

SciFinder Web

源于化学，超越化学的一站式检索平台

SciFinder Web使用介绍

俞靓

SciFinder培训专员

2013.11



提纲

- 介绍
 - SciFinder Web中的新界面及内容
- **SciFinder Web中的检索举例**
 - SciFinder中的基础检索
 - SciFinder中的结构面板使用技巧
 - SciFinder中的反应筛选
 - SciFinder中的反应设计
- **SciFinder Web网络资源**

SciFinder新界面

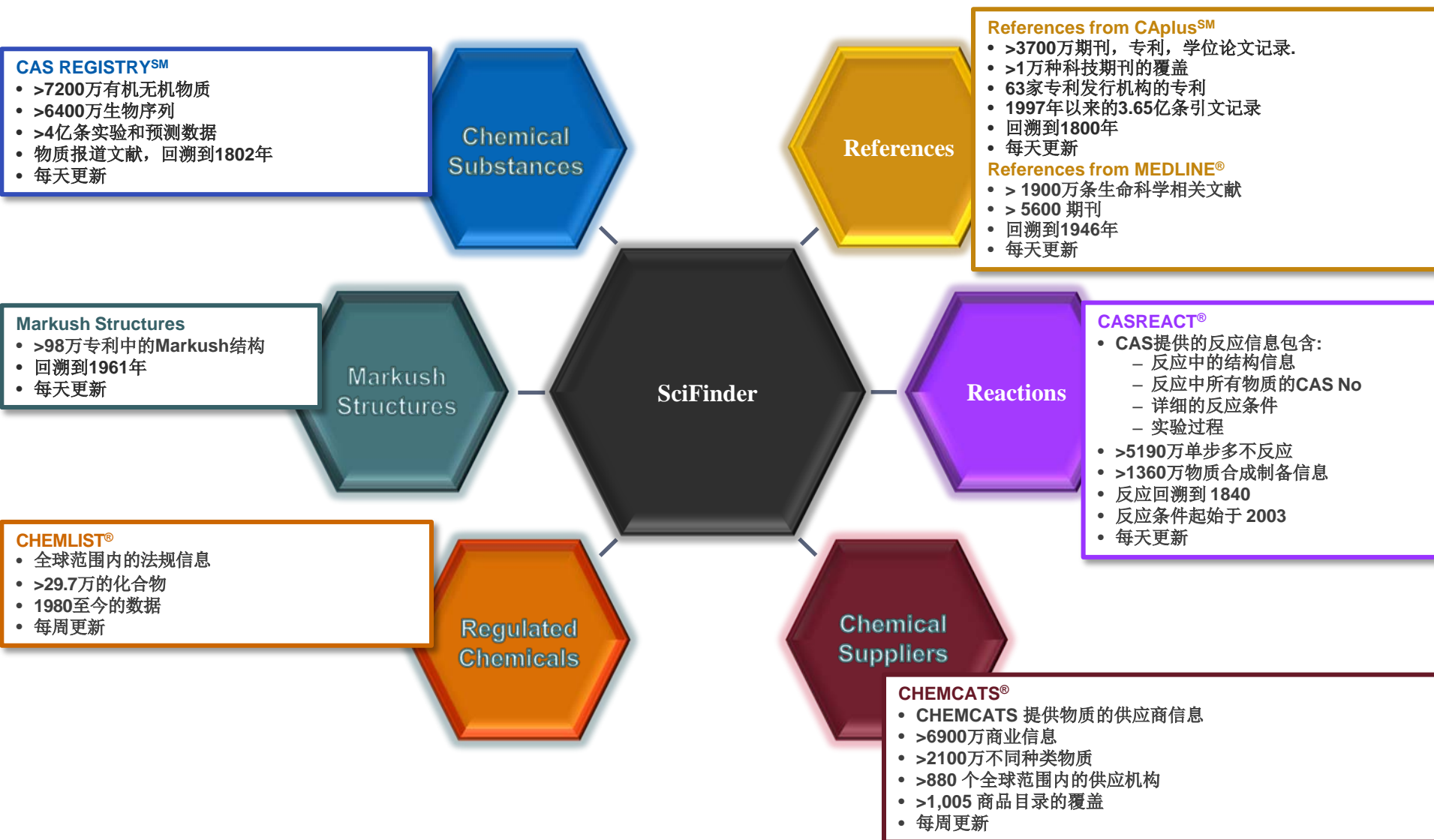
The screenshot displays the SciFinder web interface. At the top left is the SciFinder logo. The top right corner contains links for 'Preferences', 'SciFinder Help', and a 'Sign Out' button. Below the logo, there is a navigation bar with 'Explore', 'Saved Searches', and 'SciPlanner' tabs. A user greeting 'Welcome Sam Yu' is visible on the right side of the navigation bar.

