

匡金海

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如何使用SciFinder获取科技信息

郑州轻工业学院

2016.11.14



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

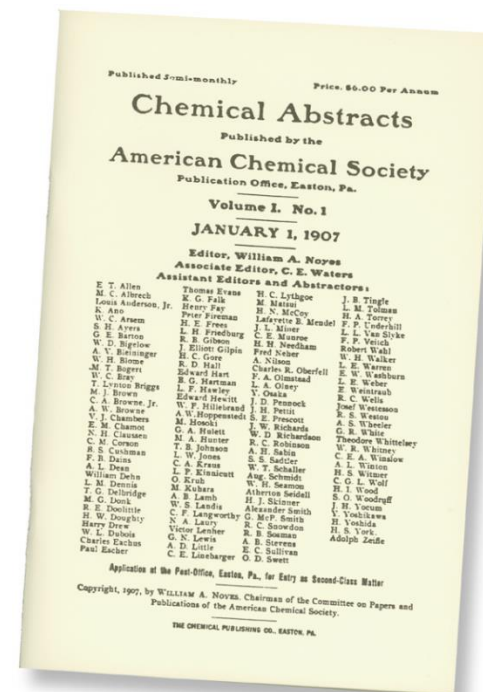


1907年，信息的汇集、管理发生了重大的变化



威廉·诺伊斯
(William A. Noyes)

- “化学文摘”创刊
- 当年编制近12,000条文摘
- 今天，CAS每年收录、创建来自期刊、专利和其他已公开信息的文摘达到了100余万条



CAS——构建最高质量的化学数据库



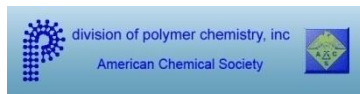
arXiv.org

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

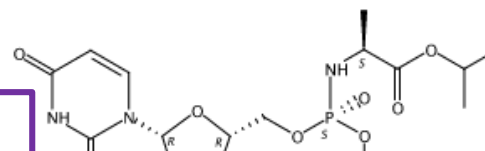
Concepts

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

Substances

1190307-88-0P Sofosbuvir 
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。

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- 极大节约用户在研究专利时的时间
- 快速查找定位专利中的关键化学信息

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

Quick View PATENTPAK

By Beigelman, Le...
From PCT Int. App...

Patent No.	Kind	Language
WO 2016100441	A1	English

Patent Family

US 20160176911	A1	English
----------------	----	---------

Disclosed he...
phosphate, R...
methods of t...
medicament

atkina, Natalia
Language: English, Database: CAPLUS

B is substituted purine and pyrimidine nucleobase; dashed bond between R and R⁴ is absent, then R is H, substituted each R⁶ and R⁷ are independently hydrogen or deuterium; R⁵ is -OH or F; methods of synthesizing nucleotide analogs and as a HCV infection with one or more nucleotide analogs. Thus, nucleotide II was prepd. and tested as antiviral agent and of a hepatitis C virus.

7. Process for preparation of sofosbuvir

Quick View PATENTPAK

By Li, Zebiao; Zhu, Mingmin; Zhang, Qinghai; Zhu, Gongfeng; Zhang, Zhaoguo; Lin, Yanfeng
From Faming Zhuanli Shenqing (2016), CN 105669804 A 20160615. | Language: Chinese, Database: CAPLUS

The prep. method comprises reaction of (2'R)-2'-deoxy-2'-fluoro-2'-methylyridine with

ZOOM: - +

DOWNLOAD PDF: [Icon]

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

(19) World Intellectual Property Organization
International Bureau

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

WIPO PCT

(51) International Patent Classification:
C07H 19/10 (2006.01) C07H 19/13 (2006.01)
C07H 19/20 (2006.01) A61K 31/7072 (2006.01)
C07H 19/11 (2006.01) A61K 31/7076 (2006.01)
C07H 19/213 (2006.01) A61K 31/708 (2006.01)
C07H 19/067 (2006.01) A61P 31/14 (2006.01)
C07H 19/073 (2006.01)

(81) Designated States (unless otherwise indicated, for every kind of national protection available): AO, AT, AU, AZ, BA, BB, BG, BR, CA, CH, CL, CN, CO, CZ, DE, DK, DR, DO, DZ, EC, EE, EG, ES, FI, FR, GB, GR, GT, HN, HR, HU, ID, IL, IN, JP, KE, KG, KH, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, NZ, OM, PA, PE, PG, PH, PL, PT, RU, SE, SG, SK, SL, SM, ST, SV, SY, TH, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW.

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

(25) Filing Language:
English

(84) Designated States (unless otherwise indicated, for every kind of regional protection available): ARIPO (BW, GH, GM, KE, LU, MG, MW, MZ, NA, NG, SD, SI, SS, SZ, TZ, UG, ZM, ZW), Eurasian (AM, AZ, BY, KG, KZ, RU, TJ, TM), European (AL, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LT, LU, LV, MA, MC, MT, NL, NO, PL, PT, RO, SE, SI, SK, SL, SM, ST, SV, SY, TH, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW), African and Asian (DZ, EG, ES, FI, FR, GB, GR, HU, IE, IT, LT, LU, LV, MA, MC, MT, NL, NO, PL, PT, RO, SE, SI, SK, SL, SM, ST, SV, SY, TH, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW), African and Asian (DZ, EG, ES, FI, FR, GB, GR, HU, IE, IT, LT, LU, LV, MA, MC, MT, NL, NO, PL, PT, RO, SE, SI, SK, SL, SM, ST, SV, SY, TH, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW).

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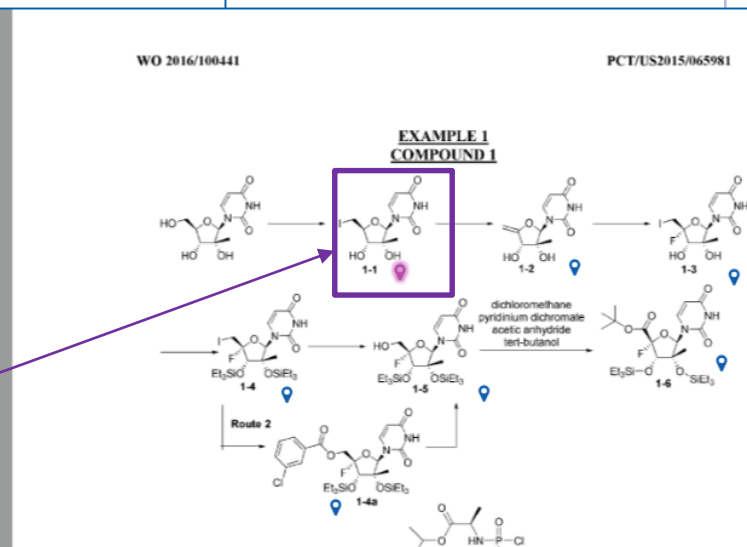
Analyst Markup Locations (1)
page 130

CAS RN 1206126-39-7

Search in SciFinder | View Detail

Analyst Markup Locations (1)
page 130

CAS RN 1206126-41-1



CAS最新动向—解决方案

- CAS于2016年2月正式发布MethodsNow™
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- 来自重要的全文信息资源：CAS高质量标引、全新的、增值的方法
- 满足合成和分析研究工作者的需求

SciFinder
SciPlanner
Reaction Structure substructure > reactions (9)
Analyze by: Reagent, E/N, K₂CO₃, EN(Ph-2)
1. View Reaction Detail [Link] [Send to SciPlanner]
Single Step viewer over any structure for more options.
Overview
Microcosm™
Procedure
1. Stir the mixture of 7-methyl-4-methoxy-ycarbonylmethyl-2H-chromen-2-one (480 mg, 1.05 mmol), 1-iodooctadecane (388 mg, 1.82 mmol), copper(II) sulfate pentahydrate (42 mg, 0.17 mmol), (+)-sodium L-ascorbate (360 mg, 1.82 mmol) in t-BuOH/water (15 mL/15 mL) at room temperature for 4 hours.
View more...
Available Experimental Data
1H NMR, 13C NMR, IR, HRMS, Mass Spec, MP
View with MethodsNow

嵌在SciFinder中的合成模块

CAS Solutions
METHODS NOW
atorvastatin
Results (528)
Sort Relevance
Analyte
Atorvastatin (227)
Atorvastatin calcium (211)
Ezetimibe (80)
Amiodipine besylate (56)
Fenofibrate (46)
View All
Method Category
Matrix
Pharmaceutical tablets (293)
Blood plasma (60)
Tablets (49)
Pharmaceutical capsules (34)
Garcinia atroviridis (20)
View All
Technique
Reversed-phase HPLC (152)
Spectrophotometry (101)
UV-visible spectroscopy (71)
HPLC (57)
Liquid chromatographic UV detectors (43)
View All
Analysis of Atorvastatin in Blood plasma by High-performance thin layer chromatography
CAS MN: 1-101-CAS-1389
View Details & Instructions
Add to Compare
Analyte: Atorvastatin
Matrix: Blood plasma
Other Materials: Material: 60 F254 silica gel HP TLC plates
Method Category: Active Pharmaceutical Ingredient and Metabolite Analysis
Technique: High-performance thin layer chromatography
Equipment Used: Automatic TLC Sampler 3
Source: HPTLC determination of atorvastatin in plasma
Jamshidi, A.; Nateghi, A. R.
Chromatographia (2007), 65 (11/12), 763-766. Vieweg Verlag/GWV Fachverlage GmbH
Document Sources
Abstract

单独的分析界面

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

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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 CAS Solutions logo and the SciFinder logo. The top right contains links for Preferences, SciFinder Help, and a Sign Out button. Below the header is a navigation bar with 'Explore', 'Saved Searches', and 'SciPlanner' options. The main content area is titled 'REFERENCES: RESEARCH TOPIC' and features a search input field with example text: 'The effect of antibiotic residues on dairy products' and 'Photocyanation of aromatic compounds'. A 'Search' button and an 'Advanced Search' link are located below the input field. On the left side, there is a sidebar menu 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). On the right side, there is a 'SAVED ANSWER SETS' section listing various saved sets like 'CSF1R', 'jmc', 'EP 19870107847', etc., and a 'KEEP ME POSTED' section with a message: 'You have no proxies. Learn how to: Create Keep Me Posted'.

已保存的结果集

检索入口

定题追踪



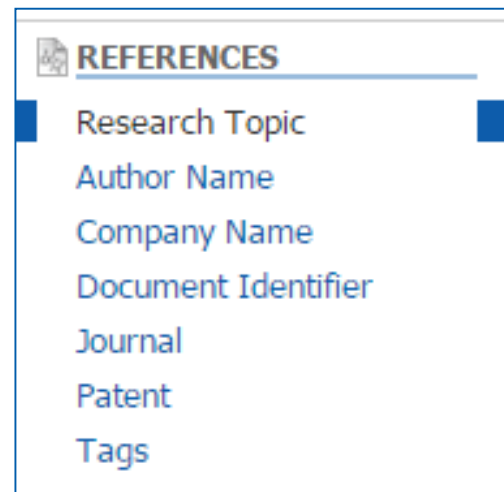
SciFinder检索——文献检索

■ 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: 薄膜技术在处理污水中的应用

The screenshot displays the SciFinder web interface. At the top, there are navigation tabs: 'Explore', 'Saved Searches', and 'SciPlanner'. Below these, the current search topic is identified as 'Research Topic "membrane process of wastewater..."'. 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', 'Property', and 'Substance Identifier'. The main content area is titled 'REFERENCES: RESEARCH TOPIC' and features a search input field containing the text 'membrane process of wastewater treatment'. Below the input field, there are 'Examples:' such as 'The effect of antibiotic residues on dairy products' and 'Photocyanation of aromatic compounds'. A prominent blue 'Search' button is located below the examples. At the bottom of the main area, there is a link for 'Advanced Search'. A purple-bordered box at the bottom of the screenshot contains the text: '关键词之间用介词连接: in, with, of...'.

