



如何利用SciFinder提高研究效率

钱欣

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美国化学文摘社北京代表处

提纲

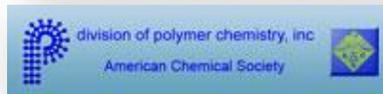
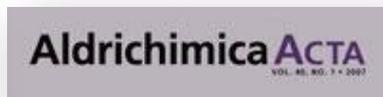
- 美国化学文摘社简介
- SciFinder简介及检索方式
 - 文献检索
 - 物质检索
 - Markush检索
 - 反应检索
 - SciPlanner使用简介
- SciFinder常见问题及解决

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
- 总部坐落于俄亥俄州的哥伦布市



CAS-构建最高质量的化学数据库

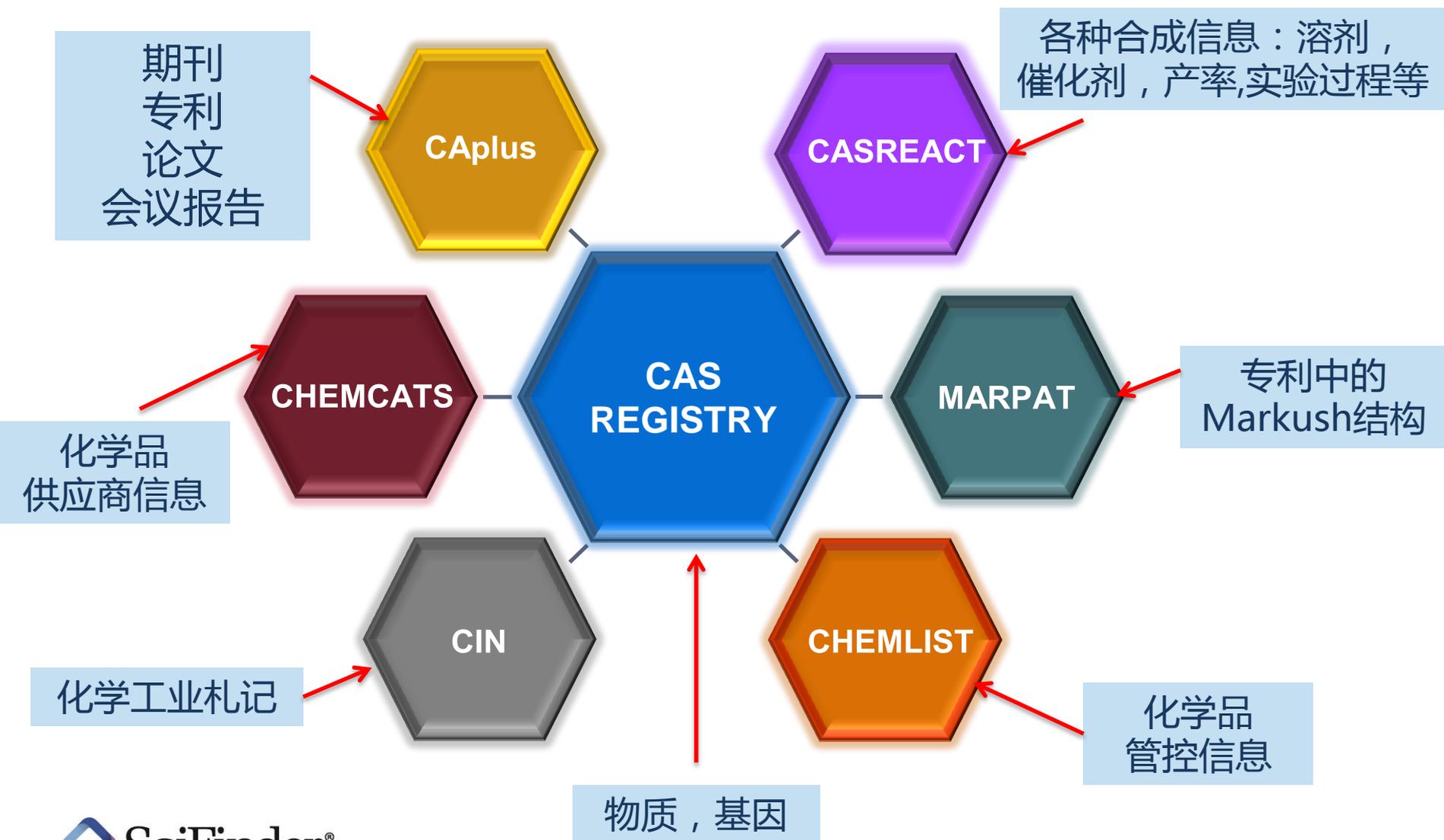


U.S. Patent Office

Patents,
journals, web,
catalogs, etc.



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

a

CAS数据库最具价值的内容—人工索引

12. Cobalt-Catalyzed Reductive Allylation of Alkyl Halides with Allylic Acetates or Carbonates

By: Qian, Xin; Auffrant, Audrey; Felouat, Abdellah; Gosmini, Corinne

A new route for the direct allylation of various alkyl halides catalyzed by simple cobalt(II) bromide has been developed. This method is efficient for the coupling of a large variety of alkyl halides (primary, secondary and tertiary) with substituted allylic acetates and carbonates and provides good to excellent yields with good functional group tolerance.

Indexing

General Organic Chemistry (Section21-2)	
Concepts	Substances
Allylic compounds acetates, carbonates; prepn. of olefins via cobalt catalyzed reductive allylation of alkyl halides with allylic acetates or allylic carbonates Reactant; Synthetic preparation; Preparation; Reactant or reagent	7789-43-7 Cobalt(II) bromide prepn. of olefins via cobalt catalyzed reductive allylation of alkyl halides with allylic acetates or allylic carbonates Catalyst use; Uses
Alcohols allyl; prepn. of olefins via cobalt catalyzed reductive allylation of alkyl halides with allylic acetates or allylic carbonates Reactant; Reactant or reagent	
Bromoalkanes	
Alkenes prepn. of olefins via cobalt catalyzed reductive allylation of alkyl halides with allylic acetates or allylic carbonates Synthetic preparation; Preparation	4407-36-7 trans-Cinnamyl alcohol 5332-06-9 4-Bromobutyronitrile 6940-78-9 1-Bromo-4-chlorobutane 7697-09-8 1-Bromobicyclo[2.2.2]octane 14660-52-7 Ethyl 5-bromopentanoate 25260-60-0 33884-43-4 2(2-Bromoethyl)-1,3-dioxane 57006-69-6 74036-95-6 166953-64-6 Benzyl 4-bromopiperidine-1-carboxylate
Allylation	Allylation catalysts prepn. of olefins via cobalt catalyzed reductive allylation of alkyl halides with allylic acetates or allylic carbonates

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

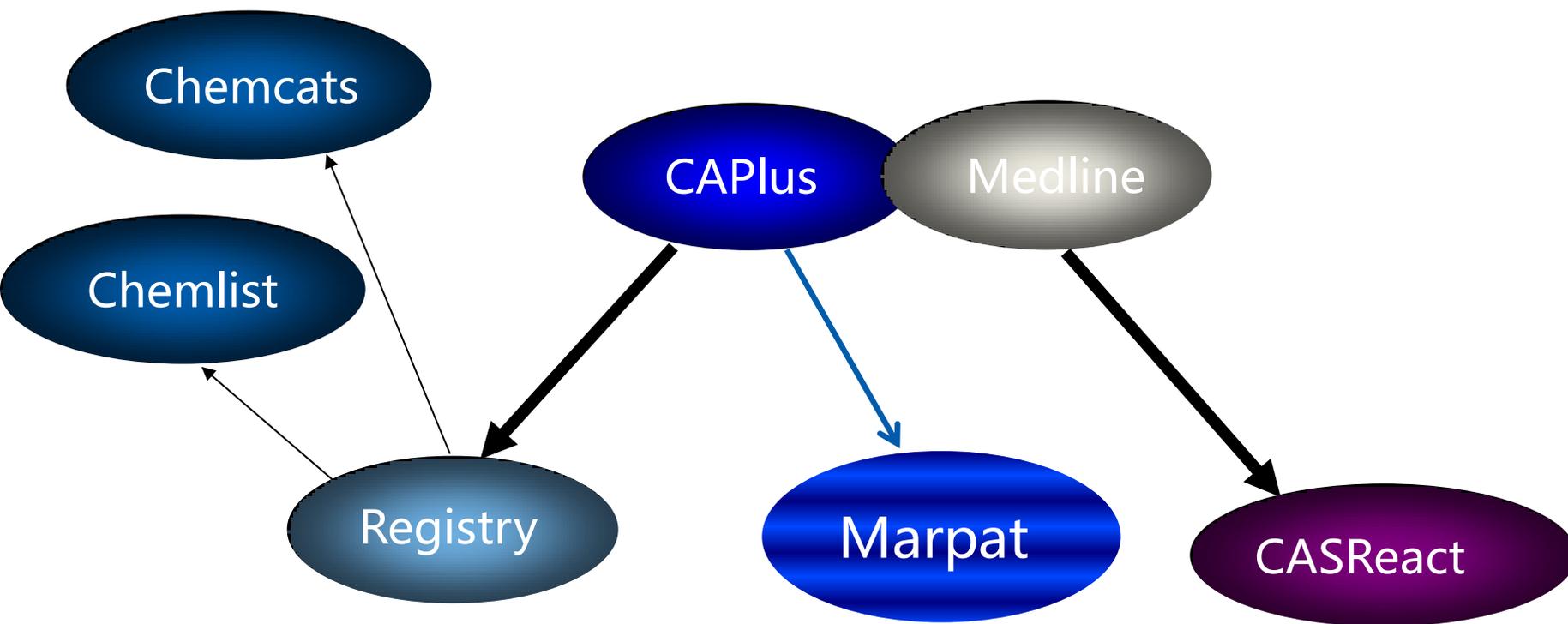
CAS人工索引解决的问题

- 检索词的同义词拓展：解决不同科研人员由于教育背景、语言、表达习惯不同导致的对同一个技术术语描述的差异。
- 用名称、分子式等检索化合物，会导致检索不全、不准的问题。CAS RN很好的解决了该问题，帮助检索人员实现精准定位化合物的目标。
- 利用SciFinder中的标引信息（Index Term，CAS RN，CAS Role），提高效率，启发思路。

提纲

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

SciFinder 的内容



SciFinder 登录界面

SciFinder®
The choice for chemistry research.™

Sign In

输入SciFinder帐号和密码

Username

Password

NEW Remember me for two weeks unless I sign out
(Do not use on a shared computer)

Sign In

[Forgot Username or Password?](#)

Your SciFinder username and password are assigned to you alone and may not be shared with anyone else.

<https://scifinder.cas.org>

News & Updates

Welcome to SciFinder

A New Non-Java Structure Editor is Now Available in SciFinder

SciFinder now features a non-Java version of the CAS Structure Editor, a new option for your substance and reaction searching! Start searching with the new editor today. Plus, we've added a new option to Analyze reaction answer sets by reagent, along with other enhancements. See [all that's new](#) in the latest release.

Learn about this year's Nobel Prize-winning chemistry research with SciFinder

By now you've heard that Martin Karplus, Michael Levitt and Arieh Warshel were awarded the 2013 Nobel Prize in Chemistry. But did you know that much of their Nobel Prize-winning research can be found in SciFinder? Check out a few examples of their [most highly cited articles](#).

