

朱传娴

客户顾问

hzhu@acs-i.org

如何使用SciFinder获取科技信息

南京工业大学



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



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

SciFinder覆盖的数据库




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

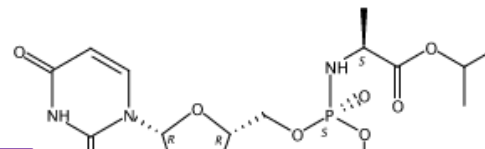
Crystallization	Drug bioavailability
Hepatitis C	Hepatitis C virus
Homo sapiens	Human
Pharmaceutical coated tablets	

prepn. of novel sofosbuvir crystal

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。

提纲

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

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What is SciFinder?
SciFinder® is a research discovery application that provides integrated access to the world's most comprehensive and authoritative source of references, substances and reactions in chemistry and related sciences.

News & Updates

Welcome to SciFinder

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

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New Commercial Source Logos



输入SciFinder帐号和密码

SciFinder主界面

检索完，请点击退出

工具栏

Sign Out

Preferences | SciFinder Help

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

Search

Advanced Search

已保存的结果集

- SAVED ANSWER SETS
- CSF1R
 - jmc
 - EP 19870107847
 - Daclatasvir-1
 - SUB result
 - EX result
 - MF result
 - polymer1
 - polymer1
 - structure search
 - Autosaved Substance Set
- View All | Import
- KEEP ME POSTED
- You have no proxies.
Learn how to:
Create Keep Me Posted

检索入口

定题追踪



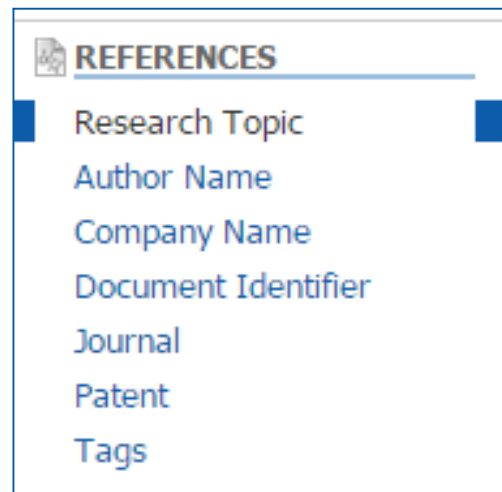
SciFinder检索——文献检索

■ 文献检索方法

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

■ 检索策略推荐

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



文献检索——主题

主题检索：离子液体催化剂

检索式： ionic liquid with catalysis

The screenshot displays the SciFinder web interface. At the top, there is a navigation bar with 'Explore', 'Saved Searches', and 'SciPlanner' tabs. Below this, the search topic 'ionic liquid with catalysis' is entered. On the left, a sidebar menu lists search criteria under 'REFERENCES' and 'SUBSTANCES'. The main content area shows the search term in a text box, followed by 'Examples:' and two sample search results. A blue 'Search' button is positioned below the examples. At the bottom of the main area, there is a link for 'Advanced Search'. A purple-bordered box highlights the search term and examples, with a text overlay: '关键词之间用介词连接: in, with, of...'.

CAS Solutions

SCIFINDER
A CAS SOLUTION

Explore ▼ Saved Searches ▼ SciPlanner

Research Topic "ionic liquid with catalysis"

REFERENCES

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

SUBSTANCES

- Chemical Structure
- Markush

REFERENCES: RESEARCH TOPIC ?

ionic liquid with catalysis

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

Search

Advanced Search

关键词之间用介词连接: in, with, of...

主题检索的候选项

Explore ▼ Saved Searches ▼ SciPlanner

Research Topic "ionic liquid with catalysis"

REFERENCES ?

Select All Deselect All

1 of 5 Research Topic Candidates Selected

		References
<input type="checkbox"/>	74 references were found containing "ionic liquid with catalysis" as entered.	74
<input checked="" type="checkbox"/>	16803 references were found containing the two concepts "ionic liquid" and "catalysis" closely associated with one another.	16803
<input type="checkbox"/>	20983 references were found where the two concepts "ionic liquid" and "catalysis" were present anywhere in the reference.	20983
<input type="checkbox"/>	91371 references were found containing the concept "ionic liquid".	91371
<input type="checkbox"/>	3150688 references were found containing the concept "catalysis".	3150688

Get References

“As entered”表示对检索式做精确文本检索；

“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

The screenshot shows the SciFinder interface for a search on "ionic liquid with catalysis". The results are sorted by "Citing References". The interface includes a navigation bar with "Explore", "Saved Searches", and "SciPlanner". The search results are displayed in a list format, with each entry showing the author, title, and a brief description. The first result is by Welton, Thomas (1999), titled "Ionic Liquids. Solvents for Synthesis and Catalysis". The second result is by Wasserscheid, Peter; Keim, Wilhelm (2000), titled "Ionic liquids - new 'solutions' for transition metal catalysis". The third result is by Dupont, Jairton; de Souza, Roberto F.; Suarez, Paulo A. Z. (2002), titled "Ionic Liquid (Molten Salt) Phase Organometallic Catalysis".

Research Topic "ionic liquid with catalysis" > references (16803)

REFERENCES

Analyze Refine Categorize

Sort by: Citing References

Accession Number
Author Name
Citing References
Publication Year
Title

Display Options

Page: 1 of 841

Analyze by: Author Name

Author Name	Citations
Wasserscheid Peter	170
Zhang Suojiang	146
Dupont Jairton	132
Li Huaming	97
Yu Shitao	96
Deng Youquan	91
Wang Jun	78
Chen Jing	76
Dyson Paul J	76
Fang Dong	75

- 1. Ionic Liquids. Solvents for Synthesis and Catalysis**
By Welton, Thomas
From Chemical Reviews (Washington, D. C.) (1999), 99(8), 2071-2083. | Language: English, Database: CAPLUS
A review with 124 refs. covering org. reactions in alkylhalo- and haloaluminate ionic liqs.
- 2. Ionic liquids - new "solutions" for transition metal catalysis**
By Wasserscheid, Peter; Keim, Wilhelm
From Angewandte Chemie, International Edition (2000), 39(21), 3772-3789. | Language: English, Database: CAPLUS
A review with 98 refs. Ionic liqs. are salts that are liq. at low temp. (<100°C), which represent a new class of solvents with nonmol., ionic character. Even though the first representative has been known since 1914, ionic liqs. have only been investigated as solvents for transition metal catalysis in the past ten years. Publications to date show that replacing an org. solvent by an ionic liq. can lead to remarkable improvements in well-known processes. Ionic liqs. form biphasic systems with many org. product mixts. This gives rise to the possibility of a multiphase reaction procedure wit...
- 3. Ionic Liquid (Molten Salt) Phase Organometallic Catalysis**
By Dupont, Jairton; de Souza, Roberto F.; Suarez, Paulo A. Z.
From Chemical Reviews (Washington, DC, United States) (2002), 102(10), 3667-3691. | Language: English, Database: CAPLUS
A review including ionic liqs.; oligomerization and polymn.; hydrogenation; dimerization and telomerization of dienes; carbonylation; oxidn. and radical reactions; Heck, Suzuki, Stille, Sonogashira, Negishi, and Ullmann coupling reactions; allylation; olefin metathesis; and mechanistic aspects of reactions in ionic liqs.

Citing Reference: 帮助找到最重要的文献

文献检索结果

CAS Solutions | SciFinder | A CAS SOLUTION

Preferences | SciFinder Help | Sign Out

Welcome Helen Zhu

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

Research Topic "ionic liquid with catalysis" > referen

REFERENCES

Substances | Reactions | Citations | Tools

Create Keep Me Posted Alert | Send to SciPlanner

Analyze | Refine | Categorize

Sort by: Accession Number

0 of 16803 References Selected

Page: 1 of 841

Analyze by: Author Name

Author Name	Count
Wasserscheid Peter	170
Zhang Suojiang	146
Dupont Jairton	132
Li Huaming	97
Yu Shitao	96
Deng Youquan	91
Wang Jun	78
Chen Jing	76
Dyson Paul J	76
Fang Dong	75

1. Significant effect of 5,10,15,20-meso-tetraarylporphyrinatoiron(III) chloride/triflate and acidic/neutral/basic imidazolium ionic liquids in catalytic oxidation of phenols

Quick View | Other Sources

By Ahmad, Sohail; Gautam, Renu; Singhal, Anchal; Chauhan, S. M. S.
From Journal of Molecular Liquids (2018), 260, 292-303. | Language: English, Database: CAPLUS

The influence of acidic, neutral and basic ionic liqs. and their binary mixt. with dichloromethane on the reactivity of iron(III)porphyrins was investigated during oxidn. of phenols with hydrogen peroxide catalyzed by 5,10,15,20-tetraarylporphyrinatoiron(III) chloride and 5,10,15,20-tetraarylporphyrinatoiron(III) triflate. The generation of different intermediates of iron(III) porphyrin in different ILs was studied through viscosity, d., UV-Vis and ¹H NMR spectroscopy. The heterolytic cleavage efficiency of (TAP) Fe^{III}-OOH and formation of quinone using iron(III)porphyrin (TAP)Fe^{III}Cl with Cl...

2. Supported ionic liquid phase (SILP) facilitated gas-phase enzyme catalysis - CALB catalyzed transesterification of vinyl propionate

Quick View | Other Sources

By Lee, Changhee; Sandig, Bernhard; Buchmeiser, Michael R.; Haumann, Marco
From Catalysis Science & Technology (2018), Ahead of Print. | Language: English, Database: CAPLUS

The supported ionic liq. phase (SILP) technol. has been used to immobilize Candida Antarctica Lipase B (CALB) within a hybrid monolith. The monolith was synthesized in-situ inside a Teflon cartridge via the 4-(dimethylamino)pyridine-catalyzed polyaddn. of 1,1,1-tris(hydroxymethyl)propane to 4,4'-methylenebis(phenylisocyanate) in the presence of porous cellulose-2.5-acetate beads. An ionic liq. contg. small amts. of CALB was impregnated into these beads and the resulting enzyme-SILP (e-SILP) catalyst was tested in the continuous gas-phase transesterification of vinyl propionate and 2-propanol...