主题检索的候选项

Select All Deselect All

0 of 5 Research Topic Candidates Selected

		Reference
<input type="checkbox"/>	3273 references were found containing "membrane process of wastewater treatment" as entered	327
<input type="checkbox"/>	16230 references were found containing the two concepts "membrane process" and "wastewater treatment" closely associated with one another.	1623
<input type="checkbox"/>	36838 references were found where the two concepts "membrane process" and "wastewater treatment" were present anywhere in the reference.	3683
<input type="checkbox"/>	291731 references were found containing the concept "membrane process".	29173
<input type="checkbox"/>	728837 references were found containing the concept "wastewater treatment".	72883

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

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Sort by: Accession Number Display Options

0 of 16230 References Selected Page: 1 of 812

1. **Preparation of graphene oxide modified poly(m-phenylene isophthalamide) nanofiltration membrane with improved water flux and antifouling property**
Quick View Other Sources
By Yang, Mei; Zhao, Changwei; Zhang, Shaofeng; Li, Pei; Hou, Deyin
From Applied Surface Science (2016), Ahead of Print. | Language: English, Database: CAPLUS
Poly (m-phenylene isophthalamide)/graphene oxide (PMIA/GO) composite nanofiltration (NF) membranes were prepd. via a facile phase inversion method. Structures, surface properties and hydrophilicities of the membrane were analyzed using FT-IR, XPS, AFM, SEM, water contact angle and Zeta-potential measurements. FTIR spectra indicated the existence of hydrophilic carboxylic acid and hydroxyl groups in the GO mols. SEM pictures revealed the large and finger-like micro-voids formed in the sublayer of the NF membranes after adding GO. The zeta-potential and water contact angle results proved tha...

2. **Cleaning method and cleaning agent of permeable membrane [Machine Translation].**
Quick View Other Sources
By Azuma, Nozomu
From Jpn. Kokai Tokkyo Koho (2016), JP 2016185514 A 20161027. | Language: Japanese, Database: CAPLUS
[Machine Translation of Descriptors]. To provide a method of cleaning the permeable membrane that can be recovered until the permeation flux of enough for example new film and the same degree contaminated permeable membrane by water treatment. A method of cleaning a permeable membrane for water treatment membrane device, a first step of a translucent over film is brought into contact with the surfactant-contg. aq. alkali soln., thereafter, the method of cleaning permeable membrane characterized by having a second step of contacting the translucent filtration membrane with the oxalic acid aq....

3. **A domestic garbage exudation wastewater treatment method [Machine Translation].**
Quick View Other Sources

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文献检索结果

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

1. **the enumeration and subculture of bacteria from potable water**
By Reasoner, D. J.; Geldreich, E. E.
From Applied and Environmental Microbiology (1985), 49(1), 1-7. | Language: English, Database: CAPLUS

A new medium was developed for use in heterotrophic plate count analyses and for subculture of bacteria isolated from potable **water** samples. The new medium, designated R2A, contains 0.5 g yeast ext., 0.5 g Difco Proteose Peptone no. 3, 0.5 g Casamino Acids, 0.5 g glucose, 0.5 g sol. starch, 0.3 g K₂HOP₄, 0.05 g MgSO₄·7H₂O, 0.3 g Na pyruvate, and 15 g agar/L of lab.-quality **water**. The pH was adjusted to 7.2 with cryst. K₂HPO₄ or KH₂PO₄ and the medium was sterilized at 121° for 15 min. Results from parallel studies with spread **membrane** filter and pour-plate procedures showed that the R2A medi...

2. **Occurrence and removal of pharmaceuticals and endocrine disruptors in South Korean surface, drinking, and waste waters**
By Kim, Sang D.; Cho, Jaeweon; Kim, In S.; Vanderford, Brett J.; Snyder, Shane A.
From Water Research (2007), 41(5), 1013-1021. | Language: English, Database: CAPLUS

Liq. chromatog./tandem mass spectrometry (LC-MS/MS) with electrospray ionization (ESI) and atm. pressure chem. ionization (APCI) were used to measure the concns. of 14 pharmaceuticals, 6 hormones, 2 antibiotics, 3 personal care products (PCPs), and 1 flame retardant in surface **waters** and **wastewater treatment** plant effluents in South Korea. Tris(2-chloroethyl) phosphate (TCEP), iopromide, naproxen, carbamazepine, and caffeine were

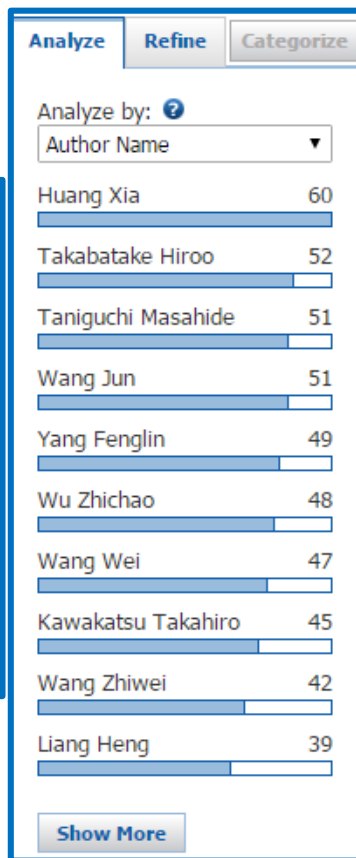
5种排序方式，可以按照进入数据库的时间、作者名、引文、公开年限、标题对文献检索结果进行重新排序

Citing Reference: 可以帮助找到最重要的文献

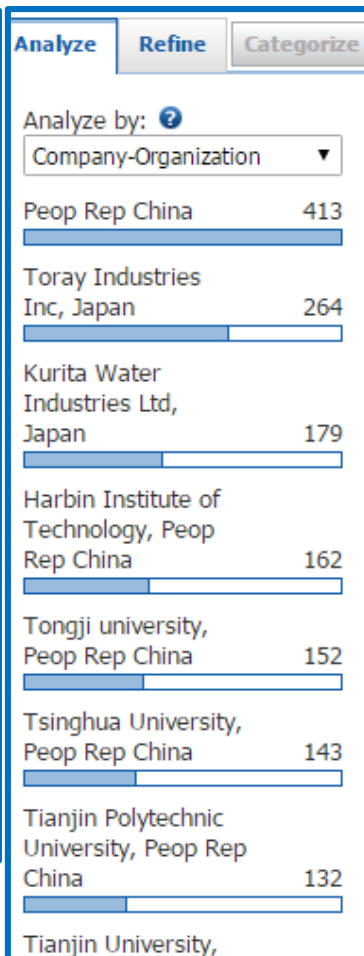
文献检索结果：Analyze

12种文献分析选项

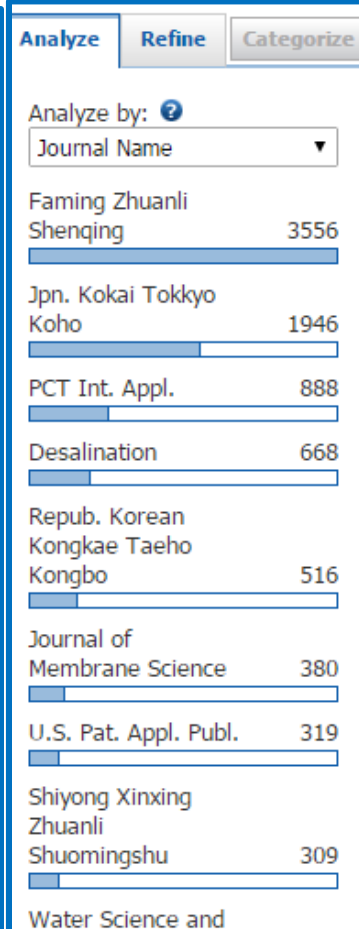
主要研究人员



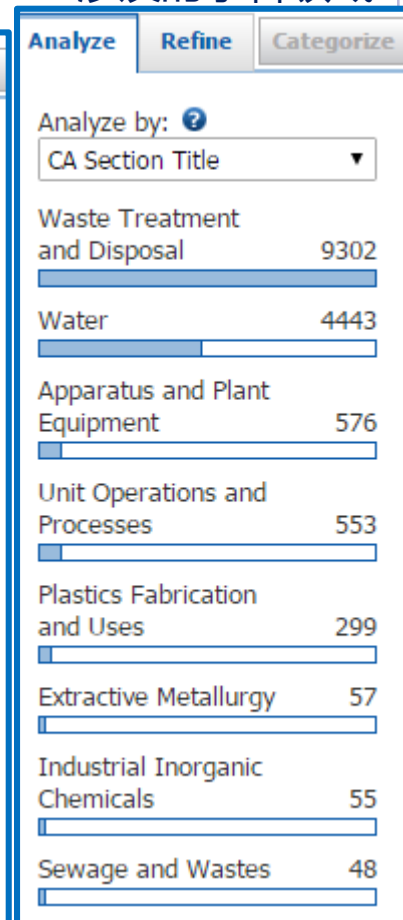
主要研究机构，合作伙伴&竞争对手



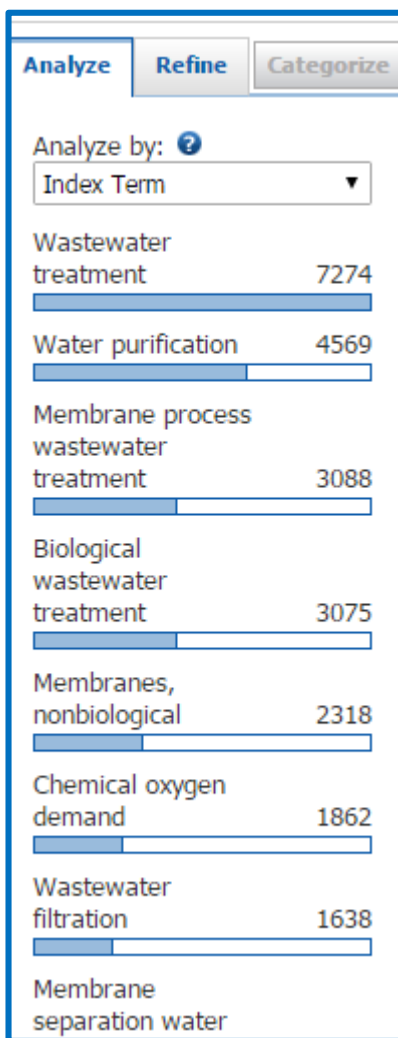
主要发表期刊



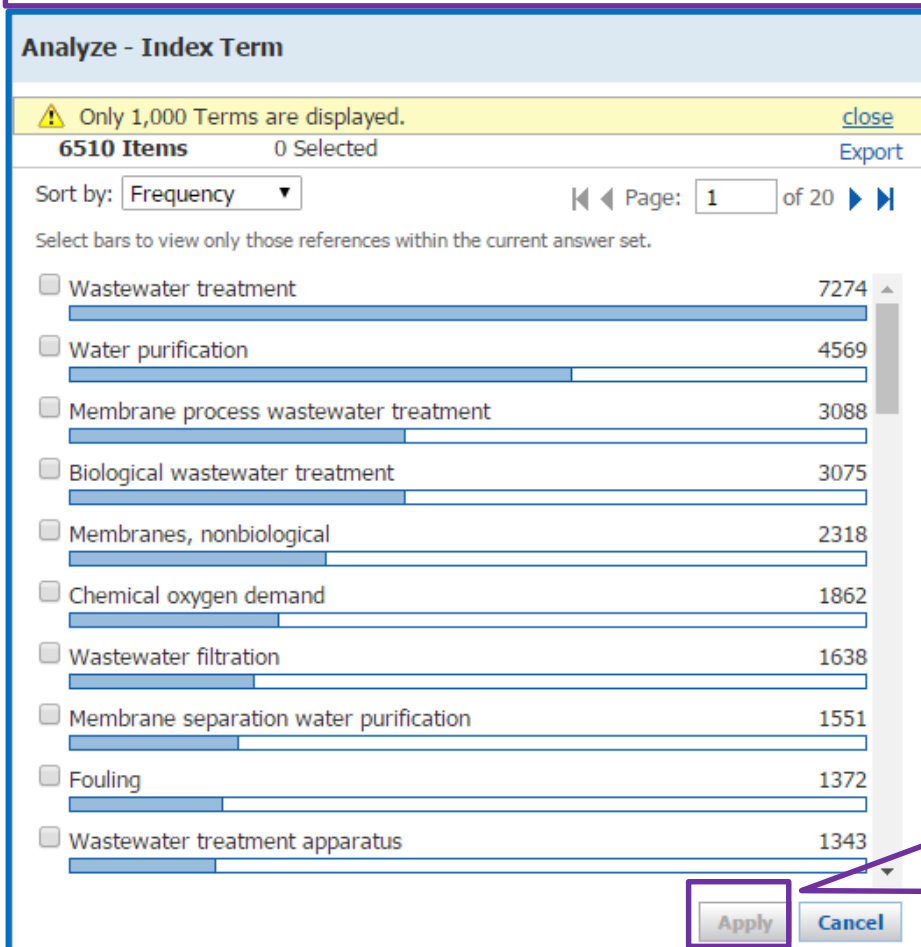
涉及的学科领域



文献检索结果：Analyze



Index Term: 帮助用户全景了解本领域涉及的重要技术术语，精选文献



选择感兴趣的技术术语，点击 Apply



文献检索结果：Refine

REFERENCES

Analyze Refine Categorize

Refine by:

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

Company Name

Examples:

3M

DuPont

Refine

Get Substances Get Reactions Get Related Citations Tools

Sort by: Citing References

0 of 6770 References Selected Page: 1 of 339

- Ultrathin Graphene Nanofiltration Membrane for Water Purification**
By Han, Yi; Xu, Zhen; Gao, Chao
From Advanced Functional Materials (2013), 23(29), 3693-3700. | Language: English, Database: CAPLUS
A method of fabricating ultrathin (~22-53 nm thick) graphene nanofiltration membranes (uGNMs) on microporous substrates is presented for efficient water purifn. using chem. converted graphene (CCG). The prepd. uGNMs show well packed layer structure formed by CCG sheets, as characterized by SEM, at. force microscopy, and transmission electron microscopy. The performance of the uGNMs for water treatment was evaluated on a dead end filtration device and the pure water flux of uGNMs was high (21.8 L /m²-h-bar). The uGNMs show high retention (>99%) for org. dyes and moderate retention (~20-60%) f...
- Photocatalytic organic pollutants degradation in metal-organic frameworks**
By Wang, Chong-Chen; Li, Jian-Rong; Lv, Xiu-Liang; Zhang, Yan-Qiu; Guo, Guangsheng
From Energy & Environmental Science (2014), 7(9), 2831-2867. | Language: English, Database: CAPLUS
A review. Efficient removal of org. pollutants from wastewater has become a hot research topic due to its ecol. and environmental importance. Traditional water treatment methods such as adsorption, coagulation, and membrane sepn. suffer from high operating costs, and even generate secondary pollutants. Photocatalysis on semiconductor catalysts (TiO₂, ZnO, Fe₂O₃, CdS, GaP, and ZnS) has demonstrated efficiency in degrading a wide range of org. pollutants into biodegradable or less toxic org. compds., as well as inorg. CO₂, H₂O, NO₃⁻, PO₄³⁻, and halide ions. However, the difficult post-sepn.,...
- Membrane fouling in a submerged membrane bioreactor (MBR) under sub-critical flux operation: Membrane foulant and gel layer characterization**

通过Refine快速获取目标信息

文献检索结果：Categorize

学科主分类

学科副分类

学科副分类涉及
的重要技术术语

选中的重要技术术语

Categorize ?

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

Category Heading	Category	Index Terms	Selected Terms
All	Environment (262)	Page: 1 of 3 Select All Deselect All	Click 'x' to remove the category from 'Selected Terms'
Technology	Formed, removed, & other substances (1393)	<input type="checkbox"/> Industrial wastewater 283	<input checked="" type="checkbox"/> Environmental chemistry > Environment (1 Terms)
Environmental chemistry	Pollutants (1135)	<input type="checkbox"/> Wastewater treatment sludge 261	
General chemistry	Geology & soil chemistry (149)	<input type="checkbox"/> Activated-sludge process wastewater treatment 258	
Physical chemistry	Substances in geology & astronomy (18)	<input checked="" type="checkbox"/> Reverse osmosis water purification 258	
Polymer chemistry	Astronomy (2)	<input type="checkbox"/> Organic matter 243	
Genetics & protein chemistry		<input type="checkbox"/> Sludges 230	
Biotechnology		<input type="checkbox"/> Wastewater reclamation 175	
Synthetic chemistry		<input type="checkbox"/> Drinking waters 144	
Biology		<input type="checkbox"/> Separatory wastewater treatment 142	
Catalysis		<input type="checkbox"/> Photocatalytic 140	
Analytical chemistry			

Environmental chemistry > Environment > 1 Index Term(s) Selected

OK **Cancel**

基于学科对文献进行自动分类，帮助用户精准定位所关注的学科和技术术语。

结果集的保存— Save, Print, Export

点击标题获取文献信息

1. Performance of UF-NF integrated membrane process for seawater softening

By Song, Yuefei; Xu, Jia; Xu, Yan; Gao, Xueli; Gao, Congjie
From Desalination (2011), 276(1-3), 109-116. | Language: English, Database: CAPLUS

Nanofiltration (NF) membranes are playing a more and more important role in brackish and seawater softening process, wastewater reclamation and other industrial sepn. Ultrafiltration (UF) and NF (ESNA3, Hydranautics) were assembled to an integrated membrane system (IMS) as pretreatment prior to seawater reverse osmosis (SWRO) to evaluate the NF efficiency of seawater softening. The influences of NF feed property (the feed from UF1 with 100 kDa MWCO and UF2 with 20 kDa MWCO, resp.), operating pressure (0.5-3.0 MPa), cross-flow velocity (0.028-0.048 m/s) and feed temp. (5-17°) on the softening...

2. Coupling of biological methods with membrane filtration using ozone as pre-treatment for water reuse

By Qi, Luqing; Wang, Xiaojun; Xu, Qikun
From Desalination (2011), 270(1-3), 264-268. | Language: English, Database: CAPLUS

This work focused on the advanced treatment of the biol. treated wastewater of a textile plant. Nowadays, treatment methods for water reuse are mainly membrane technologies. According to the difficulty of conc. stream treatment and fouling problem in membrane process, a combination pre-treatment process including ozonation, biol. aerated filter (BAF) and reverse osmosis was developed for textile wastewater treatment. Comparing different ozone dosing methods, the ozone-BAF integrated device allowed a higher COD and color redn. The optimal ozone dosage in the integrated device was 20-30 mg/L...

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

Export

Export:

- All
- Selected
- Range

Example: 2-20

For:

Citation Manager

- Citation export format (*.ris)
- Quoted Format (*.txt)
- Tagged Format (*.txt)

Offline review

- Portable Document Format (*.pdf)
- Rich Text Format (*.rtf)
- Answer Keys (*.txt)

Saving locally

- Answer Key eXchange (*.akc)

Details:

File Name: *

Reference_06_19_2012_100848

Format:

- Summary without abstracts
- Summary with partial abstracts
- Summary with full abstracts
- Detail (full record)

Include:

- Task History
- Tags
- Comments

Export Cancel

文献信息详情

标题

1. Performance of UF-NF integrated membrane process for seawater softening

By: Song, Yuefei; Xu, Jia; Xu, Yan; Gao, Xueli; Gao, Congjie

摘要

QUICK LINKS

0 Tags, 0 Comments

SOURCE

Desalination
Volume276
Issue1-3
Pages109-116
Journal; Online Computer File
2011
CODEN:DSLNAH
ISSN:0011-9164
DOI:10.1016/j.desal.2011.03.064

COMPANY/ORGANIZATION

College of Chemistry and Chemical Engineering
Ocean University of China
Qingdao, Shandong, Peop. Rep. China 266100

ACCESSION NUMBER

2011:797594
CAN156:370629
CAPLUS

Nanofiltration (NF) membranes are playing a more and more important role in brackish and seawater softening process, wastewater reclamation and other industrial sepn. Ultrafiltration (UF) and NF (ESNA3, Hydranautics) were assembled to an integrated membrane system (IMS) as pretreatment prior to seawater reverse osmosis (SWRO) to evaluate the NF efficiency of seawater softening. The influences of NF feed property (the feed from UF1 with 100 kDa MWCO and UF2 with 20 kDa MWCO, resp.), operating pressure (0.5-3.0 MPa), cross-flow velocity (0.028-0.048 m/s) and feed temp. (5-17°C) on the softening efficiency in terms of the NF flux and ion rejection were studied. The high softening efficiency of NF membrane could be achieved using UF membrane with smaller MWCO (20 kDa). NF system using UF2 as pretreatment process yielded a higher flux of 61.4 L/(m² h) with Ca²⁺, Mg²⁺, SO₄²⁻ rejection of 44.37%, 73.26% and 99.82%, resp., under the optimum operating conditions of operating pressure at 1.5 MPa, cross-flow velocity at 0.035 m/s and feed temp. at 12.5°. And, the relatively excellent selectivity of divalent ions and univalent ions can be obtained by ESNA3 membrane compared to that of other NF membranes reported in the literature, indicating that the ESNA3 membrane seems to be appropriate for seawater softening process.

Indexing

Water (Section61-4)

重要技术术语

Concepts

Water purification




nanofiltration; performance of UF-NF integrated membrane process for seawater softening

Alkalinity
Electric conductivity
Pressure
Seawater
pH

Chemical oxygen demand
Membranes, nonbiological
Reverse osmosis water purification
Turbidity




Substances

重要物质

1317-61-9 Iron oxide, uses 
1344-28-1 Aluminum oxide, uses 
7631-86-9 Silica, uses 

performance of UF-NF integrated membrane process for seawater softening

Other use, unclassified; Uses

7439-95-4 Magnesium, processes 
7440-09-7 Potassium, processes 
7440-23-5 Sodium, processes 

书目信息

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
 - 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

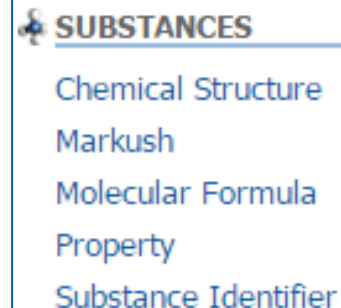
■ 物质检索方法

—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



The image shows a screenshot of the SciFinder interface. At the top, there is a purple icon of a flask and the word "SUBSTANCES" in bold purple text, underlined. Below this, there is a list of search options: "Chemical Structure", "Markush", "Molecular Formula", "Property", and "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

Substance Identifier "1190307-88-0" > substances (1)

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 ?

1190307-88-0

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

Get References Get Reactions Get Commercial Sources

Sort by: CAS Registry Number

0 of 1 Substance Selected

1. 1190307-88-0

~619 ~95

Absolute stereochemistry.

C₂₂ H₂₉ F N₃ O₉ P
L-Alanine, *N*-[[[*P*(*S*),2'*R*]-2'-deoxy-2'-fluoro-2'-methyl-*P*-phenyl-5'-uridylyl]-, 1-methylethyl ester

▶ **Key Physical Properties**
Regulatory Information

CAS Registry Number: 1190307-88-0

- 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

点击此处，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 1190307-88-0

~619 ~95

C₂₂ H₂₉ F N₃ O₉ P
L-Alanine, *N*[[*P*(*S*),2'*R*]-2'-deoxy-2'-fluoro-2'-methyl-*P*-phenyl-5'-uridylyl]-, 1-methylethyl ester

Molecular Weight
529.45

Density (Predicted)
Value: 1.41±0.1 g/cm³ | Condition: Temp: 20 °C Press: 760 Torr

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

Other Names
GS 7977
Hepcinat
Hepcvir
Isopropyl (2*S*)-2-[(2*R*,3*R*,4*R*,5*R*)-5-(2,4-dioxypyrimidin-1-yl)-4-fluoro-3-hydroxy-4-methyl-tetrahydrofuran-2-yl]methoxy-phenoxy-phosphoryl]amino]propionate
PSI 7977

[View more...](#)

由物质获得文献，反应，供应商等信息

Absolute stereochemistry.

