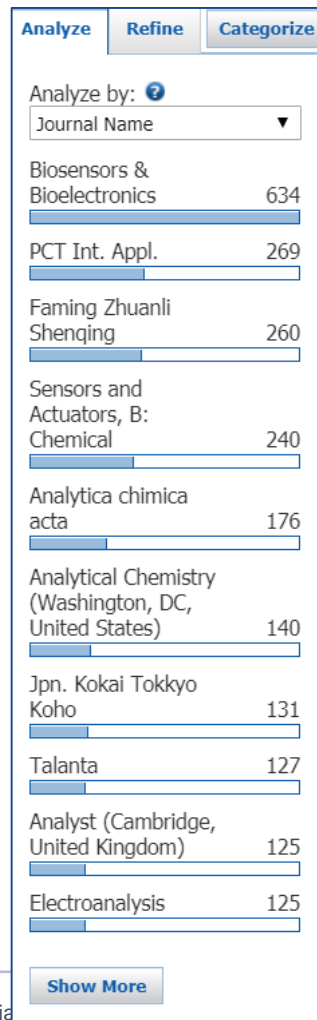
本领域研究人员



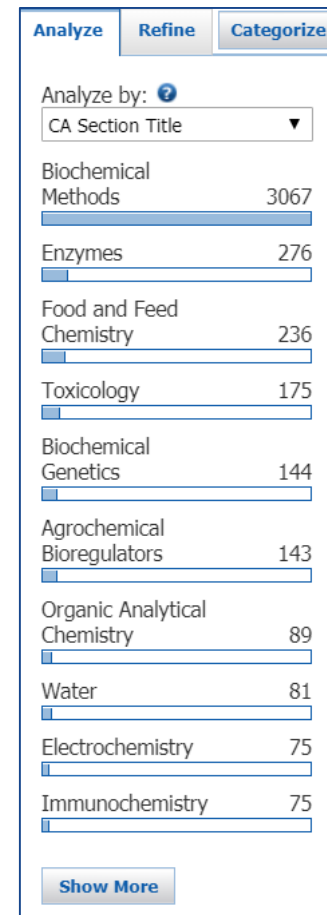
本领域研究机构、合作伙伴、竞争对手



期刊



涉及学科领域



文献检索结果的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

Analyze by: [?](#)
Index Term ▼

Biosensors	2097
Human	853
Protein immobilization	817
Chemically modified electrodes	806
Electronic device fabrication	743
Enzyme electrodes	736
Electrodes	718
Nanoparticles	625
Blood analysis	609
Amperometry	552

Show More

Analyze - Index Term

⚠ Only 1,000 Terms are displayed. [close](#)

9201 Items 1 Selected [Export](#)

Sort by: Frequency ▼ Page: 1 of 20

Select bars to view only those references within the current answer set.

<input type="checkbox"/> Biosensors	2097
<input type="checkbox"/> Human	853
<input type="checkbox"/> Protein immobilization	817
<input type="checkbox"/> Chemically modified electrodes	806
<input type="checkbox"/> Electronic device fabrication	743
<input type="checkbox"/> Enzyme electrodes	736
<input type="checkbox"/> Electrodes	718
<input type="checkbox"/> Nanoparticles	625
<input checked="" type="checkbox"/> Blood analysis	609
<input type="checkbox"/> Amperometry	552

Apply Cancel

选择感兴趣的内容，点击Apply

文献检索结果的Categorize

学科领域
主分类

学科领域
副分类

Index Term

选中的Index Term

Categorize ?

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

Category Heading	Category	Index Terms	Selected Terms
All	Processes & apparatus (818)	Page: 1 of 9 Select All Deselect All	Click 'x' to remove the category from 'Selected Terms'
Analytical chemistry	Substances in technology (3675)	<input type="checkbox"/> Biosensors 2036	<input checked="" type="checkbox"/> Technology > Processes & apparatus (1 Terms)
General chemistry	Materials & products (607)	<input type="checkbox"/> Enzyme electrodes 810	
Technology	Metallurgy (148)	<input type="checkbox"/> Chemically modified electrodes 807	
Genetics & protein chemistry	Imaging & recording (88)	<input type="checkbox"/> Electronic device fabrication 743	
Biotechnology	Formed, removed, & other substances (201)	<input type="checkbox"/> Electrodes 528	
Biology	Ceramics (20)	<input type="checkbox"/> Electrochemical biosensors 474	
Physical chemistry	Power & fuel topics (20)	<input type="checkbox"/> Amperometric biosensors 472	
Polymer chemistry	Construction (8)	<input type="checkbox"/> Enzymic biosensors 369	
Synthetic chemistry		<input checked="" type="checkbox"/> Nanoscale surface modification 366	
Catalysis		<input type="checkbox"/> Glucose sensors 330	
Environmental chemistry		<input type="checkbox"/> Surface treatment 266	
		<input type="checkbox"/> Glassy carbon 252	

Technology > Processes & apparatus > 1 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。

结果集的保存— Save, Print, Export

The screenshot shows the SciFinder search results page. At the top, there are buttons for 'Save', 'Print', and 'Export'. Below the search bar, there are navigation options like 'Get Substances', 'Get Reactions', and 'Get Related Citations'. The main content area displays a list of search results. The first result is highlighted with a purple box and labeled '文献详细信息' (Literature Detailed Information). This result includes a title, authors, a diagram of the biosensor mechanism, and a graph showing photocurrent responses. The second and third results are also visible but not highlighted.

Save : 保存在服务器上, 方便以后登陆查看, 每次可存1万条记录。

Export : 导出至本地电脑。

Print : 打印成PDF格式

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

The screenshot shows the 'Export' dialog box in SciFinder. It is divided into three main sections: 'Export:', 'For:', and 'Details:'.
- 'Export:' has radio buttons for 'All', 'Selected', and 'Range'. Below it is a text input field with the example '2-20'.
- 'For:' has a 'Citation Manager' section with radio buttons for 'Citation export format (*.ris)', 'Quoted Format (*.bt)', and 'Tagged Format (*.bt)'. It also has an 'Offline review' section with radio buttons for 'Portable Document Format (*.pdf)', 'Rich Text Format (*.rtf)', and 'Answer Keys (*.bt)'. A 'Saving locally' section has a radio button for 'Answer Key eXchange (*.akx)'.
- 'Details:' has a 'File Name:' field with the value 'Reference_06_19_2012_100848'. It also has a 'Format:' section with radio buttons for 'Summary without abstracts', 'Summary with partial abstracts', 'Summary with full abstracts', and 'Detail (full record)'. A 'Include:' section has checkboxes for 'Task History', 'Tags', and 'Comments'.
At the bottom right, there are 'Export' and 'Cancel' buttons.