3. A Phosphine-mediated Synthesis of 2,3,4,5-tetra-substituted Nhydroxypyrrroles from α-oximino Ketones and Dialkyl Acetylenedicarboxylates Under Ionic Liquid Green-media

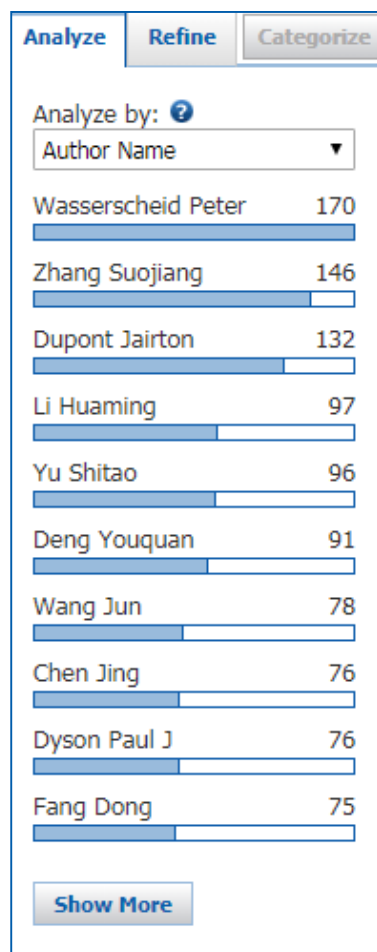
Quick View | Other Sources

By Shahvelayati, Ashraf S.; Ghazvini, Maryam; Yadollahzadeh, Khadijeh; Delbari, Akram S.
From Combinatorial Chemistry & High Throughput Screening (2018), 21(1), 14-18. | Language: English, Database: CAPLUS

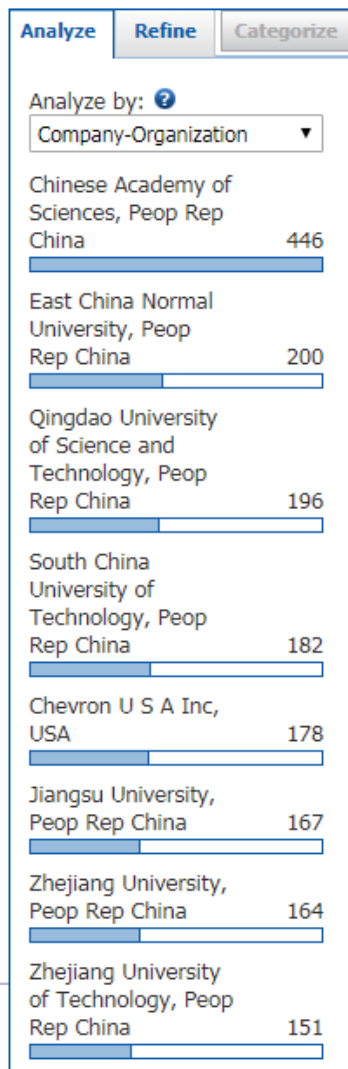
SciFinder提供强大的文献处理工具，帮助处理文献

文献检索结果的Analyze

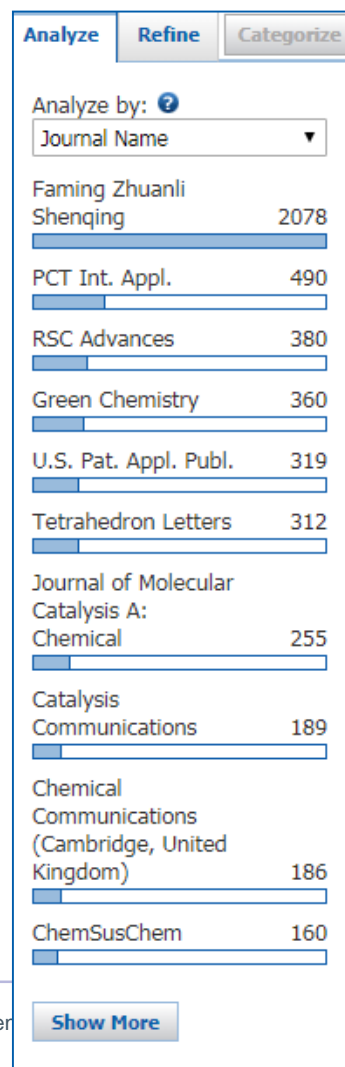
本领域研究人员



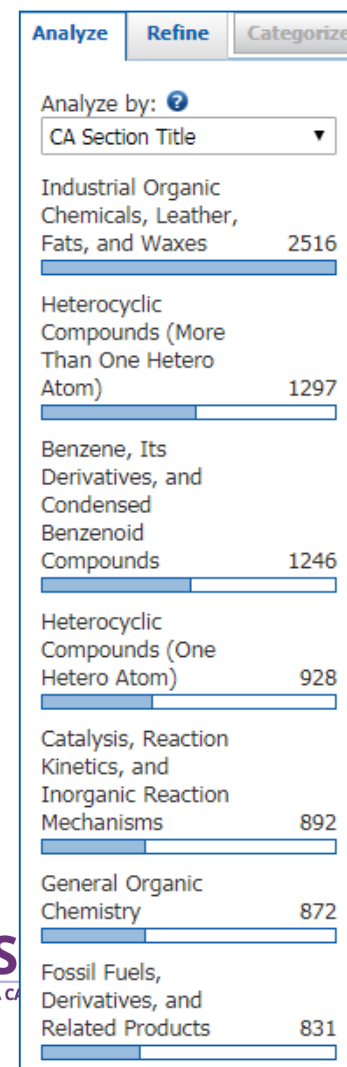
本领域研究机构、合作伙伴、竞争对手



期刊



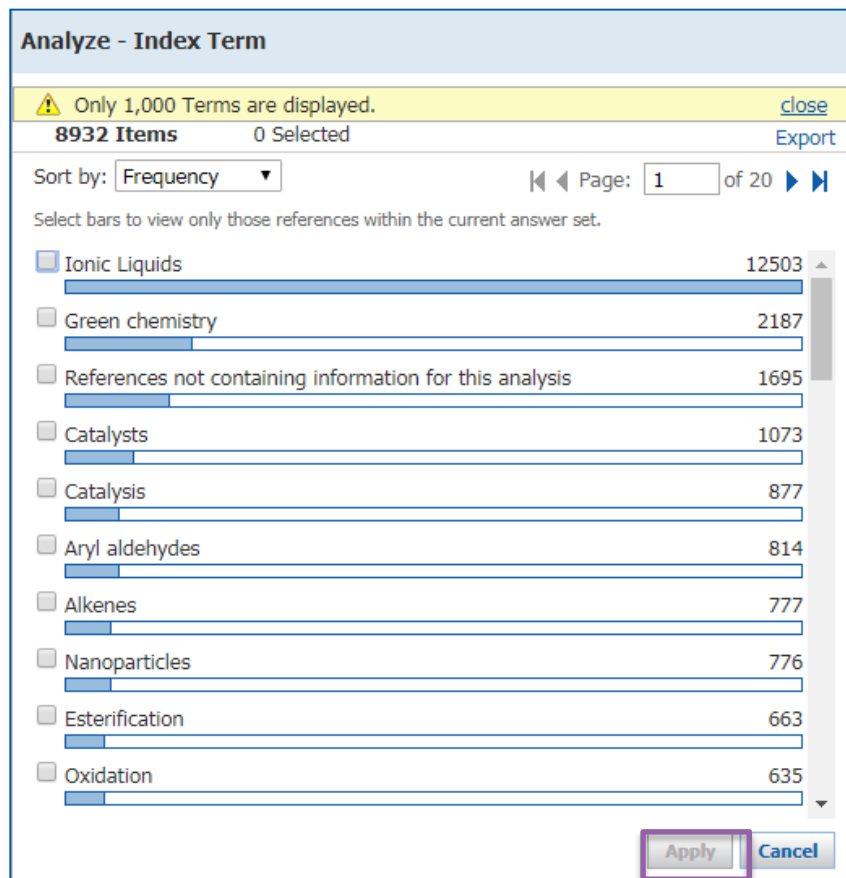
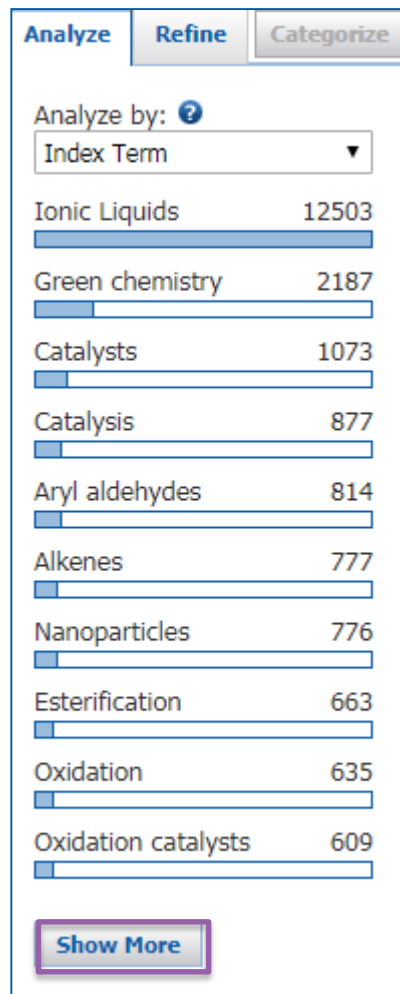
涉及学科领域



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Refine

Analyze Refine Categorize

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

Refine

Get Substances Get Reactions Get Related Citations Tools

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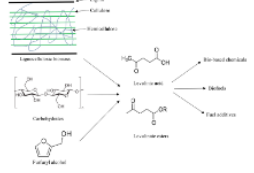
Sort by: Accession Number

0 of 1224 References Selected Page: 1 of 62

1. Conversion of Biomass and Its Derivatives to Levulinic Acid and Levulinate Esters via **Ionic Liquids**

Quick View Other Sources

By Tiong, Yong Wei; Yap, Chiew Lin; Gan, Suyin; Yap, Winnie Soo Ping
From Industrial & Engineering Chemistry Research (2018), 57(14), 4749-4766. | Language: English, Database: CAPLUS



A review. Biomass has emerged as an abundant and relatively low cost carbon resource alternative to fossil fuel resources in the sustainable prodn. of specialty chems. and biofuel. Levulinic acid is an attractive platform chem. Upgrading of levulinic acid produces levulinate esters, which serve as a transportation fuel and fuel additive. The present review focuses on the development of sustainable conversion of biomass into levulinic acid and levulinate esters via **ionic liqs.** dual solvent-**catalysts**. The synthesis routes of levulinic acid and levulinate esters and the corresponding **ionic l...**

2. Recent Advances in Pd-Catalyzed Cross-Coupling Reaction in **Ionic Liquids**

Quick View Other Sources

By Li, Jianxiao; Yang, Shaorong; Wu, Wanqing; Jiang, Huanfeng
From European Journal of Organic Chemistry (2018), 2018(11), 1284-1306. | Language: English, Database: CAPLUS

A review. **Ionic liqs. (ILs)** can behave as green solvents in comparison with conventional org. solvents, but more often they also act as ligands, co-**catalysts**, and stabilizing agents both for metal active species and for intermediates of **catalytic** systems. In this review we have mainly summarized the recent achievements (2013 to the present) in Pd-**catalyzed** cross-coupling in **ILs** for the assembly of structurally diverse and highly functionalized org. mols., with the focus on cascade **reactions** triggered by nucleopalladation, Suzuki coupling, Sonogashira coupling, allylic functionalization, and ...

3. Acid-Catalyzed Conversion of Carbohydrates into Value-Added Small Molecules in Aqueous Media and **Ionic Liquids**

Quick View Other Sources

By Bodachivskiy, Iurii; Kuzhiumparambil, Unnikrishnan; Williams, D. Bradley G.
From ChemSusChem (2018), 11(4), 642-660. | Language: English, Database: CAPLUS

A review. Biomass is the only realistic major alternative source (to crude oil) of hydrocarbon substrates for the com. synthesis of bulk and fine chems. Within biomass, terrestrial sources are the most accessible, and therein lignocellulosic materials are most abundant. Although lignin shows promise for the delivery of certain types of org. mols., cellulose is a biopolymer with significant potential for conversion into high-vol. and high-value chems. This review covers the acid-**catalyzed** conversion of lower value (poly) carbohydrates into valorized org. building-block chems. (platform mols....

Refine: 帮助用户迅速获得需要的文献

文献检索结果的Categorize

学科领域
主分类

学科领域
副分类

Index Term

选中的Index Term

Categorize ?

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

Category Heading	Category	Index Terms	Selected Terms
All	Catalysis (162)	Page: 1 of 4 Select All Deselect All	Click 'x' to remove the category from 'Selected Terms'
Synthetic chemistry	Catalysts (328)	<input type="checkbox"/> Enzymes 46	<input checked="" type="checkbox"/> Catalysis > Catalysts (1 Terms)
General chemistry		<input checked="" type="checkbox"/> Imidazolium compounds 32	
Catalysis		<input type="checkbox"/> Transition metal complexes 31	
Physical chemistry		<input type="checkbox"/> Palladium 28	
Environmental chemistry		<input type="checkbox"/> Lewis acids 25	
Technology		<input type="checkbox"/> Transition metals 25	
Genetics & protein chemistry		<input type="checkbox"/> Heteropoly acids 24	
Polymer chemistry		<input type="checkbox"/> Zeolites, synthetic 21	
Biotechnology		<input type="checkbox"/> Lipase 20	
Biology		<input type="checkbox"/> Bronsted acids 17	
Analytical chemistry		<input type="checkbox"/> Ruthenium 17	
		<input type="checkbox"/> Metals 16	
		<input type="checkbox"/> Oxides (inorganic) 16	
		<input type="checkbox"/> Quaternary ammonium compounds 16	

Catalysis > Catalysts > 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

The screenshot shows the SciFinder search results page. At the top, there are navigation buttons for 'Save', 'Print', and 'Export'. Below the search bar, there are options for 'Get Substances', 'Get Reactions', 'Get Related Citations', and 'Tools'. The search results are sorted by 'Accession Number' and show 0 of 32 references selected. The first three results are listed, with the first one highlighted. A purple box highlights the title 'Chiral Ionic Liquids: Synthesis and Role as Efficient Green Catalyst in Asymmetric Synthesis'. A purple arrow points from this box to a text box containing '文献详细信息'. Another purple box highlights the title 'Imidazolium-based ionic liquids grafted on solid surfaces'.

文献详细信息

Save: 保存在服务器上, 方便以后登陆查看, 每次可存2万条记录。

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

The screenshot shows the 'Export' dialog box in SciFinder. It has three main sections: 'Export:', 'For:', and 'Details:'. The 'Export:' section has radio buttons for 'All', 'Selected', and 'Range', with 'All' selected. The 'For:' section has radio buttons for 'Citation Manager', 'Offline review', and 'Saving locally'. Under 'Citation Manager', there are radio buttons for 'Citation export format (*.ris)', 'Quoted Format (*.txt)', and 'Tagged Format (*.txt)'. Under 'Offline review', there are radio buttons for 'Portable Document Format (*.pdf)', 'Rich Text Format (*.rtf)', and 'Answer Keys (*.txt)'. Under 'Saving locally', there is a radio button for 'Answer Key eXchange (*.akx)'. The 'Details:' section has a 'File Name:' field with the value 'Reference_06_19_2012_100848'. There are also radio buttons for 'Format:' (Summary without abstracts, Summary with partial abstracts, Summary with full abstracts, Detail (full record)) and 'Saving locally:' (Task History, Tags, Comments). At the bottom right, there are 'Export' and 'Cancel' buttons.

文献信息—题录、摘要、索引

获得引文及参考文献

REFERENCE DETAIL Get Substances Get Related Citations Link to Other Sources Send to SciFinder

Return Previous Next

4. The Partial Hydrogenation of 1,3-Dienes Catalyzed by Soluble Transition-Metal Nanoparticles

By: Luza, Leandro; Gual, Aitor; Dupont, Jairton

A review. The partial hydrogenation of a 1,3-dienes is a structure sensitive reaction that is typically catalyzed by classical heterogeneous (heterotopic) or homogeneous (homotopic) catalysts. Recently, sol. transition-metal nanoparticles (M-NPs), particularly palladium and gold-based systems, have emerged as an efficient alternative. Here, the authors review the current state of the techniques for the partial hydrogenation of 1,3-dienes by M-NPs and conclude that, from the reactivity point of view, these materials possess heterotopic-like and homotopic-like characteristics. They are heterotopic-like because the relative concn. of the monoalkene with respect to the diene does not affect the product selectivity and their catalytic performance is affected by their phys. properties (such as size and shape). Furthermore, they are easily recoverable, with long catalytic lifetimes. Addnl., as homotopic systems, their reactivity can be tuned by using an appropriate org. stabilizer, which displays substrate-selective levels that are not obsd. for classical heterotopic catalysts.

Indexing

General Organic Chemistry (Section 21.0)

Concepts

Hydrogenation
Ionic liquids
Polymer-supported catalysts

Hydrogenation catalysts
Nanoparticles
Surfactants

advances in development of methods for synthesis of alkene derivs. by transition-metal catalyst hydrogenation

Dendrimers
Transition metals

advances in development of methods for synthesis of alkene derivs. by transition-metal catalyst hydrogenation

Catalyst use; Uses

Group 10 elements

Substances

7439-89-6 Iron (nanoparticles), uses

7440-05-3 Palladium (nanoparticles), uses

7440-16-6 Rhodium (nanoparticles), uses

7440-18-8 Ruthenium (nanoparticles), uses

advances in development of methods for synthesis of alkene derivs. by transition-metal catalyst hydrogenation of alkadienes

Catalyst use; Uses

592-57-4 1,3-Cyclohexadiene

advances in development of methods for synthesis of alkene derivs. by transition-metal catalyst hydrogenation of alkadienes

Reactant; Reactant or reagent

QUICK LINKS

0 Tags, 0 Comments

SOURCE

ChemCatChem
Volume6
Issue3
Pages702-710
Journal; General Review;
Online Computer File
2014
CODEN:CHEMK3
ISSN:1867-3880
DOI:10.1002/cctc.201300673

COMPANY/ORGANIZATION

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970 RS

ACCESSION NUMBER

2013:1749284
CAN160:412993
CAPLUS

PUBLISHER

Wiley-VCH Verlag GmbH &
Co. KGaA

重要概念

重要物质

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，精准定位文献



提纲

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

SciFinder检索选项——物质检索

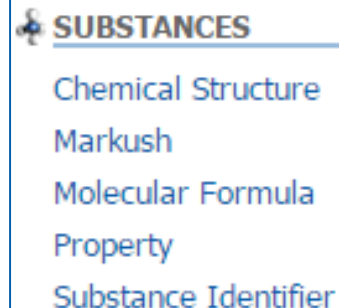
■ 物质检索方法

—结构式检索

—分子式检索

—理化性质检索

—物质标识符检索：化学名称，CAS RN



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

■ 物质检索策略推荐

—有机化合物，天然产物：结构检索

—无机物，合金：分子式检索

—高分子化合物：分子式检索和结构检索

物质检索——标识符检索

Explore ▾ Saved Searches ▾ SciPlanner

Research Topic "ionic liquid with catalysis" > references (16803) > refine "Review" (1224) > refine by c

REFERENCES

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

SUBSTANCES

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

SUBSTANCES: SUBSTANCE IDENTIFIER

UHMWPE

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

The screenshot displays the SciFinder interface for a substance record. At the top, it shows "0 of 1 Substance Selected". Below this, a search bar contains the CAS Registry Number "9002-88-4". To the left of the search bar, there are icons for "359876" and "112". The main content area shows the substance name "(C₂H₄)_x Ethene, homopolymer" and a list of "Key Physical Properties" including Regulatory Information, Spectra, and Experimental Properties. A chemical structure of ethene (CH₂=CH₂) is displayed. A context menu is open over the substance name, listing various actions: 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, and 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 9002-88-4

~359,876  ~112  

(C₂H₄)_x
Ethene, homopolymer
Polymer

Polymer Class Terms
Polyolefin

Melting Point (Experimental)
Value: 100-120 °C

Boiling Point (Experimental)
Value: 48-110 °C | Condition: Press: 9 Torr

Density (Experimental)
Value: 0.9745 g/cm³ | Condition: Temp: 25 °C

Other Names
Ethylene, polymers (8CI)
0017ZSK
0100F
0134M
030S
[View more...](#)

74-85-1
C₂H₄
C=C

物质详情

▼ EXPERIMENTAL PROPERTIES

Biological Chemical Density Electrical Electronic Flow and Diffusion Interface Magnetic Mechanical Nuclear Optical and Scattering Structure Related Thermal

Interface Properties

	Value	Condition	Note
Contact Angle	See full text	1 of 31	(12)CAS
Surface Tension	See full text	1 of 12	(872)CAS

Notes

- (12) Choi, Woo-Zin; Geosystem Engineering 2004, V7(3), P57-62 CAPLUS 🔍
- (872) Sanchis, M. R.; European Polymer Journal 2006, V42(7), P1558-1568 CAPLUS 🔍

实验数据与实验谱图

▼ EXPERIMENTAL SPECTRA

¹H NMR ¹³C NMR Hetero NMR IR Mass Raman UV and Visible X-Ray Additional Spectra

¹H NMR Properties

	Value	Condition	Note
Proton NMR Spectrum	See full text	1 of 15	(1313)CAS

Notes

- (1313) Kemmere, Maartje; DECHEMA Monographien 2004, V138(8th International Workshop on Polymer Reaction Engineering, 2004), P189-195 CAPLUS 🔍

▶ REGULATORY INFORMATION

▶ CAS REFERENCE ROLES

▶ ADDITIONAL DETAILS

物质检索——Property explore

CAS Solutions ▾

SciFINDER
A CAS SOLUTION

Explore ▾ Saved Searches ▾ SciPlanner

Substance Identifier "UHMWPE" > substances (1) > 9002-88-4

REFERENCES

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

SUBSTANCES

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

SUBSTANCES: PROPERTY ?

Experimental

Electric Resistance (ohm) ▾ >125
Examples: 44, 25-35, >125

Predicted

Select Property... ▾
Examples: 44, 25-35, >125

Search

寻找电阻率大于125ohm的含铁物质

物质结果集的筛选——Refine

SUBSTANCES ?

Get References

Get Reactions

Get Commercial Sources

Tools v

Create Keep Me Posted Alert

Send to SciPlanner

Analyze ?

Refine

Sort by: CAS Registry Number v

Display Options

0 of 137 Substances Selected

Page: 1 of 3

Analyze by: ?

Elements v

O 73

C 37

H 30

Fe 19

N 19

Mg 16

Ca 13

Cr 13

Se 13

In 12

Show More

1. 1360099-47-3 ?

~250

Component	Component Ratio
Te	x
Cd	x
Hg	x

Cd . Hg . Te

Cadmium mercury telluride

Experimental Properties

2. 1262894-47-2 ?

~2

Double bond geometry as shown.,Relative stereochemistry.

C₂₅ H₂₀ N₄ O

3. 1160936-40-2 ?

~1

Component	Component Ratio
Te	1.8
Se	0.2
In	0.1
Cu	0.1
Cd	1.8

4. 1160936-38-8 ?

~1

Component	Component Ratio
Te	1.6
Se	0.4
In	0.2
Cu	0.2
Cd	1.6

0 of 19 Substances Selected

1. 775325-57-0 ?

~1

Component	Component Ratio
O	2.82
Ca	0.02
Mg	0.1
Fe	1.8

Ca . Fe . Mg . O

Calcium iron magnesium oxide
(Ca_{0.02}Fe_{1.8}Mg_{0.1}O_{2.82})

Experimental Properties

2. 775325-56-9 ?

~1

Component	Component Ratio
O	2.74
Ca	0.14
Mg	0.2
Fe	1.6

Ca . Fe . Mg . O

Calcium iron magnesium oxide
(Ca_{0.14}Fe_{1.6}Mg_{0.2}O_{2.74})

Experimental Properties

3. 775325-55-8 ?

~1

Component	Component Ratio
O	2.67
Ca	0.07
Mg	0.2
Fe	1.6

Ca . Fe . Mg . O

Calcium iron magnesium oxide
(Ca_{0.07}Fe_{1.6}Mg_{0.2}O_{2.67})

Experimental Properties

4. 775325-54-7 ?

~1

Component	Component Ratio
O	2.64
Ca	0.04
Mg	0.2
Fe	1.6

Ca . Fe . Mg . O

Calcium iron magnesium oxide
(Ca_{0.04}Fe_{1.6}Mg_{0.2}O_{2.64})

Experimental Properties

5. 775325-53-6 ?

~1

Component	Component Ratio
O	2.44
Ca	0.14
Mg	0.35
Fe	1.3

Ca . Fe . Mg . O

Calcium iron magnesium oxide
(Ca_{0.14}Fe_{1.3}Mg_{0.35}O_{2.44})

Experimental Properties

6. 775325-52-5 ?

~1

Component	Component Ratio
O	2.37
Ca	0.07
Mg	0.35
Fe	1.3

Ca . Fe . Mg . O

Calcium iron magnesium oxide
(Ca_{0.07}Fe_{1.3}Mg_{0.35}O_{2.37})

Experimental Properties

7. 775325-51-4 ?

~1

Component	Component Ratio
O	2.34
Ca	0.04
Mg	0.35
Fe	1.3

Ca . Fe . Mg . O

Calcium iron magnesium oxide
(Ca_{0.04}Fe_{1.3}Mg_{0.35}O_{2.34})

Experimental Properties

8. 775325-50-3 ?

~1

Component	Component Ratio
O	2.14
Ca	0.14
Mg	0.5
Fe	1

Ca . Fe . Mg . O

Calcium iron magnesium oxide
(Ca_{0.14}FeMg_{0.5}O_{2.14})

Experimental Properties

如何筛选含铁物质?

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

1. 151-21-3
(Component: 151-41-7)
~84904 ~276

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

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

金属盐：金属离子和阴离子间用点 (.) 分开

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

物质检索——结构

REFERENCES

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

SUBSTANCES

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

REACTIONS

- Reaction Structure

SUBSTANCES: CHEMICAL STRUCTURE

Structure Editor:

Java Non-Java

Click to Edit

Search Type:

- Exact Structure
- Substructure
- Similarity

Show precision analysis

ChemDraw
Launch a SciFinder substance or re

Import CXF

Search

[Advanced Search](#) Always Show

物质检索——结构

The image shows a screenshot of the 'Structure Editor' software interface. The interface includes a top toolbar, a central workspace, and a right-hand panel. Various tools and features are highlighted with purple boxes and labeled in Chinese:

- 橡皮** (Eraser)
- 结构和反应切换功能** (Structure and Reaction Switching Function)
- 铅笔** (Pencil)
- 元素周期表** (Periodic Table)
- 可变基团** (Variable Group)
- 重复基团工具** (Repeat Group Tool)
- 碳链工具** (Carbon Chain Tool)
- 选择工具** (Selection Tool)
- 环锁定工具** (Ring Locking Tool)
- 旋转工具** (Rotation Tool)
- 正电子** (Positron)
- C原子和单键恢复工具** (C Atom and Single Bond Restoration Tool)
- 常用基团** (Common Group)
- R基团定义工具** (R Group Definition Tool)
- 可变位置连接工具** (Variable Position Connection Tool)
- 模版工具** (Template Tool)
- 索套选择工具** (Lasso Selection Tool)
- 原子锁定工具** (Atom Locking Tool)
- 镜面旋转工具** (Mirror Rotation Tool)
- 结构检索选择** (Structure Search Selection)
- 负电子** (Negatron)
- 单双键, RS构型, 不确定键定义工具** (Single/Double Bond, RS Configuration, Uncertain Bond Definition Tool)
- 常见环, 多元环工具** (Common Ring, Poly-ring Tool)

The right-hand panel, titled 'Drawing Editor', shows search options: 'Exact search', 'Substructure search' (selected), and 'Similarity search'. It also includes '确定' (OK) and '取消' (Cancel) buttons.

物质检索——精确结构检索

Structure Editor

Draw or change atoms or bonds. Shortcut Keys

Atom Short

-X =R

1-4

Draw or change atoms or bonds. Shortcut Keys

Ir

Ir

Ir

Get substances that match your query using:

- Exact search
- Substructure search
- Similarity search

OK

Cancel

Ir · Ir · C₁₀H₁₆ · C₁₀H₁₆ · C₈H₆N₄ 192.22 · 192.22 · 136.24 · 136.24 · 158.16


- Characteristics
- Single component
 - Commercially available
 - Included in references
- Classes
- Alloys
 - Coordination compounds
 - Incompletely defined
 - Mixtures
 - Polymers
 - Organics, and others not listed
- Studies
- Analytical
 - Biological
 - Preparation
 - Reactant or reagent


限定为单一组分


精确结构检索

物质检索——精确结构检索


0 of 4 Substances Selected


1. 1613301-57-7 

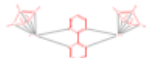
~2 




C₁₈ H₂₃ Ir N₄ O
Iridium(2+), aqua(2,2'-bipyrimidine-κN',κN'')
[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-


2. 1448751-22-1 

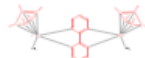
~0 




C₂₈ H₃₆ Ir₂ N₄
Iridium(4+), [μ-(2,2'-bipyrimidine-κN',
κN'':κN^δ,κN^δ)]bis[(1,2,3,4,5-η)-1,2,3,4,5-
pentamethyl-2,4-cyclopentadien-1-yl]di-


3. 1448751-19-6 


~0 



C₂₈ H₄₀ Ir₂ N₄ O₂
Iridium(4+), diaqua[μ-(2,2'-bipyrimidine-κN',
κN'':κN^δ,κN^δ)]bis[(1,2,3,4,5-η)-1,2,3,4,5-
pentamethyl-2,4-cyclopentadien-1-yl]di-

4. 920966-48-9 

~1 



C₁₈ H₂₁ Ir N₄
Iridium, (2,2'-bipyrimidine-κN',κN'')[(1,2,3,4,
5-η)-1,2,3,4,5-pentamethyl-2,4-
cyclopentadien-1-yl]-

物质检索——精确结构检索

精确结构检索：

获得被检索结构的盐，混合物，配合物，聚合物等，被检结构不能被取代

物质检索——亚结构检索

The screenshot displays the Structure Editor software interface. The main workspace shows a chemical structure of a nitro compound, CC(=O)N, with the label "Ag" next to it. The interface includes a top toolbar with various drawing and editing tools, a left sidebar with additional tools, and a right sidebar with search options. The search options are:

- Drawing Editor:**
 - Structure
 - Reaction
 - Markush
- Get substances that match your query using:**
 - Exact search
 - Substructure search
 - Similarity search

At the bottom of the interface, there is a status bar showing the chemical formula Ag . C2H5NO2 and the molecular weight 107.87 . 75.07.

物质检索——亚结构检索

Chemical Structure substructure > substances (2098)

SUBSTANCES [Get References](#) [Get Reactions](#) [Get Commercial Sources](#) [Tools](#) [Create Keep Me Posted Alert](#) [Send to SciPlanner](#)

Analyze Refine

Sort by: CAS Registry Number

0 of 2098 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: **Substructure**

Only retrieve substances that:


- Have references
- Are commercially available
- Are a single component
- Are in specific substance

1. [2247810-17-7](#) 


~1 

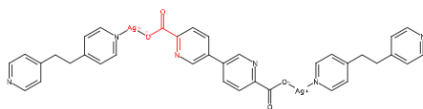
Substance
Image
Cannot Be
Displayed
2247810-17-7

$C_{23} H_{25} Ag N_3 O_9 S$
INDEX NAME NOT YET ASSIGNED

2. [2241885-38-9](#) 


(Component: 2241885-37-8)


~1 

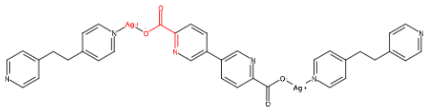


• 2 H₂O


$C_{36} H_{30} Ag_2 N_6 O_4 \cdot 2 H_2 O$
INDEX NAME NOT YET ASSIGNED


3. [2241885-37-8](#) 

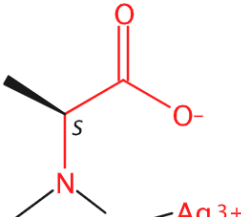
~0 



$C_{36} H_{30} Ag_2 N_6 O_4$
INDEX NAME NOT YET ASSIGNED

4. [2237966-12-8](#) 

~1 



Ag³⁺

亚结构检索结果的限定

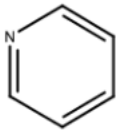
Analyze **Refine**

Refine by: ?

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

Structure Editor:

Java **Non-Java**

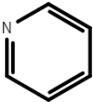


Click image to change structure or view detail.
Search type: **Substructure**

化学结构的再次限定

Structure Editor

Click a ring system to block it from further ring fusion. Click a chain to block it from ring formation.



Get substances that match your query using:

- Exact search
- Substructure search

OK
Cancel

C₅H₅N 79.10



环锁定

亚结构检索结果的限定

SUBSTANCES [Get References](#) [Get Reactions](#) [Get Commercial Sources](#) [Tools](#) [Create Keep Me Posted Alert](#) [Send to SciPlanner](#)

Analyze **Refine** Sort by: Relevance [Display Options](#)

0 of 173 Substances Selected Page: 1 of 12

Analyze by: [Substance Role](#) Properties 80 Preparation 66 Reactant or Reagent 30 Uses 18 Biological Study 17 Process 7 Analytical Study 1 [Show More](#)

1. **27876-60-4** (Component: 98-98-6) ~23

- Ag(I)

$C_6H_5NO_2 \cdot Ag$
2-Pyridinecarboxylic acid, silver(1+) salt (1:1)

2. **22721-95-5** (Component: 98-98-6) ~4

- 1/2 Ag(II)

$C_6H_5NO_2 \cdot 1/2 Ag$
2-Pyridinecarboxylic acid, silver(2+) salt (2:1)

3. **171626-32-7** (Component: 23628-31-1) ~2

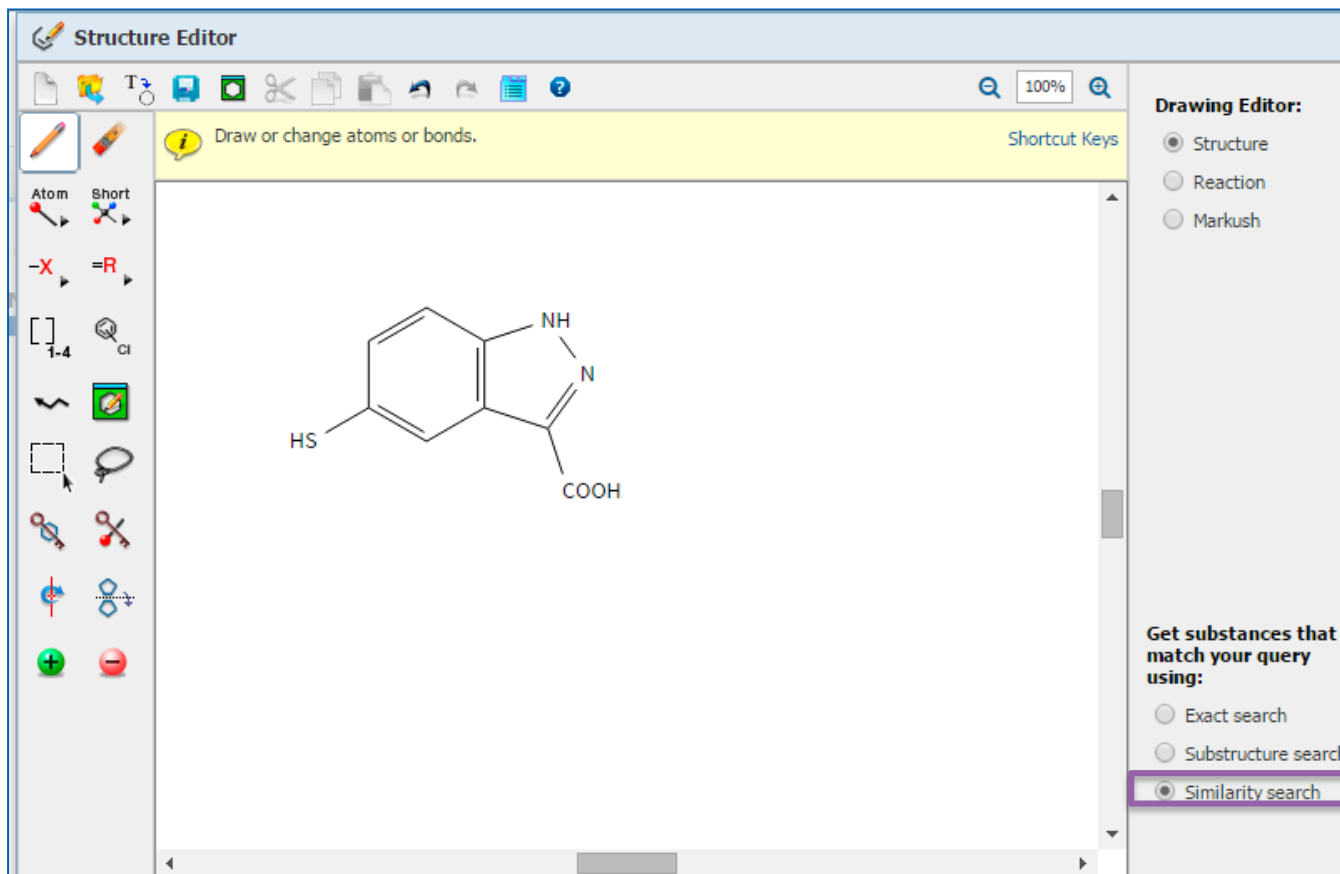
4. **1622218-89-6** (Component: 499-83-2) ~1

物质检索——亚结构检索

- 亚结构检索：

包括精确结构检索结果，及被检索结构的修饰结构

物质检索——相似结构检索



相似结构检索结果

Select All Deselect All

0 of 6 Similarity Candidates Selected

	Substances
<input type="checkbox"/> ≥ 99 (most similar)	0
<input type="checkbox"/> 95-98	0
<input type="checkbox"/> 90-94	0
<input type="checkbox"/> 85-89	11
<input type="checkbox"/> 80-84	34
<input type="checkbox"/> 75-79	84
<input type="checkbox"/> 70-74	267
<input type="checkbox"/> 65-69	696
<input type="checkbox"/> 0-64 (least similar)	1818

Get Substances

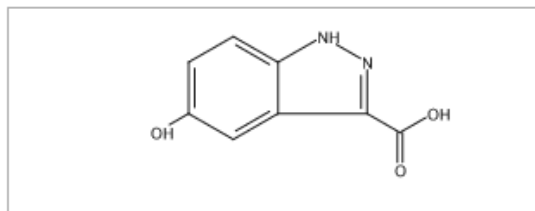
评分越高，相似度越高，结构越相似

Score: 88

1. 885518-94-5

取代基变化

~1 ~35



C₈ H₆ N₂ O₃
1*H*-Indazole-3-carboxylic acid, 5-hydroxy-

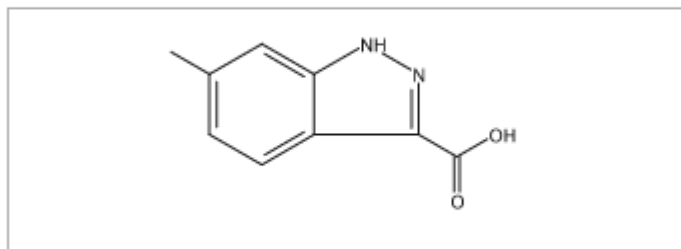
▶ Key Physical Properties

Score: 86

5. 858227-12-0

取代基位置变化

~7 ~41



C₉ H₈ N₂ O₂
1*H*-Indazole-3-carboxylic acid, 6-methyl-

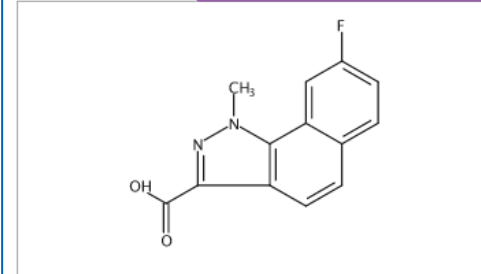
▶ Key Physical Properties

Score: 65

541. 1100422-

母体结构变化

~1



C₁₃ H₉ F N₂ O₂
1*H*-Benz[σ]indazole-3-carboxylic acid, 8-fluoro-1-methyl-

▶ Key Physical Properties

物质检索——相似结构检索

- 相似结构检索：

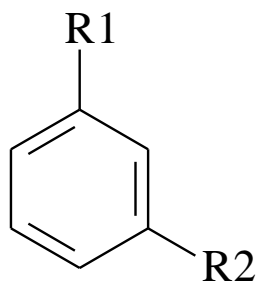
获得片段或整体结构与被检索结构相似的结果，母体结构可以被取代，也可以被改变

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
- SciFinder常见问题及解决

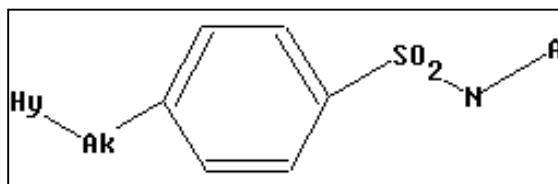
Markush检索

- 具体物质[Specific Substance]:
 - 以具体化学结构陈述的特定物质, 会被分配CAS RN
- 预测性物质[Prophetic Substance]:
 - 使用Markush结构陈述的预测物质, 一个Markush可以陈述上百或上千个化学物质
 - 专利中所陈述的预测物质, 不会被分配CAS RN
 - Markush检索, 能检索到通过结构检索检不到的专利



R1 = H, Br, Cl, I

R2 = Br, Cl, I, —CH₂—halogen, —CH—halogen,
|
CH₃



可用SciFinder中的Markush检索
查看专利中化合物结构保护范围。

Structure Editor

Draw or change atoms or bonds. Shortcut Keys

100%

Atom Short

-X =R

Hy-Ak SO₂-N-A

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

Display Options

Analyze by: Document Type

Patent	1969
Journal	1

Show More

全部是专利

1. **Compounds and methods for anticoagulation therapy**
PATENTPAK
By Allende Rodriguez, Mikel; Hermida Santos, Jose; Montes Diaz, Ramon; Oyarzabal Santamarina, Julen
From PCT Int. Appl. (2016), WO 2016120432 A1 20160804. | Language: English, Database: CAPLUS

The invention relates to certain compds. that are inducers of Heat shock 70 kDa protein 1A/1B (HSPA1A/B) and their use for anticoagulation therapy; and to a method for anticoagulation therapy that comprises the administration of one of these inducer compds. It has been here proved that induction of Heat shock 70 kDa protein 1A/1B by administration of one of these inducer compds. has antithrombotic effects without accelerating or altering bleeding time.

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

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

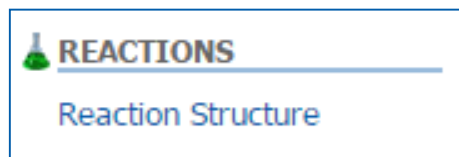
提纲

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

SciFinder检索选项——反应检索

- 反应检索方法

结构式



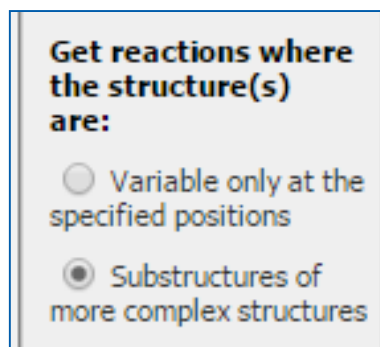
- 常用获取方法

已知物质：由物质获取反应

已知文献：从文献中获取反应

精确结构反应检索

亚结构反应检索



反应绘制工具

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

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

The interface includes a top toolbar with standard editing tools, a central drawing area with a yellow status bar that says "Draw or change atoms or bonds.", and a right-hand panel with "Drawing Editor" options (Structure, Reaction, Markush) and search filters. The bottom of the window shows a chemical formula input field with "CH₄", a periodic table, and a status bar with the version number "16.04".

SciFinder反应检索——精确反应检索

The screenshot displays the SciFinder Structure Editor interface. The central workspace shows a chemical reaction: nitrobenzene (reactant) is converted to aniline (product). The reactant is a benzene ring with an NO_2 group at the bottom, and the product is a benzene ring with an NH_2 group at the bottom. An arrow points from the reactant to the product. Below the structures, the text "reactant" and "product" are visible. The interface includes a drawing toolbar on the left with various icons for atoms, bonds, and rings. A yellow banner at the top of the workspace says "Draw or change atoms or bonds." On the right, the "Drawing Editor" panel is open, showing three radio buttons: "Structure", "Reaction" (which is selected), and "Markush". Below this, the text "Get reactions where the structure(s) are:" is followed by two radio buttons: "Variable only at the specified positions" (which is selected) and "Substructures of more complex structures". A purple callout box with the text "精确反应检索" (Precise Reaction Search) points to the "Variable only at the specified positions" option. At the bottom of the interface, there is a search bar containing "NH2", a list of elements (C, H, O, S, N, P, Cl, Br, F, I, Si), and a status bar showing the molecular formula $\text{C}_7\text{H}_7\text{NO}_2 \cdot \text{C}_7\text{H}_7\text{N}$ and the coordinates 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。

The screenshot displays the SciFinder interface. At the top, there are tabs for 'Get References' and 'Tools'. Below this, a 'Group by' dropdown menu is open, showing options: 'No Grouping', 'Document' (which is highlighted and selected), and 'Transformation'. The 'Sort by' dropdown is set to 'Relevance'. A 'Send to SciPlane' button is visible in the top right corner. The main content area shows a reaction scheme for the reduction of 4-nitrotoluene to 4-aminotoluene. The reactant is 4-nitrotoluene (SMILES: Cc1ccc([N+](=O)[O-])cc1) with a yield of ~102%. The product is 4-aminotoluene (SMILES: Cc1ccc(N)cc1) with a yield of 100% and ~122%. Below the reaction, there is an 'Overview' section with 'Steps/Stages' and 'Notes'. The 'Steps/Stages' section lists: 1.1 R:NaBH₄, C:1832616-28-0, C:Ru, S:H₂O, S:THF, 45 min, 25°C. The 'Notes' section describes the catalyst and reaction conditions. The 'References' section lists: Fabrication of Ruthenium Nanoparticles in Porous Organic Polymers: Towards Advanced Heterogeneous Catalytic Nanoreactors.

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

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

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

~102% 100%
~122%

Overview

Steps/Stages

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

Notes

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

References

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

按照反应类型排序

Group by: Transformation ▼ Sort by: Frequency ▼ ↓

0 of 560 Reactions Selected

1. Reduction of Nitro Compounds to Amines
538 Reactions

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

2. Reduction of Nitro to Azo Compounds
11 Reactions

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

3. Reduction of Nitro to Azoxy Compounds
11 Reactions

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

更精确的查找需要的反应

反应检索结果的筛选

获得特定物质做还原剂的反应

The screenshot displays the SciFinder interface for reaction search results. On the left, a sidebar titled 'REACTANTS' allows for refining results by reagent. The 'Reagent' dropdown is set to 'NaBH₄', which is highlighted with a purple box. Below this, a list of reagents and their corresponding number of reactions is shown: H₂ (148), NaBH₄ (51), N₂H₄-H₂O (43), KOH (17), CO (16), HCO₂H (16), NH₄⁺•HCO₂⁻ (16), H₂O (14), N₂H₄ (14), and NaOH (14). A 'Show More' button is located at the bottom of this list.

The main search results area shows '0 of 512 Reactions Selected'. The top result is '1. View Reaction Detail', which is expanded to show a 'Single Step' reaction. The reaction scheme shows the reduction of 4-nitrotoluene (SMILES: Cc1ccc(cc1)[N+](=O)[O-]) to 4-aminotoluene (SMILES: Cc1ccc(cc1)N). The reaction is catalyzed by Ru (indicated by a catalyst icon) and proceeds in 100% yield. The number of reactions for this step is approximately 122 (~122).

Below the reaction scheme, the 'Overview' section provides details for 'Steps/Stages':
1.1 R:NaBH₄, C:1832616-28-0, C:Ru, S:H₂O, S:THF, 45 min, 25°C

The 'Notes' section describes the catalyst: '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'.

The 'References' section lists: '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

亚结构反应检索

通过C-H活化对苯并噁唑或者恶唑进行烷基化

The screenshot displays the 'Structure Editor' interface on the left and the 'R-group Definitions' dialog box on the right. In the Structure Editor, a benzimidazole-like structure is shown with an R1 group attached to the imidazole ring. The 'R-group Definitions' dialog box is open, showing the definition for R1 as 'O, S'. A purple arrow points from the '=R' button in the Structure Editor's toolbar to the 'S' element in the periodic table within the R-group Definitions dialog. The periodic table shows 'S' highlighted in a purple box. Below the periodic table, there are sections for 'Variables' and 'Shortcuts'. At the bottom of the dialog, there are 'Close' and 'Cancel' buttons. The Structure Editor toolbar includes various drawing tools, and the status bar at the bottom left indicates 'Formula is not available'.

亚结构反应检索

The screenshot displays the SCIFINDER Structure Editor interface. The main workspace shows a chemical reaction scheme where a reactant (a benzimidazole-like structure with an R1 group and a hydrogen atom) is converted into a product (the same structure with an Ak group instead of the hydrogen). A purple arrow points from the Ak variable in the product to the Variables dialog box.

Structure Editor

Drag the reaction arrow to specify reaction direction.

Drawing Editor:

- Structure
- Reaction
- Markush

Variables

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

Get reactions where the structure(s) are:

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

Formulas: C H O S N P Cl Br F I Si

Formula is not available

通过后处理工具筛选反应--Analyze

通过催化剂筛选反应

Analyze Refine

Analyze by: ?
Catalyst

CuI	28
312696-09-6	17
AgNO ₃	17
(MeOCH ₂ CH ₂) ₂ O	16
NaI	15
1905414-33-6	14
CoBr ₂	11
Me ₃ SiCH ₂ MgCl	10
Ph ₂ P(CH ₂) ₃ PPh ₂	10
658062-48-7	9

Group by: No Grouping Sort by: Accession Number

No Grouping
Document
Transformation

1. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.

~57
~52
83%

Overview

Steps/Stages

- 1.1 R:LiO-Bu-*t* C:1905414-33-6, S:Dioxane, 16 h, 100°C
- 1.2 S:H₂O, rt
- 1.3 R:HCl, S:H₂O, neutralized

Notes

catalyst prepared and used, screw cap tube used, Reactants: 2, Reagents: 2, Catalysts: 1, Solvents: one step: 3

References

ACS / Proprietary and Confidential / Do Not Distribute

提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
 - 文献检索
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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** [Send to SciPlanner](#) [Display Options](#)

Overview

Steps/Stages

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

Notes

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

References

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

进入SciPlanner 新建文件

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

Workspace Edit View GoTo

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

Your Workspace is empty.

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

SciPlanner使用简介

SciPlanner 11_19_2015_112612

Workspace Edit View GoTo

CAS Registry Number: 13091-23-1

- View Substance Detail
- Explore by Structure
- Synthesize this...
- Get Reactions where Substance is a
- Get Commercial Sources
- Get Regulatory Information
- Get References
- Export as Image
- Export as molfile

打开中间产物的标准菜单
选择Synthesis this

1 2 3

Get References Tools

Send selected records to SciPlanner. Send to SciPlanner

Group by: No Grouping Sort by: Accession Number

1 of 34 Reactions Selected

1. View Reaction Detail

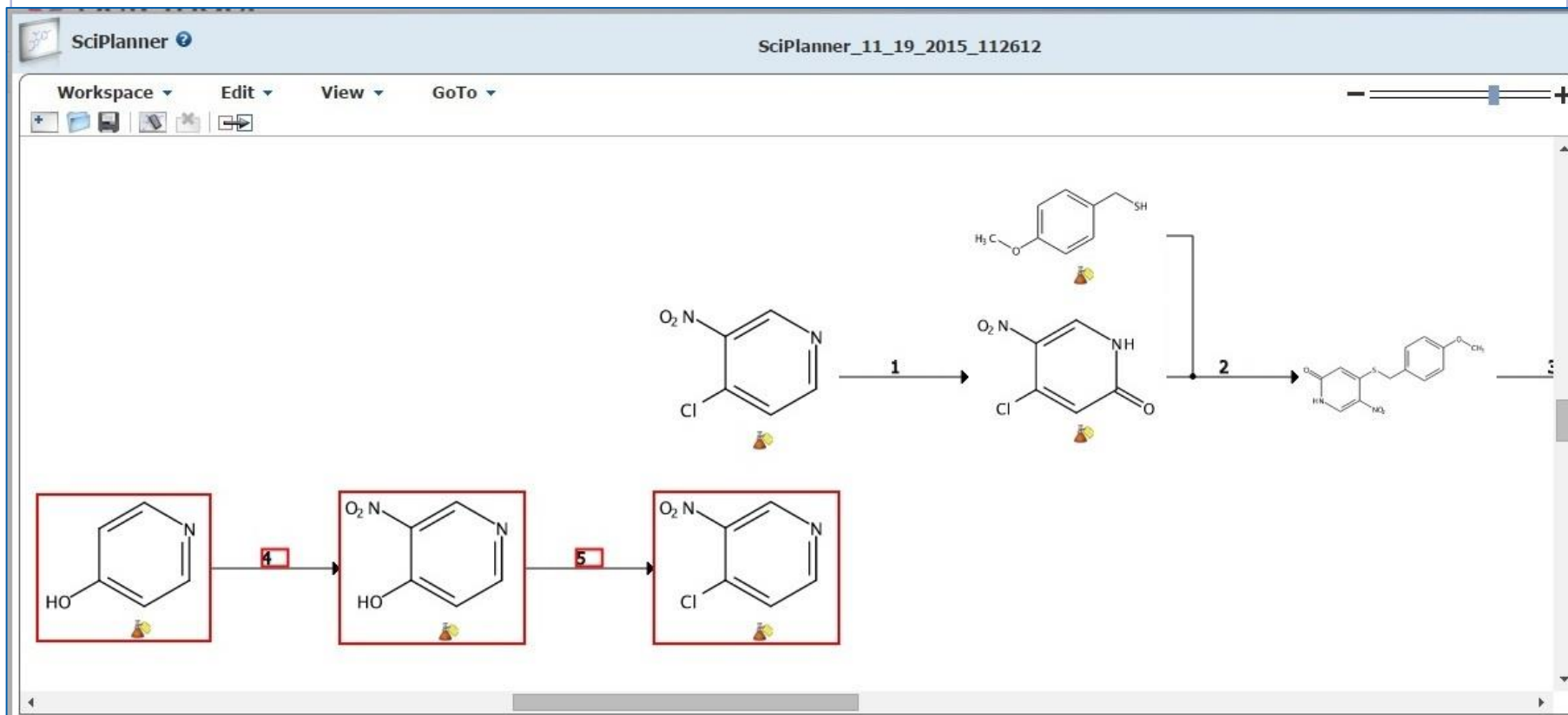
2 Steps Hover over any structure for more options.

在检索到的反应中选择感兴趣的反应

继续推送到SciPlanner

~161 ~192

SciPlanner使用简介



步骤同前，将推送过来的反应拖到编辑面板中，可以看到两条反应中存在同样的结构

SciPlanner使用简介

The screenshot displays the SciPlanner software interface. At the top, the title bar reads "SciPlanner" and "SciPlanner_11_19_2015_112612". Below the title bar is a menu bar with "Workspace", "Edit", "View", and "GoTo". A "Workspace" dropdown menu is open on the left, listing options: "New", "Open", "Save", "Duplicate", "Import", "Export" (highlighted in blue), "Print", and "Close".

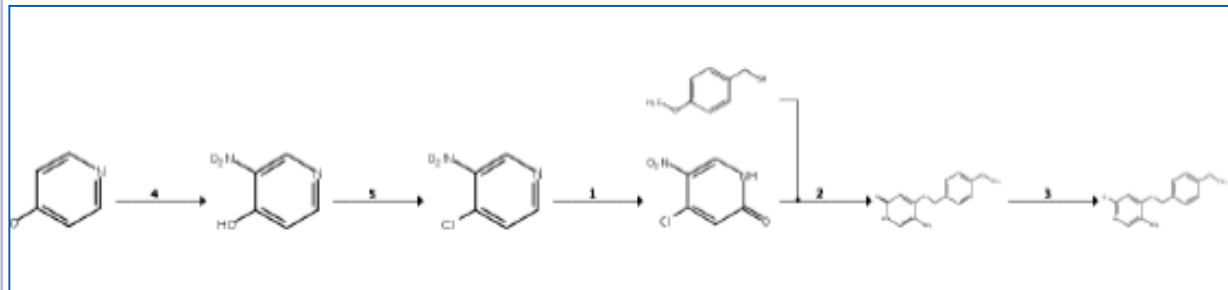
The main workspace shows a chemical reaction sequence. It starts with a pyridine ring substituted with a nitro group (O₂N) and a hydroxyl group (HO). An arrow labeled "4" points to a second pyridine ring with a nitro group (O₂N) and a chlorine atom (Cl). An arrow labeled "5" points to a third pyridine ring with a nitro group (O₂N) and a chlorine atom (Cl). An arrow labeled "1" points to a fourth pyridine ring with a nitro group (O₂N) and a chlorine atom (Cl). A pink callout box with a pointer to the second and third structures contains the text: "用鼠标将两个同样的结构拖至重叠，两条反应合并".