物质详情

通过物质获得文献

Get References

Limit results to:

- Adverse Effect, including toxicity
- Analytical Study
- Biological Study
- Combinatorial Study
- Crystal Structure
- Formation, nonpreparative
- Miscellaneous
- Occurrence
- Preparation
- Process
- Properties
- Prophetic in Patents
- Reactant or Reagent
- Spectral Properties
- Uses

For each sequence, retrieve:

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

Get **Cancel**

分析化学

晶体结构

制备

工艺

谱图性质性质

SciFinder中的物质信息

EXPERIMENTAL PROPERTIES

Structure Related

Structure Related Properties	Value	Condition	Note
Crystal Structure	See full text		(1)CAS

Notes

(1) Sofia, Michael J.; Journal of Medicinal Chemistry 2010, V53(19), P7202-7218 CAPLUS 🔍

EXPERIMENTAL SPECTRA

¹H NMR Hetero NMR Mass

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

Notes

(1) Sofia, Michael J.; Journal of Medicinal Chemistry 2010, V53(19), P7202-7218 CAPLUS 🔍

PREDICTED PROPERTIES

PREDICTED SPECTRA

实验数据和实验谱图

预测实验数据

物质检索——Property explore

CAS Solutions

SCIFINDER
A CAS SOLUTION

Explore ▾ Saved Searches ▾ SciPlanner

Opened saved answer set "c-c bond formation" (693) > Formation Mechanism of the Fir...

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) ▾ > 353400
Examples: 44, 25-35, >125

Select Property...

- Boiling Point (°C)
- Density (g/cm³)
- Electric Conductance (S)
- Electric Conductivity (S/cm)**
- Electric Resistance (ohm)
- Electric Resistivity (ohm*cm)
- Glass Transition Temp. (°C)
- Magnetic Moment (μB)
- Median Lethal Dose (LD50) (mg/kg)
- Melting Point (°C)
- Optical Rotatory Power (degrees)
- Refractive Index
- Tensile Strength (MPa)

Examples: 44, 25-35, >125

寻找导电率比铜的60%大的非金属材料

物质结果集的筛选——Refine

CAS Solutions
SCIFINDER
A CAS SOLUTION

Preferences | SciFinder Help | Sign Out

Welcome Helen Zhu

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

Property "Experimental - Electric Conduc..." > **substances (39)** > refine "exclude metal-containing" (14)

SUBSTANCES | Get References | Get Reactions | Get Commercial Sources | Tools

Create Keep Me Posted Alert | Send to SciPlanner

Analyze | **Refine** | Sort by: CAS Registry Number | Display Options

0 of 39 Substances Selected | Page: 1 of 3

Refine by:

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

Select One:

- Include only metal-containing substances
- Exclude metal-containing substances**

Refine

1. **1044804-35-4**

Substance
Image
Cannot Be Displayed
1044804-35-4

Editor Note: A sulfonated polystyrene-doped PEDOT (H.C. Starck)

Unspecified
Clevios P-VP-AI 4083
Experimental Properties

2. **943433-94-1**

210531-45-6 (Component: 625392-06-5)
C₁₃ H₈ F₂ O₇ S₂ · 2 Na

Click to view detail

0 of 14 Substances Selected

1. **1044804-35-4**

Substance
Image
Cannot Be Displayed
1044804-35-4

Click to view detail

Editor Note: A sulfonated polystyrene-doped PEDOT (H.C. Starck)

Unspecified
Clevios P-VP-AI 4083
Experimental Properties

2. **868628-72-2**

C₁₈ H₃₂ B N₂
Boron, tributyl(1-(2-propen-1-yl)-1H-imidazole-κN¹), (7-4)

Key Physical Properties
Experimental Properties

Chemical structure: CCCC[CH2-]B(3+)(CCCC[CH2-])(CCCC[CH2-])N1C=CN(C=C)C1

3. **868628-71-1**

Chemical structure: CCCC[CH2-]B(3+)(CCCC[CH2-])(CCCC[CH2-])N1C=CN(C=C)C1

4. **866023-23-6**

120120-58-3
C₁₈ H₄ O₄ S₄

Chemical structure: C1=CC2=C(C=C1)S(=O)(=O)SC2=O

如何筛选非金属材料？

物质检索——分子式

检索KAl(SO₄)₂·12H₂O, Aluminum potassium sulfate dodecahydrate

The screenshot shows the SciFinder web interface. On the left is a navigation menu with 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). The main content area is titled 'SUBSTANCES: MOLECULAR FORMULA'. It features a search input field with the text 'AlK5O8S2(C3H6O.C2H4O)x', a 'Search' button, and examples: 'AlK5O8S2', 'H4SiO4', and '(C3H6O.C2H4O)x'. A pop-up window on the right shows the search results: 'Explore Substances resulted in 0 substances' with a 'Return' link. Below this, it says 'Molecular Formula "Al K O8 S2 , 12 H2 O" > substances (0)'. There are 'SUBSTANCES' and 'Analyze' buttons, and a 'Refine' button. The 'Analyze by:' section shows 'No substances available'.

分子式书写遵守Hill排序规则：

1. 不含碳物质，按元素符号的字母顺序排列；含碳物质，“C”在前，氢在后，其它元素符号按字母顺序排列
2. 混合物：不同组份间用点（.）分开

物质检索——分子式

Explore ▾ Saved Searches ▾ SciPlanner

Molecular Formula "Al . H4 O8 S2 . 12 H2 O . K" > substances (0)

REFERENCES

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

SUBSTANCES

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

SUBSTANCES: MOLECULAR FORMULA

Al.12H2O.2H2O4S.K

Examples:
H4SiO4
(C3H6O.C2H4O)x

Search

1. 7784-24-9

(Component: 7664-93-9)

~998 ~85

• 1/2 Al

• 1/2 K

• 6 H₂O

Al . 2 H₂ O₄ S . 12 H₂ O . K
Sulfuric acid, aluminum potassium salt (2:1:1), dodecahydrate (8CI, 9CI)

Regulatory Information
Spectra

物质检索——结构

REFERENCES

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

SUBSTANCES

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

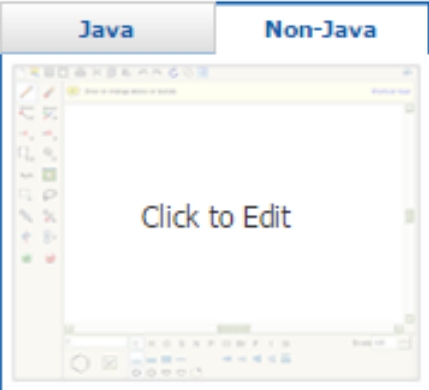
REACTIONS

- Reaction Structure

SUBSTANCES: CHEMICAL STRUCTURE

Structure Editor:

Java Non-Java



Search Type:

- Exact Structure
- Substructure
- Similarity

Show precision analysis

ChemDraw
Launch a SciFinder substance or reaction

Import CXF

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 Recovery 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)
- 负电子 (Negatron)
- 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)

物质检索——精确结构检索

The screenshot displays the 'Structure Editor' window. At the top left, a callout box points to the 'I' icon in the toolbar, containing the text: '通过CAS RN转换结构：CAS RN: 50-36-2'. The central workspace shows a chemical structure of a bicyclic amine derivative with a benzoyl group. On the right side, the 'Drawing Editor' panel is visible, with 'Structure' selected. Below it, the search options are: 'Exact search' (selected), 'Substructure search', and 'Similarity search'. A callout box highlights the 'Exact search' option with the text: '精确结构检索'. At the bottom of the window, the molecular formula $C_{17}H_{21}NO_4$ and the molecular weight 303.36 are displayed.

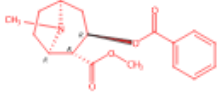
精确结构检索结果

Get References | Get Reactions | Get Commercial Sources | Tools | Create Posted

Sort by: Relevance

0 of 6 Substances Selected

1. **668-19-9**



Absolute stereochemistry.

C₁₇H₂₁N O₄
8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(benzoyloxy)-8-methyl-, methyl ester, (1*R*, 2*R*, 3*R*, 5*S*)-

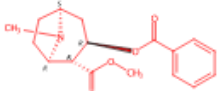
Key Physical Properties
Spectra

可卡因

2. **114599-38-1**

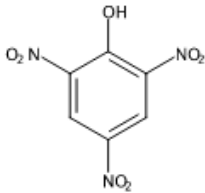
可卡因组合物

668-19-9
C₁₇H₂₁N O₄



Absolute stereochemistry.

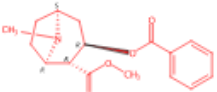
88-89-1
C₆H₃N₃O₇



C₁₇H₂₁N O₄ · C₆H₃N₃O₇
Alcocaine, picrate (6CI)

3. **109496-04-0**

(Component: 668-19-9)



* HCl

Absolute stereochemistry.

C₁₇H₂₁N O₄ · Cl H
Alcocaine, hydrochloride (6CI)

盐酸可卡因

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

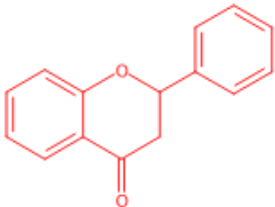
The screenshot displays the 'Structure Editor' window. The main canvas shows a chemical structure of a benzodioxane derivative with a phenyl group. The interface includes a toolbar on the left with various drawing tools, a top toolbar with file operations, and a right-hand panel with search settings. The search settings panel is titled 'Get substances that match your query using:' and has three radio buttons: 'Exact search', 'Substructure search' (which is selected and highlighted with a purple box), and 'Similarity search'. Below the search settings 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

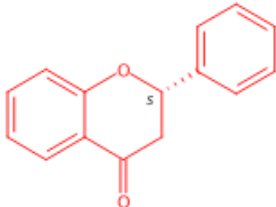


$C_{15}H_{12}O_2$
4-phenyl-4H-1-benzopyran-4-one, 2,3-dihydro-2-phenyl-

▶ Key Physical Properties
Regulatory Information
Spectra
Experimental Properties

2. 17002-31-2

~244



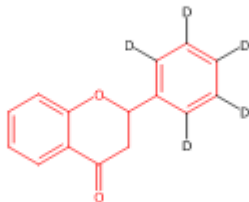
Absolute stereochemistry...Rotation (-).