文献信息—题录、摘要、索引

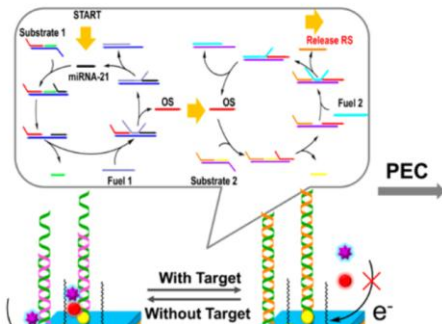
链接至原文



1. Enzyme-Free Photoelectrochemical Biosensor Based on the Co-Sensitization Effect Coupled with Dual Cascade Toehold-Mediated Strand Displacement Amplification for the Sensitive Detection of MicroRNA-21

获得引文及参考文献

The co-sensitization of biocompatible CuInS₂/ZnS quantum dots (ZCIS QDs) and N-doped carbon dots (N-CDs) coupled with dual cascade toehold-mediated strand displacement amplification (TSDA) for microRNA-21 (miRNA-21) detection. On the one hand, the TiO₂/Au hybrid structure was used to immobilize double-stranded DNA (thiolated capture strand and carboxylated signal strand), which could capture glutathione stabilized ZCIS QDs and N-CDs. The original TiO₂/Au/ZCIS/N-CDs structure formed a cascade band gap arrangement, which provided a good band position for effective charge carrier sepn., thus improving PEC performance and resulting in an evident decrease in photocurrent signal after the release of signal strands (SIG). However, the sensitivity of the biosensor was further enhanced by enzyme-free dual cascade TSDA, which was initiated by the target miRNA-21, like a mol. machine, and consumed the substrates and fuels, repeatedly used the target miRNA-21, and released a large no. of reporter strands (RS). Subsequently, the released RS replaced SIG to prevent ZCIS QDs and N-CDs from sensitizing the electrode, which remarkably suppressed the photocurrent signal. The introduction of TSDA could produce high amplification capacity and specificity for the target miRNA-21 with advantages of simple primer design and mild reaction conditions. Impressively, with the cascade band gap arrangement for enhanced PEC performance and enzyme-free dual cascade TSDA for amplification capacity and specificity, the PEC biosensor exhibited excellent application in miRNA-21 anal. with a linear range from 1 pM to 100 nM and a low detection limit of 0.31 pM. This PEC biosensor retained good specificity, stability, and reproducibility and provided an effective method for PEC biosensor construction for microRNA. Moreover, the designed PEC biosensor was environmentally friendly, green manuf., and self-powered and therefore compatible with the purpose of sustainable chem.



Indexing

Biochemical Methods	
Concepts	重要概念
Nanocrystals	Quantum dots
CuInS ₂ /ZnS; enzyme-free photoelectrochem. biosensor based on Co-sensitization effect coupled with dual cascade toehold-mediated strand displacement amplification for sensitive detection of MicroRNA-21	
Blood analysis Electronic device fabrication Photoelectrochemistry	Chemically modified electrodes Nanoscale surface modification
enzyme-free photoelectrochem. biosensor based on Co-sensitization effect coupled with dual cascade toehold-mediated strand displacement amplification for sensitive detection of MicroRNA-21	
DNA	
enzyme-free photoelectrochem. biosensor based on Co-sensitization effect coupled with dual cascade toehold-mediated strand displacement amplification for sensitive detection of MicroRNA-21	
Analytical reagent use; Biological use, unclassified; Properties; Technical or engineered material use; Analytical study; Biological study; Uses	
MicroRNA	
miRNA-21; enzyme-free photoelectrochem. biosensor based on Co-sensitization effect coupled with dual cascade toehold-mediated strand displacement amplification for sensitive detection of MicroRNA-21	
Analyte; Biological study, unclassified; Analytical study; Biological study	

Substances

重要物质

7727-37-9 Nitrogen	
dopant in carbon dot; enzyme-free photoelectrochem. biosensor based on Co-sensitization effect coupled with dual cascade toehold-mediated strand displacement amplification for sensitive detection of MicroRNA-21	
Analytical reagent use; Biological use, unclassified; Physical, engineering or chemical process; Technical or engineered material use; Analytical study; Biological study; Process; Uses	
7440-44-0 Carbon	
dot, N-doped; enzyme-free photoelectrochem. biosensor based on Co-sensitization effect coupled with dual cascade toehold-mediated strand displacement amplification for sensitive detection of MicroRNA-21	
Analytical reagent use; Biological use, unclassified; Physical, engineering or chemical process; Technical or engineered material use; Analytical study; Biological study; Process; Uses	
1314-98-3 Zinc sulfide (ZnS)	
12016-94-9 Copper indium sulfide (CuInS ₂)	
enzyme-free photoelectrochem. biosensor based on Co-sensitization effect coupled with dual cascade toehold-mediated strand displacement amplification for sensitive detection of MicroRNA-21	
Analytical reagent use; Biological use, unclassified; Physical, engineering or chemical process; Technical or engineered material use; Analytical study; Biological study; Process; Uses	
7440-57-5 Gold	
13463-67-7 Titanium oxide (TiO ₂)	
50926-11-9 ITO	

文献详情界面包括：

1. 标题
2. 摘要
3. 文献中重要的技术术语
4. 文献中重要的物质
5. 书目信息
6. 获得文献中的物质，反应
7. 参考文献
8. 链接原文



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，精准定位文献



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



SUBSTANCES

Chemical Structure

Markush

Molecular Formula

Property

Substance Identifier

■ 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 "ionic liquid with catalysis" > references (16803) > refine "Review" (1224) > refine by c

REFERENCES

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

SUBSTANCES

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

SUBSTANCES: SUBSTANCE IDENTIFIER

UHMWPE

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

Search

提示：

1. 一次最多可输入25个物质。
2. 每行一个物质标识符。

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

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 substance record. At the top, it shows "0 of 1 Substance Selected". Below this, the CAS Registry Number "9002-88-4" is highlighted. The substance is identified as "(C₂H₄)_x Ethene, homopolymer". The chemical structure C=C is shown. A context menu is open over the substance, listing various actions: "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".

74-85-1
C₂H₄
CH₂=CH₂

(C₂H₄)_x
Ethene, homopolymer

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

CAS Registry Number: 9002-88-4

- 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

SUBSTANCE DETAIL 

 **Get References**  **Get Reactions**  **Get Commercial Sources**

 [Return](#)

CAS Registry Number 9002-88-4

~359,876  ~112  

(C₂H₄)_x
Ethene, homopolymer
Polymer

Polymer Class Terms
Polyolefin

Melting Point (Experimental)
Value: 100-120 °C

Boiling Point (Experimental)
Value: 48-110 °C | Condition: Press: 9 Torr

Density (Experimental)
Value: 0.9745 g/cm³ | Condition: Temp: 25 °C

Other Names
Ethylene, polymers (8CI)
0017ZSK
0100F
0134M
030S
[View more...](#)

74-85-1
C₂H₄
C=C

物质详情

通过物质获得文献

Get References

Retrieve references for:

All substances
 Selected substances

Limit results to:

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

For each sequence, retrieve:

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

分析化学

生物研究

制备

工艺

谱图数据

用途



SCIFINDER
A CAS SOLUTION

▼ EXPERIMENTAL PROPERTIES

Biological Chemical Density Electrical Electronic Flow and Diffusion Interface Magnetic Mechanical Nuclear Optical and Scattering Structure Related Thermal

Interface Properties	Value	Condition	Note
Contact Angle	See full text	1 of 31	(12)CAS
Surface Tension	See full text	1 of 12	(872)CAS

Notes

(12) Choi, Woo-Zin; Geosystem Engineering 2004, V7(3), P57-62 CAPLUS 🔍
(872) Sanchis, M. R.; European Polymer Journal 2006, V42(7), P1558-1568 CAPLUS 🔍

实验数据与实验谱图

▼ EXPERIMENTAL SPECTRA

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

¹ H NMR Properties	Value	Condition	Note
Proton NMR Spectrum	See full text	1 of 15	(1313)CAS

Notes

(1313) Kemmere, Maartje; DECHEMA Monographien 2004, V138(8th International Workshop on Polymer Reaction Engineering, 2004), P189-195 CAPLUS 🔍

▶ REGULATORY INFORMATION

▶ CAS REFERENCE ROLES

▶ ADDITIONAL DETAILS

物质检索——Property explore

CAS Solutions ▾

SciFINDER
A CAS SOLUTION

Explore ▾ Saved Searches ▾ SciPlanner

Substance Identifier "UHMWPE " > substances (1) > 9002-88-4

REFERENCES

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

SUBSTANCES

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

SUBSTANCES: PROPERTY ?

