

匡金海

客户顾问

jkuang@acsi.info

如何使用SciFinder获取科技信息

天津师范大学

2016.11.17



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

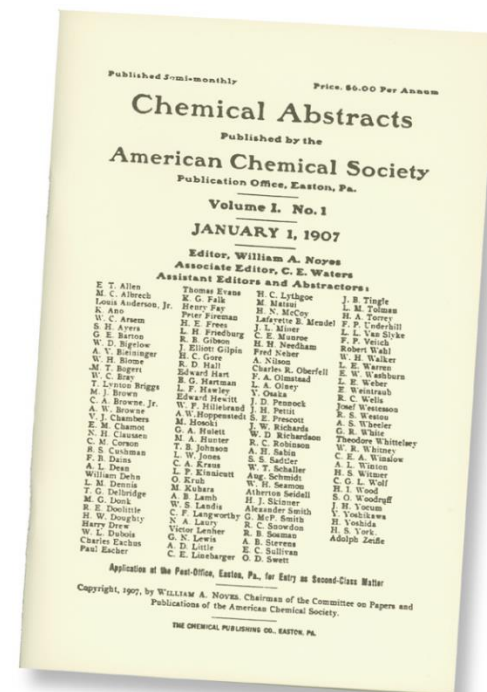


1907年，信息的汇集、管理发生了重大的变化



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



SciFinder®
A CAS SOLUTION

CAS——构建最高质量的化学数据库



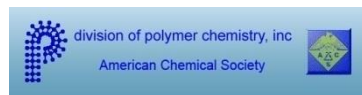
arXiv.org

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[®]
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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

12. Nucleoside Inhibitors of Hepatitis C Virus NS5B Polymerase: A Systematic Review

By: Xie, Yuanchao; Ogah, Comfort Aicha; Jiang, Xiangrui; Li, Jianfeng; Shen, Jingshan

A review. Nowadays, a large no. of people in the world are suffering from chronic Hepatitis C. HCV NS5B polymerase conserved across the identified 7 HCV genotypes is considered to be the most promising target in combating HCV. During the past decade, significant progress has been made in the discovery of novel nucleoside HCV NS5B polymerase inhibitors. A potent anti-HCV drug, sofosbuvir with high cure rates has been approved. Besides, quite a few nucleoside anti-HCV agents are being evaluated in clin. trials. The purpose of this review is to present recent progress in the development of nucleoside HCV NS5B polymerase inhibitors, focusing on lead compds. that hold great promise for medicinal use and their structure-activity relationships (SARs) in order to provide guidance for future drug design and discovery.

Indexing

Pharmacology (Section1-0)


Concepts

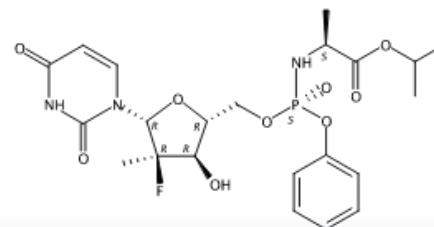
Drug design
Genotypes
Homo sapiens
Structure-activity relationship


Drug discovery
Hepatitis C virus
Human

development of novel nucleoside hepatitis C virus NS5B polymerase inhibitors for medicinal use and their structure-activity relationships for guidance future drug design and discovery for treating disease in human

Substances

1190307-88-0 Sofosbuvir 
Absolute stereochemistry.



1430213-40-3 NS5B polymerase 

development of novel nucleoside hepatitis C virus NS5B polymerase inhibitors for medicinal use and their structure-activity relationships for guidance future drug design and discovery for treating disease in human

Biological study, unclassified; Biological study

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。

CAS最新动向—解决方案

PatentPak™

 **NCI™ Global**
A Solution Powered by CAS

 **METHODSNow™**
A CAS SOLUTION

 **CHEMZENT™**
A CAS SOLUTION

 **SCIFINDER®**
A CAS SOLUTION

CAS最新动向—解决方案

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

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

Quick View PATENTPAK

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

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

Patent No.	Kind	Language
WO 2016100441	A1	English

Patent Family

Patent No.	Kind	Language
US 20160176911	A1	English

atkina, Natalia
language: English, Database: CAPLUS

B is substituted purine and pyrimidine nucleobase; dashed bond between R and R' 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'-methylduridine wit

ZOOM

DOWNLOAD PDF

8. Q...

By Fro...

(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

(10) International Patent Classification:

(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)

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

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

(25) Filing Language:
English

(81) Designated States (kind of national protection available): AO, AT, AU, AZ, BZ, CA, CH, CL, CN, DO, DZ, EC, EE, EG, HN, HR, HU, ID, IL, KZ, LA, LC, LK, LR, MK, MN, MW, MX, PA, PE, PG, PH, PL, SD, SE, SG, SK, SL, SM, ST, SV, SY, TH, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW.

(84) Designated States (unless otherwise indicated, for every kind of regional protection available): ARIPO (BW, GH, GM, KE, LU, MG, MW, MZ, NA, NG, SD, SI, SZ, TZ, UG, ZM, ZW), EPO (AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LT, LU, LV, 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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CAS RN 1206126-39-7

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Analyst Markup Locations (1)
page 130

CAS RN 1206126-41-1

Search in SciFinder | View Detail

Analyst Markup Locations (1)
page 130

WO 2016/100441

PCT/US2015/065981

EXAMPLE 1
COMPOUND 1

Route 2

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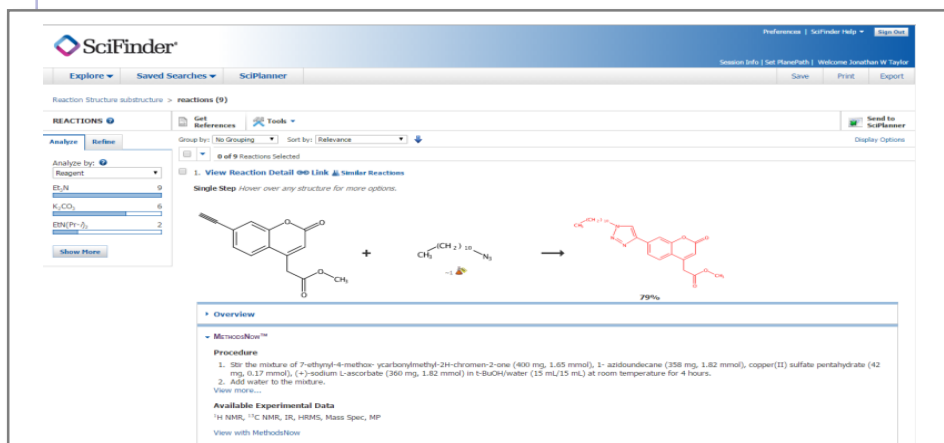
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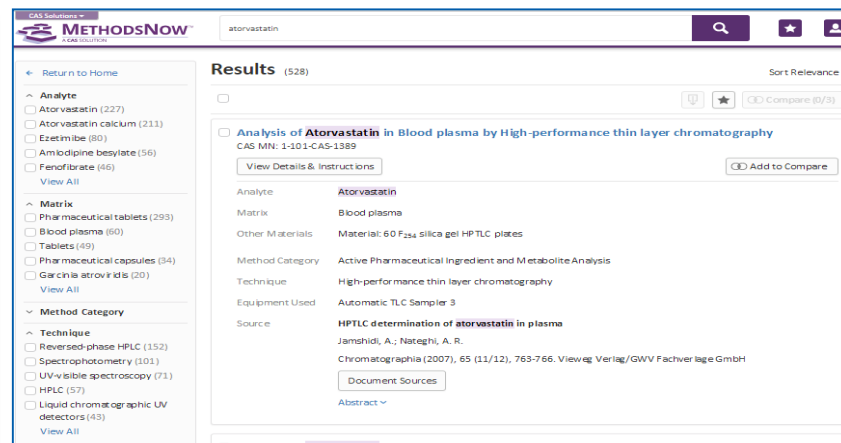
1-4zz

CAS最新动向—解决方案

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



嵌在SciFinder中的合成模块



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

CAS——构建最高质量的化学数据库



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

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Examples:
The effect of antibiotic residues on dairy products
Photocyanation of aromatic compounds

Search

Advanced Search

REFERENCES

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

SUBSTANCES

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

REACTIONS

- Reaction Structure

SAVED ANSWER SETS

- CSF1R
- jmc
- EP 19870107847
- Daclatasvir-1
- SUB result
- EX result
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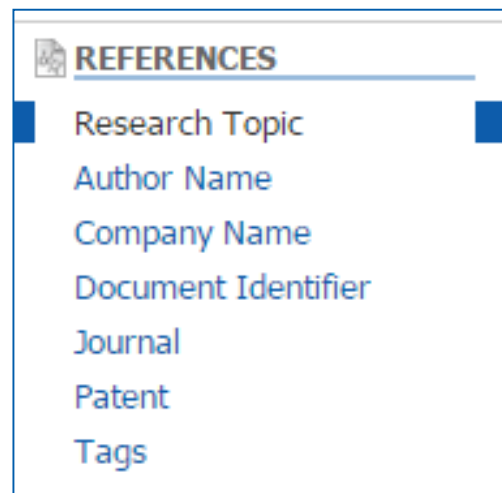
SciFinder检索——文献检索

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文献检索——主题

主题检索：三维石墨烯的制备

检索式：prepare of 3D graphene

The screenshot displays the SciFinder web interface. At the top, the 'CAS Solutions' logo and 'SciFinder A CAS SOLUTION' are visible. Below the navigation bar (Explore, Saved Searches, SciPlanner), the breadcrumb trail reads: 'Research Topic "prepare of 3D graphene" > references (767) > Facile Synthesis of 3D Graphen...'. On the left sidebar, under the 'REFERENCES' section, a list of search criteria is shown: Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, Tags, and SUBSTANCES (with sub-options: Chemical Structure, Markush). The main search area is titled 'REFERENCES: RESEARCH TOPIC'. It contains a search input field with the text 'prepare of 3D graphene', a 'Search' button, and a section for 'Examples' listing 'The effect of antibiotic residues on dairy products' and 'Photocyanation of aromatic compounds'. Below the search area is a link for 'Advanced Search'.

关键词之间用介词连接：in, with, of...

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Research Topic "prepare of 3D graphene"

REFERENCES ?

Select All Deselect All

1 of 8 Research Topic Candidates Selected

	References
<input type="checkbox"/> 1 reference was found containing "prepare of 3D graphene" as entered.	1
<input checked="" type="checkbox"/> 910 references were found containing the two concepts "prepare" and "3D graphene" closely associated with one another.	910
<input type="checkbox"/> 1603 references were found where the two concepts "prepare" and "3D graphene" were present anywhere in the reference.	1603
<input type="checkbox"/> 58400 references were found containing the concept "prepare", and either the concept "3D" or the concept "graphene". The concepts found were closely associated with one another.	58400
<input type="checkbox"/> 102301 references were found containing the concept "prepare", and either the concept "3D" or the concept "graphene". The concepts found were present anywhere (perhaps widely separated) within the reference.	102301
<input type="checkbox"/> 11876585 references were found containing the concept "prepare".	11876585
<input type="checkbox"/> 2881 references were found containing the concept "3D graphene".	2881
<input type="checkbox"/> 421680 references were found containing either the concept "3D" or the concept "graphene".	421680

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“Concepts”表示对主题词做了同义词的扩展；

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

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

按被引次数排序— Citing References

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Research Topic "prepare of 3D graphene" > references (767)

REFERENCES ?

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Analyze | Refine | Categorize

Sort by: Citing References

Analyze by: Author Name

Wei Wei 13

Huang Wei 11

Hu Yun Hang 10

Ma Jie 10

Yu Fei 10

Dong Xiaochen 9

Chen Peng 8

Zhang Hua 8

Qu Liangti 7

Shi Gaoquan 7

1. **Cobalt Oxide Electrode for High-Performance Supercapacitor and Enzymeless Glucose Detection**

By Dong, Xiao-Chen; Xu, Hang; Wang, Xue-Wan; Huang, Yin-Xi; Chan-Park, Mary B.; Zhang, Hua; Wang, Lian-Hui; Huang, Wei; Chen, Peng
From ACS Nano (2012), 6(4), 3206-3213. | Language: English, Database: CAPLUS

Using a simple hydrothermal procedure, cobalt oxide (Co₃O₄) nanowires were in situ **synthesized** on three-dimensional (3D) **graphene** foam grown by chem. vapor deposition. The structure and morphol. of the resulting **3D graphene**/Co₃O₄ composites were characterized by SEM, TEM, x-ray diffraction, and Raman spectroscopy. The **3D graphene**/Co₃O₄ composite was used as the monolithic free-standing electrode for supercapacitor application and for enzymeless electrochem. detection of glucose. The authors demonstrate that it is capable of delivering high specific capacitance of ~1100 F g⁻¹ at a c.d. of 10...

2. **A Three-Dimensional Carbon Nanotube/Graphene Sandwich and Its Application as Electrode in Supercapacitors**

By Fan, Zhuangjun; Yan, Jun; Zhi, Linjie; Zhang, Qiang; Wei, Tong; Feng, Jing; Zhang, Milin; Qian, Weizhong; Wei, Fei
From Advanced Materials (Weinheim, Germany) (2010), 22(33), 3723-3728. | Language: English, Database: CAPLUS

A **3D CNT/graphene** sandwich structures with CNT pillars grown in between the **graphene** layers had been **prepd.** by CVD. The unique structure endows the high rate transportation of electrolyte ions and electrons throughout the electrode matrix and comprehensive utilization of pseudo and double-layer capacitance, resulting in excellent electrochem. performances. The supercapacitor based on CGS exhibits 1'00 a specific capacitance of 385 F g⁻¹ at 10 mV s⁻¹ in 6 M KOH 1600 2000 soln. After 2000 cycles, a capacitance increase of ca. 20 % of the initial capacitance is obsd., indicating excellent elec...

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Analyze Refine Categorize

Sort by: Accession Number

0 of 767 References Selected

Analyze by: Author Name

Wei Wei	13
Huang Wei	11
Hu Yun Hang	10
Ma Jie	10
Yu Fei	10
Dong Xiaochen	9
Chen Peng	8
Zhang Hua	8
Qu Liangti	7
Shi Gaoquan	7

1. Edge-rich and (N, S)-doped 3D porous graphene as efficient metal-free electrocatalyst for ORR

Quick View Other Sources

By Wu, Xiaobo; Xie, Zhiyong; sun, min; lei, tin; zuo, zhenming; Xie, Xiangmin; li, liangyi; Huang, Qizhong
From RSC Advances (2016), Ahead of Print. | Language: English, Database: CAPLUS

A novel edge-rich and (N, S)-doped 3D porous graphene was synthesized by Chem. Vapor Deposition (CVD) and chem. corrosion. The hybrid material as a metal-free electrocatalyst exhibited a four-electron pathway, stronger alk. tolerance and excellent catalytic activity for oxygen redn. reaction due to the edge effect and heteroatom synergistic effect.

2. Facile Synthesis of 3D Graphene Flowers for Ultrasensitive and Highly Reversible Gas Sensing

Quick View Other Sources

By Wu, Jin; Feng, Shuanglong; Wei, Xingzhan; Shen, Jun; Lu, Wenqiang; Shi, Haoqi; Tao, Kai; Lu, Shirong; Sun, Tai; Yu, Leyong; et al
From Advanced Functional Materials (2016), Ahead of Print. | Language: English, Database: CAPLUS

Fabrication of nanostructured graphene (Gr) for gas sensing applications has become increasingly attractive. For the first time, 3D graphene flowers (GF) cluster patterns are grown directly on an Ni foam substrate by inexpensive homebuilt microwave plasma-enhanced chem. vapor deposition (MPCVD) using the gas mixt. H₂/C₂H₄O₂@Ar as a precursor. The interim morphologies of the synthesized GF are investigated and the growth mechanism of the GF film is proposed. The GF are decompd. to few-layer Gr sheets by ultrasonication in ethanol. For the first time, MPCVD-synthesized Gr is exploited to fab...

3. N-P-O co-doped high performance 3D graphene prepared through red phosphorous-assisted "cutting-thin" technique: A universal synthesis and multifunctional applications

Quick View Other Sources

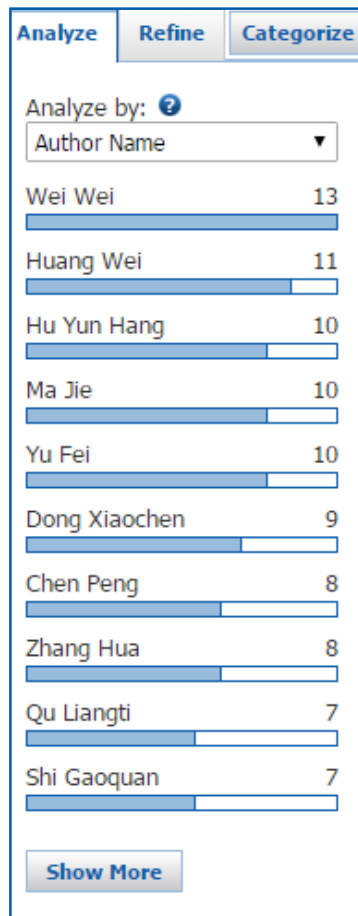
By Zhao, Yufeng; Huang, Shifei; Xia, Meirong; Rehman, Sarish; Mu, Shichun; Kou, Zongkui; Zhang, Zhi; Chen, Zhaoyang; Gao, Faming; Hou, Yanglong
From Nano Energy (2016), 28, 346-355. | Language: English, Database: CAPLUS

Large scale prodn. of three dimensional (3D) graphene materials with high d. and low degree of defects stands for the main challenge hindering their practical applications.

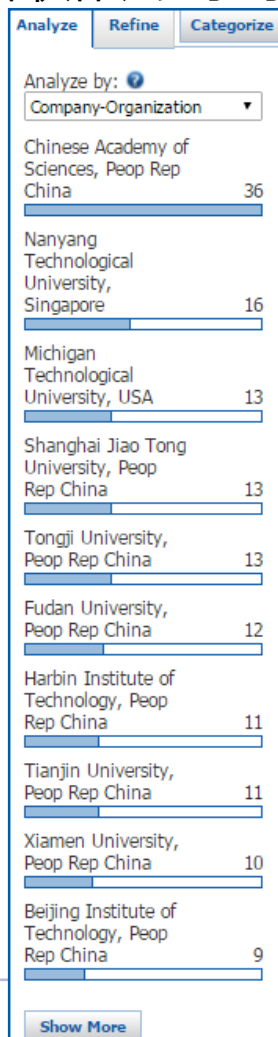
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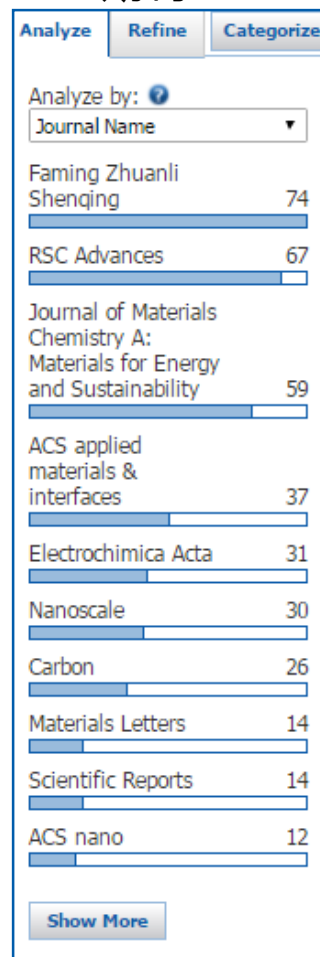
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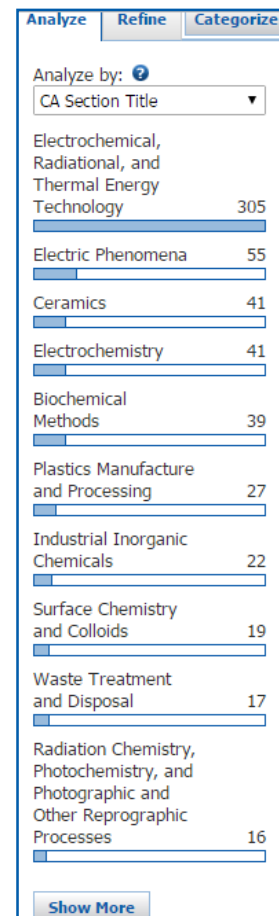
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涉及学科领域

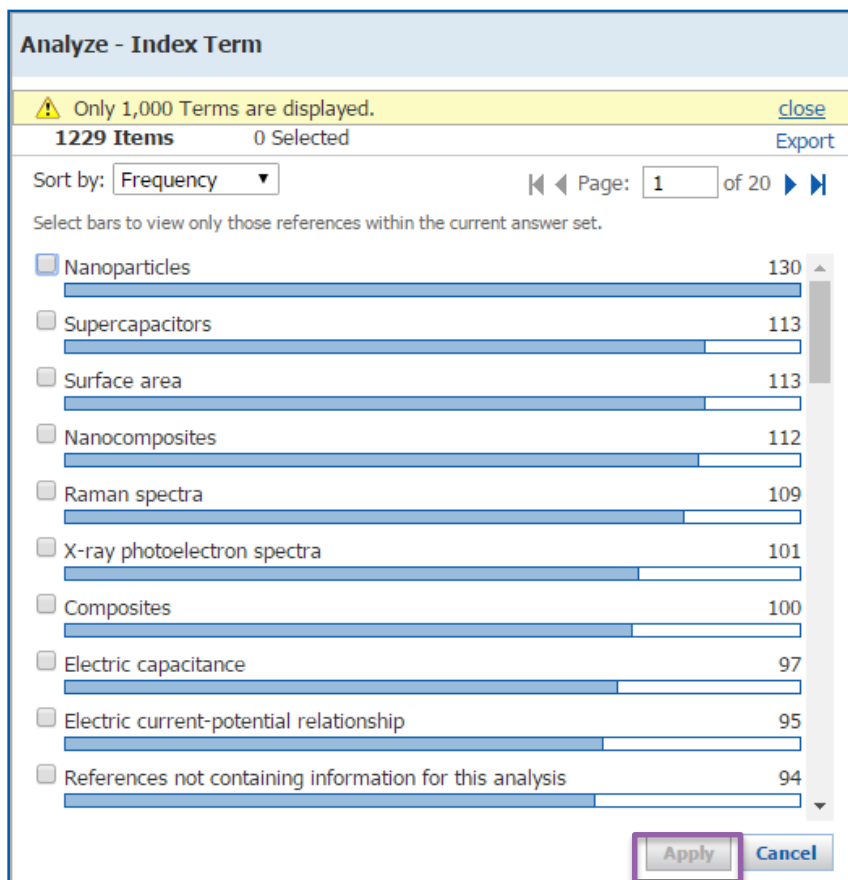
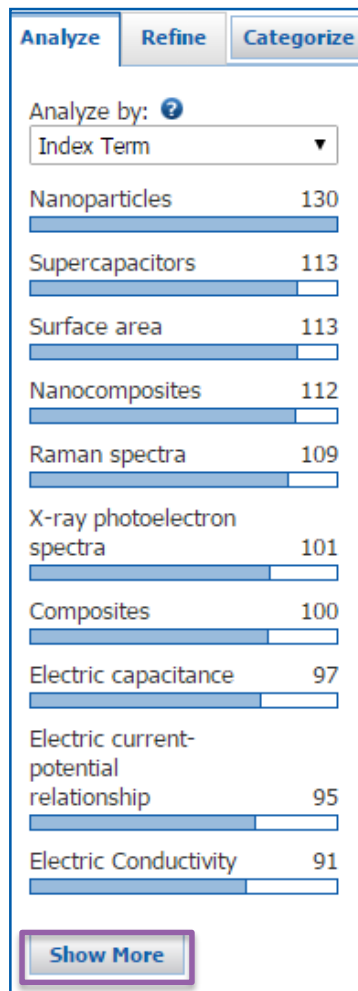


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Company Name
china

Examples:
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Refine

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1. N-P-O co-doped high performance 3D graphene prepared through red phosphorous-assisted "cutting-thin" technique: A universal synthesis and multifunctional applications
Quick ViewOther Sources
By Zhao, Yufeng; Huang, Shifei; Xia, Meirong; Rehman, Sarish; Mu, Shichun; Kou, Zongkui; Zhang, Zhi; Chen, Zhaoyang; Gao, Faming; Hou, Yanglong
From Nano Energy (2016), 28, 346-355. | Language: English, Database: CAPLUS
Large scale prodn. of three dimensional (3D) graphene materials with high d. and low degree of defects stands for the main challenge hindering their practical applications. Herein, we report a universal and readily scalable strategy to produce an N-P-O co-doped free standing 3D graphene through a one-pot red phosphorus-assisted "cutting-thin" technique. The solid carbon precursor is gradually exfoliated through the slowly released gases (e.g. PH_3 , H_2 , CO_2) and metallic K during the reaction, which allows the formation of dominant amt. nanopores, and ensures the high d. of the products. The ...

2. Rational construction of graphene oxide with MOF-derived porous NiFe@C nanocubes for high-performance microwave attenuation
Quick ViewOther Sources
By Yang, Zhihong; Lv, Hualiang; Wu, Renbing
From Nano Research (2016), Ahead of Print. | Language: English, Database: CAPLUS
Exploring lightwt. microwave attenuation materials with strong and tunable wideband microwave absorption is highly desirable but remains a significant challenge. Herein, three-dimensional (3D) porous hybrid composites consisting of NiFe nanoparticles embedded within carbon nanocubes decorated on graphene oxide (GO) sheets (NiFe@C nanocubes@GO) as high-performance microwave attenuation materials have been rationally synthesized. The 3D porous hybrid composites are fabricated by a simple method, which involves one-step pyrolysis of NiFe Prussian blue analog nanocubes in the presence of GO shee...

3. Facile self-assembly N-doped graphene quantum dots/graphene for oxygen reduction reaction
Quick ViewOther Sources
By Fan, Mengmeng; Zhu, Chunlin; Yang, Jiazhi; Sun, Dongping
From Electrochimica Acta (2016), 216, 102-109. | Language: English, Database: CAPLUS
Nitrogen doping carbon nanomaterial has become an important metal-free electrocatalyst for oxygen redn. reaction (ORR) in fue cells. N-doped graphene quantum dots (N-GQDs) are one of the most promising nanomaterials due to abundant electrocatalytic edging and N doping active sites, but low yield, high dispersity and no forming efficient percolative conductive network hinder their direct application as the electrocatalyst. Hydrothermal method is an effective route for prepg. high-quality N-GQDs and meanwhile, overcomes the drawbacks of complicated prepg. progress and low yield. We further hy...

4. High performance agar/graphene oxide composite aerogel for methylene blue removal
Quick ViewOther Sources
By Chen, Long; Li, Yanhui; Du, Qiuju; Wang, Zonghua; Xia, Yanzhi; Yedinak, Emily; Lou, Jun; Ci, Lijie
From Carbohydrate Polymers (2017), 155, 345-353. | Language: English, Database: CAPLUS

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文献检索结果的Categorize

学科领域
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学科领域
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Index Term

选中的Index Term

Categorize ?

1. Select a heading and category.

Category Heading	Category
All	Substances in technology (716)
Technology	Materials & products (203)
General chemistry	Processes & apparatus (202)
Physical chemistry	Metallurgy (52)
Synthetic chemistry	Power & fuel topics (25)
Polymer chemistry	Formed, removed, & other substances (106)
Catalysis	Construction (11)
Biotechnology	Imaging & recording (12)
Analytical chemistry	Ceramics (8)
Environmental chemistry	
Genetics & protein chemistry	
Biology	

2. Select index terms of interest.

Index Terms	
Page: 1 of 3	
Select All Deselect All	
<input type="checkbox"/> Graphene	427
<input type="checkbox"/> Nanocomposites	86
<input type="checkbox"/> Composites	85
<input type="checkbox"/> Graphite	83
<input type="checkbox"/> Platinum	31
<input type="checkbox"/> Hydrogen	26
<input type="checkbox"/> Carbon black	21
<input type="checkbox"/> Oxygen	20
<input checked="" type="checkbox"/> Nanostructured materials	19
<input type="checkbox"/> Porous materials	16
<input type="checkbox"/> Adsorbents	13
<input type="checkbox"/> Solar cells	12
<input type="checkbox"/> Nanowires	11
<input type="checkbox"/> Sulfur	11
<input type="checkbox"/> Argon	10

Selected Terms

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

- Technology > Materials & products (1 Terms)

Technology > Materials & products > 1 Index Term(s) Selected

OK Cancel

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aphene" > references (767) > refine "china" (534) > refine by categories

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0 of 19 References Selected

1. A green and simple strategy to prepare graphene foam-like three-dimensional porous carbon/Ni nanoparticles for glucose sensing

Quick View Other Sources

By Wang, Li; Zhang, Yayun; Yu, Jie; He, Juan; Yang, Han; Ye, Yihan; Song, Yonghai

From Sensors and Actuators, B: Chemical (2017), 239, 172-179. | Language: English, Database: CAPLUS

A green and simple strategy to prep. graphene foam-like three-dimensional (3D) porous carbon/Ni nanoparticles (NINPs) nanocomposites was developed for glucose detection. The discarded sponge-like natural product, pomelo peel, was employed as novel supporting materials. The pomelo peel was carbonized to construct the graphene foam-like 3D porous carbon/NINPs nanocomposites. The nanocomposites were carefully characterized by SEM, transmission electron microscopy, N₂ adsorption/desorption isotherms, X-ray powder...

2. Facile synthesis of flower-like platinum nanostructures as an efficient electrocatalyst for methanol electro-oxidation

Quick View Other Sources

By Zhang, Jie; Chen, Jinwei; Jiang, Yiwu; Zhou, Feilong; Zhong, Jing; Wang, Gang; Kiani, Maryam; Wang, Rulin

From Journal of Colloid and Interface Science (2016), 479, 64-70. | Language: English, Database: CAPLUS

This paper presents a facile approach for the synthesis of a novel Pt/graphene-nickel foam (Pt/GNF) electrode composed of flower-like Pt nanoparticles (NPs) and 3D graphene. The fabrication process involved the chem. vapor deposition of graphene onto Ni foam as a substrate and the subsequent growth of Pt NPs via a galvanic replacement reaction without using any seed and org. solvent. The surface morphol. and compn. of the prepd. materials were characterized. Meanwhile, cyclic voltammetry and electrochem. impedance spectroscopy were employed to confirm their typical electrochem. characterist...

3. Extremely Weak van der Waals Coupling in Vertical ReS₂ Nanowalls for High-Current-Density Lithium-Ion Batteries

Quick View Other Sources

By Zhang, Qin; Tan, Shuangjie; Mendes, Rafael G.; Sun, Zhongti; Chen, Yongting; Kong, Xin; Xue, Yinghui; Ruenmell, Mark H.; Wu, Xiaojun; Chen, Shengli; et al

From Advanced Materials (Weinheim, Germany) (2016), 28(13), 2616-2623. | Language: English, Database: CAPLUS

In addn. to the weak interlayer coupling, ReS₂ possesses the highest anisotropic ratio along its two principle axes as compared to all exptl. investigated 2D layered materials. As shown in early studies, the direction of the Re-Re at. chain is more conductive than other cryst. orientations. However, 2D layered materials, including ReS₂, are oriented in a conventional stacked geometry. Therefore, we first synthesized ultrauniformly distributed vertical ReS₂ nanowalls (V-ReS₂) grown on 3D Ni foam...

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☐ Summary with partial abstracts

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文献信息一题录、摘要、索引

3. Extremely Weak van der Waals Coupling in Vertical ReS₂ Nanowalls for High-Current-Density Lithium-Ion Batteries

By: Zhang, Qin; Tan, Shuangjie; Mendes, Rafael G.; Sun, Zhongti; Chen, Yongting; Kong, Xin; Xue, Yinghui; Ruemmel, Mark H.; Wu, Xiaojun; Chen, Shengli; Fu, Lei

In addn. to the weak interlayer coupling, ReS₂ possesses the highest anisotropic ratio along its two principle axes as compared to all exptl. investigated 2D layered materials. As shown in early studies, the direction of the Re-Re at. chain is more conductive than other cryst. orientations. However, 2D layered materials, including ReS₂, are always randomly oriented in a conventional stacked geometry. Therefore, we first synthesized ultrauniformly distributed vertical ReS₂ nanowalls (V-ReS₂) grown on 3D graphene foam (3DGF) by chem. vapor deposition with Re-Re sites adjacent to the graphene for the purpose of enhancing the cond. Meanwhile, the ReS₂ nanowalls expose more active sulfur edge sites, which improves easy lithium intercalation and deintercalation. To enhance the cond. of the whole electrode material, 3DGF was selected as template due to its high cond. and high-sp. surface area. Moreover, this favorable vertical structure shortens the pathways and facilitates fast diffusion of both Li⁺ and electrolyte ions. As expected, the V-ReS₂/3DGF composite demonstrated good cycling stability at high-current-densities when serving as anode material for LIBs. At the high c.d. of 1000 mA/g, the capacity of our ReS₂/3DGF anodes still maintained over 200 mAh/g even after 500 cycles. The extremely weak vdW coupling material of ReS₂ holds great promise for practical applications in LIBs. In addn., it broadens the material choice of anode materials for other alk.-ion batteries.

Indexing

Electrochemistry / Energy Technology (Section52-2)

Concepts

重要概念

Battery anodes
Delithiation
Lithiation
Nanostructured materials
Current density
Intercalation
Lithium-ion secondary batteries

extremely weak van der Waals coupling in vertical ReS₂ nanowalls for high-current-d. lithium-ion batteries

Substances

重要物质

12038-63-0P Rhenium sulfide

extremely weak van der Waals coupling in vertical ReS₂ nanowalls for high-current-d. lithium-ion batteries

Synthetic preparation; Technical or engineered material use; Preparation; Uses

7439-93-2 Lithium, uses
1034343-98-0 Graphene

extremely weak van der Waals coupling in vertical ReS₂ nanowalls for high-current-d. lithium-ion batteries

Technical or engineered material use; Uses

QUICK LINKS

0 Tags, 0 Comments

SOURCE

Advanced Materials
(Weinheim, Germany)
Volume28
Issue13
Pages2616-2623
Journal; Online Computer File
2016
CODEN:ADVMEW
ISSN:0935-9648
DOI:10.1002/adma.201505498

COMPANY/ORGANIZATION

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Wuhan University
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ACCESSION NUMBER

2016:170829
CAN164:397211
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PUBLISHER

Wiley-VCH Verlag GmbH & Co. KGaA

LANGUAGE

English

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1. 标题
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3. 文献中重要的技术术语
4. 文献中重要的物质
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6. 获得文献中的物质，反应
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- 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

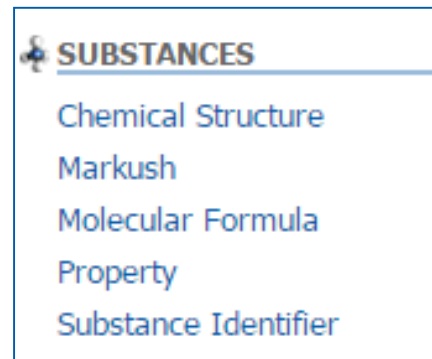
提纲

- 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



■ 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

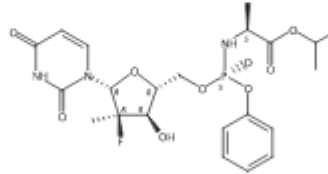
Get References Get Reactions Get Commercial Sources

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*[[*R*(*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:

<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.

Get **Cancel**

Chinese Annotations:

- 分析化学 (Analytical Chemistry) points to Analytical Study
- 晶体结构 (Crystal Structure) points to Crystal Structure
- 制备 (Preparation) points to Preparation
- 工艺 (Process) points to Process
- 谱图性质性质 (Spectral Properties) points to Spectral Properties

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

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

Analyze | Refine

Sort by: CAS Registry Number

0 of 39 Substances Selected

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
~929
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
~2
210531-45-6 (Component: 625392-06-5)
 $C_{13}H_8F_2O_7S_2 \cdot 2Na$
Click to view detail

如何筛选非金属物质？

0 of 14 Substances Selected

1. 1044804-35-4
~929
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
~2
Chemical structure: CCCC[CH2-]B(3+)(CCCC[CH2-])CCCC[CH2-]N1C=CC=C(C=C1)CC=C

$C_{18}H_{32}BN_2$
Boron, tributyl(1-(2-propen-1-yl)-1H-imidazole- κ^N), (7-4)-
Key Physical Properties
Experimental Properties

3. 868628-71-1
~2
Chemical structure: CCCC[CH2-]B(3+)(CCCC[CH2-])CCCC[CH2-]N1C=CC=C(C=C1)CC=C

4. 866023-23-6
~3
120120-58-3
 $C_{18}H_8O_4S_4$
Chemical structure: O=C1C(=O)SC2=C(S1)SC3=C2C(=O)SC3=O

物质检索——分子式

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

The screenshot displays the SciFinder web interface. On the left, there are navigation tabs: 'Explore', 'Saved Searches', and 'SciPlanner'. Below these, there are sections for 'REFERENCES' and 'SUBSTANCES'. The 'SUBSTANCES' section is active, showing a search for the molecular formula 'AlK5O8S2.12H2O'. The search results show '0 substances'. A message box states: 'Explore Substances resulted in 0 substances'. Below this, it says 'Molecular Formula "Al K O8 S2 . 12 H2 O" > substances (0)'. There are buttons for 'Analyze' and 'Refine'. A message box at the bottom of the search results area says 'Analyze by: 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

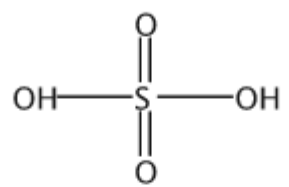
Examples:
H4SiO4
(C3H6O.C2H4O)x

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

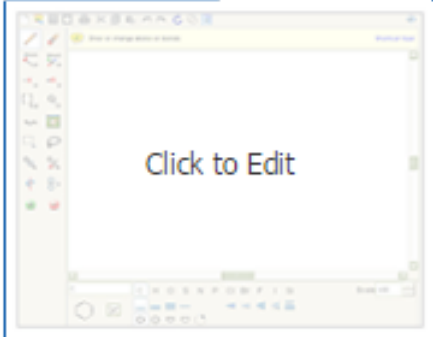
REACTIONS

- 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

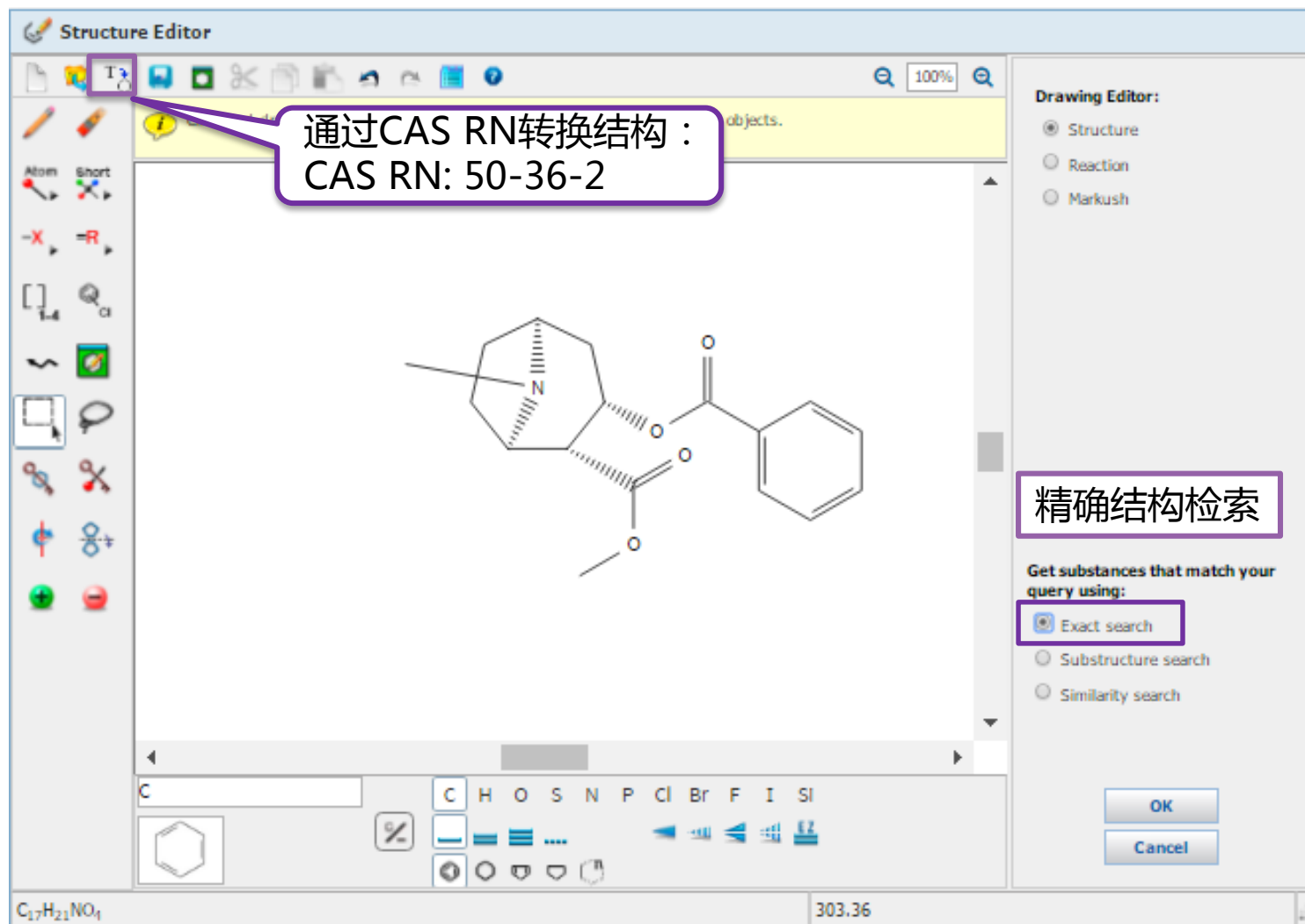
物质检索——结构

The image shows the SciFinder Structure Editor window with various tools and features labeled in Chinese:

- 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)
- 负电子** (Electron)
- C原子和单键恢复工具** (C Atom and Single Bond Restoration Tool)
- 常用基团** (Common Groups)
- 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** (Snare Selection Tool)
- 原子锁定工具** (Atom Locking Tool)
- 镜面旋转工具** (Mirror Rotation Tool)
- 单双键，RS构型，不确定键定义工具** (Single/Double Bond, RS Configuration, Uncertain Bond Definition Tool)
- 结构检索选择** (Structure Search Selection)
- 常见环，多元环工具** (Common Rings, Polycyclic Rings Tool)

The interface includes a toolbar with icons for drawing and editing, a central workspace for the chemical structure, and a right-hand panel for search options (Exact search, Substructure search, Similarity search) and buttons for '确定' (OK) and '取消' (Cancel).

物质检索——精确结构检索



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.

$C_{17}H_{21}NO_4$
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

Absolute stereochemistry.

$C_{17}H_{21}NO_4$

可卡因组合物

88-89-1

Absolute stereochemistry.

$C_6H_3N_3O_7$

$C_{17}H_{21}NO_4 \cdot C_6H_3N_3O_7$
Alcococaine, picrate (6CI)

3. 109496-04-0

Absolute stereochemistry.

$C_{17}H_{21}NO_4 \cdot ClH$
(Component: 668-19-9)
Alcococaine, hydrochloride (6CI)

盐酸可卡因

SciFinder®
A CAS SOLUTION

ACS / Proprietary and Confidential / Do Not Distribute

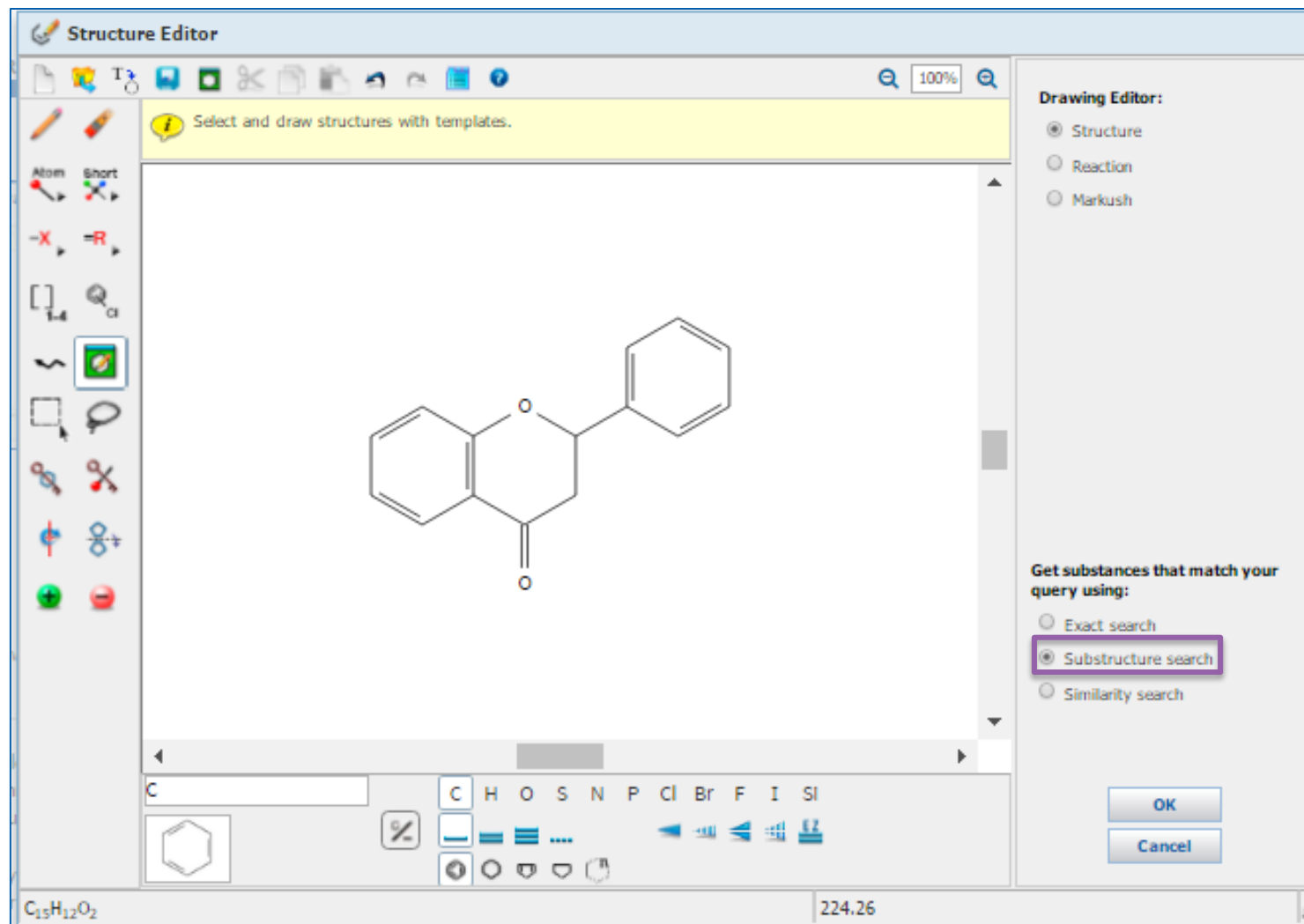
43

物质检索——精确结构检索

- 精确结构检索：

获得被检索结构的盐，混合物，配合物，聚合物等，被检结构不能被取代

物质检索——亚结构检索

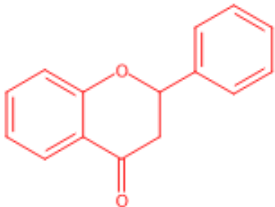


物质检索——亚结构检索

0 of 23824 Substances Selected

1. 487-26-3

~2093

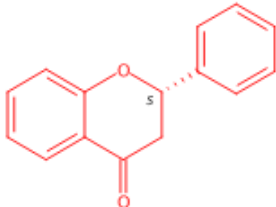


C₁₅H₁₂O₂
4-phenyl-4H-benzopyran-4-one, 2,3-dihydro-2-phenyl-

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

2. 17002-31-2

~244



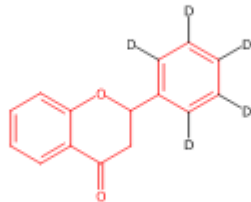
Absolute stereochemistry...Rotation (-).

C₁₅H₁₂O₂
4-phenyl-4H-benzopyran-4-one, 2,3-dihydro-

▶ **Key Physical Properties**
Experimental Properties

10. 146196-91-0

~1 ~5



C₁₅H₇D₅O₂
4-(2,3,4,5-tetradeuteriophenyl)-4H-benzopyran-4-one, 2,3-dihydro- (9CI)

Spectra

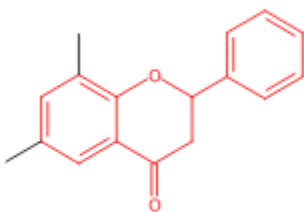
同位素

亚结构检索结果

281. 123251-10-5

~3   ~1 

取代物



$C_{17}H_{16}O_2$

4H-1-Benzopyran-4-one, 2,3-dihydro-6,8-dimethyl-

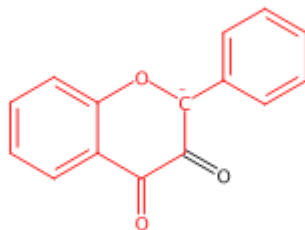
► Key Physical Properties

Experimental Properties

295. 780723-19-5

~0 

离子



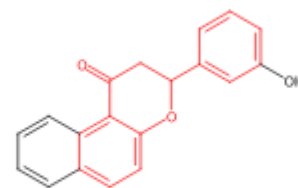
$C_{15}H_9O_3$

2H-1-Benzopyran-3,4-dione, 2-phenyl-, ion(1-)

284. 136116-23-9

~2 

稠环物质



$C_{19}H_{14}O_3$

1H-Naphtho[2,1-b]pyran-1-one, 2,3-dihydro-3-(3-hydroxyphenyl)-

► Key Physical Properties



SCIFINDER®
A CAS SOLUTION

亚结构检索结果的限定

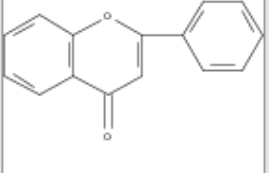
化学结构的再次限定

Analysis Refine

Refine by: ⓘ

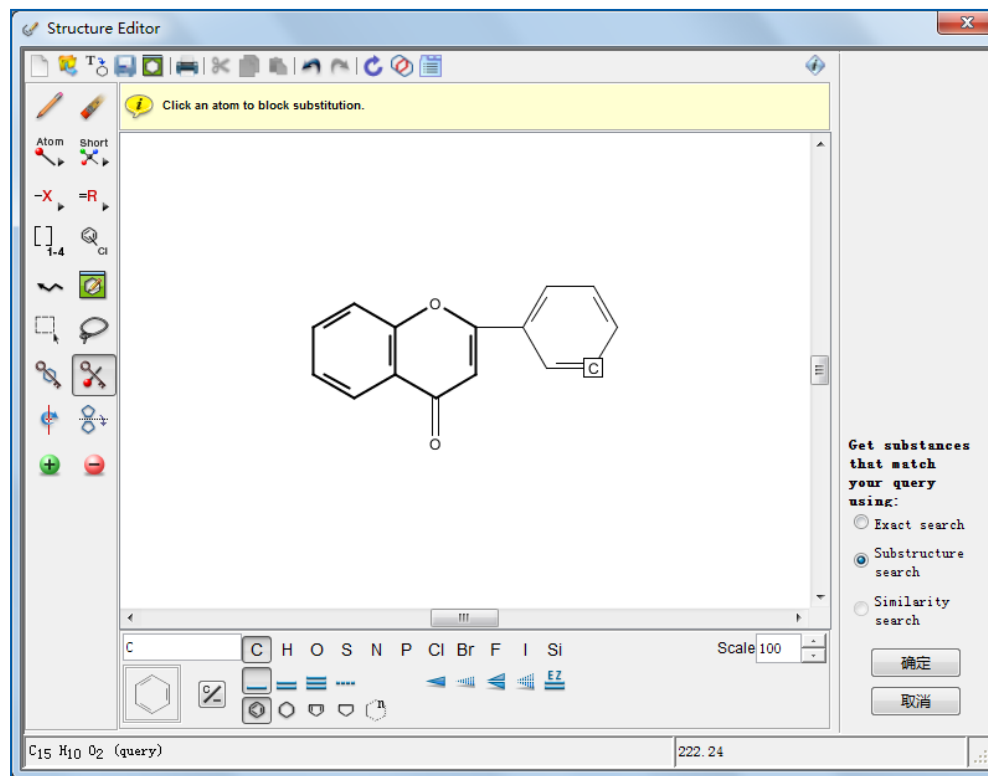
- ☒ Chemical Structure
- ☐ Isotope-Containing
- ☐ Metal-Containing
- ☐ Commercial Availability
- ☐ Property Availability
- ☐ Property Value
- ☐ Reference Availability
- ☐ Atom Attachment

Chemical Structure:



Click image to change structure or view detail

Search type: **Substructure**



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

1. **487-26-3**

~2093

C₁₅H₁₂O₂
4H-1-Benzopyran-4-one, 2,3-dihydro-2-phenyl-

Key Physical Properties
Regulatory Information
Spectra
Experimental Properties

2. **17002-31-2**

~244

C₁₅H₁₂O₂
4H-1-Benzopyran-4-one, 2,3-dihydro-2-phenyl-, (2S)-

Key Physical Properties
Experimental Properties

Absolute stereochemistry, Rotation (-).

4. **104550-32-5**

~3

5. **75524-43-5**

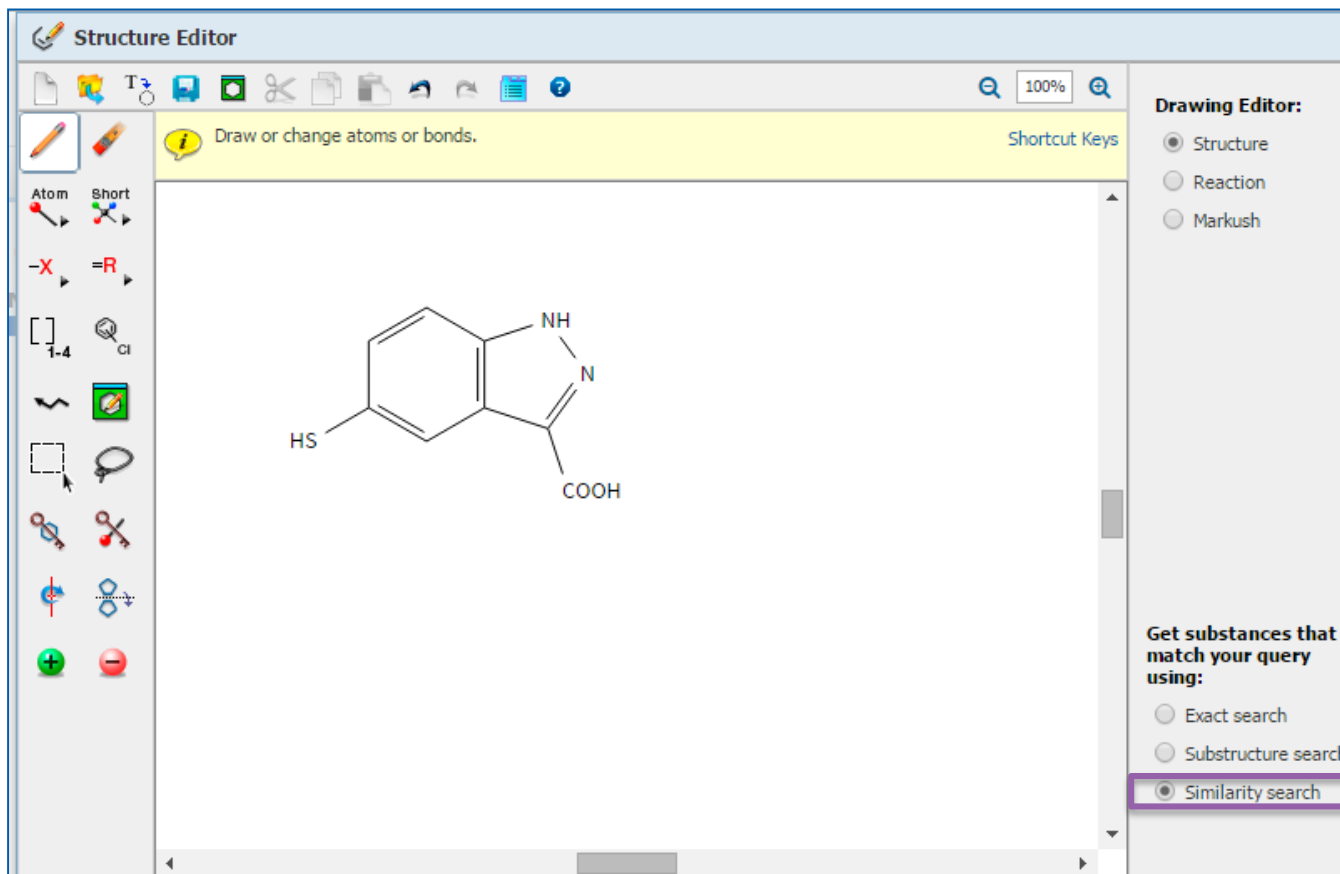
~2

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

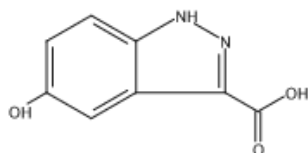
评分越高，相似度越高，结构越相似

Score: 88

☐ 1. 885518-94-5

取代基变化

~1 ~35



$C_8H_6N_2O_3$

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

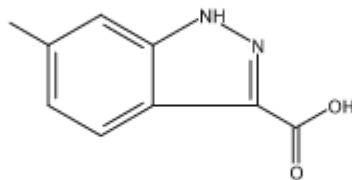
► Key Physical Properties

Score: 86

☐ 5. 858227-12-0

取代基位置变化

~7 ~41



$C_9H_8N_2O_2$

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

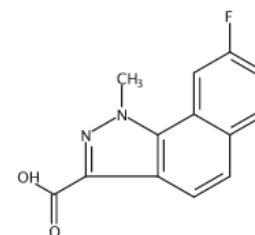
► Key Physical Properties

Score: 65

☐ 541. 1100422-

母体结构变化

~1



$C_{13}H_9FN_2O_2$

1H-Benz[7]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：

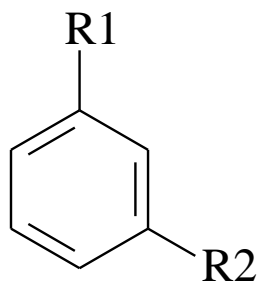
获得片段或整体结构与被检索结构相似的结果，母体结构可以被取代，也可以被改变

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

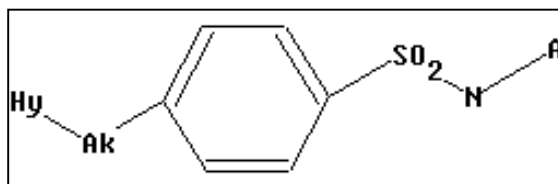
Markush检索

- 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(CH₃)—halogen,



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%

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

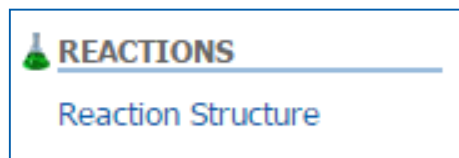
提纲

- 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



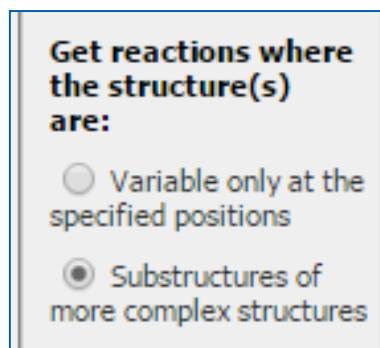
- 常用获取方法

已知物质：由物质获取反应

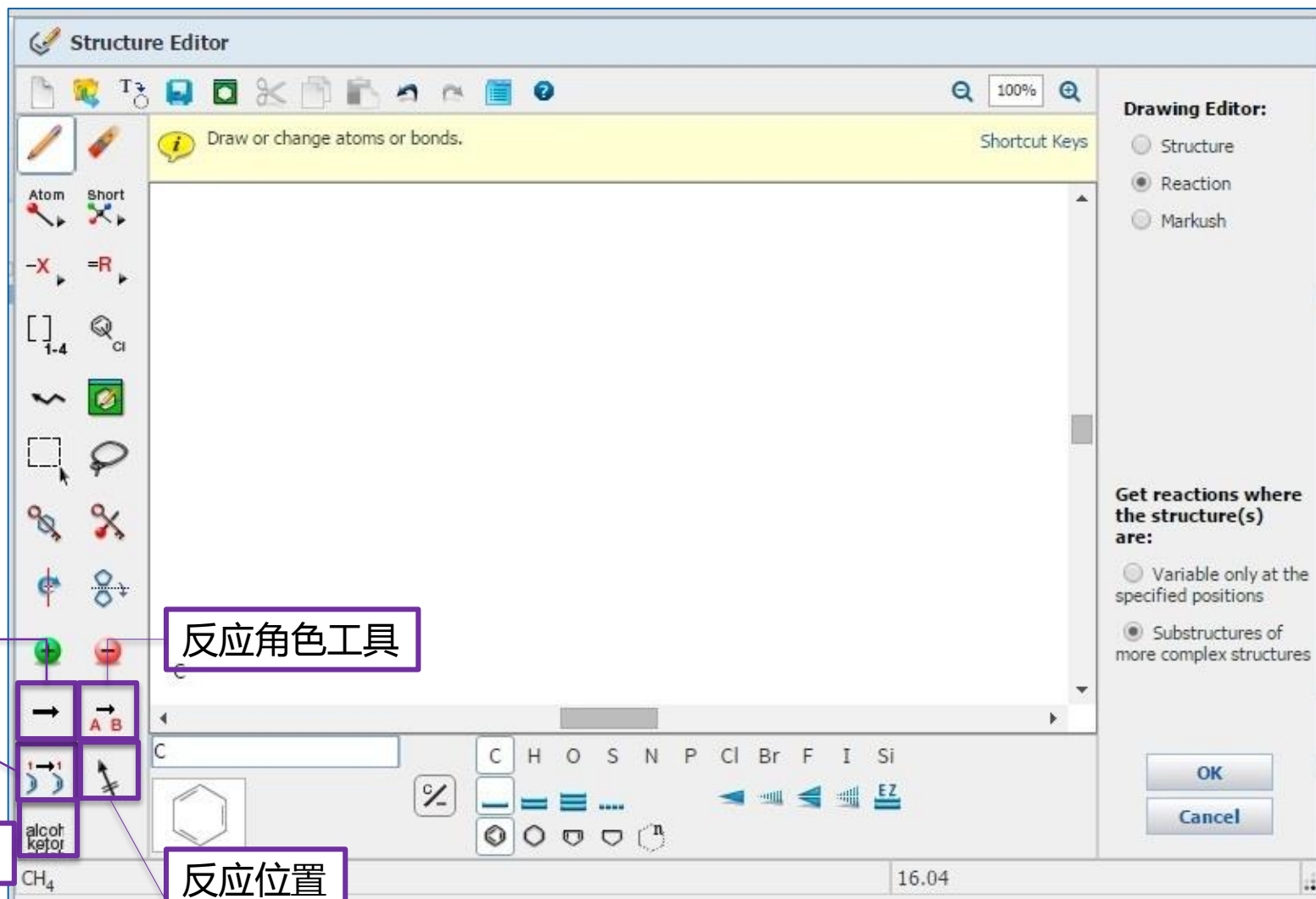
已知文献：从文献中获取反应

精确结构反应检索

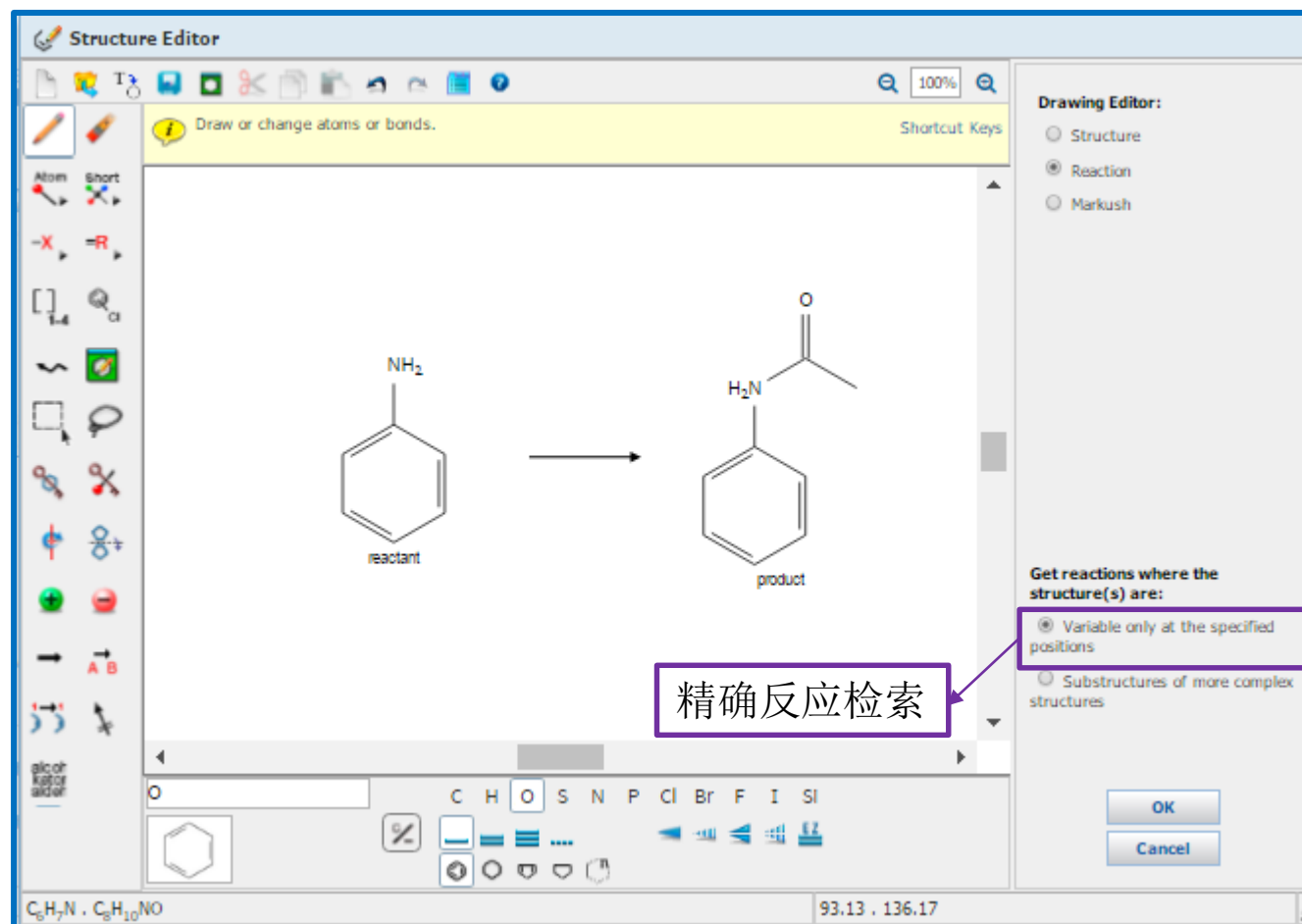
亚结构反应检索



反应绘制工具



SciFinder反应检索——精确反应检索



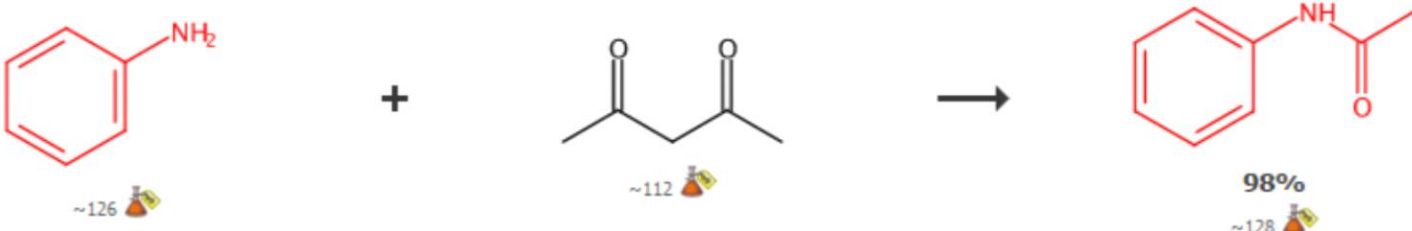
反应检索结果

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

Group by: No Grouping No Grouping Document Transformation Sort by: Relevance ↓

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

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


~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

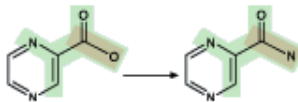
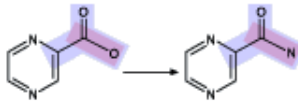
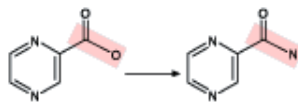
☐ Current answer set

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 ReactionsCancel

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

Analyze by: ?

Solvent

H₂O 99

CH₂Cl₂ 65

MeCN 55

THF 27

PhMe 26

AcOH 25

CHCl₃ 22

DMF 15

DMSO 15

Me₂CO 15

Show More

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.

Nc1ccccc1

~126

+

CC(=O)CC(=O)C

~112

→

CC(=O)Nc1ccccc1

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

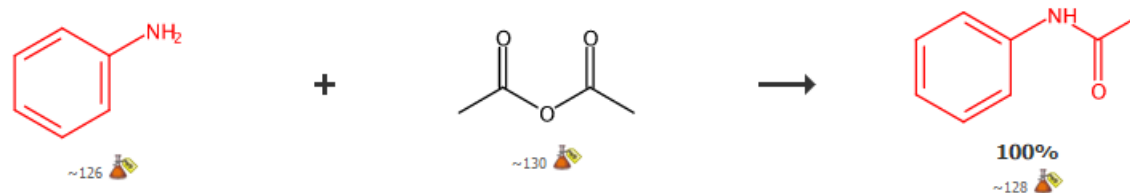
green chemistry-reagent, silica supported and used, no solvent, aerobic, optimization optimized on temperature, Reactants: 2, Most stages in any one step: 1

References

Silica sulfuric acid mediated acylation of a

筛选用水作溶剂的反应

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

Q 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

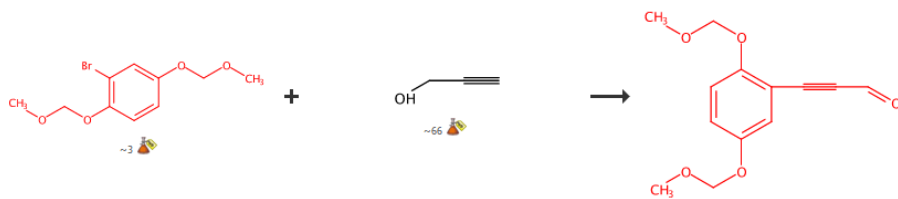
▼ Experimental Procedure



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.



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 in any one step: 4

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。

Experimental Procedure

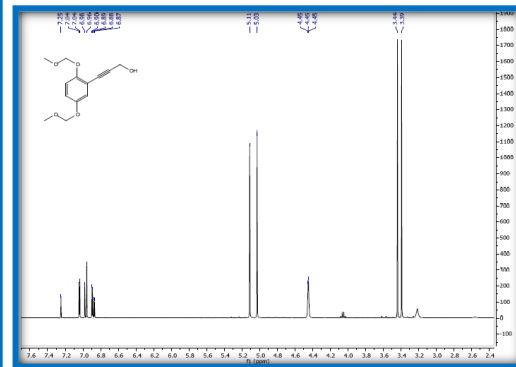
NATURAL PRODUCTS

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(PPh₃)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-ol (**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), 95.88 (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).



SCIFINDER®
A CAS SOLUTION

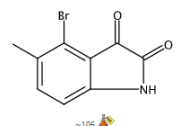
MethodsNow Synthesis

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

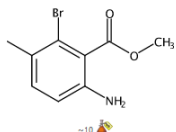
Reaction Steps 1 2 3



+



→



Products	Benzoic acid, 6-amino-2-bromo-3-methyl-, methyl ester, 84%, CAS RN: 147149-88-0
Reactants	1#-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, J = 8.2 Hz, 1 H, Ar-H), 7.00 (d, J = 8.2 Hz, 1 H, Ar-H).
IR	KBr cm ⁻¹ : 3472, 3382, 2953, 2924, 1716, 1622, 1480, 1277, 816.

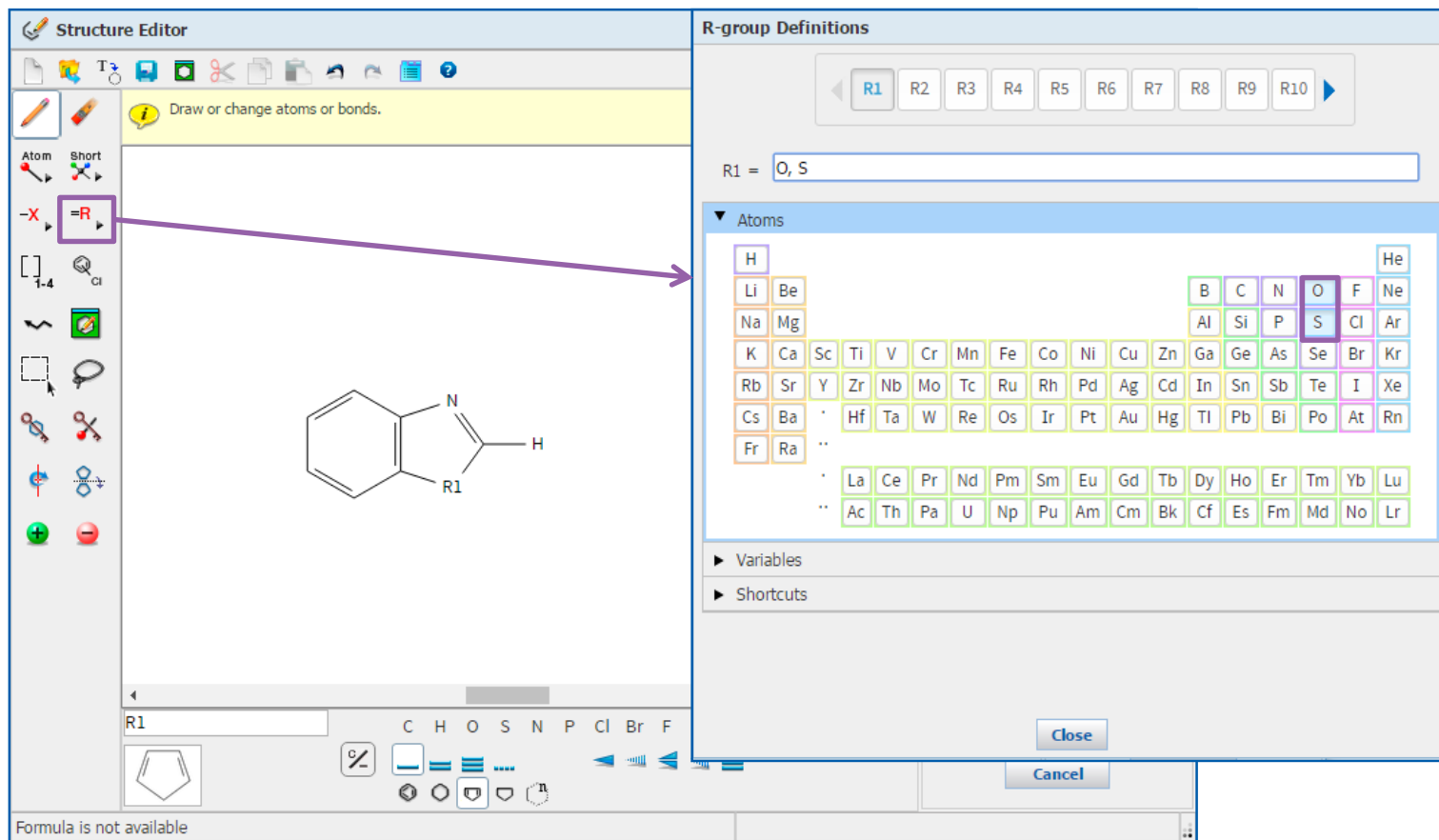
物质信息

实验过程

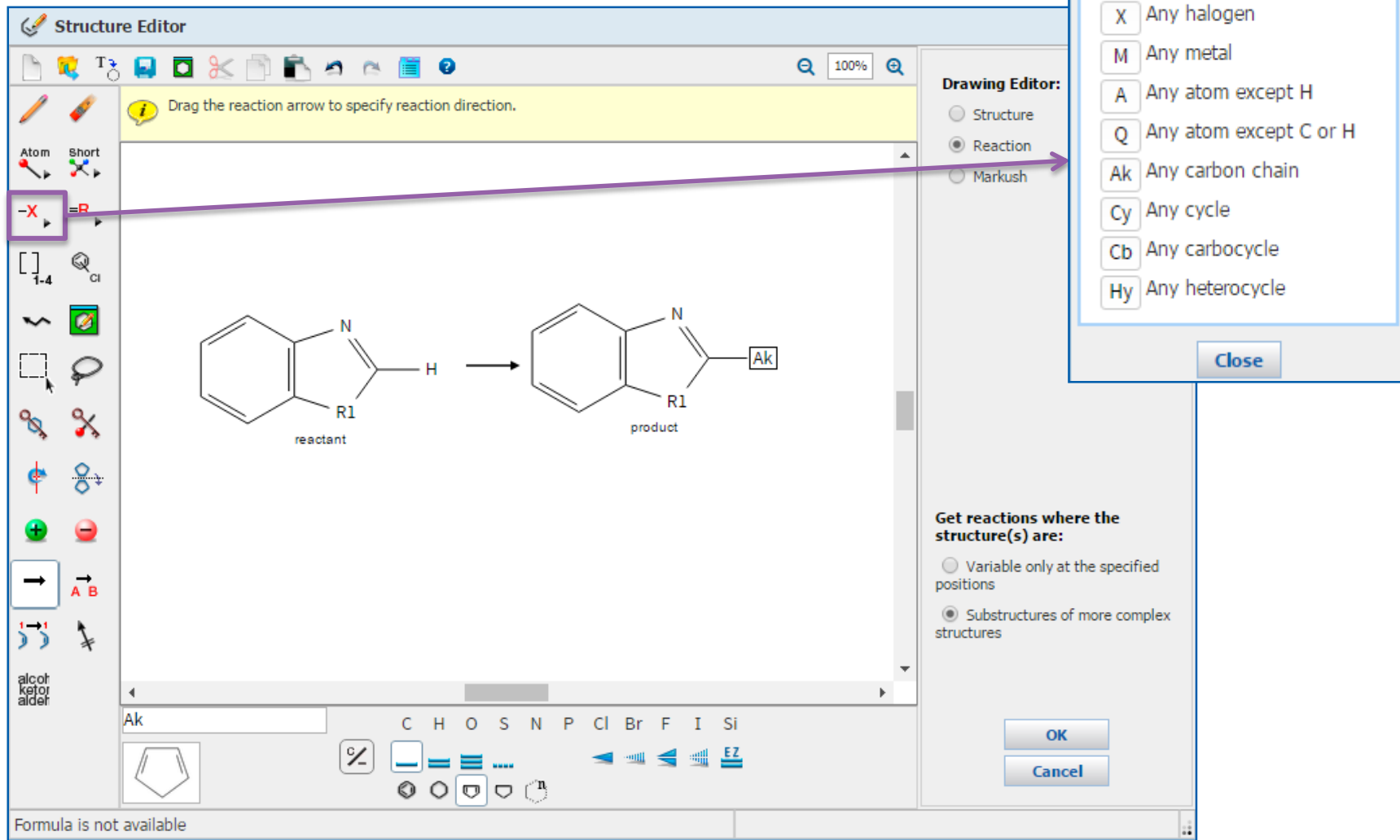
图谱信息

亚结构反应检索

通过C-H活化对苯并噻唑或者恶唑进行烷基化



亚结构反应检索



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.*

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
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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

进入SciPlanner 新建文件

将刚推送过来的反应拖至编辑面板

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

SciPlanner

SciPlanner_11_19_2015_112612

Workspace Edit View GoTo

New
Open
Save
Duplicate
Import
Export
Print
Close

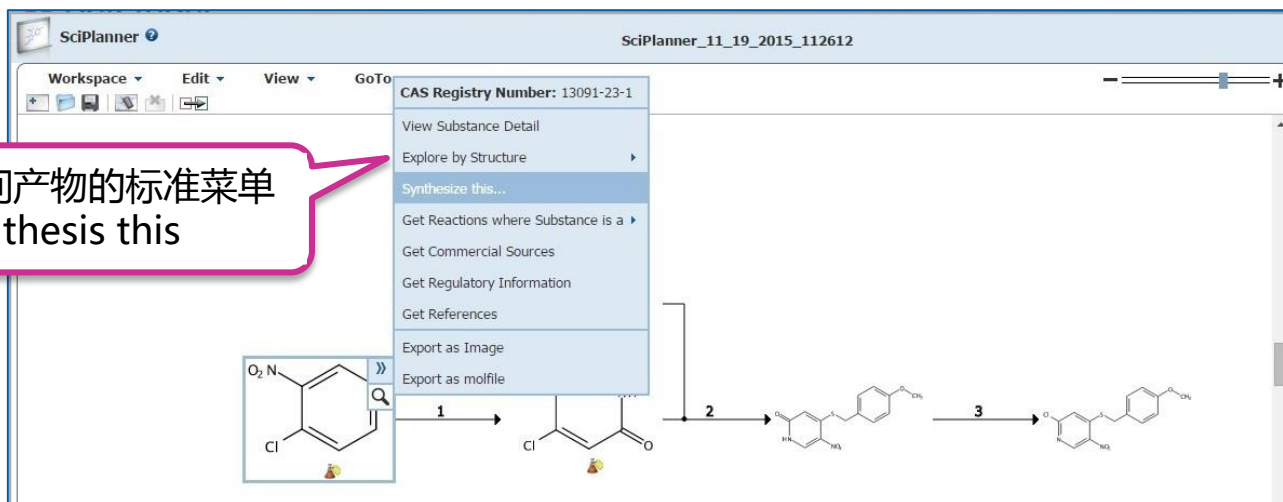
Your Workspace is empty.

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

SCI FINDER®
A CAS SOLUTION

SciPlanner使用简介

打开中间产物的标准菜单
选择Synthesize this



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Tools

Send selected records to SciPlanner.

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Group by: No Grouping Sort by: Accession Number

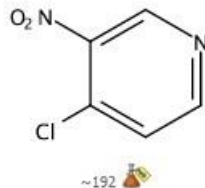
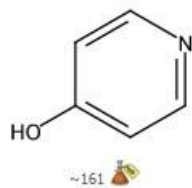
1 of 34 Reactions Selected

在检索到的反应中选择感兴趣的反应

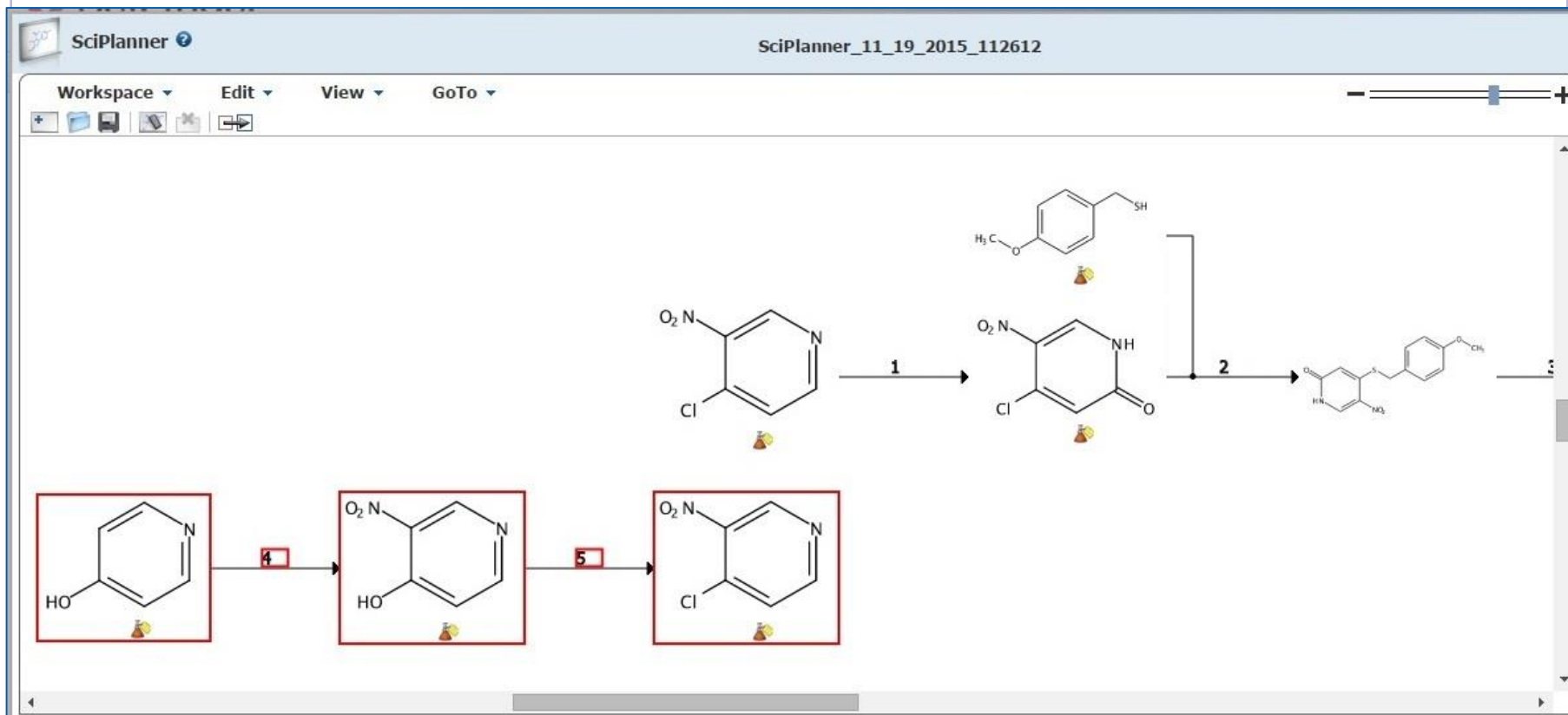
继续推送到SciPlanner

1. View Reaction Detail

2 Steps Hover over any structure for more options.



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

SciPlanner 11_19_2015_112612

Workspace Edit View GoTo

New
Open
Save
Duplicate
Import
Export
Print
Close

点击 Workspace, 选择 Export 导出结果

用鼠标将两个同样的结构拖至重叠, 两条反应合并

选择适当的输出格式, 输出结果

Export

For:

Offline Review

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

Saving Locally

- ☐ SciPlanner eXchange (*.pkx)

Details:

File Name: *

SciPlanner_11_19_2015_112612

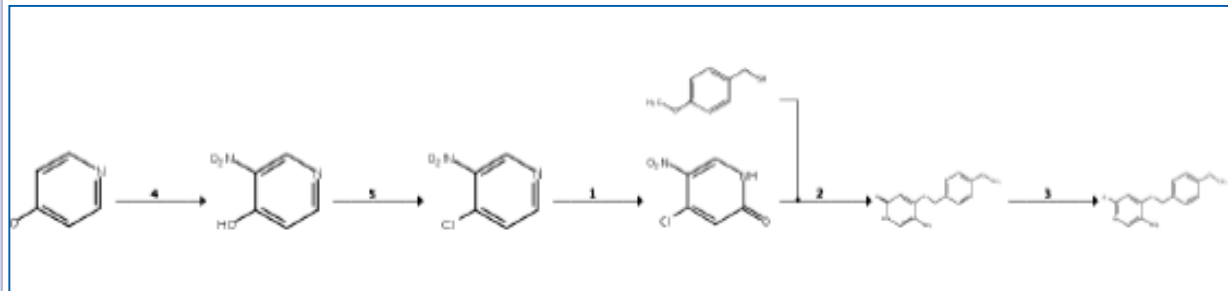
Title

Include:

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

Export **Cancel**

SciPlanner导出结果



Reaction	Stages	Notes	Yield
5	1.1 R:POCl ₃ , S:PhMe, 0°C → rt; 16 h, rt → 110°C	Reactants: 1, Reagents: 2, Solvents: 2, Steps: 1, Stages: 2	90%
	1.2 R:K ₂ CO ₃ , S:H ₂ O, cooled, pH 10	Transformation: 1. Formation of Alkyl Halides from Alcohols	

References

High color rendering index and color stable hybrid white efficient OLEDs with a double emitting layer structure using a single phosphorescence dopant of heteroleptic platinum complexes

By Poloek, Anurach et al

From Journal of Materials Chemistry C: Materials for Optical and Electronic Devices, 2(48), 10343-10356; 2014

Substance Information		
<p>1228150-22-8</p> <p>C₁₃H₁₂N₂O₄S 2(1H)-Pyridine, 4-[[4-methoxyphenyl]methyl]thio-5-nitro- Related Info: ~ 2 References Reactions</p>	<p>1228150-23-9</p> <p>C₁₃H₁₁ClN₂O₄S Pyridine, 2-chloro-4-[[4-methoxyphenyl]methyl]thio-5-nitro- Related Info: ~ 2 References Reactions</p>	<p>13091-23-1</p> <p>C₅H₃ClN₂O₂ Pyridine, 4-chloro-3-nitro- Related Info: ~ 301 References Reactions ~ 100 Commercial Sources Regulatory Information</p>
<p>5435-54-1</p> <p>C₅H₄N₂O₃ 4-Pyridinol, 3-nitro- Related Info: ~ 113 References Reactions ~ 197 Commercial Sources Regulatory Information</p>	<p>6258-60-2</p> <p>C₈H₁₀O S Benzenemethanethiol, 4-methoxy- Related Info: ~ 749 References Reactions ~ 71 Commercial Sources Regulatory Information</p>	<p>626-64-2</p> <p>C₅H₅N O 4-Pyridinol Related Info: ~ 1351 References Reactions ~ 160 Commercial Sources Regulatory Information</p>
<p>850663-54-6</p> <p>C₁₃H₉ClN₂O₄ 2(1H)-Pyridine, 4-chloro-5-nitro- Related Info: ~ 22 References Reactions ~ 138 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



天津师范大学
Tianjin Normal University

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讲座-SciFinder 化学学科的...

掌上学习平台开通试用

民国书库试用

公报》(1902-1949)全文...

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SciFinder Web 数据库

2012-10-06 10:36 图书馆

各位老师同学:

美国化学文摘社现使用的SciFinder Client升级为SciFinder Web, SciFinder Web将提供更为方便的访问方式、强大的功能和个性化的服务。

SciFinder Web的主要访问方式是每个用户在校园网IP范围内注册个人用户名和密码:

注册地址:

<https://scifinder.cas.org/registration/index.html?corpKey=929CB882X86F35055X20E7407C14AD544E21>

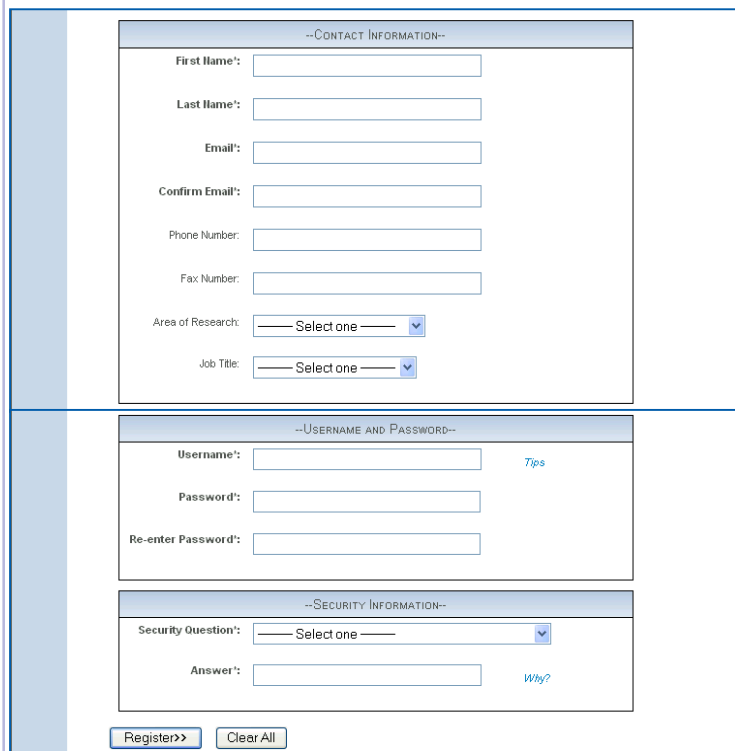
访问地址: <https://scifinder.cas.org> <https://origin-scifinder.cas.org> (教育网)

访问方式: 读者必须使用学校的email邮箱地址注册, 无并发用户限制。

使用指南: 附件

培训资料: 附件

如何获取SciFinder账号



The registration form is divided into three main sections: Contact Information, Username and Password, and Security Information. The Contact Information section includes fields for First Name, Last Name, Email, Confirm Email, Phone Number, Fax Number, Area of Research (a dropdown menu), and Job Title (a dropdown menu). The Username and Password section includes fields for Username, Password, and Re-enter Password, with a 'Tips' link next to the Password field. The Security Information section includes a Security Question (a dropdown menu) and an Answer field, with a 'Why?' link next to the Answer field. At the bottom of the form are two buttons: 'Register>>' and 'Clear All'.

--CONTACT INFORMATION--

First Name:

Last Name:

Email:

Confirm Email:

Phone Number:

Fax Number:

Area of Research:

Job Title:

--USERNAME AND PASSWORD--

Username:

Password: [Tips](#)

Re-enter Password:

--SECURITY INFORMATION--

Security Question:

Answer: [Why?](#)

请注意：

1.必须输入真实姓名和**学校域名**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

From: CAS

Dear user,

To complete your SciFinder registration, you must click the link provided below. By clicking the link, you agree to all of the following terms and conditions:

- I will not share my username and password with any other person.
- I will search only for myself and not for others or other organizations.
- I will not use any automated program or script for extracting or downloading CAS data, or any other systematic retrieval of data.
- I may retain a maximum of 5,000 Records at any given time for personal use or to share within a Project team for the duration of the Project.
- My organization's SciFinder License and the CAS Information Use Policies (<http://www.cas.org/legal/infopolicy.html>) apply to my use of SciFinder.
- I will contact my SciFinder Key Contact if I have questions.

If you do not accept these terms and conditions, do not click the link and delete this e-mail message.

<https://scifinder.cas.org/registration/completeRegistration.html?respKey=B8CB6727-86F3-F014-11E6-D312D80AC094>

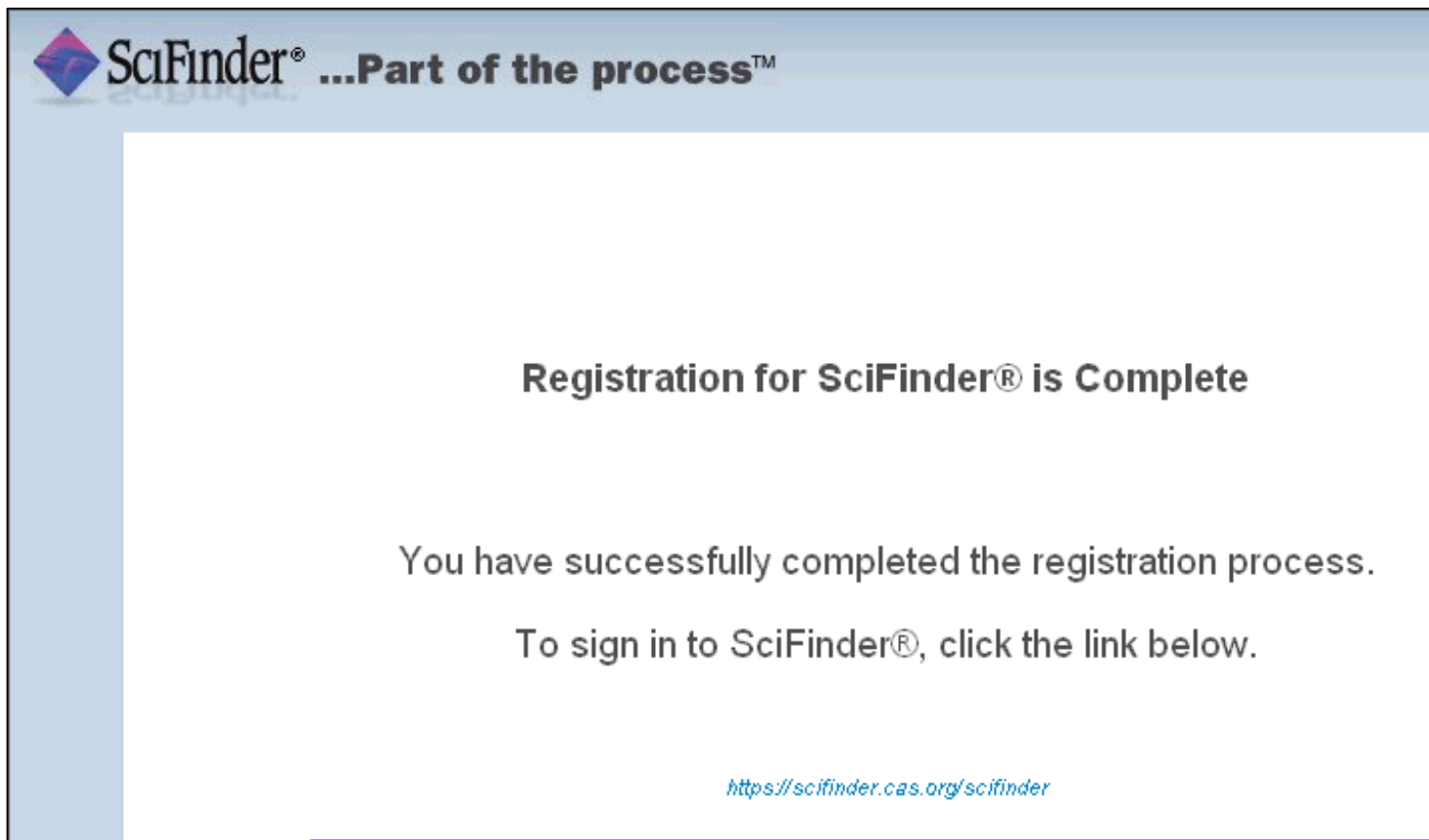
This link is valid for only one use and will expire within 48 hours.

If you need assistance at any time, consult the key contact at your organization.

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

美国化学文摘社北京代表处

010-62508026

china@acsi.info