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

▶ Key Physical Properties
Experimental Properties

10. 146196-91-0

~1 ~5



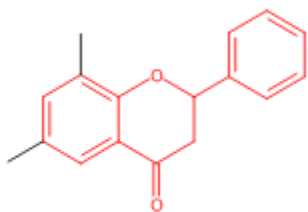
$C_{15}H_7D_5O_2$
4-phenyl-4H-1-benzopyran-4-one, 2,3-dihydro-2-(phenyl- d_5)- (9CI)

Spectra

同位素

亚结构检索结果

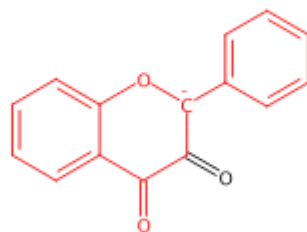
取代物



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

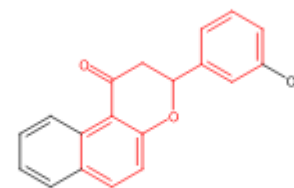
▶ Key Physical Properties
Experimental Properties

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

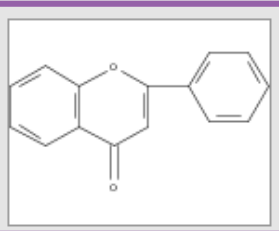
亚结构检索结果的限定

Analysis **Refine**

Refine by: ⓘ

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

Chemical Structure:



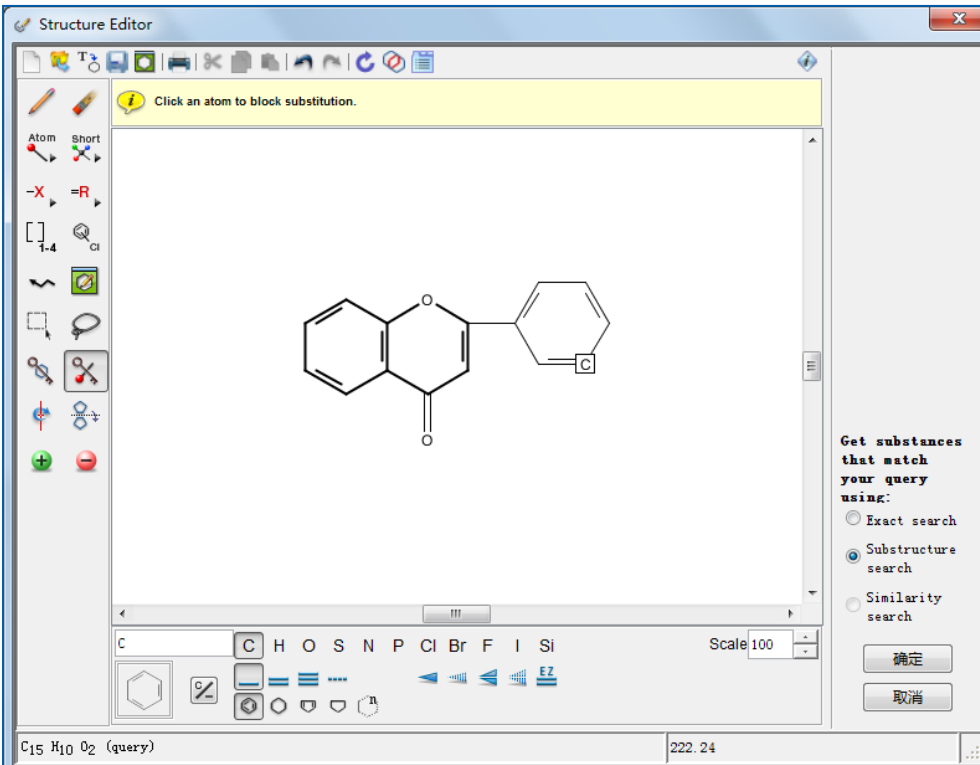
Click image to change structure or view detail

Search type: **Substructure**

化学结构的再次限定

Structure Editor

Click an atom to block substitution.



Get substances that match your query using:

- Exact search
- Substructure search
- Similarity search

确定 取消

C₁₅ H₁₀ O₂ (query) 222.24



环锁定



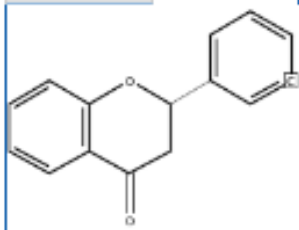
原子锁定

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

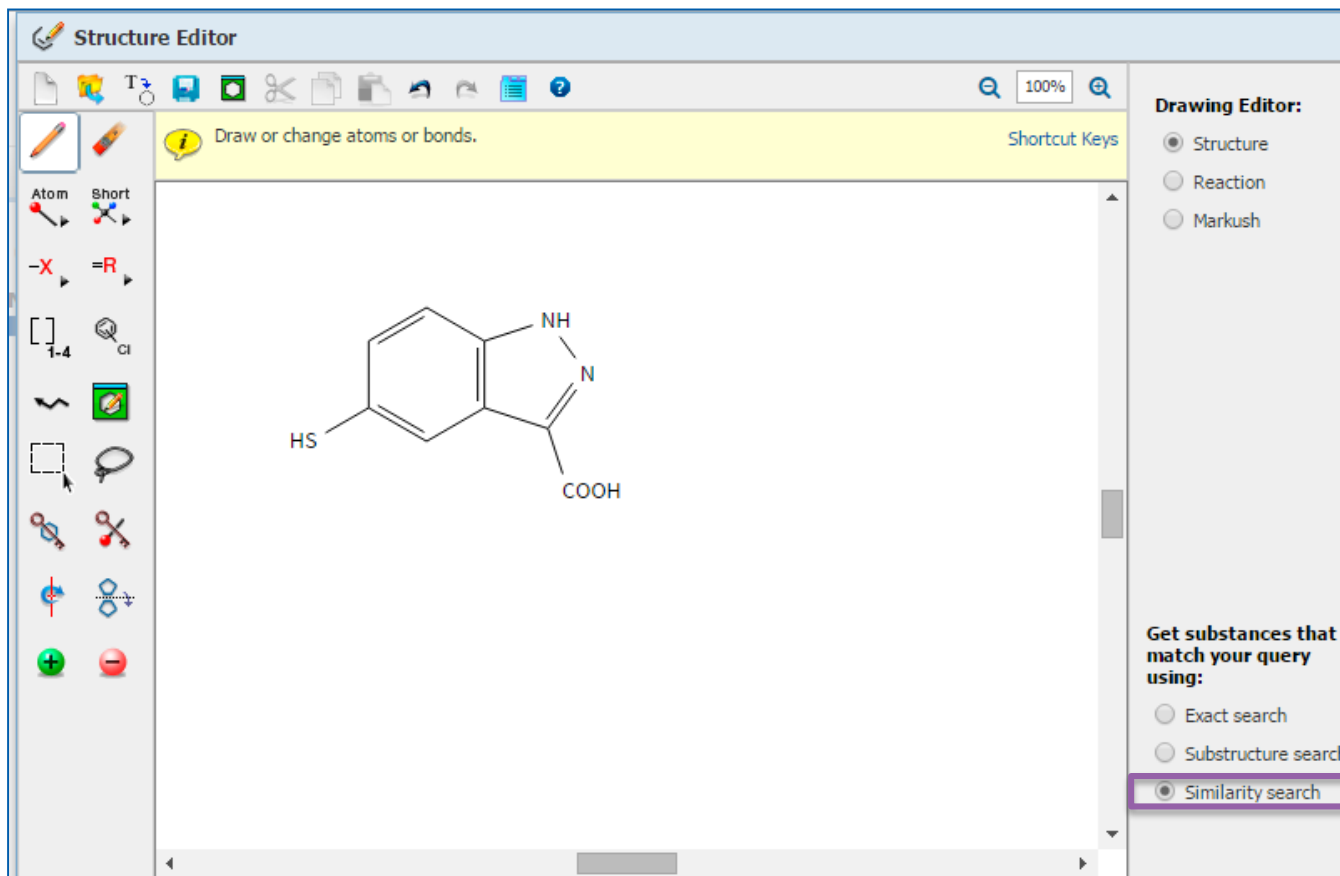
C₁₅H₁₂O₂
4H-1-Benzopyran-4-one, 2,3-dihydro-2-phenyl-, (2S)-
Absolute stereochemistry, Rotation (-).
Key Physical Properties
Experimental Properties

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

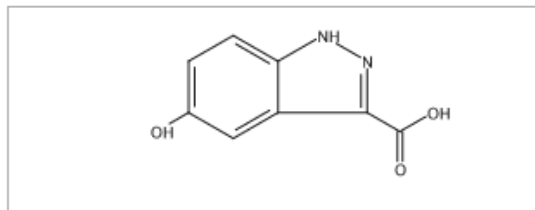
评分越高，相似度越高，结构越相似

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-

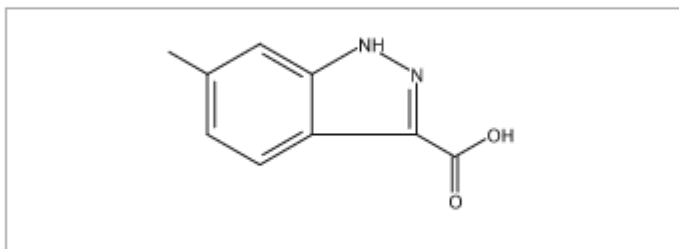
▶ Key Physical Properties

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-

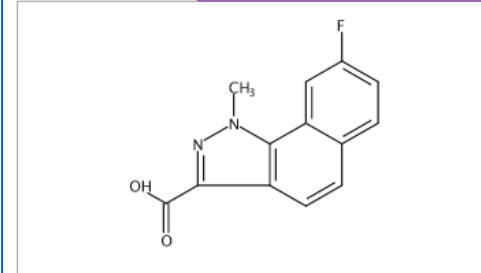
▶ Key Physical Properties

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：

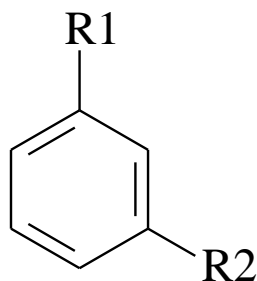
获得片段或整体结构与被检索结构相似的结果，母体结构可以被取代，也可以被改变

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

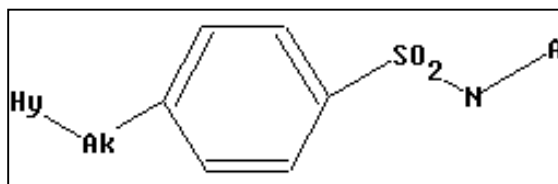
Markush检索

- 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

Drawing Editor:

- Structure
- Reaction
- Markush

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

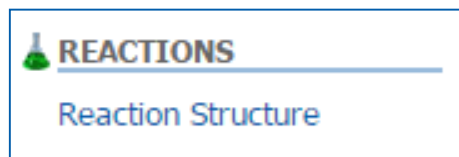
提纲

- 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



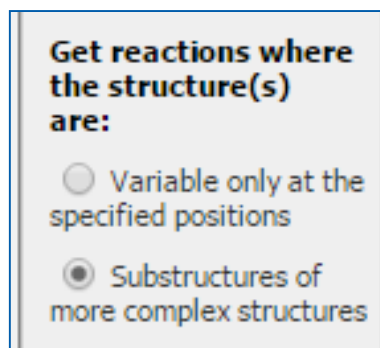
- 常用获取方法

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 window with various toolbars and panels. The main drawing area is empty. The left toolbar contains icons for drawing atoms, bonds, and reaction arrows. The right panel shows the Drawing Editor settings, with 'Reaction' selected. The bottom status bar displays 'CH₄' and '16.04'.