An "Export" dialog box is open on the right side of the interface. It has a title bar "Export" and a question mark icon. The dialog is divided into sections: "For:", "Offline Review", "Saving Locally", "Details:", and "Include:".

- For:** This section is currently empty.
- Offline Review:** Contains three radio button options: "Portable Document Format (*.pdf)", "Citations (*.ris)", and "Image (*.png)".
- Saving Locally:** Contains one radio button option: "SciPlanner eXchange (*.pkx)".
- Details:** Contains a "File Name:" field with the text "SciPlanner_11_19_2015_112612" and a "Title" field.
- Include:** Contains four checked checkboxes: "SciPlanner Image", "Reaction Details", "Substance Details", and "Reference Details".

At the bottom right of the dialog box are "Export" and "Cancel" buttons. A pink callout box with a pointer to the "Offline Review" section contains the text: "选择适当的输出格式，输出结果".

SciPlanner导出结果



Reaction	Stages	Notes	Yield
5	<p>1.1 R:POCl₃, S:PhMe, 0°C → rt; 16 h, rt → 110°C</p> <p>1.2 R:K₂CO₃, S:H₂O, cooled, pH 10</p>	<p>Reactants: 1, Reagents: 2, Solvents: 2, Steps: 1, Stages: 2</p> <p>Transformation:</p> <p>1. Formation of Alkyl Halides from Alcohols</p>	90%
<p>References</p> <p>High color rendering index and color stable hybrid white efficient OLEDs with a double emitting layer structure using a single phosphorescence dopant of heteroleptic platinum complexes</p> <p>By Poloek, Anurach et al</p> <p>From Journal of Materials Chemistry C: Materials for Optical and Electronic Devices, 2(48), 10343-10356; 2014</p>			

Substance Information		
<p>1228150-22-8</p> <p>C₁₃H₁₂N₂O₄S 2-(1H)-Pyridinone, 4-[[4-methoxyphenyl)methyl]thio]-5-nitro-</p> <p>Related Info: ~ 2 References Reactions</p>	<p>1228150-23-9</p> <p>C₁₃H₁₁ClN₂O₃S Pyridine, 2-chloro-4-[[4-methoxyphenyl)methyl]thio]-5-nitro-</p> <p>Related Info: ~ 2 References Reactions</p>	<p>13091-23-1</p> <p>C₅H₃ClN₂O₂ Pyridine, 4-chloro-3-nitro-</p> <p>Related Info: ~ 301 References Reactions ~ 100 Commercial Sources Regulatory Information</p>
<p>5435-54-1</p> <p>C₅H₄N₂O₃ 4-Pyridinol, 3-nitro-</p> <p>Related Info: ~ 113 References Reactions ~ 197 Commercial Sources Regulatory Information</p>	<p>6258-60-2</p> <p>C₈H₁₀O S Benzenemethanethiol, 4-methoxy-</p> <p>Related Info: ~ 749 References Reactions ~ 71 Commercial Sources Regulatory Information</p>	<p>626-64-2</p> <p>C₅H₅N O 4-Pyridinol</p> <p>Related Info: ~ 1351 References Reactions ~ 160 Commercial Sources Regulatory Information</p>
<p>850663-54-6</p> <p>C₆H₃ClN₂O₃ 2-(1H)-Pyridinone, 4-chloro-5-nitro-</p> <p>Related Info: ~ 22 References Reactions ~ 136 Commercial Sources</p>		

提纲

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

SciFinder浏览器选择建议

- Windows 7以上用户升级IE到10以上，不支持IE7、IE8
- Chrome和FireFox浏览器在所有系统上的表现都优于IE浏览器
- 不建议使用360浏览器检索SciFinder，会被自动拦截相关功能或插件

如何获取SciFinder账号

资源

版权公告

馆藏资源

电子资源

外文数据库

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SciFinder Web (网络版)

发布时间:2015-01-01 00:00:00 【大 中 小】 浏览:135769次

访问链接:

(首先需要用校内邮箱进行用户注册, 校园网IP范围内访问)

链接1: <https://scifinder.cas.org/>

链接2: <https://origin-scifinder.cas.org/>

数据库简介:

SciFinder由美国化学会 (American Chemical Society, ACS) 旗下的美国化学文摘社 (Chemical Abstracts Service, CAS) 出品, 是一个研发应用平台, 提供全球最大、最权威的化学及相关学科文献、物质和反应信息。SciFinder涵盖了化学及相关领域如化学、生物、医药、工程、农学、物理等多学科、跨学科的科技信息。SciFinder收录的文献类型包括期刊、专利、会议论文、学位论文、图书、技术报告、评论和网络资源等。

1、检索功能及使用技巧 ([点击下载](#)), 更多的使用指南, 请登陆 <http://www.cas-china.org/index.php?c=list&cs=scifinder-train>, 就可以看到相关功能的介绍及使用演示。

2. 用户注册指南 ([点击下载](#))

(1) 读者在使用之前必须先用email (@njtech.edu.cn) 邮箱地址进行注册, 注册后系统将自动发送一个链接到您所填写的email邮箱中, 激活此链接即可完成注册。(注意: 该链接有效期为48小时, 若未在有效期内确认, 48小时过后需重新注册)。

备注: 已经用@njut.edu.cn邮箱注册过的读者, 无须重复注册, 用之前的账号可以正常访问, 可以登录后修改注册邮箱。

用户注册链接:

<https://scifinder.cas.org/registration/index.html?corpKey=25F0D4A1X86F35055X4FCCACB937E8C4693F>

如何获取SciFinder账号

The screenshot displays the SciFinder registration interface, divided into three main sections:

- CONTACT INFORMATION--**: Includes input fields for First Name, Last Name, Email, Confirm Email, Phone Number, and Fax Number. It also features dropdown menus for Area of Research and Job Title.
- USERNAME AND PASSWORD--**: Includes input fields for Username (with a '7ps' tip), Password, and Re-enter Password.
- SECURITY INFORMATION--**: Includes a dropdown menu for Security Question and an input field for Answer (with a 'Why?' tip).

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

请注意：

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

- - (破折号)
- _ (下划线)
- . (句点)

• @ (表示 “at” 的符号)

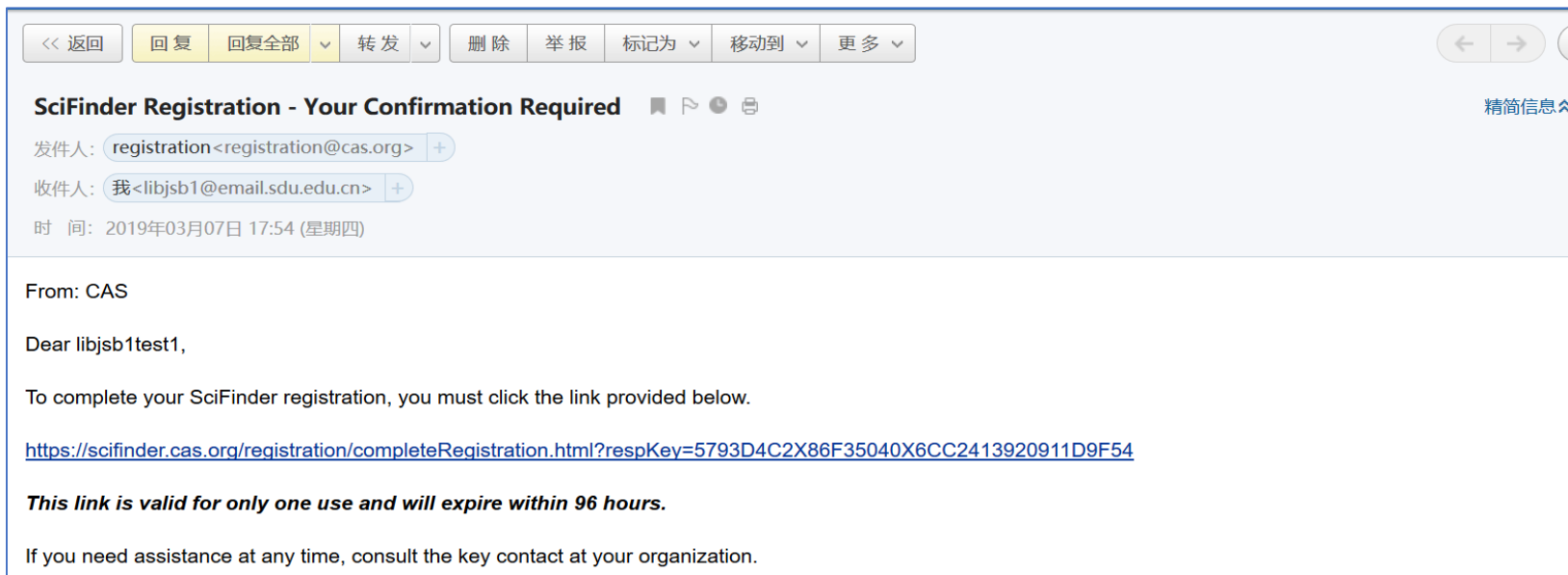
3. 密码必须包含 7-15 个字符，并且至少**包含三种以下字符**：

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

例：abc@123

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

如何获取SciFinder账号



打开并阅读 CAS 的电子邮件（必须在48小时内点击，否则需要重新注册）

注意垃圾邮件、未知邮件、订阅邮件等来自@cas.org的邮件



如何获取SciFinder账号



Registration Already Complete

You have already completed your registration. For assistance with accessing SciFinder, consult the key contact for your organization.

注册成功后直接点击<https://SciFinder.cas.org>即可访问SciFinder数据库



SciFinder使用注意事项

- 在校内完成注册（教学楼、图书馆、实验室）
- 一人注册一个帐号
- 请提供真实姓名信息（中文名的汉语拼音全拼）
- 严禁过量下载
- 严禁账号分享
- 严禁将账号用于非学术研究

更多培训资料请访问

www.cas-china.org

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