Experimental

Electric Resistance (ohm) ▾ >125
Examples: 44, 25-35, >125

Predicted

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

Search

寻找电阻率大于125ohm的含铁物质

物质结果集的筛选——Refine

SUBSTANCES ?

Get References
Get Reactions
Get Commercial Sources
Tools v

Create Keep Me Posted Alert
Send to SciPlanner

Analyze ?
Refine

Sort by: CAS Registry Number v
Display Options

0 of 137 Substances Selected
Page: 1 of 3

Analyze by: ?

Elements v

O 73

C 37

H 30

Fe 19

N 19

Mg 16

Ca 13

Cr 13

Se 13

In 12

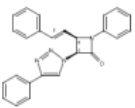
Show More

1. 1360099-47-3 ?
~250

Component	Component Ratio
Te	x
Cd	x
Hg	x

Cd . Hg . Te
Cadmium mercury telluride
Experimental Properties

2. 1262894-47-2 ?
~2



Double bond geometry as shown.,Relative stereochemistry.

C₂₅ H₂₀ N₄ O

3. 1160936-40-2 ?
~1

Component	Component Ratio
Te	1.8
Se	0.2
In	0.1
Cu	0.1
Cd	1.8

4. 1160936-38-8 ?
~1

Component	Component Ratio
Te	1.6
Se	0.4
In	0.2
Cu	0.2
Cd	1.6

0 of 19 Substances Selected

1. 775325-57-0 ?
~1

Component	Component Ratio
O	2.82
Ca	0.02
Mg	0.1
Fe	1.8

Ca . Fe . Mg . O
Calcium iron magnesium oxide
(Ca_{0.02}Fe_{1.8}Mg_{0.1}O_{2.82})
Experimental Properties

2. 775325-56-9 ?
~1

Component	Component Ratio
O	2.74
Ca	0.14
Mg	0.2
Fe	1.6

Ca . Fe . Mg . O
Calcium iron magnesium oxide
(Ca_{0.14}Fe_{1.6}Mg_{0.2}O_{2.74})
Experimental Properties

3. 775325-55-8 ?
~1

Component	Component Ratio
O	2.67
Ca	0.07
Mg	0.2
Fe	1.6

Ca . Fe . Mg . O
Calcium iron magnesium oxide
(Ca_{0.07}Fe_{1.6}Mg_{0.2}O_{2.67})
Experimental Properties

4. 775325-54-7 ?
~1

Component	Component Ratio
O	2.64
Ca	0.04
Mg	0.2
Fe	1.6

Ca . Fe . Mg . O
Calcium iron magnesium oxide
(Ca_{0.04}Fe_{1.6}Mg_{0.2}O_{2.64})
Experimental Properties

5. 775325-53-6 ?
~1

Component	Component Ratio
O	2.44
Ca	0.14
Mg	0.35
Fe	1.3

Ca . Fe . Mg . O
Calcium iron magnesium oxide
(Ca_{0.14}Fe_{1.3}Mg_{0.35}O_{2.44})
Experimental Properties

6. 775325-52-5 ?
~1

Component	Component Ratio
O	2.37
Ca	0.07
Mg	0.35
Fe	1.3

Ca . Fe . Mg . O
Calcium iron magnesium oxide
(Ca_{0.07}Fe_{1.3}Mg_{0.35}O_{2.37})
Experimental Properties

7. 775325-51-4 ?
~1

Component	Component Ratio
O	2.34
Ca	0.04
Mg	0.35
Fe	1.3

Ca . Fe . Mg . O
Calcium iron magnesium oxide
(Ca_{0.04}Fe_{1.3}Mg_{0.35}O_{2.34})
Experimental Properties

8. 775325-50-3 ?
~1

Component	Component Ratio
O	2.14
Ca	0.14
Mg	0.5
Fe	1

Ca . Fe . Mg . O
Calcium iron magnesium oxide
(Ca_{0.14}FeMg_{0.5}O_{2.14})
Experimental Properties

如何筛选含铁物质？

物质检索——分子式

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

CAS Solutions

SCIFINDER[®]
A CAS SOLUTION

Explore ▾ Saved Searches ▾ SciPlanner

REFERENCES

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

SUBSTANCES

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

REACTIONS

- Reaction Structure

SUBSTANCES: MOLECULAR FORMULA

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

Examples:
H4SiO4
(C3H6O.C2H4O)x

Search

1. 34370-41-7
(Component: 7664-93-9)

- 1/2 NH₃
- 2 H₂O
- 1/2 Sm(III)

H₃N · 2H₂O₄S · 4H₂O · Sm
Sulfuric acid, ammonium samarium(3+) salt (2:1:1), tetrahydrate (8CI,9CI)

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

物质检索——结构

The screenshot displays the SciFinder web interface for chemical structure search. On the left is a navigation menu with three main sections: REFERENCES, SUBSTANCES, and REACTIONS. Under SUBSTANCES, 'Chemical Structure' 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. The editor contains a large white area with the text 'Click to Edit'. To the right of the editor are search options: 'Search Type' with radio buttons for 'Exact Structure', 'Substructure' (selected), and 'Similarity'; and a checkbox for 'Show precision analysis'. Below these is a 'ChemDraw' logo and the text 'Launch a SciFinder substance or re'. At the bottom of the main area is a blue 'Search' button, an 'Advanced Search' link, and a checked 'Always Show' checkbox.

REFERENCES

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

SUBSTANCES

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

REACTIONS

- Reaction Structure

SUBSTANCES: CHEMICAL STRUCTURE

Structure Editor:

Java Non-Java

Click to Edit

Search Type:

- Exact Structure
- Substructure
- Similarity

Show precision analysis

ChemDraw

Launch a SciFinder substance or re

Search

[Advanced Search](#) Always Show

物质检索——结构

The image shows a screenshot of the 'Structure Editor' software interface. The interface includes a toolbar on the left with various drawing and editing tools, a central workspace for drawing chemical structures, and a 'Drawing Editor' panel on the right. The 'Drawing Editor' panel has radio buttons for 'Structure', 'Reaction', and 'Markush', and search options for 'Exact search', 'Substructure search', and 'Similarity search'. The interface is annotated with numerous Chinese labels pointing to specific tools and features.

Labels and their corresponding functions:

- 橡皮 (Eraser)
- 结构和反应切换功能 (Structure and Reaction Switching Function)
- 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 (Selection Tool)
- 环锁定工具 (Ring Locking Tool)
- 旋转工具 (Rotation Tool)
- 正电子 (Positron)
- C原子和单键恢复工具 (C Atom and Single Bond Restoration Tool)
- 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 (Lasso Selection Tool)
- 原子锁定工具 (Atom Locking Tool)
- 镜面旋转工具 (Mirror Rotation Tool)
- 结构检索选择 (Structure Search Selection)
- 单双键, RS构型, 不确定键定义工具 (Single/Double Bond, RS Configuration, Uncertain Bond Definition Tool)
- 常见环, 多元环工具 (Common Ring, Poly-ring Tool)
- 负电子 (Negatron)

物质检索——精确结构检索

Structure Editor

Draw or change atoms or bonds. Shortcut Keys

Sm

H
|
H—N—H
|
H

O
||
O=S=O
|
O

H—O—H

Sm . H₄N . H₂O₅ . H₂O

150.36 . 18.04 . 98.08 . 18.02




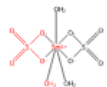

限定为单一组分

精确结构检索

物质检索——精确结构检索

Sort by: CAS Registry Number 倒序排列 Display Options

0 of 5 Substances Selected

<p>1. 34370-41-7 </p> <p>(Component: 7664-93-9)</p> <p>~12 </p>  <ul style="list-style-type: none"> • 1/2 NH₄⁺ • 2 H₂O • 1/2 Sm(III) <p>H₃N · 2 H₂O₄S · 4 H₂O · Sm Sulfuric acid, ammonium samarium(3+) salt (2:1:1), tetrahydrate (8CI,9CI)</p>	<p>2. 40148-71-8 </p> <p>(Component: 7664-93-9)</p> <p>~1 </p>  <ul style="list-style-type: none"> • NH₄⁺ • 1/3 H₂O • 1/3 Sm(III) <p>H₃N · H₂O₄S · 1/3 H₂O · 1/3 Sm Sulfuric acid, ammonium samarium(3+) salt (3:3:1), monohydrate (9CI)</p>	<p>3. 40148-74-1 </p> <p>(Component: 7664-93-9)</p> <p>~1 </p>  <ul style="list-style-type: none"> • 1/2 NH₄⁺ • H₂O • 1/2 Sm(III) <p>H₃N · 2 H₂O₄S · 2 H₂O · Sm Sulfuric acid, ammonium samarium(3+) salt (2:1:1), dihydrate (9CI)</p>	<p>4. 42949-48-4 </p> <p>~1 </p> <div style="border: 1px solid black; padding: 5px;"> <p>49856-58-8 (Component: 736080-59-4) H₈O₁₁S₂Sm · H₄N · H₂O</p>  <ul style="list-style-type: none"> • NH₄⁺ • H₂O </div> <p>(H₈O₁₁S₂Sm · H₄N · H₂O) Samarate(1-), triaquabis[sulfato(2-)-O,O']-, ammonium monohydrate, homopolymer (9CI)</p>
<p>5. 49856-58-8 </p> <p>(Component: 736080-59-4)</p> <p>~0 </p>  <ul style="list-style-type: none"> • NH₄⁺ • H₂O <p>H₈O₁₁S₂Sm · H₄N · H₂O Samarate(1-), triaquabis[sulfato(2-)-O,O']-, ammonium monohydrate (9CI)</p>			

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

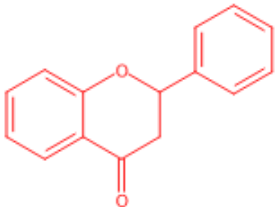
The screenshot displays the 'Structure Editor' window. The central workspace shows a chemical structure of a benzodioxane derivative with a phenyl group. The interface includes a toolbar on the left with various drawing tools, a top toolbar with file operations, and a right-hand panel with search settings. The search settings panel is titled 'Get substances that match your query using:' and has three radio button options: 'Exact search', 'Substructure search' (which is selected and highlighted with a purple box), and 'Similarity search'. Below these options are 'OK' and 'Cancel' buttons. At the bottom of the window, the molecular formula $C_{15}H_{12}O_2$ and the molecular weight 224.26 are displayed.

物质检索——亚结构检索

0 of 23824 Substances Selected

1. 487-26-3

~2093

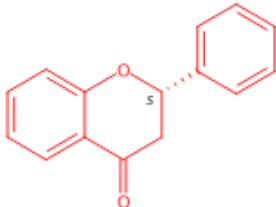


$C_{15}H_{12}O_2$
4-phenyl-4H-1-benzopyran-4-one, 2,3-dihydro-2-phenyl-

▶ Key Physical Properties
Regulatory Information
Spectra
Experimental Properties

2. 17002-31-2

~244



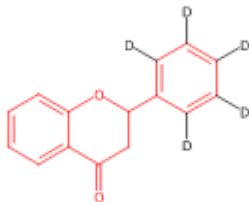
Absolute stereochemistry...Rotation (-).

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

▶ Key Physical Properties
Experimental Properties

10. 146196-91-0

~1 ~5



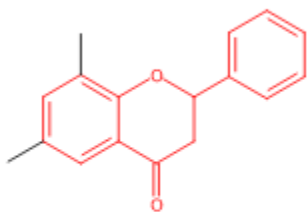
$C_{15}H_7D_5O_2$
4-phenyl-4H-1-benzopyran-4-one, 2,3-dihydro-2-(phenyl- d_5)- (9CI)

Spectra

同位素

亚结构检索结果

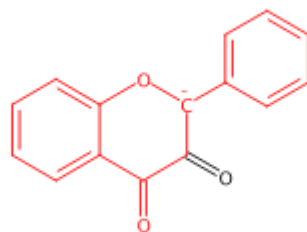
取代物



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

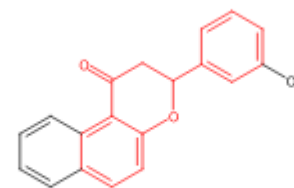
▶ Key Physical Properties
Experimental Properties

离子



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

稠环物质



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

▶ Key Physical Properties

亚结构检索结果的限定

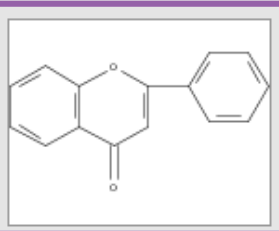
化学结构的再次限定

Analysis Refine

Refine by: ⓘ

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

Chemical Structure:

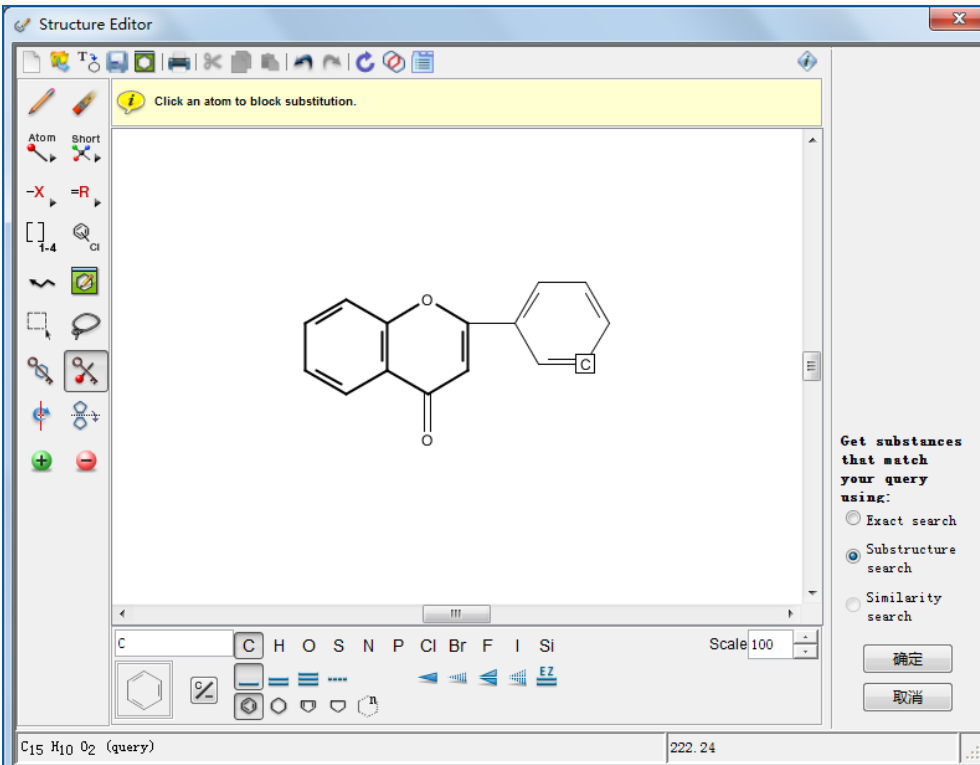


Click image to change structure or view detail

Search type: **Substructure**

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



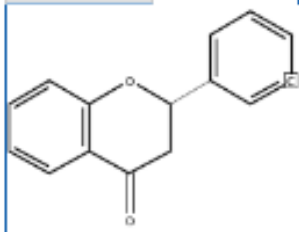
原子锁定

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

<p>1. 487-26-3</p> <p>~2093</p>	<p>2. 17002-31-2</p> <p>~244</p>
<p>4. 104550-32-5</p> <p>~3</p>	<p>5. 75524-43-5</p> <p>~2</p>