Reaction Arrow: 反应箭头

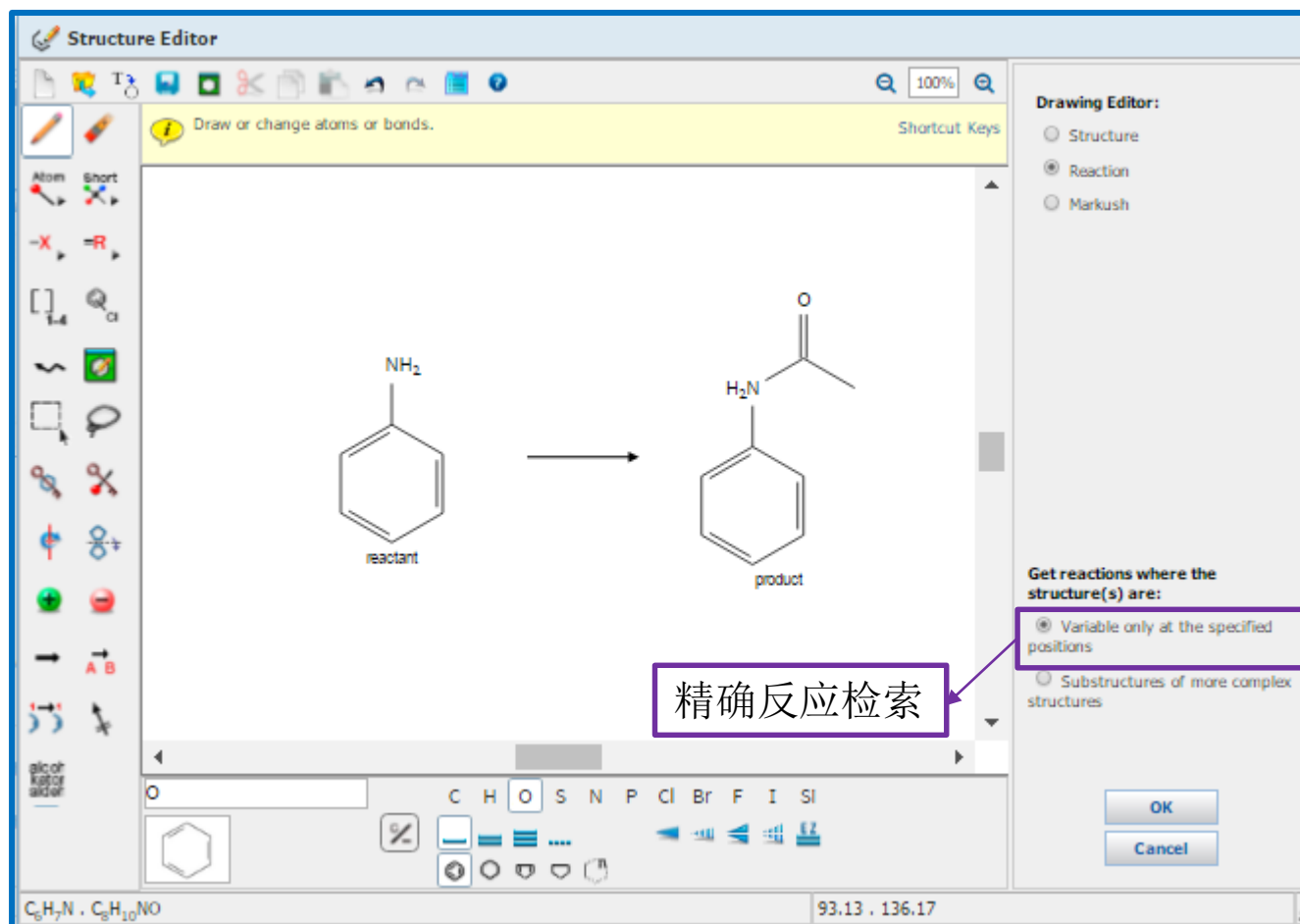
Reaction Role Tools: 反应角色工具

Reaction Atom Marking Tools: 反应原子标记工具

Functional Group List: 官能团列表

Reaction Position Marking Tools: 反应位置标记工具

SciFinder反应检索——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章，
通过Group by Document合并。

Group by: No Grouping Sort by: Relevance

No Grouping
 Document 0 Items Selected
 Transformation

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

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

Nc1ccc(cc1) + CC(=O)CC(=O)C >> CC(=O)Nc1ccc(cc1)

~126 ~112 98% ~128

Overview

Steps/Stages

1.1 R:H₂O, R:O₂, C:SiO₂ (sulfuric acid), C:H₂SO₄ (silica), 2 h, 120°C, 1 atm

Notes

green chemistry-reagent, silica supported and used, no solvent, aerobic, optimization optimized on temperature, Reactants: 2, Most stages in any one step: 1

References

获取相似反应

获取相似反应

选择相似反应的相似限制：

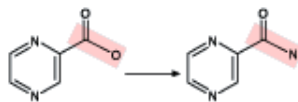
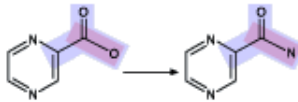
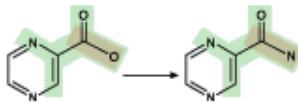
- Broad：仅反应中心相似
- Medium：反应中心及附属原子和键
- Narrow：反应中心及扩展的原子和键

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)


[Get Reactions](#) [Cancel](#)

按照反应类型排序

Group by: Transformation Sort by: Frequency

0 of 605 Reactions Selected

1. Acylation of Nitrogen Nucleophiles by Anhydrides or Dicarboxates
188 Reactions

$$\text{R}-\text{C}(=\text{O})-\text{O}-\text{C}(=\text{O})-\text{R}^2 + \text{R}^1-\text{NH}-\text{R}^1 \longrightarrow \text{R}-\text{C}(=\text{O})-\text{N}(\text{R}^1)_2 + \text{R}^2-\text{C}(=\text{O})-\text{OH}$$

2. Acylation of Nitrogen Nucleophiles by Carboxylic Acids
81 Reactions

$$\text{R}-\text{C}(=\text{O})-\text{OH} + \text{R}^1-\text{NH}-\text{R}^1 \longrightarrow \text{R}-\text{C}(=\text{O})-\text{N}(\text{R}^1)_2$$

更精确的查找需要的反应

3. Acylation of Nitrogen Nucleophiles by Acyl/ Thioacyl/ Carbamoyl Halides and Analogs
55 Reactions

$$\text{R}-\text{C}(=\text{Y})-\text{X} + \text{R}^1-\text{NH}-\text{R}^1 \longrightarrow \text{R}-\text{C}(=\text{Y})-\text{N}(\text{R}^1)_2$$

Y = O, S, NR'

反应检索结果的筛选

Analyze Refine

Group by: No Grouping Sort by: Relevance

0 of 606 Reactions Selected

1. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.

筛选用水作溶剂的反应

Analyze by: Solvent

H ₂ O	99
CH ₂ Cl ₂	65
MeCN	55
THF	27
PhMe	26
AcOH	25
CHCl ₃	22
DMF	15
DMSO	15
Me ₂ CO	15

Show More

~126 ~112 98% ~128

Overview

Steps/Stages

1.1 R:H₂O, R:O₂, C:SiO₂ (sulfuric acid), C:H₂SO₄ (silica), 2 h, 120°C, 1 atm

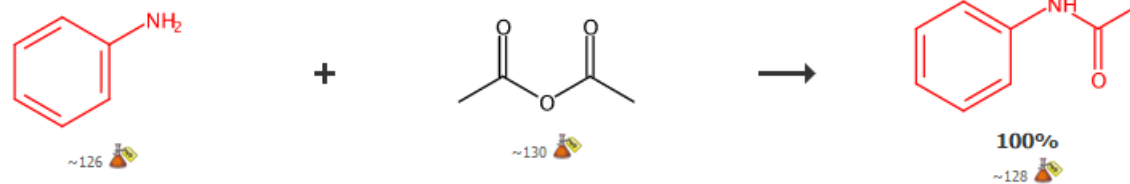
Notes

green chemistry-reagent, silica supported and used, no solvent, aerobic, optimization optimized on temperature, Reactants: 2, Most stages in any one step: 1

References

Silica sulfuric acid mediated acylation of a

SciFinder囊括最大的反应实验过程合集



▼ Overview

Steps/Stages

1.1 S:CH₂Cl₂, 20-120 min, rt

Notes

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

References

Indole Synthesis via Rhodium Catalyzed Oxidative Coupling of Acetanilides and Internal Alkynes

Quick View [Other Sources](#)

By Stuart, David R. et al

From Journal of the American Chemical Society, 130(49), 16474-16475; 2008

不用阅读全文，直接获得包含
实验过程的反应记录

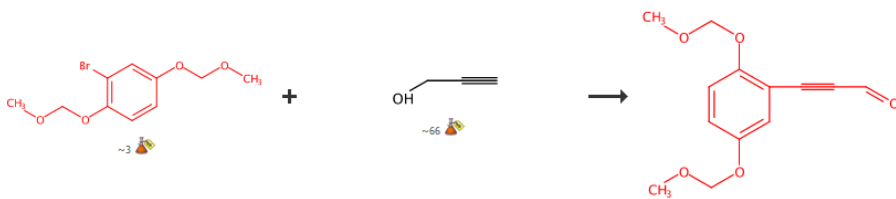
▼ Experimental Procedure



Representative procedure for the preparation of acetanilides: Aniline (10.1 mL, 109.7 mmol, 1 eq) was added to a round-bottom flask via syringe and fitted with a rubber septum. The flask was purged with argon and dry DCM (300 mL, 0.4 M) was added. Acetic anhydride (12.5 mL, 132.2 mmol, 1.2 eq) was added and the reaction was stirred at room temperature and monitored by TLC. Upon completion (generally a couple of hours, but as short as 20 minutes) the reaction mixture was washed with a saturated solution of sodium carbonate, the organic layers dried with MgSO₄ and the solvent removed under reduced pressure. The product was obtained in quantitative yield (14.8 g). In most cases analytically pure acetanilides can be obtained after extraction however if necessary purification by flash chromatography with ethyl acetate/pet. ether was used (see below for specific conditions). **Acetanilide (1a):** The above procedure was followed to afford the product in quantitative yield. This compound can also be purchased from commercial sources (CAS: 103-84-4). ¹H NMR (400 MHz, CDCl₃, 293 K): δ 7.50 (d, J = 7.8 Hz, 2H), 7.32 (t, J = 7.9 Hz, 2H), 7.10 (t, J = 7.4 Hz, 1H), 2.17 (s, 3H). The signal for the exchangeable NH does not appear in the spectrum.

SciFinder囊括最大的反应实验过程合集

2 Steps Hover over any structure for more options.



Experimental Procedure: 我们可以做得更好

- 更好的阅读体验?
- 这些数字代表什么?
- 去免费的Supporting Information查? 可能只有图谱。

Overview

Steps/Stages

- 1.1 C: Pd(PPh₃)₄; S: BuNH₂; 21 h, 100°C
- 2.1 R: DMSO; R: Cl(O=)CC(=O)Cl; S: CH₂Cl₂; 15 min, -78°C
- 2.2 S: CH₂Cl₂; -78°C; 2 h, -78°C
- 2.3 R: Et₃N; 30 min, -78°C; -78°C → rt

Notes

- 1) key step, alternate catalyst concentration, catalyst (CuI) and temperature, Sonogashira coupling, 2) key intermediate, Swern oxidation, scale method shown, Reactants: 2, Reagents: 5, Catalysts: 1, Solvents: 2, Stages: 4

Experimental Procedure

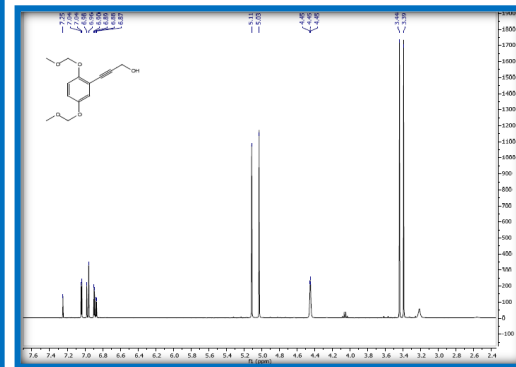
NATURAL PRODUCTS

Step 1

General Procedure for the Sonogashira Coupling.^{8,10,11} Compounds **6a**³¹ and **16**⁸ were synthesized according to literature procedures. Aryl halide **6a** or **16** (9.21 mmol) in n-butylamine (6.4 mL) was placed in a flame-dried round-bottomed flask under an argon atmosphere. A mixture of terminal alkynes **7**, **25**, **26**, or **27** (9.21 mmol) in n-butylamine (10 mL) and Pd(Ph₃)₄ (5% or 3%) was added, with the optional addition of CuI (3%) where appropriate. The mixture was heated for 21 h at 98 °C and poured into H₂O (80 mL). The product was extracted with EtOAc (3 × 80 mL). The combined organic layers were washed with brine, dried over anhydrous Na₂SO₄, and evaporated under reduced pressure. The crude product was purified by silica gel column chromatography (EtOAc/hexanes, 10-50%). 3-[2,5-Bis(methoxymethoxy)phenyl]prop-2-yn-1-ol² (**8**). Yield 96%; colorless oil. IR (KBr) ν_{max} 3310, 2230 cm⁻¹; ¹H NMR (CDCl₃, 400 MHz) δ 3.46 (3H, s, H-4b), 3.51 (3H, s, H-1b), 4.51 (2H, s, H-1a), 5.09 (2H, s, H-4a), 5.17 (2H, s, H-1a), 6.95 (1H, dd, *J* = 9 and 3.0 Hz, H-5), 7.03 (1H, d, *J* = 9.0 Hz, H-6), 7.10 (1H, d, *J* = 3.0 Hz, H-3); ¹³C NMR (CDCl₃, 100 MHz) δ 51.81 (C-9), 56.05 (C-4b), 56.38 (C-1b), 81.74 (C-7), 91.56 (C-8), 95.14 (C-4a), 95.88 (C-4b), 114.19 (C-2), 117.13 (C-5), 118.50 (C-3), 121.20 (C-6), 151.95 (C-4), 153.06 (C-1); HRESIMS *m/z* 275.0900 [M + Na]⁺ (calcd for C₁₃H₁₆O₅ 275.0896).