Watch Part 3 of Our New Science in the News Podcast on Molecular Gastronomy

In part 3 of our Science in the News podcast on molecular gastronomy, find out why SciFinder is essential to food chemistry research. [Watch it now](#) and don't forget to catch all three parts of

SciFinder主界面

检索完，请点击退出

工具栏

The screenshot shows the SciFinder main interface. At the top left is the SciFinder logo. Below it is a navigation bar with 'Explore', 'Saved Searches', and 'SciPlanner'. On the right, there are links for 'Preferences', 'SciFinder Help', and 'Sign Out', along with a user profile for 'Helen Zhu'. The main content area is titled 'REFERENCES: RESEARCH TOPIC' and features a search input field with examples: 'The effect of antibiotic residues on dairy products' and 'Photocyanation of aromatic compounds'. A 'Search' button and an 'Advanced Search' link are also present. On the left, a sidebar lists categories: 'REFERENCES' (with sub-items: Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, Tags), 'SUBSTANCES' (with sub-items: Chemical Structure, Markush, Molecular Formula, Property, Substance Identifier), and 'REACTIONS' (with sub-item: Reaction Structure). On the right, there are two panels: 'SAVED ANSWER SETS' listing various saved sets like 'all', '聚芳醚', '1', 'HFUT', 'yanghua', 'pyrazole', 'Wuhan Institute of Tech', 'modification of chemical fiber organosilicon', 'Ba', and 'Autosaved Substance Set'; and 'KEEP ME POSTED' which states 'You have no profiles.' and provides a link to 'Learn how to: Create Keep Me Posted'.

工具栏

References | SciFinder Help | Sign Out

Help
Training
What's New
Contact Us

Helen Zhu

Explore | Saved Searches | SciPlanner

REFERENCES: RESEARCH TOPIC

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

Search

Advanced Search

REFERENCES

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

SUBSTANCES

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

REACTIONS

- Reaction Structure

SAVED ANSWER SETS

- all
- 聚芳醚
- 1
- HFUT
- yanghua
- pyrazole
- Wuhan Institute of Tech
- modification of chemical fiber organosilicon
- Ba
- Autosaved Substance Set

View All | Import

KEEP ME POSTED

You have no profiles.

Learn how to:
Create Keep Me Posted

检索入口

检索页面

已保存的结果集

定题跟踪，及时捕捉最新动态

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
- 文献标示符检索
- 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

REFERENCES

Research Topic

Author Name

Company Name

Document Identifier

Journal

Patent

Tags

文献检索—主题: Suzuki催化反应

检索式: Suzuki reaction with catalyst

The screenshot displays the SciFinder search interface. At the top, there is a navigation bar with the SciFinder logo, user information (Welcome Cyrene Qian), and links for Preferences, SciFinder Help, and Sign Out. Below the navigation bar are tabs for Explore, Saved Searches, and SciPlanner. The main content area is titled 'REFERENCES: RESEARCH TOPIC' and features a search input field containing 'suzuki reaction with catalyst'. Below the input field, there are examples of search results: 'The effect of antibiotic residues on dairy products' and 'Photocyanation of aromatic compounds'. A blue 'Search' button is visible, along with an 'Advanced Search' link. A blue callout box highlights the text: '关键词之间可用介词连接: in, with, of...'. On the left side, there is a sidebar with navigation options under 'REFERENCES', 'SUBSTANCES', and 'REACTIONS'. On the right side, there are sections for 'SAVED ANSWER SETS' and 'KEEP ME POSTED'.

文献检索—主题: Suzuki催化反应

检索式: Suzuki reaction with catalyst

Advanced Search Always Show

Publication Years

Examples: 1995, 1995-1999, 1995-, -1995

Document Types

- | | |
|---|-------------------------------------|
| <input type="checkbox"/> Biography | <input type="checkbox"/> Historical |
| <input type="checkbox"/> Book | <input type="checkbox"/> Journal |
| <input type="checkbox"/> Clinical Trial | <input type="checkbox"/> Letter |
| <input type="checkbox"/> Commentary | <input type="checkbox"/> Patent |
| <input type="checkbox"/> Conference | <input type="checkbox"/> Preprint |
| <input type="checkbox"/> Dissertation | <input type="checkbox"/> Report |
| <input type="checkbox"/> Editorial | <input type="checkbox"/> Review |

Languages

- | | |
|----------------------------------|-----------------------------------|
| <input type="checkbox"/> Chinese | <input type="checkbox"/> Japanese |
| <input type="checkbox"/> English | <input type="checkbox"/> Polish |
| <input type="checkbox"/> French | <input type="checkbox"/> Russian |
| <input type="checkbox"/> German | <input type="checkbox"/> Spanish |
| <input type="checkbox"/> Italian | |

Author

Last Name *

First

Middle

<input type="text"/>	<input type="text"/>	<input type="text"/>
----------------------	----------------------	----------------------

Company

Examples:

Minnesota Mining and Manufacturing
DuPont

提前限制出版年限、
文献类型、语言等

主题检索的候选项

REFERENCES ?	
Select All Deselect All	
1 of 5 Research Topic Candidates Selected	
	References
<input type="checkbox"/> 79 references were found containing "suzuki reaction with catalyst" as entered.	79
<input checked="" type="checkbox"/> 8135 references were found containing the two concepts "suzuki reaction" and "catalyst" closely associated with one another.	8135
<input type="checkbox"/> 9943 references were found where the two concepts "suzuki reaction" and "catalyst" were present anywhere in the reference.	9943
<input type="checkbox"/> 17388 references were found containing the concept "suzuki reaction".	17388
<input type="checkbox"/> 2398660 references were found containing the concept "catalyst".	2398660

[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或同时作为索引词；

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

文献检索结果

文献处理工具

The screenshot displays the SciFinder web interface. At the top, there are navigation links for 'Preferences', 'SciFinder Help', and 'Sign Out'. Below this, a navigation bar includes 'Explore', 'Saved Searches', and 'SciPlanner'. The main content area shows search results for the topic 'Suzuki reaction with catalyst' with 8135 references. A red arrow points from the '文献处理工具' (Literature Processing Tools) header to the 'REFERENCES' tab, which is highlighted with a red box. Below the 'REFERENCES' tab are sub-tabs for 'Analyze', 'Refine', and 'Categorize'. On the left, an 'Analyze by:' section lists authors with their respective counts: Zhou Mingjie (146), Wang Ping (114), Zhang Zhenhua (81), Molander Gary A (67), Liu Chun (52), and Zhang Juanjuan (42). The main results list shows two entries. The first entry is 'Suzuki-Miyaura Reaction for Efficient Construction of Biaryls' by Liu, Chun; Li, Xinmin. A blue box labeled '获取原文' (Get Full Text) has an arrow pointing to the 'Quick View' link. The second entry is 'Iron Oxide Nanoparticles Modified with Carbon Quantum Nanodots for the Stabilization of Palladium Nanoparticles: An Efficient Catalyst for the Suzuki Reaction in Aqueous Media under Mild Conditions' by Gholinejad, Mohammad; Sayedhamzeh, Mohammed; Razeghi, Mehran; Najera, Carmen; Kompany-Zareh, Mohsen. A blue box labeled '涉及物质及引文链接' (Involving Substances and Citation Links) has an arrow pointing to the 'Other Sources' link. A red box highlights the 'Other Sources' link in the first entry. On the right side of the interface, there are buttons for 'Create Keep Me Posted Alert' and 'Send to SciPlanner'. A red arrow points from the '涉及物质及引文链接' box to a small icon in the top right corner.

REFERENCES

Analyze Refine Categorize

Analyze by: Author Name

Zhou Mingjie	146
Wang Ping	114
Zhang Zhenhua	81
Molander Gary A	67
Liu Chun	52
Zhang Juanjuan	42

Sort by: Accession Number

Get Substances Get Reactions Get Related Citations Tools

1. Suzuki-Miyaura Reaction for Efficient Construction of Biaryls

By Liu, Chun; Li, Xinmin

From Chemical Record (2015), Ahead of Print. | Language: English, Database: CAPLUS

2. Iron Oxide Nanoparticles Modified with Carbon Quantum Nanodots for the Stabilization of Palladium Nanoparticles: An Efficient Catalyst for the Suzuki Reaction in Aqueous Media under Mild Conditions

By Gholinejad, Mohammad; Sayedhamzeh, Mohammed; Razeghi, Mehran; Najera, Carmen; Kompany-Zareh, Mohsen

From ChemCatChem (2015), Ahead of Print. | Language: English, Database: CAPLUS

获取原文

涉及物质及引文链接

文献结果的排序功能

Research Topic "suzuki reaction with catalyst" > references (8135)

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

Analyze Refine Categorize Sort by: Accession Number ↓

Analyze by: Author Name

Zhou Mingjie	146
Wang Ping	114
Zhang Zhenhua	81
Molander Gary A	67
Liu Chun	52
Zhang Juanjuan	42

1. **Suzuki-Miyaura Reaction for Efficient Construction of Biaryls**
By Liu, Chun; Li, Xinmin
From Chemical Record (2015), Ahead of Print. | Language: English, Database: CAPLUS

2. **Iron Oxide Nanoparticles Modified with Carbon Quantum Nanodots for the Stabilization of Palladium Nanoparticles: An Efficient Catalyst for the Suzuki Reaction in Aqueous Media under Mild Conditions**
By Gholinejad, Mohammad; Seyedhamzeh, Mohammed; Razeghi, Mehran; Najera, Carmen; Kompany-Zareh, Mohsen
From ChemCatChem (2015), Ahead of Print. | Language: English, Database: CAPLUS

Accession Number
Author Name
Citing References
Publication Year
Title

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

Citing Reference: 可能帮助找到最重要的文献

文献检索结果：Analyze

领域内主要研究人员，专家

主要研究机构，合作伙伴，竞争对手

主要的期刊

12种文献分析工具

Analyze Refine Categorize

Analyze by: ?

- Author Name
- Author Name
- CAS Registry Number
- CA Section Title
- Company-Organization
- Database
- Document Type
- Index Term
- CA Concept Heading
- Journal Name
- Language
- Publication Year
- Supplementary Terms

REFERENCES ?

Analyze Refine Categorize

Analyze by: ?

Author Name

Zhou Mingjie	146
Wang Ping	114
Zhang Zhenhua	81
Molander Gary A	67
Liu Chun	52
Zhang Juanjuan	42
Langer Peter	41
Wu Yangjie	41
Buchwald Stephen L	40
Cao Yong	40

Show More

Analyze Refine Categorize

Analyze by: ?

Company-Organization

Chinese Academy of Sciences, Peop Rep China	156
Ocean's King Lighting Science & Technology Co Ltd, Peop Rep China	146
Shenzhen Ocean's King Lighting Science & Technology Co Ltd	142
Shenzhen Ocean's King Lighting Engineering Co Ltd	78
Dalian University of Technology, Peop Rep China	77
Massachusetts Institute of Technology, USA	64

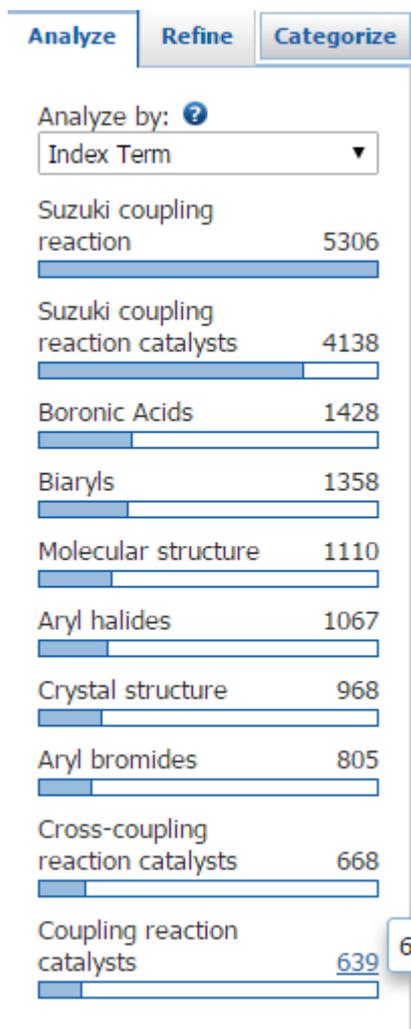
Analyze Refine Categorize

Analyze by: ?

