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如何使用SciFinder获取科技信息

中国科技大学

2017.3.21



提纲

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

美国化学文摘社—Chemical Abstracts Service

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

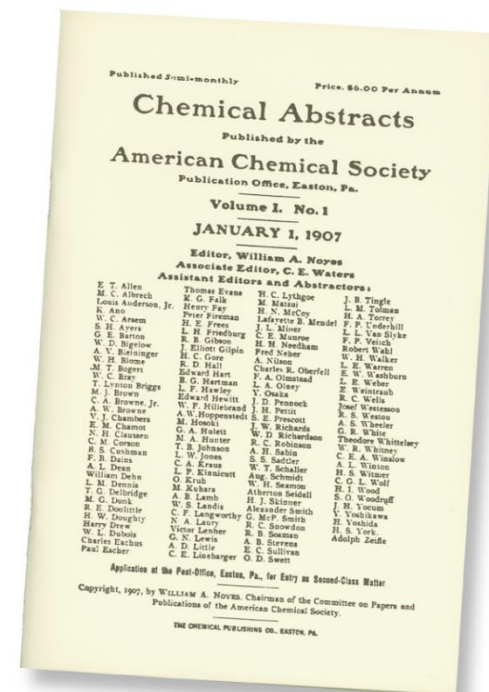


1907年，信息的汇集、管理发生了重大的变化



威廉·诺伊斯
(William A. Noyes)

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



CAS——构建最高质量的化学数据库



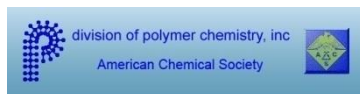
arXiv.org

Aldrichimica ACTA

ACS
chemical
biology



BEILSTEIN JOURNAL
OF ORGANIC CHEMISTRY



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

ACS Chemical
Neuroscience



THE JOURNAL OF
PHYSICAL CHEMISTRY
Letters

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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


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 |
|------------------|-------------|

Indexing


Carbohydrates (Section33-9)

Section cross-reference(s): 34, 63

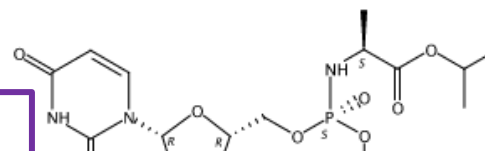
Concepts

| | |
|-------------------------------|----------------------|
| 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。

CAS最新动向—解决方案

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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...

Disclosed he...
phosphate, R...
methods of...
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 for 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'-methyluridine with

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

(19) World Intellectual Property Organization
International Bureau

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

WIPO PCT

(51) International Patent Classification:
C07H 19/10 (2006.01) C07H 19/13 (2006.01)
C07H 19/20 (2006.01) A61K 31/702 (2006.01)
C07H 19/11 (2006.01) A61K 31/706 (2006.01)
C07H 19/213 (2006.01) A61K 31/708 (2006.01)
C07H 19/067 (2006.01) A61P 31/14 (2006.01)
C07H 19/073 (2006.01)

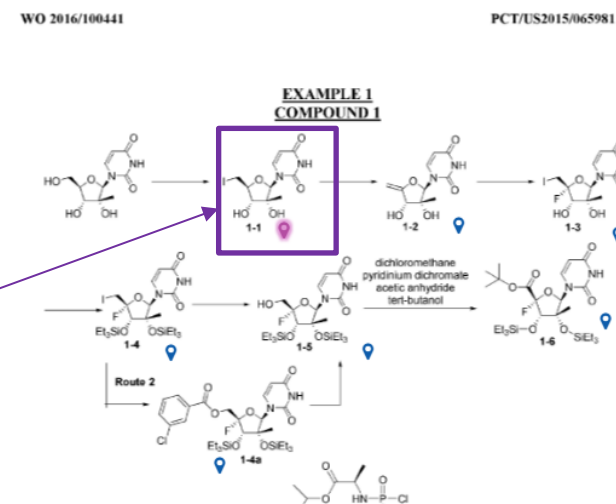
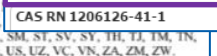
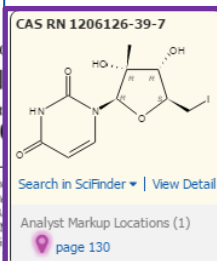
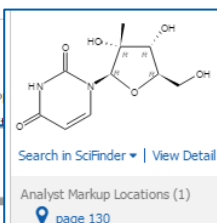
(81) Designated States (kind of national protection):
AO, AT, AU, AZ, BA, BB, BG, CA, CH, CL, CN, CZ, DE, DK, EC, EE, EG, ES, FI, FR, GB, GR, HK, HU, IL, IN, JP, KZ, LA, LC, LK, LT, LU, LV, MA, MD, ME, MK, MN, MW, MX, MY, NG, NI, NO, NZ, OM, PA, PE, PG, PH, PL, PT, RO, RU, SE, SG, SK, SL, SM, ST, SV, SY, TH, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW.

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

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

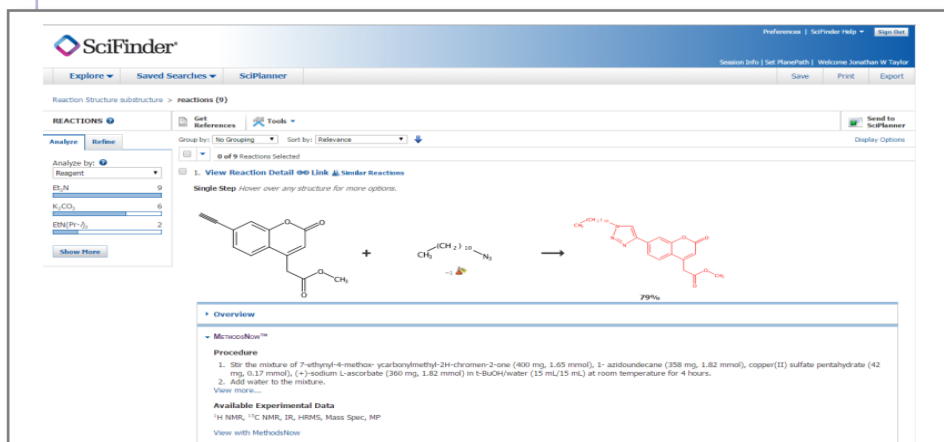
(25) Filing Language:
English

(84) Designated States (unless otherwise indicated, for every kind of regional protection available): ARIPO (BW, GH, GM, KE, LU, MG, MW, MZ, NA, NG, SD, SI, SZ, TZ, UG, ZM, ZW), EPO (AL, AT, AU, BA, BB, BG, CA, CH, CL, CN, CZ, DE, DK, EC, EE, EG, ES, FI, FR, GB, GR, HK, HU, IL, IN, JP, KZ, LA, LC, LK, LT, LU, LV, MA, MD, ME, MK, MN, MW, MX, MY, NG, NI, NO, NZ, OM, PA, PE, PG, PH, PL, PT, RO, RU, SE, SG, SK, SL, SM, ST, SV, SY, TH, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW).

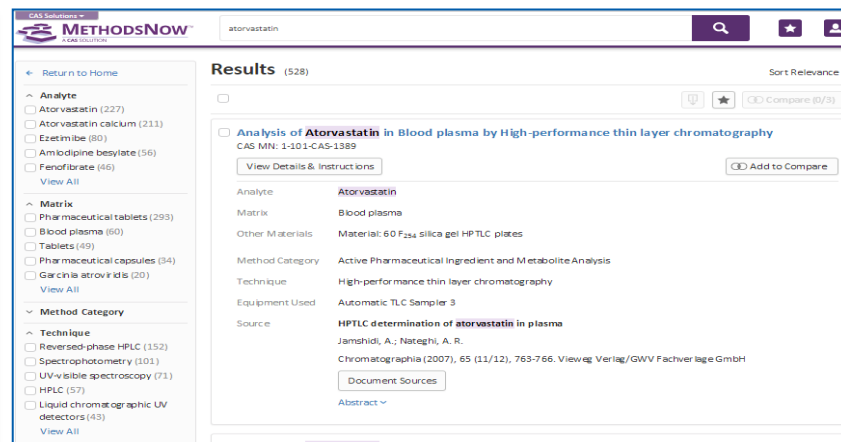


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- CAS于2016年2月正式发布MethodsNow™
- 最大方法信息合集
- 来自重要的全文信息资源：CAS高质量标引、全新的、增值的方法
- 满足合成和分析研究工作者的需求



嵌入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

SciFinder覆盖的数据库



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检索完，请点击退出

工具栏

The screenshot shows the SciFinder web interface. At the top, there is a header bar with the SciFinder logo, navigation links (Explore, Saved Searches, SciPlanner), and user information (Welcome Helen Zhu). A search bar is prominently displayed in the center. To the left, a sidebar lists various search categories: REFERENCES (Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, Tags), SUBSTANCES (Chemical Structure, Markush, Molecular Formula, Property, Substance Identifier), and REACTIONS (Reaction Structure). On the right, there is a section for 'SAVED ANSWER SETS' listing several saved searches, and a 'KEEP ME POSTED' section. Annotations in Chinese point to specific features: '检索完，请点击退出' points to the 'Sign Out' button; '工具栏' points to the top navigation bar; '检索入口' points to the search bar; '已保存的结果集' points to the 'SAVED ANSWER SETS' section; and '定题追踪' points to the 'KEEP ME POSTED' section.

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Welcome Helen Zhu

Explore | Saved Searches | SciPlanner

REFERENCES

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

SUBSTANCES

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

REACTIONS

- Reaction Structure

REFERENCES: RESEARCH TOPIC

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

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SAVED ANSWER SETS

- CSF1R
- jmc
- EP 19870107847
- Daclatasvir-1
- SUB result
- EX result
- MF result
- polymer1
- polymer1
- structure search
- Autosaved Substance Set

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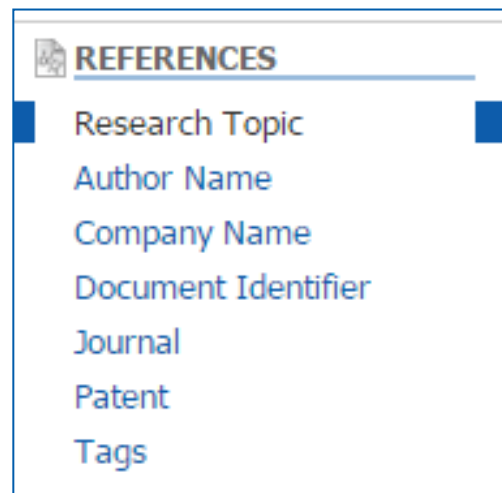
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- 机构名检索
- 文献标识符检索
- 期刊名称和专利信息（公开号，申请号等）
- 从物质，反应获得文献



■ 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 '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, the 'REFERENCES' section is active, listing search criteria: Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, and Tags. Below this, the 'SUBSTANCES' section lists 'Chemical Structure' and 'Markush'. The main search area on the right is titled 'REFERENCES: RESEARCH TOPIC' and contains a search box with the text 'prepare of 3D graphene'. Below the search box, it provides 'Examples:' such as 'The effect of antibiotic residues on dairy products' and 'Photocyanation of aromatic compounds'. A blue 'Search' button is positioned below the examples, followed by a link to 'Advanced Search'.

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

REFERENCES

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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

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

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REFERENCES | Get Substances | Reactions | Citations | Tools

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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**
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**
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. $H_2/C_2H_4O_2@Ar$ 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...

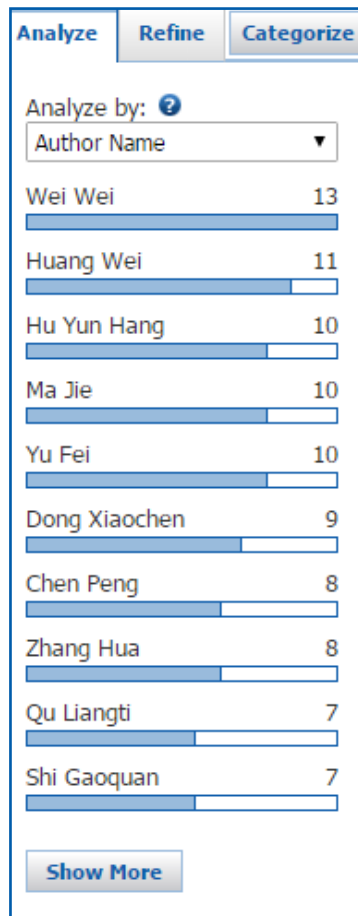
3. **N-P-O co-doped high performance 3D graphene prepared through red phosphorous-assisted "cutting-thin" technique: A universal synthesis and multifunctional applications**
By Zhao, Yufeng; Huang, Shifei; Xia, Meirong; Rehman, Sarish; Mu, Shichun; Kou, Zongkui; Zhang, Zhi; Chen, Zhaoyang; Gao, Faming; 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.

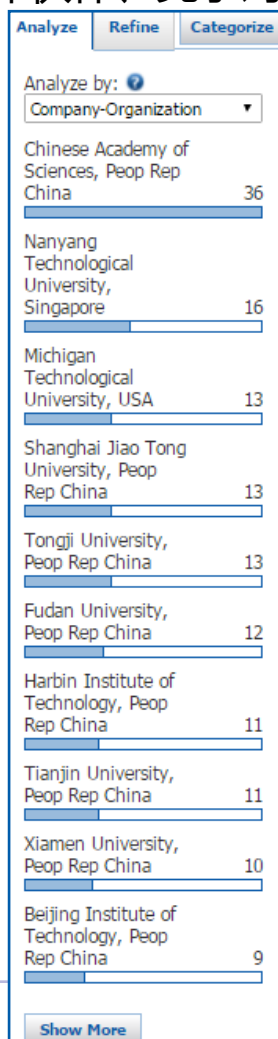
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文献检索结果的Analyze

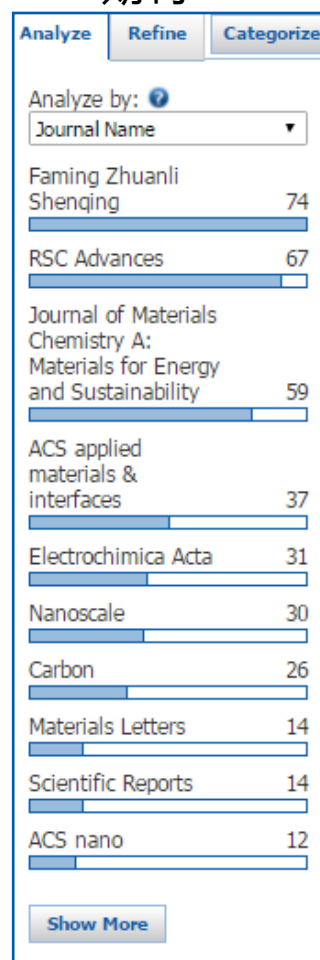
本领域研究人员



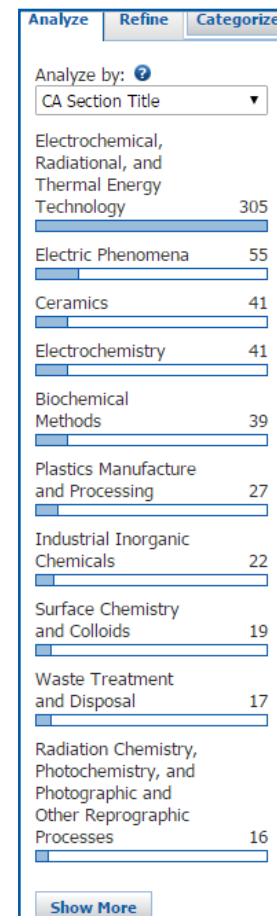
本领域研究机构、 合作伙伴、竞争对手



期刊



涉及学科领域

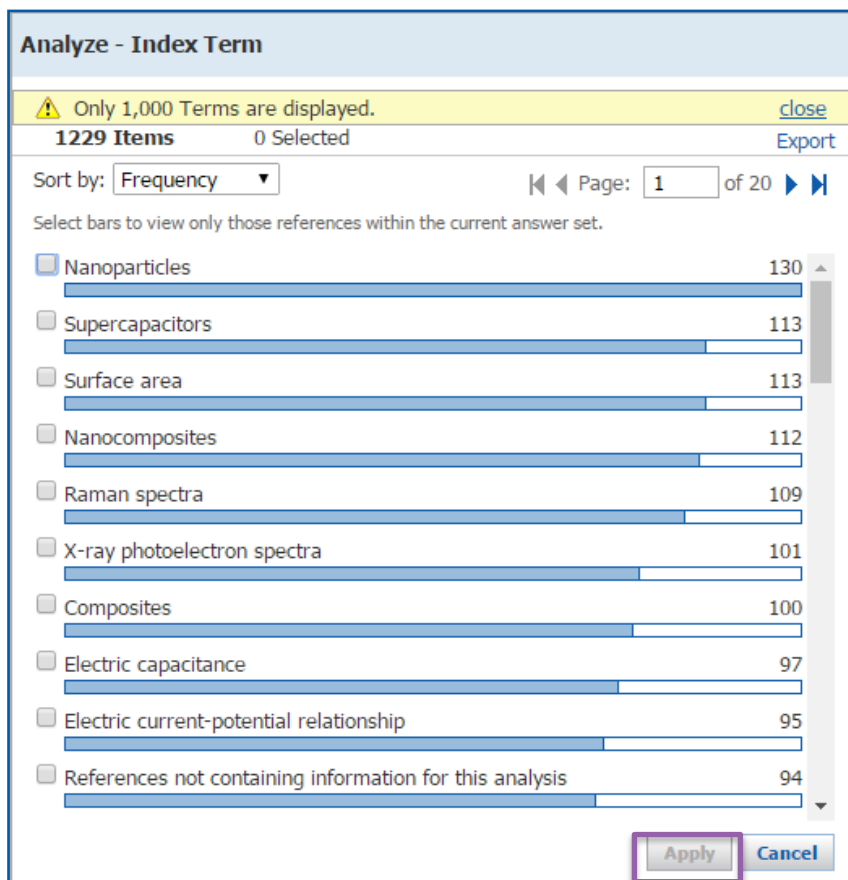
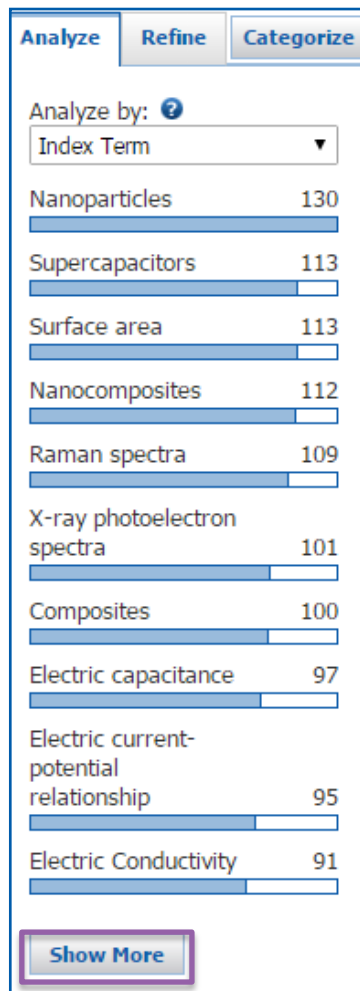


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文献检索结果的Analyze

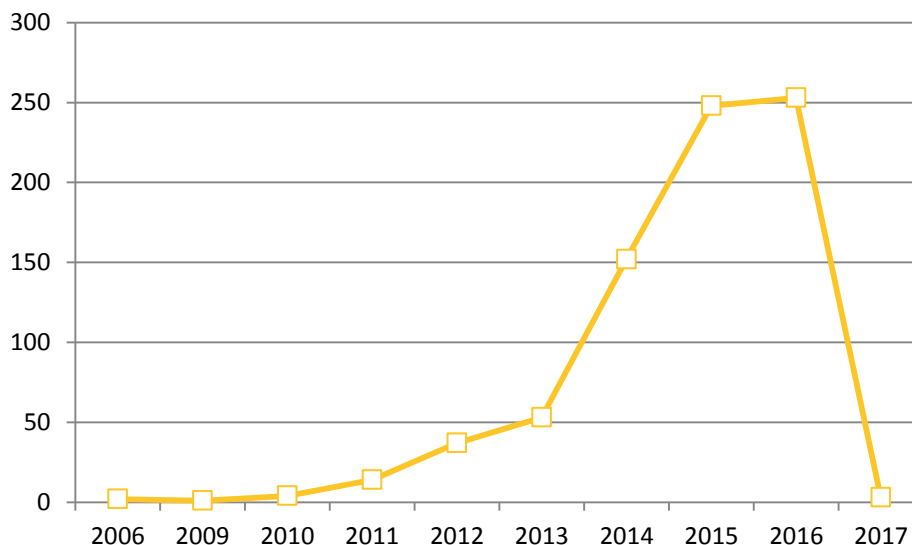
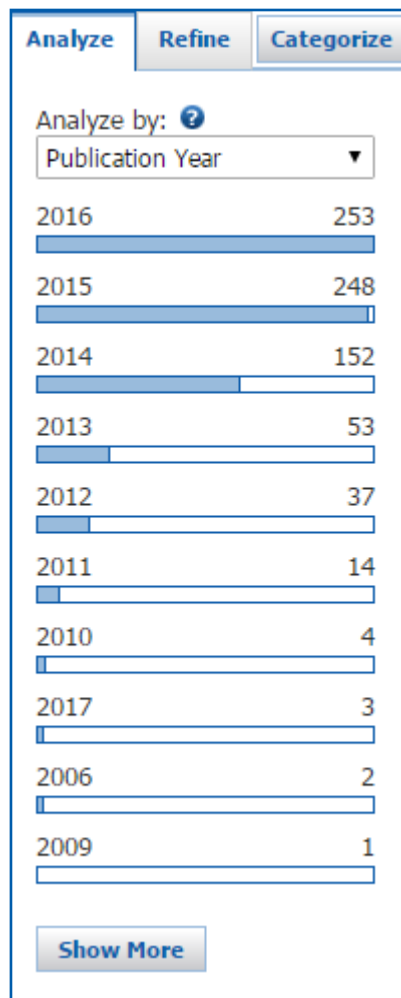
Index Term :

帮助用户了解涉及到的重要技术术语，并修正检索词



选择感兴趣的内容，点击Apply

文献检索结果的Analyze



Publication Year: 分析领域发展趋势

文献检索结果的Refine

AnalyzeRefineCategorize

Refine by: ?

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

Company Name
china

Examples:
3M
DuPont

Refine

Get SubstancesGet ReactionsGet Related CitationsTools

Create Keep Me Posted AlertSend to SciFinder

Sort by: Accession Number

0 of 534 References Selected

Display Options

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 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

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

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.

| 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

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.

aphene" > 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 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 carbon foam...

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

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Export:

☒ All
☐ Selected
☐ Range

Example: 2-20

For:

Citation Manager

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☐ Quoted Format (*.txt)
☐ Tagged Format (*.txt)

Offline review

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

Saving locally

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* Required

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

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
- 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

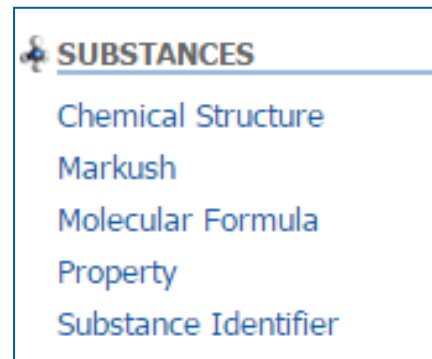
提纲

- 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

 **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。

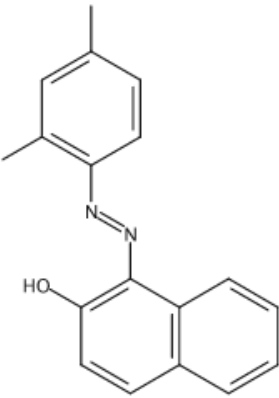
物质标识符包括CAS RN和化学名称，化学名称可以是通用名称、商品名、俗名。

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



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

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

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

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

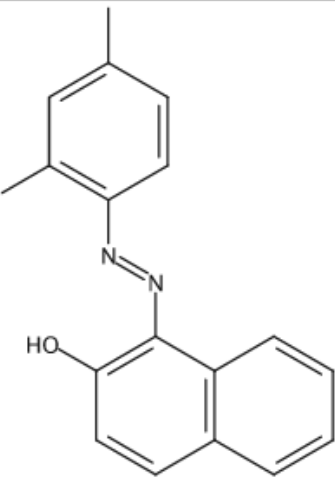
Melting Point (Experimental)
Value: 166 °C

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...](#)



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物质详情

通过物质获得文献

分析化学
生物研究

Get References

Retrieve references for:

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Limit results to:

| | |
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| <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.

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

¹H NMR Properties

Proton NMR Spectrum

Value

See spectrum

Condition

Note

(13) BIORAD

Notes

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

PREDICTED PROPERTIES

Biological Chemical Density Lipinski Structure Related Thermal

Lipinski Properties

Freely Rotatable Bonds

3

Condition

Note

(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)

Notes

(21) Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994-2015 ACD/Labs)

预测数据与预测谱图

PREDICTED SPECTRA



SCIFINDER®
A CAS SOLUTION

物质检索——Property explore

The screenshot shows the SciFinder web interface for property exploration. The browser address bar displays <https://scifinder.cas>. The SciFinder logo is prominently displayed. The 'Explore' tab is selected, and the 'SUBSTANCES' section is active. A dropdown menu for 'Select Property...' is open, listing various properties such as Boiling Point, Density, and Molecular Weight. 'Molecular Weight' is highlighted. Below the dropdown, a search criteria input field shows '250-400' with examples '44, 25-35, >125'. A blue 'Search' button is located at the bottom center of the interface.

Search criteria: 250-400
Examples: 44, 25-35, >125

Search

寻找分子量在250-400之间的物质

物质结果集的筛选——Refine

SUBSTANCES ?

Get References Get Reactions Get Commercial Sources Tools ▾

Analyze **Refine**

Sort by: CAS Registry Number ▾

☐ 0 of 45142315 Substances Selected

Refine by: ?

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

Structure Editor:

Java Non-Java

Click to Edit

Search type: **Exact Structure**

Only retrieve substances

1. **1986293-22-4** 🔍

~0

C₁₅ H₁₇ Br N₂
3-Pyridinamine, 2-bromo-*N*-(3-phenylbutyl)-
▶ **Key Physical Properties**

2. **1986293-21-3** 🔍

~0

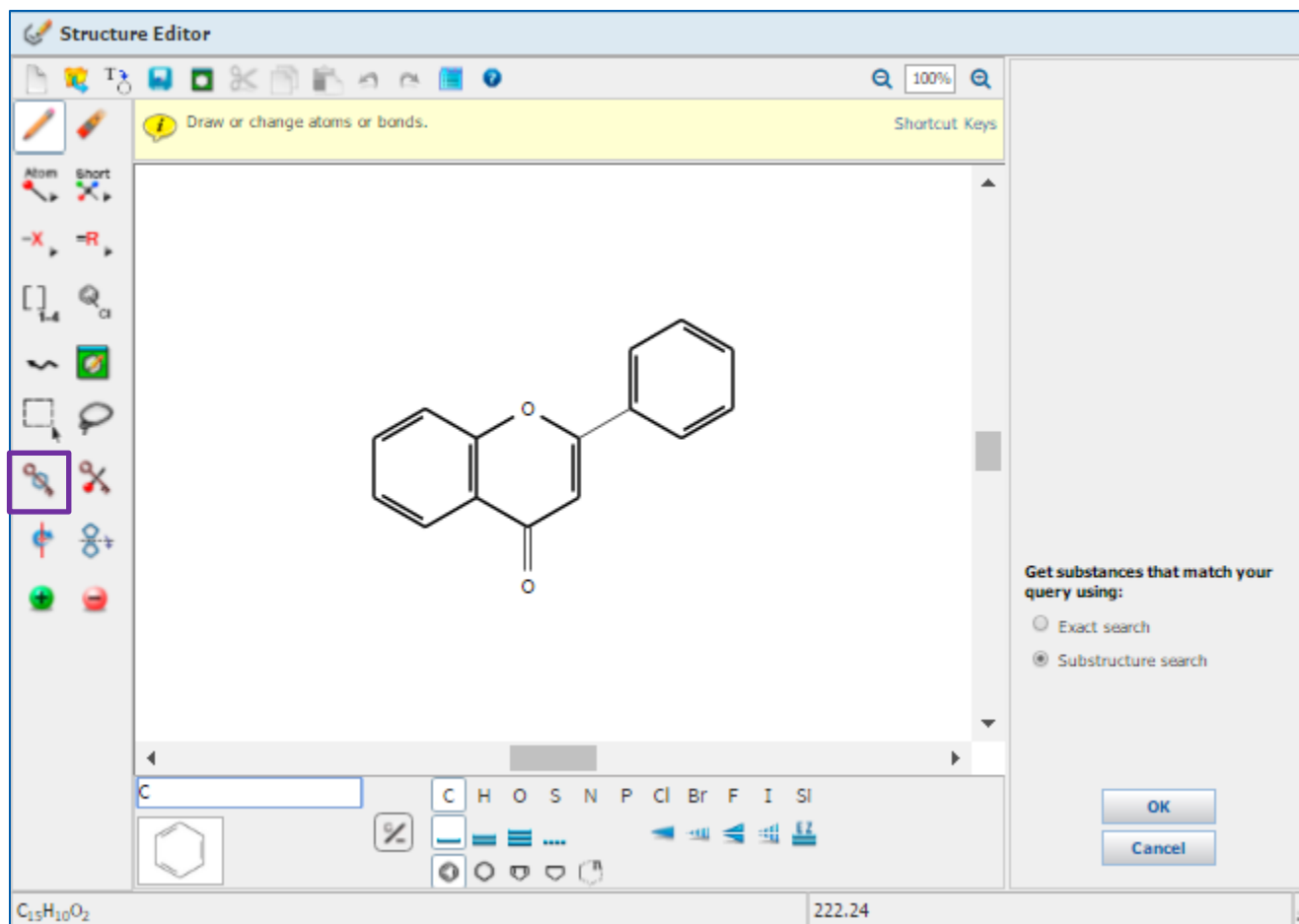
C₁₁ H₁₆ Cl F₂ N₃ O
4-Pyrimidinamine, *N*-(2-chloroethyl)-*N*-(2,2-difluoroethyl)-6-ethoxy-5-methyl-
▶ **Key Physical Properties**

4. **1986293-16-6** 🔍

5. **1986293-14-4** 🔍

4500多万个结构，
如何筛选黄酮类物质？

物质结果集的筛选——Refine



锁环工具：避免在被锁定的环结构上出现新的环结构

SUBSTANCES ?

Analyze Refine

Refine by: ?

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

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

物质检索结果集

Explore ▾ Saved Searches ▾ SciPlanner

Property "Predicted - Molecular Weight, ..." > substances (45142315) > refine "substructure" (16901)

SUBSTANCES ⓘ

Get References Get Reactions Get Commercial Sources Tools ▾

Analyze Refine

Sort by: Relevance ▾

0 of 16901 Substances Selected

Refine by: ⓘ

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

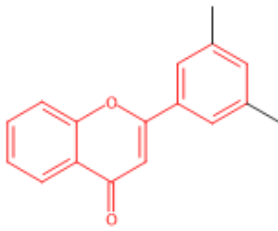
Structure Editor:

Java Non-Java

Click image to change structure or view detail.
Search type: Substructure

1. 1373355-19-1

~3

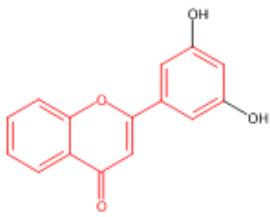


$C_{17}H_{14}O_2$
4/4'-1-Benzopyran-4-one, 2-(3,5-dimethylphenyl)-

Key Physical Properties

2. 912915-64-1

~6 ~3

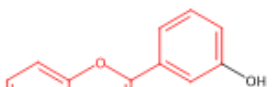


$C_{15}H_{10}O_4$
4/4'-1-Benzopyran-4-one, 2-(3,5-dihydroxyphenyl)-

Key Physical Properties

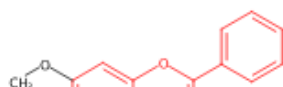
4. 6665-68-5

~38 ~7



5. 22395-22-8

~269 ~67



从4500多万个结构中
筛选出16901个黄酮类物质

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

金属盐：金属离子和阴离子间用点 (.) 分开

1. **151-21-3**

(Component: 151-41-7)

~84904 ~276

Chemical structure diagram showing the structure of Sulfuric acid monododecyl ester sodium salt (1:1). The structure consists of a central sulfur atom (S) double-bonded to two oxygen atoms (O) and single-bonded to a hydroxyl group (OH) and an ester group (O-CH2-CH2-...-CH2-CH3). The ester chain is represented as (CH2)11-CH3. Below the structure, the sodium ion (Na+) is indicated.

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

Key Physical Properties

- Regulatory Information
- Spectra
- Experimental Properties

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

REFERENCES

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

SUBSTANCES

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

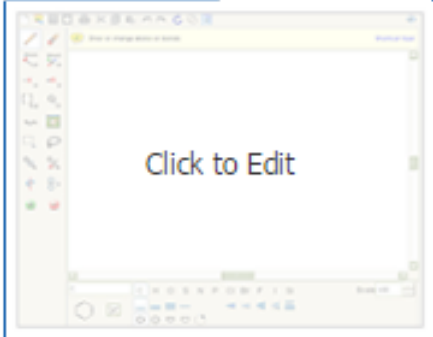
REACTIONS

- 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

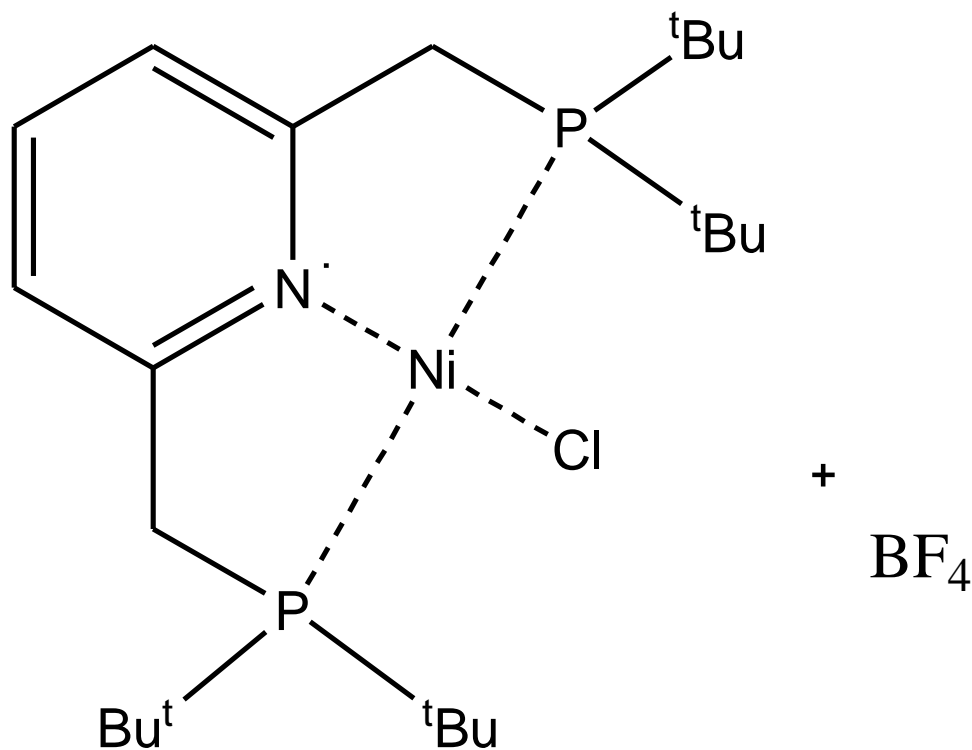
 Advanced Search ☒ Always Show

物质检索——结构

The image shows the SciFinder Structure Editor interface with various tools labeled in Chinese. The labels are as follows:

- 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 (Negatron)
- 常用基团 (Common Group)
- R基团定义工具 (R-Group Definition Tool)
- 可变位置连接工具 (Variable Position Connection Tool)
- 模版工具 (Template Tool)
- 索套选择工具 (Loop Selection Tool)
- 原子锁定工具 (Atom Locking Tool)
- 镜面旋转工具 (Mirror Rotation Tool)
- 结构检索选择 (Structure Search Selection)
- 单双键，RS构型，不确定键定义工具 (Single/Double Bond, RS Configuration, Uncertain Bond Definition Tool)
- C原子和单键恢复工具 (C-Atom and Single Bond Restoration Tool)
- 常见环，多元环工具 (Common Ring, Polycyclic Ring Tool)

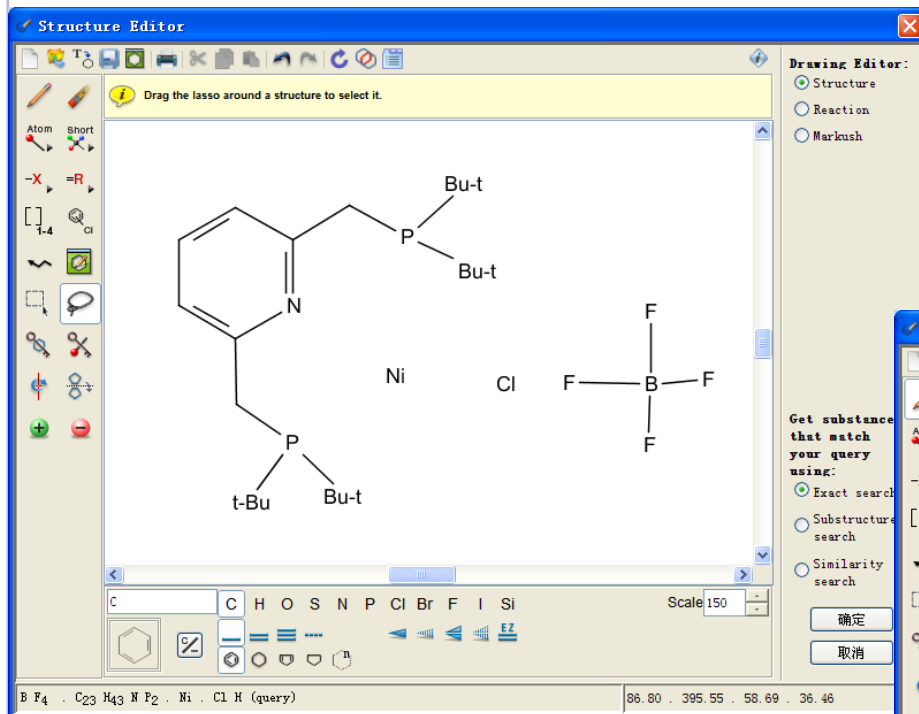
物质检索——精确结构检索



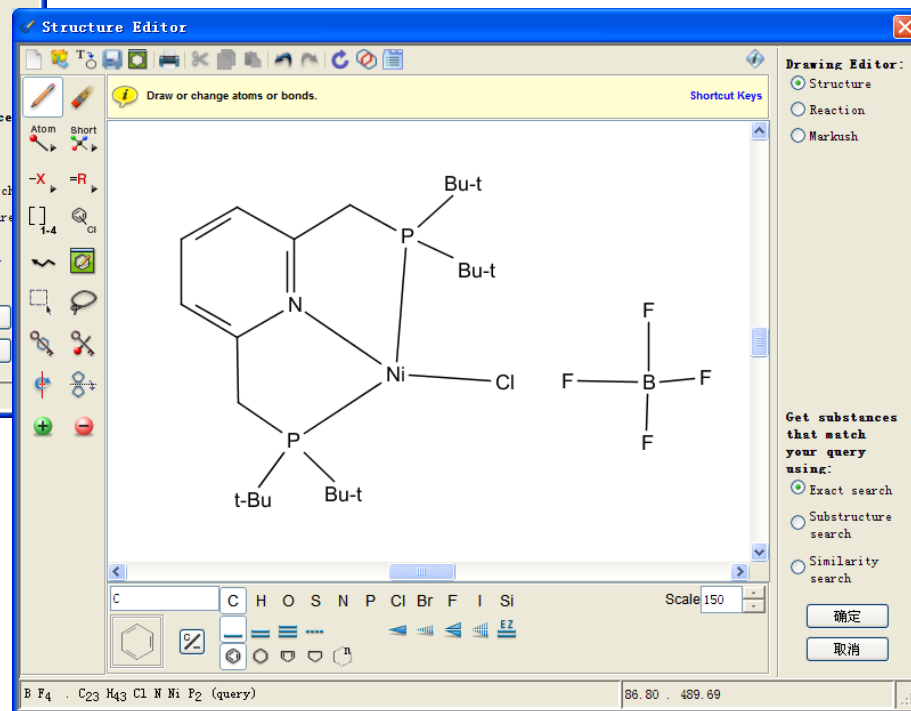
该结构中包含：

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

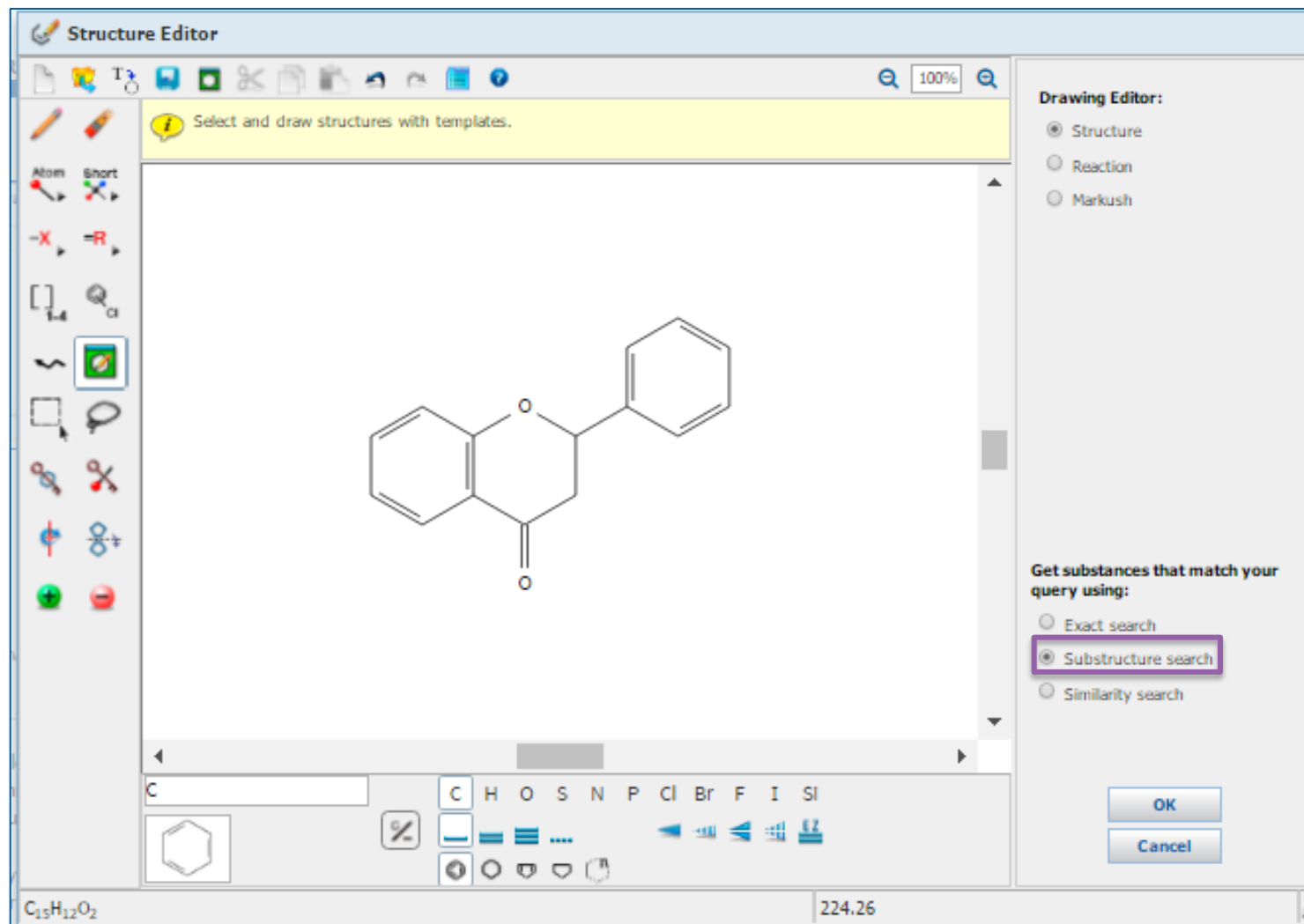


物质检索——精确结构检索

- 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

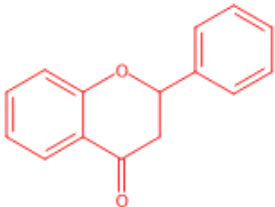


物质检索——亚结构检索

0 of 23824 Substances Selected

1. 487-26-3

~2093

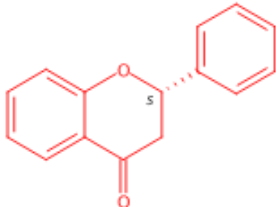


C₁₅H₁₂O₂
4-phenyl-4H-benzopyran-4-one, 2,3-dihydro-2-phenyl-

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

2. 17002-31-2

~244



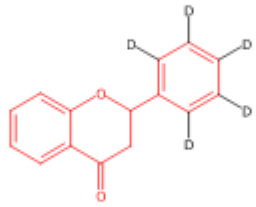
Absolute stereochemistry...Rotation (-).

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

► **Key Physical Properties**
Experimental Properties

10. 146196-91-0

~1



C₁₅H₇D₅O₂
4-(2,3,4,5-tetradeuteriophenyl)-4H-benzopyran-4-one, 2,3-dihydro-2-(phenyl-d₄)- (9CI)

Spectra

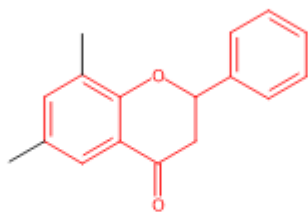
同位素

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-

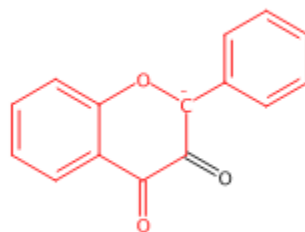
Key Physical Properties

Experimental Properties

295. 780723-19-5

~0

离子



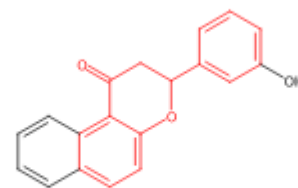
$C_{15}H_9O_3$

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

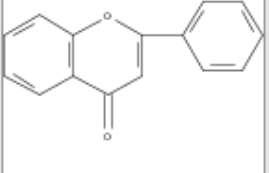
化学结构的再次限定

Analysis Refine

Refine by: ⓘ

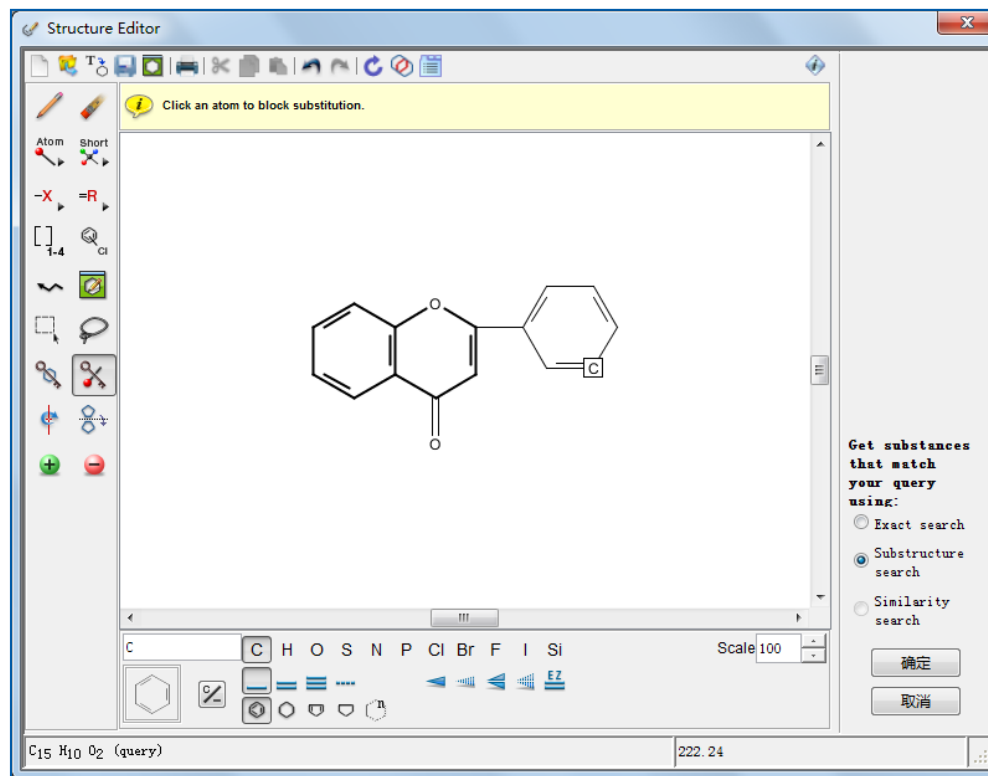
- ☒ Chemical Structure
- ☐ Isotope-Containing
- ☐ Metal-Containing
- ☐ Commercial Availability
- ☐ Property Availability
- ☐ Property Value
- ☐ Reference Availability
- ☐ Atom Attachment

Chemical Structure:



Click image to change structure or view detail

Search type: **Substructure**



环锁定

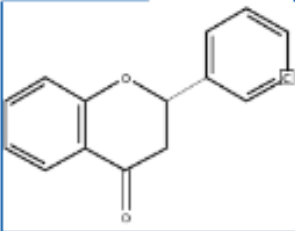


原子锁定

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

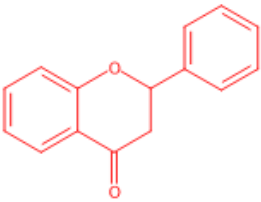
Get References Get Reactions Get Commercial Sources Tools

Sort by: Relevance

0 of 13826 Substances Selected

1. **487-26-3**

~2093

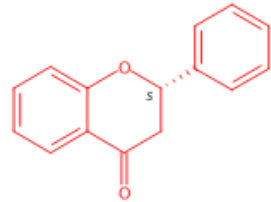


C₁₅H₁₂O₂
4H-1-Benzopyran-4-one, 2,3-dihydro-2-phenyl-

Key Physical Properties
Regulatory Information
Spectra
Experimental Properties

2. **17002-31-2**

~244



Absolute stereochemistry., Rotation (-).

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

Key Physical Properties
Experimental Properties

4. **104550-32-5**

~3

5. **75524-43-5**

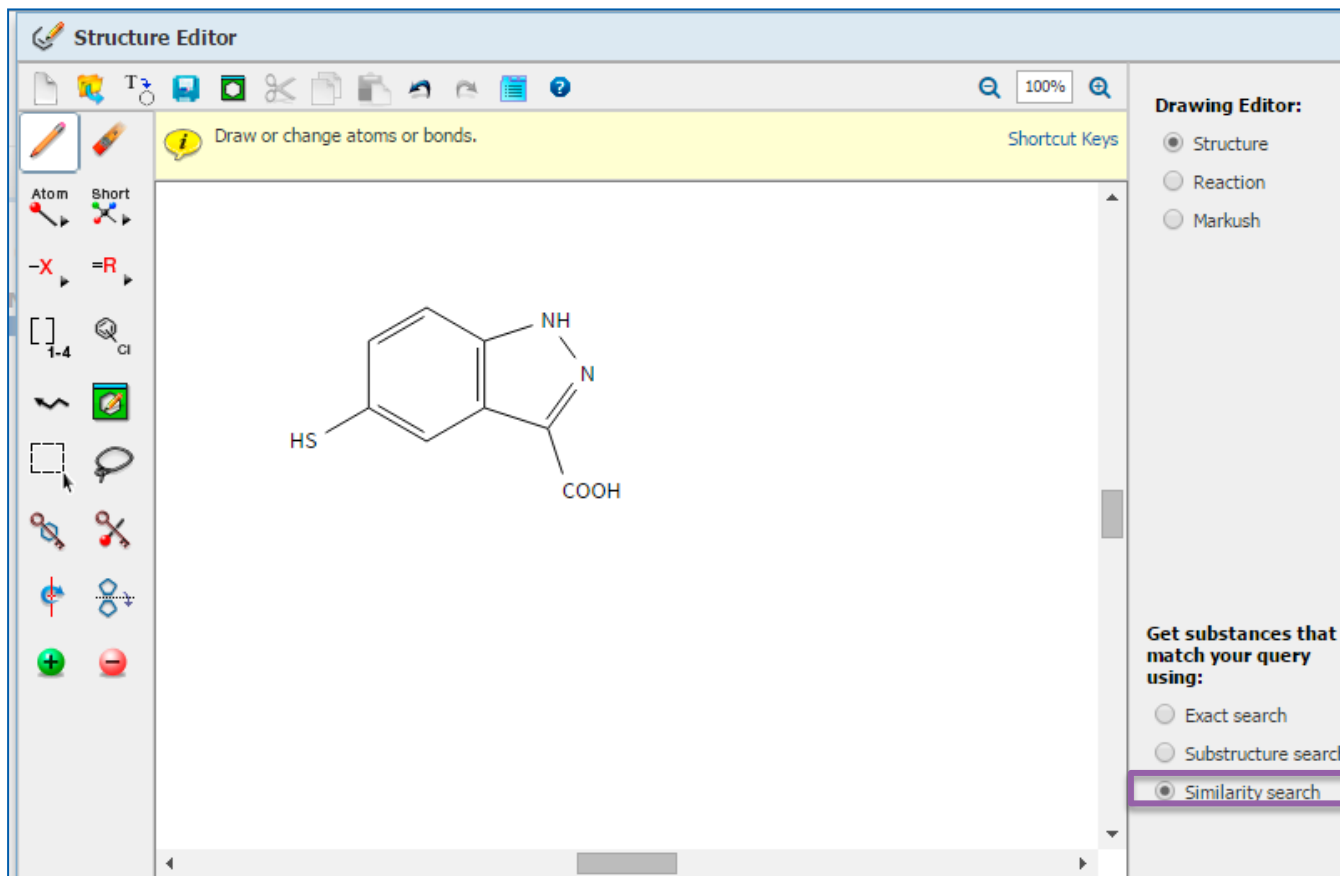
~2

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 |

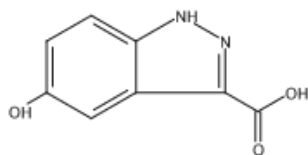
Get Substances

评分越高，相似度越高，结构越相似

Score: 88

☐ 1. 885518-94-5

~1 ~35



$C_8 H_6 N_2 O_3$

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

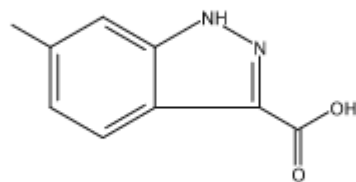
► Key Physical Properties

取代基变化

Score: 86

☐ 5. 858227-12-0

~7 ~41



$C_9 H_8 N_2 O_2$

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

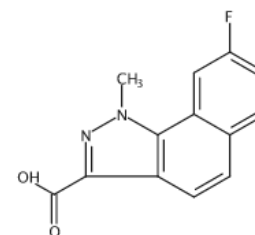
► Key Physical Properties

取代基位置变化

Score: 65

☐ 541. 1100422-

~1



$C_{13} H_9 F N_2 O_2$

1H-Benz[7]indazole-3-carboxylic acid, 8-fluoro-1-methyl-

► Key Physical Properties

母体结构变化



SCIFINDER®
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物质检索——相似结构检索

- 相似结构检索：

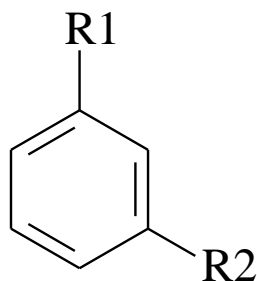
获得片段或整体结构与被检索结构相似的结果，母体结构可以被取代，也可以被改变

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

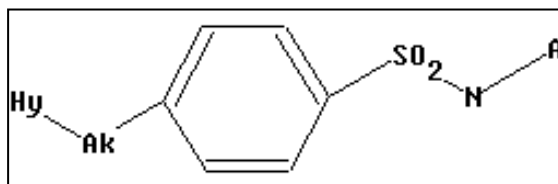
Markush检索

- 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%

Atom Short

-X =R

1-4 Cl

Hy-Ak

SO₂-N-A

Drawing Editor:

- ☐ Structure
- ☐ Reaction
- ☒ Markush


Get Markush patents where the structure(s) are:

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

OK Cancel

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

Markush检索

 **SCIFINDER**
A CAS SOLUTION

Welcome Helen Zhu

Explore ▾ Saved Searches ▾ SciPlanner Save Print Export

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

REFERENCES ⓘ

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

Analyze Refine Categorize

Sort by: Accession Number ▾

0 of 1969 References Selected

Page: 1 of 99

Analyze by: Document Type ▾

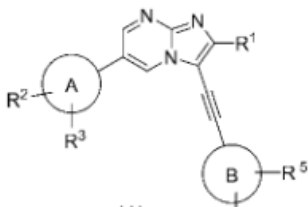
Patent 1969

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^aR^b, SO₃H, SO₂NR^aR^b, SO₂R^b, or NR^aSO₂R^b; R^a, R^b (same...

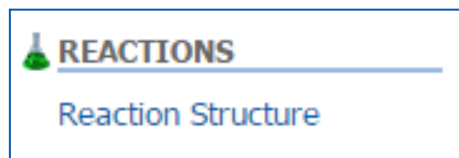
提纲

- 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



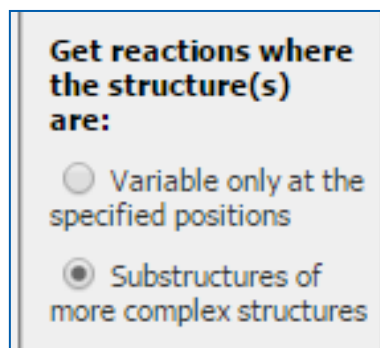
- 常用获取方法

已知物质：由物质获取反应

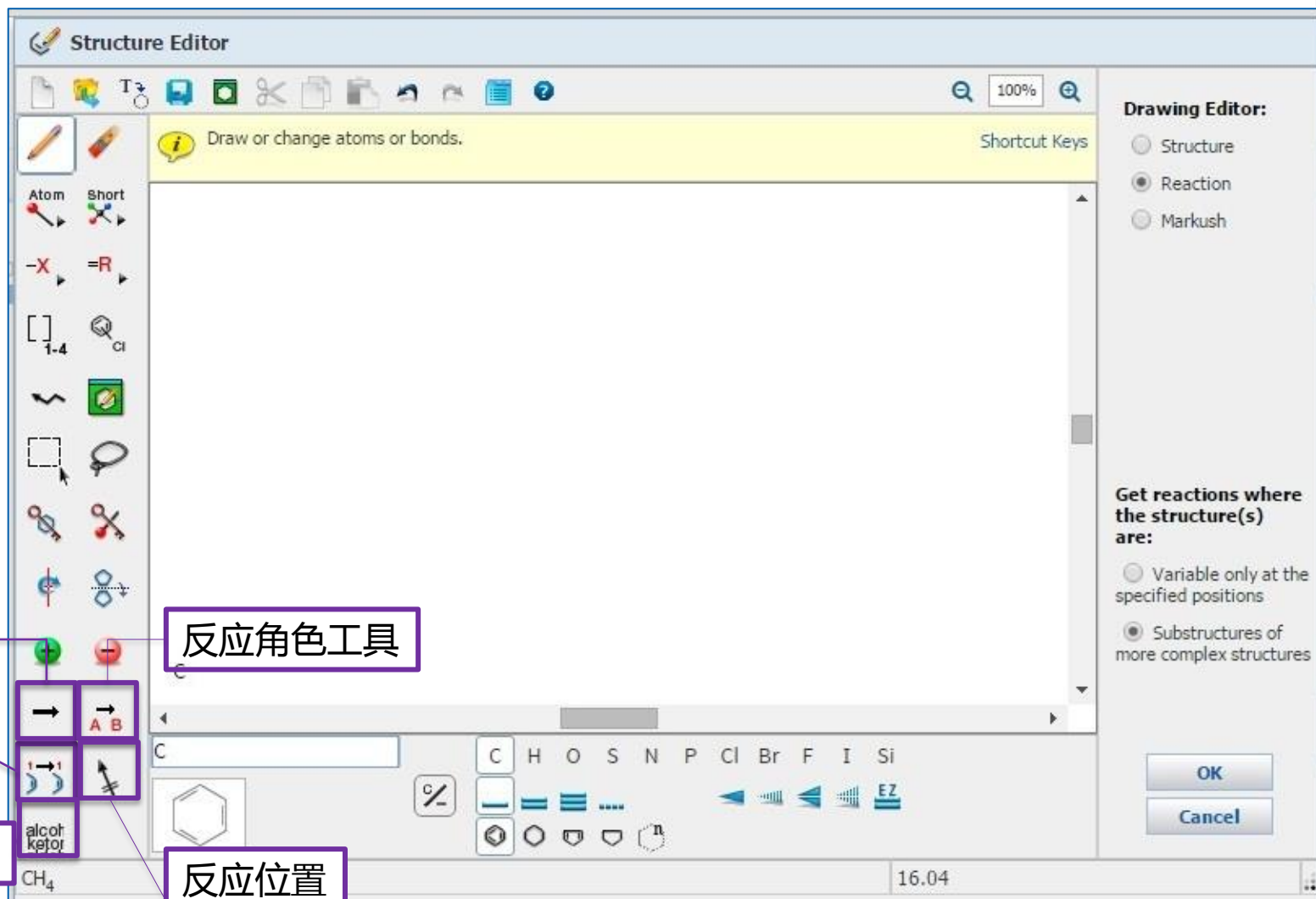
已知文献：从文献中获取反应

精确结构反应检索

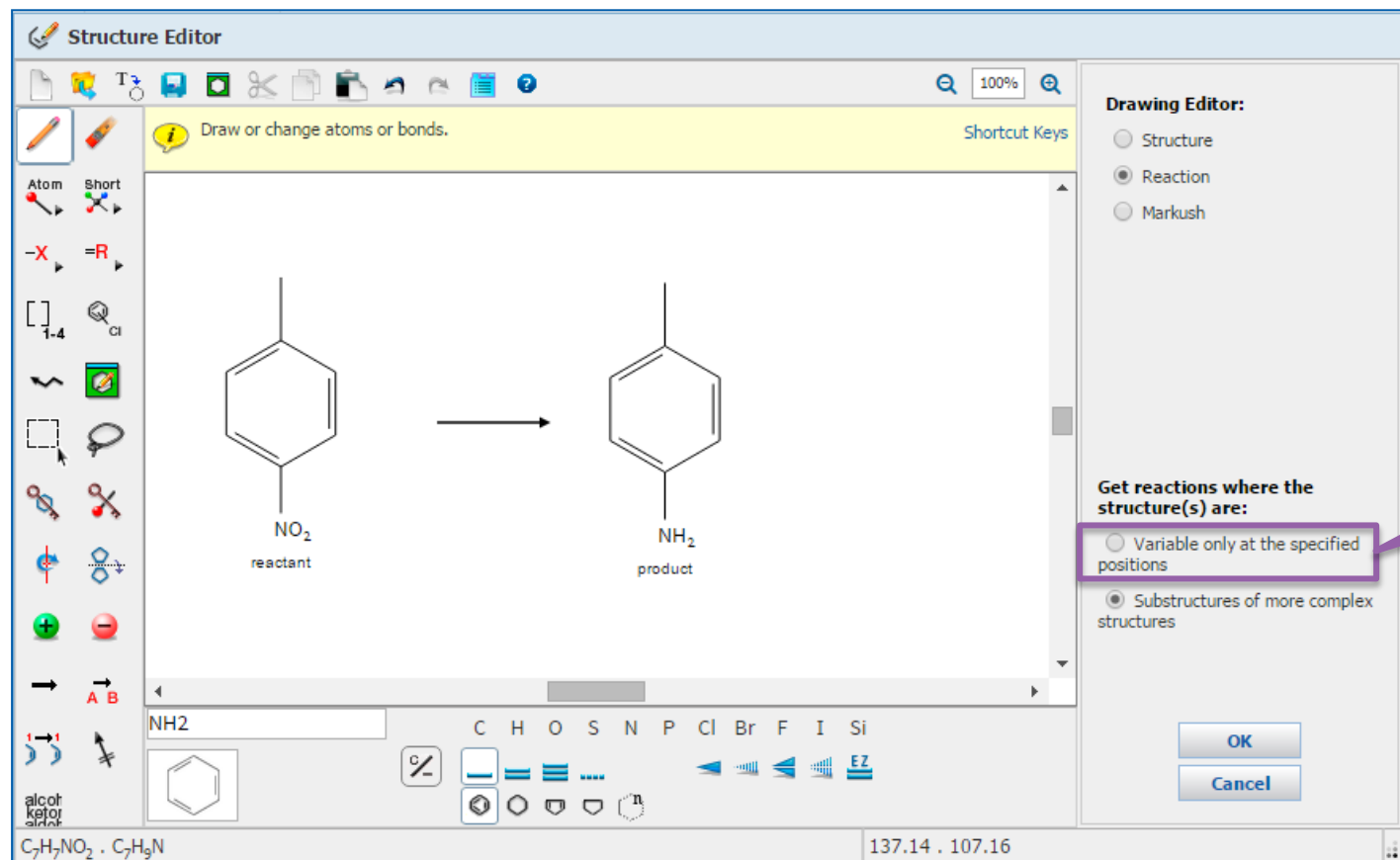
亚结构反应检索



反应绘制工具



SciFinder反应检索——精确反应检索



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。

Get References Tools

Group by: No Grouping Document Transformation Sort by: Relevance Selected Send to SciPlane Display Options 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

获取相似反应

选择相似反应的相似限制：

Broad：仅反应中心相似

Medium：反应中心及附属原子和键

Narrow：反应中心及扩展的原子和键

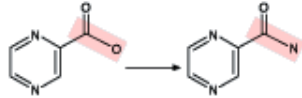
Get Similar Reactions ?

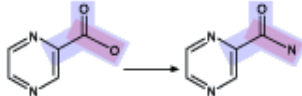
Retrieve similar reactions from:

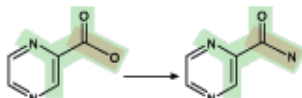
- ☒ All reactions
- ☐ Current answer set

Include this level of similarity:

- ☒ Broad - Reaction centers only (2934)


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


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



Get Reactions

Cancel

按照反应类型排序

Group by: Transformation ▼ Sort by: Frequency ▼ ↓

☐ 0 of 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

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

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

Analyze Refine

Analyze by: Reagent

H₂ 148

NaBH₄ 51

N₂H₄·H₂O 43

KOH 17

CO 16

HCO₂H 16

NH₄⁺·HCO₂⁻ 16

H₂O 14

N₂H₄ 14

NaOH 14


Show More

Group by: No Grouping Sort by: Relevance

0 of 512 Reactions Selected

1. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.



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

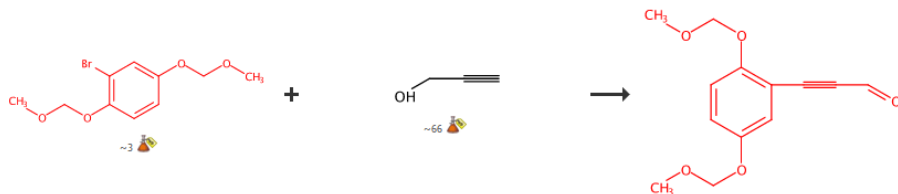


General/Typical Procedure: **General Procedure for Nitroarene Reductions.** Molecular hydrogen was added with a balloon filled with 1 atm of H₂ to a mixture of nitroarene (0.3 mmol), Cs₂CO₃ (0.3 mmol), anisole as internal standard (0.3 mmol), and NHC-Pd-rGO (6 × 10⁻³ mmol, based on metal) in toluene (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: 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, 3) 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:

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Experimental Procedure

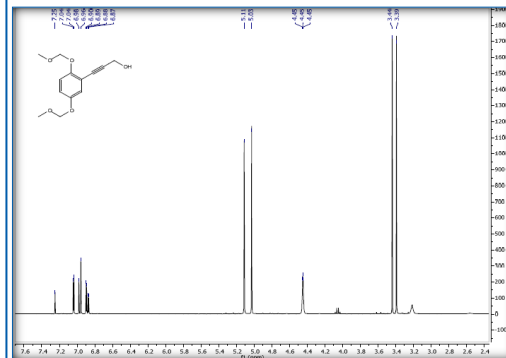


Step 1

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-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), 95.58 (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).



SCIFINDER
 A CAS SOLUTION

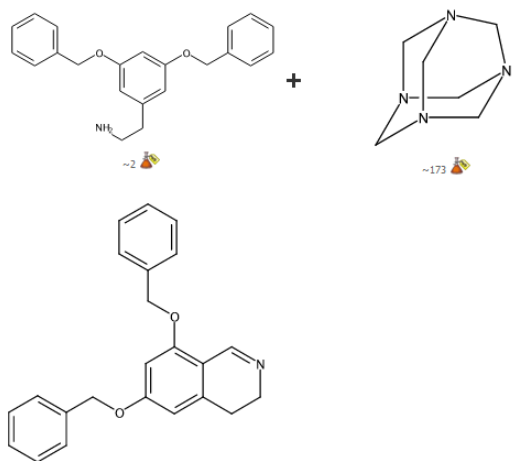
MethodsNow Synthesis

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 | 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 H ₂ O. 4. Basify with potassium carbonate and extract with CH ₂ Cl ₂ . 5. Wash the combined organic layers with brine. 6. Dry over MgSO ₄ 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 |
| ¹ H 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) |
| ¹³ C 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 O 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

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 - 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

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**

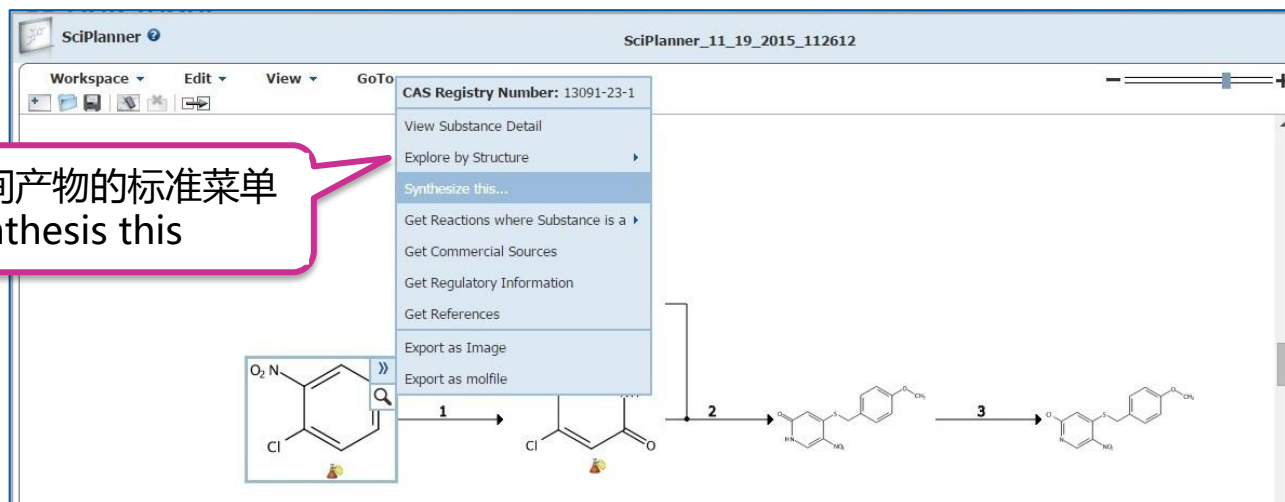
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Your Workspace is empty.

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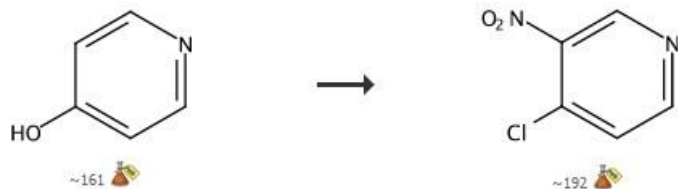
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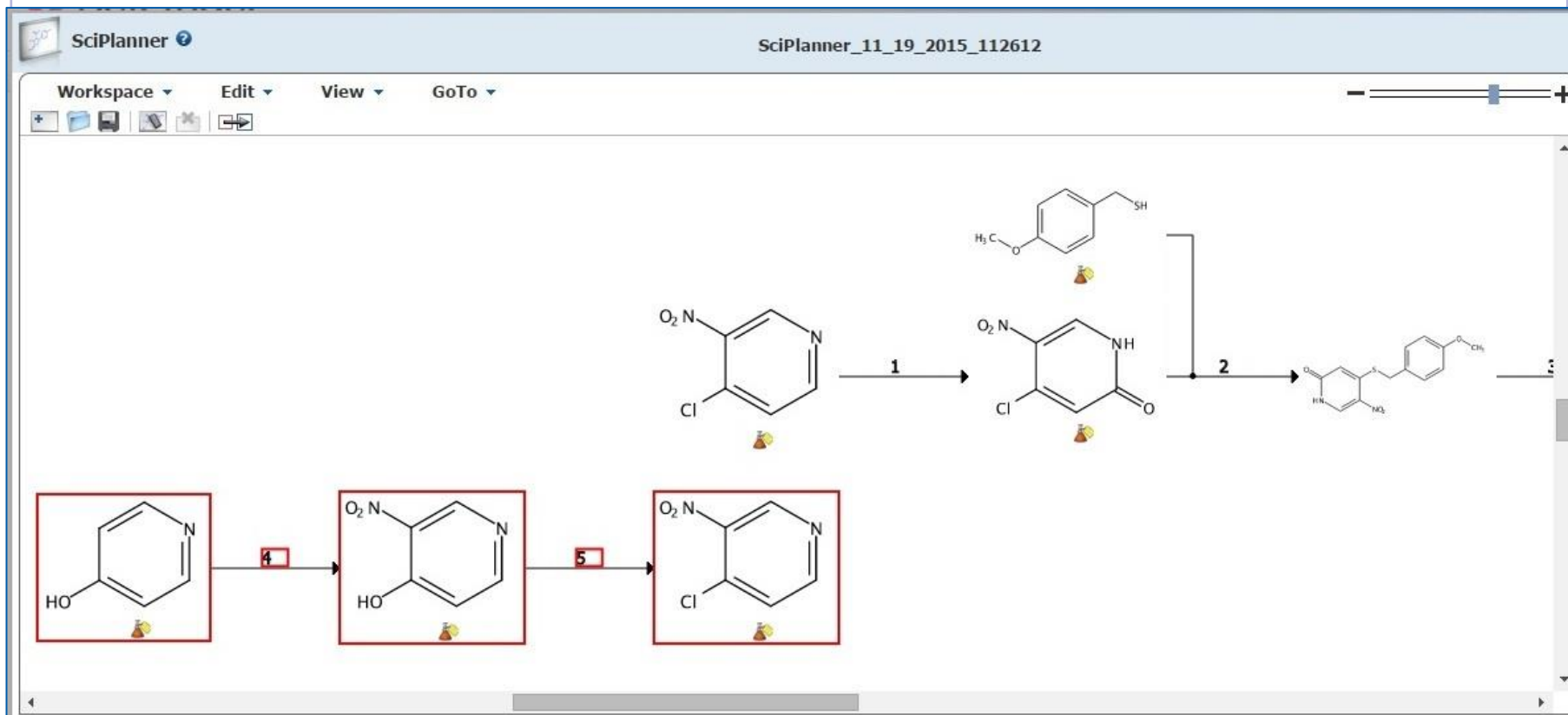


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继续推送到SciPlanner



SciPlanner使用简介



步骤同前，将推送过来的反应拖到编辑面板中，可以看到两条反应中存在同样的结构

SciPlanner使用简介

SciPlanner 11_19_2015_112612

Workspace Edit View GoTo

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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

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SciPlanner_11_19_2015_112612

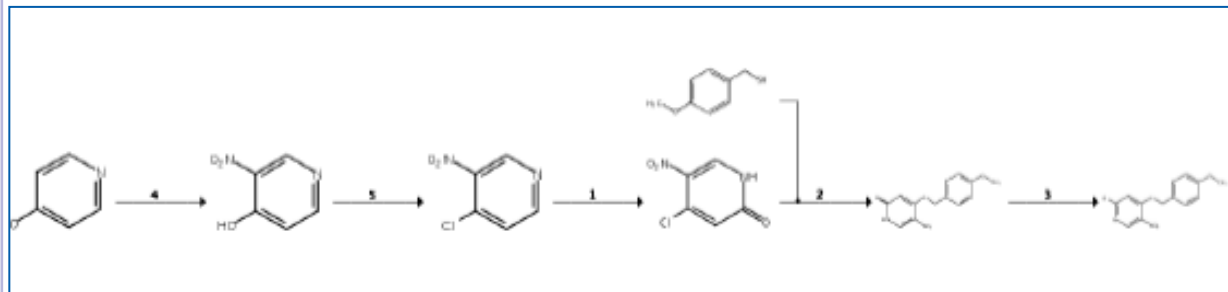
Title

Include:

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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)-Pyridone, 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: ~ 391 References Reactions ~ 190 Commercial Sources Regulatory Information</p> |
| <p>5435-54-1</p> <p>C₆H₄N₂O₃ 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>C₆H₃ClN₂O₃ 2(1H)-Pyridone, 4-chloro-5-nitro- Related Info: ~ 22 References Reactions ~ 136 Commercial Sources</p> | | |

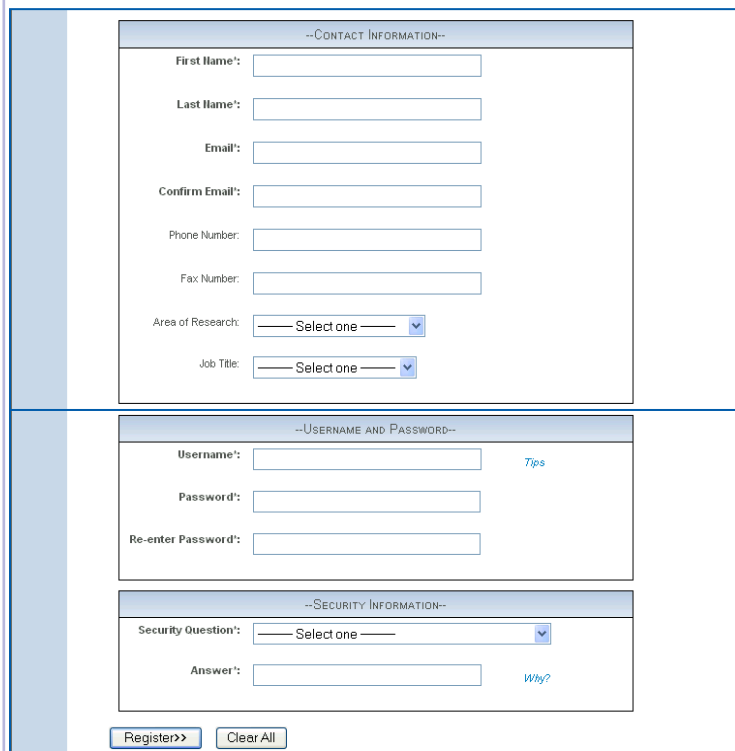
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 - SciPlanner
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Job Title:

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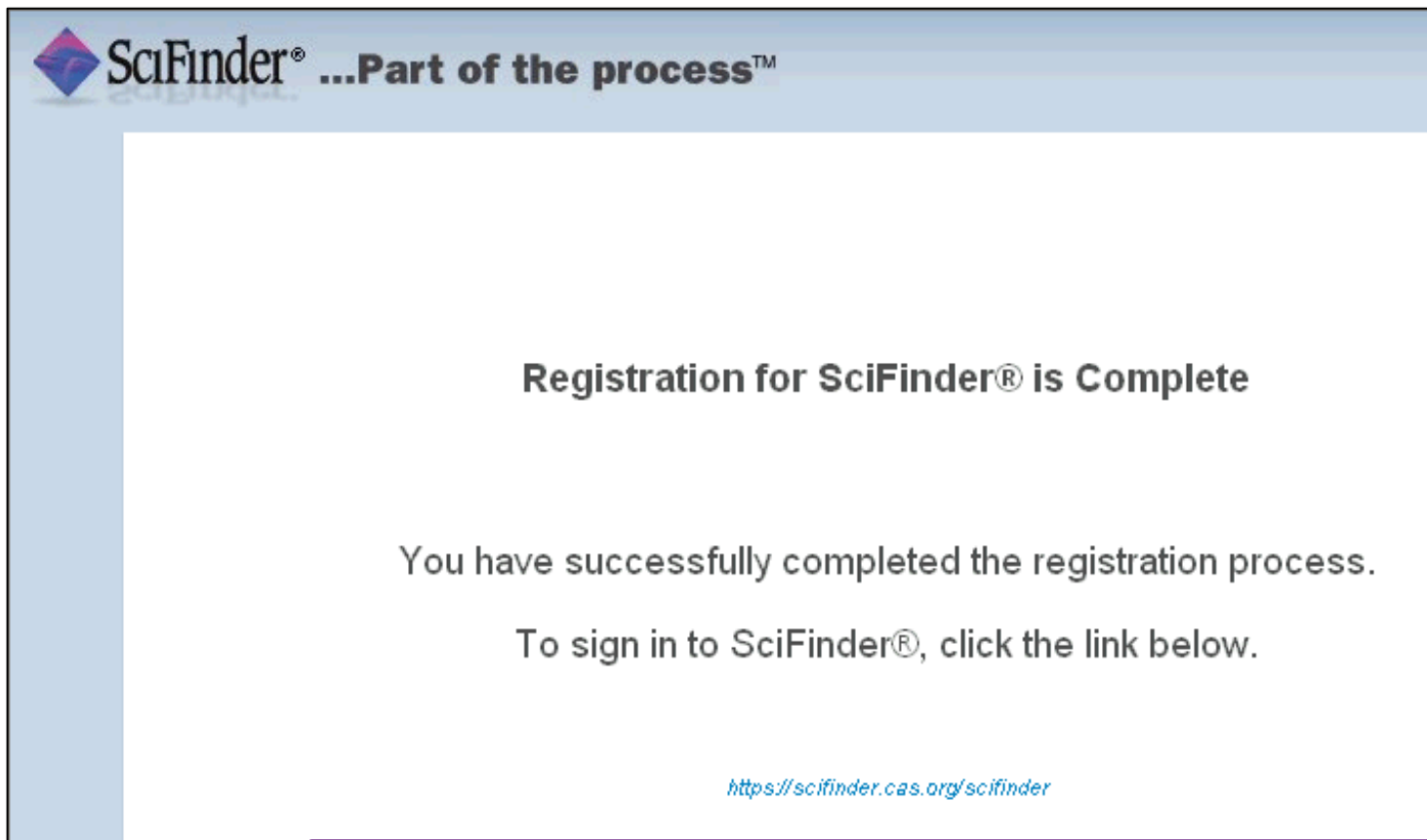
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