Step 2

Generation of the Key Aldehyde.¹⁷ Oxalyl chloride (272.3 μ L, 3.12 mmol) in dry CH₂Cl₂ (9 mL) was added to a stirred solution of DMSO (332 μ L, 4.68 mmol) in dry CH₂Cl₂ (1.5 mL) under an argon atmosphere at -78 °C. The mixture was stirred for 15 min, and the alcohol **8** (393.5 mg, 1.56 mmol) or alcohol **17** (300 mg, 1.56 mmol) in dry CH₂Cl₂ (12 mL) was added dropwise (Note: Swern oxidation could be scaled-up to 1.56 mmol of starting material). After the starting material had been consumed (nearly 2 h), Et₃N (1.88 mL, 7.8 mmol) was added. The reaction mixture was stirred at -78 °C for a further 30 min and was allowed to warm to rt and quenched with saturated NH₄Cl and H₂O, and the mixture was stirred for 30 min. The organic phase was decanted off, and the aqueous layer was extracted with CH₂Cl₂ (3 × 30 mL). The combined organic layers were washed with brine, dried over anhydrous Na₂SO₄, and evaporated under reduced pressure. 3-[2,5-Bis(methoxymethoxy)phenyl]prop-2-ynal (**9**). Yield 91%; colorless oil. IR (KBr) ν_{max} 1660, 2194 cm⁻¹; ¹H NMR (CDCl₃, 400 MHz) δ 3.46 (3H, s, H-4b), 3.51 (3H, s, H-1b), 5.10 (2H, s, H-4a), 5.21 (2H, s, H-1a), 7.09 (1H, dd, *J* = 9.2 and 1.2 Hz, H-6), 7.12 (1H, dd, *J* = 9.1 and 2.2 Hz, H-5), 7.22 (1H, dd, *J* = 2.2 and 1.3 Hz, H-3), 9.44 (1H, s, H-9); ¹³C NMR (CDCl₃, 100 MHz) δ 56.18 (C-4b), 56.54 (C-1b), 92.05 (C-8), 92.27 (C-7), 95.22 (C-4a), 95.58 (C-1a), 110.70 (C-2), 116.72 (C-6), 122.0 (C-5), 122.09 (C-3), 151.85 (C-4), 154.88 (C-1), 176.92 (C-9); HRESIMS *m/z* 273.0741 [M + Na]⁺ (calcd for C₁₃H₁₄O₅ 273.0739).



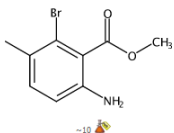
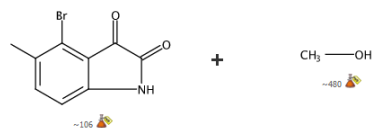
MethodsNow Synthesis

MethodsNow

A New Method for Synthesis of Nolatrexed Dihydrochloride

By Zhao, Xueqing; Li, Fei; Zhuang, Weiping; Xue, Xiaowen; Lian, Yuanyang; Fan, Jianhui; Fang, Dongsheng
 From Organic Process Research & Development, 14(2), 346-350; 2010
 Published by American Chemical Society

Reaction Steps 1 2 3



Products	Benzoic acid, 6-amino-2-bromo-3-methyl-, methyl ester, 84%, CAS RN: 147149-88-0
Reactants	1 <i>H</i> -Indole-2,3-dione, 4-bromo-5-methyl-, CAS RN: 147149-84-6 Methanol, CAS RN: 67-56-1
Reagents	Potassium persulfate, CAS RN: 7727-21-1 Sodium methoxide, CAS RN: 124-41-4 Hydrochloric acid, CAS RN: 7647-01-0 Sodium dithionite, CAS RN: 7775-14-6
Solvents	Methanol, CAS RN: 67-56-1 Water, CAS RN: 7732-18-5
Procedure	<ol style="list-style-type: none"> 1. Add sodium methoxide (22.6%, 4.80 kg, 20.1 mol) to a mixture of 4-bromo-5-methylisatin (6.67 mol) and anhydrous methanol (6.70 L). 2. Add K₂S₂O₈ (1.90 kg, 7.03 mol) to the mixture in parts 10°C with an ice-water bath. 3. After addition the reactant mixture turns yellow, continue the stirring for 1 hour at room temperature. 4. Adjust the reaction mixture to pH 8-9 with aqueous 36% HCl (1.24 L) 15 °C. 5. Destroy the excessive K₂S₂O₈ by aqueous 5% Na₂S₂O₄ solution (450 mL). 6. After rotary evaporation under a reduced pressure at 55 °C, Leave a brown liquid. 7. Mix the mixture with CH₂Cl₂ (6 L) and H₂O (4 L). 8. Separate the organic phase. 9. Extract the aqueous phase with CH₂Cl₂ (4 L). 10. Dry the combined organic phases over Na₂SO₄. 11. Concentrate the combined organic phases with a rotavapor. 12. Distill the resulted brown liquid under high vacuum.
Scale	milligram
¹H NMR	CDCl ₃ : δ 2.28 (s, 3 H, Ar-CH ₃), 3.91 (s, 3 H, -OCH ₃), 4.26 (br s, 2 H, NH ₂), 6.54 (d, <i>J</i> = 8.2 Hz, 1 H, Ar-H), 7.00 (d, <i>J</i> = 8.2 Hz, 1 H, Ar-H).
IR	KBr cm ⁻¹ : 16472, 3382, 2953, 2924, 1716, 1622, 1480, 1277, 816.

物质信息

实验过程

图谱信息

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 image shows a screenshot of a chemical software interface. On the left is the "Structure Editor" window, which contains a toolbar with various drawing tools and a central workspace displaying a chemical structure of a benzimidazole derivative. The structure has a benzene ring fused to a five-membered imidazole ring. One of the imidazole ring's nitrogen atoms is labeled "N", and the carbon atom at the 2-position is labeled "R1". A purple arrow points from the "R1" label in the structure to the "S" atom in the periodic table shown in the "R-group Definitions" dialog on the right.

The "R-group Definitions" dialog is open, showing a list of R-groups (R1 to R10) at the top. Below this, there is a text input field for "R1 =" containing "O, S". The main part of the dialog is a periodic table of elements. The "S" atom (Sulfur) is highlighted with a purple border. Below the periodic table are sections for "Variables" and "Shortcuts". At the bottom of the dialog are "Close" and "Cancel" buttons.

At the bottom of the Structure Editor window, there is a status bar that says "Formula is not available".

亚结构反应检索

The screenshot displays the SCIFINDER Structure Editor interface. The main workspace shows a chemical reaction where a reactant (a benzimidazole-like structure with an R1 group and a hydrogen atom) is converted into 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

- 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 (MethodsNow Synthesis)
 - 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** [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

SciPlanner 11_19_2015_112612

Workspace Edit View GoTo

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
- Export as molfile

打开中间产物的标准菜单
选择Synthesis this

1 2 3

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

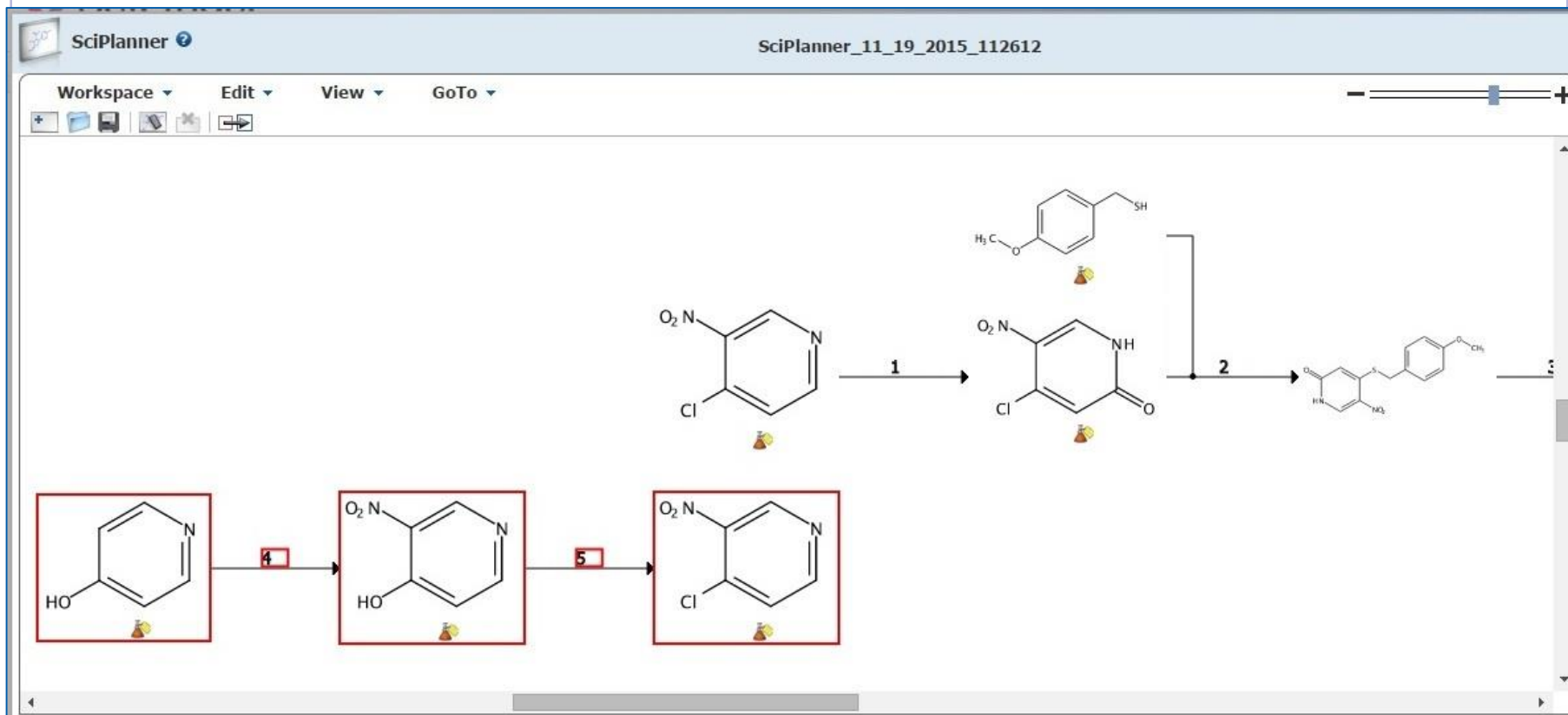
2 Steps Hover over any structure for more options.