C₁₅H₁₂O₂
4H-1-Benzopyran-4-one, 2,3-dihydro-2-phenyl-
Key Physical Properties
Regulatory Information
Spectra
Experimental Properties

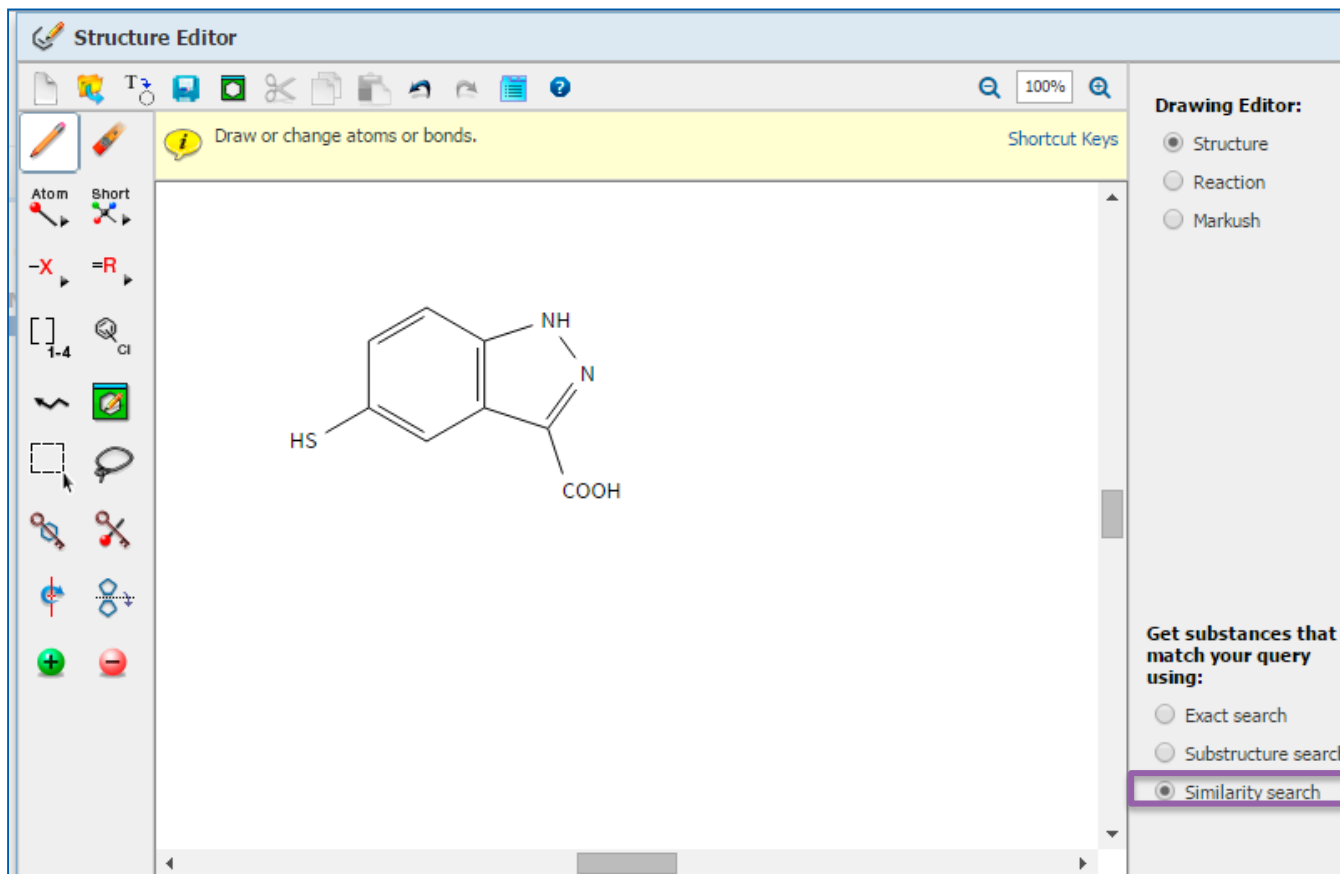
C₁₅H₁₂O₂
4H-1-Benzopyran-4-one, 2,3-dihydro-2-phenyl-, (2S)-
Absolute stereochemistry, Rotation (-).
Key Physical Properties
Experimental Properties

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

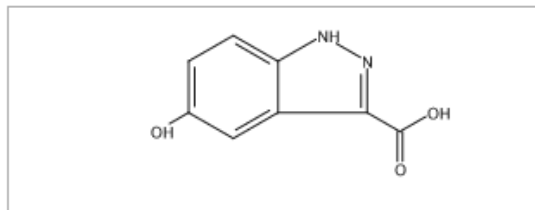
评分越高，相似度越高，结构越相似

Score: 88

1. 885518-94-5

取代基变化

~1 ~35



$C_8 H_6 N_2 O_3$

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

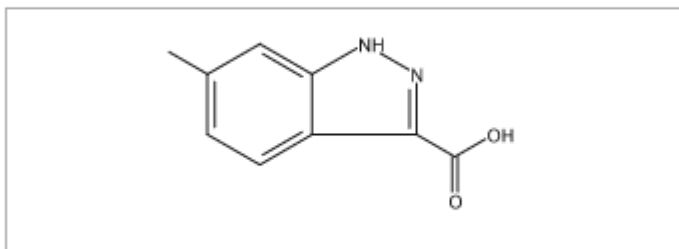
▶ Key Physical Properties

Score: 86

5. 858227-12-0

取代基位置变化

~7 ~41



$C_9 H_8 N_2 O_2$

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

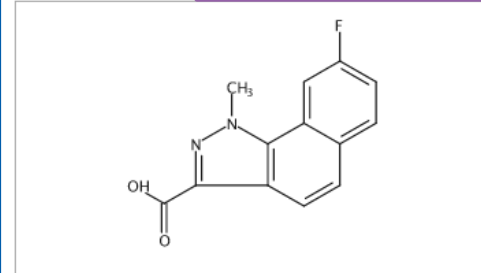
▶ Key Physical Properties

Score: 65

541. 1100422-

母体结构变化

~1



$C_{13} H_9 F N_2 O_2$

1H-Benz[σ]indazole-3-carboxylic acid, 8-fluoro-1-methyl-

▶ Key Physical Properties



SCIFINDER[®]
A CAS SOLUTION

物质检索——相似结构检索

- 相似结构检索：

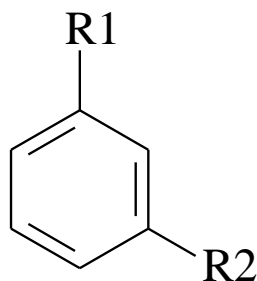
获得片段或整体结构与被检索结构相似的结果，母体结构可以被取代，也可以被改变

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

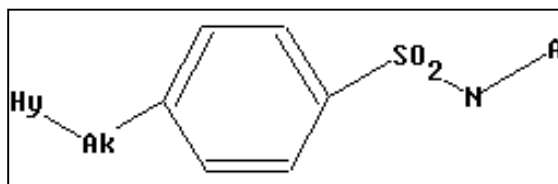
Markush检索

- 具体物质[Specific Substance]：
 - 以具体化学结构陈述的特定物质，会被分配CAS RN
- 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



R1 = H, Br, Cl, I

R2 = Br, Cl, I, —CH₂—halogen, —CH—halogen,
|
CH₃



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

Hy-Ak SO₂-N-A

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

Markush检索

SCIFINDER
A CAS SOLUTION

Welcome Helen Zhu

Explore ▾ Saved Searches ▾ SciPlanner Save Print Export

Markush substructure > references (1969) > Compounds and methods for anti...