Journal Name

Faming Zhuanli Shenqing	396
Tetrahedron Letters	391
Organic letters	352
Journal of Organic Chemistry	314
Tetrahedron	267
Journal of the American Chemical Society	224
Organometallics	204
Journal of Organometallic Chemistry	191
PCT Int. Appl.	190
European Journal of	

文献检索结果的Analyze



Index Term :

帮助用户全景了解文献内容，精选文献

Analyze - Index Term

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

3048 Items

1 Selected

[Export](#)

Sort by: Frequency ▼

Page: 1 of 20

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

<input type="checkbox"/>	Suzuki coupling reaction	5306
<input type="checkbox"/>	Suzuki coupling reaction catalysts	3474
<input type="checkbox"/>	Boronic acids	1242
<input type="checkbox"/>	Biaryls	1209
<input type="checkbox"/>	Aryl halides	913
<input type="checkbox"/>	Crystal structure	705
<input type="checkbox"/>	Molecular structure	702
<input type="checkbox"/>	Aryl bromides	698
<input type="checkbox"/>	Heck reaction	582
<input checked="" type="checkbox"/>	Nanoparticles	454

Apply

Cancel

文献检索结果的Refine

六种限定工具，包括主题词、作者姓名、机构名称、出版年代、语言、所属数据库

在结果中筛选主题带有“ionic liquid”的文献

The screenshot displays the SciFinder search results page. At the top, there are navigation tabs: 'Analyze', 'Refine', and 'Categorize'. The 'Refine' tab is active. Below the tabs, there are buttons for 'Get Substances', 'Get Reactions', 'Get Related Citations', and 'Tools'. A 'Sort by' dropdown menu is set to 'Accession Number'. The main content area shows a list of search results. The first result is titled '1. Composition Control Synthesis and Catalytic Properties in the Suzuki Reaction of Bimetallic PdSn Nanoparticles'. The second result is '2. POPd/TBAB co-catalyzed Suzuki cross-coupling reaction of heteroaryl chlorides/bromides with 4-fluorophenylboronic acid in water'. The third result is '3. Acyclic aminocarbene-like palladium complex-catalyzed Suzuki-Miyaura reaction at low catalyst loadings'. On the left side, there is a 'Refine by:' section with a list of categories: Research Topic, Author, Company Name, Document Type, Publication Year, Language, and Database. The 'Research Topic' category is selected, and a text input field contains the text 'ionic liquid'. A red arrow points from the text '在结果中筛选主题带有“ionic liquid”的文献' to this input field. Below the input field, there are examples of research topics: 'The effect of antibiotic residues on dairy products' and 'Photocyanation of aromatic compounds'. A 'Refine' button is located at the bottom of the 'Refine by:' section.

文献检索结果的Refine

在结果中筛选专利文献

Analyze Refine Categorize

Sort by: Accession Number ↓

0 of 222 References Selected

Page: 1 of 3

Refine by:

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

Document Type(s)

- Biography
- Book
- Clinical Trial
- Commentary
- Conference
- Dissertation
- Editorial
- Historical
- Journal
- Letter
- Patent**
- Preprint
- Report
- Review

1. **A one-step co-condensation method for the synthesis of well-defined functionalized mesoporous SBA-15 using trimethylsilanes as organosilane sources**
Quick View Other Sources
By Han, Ye Ri; Park, Jung-Woo; Kim, Hanil; Ji, Hyejeong; Lim, Soo Hyun; Jun, Chul-Ho
From Chemical Communications (Cambridge, United Kingdom) (2015), 51(96), 17084-17087. | Language: English, Database: CAPLUS
A new method for the prepn. of well-defined functionalized mesoporous SBA-15 has been developed by a one-step co-condensation method using trimethylsilanes as organosilane sources. This new method enables the incorporation of various bulky org. functional groups with long alkyl chain tethers into the mesoporous silica network.

2. **Catalyst from transition metal complex with imidazolium ionic liquid**
Quick View Other Sources
By Rodrigues dos Santos, Marcelo; Feitosa de Oliveira, Felipe; Amaro da Silveira Neto, Breno
From Braz. Pedido PI (2014), BR 102012027220 A2 20140722. | Language: Portuguese, Database: CAPLUS
This invention relates to transition metal **catalysts** with imidazolium **ionic liq.** complex comprising cations for use in **cross-coupling reactions** such as Heck or **Suzuki reactions**. Another aspect of the invention relates to the process of obtaining these transition metal **catalysts** based on imidazolium **ionic liqs.** More specifically, the present invention discloses the extrn. and characterization of members of a new class of metal complex ionically labeled derivs. of **reaction** between the **ionic liq.** 1-methyl-3-carboxymethylimidazolium chloride and metal **salts** of transition, for example, M (OAc) ~ 2...

3. **Palladium supported on Halloysite-triazolium salts as catalyst for ligand free Suzuki cross-coupling in water under microwave irradiation**
Quick View Other Sources
By Massaro, M.; Riel, S.; Cavallaro, G.; Colletti, C. G.; Milioto, S.; Noto, R.; Parisi, F.; Lazzara, G.
From Journal of Molecular Catalysis A: Chemical (2015), 408, 12-19. | Language: English, Database: CAPLUS
Environmental friendly halloysite-dicationic triazolium **salts** (second generation) obtained by subsequent click **reactions** of a diyne deriv. in the presence of 2-azidopropyl-modified halloysite nanotubes, were used as supports for palladium **catalyst**. Thanks to the high triazolium loading (25%) these materials were able to support higher amt. of the metal than that on the monocationic deriv. [i.e., first generation ligand, 4-(hydroxymethyl)-3-methyl-1-[3-(trimethoxysilyl)propyl]-1H-1,2,3-triazolium iodide, halloysite-nanotube-supported palladium-triazolium compd.]. Such materials were character...

4. **Functionalized Phosphonium Ionic Liquids: Synthesis and Application**
Quick View Other Sources

文献检索结果的Categorize

学科主分类

学科副分类

学科副分类涉及的重要技术术语

选中的重要技术术语

Categorize ?

1. Select a heading and category.

Category Heading	Category
All	Catalysts (10295)
General chemistry	Catalysis (216)
Synthetic chemistry	
Catalysis	
Physical chemistry	
Technology	
Biotechnology	
Polymer chemistry	
Genetics & protein chemistry	
Environmental chemistry	
Biology	
Analytical chemistry	

2. Select index terms of interest.

Index Terms	Selected Terms
Page: 1 of 103 Select All Deselect All	Click 'X' to remove the category from 'Selected Terms'
<input type="checkbox"/> Palladium	<input checked="" type="checkbox"/> Catalysis > Catalysts (1 Terms)
<input type="checkbox"/> Palladium diacetate	
<input type="checkbox"/> Tetrakis(triphenylphosphine)Pd	
<input type="checkbox"/> Tris(dibenzylideneacetone)dipalladium	
<input type="checkbox"/> Dichlorobis(triphenylphosphine)Pd	
<input type="checkbox"/> Carbene complexes	
<input type="checkbox"/> Palladium dichloride	
<input type="checkbox"/> Transition metal complexes	
<input type="checkbox"/> Triphenylphosphine	
<input checked="" type="checkbox"/> Ligands	
<input type="checkbox"/> Silica	
<input type="checkbox"/> Phosphines	
<input type="checkbox"/> PdCl2(dppf)	
<input type="checkbox"/> 2-Dicyclohexylphosphino-2',6'-dimethoxybiphenyl	

Catalysis > Catalysts > 1 Index Term(s) Selected

OK Cancel

文献信息详情

REFERENCE DETAIL [Get Substances](#) [Get Related Citations](#) [View with PatentPak](#) [Link to Other Sources](#)

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3. Method using potassium channel agonists for delivering a medicant to an abnormal brain region and/or a malignant tumor

By: Black, Keith L.; Ningaraj, Nagendra S.
Assignee: Cedars-Sinai Medical Center, USA

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Methods are disclosed for selectively delivering a medicant to an abnormal brain region and/or to a malignant tumor in a mammalian subject, including a human. A medicant is delivered simultaneously or substantially simultaneously with a calcium- or ATP-dependent potassium channel [K_{Ca} or K_{ATP}] activator (other than bradykinin or a bradykinin analog), such as an activator of sol. guanylyl cyclase (e.g., nitric oxide or a nitric oxide donor) or an activator of protein kinase, whereby the medicant is delivered selectively to the cells of the abnormal brain region and/or to the tumor, compared to normal tissues. Thus, among the disclosed methods of treating a malignant tumor in a human subject. Also disclosed are pharmaceutical compns. that combine a potassium channel activator together with a medicant and a kit for the delivery of a medicant to an abnormal brain region and/or to a malignant tumor.

Patent Information

Patent No.	Kind	Language	Date	Application No.	Date
WO 2001054771	PatentPak A2		Aug 2, 2001	WO 2001-US2743	Jan 26, 2001
WO 2001054771	A3		Jun 20, 2002		
US 7018979	B1		Mar 28, 2006	US 2000-491500	Jan 26, 2001
AU 2001034602	A		Aug 7, 2001	AU 2001-34602	Jan 26, 2001
EP 1251838	A2		Oct 30, 2002	EP 2001-906729	Jan 26, 2001
JP 2003523965	T		Aug 12, 2003	JP 2001-554753	Jan 26, 2001
US 20050153940	A1		Jul 14, 2005	US 2004-998866	Nov 29, 2004
US 20080050337	A1		Feb 28, 2008	US 2007-856654	Sep 17, 2007

Priority Application

US 2000-491500	A	Jan 26, 2000
US 2000-615854	A	Jul 14, 2000
WO 2001-US2743	W	Jan 26, 2001
US 2004-998866	B1	Nov 29, 2004

Indexing

Pharmacology (Section1-12)

Section cross-reference(s): 63

Concepts 重要技术术语

HSV-derived vector; potassium channel agonists for delivering medicant to abnormal brain region and/or malignant tumor

Glutamate antagonists

NMDA antagonists; potassium channel agonists for delivering medicant to abnormal brain region and/or malignant tumor

Diagnosis

agents; potassium channel agonists for delivering medicant to abnormal brain region

Substances 重要物质

56-65-5 Adenosine triphosphate

ATP-sensitive potassium channel; potassium channel agonists for delivering medicant to abnormal brain region and/or malignant tumor

Biological study, unclassified; Biological study

9054-75-5 Guanyl cyclase

activators; potassium channel agonists for delivering medicant to abnormal brain region and/or malignant tumor

Biological study, unclassified; Biological study

CAS Full Text Options

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Method using potassium channel agonists for delivering a medicant to an abnormal brain region and/or a malignant tumor
PCT Int. Appl. (2001), 62 pp. CODEN:PIXXD2: WO2001054771

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7. 参考文献

PatentPak——专利流程解决方案

Cai Yueqin	2
Gonell Gomez Sergio	2
Hagiwara Hisahiro	2
Liu Shenghua	2
Peris Fajarnes Eduardo Victor	2
Poyatos De Lorenzo Macarena	2
Ren Yong	2
Amaro Da Silveira Neto Breno	1
Dyson Paul	1
Earle Martyn John	1

Show More

By Rodrigues dos Santos, Marcelo; Feitosa de Oliveira, Felipe; Amaro da Silveira Neto, Breno
From Braz. Pedido PI (2014), BR 102012027220 A2 20140722. | Language: Portuguese, Database: CAPLUS

This invention relates to transition metal **catalysts** with imidazolium **ionic liq.** complex comprising cations for use in **cross-coupling reactions** such as Heck or **Suzuki reactions**. Another aspect of the invention relates to the process of obtaining these transition metal **catalysts** based on imidazolium **ionic liqs.** More specifically, the present invention discloses the extn. and characterization of members of a new class of metal complex ionically labeled derivs. of **reaction** between the **ionic liq.** 1-methyl-3-carboxymethylimidazolium chloride and metal **salts** of transition, for example, M (OAc) ~ 2...

2. Tris-imidazolium derivatives

Quick View PatentPak

By Peris Fajarnes, Eduardo Victor; Poyatos de Lorenzo, Macarena; Gonell Gomez, Sergio
From Span. (2014), ES 2478697 A1 20140722. | Language: Spanish, Database: CAPLUS

The invention relates to derivs. of highly sym. tris-imidazolium **salts** of formula I, that have a central triphenylene nucleus, where R¹ is C₁-C₁₀ alkyl or Ph, X is R², B(R³)₄, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate or P(R³)₆, R² and R³ are F, Cl or I. The invention also relates to a method for the prodn. thereof from hexamine, and to the use of same as tris-NHC ligands for producing homo-hetero-trimetal complexes in tandem catalysis **reactions** and in the prepn. of two-dimensional metal-org. frameworks (MOFs).

3. Tris-imidazolium derivatives

Quick View PatentPak

By Peris Fajarnes, Eduardo Victor; Poyatos de Lorenzo, Macarena; Gonell Gomez, Sergio
From PCT Int. App. No. WO/2014/096478. | Language: Spanish, Database: CAPLUS

The invention relates to derivs. of highly sym. tris-imidazolium **salts** of formula I, that have a central triphenylene nucleus, where R¹ is C₁-C₁₀ alkyl or Ph, X is R², B(R³)₄, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate or P(R³)₆, R² and R³ are F, Cl or I. The invention also relates to a method for the prodn. thereof from hexamine, and to the use of same as tris-NHC ligands for producing homo-hetero-trimetal complexes in tandem catalysis **reactions** and in the prepn. of two-dimensional metal-org. frameworks (MOFs).

4. A method for preparing diaryl compound in pure water

Quick View PatentPak

By Liu, Chun; Fu, Yao
From Famin Zhuanli Shennin (2014). CN 103588597 A 20140219. | Language: Chinese, Database: CAPLUS

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PatentPak——专利流程解决方案

PatentPak浏览器

The screenshot displays the PatentPak Viewer interface. At the top, there are navigation controls: a 'PAGE' dropdown set to 20 of 44, 'ZOOM' in and out buttons, and 'DOWNLOAD PDF' with a search icon. The main content area shows a patent document page with a chemical structure of a hexamine salt. The structure is a central benzene ring with two imidazole rings attached at the 2 and 6 positions. Each imidazole ring has two methyl groups on its nitrogen atoms. The entire structure is shown as a 3+ cation with three tetrafluoroborate (BF4-) counterions. A red arrow points from the 'Analyst Markup Location' section on the left to a location pin on the page number '20' in the text. The text describes the synthesis of compound I from hexamine IV.

15 **Ejemplo 1. Obtención de I (R₁ = *terc*-butilo)**

CAS RN 1448428-20-3

Analyst Markup Location
page 20

CAS RN 1448428-12-3
1*H*-Triphenyleno[2,3-*a*6,7-*d*
'10,11-*d*']triazolium,
1,3,6,8,11,13-hexakis(1,1-
dimethylethyl)-8,13-dihydro-,
tetrafluoroborate(1-) (1:3)

Analyst Markup Location
page 20

En un matraz de fondo redondo se disuelve la hexaamina **IV** (R = *terc*-butilo) (590 mg, 0,902 mmol) en 40 mL de HC(OEt)₃. Seguidamente se añade ácido tetrafluorobórico (solución etérea al 54 %; 0,36 mL, 2,977 mmol) y se deja agitando a 110°C durante 16 horas. A continuación, se añaden 100 mL de dietil éter. La sal formada se separa mediante filtración. Tras precipitar con acetonitrilo/dietil éter, el compuesto **I** se obtiene puro como un sólido beige. Rendimiento: 820 mg, 95 %.

20

¹H NMR (300 MHz, DMSO-*d*₆, 303 K): δ 9.19 (s, 6H, CH₃), 9.16 (s, 3H

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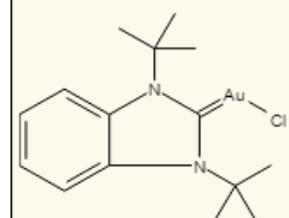
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Key Substances in Patent

CAS RN 1504582-75-5

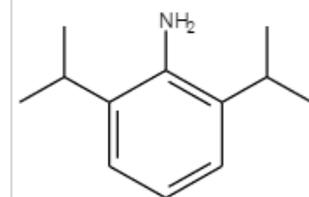


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page 25

CAS RN 24544-04-5



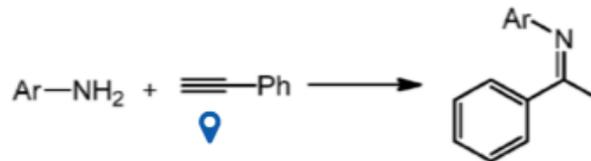
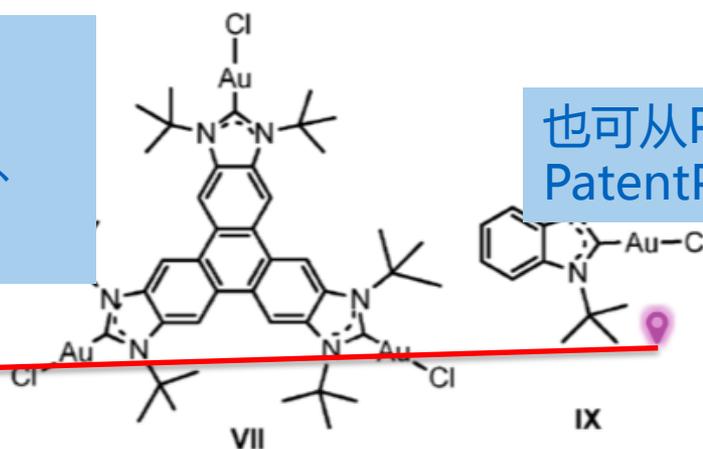
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page 29

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2	2,6- <i>i</i> Pr ₂ C ₆ H ₃	IX	82

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Research Topic "potassium channel with antican..." > references (295) > refine "Patents only" (133) > refine by categories

REFERENCES

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0 of 8 References Selected

1. Calcium-activated potassium channel-modulating agents for therapeutic use
By Jensen, Bo Skaaning; Teuber, Lene; Strobaek, Dorte; Christophersen, Palle; Olesen, Soren Peter
From PCT Int. Appl. (2000), WO 2000069794 A2 20001123. | Language: English, Database: CAPLUS
The invention discloses the use of a particular class of chem. compds. as modulators of SK₁, IK₁, and BK₁ calcium-activated potassium channels, as well as pharmaceutical compns. comprising the SK/IK/BK channel-modulating agents.

2. Potassium channel mediated delivery of agents through the blood-brain barrier
By Black, Keith L; Ningaraj, Nagendra S.
From PCT Int. Appl. (2005), WO 2005025511 A2 20050324. | Language: English, Database: CAPLUS
This invention includes pharmaceutical compns., methods and kits for the treatment or diagnosis of a malignant tumors, including brain tumors, and diseases or disorders characterized by abnormal brain tissue.

3. Method using potassium channel agonists for delivering a medicant to an abnormal brain region and/or a malignant tumor
By Black, Keith L; Ningaraj, Nagendra S.
From PCT Int. Appl. (2001), WO 2001054771 A2 20010802. | Language: English, Database: CAPLUS
Methods are disclosed for selectively delivering a medicant to an abnormal brain region and/or to a malignant tumor in a mammalian sub administered simultaneously or substantially simultaneously with a calcium- or ATP-dependent potassium channel [K_v or K_{ATP}] activator (analog), such as a direct potassium channel agonist or an indirect potassium channel activator, such as an activator of sol. guanylyl cyclase.

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- 可用Categorize实现精准定位学科信息
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提纲

- 美国化学文摘社及SciFinder简介
- SciFinder的检索和后处理
 - 文献检索
 - 物质检索
 - Markush检索
 - 反应检索
 - SciPlanner使用简介
- SciFinder常见问题及解决

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- 物质检索方法

- 结构式检索
- Markush结构检索
- 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

- 有机物化合物、天然产物：结构检索
- 无机化合物、合金：分子式检索
- 高分子化合物：分子式检索和结构检索

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

SUBSTANCES

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

REACTIONS

- Reaction Structure

SUBSTANCES: SUBSTANCE IDENTIFIER

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

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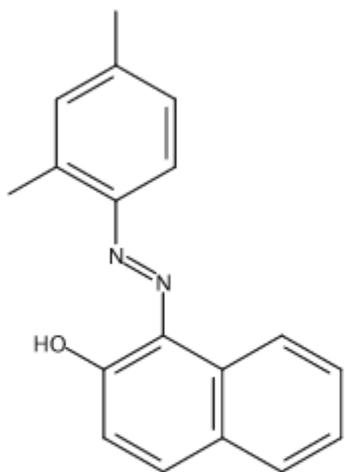
物质标识符包括CAS RN和化学名称，化学名称可以是通用名称、商品名、俗名。

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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



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SUBSTANCE DETAIL 



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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)

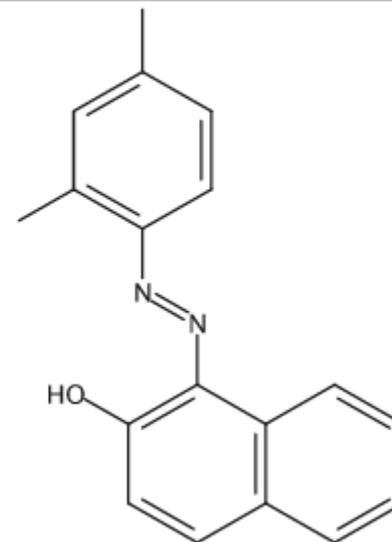
Sudan Red (6CI)

1-[2-(2,4-Dimethylphenyl)diazenyl]-2-naphthalenol

AF Red No. 5

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物质详情



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	278.33		(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

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- Document Identifier
- Journal
- Patent
- Tags

SUBSTANCES

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

REACTIONS

- Reaction Structure

SUBSTANCES: PROPERTY ?

Experimental

Select Property... ▾

- 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

Examples: 44, 25-35, >125

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- Author Name
- Company Name
- Document Identifier
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- Patent
- Tags

SUBSTANCES

Select Property...

- Bioconcentration Factor
- Boiling Point (°C)
- Density (g/cm³)
- Enthalpy of Vaporization (kJ/mol)
- Flash Point (°C)
- Freely Rotatable Bonds
- H Donor/Acceptor sum
- H Acceptors
- H Donors
- Koc
- logD
- logP
- Mass Intrinsic Solubility (g/L)
- Mass Solubility (g/L)
- Molar Intrinsic Solubility (mol/L)
- Molar Solubility (mol/L)
- Molar Volume (cm³/mol)
- Molecular Weight**
- pKa
- Molecular Weight

Examples: 44, 25-35, >125

Examples: 44, 25-35, >125

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- Metal-Containing
- Commercial Availability
- Property Availability
- Property Value
- Reference Availability
- Atom Attachment

Structure Editor: Java Non-Java

Click to Edit

1. **1817853-33-0**

$C_{17}H_{26}NO_5PS$
INDEX NAME NOT YET ASSIGNED

▶ Key Physical Properties

2. **1817853-23-0**

$C_{20}H_{20}N_2O_3S$
INDEX NAME NOT YET ASSIGNED

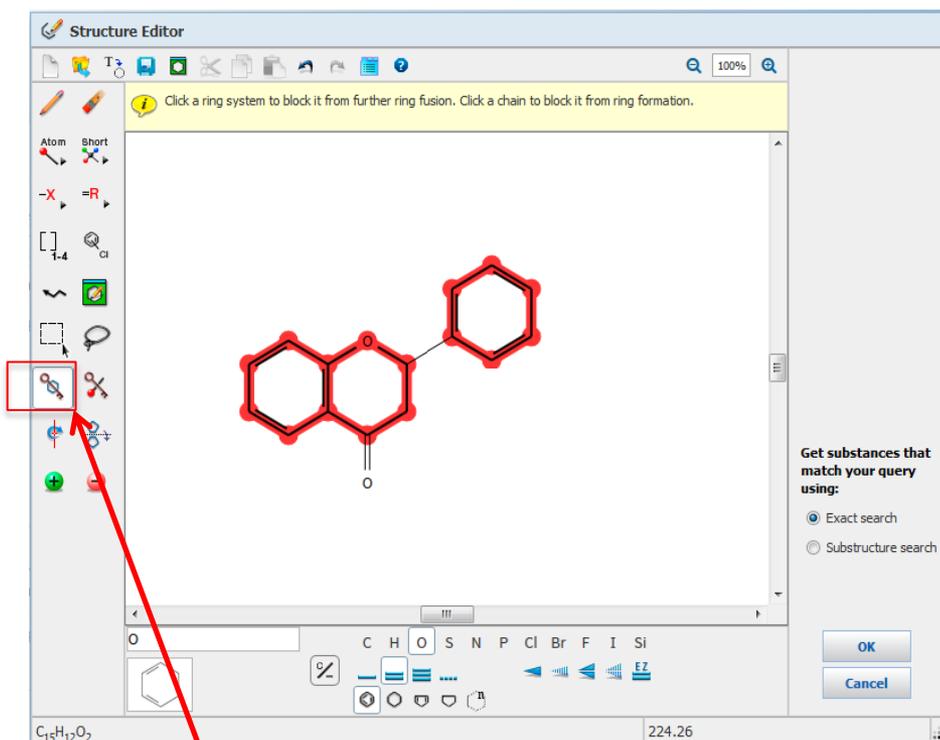
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5. **1817853-08-9**

6. **1817853-01-2**

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锁环工具：避免在现有环结构基础上出现新的稠环结构

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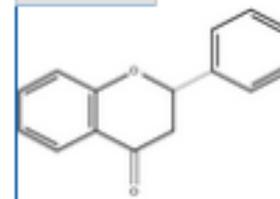
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Refine by: ?

- Chemical Structure
- Isotope-Containing
- Metal-Containing
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- Property Availability
- Property Value
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Structure Editor:

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Refine

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从3500多万个结构筛选出7800个黄酮类物质

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Property "Predicted - Molecular Weight, ..." > **refine "substructure" (7896)**

SUBSTANCES Get References Get Reactions Get Commercial Sources Tox

Analyze **Refine**

Sort by: Relevance ▾ ↓

0 of 7896 Substances Selected

1. **1772897-96-7** 🔍
~0 ~1

C₁₇ H₁₆ O₂
4#-1-Benzopyran-4-one, 2-(3,5-dimethylphenyl)-2,3-dihydro-
▶ **Key Physical Properties**

2. **1438763-**
~2

C₁₇ H₁₆ O₂
4#-1-Benzopyran-4-one, 2,3-dihydro-, (2R)
▶ **Key Physical P**

5. **21785-09-1** 🔍
~156 ~27

6. **72984-48**
~27

Refine by:
 Chemical Structure
 Isotope-Containing
 Metal-Containing
 Commercial Availability
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物质检索—分子式

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SUBSTANCES

Chemical Structure
Markush
Molecular Formula
Property
Substance Identifier

REACTIONS

Reaction Structure

SUBSTANCES: MOLECULAR FORMULA

Examples:

H4SiO4

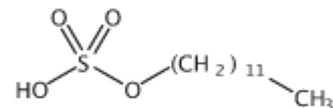
(C3H6O.C2H4O)x

Search

无机金属盐：金属离子和阴离子间用点 (.) 分开

(Component: 151-41-7)

~79363   ~283 



• Na

C₁₂ H₂₆ O₄ S . 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

The screenshot displays the SciFinder web interface. At the top, there are navigation tabs: 'Explore', 'Saved Searches', and 'SciPlanner'. Below the navigation, the breadcrumb path reads 'author Name "yan, d" > references (1019)'. On the left side, there is a sidebar menu with three main sections: 'REFERENCES', 'SUBSTANCES', and 'REACTIONS'. Under 'REFERENCES', options include Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, and Tags. Under 'SUBSTANCES', 'Chemical Structure' is highlighted with a blue box, and other options include Markush, Molecular Formula, Property, and Substance Identifier. Under 'REACTIONS', the option is Reaction Structure. The main content area is titled 'SUBSTANCES: CHEMICAL STRUCTURE' and features a 'Structure Editor' window with 'Java' and 'Non-Java' tabs and a 'Click to Edit' prompt. To the right of the editor, the 'Search Type' section includes radio buttons for 'Exact Structure', 'Substructure' (which is selected), and 'Similarity'. Below this is a checkbox for 'Show precision analysis'. At the bottom of the main area, there is an 'Import CXF' link, a blue 'Search' button, and a link for 'Advanced Search'.

SciFinder结构编辑器

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

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

The interface includes a toolbar with icons for drawing and editing, a central workspace for the chemical structure, and a right-hand panel for search options and drawing editor settings. The search options include Exact search, Substructure search (selected), and Similarity search. The drawing editor settings include Structure (selected), Reaction, and Markush. The interface also features a status bar at the bottom with a query input field and a scale control.

物质检索——精确结构检索

The screenshot displays a chemical structure editor window titled "Structure Editor". The main workspace shows a complex organic molecule consisting of a bicyclic system (a bicyclo[2.2.1]heptane derivative) with a nitrogen atom, and two ester groups attached to it. One ester group is linked to a benzene ring, and the other is linked to a methoxy group. A red arrow points from a text box to the "Delete atoms or bonds" icon in the top toolbar.

可以通过CAS RN转换结构：
CAS RN: 50-36-2

Drawing Editor:

- Structure
- Reaction
- Markush

Get substances that match your query using:

- Exact search
- Substructure search
- Similarity search

Buttons: 确定, 取消

Scale: 100

Bottom status bar: C₁₇ H₂₁ N O₄ (query) | 303.36

精确结构检索

浏览精确结构检索结果

可以通过分析限定再处理检索结果

Analyze Refine

Sort by: Relevance

0 of 80 Substances Selected

Display Options Page: 1 of 2

Refine by:

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

Select One:

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

Refine

1. 50-36-2
~20889
~23

Absolute stereochemistry.,Rotation (-).

C₁₇ H₂₁ N O₄
8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(benzoyloxy)-8-methyl-, methyl ester, (1*R*,2*R*,3*S*,5*S*)-

Key Physical Properties
Regulatory Information
Spectra
Experimental Properties

2. 53-21-4
~1700
~27

Absolute stereochemistry.,Rotation (-).

C₁₇ H₂₁ N O₄ · Cl H
8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(benzoyloxy)-8-methyl-, methyl ester, hydrochloride (1:1), (1*R*,2*R*,3*S*,5*S*)-

Key Physical Properties
Regulatory Information
Spectra
Experimental Properties

3. 52748-70-6
~11

88-89-1
C₆ H₃ N₃ O₇

50-36-2
C₁₇ H₂₁ N O₄

Absolute stereochemistry.,Rotation (-).

可卡因
盐酸可卡因
可卡因
组合物

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 image shows the SciFinder Drawing Editor interface. The central workspace displays a chemical structure of a benzofuran derivative with a phenyl group at the 3-position. The interface includes a toolbar on the left with various drawing tools, a top status bar with a zoom level of 100%, and a right-hand panel with search options. The search options are:

- Structure
- Reaction
- Markush

Below these are search criteria options:

- Exact search
- Substructure search
- Similarity search

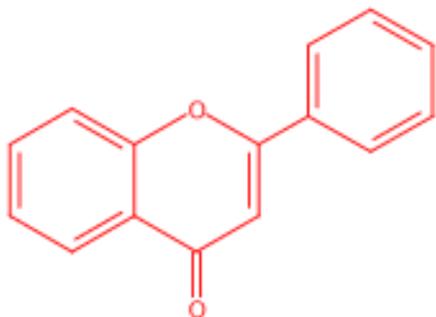
The "Substructure search" option is highlighted with a red box. At the bottom of the interface, there is a text input field containing the letter "O" and a horizontal menu with chemical elements: C, H, O, S, N, P, Cl, Br, F, I, Si.

物质检索——亚结构检索

0 of 63231 Substances Selected

1. 525-82-6

~3509   ~78 



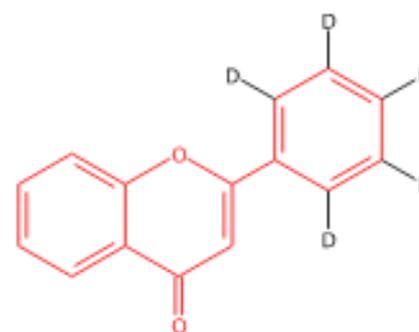
$C_{15} H_{10} O_2$
4*H*-1-Benzopyran-4-one, 2-phenyl-

Key Physical Properties

Regulatory Information
Spectra
Experimental Properties

2. 54849-75-1

~6  



同位素

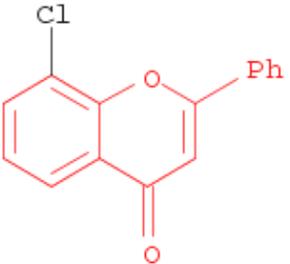
$C_{15} H_5 D_5 O_2$
4*H*-1-Benzopyran-4-one, 2-(phenyl-*d*₅)-

Spectra

浏览亚结构检索结果

251. Substance Detail
1148-20-5

取代物



ClC1=CC=C2C(=C1)OC(=O)C=C2C3=CC=CC=C3

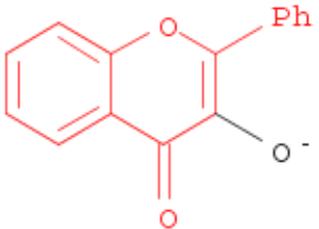
C₁₅ H₉ Cl O₂
4H-1-Benzopyran-4-one, 8-chloro-2-phenyl-

Exp

~16 


261. Substance Detail
85481-91-0

离子



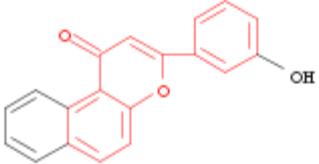
O=C1C=C(C2=CC=CC=C2)OC3=CC=CC=C3O1

C₁₅ H₉ O₃
4H-1-Benzopyran-4-one, 3-hydroxy-2-phenyl-, ion

~8 

273. Substance Detail
136116-17-1

稠环物质



O=C1C=C(C2=CC=CC=C2)OC3=CC=CC=C3O1C4=CC=C(O)C=C4

C₁₉ H₁₂ O₃
1H-Naphtho[2,1-*b*]pyran-1-one, 3-(3-hydroxyphenyl)-

~2 


亚结构检索结果的限定工具

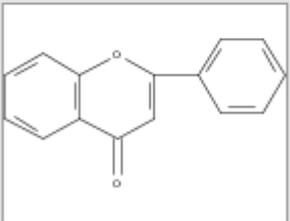
化学结构的再次限定

Analysis Refine

Refine by: ⓘ

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

Chemical Structure:

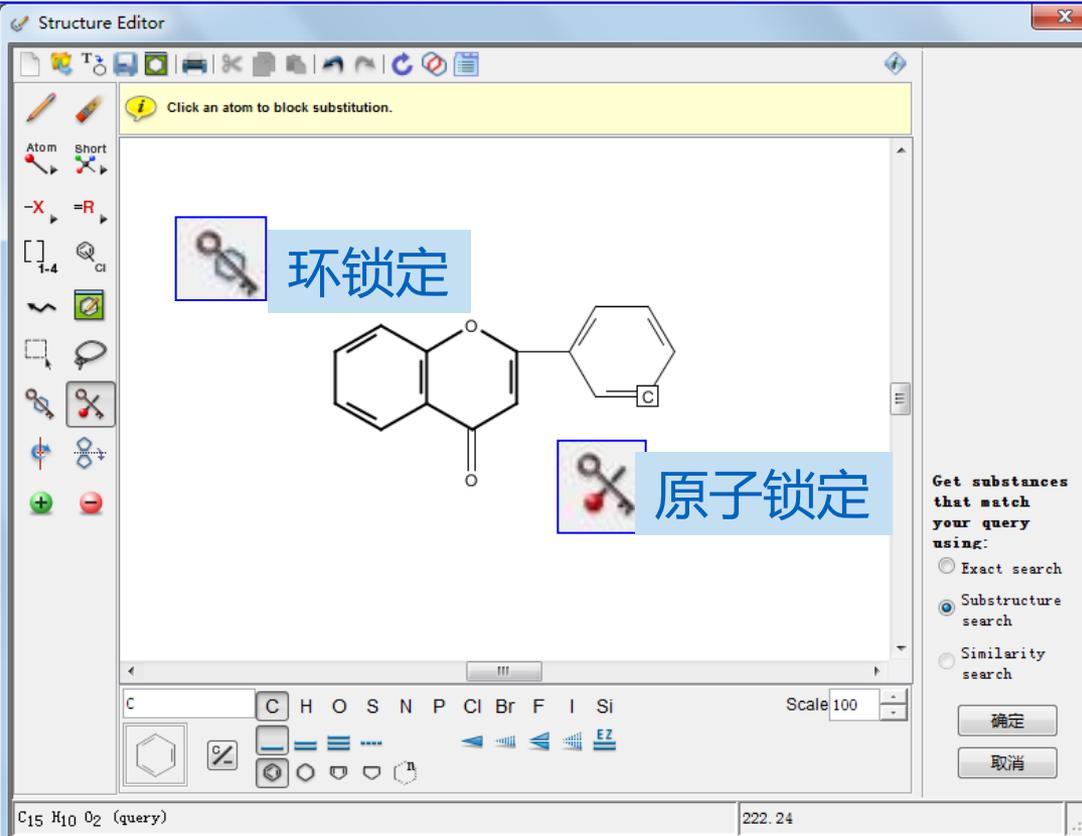


Click image to change structure or view detail

Search type: **Substructure**

Structure Editor

Click an atom to block substitution.



环锁定

原子锁定

Get substances that match your query using:

- Exact search
- Substructure search
- Similarity search

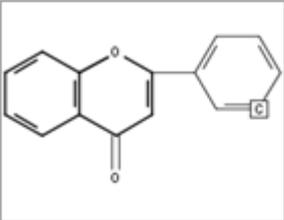
确定 取消

C H O S N P Cl Br F I Si Scale 100

C₁₅ H₁₀ O₂ (query) 222.24

化学结构的再次限定

Chemical Structure:



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

SciFinder®

Welcome Amy Qi | Sign Out

Explore References | Explore Substances | Explore Reactions

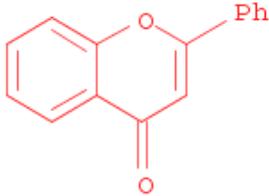
Add KMP Alert | Chemical Structure substructure > substances (52072) > refine "substructure" (28699)

Substances | Get References | Get Reactions | Tools | Send to SciPlanner

28699 Substances | 0 Selected

Select All | Deselect All | Sort by: Relevance (New)

1. Substance Detail
525-82-6

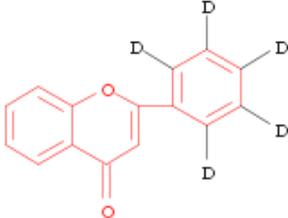


~2568

C₁₅ H₁₀ O₂
4#1-Benzopyran-4-one, 2-phenyl-

Spectra
Experimental Properties

2. Substance Detail
54849-75-1



~5

C₁₅ H₅ D₅ O₂
4#1-Benzopyran-4-one, 2-(phenyl-*d*₅)-

Spectra

同位素去除

Analysis Refine

Refine by:

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

Select One:

- Include only isotope-containing substances
- Exclude isotope-containing substances

去除同位素

SciFinder®

Welcome Amy Qi | Sign Out

Chemical Structure substructure > substances (52072) > refine "substructure" (28699) > refine "exclude isotope-containing" (28547)

Substances

28547 Substances 0 Selected

Select All Deselect All Sort by: Relevance (New)

Answers per Page [50] 1 2 3 4 5 6 ... 571

View:

1. Substance Detail
525-82-6

~2568

C15 H10 O2
4#1-Benzopyran-4-one, 2-phenyl-

2. Substance Detail
66585-04-4

~1

C15 H10 O2
4#1-Benzopyran-4-one, 2-phenyl-, radical ion(1+) (9CI)

3. Substance Detail
64586-87-4
(Component: 525-82-6)

~5

C15 H10 O2 . H
4#1-Benzopyran-4-one, 2-phenyl-, conjugate acid (1:1)

• H⁺

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

The screenshot displays the SciFinder Structure Editor interface. The central workspace shows the chemical structure of 5-mercapto-1H-benzotriazole-4-carboxylic acid, with a thiol group (-SH) at the 5-position and a carboxylic acid group (-COOH) at the 4-position of the benzotriazole ring system. The interface includes a top toolbar with various editing tools, a left sidebar with atom and bond selection options, and a right sidebar with search settings. The search settings on the right include radio buttons for 'Structure', 'Reaction', and 'Markush', and a section for 'Get substances that match your query using:' with radio buttons for 'Exact search', 'Substructure search', and 'Similarity search'. The 'Similarity search' option is selected and highlighted with a red box.

Structure Editor

Draw or change atoms or bonds. Shortcut Keys

Atom Short

-X =R

[] 1-4 Cl

HS NH COOH

Drawing Editor:

- Structure
- Reaction
- Markush

Get substances that match your query using:

- Exact search
- Substructure search
- Similarity search

相似结构检索候选项

Select All Deselect All

1 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 checked="" type="checkbox"/> 80-84	34
<input type="checkbox"/> 75-79	82
<input type="checkbox"/> 70-74	254
<input type="checkbox"/> 65-69	633
<input type="checkbox"/> 0-64 (least similar)	1636

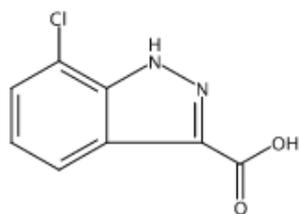
相似度越高，
结构越相似

Get Substances

相似结构检索结果

1. 129295-32-5

~3 ~96



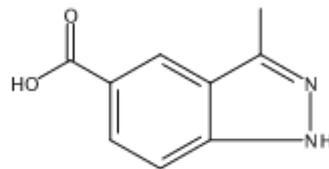
$C_8 H_5 Cl N_2 O_2$
1#Indazole-3-carboxylic acid, 7-chloro-

▶ Key Physical Properties **取代基变化**

Score: 79

3. 885223-58-5

~11 ~34



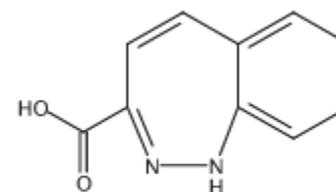
$C_9 H_8 N_2 O_2$
1#Indazole-5-carboxylic acid, 2-methyl-

▶ Key Physical Properties **取代基位置变化**

Score: 71

117. 72119-92-7

~1



$C_{10} H_8 N_2 O_2$
1#1,2-Benzodiazepine-3-carboxylic acid

▶ Key Physical Properties **母体结构变化**
[Experimental Properties](#)

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使用简介
- SciFinder常见问题及解决

➤ 具体物质[Specific Substance] :

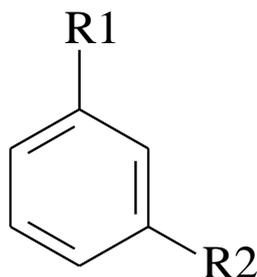
以具体化学结构陈述的特定物质，会被标示CAS RN

➤ 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

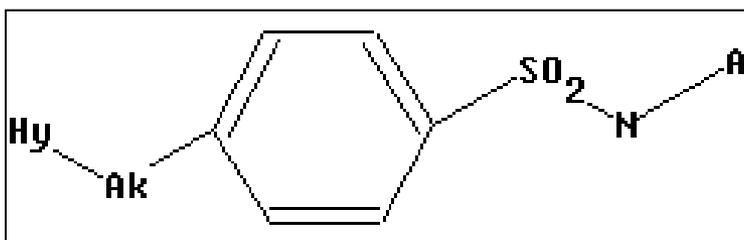
专利中所陈述的预测物质，不会被标示CAS RN

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。

Explore ▾ Saved Searches ▾ SciPlanner

Chemical Structure similarity > substances (127) > 1027511-99-4

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: MARKUSH ?

Search Type:

- Allow variability only as specified
- Substructure

Click image to change structure or view detail.

Import CXF

Search

全部是专利文献

Explore ▾ Saved Searches ▾ SciPlanner Save Print Export

Markush structure variable only at spe... > references (119)

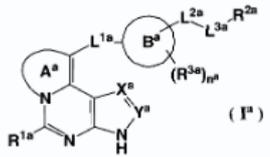
REFERENCES ⓘ Get Substances Get Reactions Get Related Citations Get Full Text Tools ▾ Create Keep Me Posted Alert Send to SciPlanner

Analyze Refine Categorize Sort by: Accession Number ▾ ↓ Answers per Page [20] Display: — = ≡

Analyze by: Document Type Patent 119 Show More

0 of 119 References Selected Page: 1 of 6

- 1. Substituted piperidine derivatives as a GPR119 agonist useful in treatment of metabolism related diseases and their preparation** Full Text
By Yang, Jin; Kim, Jinwoong; Lee, Hankyu; Kim, Jaehyun; Son, Changmo; Lee, Kyuhwan; Choi, Hyungho; Kim, Daehoon; Choi, Hyosun; Rhee, Jaekool
From PCT Int. Appl. (2013), WO 2013105753 A1 20130718. | Language: English, Database: CAPLUS
The invention is related to substituted piperidine derivs. of formula I as a GPR119 agonist useful in treatment of metab. related diseases such as diabetes or obesity and their prepn. The invention compds. I, wherein A is (un)substituted Ph or heterocyclic group; R¹ is COOR₃, or a (un)substituted heterocyclic group; R² and R³ are each independently a straight or branched chain, or a(un)substituted C₁₋₅ alkyl group; m is 0, 1, 2, 3; n is 1, 2, 3; their pharmaceutically acceptable salts are claimed. Compd. II was prepd. by multi-step procedure (procedure given). The invention compds. were eva...
- 2. Preparation of tricyclic heterocyclic compounds as JAK inhibitors** Full Text
By Hayashi, Keishi; Watanabe, Tsuneo; Toyama, Koji; Kamon, Junji; Minami, Masataka; Uni, Miyuki; Nasu, Mariko
From PCT Int. Appl. (2013), WO 2013024895 A1 20130221. | Language: English, Database: CAPLUS
Title compds. I [A^a = 5- to 6-membered heteroaryl contg. one or two N atom; X^a = H or CR^{3a}; R^{1a} = H, halo, alkyl or haloalkyl; ring B^a = cycloalkane, cycloalkene, 3- to 14-membered nonarom. heterocycle, arom. carbocycle or 5- to 10-membered arom. heterocycle; R^{2a} = H, halo, azido, cycloalkyl, etc.; L^{1a} = single bond, alkylene, alkenylene or alkynylene; L^{2a} = single bond, alkylene, alkenylene, or alkynylene; L^{3a} = single bond, O, S, etc.; Y^a = CR^{10a}; n = 0, 1 or 2, R^{3a} = hydroxy, amino, carboxy, carbamoyl, each of R^{3a} and R¹⁰ independently = H, halogen, cyano, carbamoyl, etc.], and their pharma...



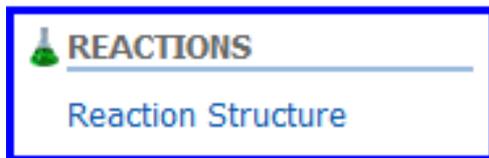
提纲

- 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使用简介
- SciFinder常见问题及解决

SciFinder检索选项——反应检索

- 功能方面

- 结构式



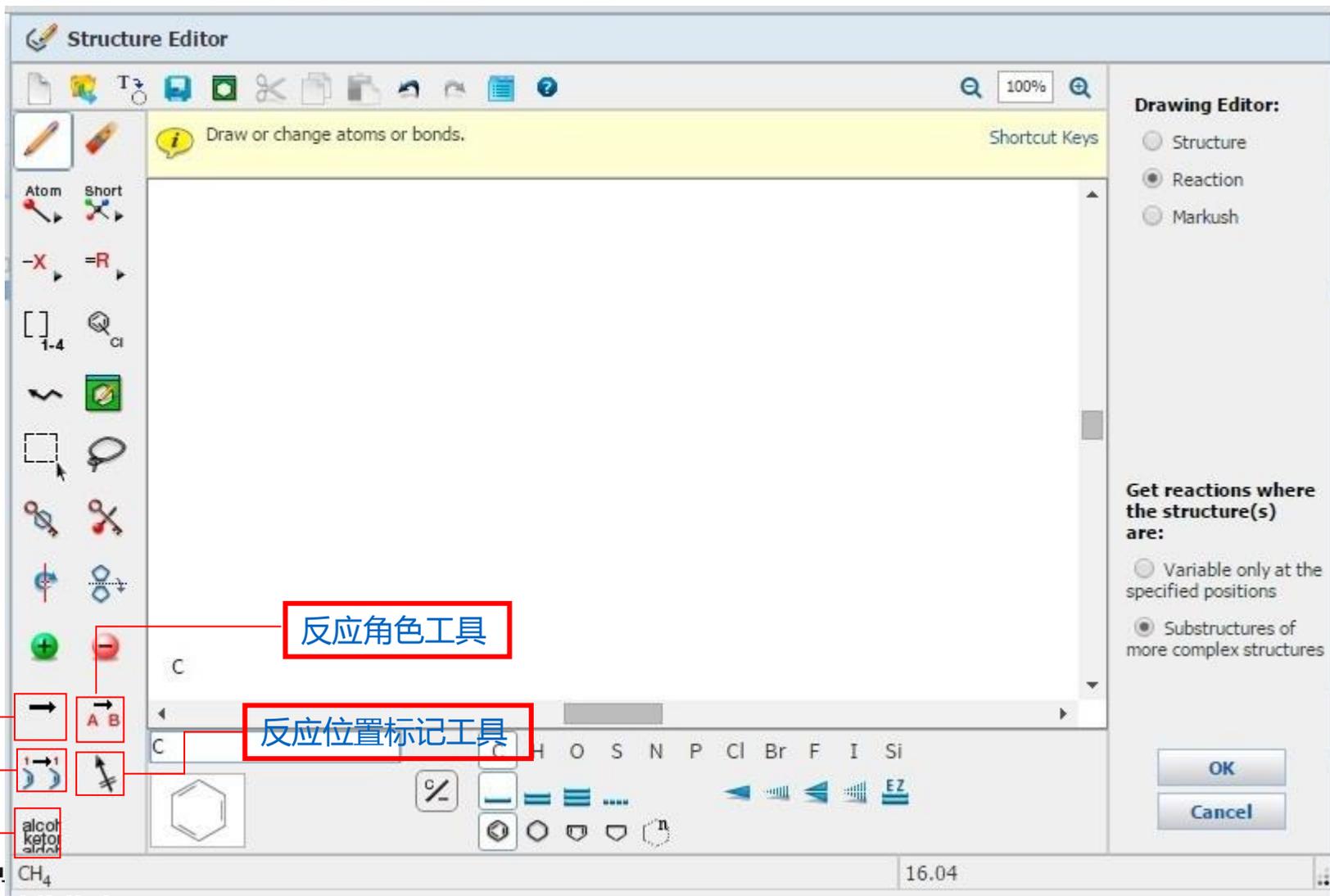
- 常用检索方法

- 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

Get reactions where the structure(s) are:

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

Scifinder 中反应定义工具



SciFinder反应检索——精确反应检索

The screenshot displays the SciFinder Reaction Editor window. The main workspace shows a chemical reaction: nitrobenzene (reactant) is converted to aniline (product). The interface includes a toolbar on the left with various drawing tools, a top menu bar, and a right-hand 'Drawing Editor' panel. In the 'Drawing Editor' panel, the 'Reaction' radio button is selected. Below it, the search criteria 'Variable only at the specified positions' is highlighted with a red box. The bottom status bar shows the reaction query: C7 H7 N O2 . C7 H9 N (reaction query) 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。

Reaction Structure structure variable only at spe... > reactions (383)

REACTIONS

Get References Tools

Analyze Refine

Analyze by: Reagent

H ₂	106
N ₂ H ₄ ·H ₂ O	32
NaBH ₄	25
CO	14
H ₂ O	14
KOH	14
N ₂ H ₄	12
HCl	11
Me ₂ CHOH	11
HCO ₂ H	10

Show More

Group by: No Grouping
No Grouping
Document Selected
Transformation

Sort by: Relevance

Display Options

Page: 1 of 8

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

Single Step Hover over any structure for more options.

Cc1ccc(cc1[N+](=O)[O-])>>Cc1ccc(cc1)N
~88 100% ~124

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

Single Step Hover over any structure for more options.

Cc1ccc(cc1[N+](=O)[O-])>>Cc1ccc(cc1)N
~88 100%

获取相似反应

按照反应类型排序

Explore ▾ Saved Searches ▾ SciPlanner Save Print Export

Reaction Structure structure variable only at spe... > reactions (383) > find additional reactions (621)

REACTIONS ⓘ Get References Tools ▾ Send to SciPlanner

Analyze Refine

Group by Transformation ▾ Sort by: Frequency ▾ ↓ Display Options

0 of 383 Reactions Selected

Analyze by: Reagent ▾

H ₂	106
N ₂ H ₄ -H ₂ O	32
NaBH ₄	25
CO	14
H ₂ O	14
KOH	14
N ₂ H ₄	12
HCl	11
Me ₂ CHOH	11
HCO ₂ H	10

Show More

1. Reduction of Nitro Compounds to Amines
373 Reactions
$$\text{R-NO}_2 \longrightarrow \text{R-NH}_2$$

2. Reduction of Nitro to Azoxy Compounds
6 Reactions
$$\text{Ar-NO}_2 \longrightarrow \text{Ar-N}^+\text{=N}^-\text{Ar}$$

3. Reduction of Nitro to Azo Compounds
5 Reactions
$$\text{Ar-NO}_2 \longrightarrow \text{Ar-N=N-Ar}$$

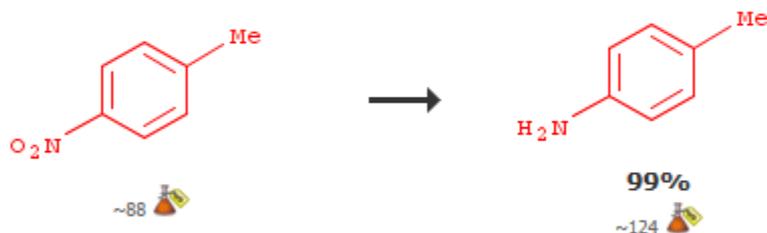
4. Formation of C=C from Alcohols via Dehydration
2 Reactions
$$\begin{array}{c} \text{R}^1 \quad \text{R}^3 \\ | \quad | \\ \text{C} - \text{C} \\ | \quad | \\ \text{H} \quad \text{OH} \end{array} \longrightarrow \begin{array}{c} \text{R}^1 \quad \text{R}^3 \\ \backslash \quad / \\ \text{C} = \text{C} \\ / \quad \backslash \\ \text{R}^2 \quad \text{R}^4 \end{array}$$

更精确的查找需要的反应

反应过程

37. **Polymeric PEG35k-Pd Nanoparticles: Efficient and Recyclable Catalyst for Reduction of Nitro Compounds** [Quick View](#) [Full Text](#)
1 Reaction [Similar Reactions](#)

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



Overview

Experimental Procedure



General/Typical Procedure: **Typical Experiment Procedure for the Reduction of Aromatic Reduction Compounds**

Reduction of nitroarenes was performed in a 10 ml, round-bottom flask in the presence of nitroarenes (entries 1-14) (1.0 mmol), polymeric PEG35k-Pd NPs (1 mol % polymeric PEG35k-Pd NPs), and hydrazine hydrate (5 equivalents) in an open atmosphere at 90 °C. After the reaction was completed, polymeric PEG35k-Pd NPs were removed by centrifugation. The solution was filtered through a pad of Celite, and then saturated aqueous NaHCO₃ (10 ml) was added to the filtrate and extracted with ethyl acetate. The combined organic layers were dried over anhydrous Na₂SO₄, concentrated under reduced pressure, and purified by the column chromatography to give the aniline derivatives. Products were characterized by ¹H NMR and ¹³C NMR and mass spectra. The removed polymeric PEG35k-Pd NPs were washed with water and diethyl ether, dried under vacuum, and then reused. Entry 2: Yield: 99%.

不用阅读全文，直接获得包含实验过程的反应记录

反应检索结果的筛选

Explore ▾ Saved Searches ▾ SciPlanner Save Print Export

32 reactions with the Reagent **N₂H₄-H₂O** are displayed **Keep Analysis** Clear Analysis

Reaction Structure structure variable only at spe... > reactions (383) > find additional reactions (621)

REACTIONS ? Get References Tools ▾ Send to SciPlanner

Analyze Refine Group by: No Grouping Sort by: Relevance Display Options

0 of 383 Reactions Selected

1. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.

获得特定物质做还原剂的反应

100%

Overview

9. Steps/Stages

1.1 R: N₂H₄-H₂O, C: CeO₂, S: H₂O, S: EtOH, 4 h, 80°C

Notes

green chemistry-catalyst, chemoselective, solid-supported catalyst, reusable catalyst, catalyst prepared and used, selectivity 100%, nanoparticle support used, Reactants: 1, Reagents: 2, Catalysts: 1, Solvents: 2, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Selective hydrogenation of nitroaromatics by ceria nanorods
Quick View Full Text
By Zhu, Hai-Zhou et al
From Nanoscale, 5(16), 7219-7223; 2013

Analyze by: Reagent

H ₂	106
N₂H₄-H₂O	32
NaBH ₄	25
CO	14
H ₂ O	14
KOH	14
N ₂ H ₄	12
HCl	11
Me ₂ CHOH	11
HCO ₂ H	10

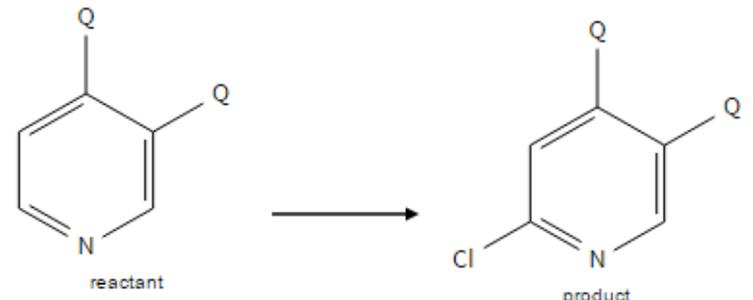
Show More

SciFinder反应检索——亚结构反应检索

Structure Editor

Drag the reaction arrow to specify reaction direction.

吡啶环的3,4位存在任意的非C,H原子或基团
检索在6位引入Cl的反应



reactant

product

Drawing Editor:

- Structure
- Reaction
- Markush

Get reactions where the structure(s) are:

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

Variables

- X Any halogen
- M Any metal
- A Any atom except H
- Q Any atom except C or H
- Ak Any alkyl chain
- Cy Any cycle
- Cb Any carbocycle
- Hy Any heterocycle

Close

Create Saved Answer

View All | Import

KEEP ME POSTED

C-N bond activation
Nov 21, 2015(1)
Nov 14, 2015(2)

View All

SciFinder反应检索——亚结构反应检索

Structure Editor

Drag the reaction arrow to specify reaction direction.

环锁定工具，当使用亚结构检索时，不允许发生稠环

reactant

product

Drawing Editor:

- Structure
- Reaction
- Markush

Get reactions where the structure(s) are:

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

亚结构反应检索结果

通过Analyze或者Refine处理检索结果

REACTIONS

Get References Tools

Group by: No Grouping Sort by: Accession Number

0 of 133 Reactions Selected

1. View Reaction Detail

3 Steps *Hover over any structure for more options.*

~192

[Step 3.1] ~106

~11

Number of Steps:
Examples: 1, 1 - 3, 1 2 - 3

Refine

Refine by:

- Reaction Structure
- Product Yield
- Number of Steps
- Reaction Classification
- Excluding Reaction Classification
- Non-participating functional groups

Overview

Steps/Stages

- 1.1 R: t-BuOK, S: THF, -78°C → -35°C
- 1.2 R: H₂O₂, S: THF, 0°C
- 1.3 S: 30 min, -35°C; 30 min, -35°C; -35°C → -78°C
- 1.4 R: NH₄Cl, S: H₂O, -78°C → rt
- 2.1 R: POCl₃, S: PhMe, 6 h, reflux; overnight, 60°C; cooled

Notes

Reactants: 2, Reagents: 6, Solvents: 4, Steps: 3, Stages: 7, Most stages in any one step: 4

References

Identification and Optimization of Benzimidazole Sulfonamides as Orally Bioavailable Sphingosine 1-Phosphate Receptor 1 Antagonists with in Vivo Activity

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
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 - 反应检索
 - SciPlanner使用简介
- SciFinder常见问题及解决

关于SciPlanner使用简介

3. View Reaction Detail Link

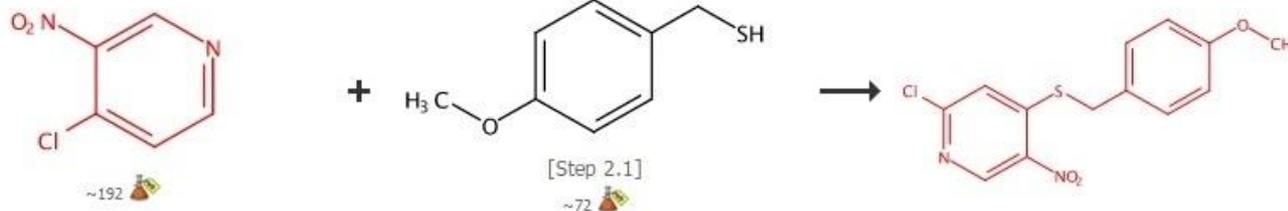
勾选想要的反应

点击Send to SciPlanner

Send to SciPlanner

Display Options

3 Steps Hover over any structure for more 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
Quick View Other Sources
By Huang, Yuhua et al
From Tetrahedron Letters, 51(21), 2800-2802; 2010

SciPlanner

SciPlanner_11_19_2015_112612

Workspace Edit View GoTo

New
Open
Save
Duplicate
Import
Export
Print
Close

workspace 下新建一个文件

Your Workspace is empty.

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

Clear Reactions

进入SciPlanner，将刚推送过来的反应拖动到屏幕中间

点击反应中的一个中间产物，单击上面的双向箭头，选择Synthesis this

在检索到的反应中，选择感兴趣的一条反应

Get References Tools

Group by: No Grouping Sort by: Accession Number

1 of 34 Reactions Selected

1. View Reaction Detail Link

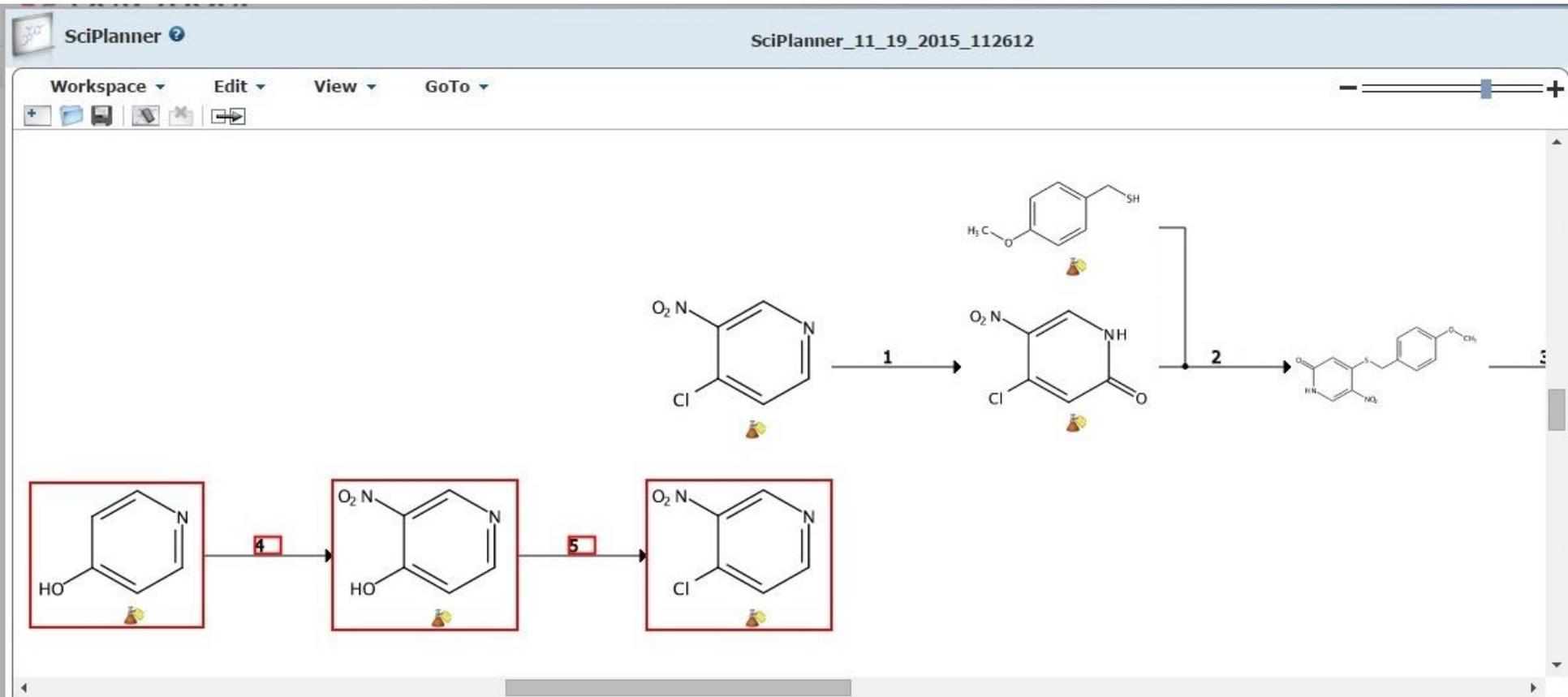
2 Steps Hover over any structure for more options.

Send selected records to SciPlanner. Send to SciPlanner

Display Options Page: 1 of 3

~161 ~192

将该条反应继续推送到SciPlanner中



同前页步骤，将推送过来的反应拖动到SciPlanner中，可以看到两条反应中存在同样的结构

SciPlanner 11_19_2015_112612

Workspace Edit View GoTo

New
Open
Save
Duplicate
Import
Export
Print
Close

4

5

1

2

3

Export ?

* Required

Details:

File Name: *
SciPlanner_11_19_2015_112612

Title

Include:

SciPlanner Image
 Reaction Details
 Substance Details
 Reference Details

Review

Portable Document Format (.pdf)
Reactions (*.ris)
Image (*.png)

Saving Locally

SciPlanner eXchange (*.pkx)

Export **Cancel**

• 用鼠标将两个同样的结构拖动至重叠状态，两条反应合并

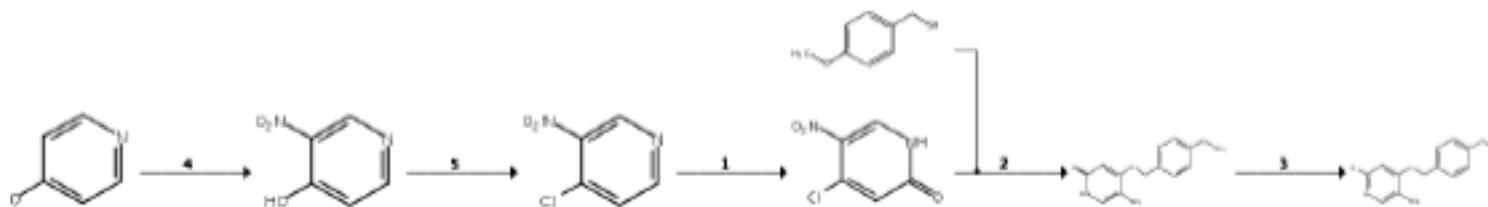
• 点击 Workspace，选择其中的 Export 输出结果

选择适当的输出格式，输出结果

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6

SciPlanner导出结果



Reaction Stages

5

- 1.1 R:POCl₃, S:PhMe, 0°C → rt; 16 h, rt → 110°C
 1.2 R:K₂CO₃, S:H₂O, cooled, pH 10

Notes

Reactants: 1, Reagents: 2
 Solvents: 2, Steps: 1, Sta

Transformation:

1. Formation of Alkyl Hal from Alcohols

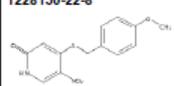
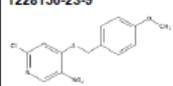
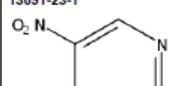
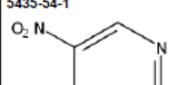
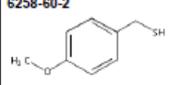
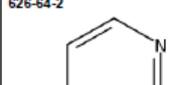
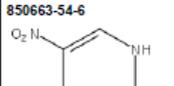
References

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

By Polek, Anurach et al

From Journal of Materials Chemistry C: Materials for Optical and Electronic Devices, 2(4) 2014

Substance Information

<p>1228150-22-8</p>  <p>C₁₃ H₁₂ N₂ O₄ S 2-((4-methoxyphenyl)methylthio)-5-nitro-2,1H-pyridin-4(1H)-one Related Info: ~ 2 References Reactions</p>	<p>1228150-23-9</p>  <p>C₁₃ H₁₁ Cl N₂ O₃ S Pyridine, 2-chloro-4-((4-methoxyphenyl)methylthio)-5-nitro- Related Info: ~ 2 References Reactions</p>	<p>13091-23-1</p>  <p>C₅ H₃ Cl N₂ O₂ Pyridine, 4-chloro-3-nitro- Related Info: ~ 391 References Reactions ~ 190 Commercial Sources Regulatory Information</p>
<p>5435-54-1</p>  <p>C₅ H₄ N₂ O₃ 4-Pyridinol, 3-nitro- Related Info: ~ 113 References Reactions ~ 197 Commercial Sources Regulatory Information</p>	<p>6258-60-2</p>  <p>C₈ H₁₀ O S Benzenemethanethiol, 4-methoxy- Related Info: ~ 749 References Reactions ~ 71 Commercial Sources Regulatory Information</p>	<p>626-64-2</p>  <p>C₅ H₅ N O 4-Pyridinol Related Info: ~ 1351 References Reactions ~ 160 Commercial Sources Regulatory Information</p>
<p>850663-54-6</p>  <p>C₉ H₇ Cl N₂ O₃ 2-((4-chloro-5-nitrophenyl)methylthio)-2,1H-pyridin-4(1H)-one Related Info: ~ 22 References Reactions ~ 136 Commercial Sources</p>		

提纲

- 美国化学文摘社简介
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 - 物质检索
 - Markush检索
 - 反应检索
 - SciPlanner使用简介
- 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

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Last Name:	<input type="text"/>
Email:	<input type="text"/>
Confirm Email:	<input type="text"/>
Phone Number:	<input type="text"/>
Fax Number:	<input type="text"/>
Area of Research:	<input type="text" value="Select one"/>
Job Title:	<input type="text" value="Select one"/>

--USERNAME AND PASSWORD--	
Username:	<input type="text"/>
Password:	<input type="text"/>
Re-enter Password:	<input type="text"/>

--SECURITY INFORMATION--	
Security Question:	<input type="text" value="Select one"/>
Answer:	<input type="text"/>

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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：

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- _ (下划线)
- . (句点)
- @ (表示“at”的符号)

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

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