在检索到的反应中选择感兴趣的反应

继续推送到SciPlanner

~161 ~192

SciPlanner使用简介

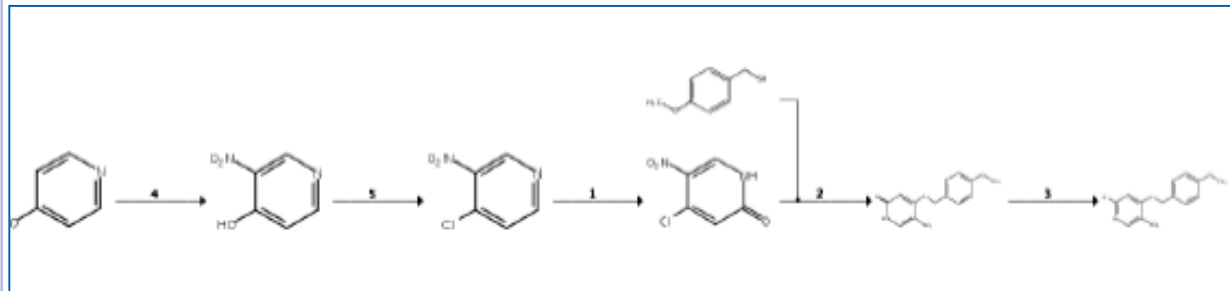


步骤同前，将推送过来的反应拖到编辑面板中，可以看到两条反应中存在同样的结构

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 dropdown menu is open under "Workspace", listing options: "New", "Open", "Save", "Duplicate", "Import", "Export", "Print", and "Close". The "Export" option is highlighted in blue. In the main workspace, a chemical reaction sequence is shown: a starting material (a pyridine ring with a nitro group and a hydroxyl group) reacts (step 4) to form a product (a pyridine ring with a nitro group and a chlorine atom). This product then reacts (step 5) to form another intermediate (a pyridine ring with a nitro group and a chlorine atom). Finally, this intermediate reacts (step 1) to form the final product (a pyridine ring with a nitro group and a chlorine atom, and a side chain with a thiol group). 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 reaction step 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, 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:" (empty). The "Include:" section has checkboxes for "SciPlanner Image", "Reaction Details", "Substance Details", and "Reference Details", all of which are checked. "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>C₁₃H₁₂N₂O₄S 2-(1H)-Pyridinone, 4-[[4-methoxyphenyl)methyl]thio]-5-nitro-</p> <p>Related Info: ~ 2 References Reactions</p>	<p>1228150-23-9</p> <p>C₁₃H₁₁ClN₂O₃S Pyridine, 2-chloro-4-[[4-methoxyphenyl)methyl]thio]-5-nitro-</p> <p>Related Info: ~ 2 References Reactions</p>	<p>13091-23-1</p> <p>C₆H₃ClN₂O₂ Pyridine, 4-chloro-3-nitro-</p> <p>Related Info: ~ 301 References Reactions ~ 100 Commercial Sources Regulatory Information</p>
<p>5435-54-1</p> <p>C₆H₄N₂O₃ 4-Pyridinol, 3-nitro-</p> <p>Related Info: ~ 113 References Reactions ~ 197 Commercial Sources Regulatory Information</p>	<p>6258-60-2</p> <p>C₈H₁₀O S Benzenemethanethiol, 4-methoxy-</p> <p>Related Info: ~ 749 References Reactions ~ 71 Commercial Sources Regulatory Information</p>	<p>626-64-2</p> <p>C₆H₇N O 4-Pyridinol</p> <p>Related Info: ~ 1351 References Reactions ~ 160 Commercial Sources Regulatory Information</p>
<p>850663-54-6</p> <p>C₆H₃ClN₂O₃ 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
- SciFinder简介及检索方式
 - 文献检索
 - 物质检索
 - Markush检索
 - 反应检索
 - SciPlanner
- SciFinder常见问题及解决

SciFinder浏览器选择建议

- Windows 7以上用户建议升级IE到10以上
- 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

SciFinder Academic (美国化学文摘网络版) 数据库

发布部门: 发布时间: 2014-09-11 浏览次数: 6657

SciFinder Academic (美国化学文摘网络版) 数据库

【数据库介绍】

SciFinder是美国化学学会 (ACS) 旗下的化学文摘服务社CAS (ChemicalAbstractService) 所出版的化学资料电子数据库。它是全世界最大、最全面的化学和科学信息数据库。SciFinder数据库整合了Medline医学数据库、全球180多个国家和地区的50多种语言的1万多份期刊、63家专利机构的专利、评论、会议录、论文、技术报告和图书中的各种化学研究成果。内容不仅涵盖了CA从1907至今的所有内容,更整合了其他5个数据库(包括生物医学,物质,反应数据库),能通过主题、分子式、结构式和反应式等多种方式进行检索。SciFinder报道的内容几乎涉及了化学家感兴趣的所有领域,其中除包括无机化学、有机化学、分析化学、物理化学、高分子化学外,还包括冶金学、地球化学、药理学、毒理学、环境化学、生物学以及物理学等诸多学科领域。

【访问方式】

使用SciFinder是以互联网的用户形式注册,允许每个用户在学校IP地址内范围内注册SciFinder 用户名和密码:

注册地址:

<https://scifinder.cas.org/registration/index.html?corpKey=43B73C05X86F35055X117ACB67551FF9932F>

如果以上网址无法注册,将自己的单位名称、职位(老师、学生)、邮箱、电话信息发送到邮箱: cas@cas.org 或者直接联系客服人员: 408-853-8888-888



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 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)

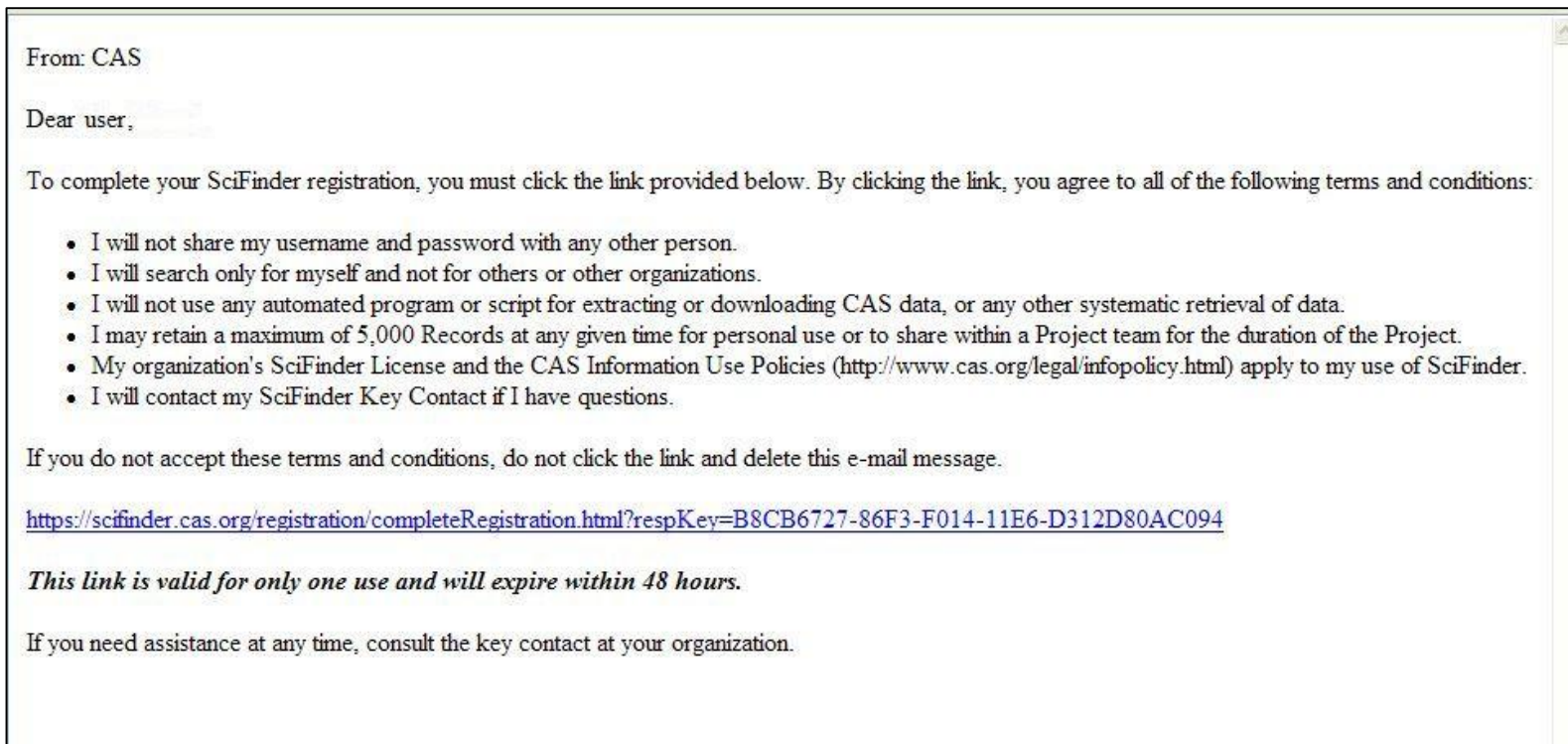
3. 密码必须包含 7-15 个字符，并且至少**包含三种以下字符**：

- 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

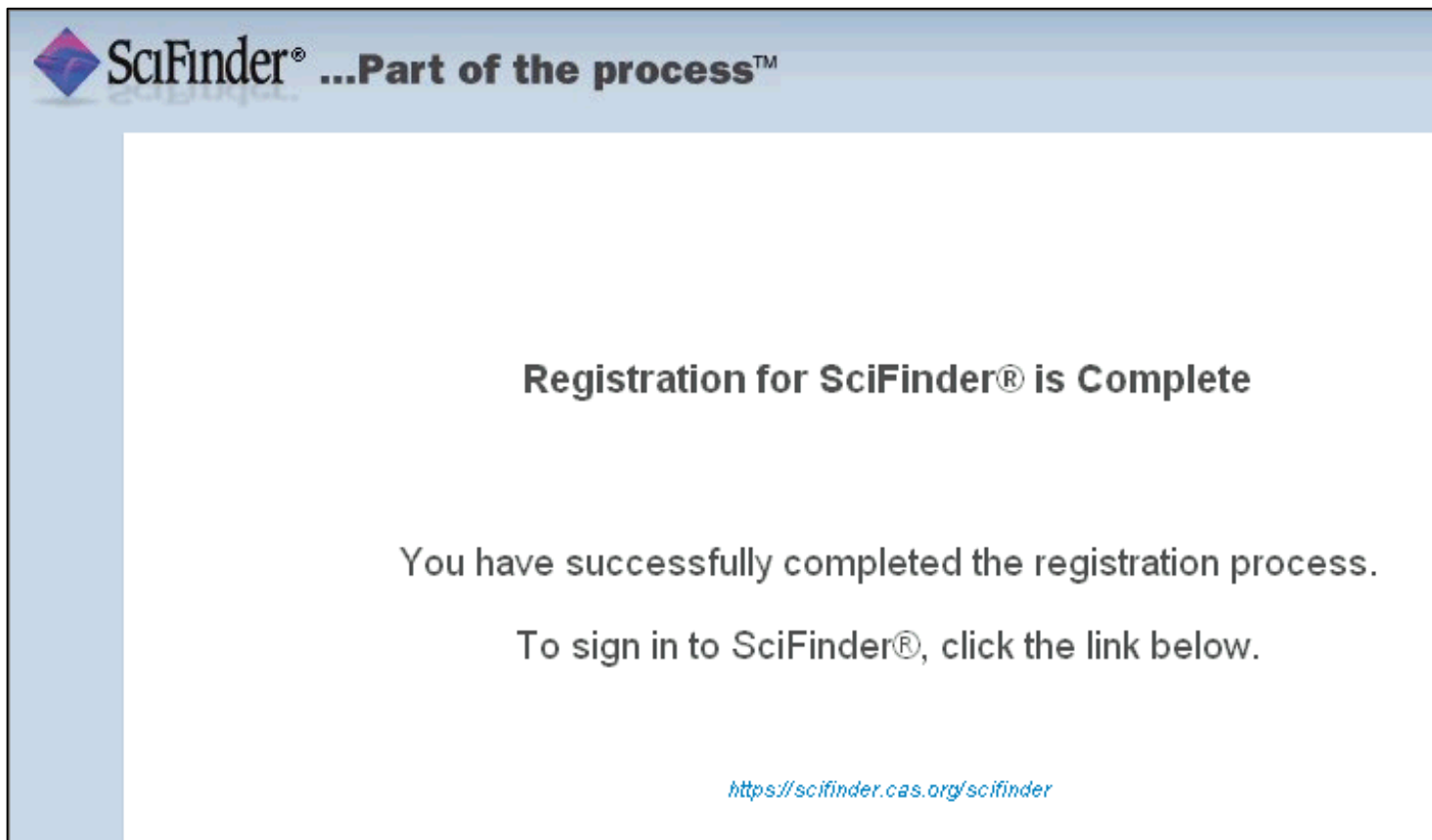


打开并阅读 CAS 的电子邮件（必须在48小时内点击，否则需要重新注册）

注意垃圾邮件、未知邮件、订阅邮件等来自@cas.org的邮件



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

- 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

www.cas-china.org

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