REFERENCES ⓘ

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

Analyze Refine Categorize

Sort by: Accession Number ▾

0 of 1969 References Selected

Display Options

Analyze by: Document Type

Patent	1969
Journal	1

Show More

全部是专利

1. **Compounds and methods for anticoagulation therapy**
PATENTPAK
By Allende Rodriguez, Mikel; Hermida Santos, Jose; Montes Diaz, Ramon; Oyarzabal Santamarina, Julen
From PCT Int. Appl. (2016), WO 2016120432 A1 20160804. | Language: English, Database: CAPLUS

The invention relates to certain compds. that are inducers of Heat shock 70 kDa protein 1A/1B (HSPA1A/B) and their use for anticoagulation therapy; and to a method for anticoagulation therapy that comprises the administration of one of these inducer compds. It has been here proved that induction of Heat shock 70 kDa protein 1A/1B by administration of one of these inducer compds. has antithrombotic effects without accelerating or altering bleeding time.

2. **Preparation of new imidazopyrimidine derivatives as negative allosteric modulators of metabotropic glutamate receptor subtype 2 (mGlu2 receptor)**
PATENTPAK
By Urashima, Kuniko; Tojo, Kengo; Koike, Shoko; Masumoto, Shuji
From Jpn. Kokai Tokkyo Koho (2016), JP 2016132660 A 20160725. | Language: Japanese, Database: CAPLUS

The title imidazo[1,2-a]pyrimidine derivs. I [R¹ = H or halogen; ring A Ph or pyridyl; R², R³ (same or different) = hydrogen, halogen, C₁₋₄ alkyl or C₁₋₄ alkoxy each optionally substituted with 1-5 halogen atoms; or in case where R² and R³ are at the adjacent substitution position, R² and R³ together with ring A form C₅₋₈ carbocyclic ring (optionally substituted with 1-5 halogen or 1-2 hydroxy group) or 5- or 6-membered satd. heterocyclic ring; ring B = Ph or pyridyl; R⁴, R⁵ (same or different) = H, halogen, hydroxy, amino, -C(O)OR^a, -C(O)NR^b, SO₃H, SO₂NR^aR^b, SO₂R^b, or NR^aSO₂R^b; R^a, R^b (same...

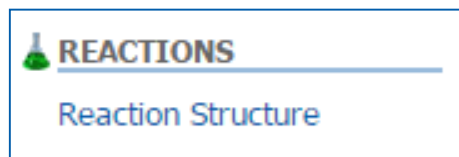
提纲

- 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



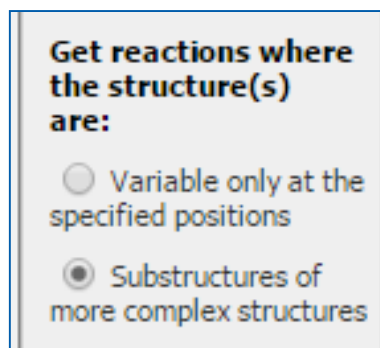
- 常用获取方法

已知物质：由物质获取反应

已知文献：从文献中获取反应

精确结构反应检索

亚结构反应检索



反应绘制工具

The screenshot shows the Structure Editor interface with the following components and annotations:

- Reaction Arrow:** A green arrow icon in the left toolbar, labeled "反应箭头".
- Reaction Role Tools:** A red plus sign and a red minus sign icon in the left toolbar, labeled "反应角色工具".
- Reaction Atom Marking Tools:** A black arrow pointing to the right and a red arrow pointing to the right with "A" and "B" labels, labeled "反应原子标记工具".
- Functional Group List:** A list of functional groups including "alcohol" and "ketone" in the left toolbar, labeled "官能团列表".
- Reaction Position Marking Tools:** A blue curved arrow and a black arrow pointing to a specific atom, labeled "反应位置标记工具".

The interface includes a top toolbar with standard editing tools, a central drawing area with a yellow status bar that says "Draw or change atoms or bonds.", and a right-hand panel with "Drawing Editor" options (Structure, Reaction, Markush) and search filters. The bottom of the window shows a chemical formula input field with "CH₄", a list of elements (C, H, O, S, N, P, Cl, Br, F, I, Si), and a version number "16.04".

SciFinder反应检索——精确反应检索

The screenshot displays the SciFinder Structure Editor. The central workspace shows a chemical reaction: nitrobenzene (reactant) is converted to aniline (product). The reactant is a benzene ring with an NO_2 group at the bottom, and the product is a benzene ring with an NH_2 group at the bottom. An arrow points from the reactant to the product. Below the structures, the text "reactant" and "product" are visible. The interface includes a top toolbar with various drawing tools, a left sidebar with additional tools, and a right sidebar titled "Drawing Editor". In the "Drawing Editor" panel, the "Reaction" radio button is selected. Below this, the text "Get reactions where the structure(s) are:" is followed by two radio button options: "Variable only at the specified positions" (which is highlighted by a purple callout box) and "Substructures of more complex structures". At the bottom of the panel are "OK" and "Cancel" buttons. The status bar at the bottom of the window shows the chemical formula $\text{C}_7\text{H}_7\text{NO}_2 \cdot \text{C}_7\text{H}_7\text{N}$ and the coordinates 137.14 . 107.16.

精确反应检索

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](#) [Link](#) [Similar Reactions](#)

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

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

~102 100% ~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

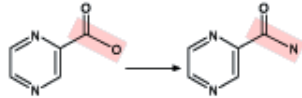
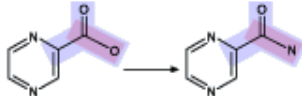
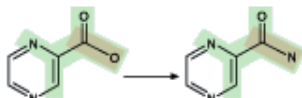
Narrow：反应中心及扩展的原子和键

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

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

3. Reduction of Nitro to Azoxy Compounds
11 Reactions

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

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

REACTIIONS [?](#) [Get References](#) [Tools](#) [Send to SciPlann](#)

Analyze **Refine**

Analyze by: [?](#)
Reagent

H ₂	148
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

[Show More](#)

Group by: No Grouping Sort by: Relevance

0 of 512 Reactions Selected

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

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

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

~102 ~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

SciFinder囊括最大的反应实验过程合集

Single Step Hover over any structure for more options.



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



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

The screenshot displays the Structure Editor interface. The main workspace shows a chemical reaction: a reactant (a benzimidazole-like structure with an R1 group and a hydrogen atom) reacting to form a product (the same structure with an Ak group instead of the hydrogen). A purple arrow points from the Ak variable in the product to the Variables dialog box.

Structure Editor

Drag the reaction arrow to specify reaction direction.

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

Formulas: C H O S N P Cl Br F I Si

Formula is not available

通过后处理工具筛选反应--Analyze

通过催化剂筛选反应

Analyze Refine

Analyze by: ?
Catalyst

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 ₃ SiCH ₂ MgCl	10
Ph ₂ P(CH ₂) ₃ PPh ₂	10
658062-48-7	9

Group by: No Grouping Sort by: Accession Number

No Grouping
Document
Transformation

1. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.

~57 ~52 83%

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

ACS / Proprietary and Confidential / Do Not Distribute

提纲

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 - 文献检索
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 - 反应检索
 - SciPlanner
- SciFinder常见问题及解决

SciPlanner使用简介

3. View Reaction Detail [Link](#) **勾选想要的反应**

3 Steps *Hover over any structure for more options.* **点击Send to SciPlanner** [Display Options](#)

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

进入SciPlanner 新建文件

SciPlanner SciPlanner_11_19_2015_112612 **将刚推送过来的反应拖至编辑面板**

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.

SciPlanner使用简介

The screenshot shows the SciPlanner software interface. At the top, the title bar reads "SciPlanner" and "SciPlanner_11_19_2015_112612". Below the title bar are menu options: "Workspace", "Edit", "View", and "GoTo". A context menu is open over a chemical structure, listing options such as "CAS Registry Number: 13091-23-1", "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", and "Export as molfile". The "Synthesize this..." option is highlighted. Below the menu, a reaction sequence is shown with three steps: 1, 2, and 3. Step 1 shows a starting material (a benzene ring with a nitro group and a chlorine atom) reacting to form an intermediate (a benzene ring with a nitro group, a chlorine atom, and a carbonyl group). Step 2 shows the intermediate reacting to form a more complex product (a benzene ring with a nitro group, a chlorine atom, and a methoxy group). Step 3 shows the final product (a benzene ring with a nitro group, a chlorine atom, and a methoxy group).

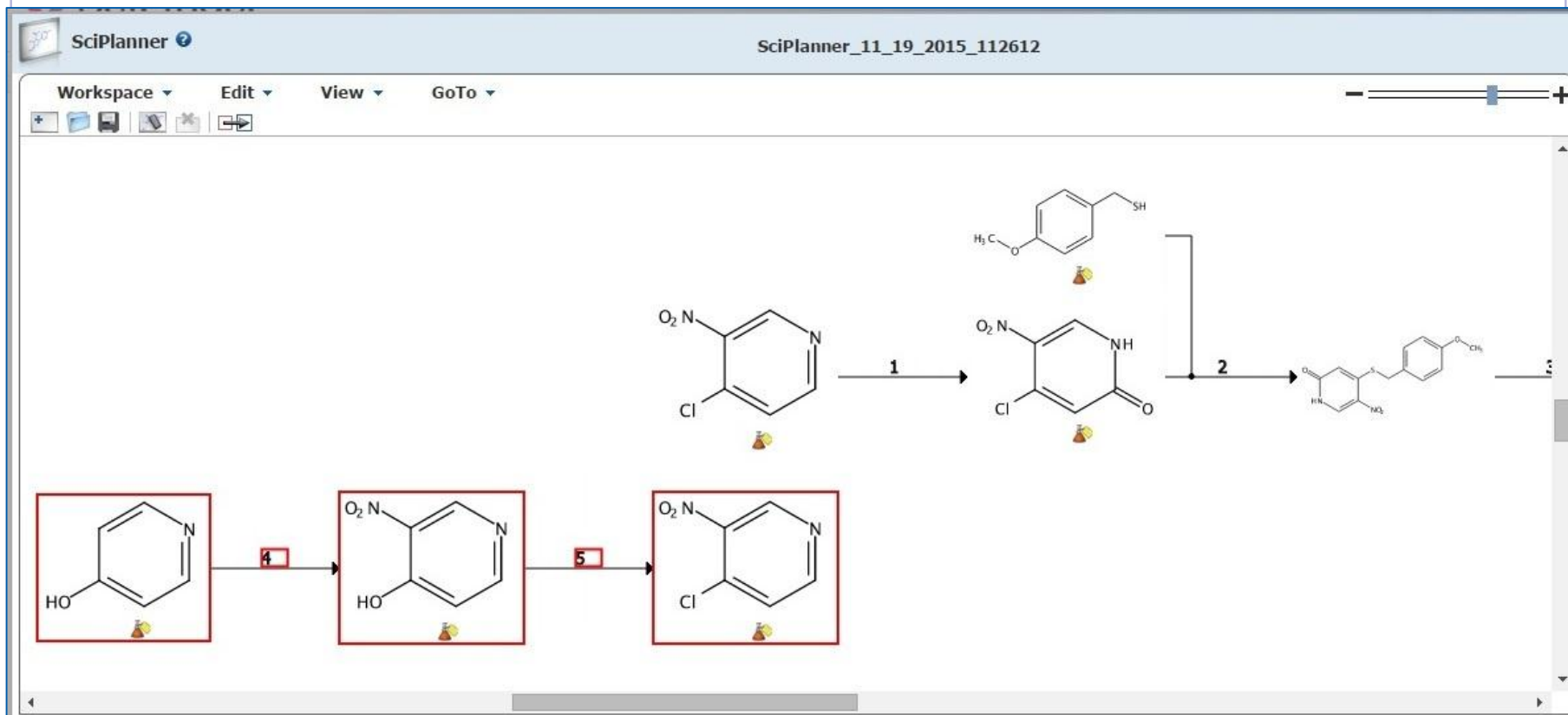
打开中间产物的标准菜单
选择Synthesize this

The screenshot shows the SciPlanner interface displaying a list of reactions. The top bar includes "Get References" and "Tools". Below the top bar, there are filters for "Group by: No Grouping" and "Sort by: Accession Number". A button "Send selected records to SciPlanner." is visible. The main area shows "1 of 34 Reactions Selected". A list of reactions is displayed, with the first one selected: "1. View Reaction Detail". Below the list, a reaction detail is shown: "2 Steps Hover over any structure for more options." The reaction shows a starting material (a benzene ring with a hydroxyl group) reacting to form a product (a benzene ring with a nitro group and a chlorine atom). The number of results for each is indicated as "~161" for the starting material and "~192" for the product.

在检索到的反应中选择感兴趣的反应

继续推送到SciPlanner

SciPlanner使用简介

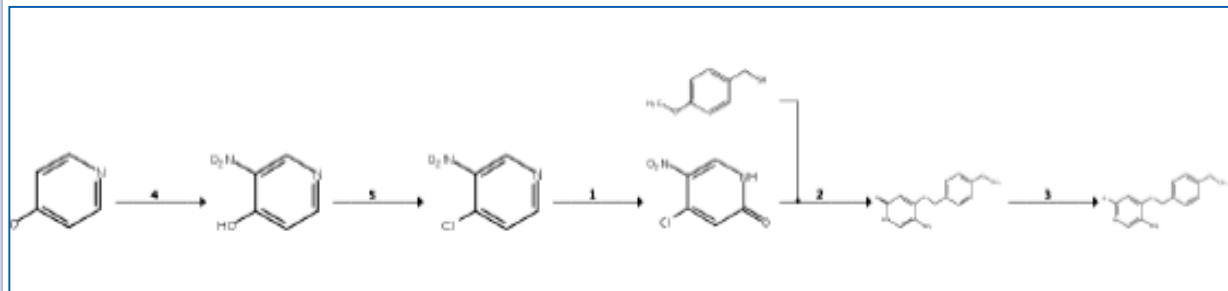


步骤同前，将推送过来的反应拖到编辑面板中，可以看到两条反应中存在同样的结构

SciPlanner使用简介

The screenshot displays the SciPlanner software interface. At the top, the title bar reads "SciPlanner" and "SciPlanner_11_19_2015_112612". Below the title bar is a menu bar with "Workspace", "Edit", "View", and "GoTo". A "Workspace" dropdown menu is open on the left, listing options: "New", "Open", "Save", "Duplicate", "Import", "Export", "Print", and "Close". The "Export" option is highlighted in blue. In the center, a chemical reaction workflow is shown with three chemical structures connected by arrows labeled "4", "5", and "1". A pink callout box points to the "Export" menu item with the text: "点击 Workspace, 选择 Export 导出结果". Another pink callout box points to the second chemical structure with the text: "用鼠标将两个同样的结构拖至重叠, 两条反应合并". A third pink callout box points to the "Export" dialog box with the text: "选择适当的输出格式, 输出结果". The "Export" dialog box is open on the right, showing options for "Offline Review" (Portable Document Format (*.pdf), Citations (*.ris), Image (*.png)) and "Saving Locally" (SciPlanner eXchange (*.pkx)). The "Details" section includes "File Name:" (SciPlanner_11_19_2015_112612) and "Title". The "Include:" section has checkboxes for "SciPlanner Image", "Reaction Details", "Substance Details", and "Reference Details". "Export" and "Cancel" buttons are at the bottom right of the dialog.

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 Poloek, 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>C₁₃ H₁₂ N₂ O₄ S 2-(1H)-Pyridinone, 4-[[[4-methoxyphenyl]methyl]thio]-5-nitro-</p> <p>Related Info: ~ 2 References Reactions</p>	<p>1228150-23-9</p> <p>C₁₃ H₁₁ Cl N₂ O₃ S Pyridine, 2-chloro-4-[[[4-methoxyphenyl]methyl]thio]-5-nitro-</p> <p>Related Info: ~ 2 References Reactions</p>	<p>13091-23-1</p> <p>C₈ H₃ Cl N₂ O₂ Pyridine, 4-chloro-3-nitro-</p> <p>Related Info: ~ 301 References Reactions ~ 100 Commercial Sources Regulatory Information</p>
<p>5435-54-1</p> <p>C₆ H₄ N₂ O₃ 4-Pyridinol, 3-nitro-</p> <p>Related Info: ~ 113 References Reactions ~ 197 Commercial Sources Regulatory Information</p>	<p>6258-60-2</p> <p>C₈ H₁₀ O S Benzenemethanethiol, 4-methoxy-</p> <p>Related Info: ~ 749 References Reactions ~ 71 Commercial Sources Regulatory Information</p>	<p>626-64-2</p> <p>C₆ H₅ N O 4-Pyridinol</p> <p>Related Info: ~ 1351 References Reactions ~ 160 Commercial Sources Regulatory Information</p>
<p>850663-54-6</p> <p>C₆ H₃ Cl N₂ O₃ 2-(1H)-Pyridinone, 4-chloro-5-nitro-</p> <p>Related Info: ~ 22 References Reactions ~ 136 Commercial Sources</p>		

提纲

- 美国化学文摘社简介
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 - 物质检索
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 - 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
- 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 displays the SciFinder registration interface, 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 'Tips' link), Password, and Re-enter Password.
- SECURITY INFORMATION--**: Includes a dropdown menu for Security Question and an input field for Answer (with a 'Why?' link).

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)

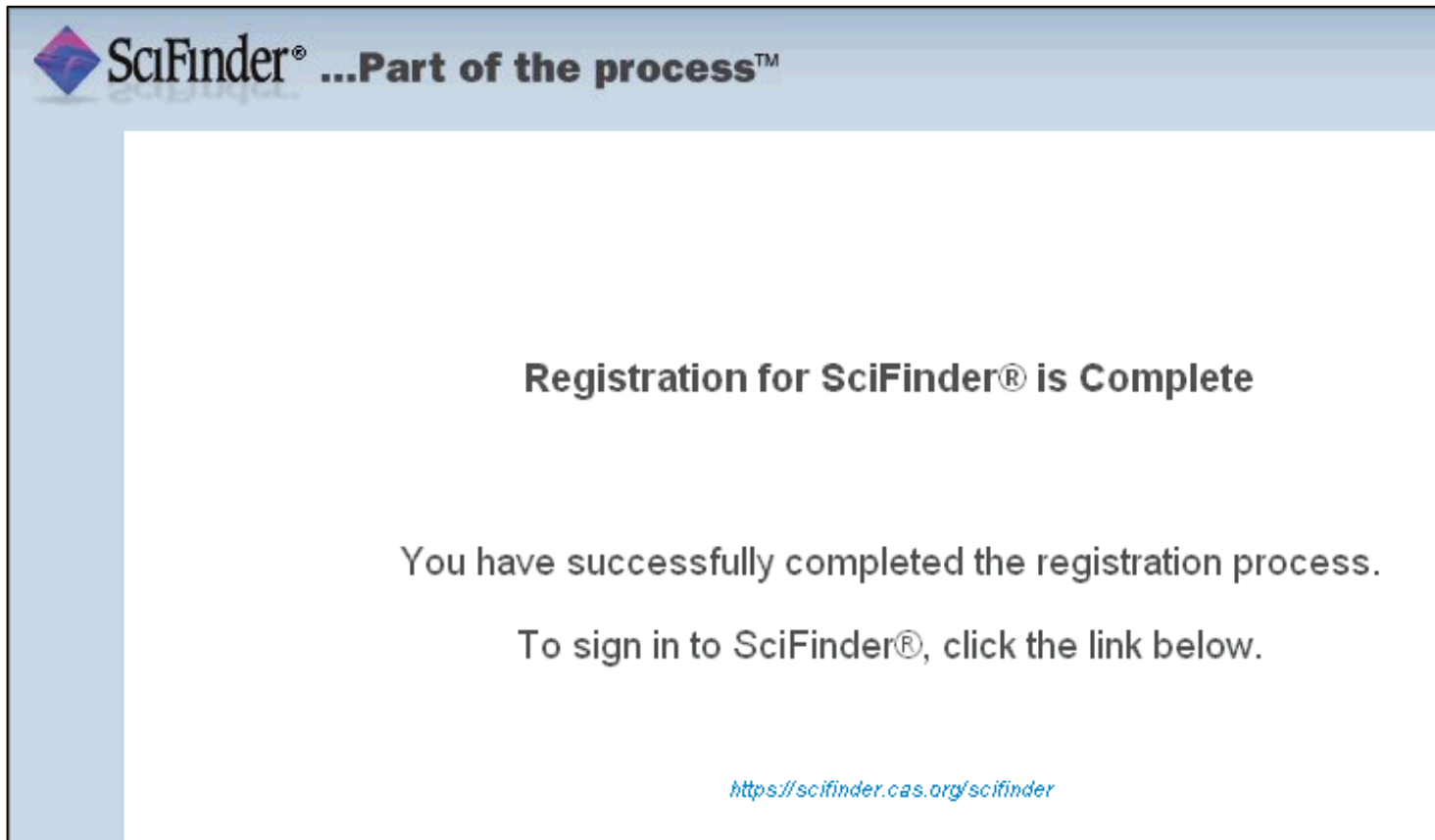
3. 密码必须包含 7-15 个字符，并且至少**包含三种以下字符**：

- 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



账号注册成功，登录scifinder.cas.org开始使用SciFinder

SciFinder使用注意事项

- 在校内完成注册（教学楼、图书馆、实验室）
- 一人注册一个帐号
- 请提供真实姓名信息
- 严禁过量下载
- 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

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