The main content area is titled 'REFERENCES: RESEARCH TOPIC'. It features a search input field with a placeholder and a 'Search' button. Below the input field, there are 'Examples:' such as 'The effect of antibiotic residues on dairy products' and 'Photocyanation of aromatic compounds'. A link for 'Advanced Search' is located below the search button.

On the left side, there is a sidebar menu with three main categories: 'REFERENCES', 'SUBSTANCES', and 'REACTIONS'. Under 'REFERENCES', there are sub-items: 'Research Topic', 'Author Name', 'Company Name', 'Document Identifier', 'Journal', 'Patent', and 'Tags'. Under 'SUBSTANCES', there are: 'Chemical Structure', 'Markush', 'Molecular Formula', 'Property', and 'Substance Identifier'. Under 'REACTIONS', there is: 'Reaction Structure'.

On the right side, there is a 'SAVED ANSWER SETS' section with a list of saved sets: '4 step ref', '3 step-ref', '4 Step', '3130', 'fluorescence with biosensor3128', 'RCM-1816ref', '646Ref', 'Luminescent substances with organic refined', 'Total reaction', and 'Autosaved Reaction Set'. At the bottom of this section are 'View All' and 'Import' links. Below that is a 'KEEP ME POSTED' section with the text 'You have no profiles.'

SciFinder的覆盖内容



提纲

- 介绍
 - SciFinder Web中的新界面及内容
- **SciFinder Web中的检索举例**
 - SciFinder中的基础检索
 - SciFinder中的结构面板使用技巧
 - SciFinder中的反应筛选
 - SciFinder中的反应设计
- **SciFinder Web网络资源**

SciFinder Web中的常规检索

主题: suzuki reaction with catalyst

The screenshot displays the SciFinder web interface. At the top left is the SciFinder logo. Below it are navigation tabs: 'Explore', 'Saved Searches', and 'SciPlanner'. On the left side, there are two main sections: 'REFERENCES' and 'SUBSTANCES'. Under 'REFERENCES', there are several search criteria listed: 'Research Topic', 'Author Name', 'Company Name', 'Document Identifier', 'Journal', 'Patent', and 'Tags'. Under 'SUBSTANCES', there are 'Chemical Structure', 'Markush', and 'Molecular Formula'. The main content area is titled 'REFERENCES: RESEARCH TOPIC'. It features a search input field containing the text 'suzuki reaction with catalyst'. Below the input field, there are 'Examples:' listed as 'The effect of antibiotic residues on dairy products' and 'Photocyanation of aromatic compounds'. A blue 'Search' button is positioned below the examples. A blue arrow points from the text '使用介词来连接关键词，点击Search' at the bottom of the screenshot to the search input field. The text 'Advanced Search' is also visible below the search button.

REFERENCES: RESEARCH TOPIC ?

suzuki reaction with catalyst

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

Search

Advanced Search

使用介词来连接关键词，点击Search

主题检索的候选项

SciFinder®

Preferences | SciFinder Help | Sign Out

Welcome Sam Yu

Explore | Saved Searches | SciPlanner

Research Topic "suzuki reaction with catalyst"

REFERENCES ⓘ

Select All Deselect All

1 of 5 Research Topic Candidates Selected

	References
<input type="checkbox"/> 64 references were found containing "suzuki reaction with catalyst" as entered.	64
<input checked="" type="checkbox"/> 6154 references were found containing the two concepts "suzuki reaction" and "catalyst" closely associated with one another .	6154
<input type="checkbox"/> 7611 references were found where the two concepts "suzuki reaction" and "catalyst" were present anywhere in the reference .	7611
<input type="checkbox"/> 13168 references were found containing the concept "suzuki reaction".	13168
<input type="checkbox"/> 2142096 references were found containing the concept "catalyst".	2142096

Get References

“Concept”表示做了同意词的扩展

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

“present anywhere in the reference”表示同时出现在一段话中

SciFinder 中的文献检索结果

文献分析工具

SciFinder®

Preferences | SciFinder Help ▾ Sign Out

Welcome Sam Yu

Explore ▾ Saved Searches ▾ SciPlanner Save Print Export

Research Topic "suzuki reaction with catalyst" > references (6154)

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: — = ≡

0 of 6154 References Selected Page: 1 of 308

Analyze by: ⓘ

Author Name	Count
Zhou Mingjie	62
Molander Gary A	56
Liu Chun	41
Buchwald Stephen L	39
Cao Yong	37
Huang Jie	33
Cetinkaya Bekir	32
Wang Ping	32
Beller Matthias	31

- 1. A simple catalytic system based on PdCl₂(CH₃CN)₂ in water for cross-coupling reactions using diazonium salts** ⓘ Full Text

By El Bakouri, Ouissam; Fernandez, Marti; Brun, Sandra; Pla-Quintana, Anna; Roglans, Anna
From Tetrahedron, Ahead of Print. | Language: English, Database: CAPLUS

Aryl-heteroaryl and heteroaryl-heteroaryl compds. are obtained through the **Suzuki-Miyaura cross-coupling reactions** between diazonium salts and potassium trifluoroborates using PdCl₂(CH₃CN)₂ as the **catalyst** in water and in the absence of any additive, ligand or base. In addn., the same mild **catalytic** system is effective for the Matsuda-Heck **reaction** between several monoolefins with aryl diazonium salts.
- 2. Fabrication of Macroporous/Mesoporous Carbon Nanofiber using CaCO₃ Nanoparticles as Dual Purpose Template and Its Application as Catalyst Support** ⓘ Full Text

By Liu, Hua; Cao, Chang-Yan; Wei, Fang-Fang; Jiang, Yan; Sun, YongBin; Huang, Peipei; Song, Wei-Guo
From Journal of Physical Chemistry C, Ahead of Print. | Language: English, Database: CAPLUS

1D hierarchical macroporous/mesoporous carbon nanofibers were prepd. via electrospinning using PAN as carbon precursor and com. available nano-CaCO₃ as dual purpose template. During the carbonization process, nano-CaCO₃ template decompd. and released CO₂ to develop mesopores, and macropores were generated by subsequent acid removal of the as-formed CaO nanoparticles. This method is facile and low cost, allowing high-yield prodn. of 1D hierarchical porous carbon nanofibers. The unique macro-/mesoporous structure of the nanofibers makes them a good support for anchoring palladium nanoparticle...

SciFinder提供的引文排序— Citing Reference

SciFinder®

Preferences | SciFinder Help ▾ Sign Out

Welcome Sam Yu

Explore ▾ Saved Searches ▾ SciPlanner Save Print Export

Research Topic "suzuki reaction with catalyst" > references (6154)

REFERENCES ⓘ

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

Analyze Refine Categorize

Analyze by: ⓘ

Author Name ▾

Zhou Mingjie 62

Molander Gary A 56

Liu Chun 41

Buchwald Stephen L 39

Cao Yong 37

Huang Jie 33

Cetinkaya Bekir 32

Wang Ping 32

Beller Matthias 31

Sort by: Citing References ▾ ↓

Accession Number

Author Name

Citing References

Publication Year

Title

Answers per Page [20] Display: — = ≡

Page: 1 of 308

1. **Reaction one century after the discovery of the Ullmann reaction** Full Text

By Hassan, Iwanoro; Sevignon, Marc; Gozzi, Christel; Schulz, Emmanuelle; Lemaire, Marc

From Chemical Reviews (Washington, D. C.) (2002), 102(5), 1359-1469. | Language: English, Database: CAPLUS

~1948

A review discusses the use of metal-catalyzed coupling reactions in the prepn. of biaryls. The use of copper, nickel, and palladium catalysts in coupling reactions such as the Ullman, Pschorr, Stille, and Suzuki coupling reactions for the prepn. of biaryls is discussed extensively; the use of other reactions such as nucleophilic arom. substitution and oxidative coupling to prep. biaryls is also discussed. The coupling reactions of aryl halides, arylstannanes, arylboronic acids, aryl silanes, and of aryl derivs. of zinc, germanium, lead, bismuth, antimony, copper, manganese, zirconium, and in...

2. **Synthetic methods. Controlled microwave heating in modern organic synthesis** Full Text

By Kappe, C. Oliver

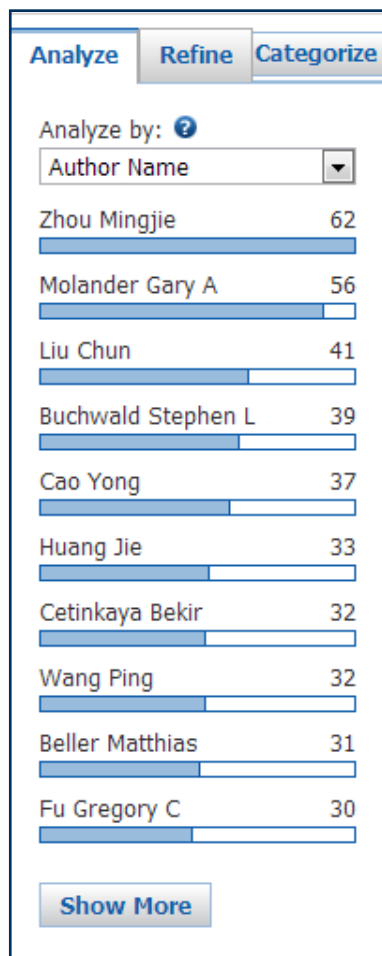
From Angewandte Chemie, International Edition (2004), 43(46), 6250-6284. | Language: English, Database: CAPLUS

~1898

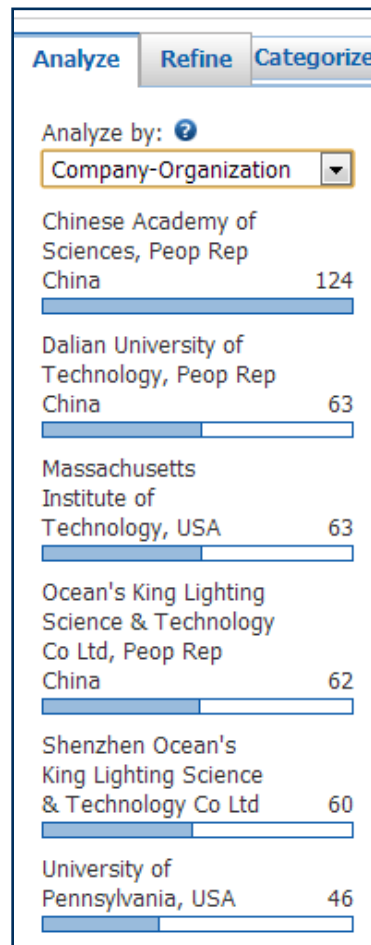
A review. Although fire is now rarely used in synthetic chem., it was not until Robert Bunsen invented the burner in 1855 that the energy from this heat source could be applied to a reaction vessel in a focused manner. The Bunsen burner was later superseded by the isomantle, oil bath, or hot plate as a source for applying heat to a chem. reaction. In the past few years, heating and driving chem. reactions by microwave energy was an increasingly popular theme in the scientific community. This nonclassical heating technique that is heavily used in both academia and industry. The efficiency ...

SciFinder中的Analysis

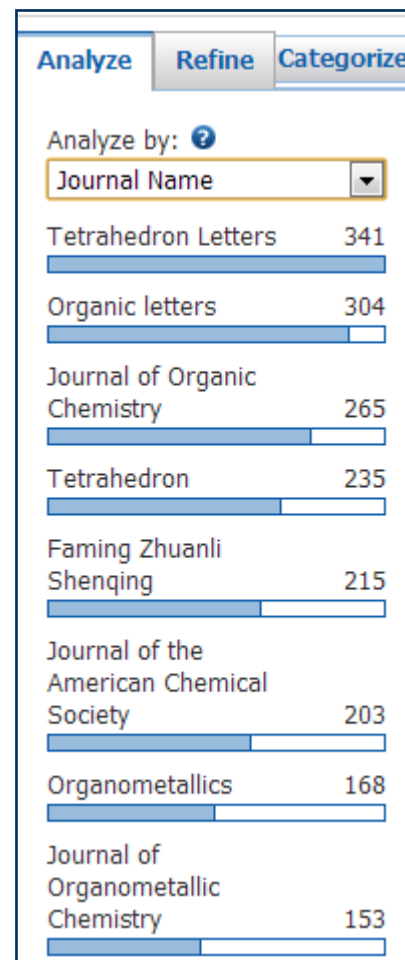
领域内主要研究人员，专家



主要研究机构，合作伙伴，竞争对手





主要出版杂志，机构，潜在投稿期刊



SciFinder中的Analysis

Analyze Refine Categorize

Analyze by: 


Index Term 

Suzuki coupling reaction	3818
Suzuki coupling reaction catalysts	2975
Boronic acids	1048
Biaryls	954
Aryl halides	848
Molecular Structure	831
Crystal structure	703
Aryl bromides	596
Cross-coupling reaction catalysts	556
Coupling reaction catalysts	555




[Show More](#)

索引词（Index Term）：可以帮助我们大致了解文献的内容

Analyze - Index Term

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

4101 Items 0 Selected [Export](#)

Sort by: Frequency  Page: 1 of 20  

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

<input checked="" type="checkbox"/> Suzuki coupling reaction	3818
<input type="checkbox"/> Suzuki coupling reaction catalysts	2975
<input type="checkbox"/> Boronic acids	1048
<input type="checkbox"/> Biaryls	954
<input type="checkbox"/> Aryl halides	848
<input type="checkbox"/> Molecular Structure	831
<input type="checkbox"/> Crystal structure	703
<input type="checkbox"/> References not containing information for this analysis	701
<input type="checkbox"/> Aryl bromides	596
<input type="checkbox"/> Cross-coupling reaction catalysts	556

[Apply](#) [Cancel](#)

选择感兴趣的内容，
点击Apply

SciFinder中的Refine

Refine : 帮助用户迅速获得需要的文献
中科院

Analyze Refine Categorize

Refine by: ?

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

Company Name

china

Examples:

3M

DuPont

Refine

SciFinder®

Preferences | SciFinder Help | Sign Out

Welcome Sam Yu

Explore Saved Searches SciPlanner Save Print Export

Research Topic: "suzuki reaction with catalyst" > references (6154) > refine "china" (1297)

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: Citing References ↓

0 of 1297 References Selected


Answers per Page [20] Display: — = ≡

Analyze by: Company-Organization

Chinese Academy of Sciences, Peop Rep China	124
Dalian University of Technology, Peop Rep China	63
Ocean's King Lighting Science & Technology Co Ltd, Peop Rep China	62
Shenzhen Ocean's King Lighting Science & Technology Co Ltd	60

1. Chiral Phosphine Lewis Bases Catalyzed Asymmetric aza-Baylis-Hillman Reaction of N-Sulfonated Imines with Activated Olefins

By Shi, Min; Chen, Lian-Hui; Li, Chao-Qun
From Journal of the American Chemical Society (2005), 127(11), 3790-3800. | Language: English, Database: CAPLUS

Ar-CH=NR' +  In the aza-Baylis-Hillman reaction of N-sulfonated imines (N-arylmethylidene-4-methylbenzenesulfonamides and others) with Me vinyl ketone, Et vinyl ketone, and acrolein, we found that, in the presence of a catalytic amt. of chiral phosphine Lewis base such as (R)-2'-diphenylphosphanyl-[1,1'] binaphthalenyl-2-ol LB1 (10 mol %) and mol. sieve 4A, the corresponding aza-Baylis-Hillman adducts could be obtained in good yields with good to high ee (70-95% ee) at low temp. (~-30 to -20 °C) or at room temp. in THF, resp. In CH2Cl2 upon heating at 40 °C, the aza-Baylis-Hillman reaction of N-sulfonated ...

2. Deep-Red Electroluminescent Polymers: Synthesis and Characterization of New Low-Band-Gap Conjugated Copolymers for Light-Emitting Diodes and Photovoltaic Devices

By Yang, Renqiang; Tian, Renyu; Yan, Jingai; Zhang, Yong; Yang, Jian; Hou, Qiong; Yang, Wei; Zhang, Chi; Cao, Yong
From Macromolecules (2005), 38(2), 244-253. | Language: English, Database: CAPLUS

结果集的保存

SciFinder® interface showing search results for "suzuki reaction with catalyst" refined to "china". The interface includes navigation tabs, search filters, and a list of references. A specific reference is highlighted with a chemical reaction scheme and text description.

Export:
Citation manager: 保存成RIS格式,
用于导入EndNote等文献管理工具

Offline Review:保存过成PDF, RTF
格式, 用于脱机浏览

Save This Answer Set

Save:

All answers

Only selected answers

Title: *

Description:

OK Cancel

Save:
保存在服务器上, 可登陆后查看

Export

Export:

All

Selected

Range

Example: 2-20

For:

Citation Manager

Citation export format (*.ris)

Quoted Format (*.bt)

Tagged Format (*.bt)

Offline review

Portable Document Format (*.pdf)

Rich Text Format (*.rtf)

Answer Keys (*.bt)

Saving locally

Answer Key eXchange (*.akx)

Details:

File Name: *

Reference_06_26_2012_150931

Export Cancel

SciFinder 中的Categorize

通过历史导航条回到任一检索界面

SciFinder®

Preferences | SciFinder Help ▾ Sign Out

Welcome Sam Yu

Explore ▾ Saved Searches ▾ SciPlanner Save Print Export

Research Topic "suzuki reaction with catalyst" > references (6154) > refine "china" (1297)

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: Citing References ▾ ↓ Answers per Page [20] Display: — = ≡

0 of 1297 References Selected Page: 1 of 65

Analyze by: Company-Organization ▾

Chinese Academy of Sciences, Peop Rep China	124
Dalian University of Technology, Peop Rep China	63
Ocean's King Lighting Science & Technology Co Ltd, Peop Rep China	62
Shenzhen Ocean's King Lighting Science & Technology Co Ltd	60

1. Chiral Phosphine Lewis Bases Catalyzed Asymmetric aza-Baylis-Hillman Reaction of N-Sulfonated Imines with Activated Olefins [Full Text](#)

By Shi, Min; Chen, Lian-Hui; Li, Chao-Qun
From Journal of the American Chemical Society (2005), 127(11), 3790-3800. | Language: English, Database: CAPLUS ~251

Ar-CH=NR' + $\begin{matrix} \text{R} \\ \text{C} \\ \text{O} \end{matrix}$ $\xrightarrow[\text{solvent}]{\text{chiral phosphine Lewis base}}$ $\begin{matrix} \text{NHR}'\text{O} \\ \text{C} \\ \text{R} \end{matrix}$

R' = Ts, Ms, p-ClC₆H₄SO₂, SES.
R = Me, Et, OPh, ONaph, H up to 95% ee

In the aza-Baylis-Hillman **reaction** of N-sulfonated imines (N-arylmethylidene-4-methylbenzenesulfonamides and others) with Me vinyl ketone, Et vinyl ketone, and acrolein, we found that, in the presence of a **catalytic** amt. of chiral phosphine Lewis base such as (R)-2'-diphenylphosphanyl-[1,1'] binaphthalenyl-2-ol LB1 (10 mol %) and mol. sieve 4A, the corresponding aza-Baylis-Hillman adducts could be obtained in good yields with good to high ee (70-95% ee) at low temp. (~-30 to -20 °C) or at room temp. in THF, resp. In CH₂Cl₂ upon heating at 40 °C, the aza-Baylis-Hillman **reaction** of N-sulfonated ...

2. Deep-Red Electroluminescent Polymers: Synthesis and Characterization of New Low-Band-Gap Conjugated Copolymers for Light-Emitting Diodes and Photovoltaic Devices [Full Text](#)

By Yang, