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如何使用SciFinder获取科技信息

吉林大学

2016.10.14



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

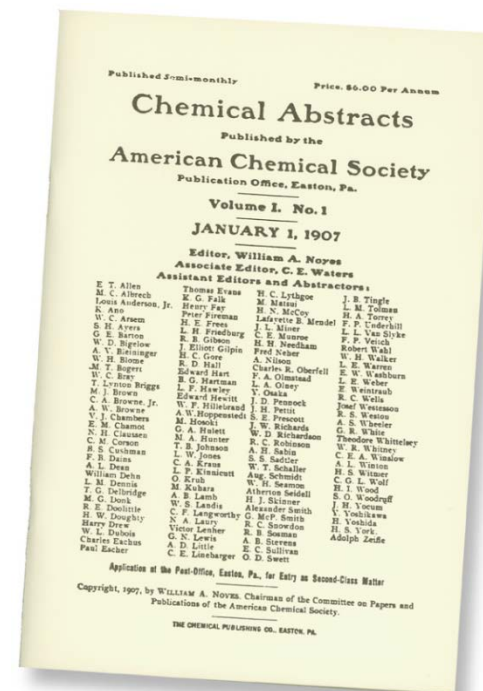


1907年，信息的汇集、管理发生了重大的变化



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



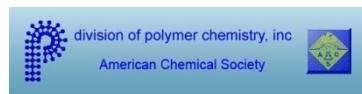
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CAS数据库——源于化学，超越化学

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

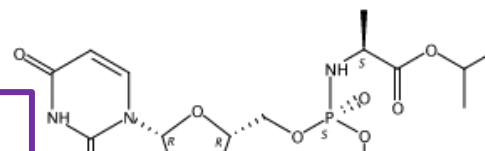
Concepts

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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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...

Patent No.	Kind	Language
WO 2016100441	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 R¹ 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 wit...

ZOOM DOWNLOAD PDF

Search in SciFinder | View Detail

Analyst Markup Locations (1)
page 130

CAS RN 1206126-39-7

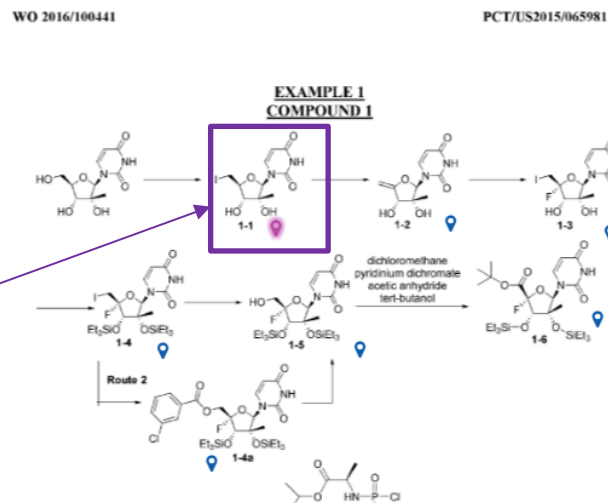
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Analyst Markup Locations (1)
page 130

CAS RN 1206126-41-1

Search in SciFinder | View Detail

Analyst Markup Locations (1)
page 130



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- 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

SciFinder interface showing a chemical synthesis reaction. The reaction involves a substituted benzofuran derivative reacting with a methylamine derivative to form a product in 70% yield. The interface includes search filters, reagent lists, and a detailed procedure section.

嵌在SciFinder中的合成模块

MethodsNow interface showing search results for 'Atorvastatin'. The results list various methods, including 'Analysis of Atorvastatin in blood plasma by High-performance thin layer chromatography'. The interface includes filters for analyte, matrix, and method category.

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

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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, there is a navigation bar with the SciFinder logo and the text 'A CAS SOLUTION'. On the right side of the navigation bar, there are links for 'Preferences', 'SciFinder Help', and a 'Sign Out' button. Below the navigation bar, there is a secondary menu with 'Explore', 'Saved Searches', and 'SciPlanner'. The main content area is titled 'REFERENCES: RESEARCH TOPIC'. It features a search input field with a 'Search' button and an 'Advanced Search' link. On the left side, there is a sidebar menu with categories: 'REFERENCES' (including Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, Tags), 'SUBSTANCES' (including Chemical Structure, Markush, Molecular Formula, Property, Substance Identifier), and 'REACTIONS' (including Reaction Structure). On the right side, there is a 'SAVED ANSWER SETS' section listing various saved sets like 'CSF1R', 'jmc', 'EP 19870107847', etc. Below that is a 'KEEP ME POSTED' section with a message: 'You have no proxies. Learn how to: Create Keep Me Posted'. Chinese annotations with callout boxes point to the 'Sign Out' button, the top navigation bar, the search input field, the left sidebar, the 'SAVED ANSWER SETS' list, and the 'KEEP ME POSTED' section.

已保存的结果集

检索入口

定题追踪



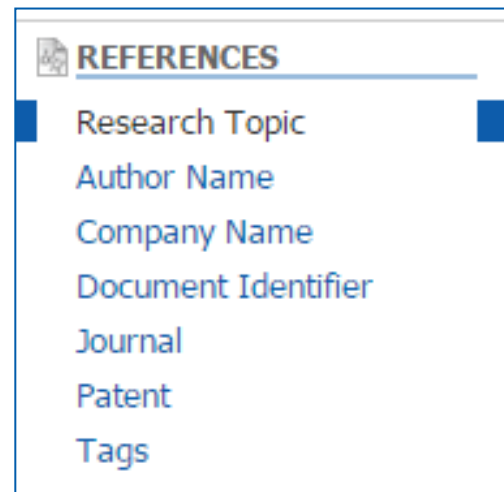
SciFinder检索——文献检索

■ 文献检索方法

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

■ 检索策略推荐

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



文献检索——主题

主题检索：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 SciFinder logo is visible, along with navigation tabs for 'Explore', 'Saved Searches', and 'SciPlanner'. The breadcrumb trail indicates the search path: 'Research Topic "prepare of 3D graphene" > references (767) > Facile Synthesis of 3D Graphen...'. On the left, a sidebar menu lists search criteria under 'REFERENCES' (Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, Tags) and 'SUBSTANCES' (Chemical Structure, Markush). The main search area contains a text input field with 'prepare of 3D graphene', a 'Search' button, and a link to 'Advanced Search'. A purple box highlights the text '关键词之间用介词连接：in, with, of...'.

主题检索的候选项

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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

Get References

“Concepts”表示对主题词做了同义词的扩展；

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

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

按被引次数排序— Citing References

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

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

REFERENCES | Get Substances | Get Reactions | Get Related Citations | Tools

Analyze | Refine | Categorize

Sort by: Citing References

Analyze by: Author Name

Author Name	Citations
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...

Citing Reference: 帮助找到最重要的文献

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Research Topic "prepare of 3D graphene" > references

REFERENCES

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Analyze Refine Categorize

Sort by: Accession Number

0 of 767 References Selected

Analyze by: Author Name

Author Name	Count
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, Haoifei; 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 a 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

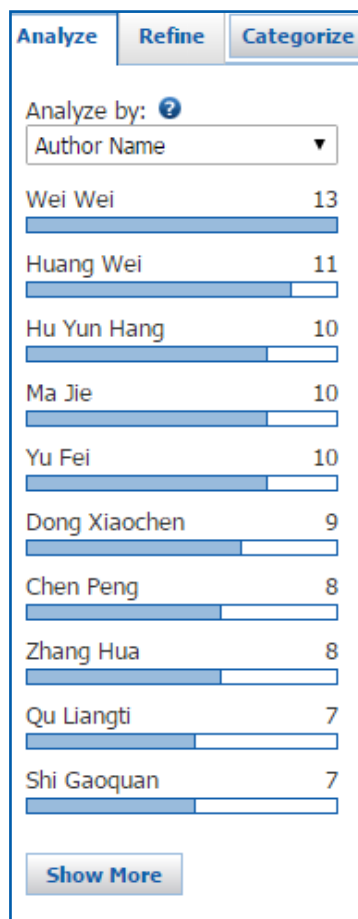
By Zhao, Yufeng; Huang, Shifei; Xia, Meirong; Rehman, Sarish; Mu, Shichun; Kou, Zongkui; Zhang, Zhi; Chen, Zhaoyang; Gao, Faming; Hou, Yanglong
From Nano Energy (2016), 28, 346-355. | Language: English, Database: CAPLUS

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.

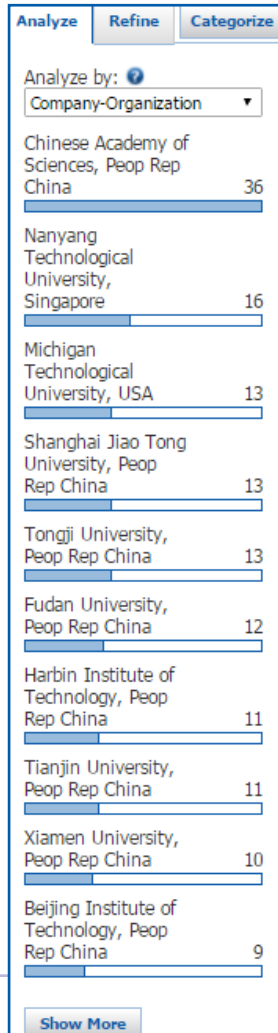
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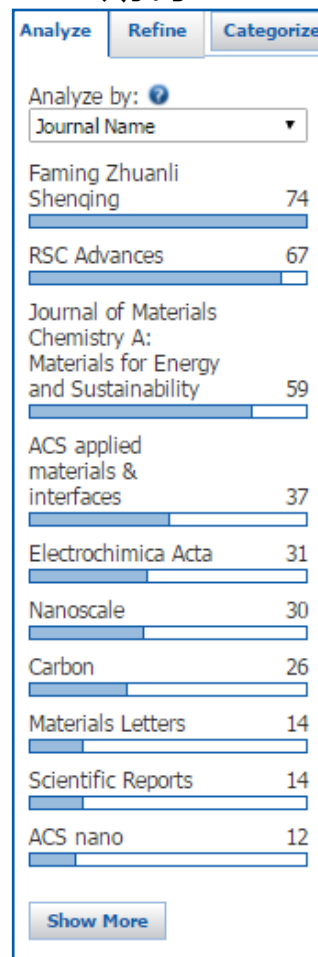
本领域研究人员



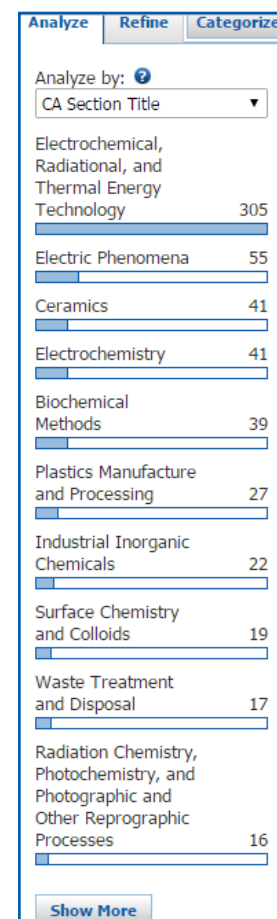
本领域研究机构、 合作伙伴、竞争对手



期刊



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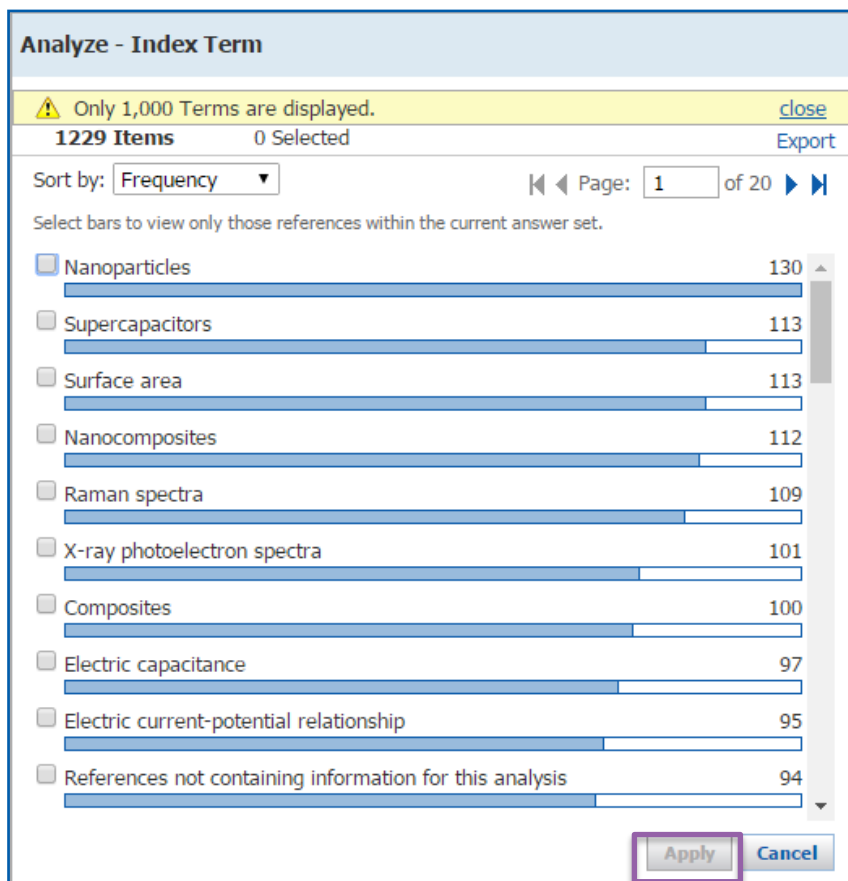
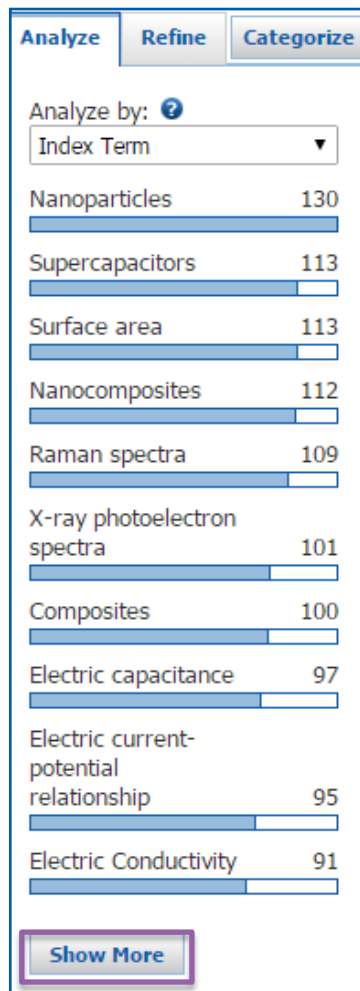


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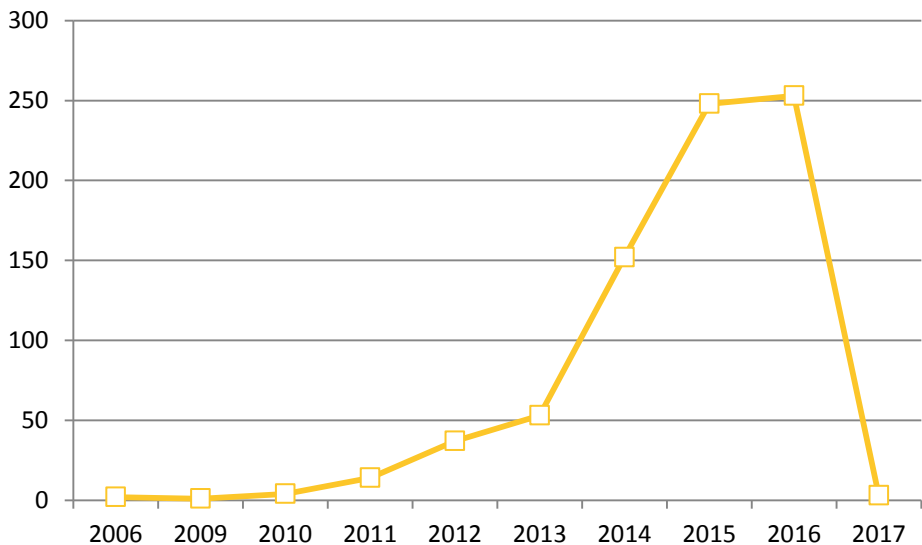
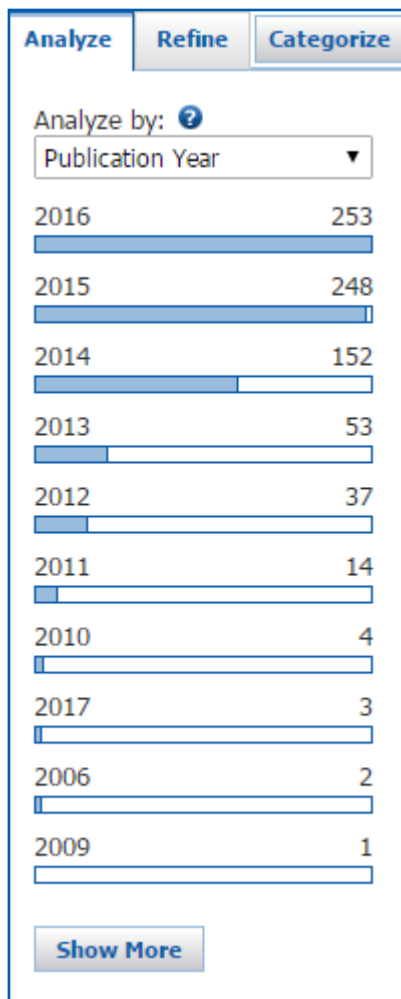
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Publication Year: 分析领域发展趋势

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Company Name

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0 of 534 References Selected Page: 1 of 27

- 1. N-P-O co-doped high performance 3D graphene prepared through red phosphorous-assisted "cutting-thin" technique: A universal synthesis and multifunctional applications**
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. PH₃, H₂, CO₂) 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**
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**
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 prep. high-quality N-GQDs and meanwhile, overcomes the drawbacks of complicated prep. progress and low yield. We further hy...
- 4. High performance agar/graphene oxide composite aerogel for methylene blue removal**
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

Refine : 帮助用户迅速获得需要的文献

文献检索结果的Categorize

学科领域
主分类

学科领域
副分类

Index Term

选中的Index Term

Categorize ⓘ

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

Category Heading	Category	Index Terms	Selected Terms
All	Substances in technology (716)	Page: 1 of 3 Select All Deselect All	Click 'x' to remove the category from 'Selected Terms'
Technology	Materials & products (203)	<input type="checkbox"/> Graphene 427	<input checked="" type="checkbox"/> Technology > Materials & products (1 Terms)
General chemistry	Processes & apparatus (202)	<input type="checkbox"/> Nanocomposites 86	
Physical chemistry	Metallurgy (52)	<input type="checkbox"/> Composites 85	
Synthetic chemistry	Power & fuel topics (25)	<input type="checkbox"/> Graphite 83	
Polymer chemistry	Formed, removed, & other substances (106)	<input type="checkbox"/> Platinum 31	
Catalysis	Construction (11)	<input type="checkbox"/> Hydrogen 26	
Biotechnology	Imaging & recording (12)	<input type="checkbox"/> Carbon black 21	
Analytical chemistry	Ceramics (8)	<input type="checkbox"/> Oxygen 20	
Environmental chemistry		<input checked="" type="checkbox"/> Nanostructured materials 19	
Genetics & protein chemistry		<input type="checkbox"/> Porous materials 16	
Biology		<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	

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

OK Cancel

Categorize学科分类功能，基于Index Term，根据大学科方向对文献进行自动分类。

结果集的保存— Save, Print, Export

Searches ▾ SciPlanner Save Print Export

ally removed.

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

Get Substances Get Reactions Get Related Citations Tools

Create Keep Me Posted Alert Send to SciPlanner

Sort by: Accession Number ↓ Display Options

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 morphology and electrochemical properties 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; Ruemmel, 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 graphite, are usually oriented in a conventional stacked geometry. Therefore, we first **synthesized** ultrauniformly distributed vertical ReS₂ nanowalls (V-ReS₂) grown on...

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 (*.akx)

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—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 and 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

College of Chemistry and Molecular Science
Wuhan University
Wuhan, Peop. Rep. China
430072

ACCESSION NUMBER

2016:170829
CAN164:397211
CAPLUS

PUBLISHER

Wiley-VCH Verlag GmbH & Co. KGaA

LANGUAGE

English

文献详情界面包括：

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

文献检索小结

- 主题检索时，使用介词 **in, with, of** 等作为连接词
- 根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

SUBSTANCES

Chemical Structure

Markush

Molecular Formula

Property

Substance Identifier

■ 物质检索策略推荐

—有机化合物，天然产物：结构检索

—无机物，合金：分子式检索

—高分子化合物：分子式检索和结构检索

物质检索——标识符检索

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 ?

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

1 3118-97-6

~894 ~58

CAS Registry Number: 3118-97-6

- » 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

C₁₈ H₁₆ N₂ O
2-Naphthalenol, 1-[2-(2,4-dimethylphenyl)diazenyl]-

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

在SciFinder中，鼠标滑过物质，即可打开物质标准菜单，获得与物质相关的所有内容

SciFinder中的物质记录

SUBSTANCE DETAIL ⓘ

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

[Return](#)

CAS Registry Number 3118-97-6

~894 ~58

C₁₈ H₁₆ N₂ O
2-Naphthalenol, 1-[2-(2,4-dimethylphenyl)diazenyl]-

Molecular Weight
276.33

Melting Point (Experimental)
Value: 166 °C

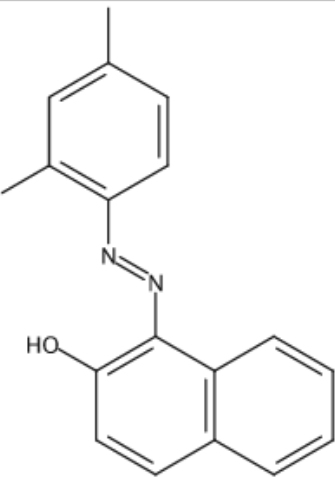
Boiling Point (Predicted)
Value: 476.7±40.0 °C | Condition: Press: 760 Torr

Density (Predicted)
Value: 1.14±0.1 g/cm³ | Condition: Temp: 20 °C Press: 760 Torr

pKa (Predicted)
Value: 13.52±0.50 | Condition: Most Acidic Temp: 25 °C

Other Names
2-Naphthalenol, 1-[(2,4-dimethylphenyl)azo]- (9CI)
C.I. Solvent Orange 7 (7CI,8CI)
Sudan Red (6CI)
1-[2-(2,4-Dimethylphenyl)diazenyl]-2-naphthalenol
AF Red No. 5
[View more...](#)

由物质获得文献，反应，供应商等信息



The chemical structure shows a naphthalene ring system with a hydroxyl group at the 2-position and an azo group at the 1-position. The azo group is connected to a 2,4-dimethylphenyl ring.

物质详情

通过物质获得文献

Get References

Retrieve references for:

All substances
 Selected substances

Limit results to:

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

For each sequence, retrieve:

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

分析化学

生物研究

制备

工艺

谱图数据

用途



SCIFINDER[®]
A CAS SOLUTION

EXPERIMENTAL PROPERTIES

EXPERIMENTAL SPECTRA

实验数据与实验谱图

¹H NMR IR Mass Raman UV and Visible

¹ H NMR Properties	Value	Condition	Note
Proton NMR Spectrum	See spectrum		(13)BIORAD

Notes

(13) BIORAD: Copyright Bio-Rad Laboratories. All Rights Reserved.

PREDICTED PROPERTIES

Biological Chemical Density Lipinski Structure Related Thermal

Lipinski Properties	Value	Condition	Note
Freely Rotatable Bonds	3		(21)
H Acceptors	3		(21)
H Donors	1		(21)
H Donor/Acceptor Sum	4		(21)
logP	5.471±1.252	Temp: 25 °C	(21)
Molecular Weight	276.33		(21)

预测数据与预测谱图

PREDICTED SPECTRA

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)

Get References | Get Reactions | Get Commercial Sources | Tools

Create Keep Me Posted Alert | Send to SciPlanner

Analyze | Refine

Sort by: CAS Registry Number

0 of 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

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

Substance
Image
Cannot Be Displayed
1044804-35-4

Click to view detail

0 of 14 Substances Selected

1. 1044804-35-4

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

Unspecified
Clevios P-VP-AI 4083
Experimental Properties

Substance
Image
Cannot Be Displayed
1044804-35-4

Click to view detail

2. 868628-72-2

$C_{18}H_{28}BN_2$
Boron, tributyl(1-(2-propen-1-yl)-1H-imidazole- κ^N), (7-4)

Key Physical Properties
Experimental Properties

Chemical structure of a boron tributyl imidazolium salt.

3. 868628-71-1

Chemical structure of a boron tributyl imidazolium salt.

4. 866023-23-6

120120-59-3
 $C_{18}H_{14}O_4S_4$

Chemical structure of a complex heterocyclic compound.

如何筛选非金属材料？

物质检索——分子式

REFERENCES

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

SUBSTANCES

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

REACTIONS

- Reaction Structure

SUBSTANCES: MOLECULAR FORMULA

Examples:
H4SiO4
(C3H6O.C2H4O)x

Search

1. 151-21-3

(Component: 151-41-7)

~84904 ~276

• Na

C₁₂H₂₆O₄S.Na
Sulfuric acid monododecyl ester sodium salt (1:1)

► **Key Physical Properties**

- Regulatory Information
- Spectra
- Experimental Properties

金属盐：金属离子和阴离子间用点 (.) 分开

分子式输入需要遵守Hill排序规则：不含碳化合物，按元素符号的字母顺序排列；分子式为含碳化合物时，则“C”在前；如有氢则紧随其后，其它元素符号按字母顺序排在氢的后面

物质检索——结构

The screenshot displays the SciFinder web interface for searching chemical structures. On the left, a navigation menu is visible with three main sections: REFERENCES, SUBSTANCES, and REACTIONS. The SUBSTANCES section is expanded, and 'Chemical Structure' is highlighted with a purple box. The main content area is titled 'SUBSTANCES: CHEMICAL STRUCTURE' and features a 'Structure Editor' window with 'Java' and 'Non-Java' tabs. The editor contains a large white area with the text 'Click to Edit'. To the right of the editor, the 'Search Type' options are listed: 'Exact Structure', 'Substructure' (selected), and 'Similarity'. Below these, there is a checkbox for 'Show precision analysis'. At the bottom right, there is a 'ChemDraw' logo and a button to 'Launch a SciFinder substance or re...'. A large blue 'Search' button is positioned below the 'Import CXF' text. At the very bottom, there are links for 'Advanced Search' and a checked 'Always Show' checkbox.

REFERENCES

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

SUBSTANCES

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

REACTIONS

- Reaction Structure

SUBSTANCES: CHEMICAL STRUCTURE

Structure Editor:

Java Non-Java

Click to Edit

Search Type:

- Exact Structure
- Substructure
- Similarity

Show precision analysis

ChemDraw

Launch a SciFinder substance or re...

Import CXF

Search

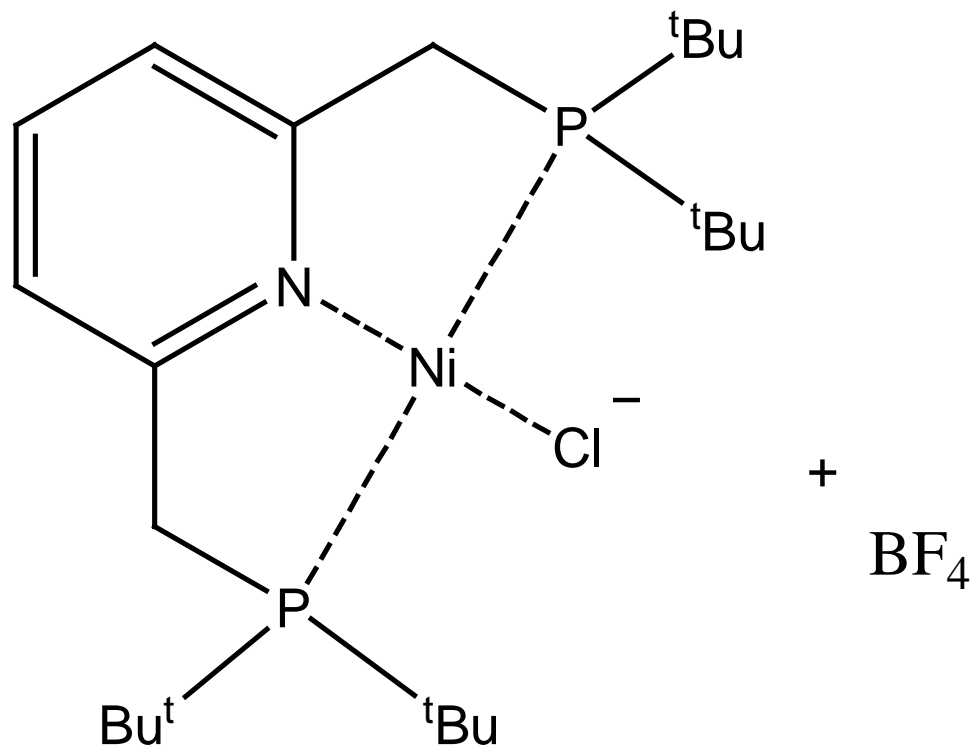
[Advanced Search](#) Always Show

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 also features a command line at the bottom with a chemical formula 'C H O S N P Cl Br F I Si' and a 'Scale' dropdown set to '100'. The labels point to the following features:

- 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)

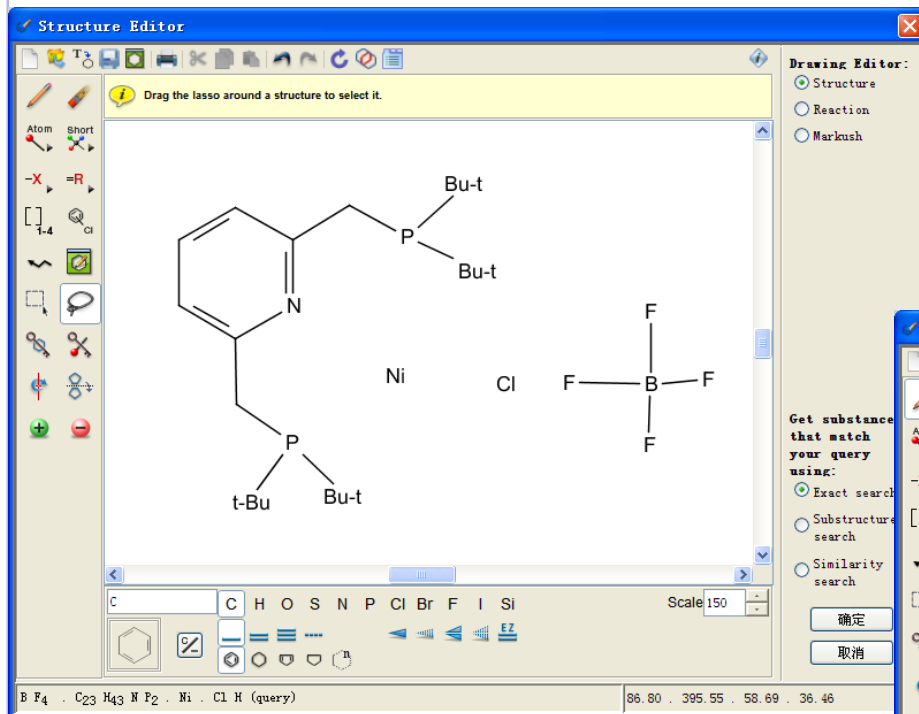
物质检索——精确结构检索



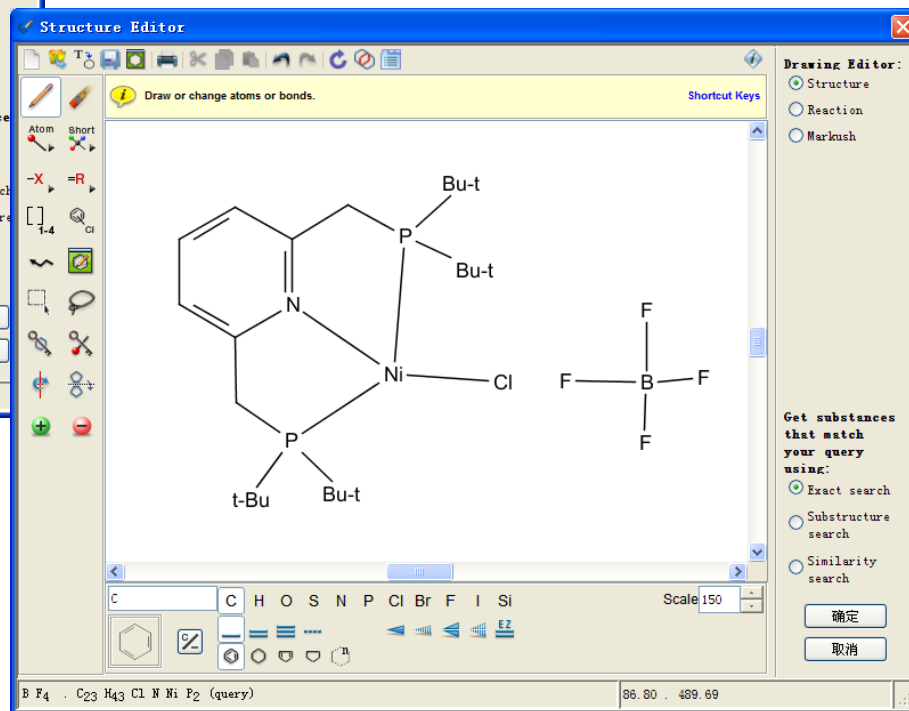
该结构中包含：

配体
金属
阳离子
阴离子

物质检索——精确结构检索



任何一种结构,使用精确结构都可以检索到



物质检索——精确结构检索

- 精确结构检索：

获得被检索结构的盐，混合物，配合物，聚合物等，被检结构不能被取代

物质检索——亚结构检索

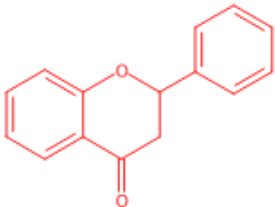
The screenshot displays the 'Structure Editor' window. The central workspace shows a chemical structure of a benzodioxane derivative with a phenyl group. The interface includes a toolbar on the left with various drawing and editing tools, a top toolbar with a search icon and a '100%' zoom level, and a right-hand panel with search options. A yellow message box at the top reads 'Select and draw structures with templates.' The search options on the right are: 'Structure' (selected), 'Reaction', 'Markush', 'Exact search', 'Substructure search' (highlighted with a purple box), and 'Similarity search'. At the bottom, there is a chemical formula input field containing 'C', a periodic table of elements, and a status bar showing the molecular formula $C_{15}H_{12}O_2$ and a numerical value 224.26.

物质检索——亚结构检索

0 of 23824 Substances Selected

1. 487-26-3

~2093

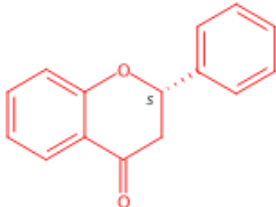


$C_{15}H_{12}O_2$
4-phenyl-4H-1-benzopyran-4-one, 2,3-dihydro-2-phenyl-

▶ Key Physical Properties
Regulatory Information
Spectra
Experimental Properties

2. 17002-31-2

~244



Absolute stereochemistry: Rotation (-).

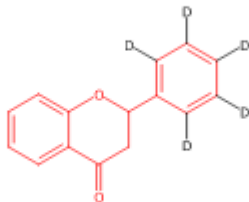
$C_{15}H_{12}O_2$
4-phenyl-4H-1-benzopyran-4-one, 2,3-dihydro-

▶ Key Physical Properties
Experimental Properties

10. 146196-91-0

~1

~5



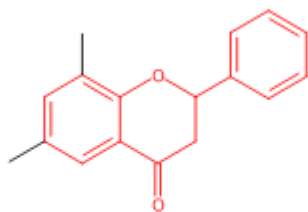
$C_{15}H_7D_5O_2$
4-(phenyl-d₅)-4H-1-benzopyran-4-one, 2,3-dihydro-2-(phenyl-d₅)- (9CI)

Spectra

同位素

亚结构检索结果

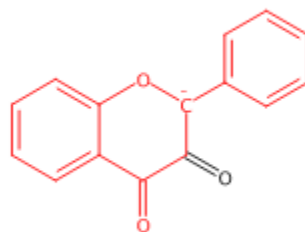
取代物



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

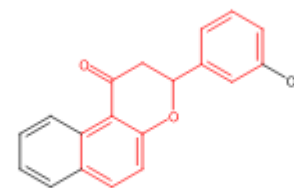
▶ Key Physical Properties
Experimental Properties

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

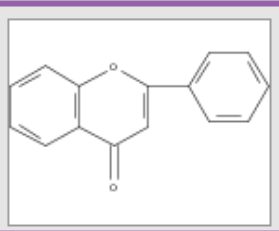
亚结构检索结果的限定

Analysis **Refine**

Refine by: ⓘ

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

Chemical Structure:



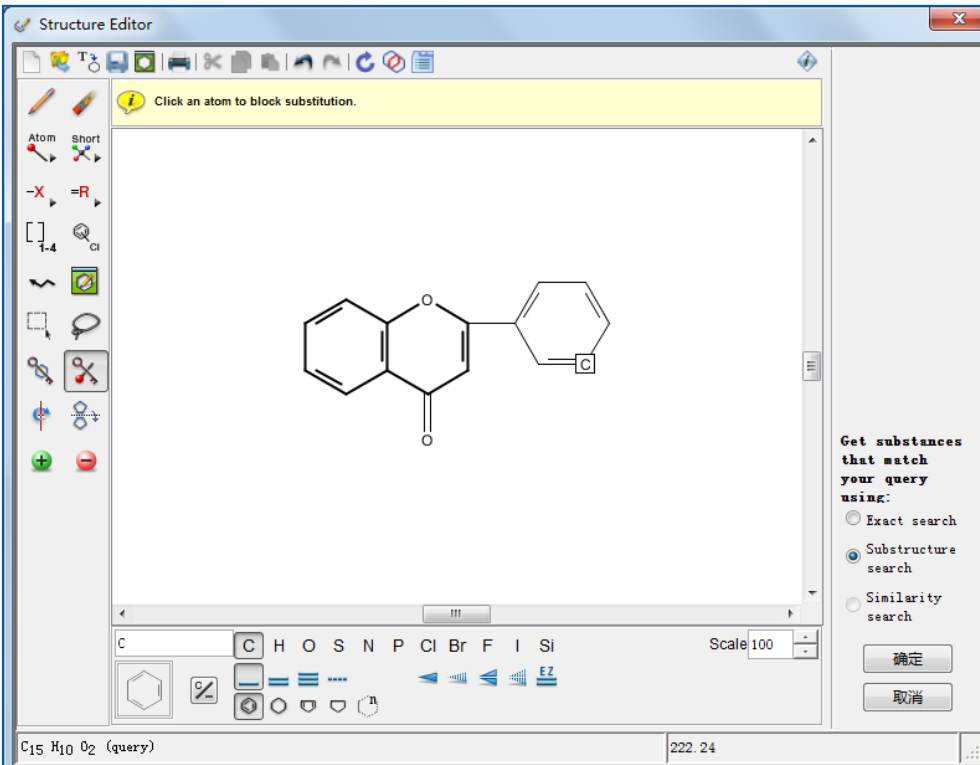
Click image to change structure or view detail

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



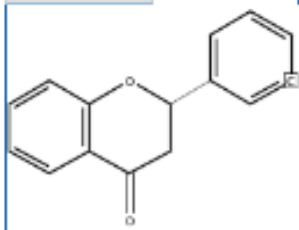
原子锁定

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

1. 487-26-3
~2093 ~69

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

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

2. 17002-31-2
~244 ~4

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

▶ **Key Physical Properties**
Experimental Properties

4. 104550-32-5
~3

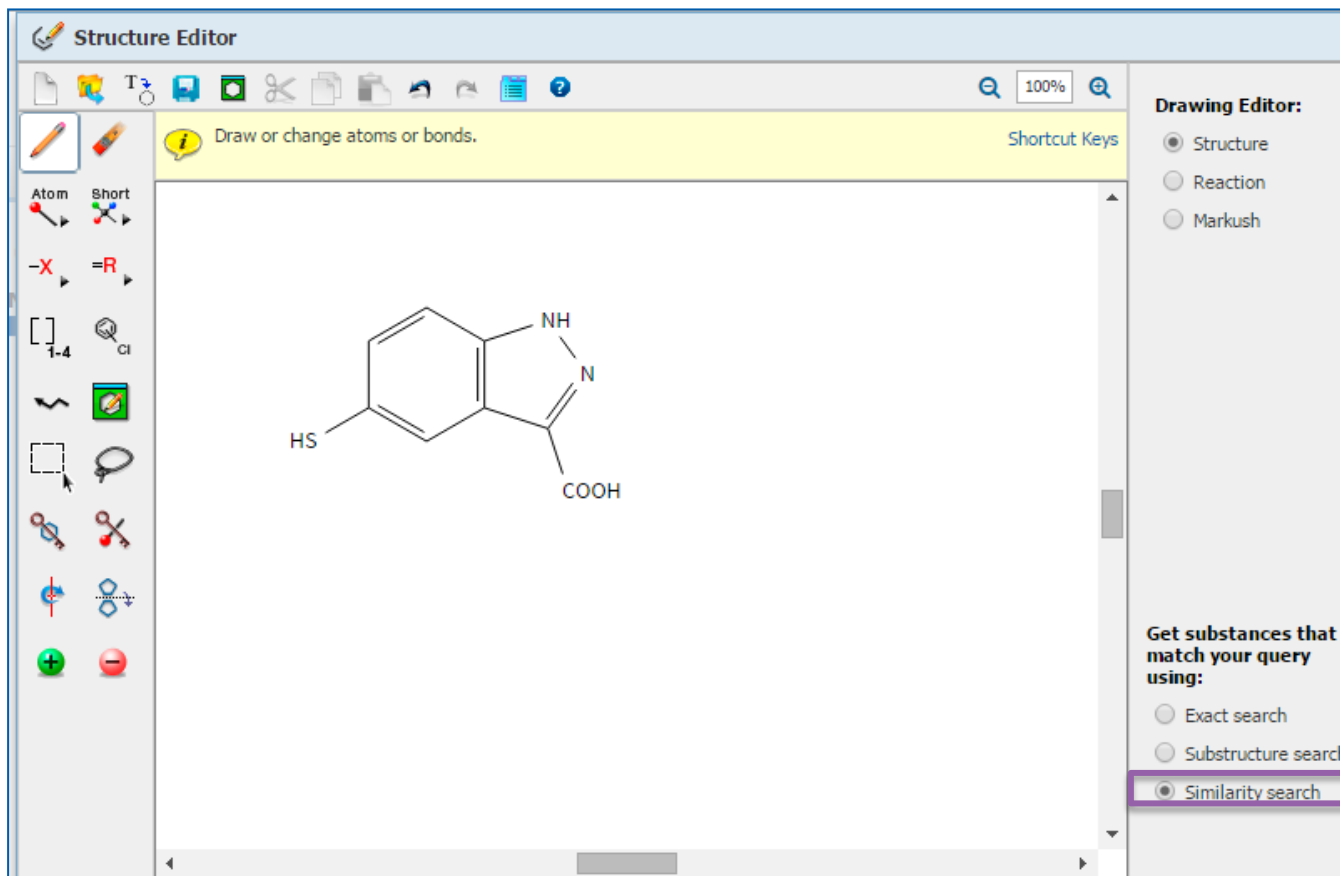
5. 75524-43-5
~2

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

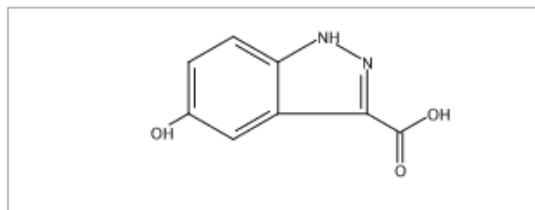
评分越高，相似度越高，结构越相似

Score: 88

1. 885518-94-5

取代基变化

~1 ~35



$C_8 H_6 N_2 O_3$

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

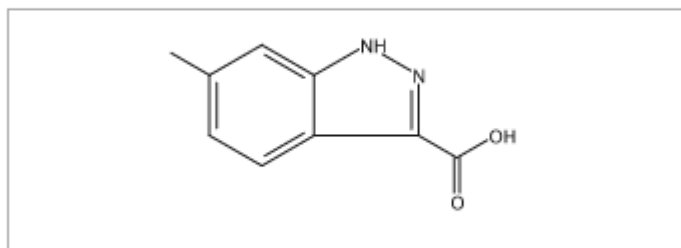
▶ Key Physical Properties

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-

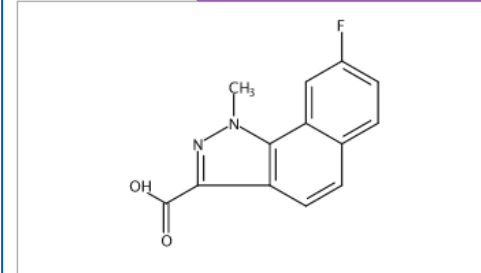
▶ Key Physical Properties

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：

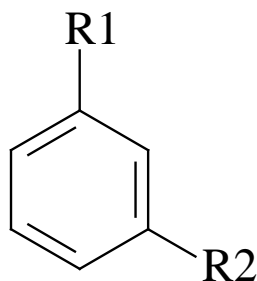
获得片段或整体结构与被检索结构相似的结果，母体结构可以被取代，也可以被改变

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

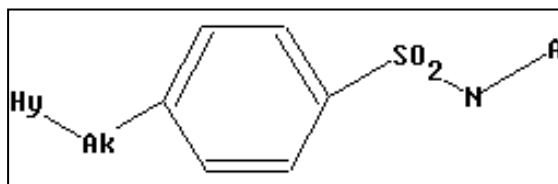
Markush检索

- 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

Get Markush patents where the structure(s) are:


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

OK

Cancel

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

Markush检索



WELCOME Helen Zhu

Explore ▾ Saved Searches ▾ SciPlanner Save Print Export

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

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

Analyze Refine Categorize Sort by: Accession Number ▾ ↓ Display Options

0 of 1969 References Selected

Analyze by: Document Type

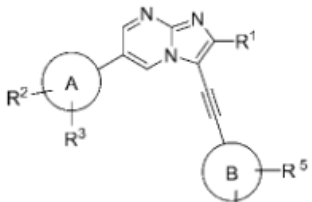
Patent	1969
Journal	1

Show More

全部是专利

1. **Compounds and methods for anticoagulation therapy**
PATENTPAK
By Allende Rodriguez, Mikel; Hermida Santos, Jose; Montes Diaz, Ramon; Oyarzabal Santamarina, Julen
From PCT Int. Appl. (2016), WO 2016120432 A1 20160804. | Language: English, Database: CAPLUS
The invention relates to certain compds. that are inducers of Heat shock 70 kDa protein 1A/1B (HSPA1A/B) and their use for anticoagulation therapy; and to a method for anticoagulation therapy that comprises the administration of one of these inducer compds. It has been here proved that induction of Heat shock 70 kDa protein 1A/1B by administration of one of these inducer compds. has antithrombotic effects without accelerating or altering bleeding time.

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



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

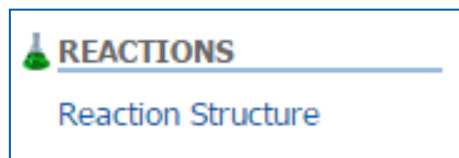
提纲

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

SciFinder检索选项——反应检索

- 反应检索方法

结构式



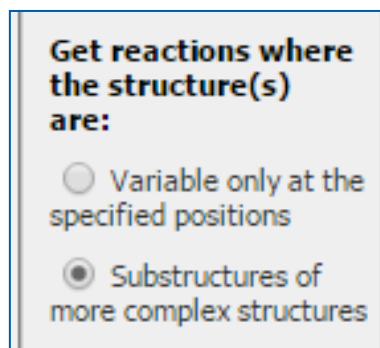
- 常用获取方法

已知物质：由物质获取反应

已知文献：从文献中获取反应

精确结构反应检索

亚结构反应检索



反应绘制工具

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

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

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

SciFinder反应检索——精确反应检索

The screenshot displays the SciFinder Structure Editor interface. The main workspace shows a chemical reaction: nitrobenzene (reactant) is converted to aniline (product). The search panel on the right is titled "Drawing Editor:" and has three radio buttons: "Structure", "Reaction" (which is selected), and "Markush". Below this, the section "Get reactions where the structure(s) are:" contains two radio buttons: "Variable only at the specified positions" (which is selected and highlighted by a purple callout box) and "Substructures of more complex structures". The status bar at the bottom shows the chemical formula $C_7H_7NO_2 \cdot C_7H_9N$ and the reaction ID 137.14 . 107.16.

精确反应检索

反应检索结果

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

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

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

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

~102 100%
~122

Overview

Steps/Stages

1.1 R:NaBH₄, C:1832616-28-0, C:Ru, S:H₂O, S:THF, 45 min, 25°C

Notes

solid-supported catalyst, ruthenium supported on porous organic polymer used, reusable catalyst, sealed tube used, scalable, Reactants: 1, Reagents: 1, Catalysts: 2, Solvents: 2, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Fabrication of Ruthenium Nanoparticles in Porous Organic Polymers: Towards Advanced Heterogeneous Catalytic Nanoreactors

获取相似反应

选择相似反应的相似限制：

Broad：仅反应中心相似

Medium：反应中心及附属原子和键

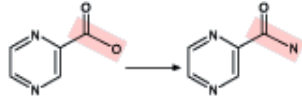
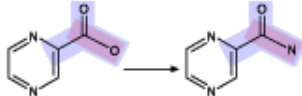
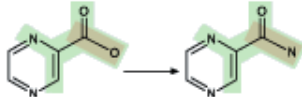
Narrow：反应中心及扩展的原子和键

Get Similar Reactions ?

Retrieve similar reactions from:

- All reactions
- Current answer set

Include this level of similarity:

- Broad - Reaction centers only (2934)

- Medium - Reaction centers plus adjacent atoms and bonds (109)

- Narrow - Reaction centers plus extended atoms and bonds (95)


按照反应类型排序

Group by: Transformation ▾ Sort by: Frequency ▾ ↓

▾ 0 of 560 Reactions Selected

1. Reduction of Nitro Compounds to Amines
538 Reactions

$$\text{R-NO}_2 \longrightarrow \text{R-NH}_2$$

2. Reduction of Nitro to Azo Compounds
11 Reactions

$$\text{Ar-NO}_2 \longrightarrow \text{Ar-N=N-Ar}$$

3. Reduction of Nitro to Azoxy Compounds
11 Reactions

$$\text{Ar-NO}_2 \longrightarrow \text{Ar-N}^+\text{=N-Ar} \text{O}^-$$

更精确的查找需要的反应

反应检索结果的筛选

获得特定物质做还原剂的反应

REACTIONS ? Get References Tools Send to SciPlann

Analyze Refine

Analyze by: ?
Reagent

H ₂	148
NaBH ₄	51
N ₂ H ₄ ·H ₂ O	43
KOH	17
CO	16
HCO ₂ H	16
NH ₄ ⁺ ·HCO ₂ ⁻	16
H ₂ O	14
N ₂ H ₄	14
NaOH	14

Show More

Group by: No Grouping Sort by: Relevance ↓

0 of 512 Reactions Selected Page: 1 of 11

1. View Reaction Detail Link Similar Reactions

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

Overview

Steps/Stages

1.1 R:NaBH₄, C:1832616-28-0, C:Ru, S:H₂O, S:THF, 45 min, 25°C

Notes

solid-supported catalyst, ruthenium supported on porous organic polymer used, reusable catalyst, sealed tube used, scalable, Reactants: 1, Reagents: 1, Catalysts: 2, Solvents: 2, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Fabrication of Ruthenium Nanoparticles in Porous Organic Polymers: Towards Advanced Heterogeneous Catalytic Nanoreactors

SciFinder囊括最大的反应实验过程合集

Single Step Hover over any structure for more options.



▼ Overview

Steps/Stages

1.1 R:H₂, R:Cs₂CO₃, C:1610424-70-8, C:1034343-98-0 (oxide), S:PhMe, 2 h, 100°C, 1 atm

Notes

solid-supported catalyst, palladium catalyst supported on graphene oxide prepared and used, reusable catalyst, Reactants: 1, Reagents: 2, Catalysts: 2, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Catalyst Enhancement and Recyclability by Immobilization of Metal Complexes onto Graphene Surface by Noncovalent Interactions

[Quick View](#) [Other Sources](#)

By Sabater, Sara et al

From ACS Catalysis, 4(6), 2038-2047; 2014

▼ Experimental Procedure

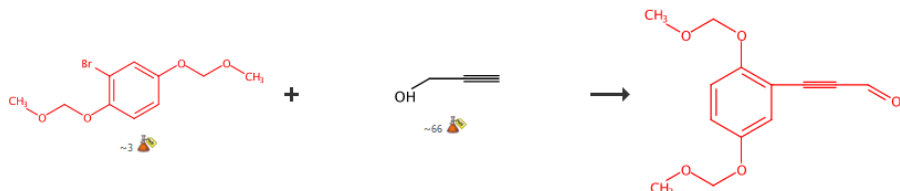


General/Typical Procedure: **General Procedure for Nitroarene Reductions.** Molecular hydrogen was added with a balloon filled with 1 atm of H₂ to a mixture of nitroarene (0.3 mmol), Cs₂CO₃ (0.3 mmol), anisole as internal standard (0.3 mmol), and NHC-Pd-rGO (6 × 10⁻³ mmol, based on metal) in toluene (5 mL). The system was then evacuated and backfilled with H₂ in cycles for three times before putting the reaction vessel in an oil bath at 100°C for 2h. Yields were determined by GC analyses using anisole (0.3 mmol) as internal standard. Products were identified according to spectroscopic data of the commercially available compounds. Entry: 4; Yield 100%.

不用阅读全文，直接获得包含实验过程的反应记录

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: t-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
- 2.4 R: H₂O, R: NH₄Cl, 30 min, rt

Notes

1) key step, alternate catalyst concentration, catalyst (CuI) and temperature, Sonogashira coupling, 2) key intermediate, Swern oxidation, see method shown, Reactants: 2, Reagents: 5, Catalysts: 1, Solvents: 2, 5. Most stages in any one step: 4

References

Synthesis of Bioactive Speciosins G and P from *Hexagonia speciosa*
[Quick View](#) [Other Sources](#)
 By Guerrero-Vasquez, Guillermo A. et al
 From Journal of Natural Products, 77(9), 2029-2036; 2014

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?
- 查免费的Supporting Information? 可能只有图谱。

Experimental Procedure

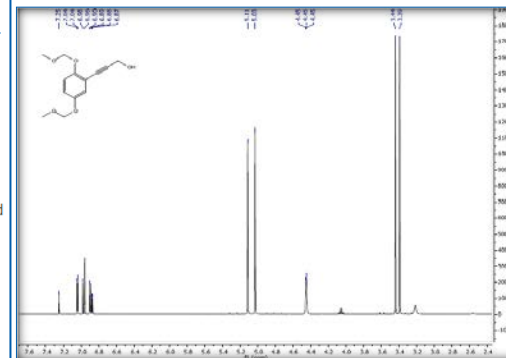


Step 1

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).



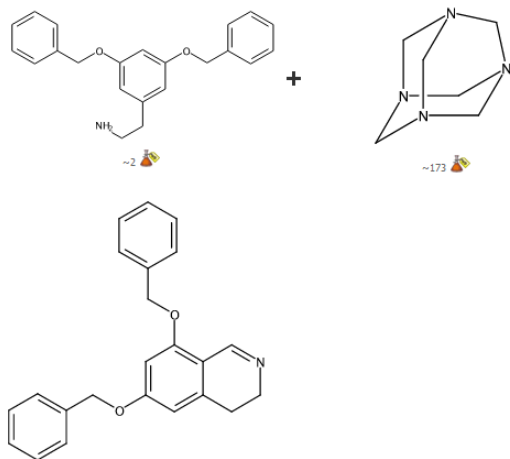
MethodsNow Synthesis

MethodsNow

Asymmetric formal synthesis of schulzeines A and C

By Jang, Jaebong; Jung, Jong-Wha; Ahn, Jaeseung; Sim, Jaehoon; Chang, Dong-Jo; Kim, Dae-Duk; Suh, Young-Ger
From Organic & Biomolecular Chemistry, 10(27), 5202-5204; 2012
Published by Royal Society of Chemistry

Reaction Steps 1 2 3 4 5 6 7 8 9 10 11



多步反应中，原文没有描述
的实验过程以灰色标示

Products	Isoquinoline, 3,4-dihydro-6,8-bis(phenylmethoxy)-, 95%, CAS RN: 1384461-35-1
Reactants	Benzeneethanamine, 3,5-bis(phenylmethoxy)-, CAS RN: 188662-05-7 Hexamethylenetetramine, CAS RN: 100-97-0
Solvents	Trifluoroacetic acid, CAS RN: 76-05-1 Acetic acid, CAS RN: 64-19-7
Procedure	<ol style="list-style-type: none"> 1. Add hexamethylenetetramine (3.1 g, 22.1 mmol) to the mixture of 2-(3,5-bis(benzyloxy)phenyl)ethanamine (2.0 g, 11.0 mmol), AcOH (12 mL) and TFA (3 mL) under argon 2. Stir the mixture for 3 hours at 90°C. 3. Dilute the reaction mixture with H₂O. 4. Basify with potassium carbonate and extract with CH₂Cl₂. 5. Wash the combined organic layers with brine. 6. Dry over MgSO₄ and concentrate in vacuo. 7. Purify the residue by column chromatography on silica gel (5 to 10% EtOAc in hexane) to obtain 6,8-bis(benzyloxy)-3,4-dihydroisoquinoline.
Scale	gram
¹H NMR	(CDCl ₃ , 400 MHz) δ 8.69 (s, 1H), 7.43 - 7.29 (m, 10H), 6.45 (d, <i>J</i> = 1.88 Hz, 2H), 6.36 (s, 1H), 5.05 (s, 2H), 5.04 (s, 2H), 3.67 (t, 2H), 2.65 (t, 2H)
¹³C NMR	(CDCl ₃ , 100 MHz) δ 161.9, 157.7, 155.2, 140.0, 136.3, 128.6, 128.5, 128.1, 128.0, 127.4, 127.1, 111.9, 105.3, 98.5, 70.1, 46.5, 26.0
IR	(thin film, neat) ν _{max} 3062, 3032, 2935, 1736, 1620, 1603, 1575, 1497, 1442, 1377, 1351, 1309 cm ⁻¹
HRMS	(FAB+) calcd for C ₂₃ H ₂₂ N ₂ (M+H ⁺) 344.1651; found 344.1658
Mass Spec	(FAB+) <i>m/z</i> 344 (M+H ⁺)
State	yellow solid
CAS Method Number	3-614-CAS-200055

物质信息

实验过程

图谱信息

保存/导出方法

Print/Export Close

亚结构反应检索

通过C-H活化对苯并噁唑或者恶唑进行烷基化

The screenshot displays the 'Structure Editor' and 'R-group Definitions' dialog. The Structure Editor shows a benzimidazole-like structure with an R1 group. The R-group Definitions dialog is open, showing the R1 definition as 'O, S' and a periodic table where the 'S' atom is highlighted. A purple arrow points from the 'R' button in the Structure Editor toolbar to the 'S' atom in the periodic table.

R-group Definitions

R1 = O, S

▼ Atoms

H																			He
Li	Be										B	C	N	O	F				Ne
Na	Mg										Al	Si	P	S	Cl			Ar	
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br		Kr	
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I		Xe	
Cs	Ba	*	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At		Rn	
Fr	Ra	**																	

▼ Variables

▼ Shortcuts

Close

Cancel

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
 - SciPlanner
- SciFinder常见问题及解决

SciPlanner使用简介

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

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

Overview

Steps/Stages

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

Notes

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

References

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

进入SciPlanner 新建文件

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

Workspace Edit View GoTo

- New
- Open
- Save
- Duplicate
- Import
- Export
- Print
- Close

Your Workspace is empty.

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

SciPlanner使用简介

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Synthesize 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

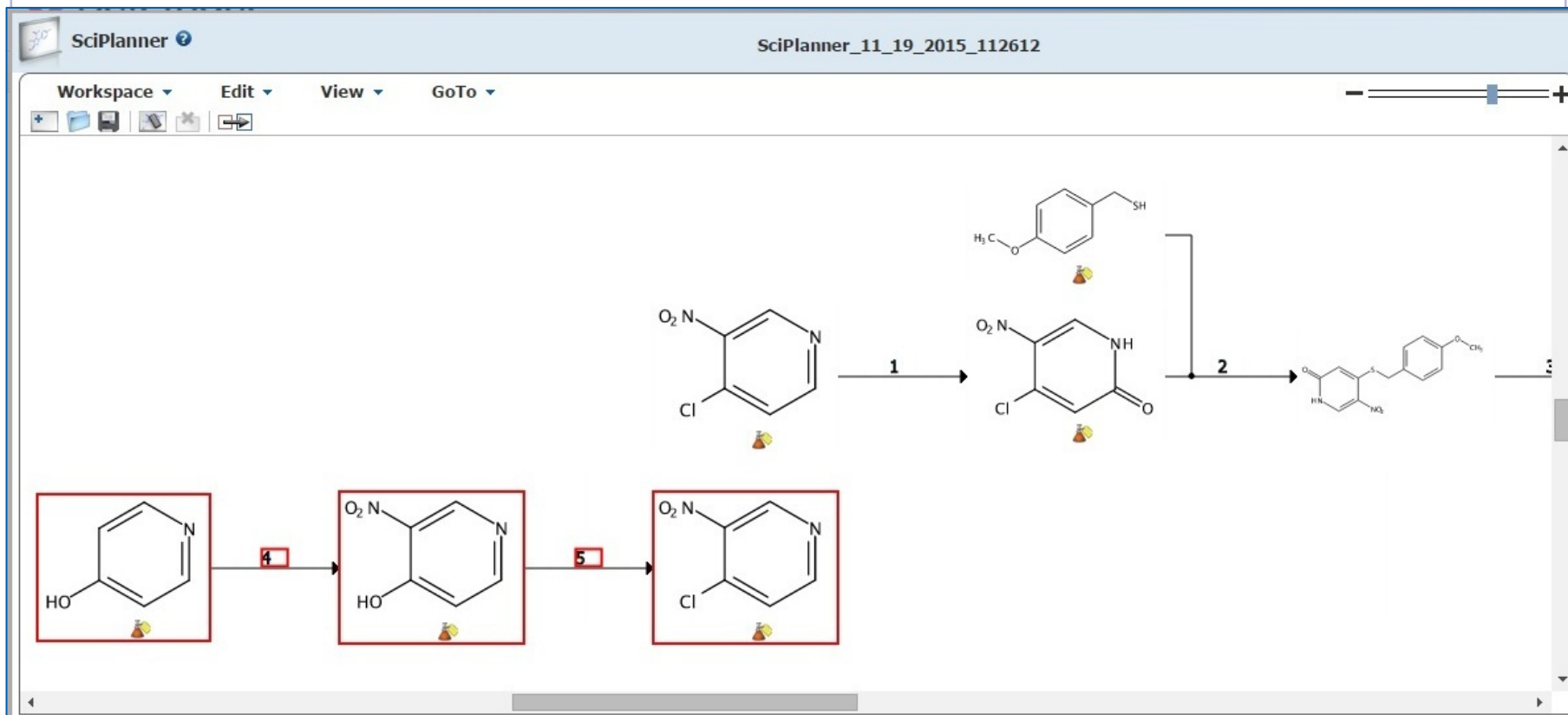
2 Steps Hover over any structure for more options.

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. The main workspace shows a chemical reaction sequence: 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).

Three callout boxes provide instructions:

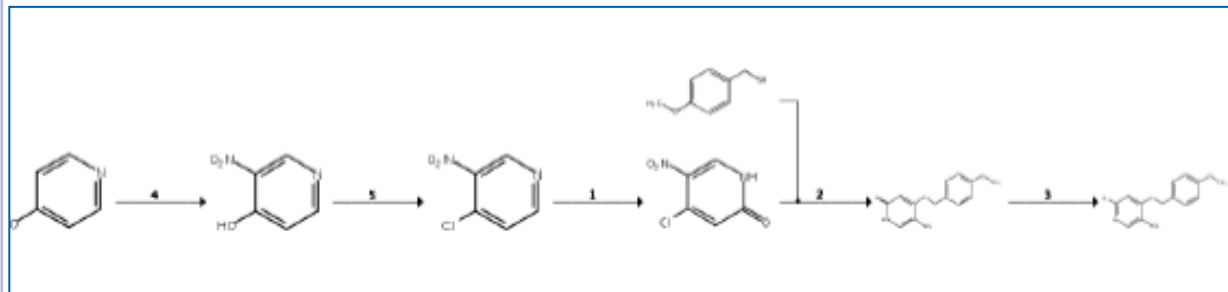
- Click **Workspace**, select **Export** to export results.
- Use the mouse to drag two identical structures to overlap, merging the two reactions.
- Select an appropriate output format to output results.

The **Export** dialog box is open, showing the following options:

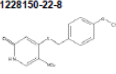
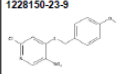
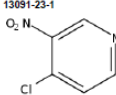
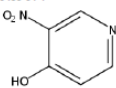
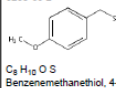
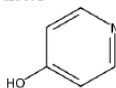
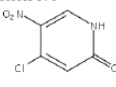
- For:**
 - Portable Document Format (*.pdf)
 - Citations (*.ris)
 - Image (*.png)
- Saving Locally:**
 - SciPlanner eXchange (*.pkx)
- Details:**
 - File Name:** * (Required) SciPlanner_11_19_2015_112612
 - Title:** (Empty field)
- Include:**
 - SciPlanner Image
 - Reaction Details
 - Substance Details
 - Reference Details

Buttons: **Export** and **Cancel**

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>C₅H₃ClN₂O₂ Pyridine, 4-chloro-3-nitro-</p> <p>Related Info: ~ 391 References Reactions ~ 190 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>C₅H₅N 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

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 two dropdown menus for 'Area of Research' and 'Job Title', both currently set to 'Select one'.
- USERNAME AND PASSWORD--**: Contains fields for Username (with a '7ps' tip), Password, and Re-enter Password.
- SECURITY INFORMATION--**: Features a dropdown menu for 'Security Question' (set to 'Select one') and an 'Answer' field (with a 'Why?' tip).

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

请注意：

1. 必须输入真实姓名和**学校**邮箱。
2. 用户名必须是唯一的，且包含 5-15 个字符。它可以只包含字母或字母组合、数字和/或以下特殊字符：

- - (破折号)
- _ (下划线)
- . (句点)
- @ (表示“at”的符号)

3. 密码必须包含 7-15 个字符，并且至少**包含三种以下字符**：

- 字母
- 混合的大小写字母
- 数字
- 非字母数字的字符 (例如 @、#、%、&、*)

例：abc@123

4. 从下拉列表中选择一个密码提示问题并给出答案。
单击 Register (注册)。

如何获取SciFinder账号

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.
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- I will not use any automated program or script for extracting or downloading CAS data, or any other systematic retrieval of data.
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- 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.

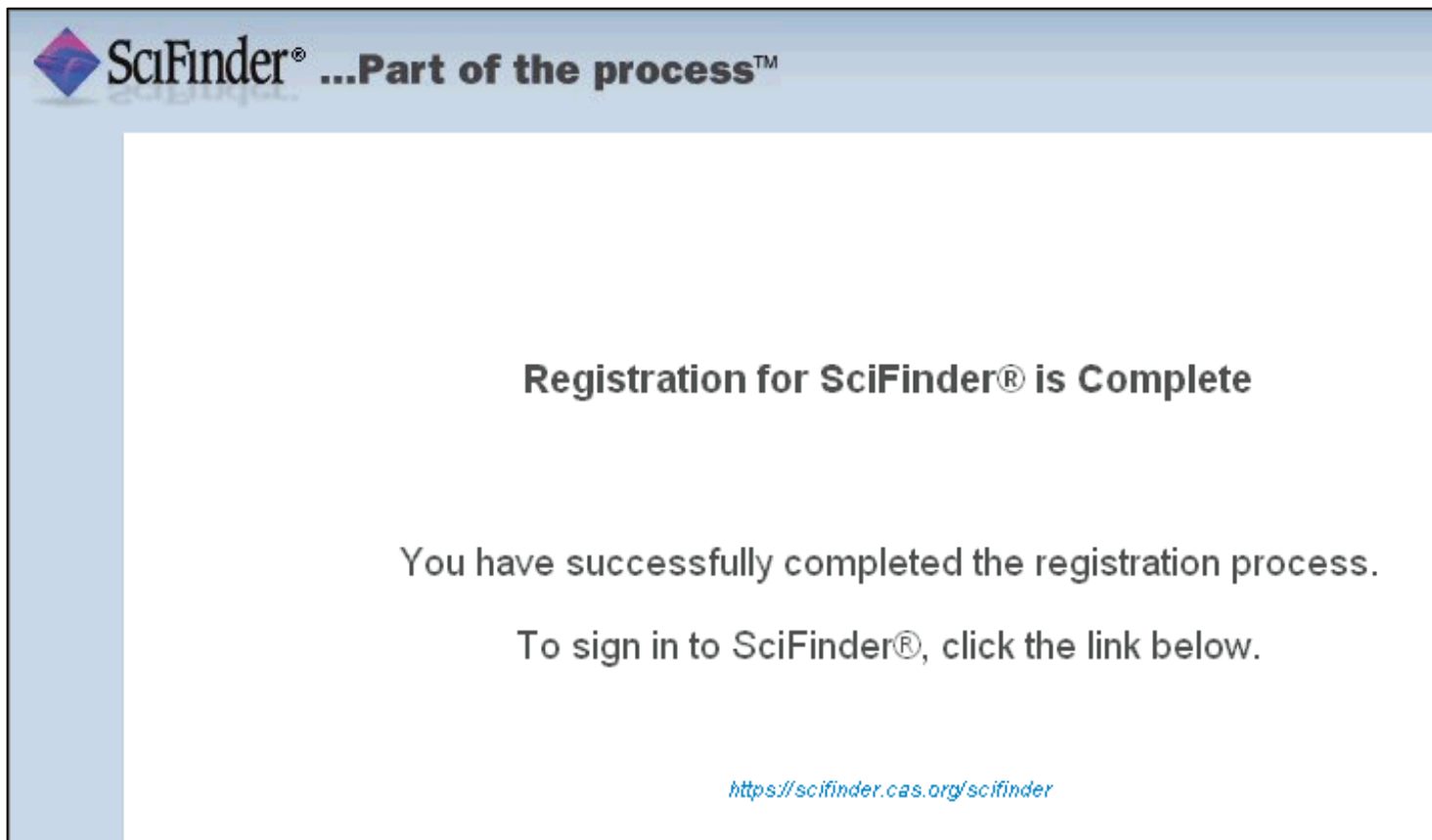
If you need assistance at any time, consult the key contact at your organization.

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注意垃圾邮件、未知邮件、订阅邮件等来自@cas.org的邮件



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

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- 严禁账号分享
- 严禁将账号用于非学术研究

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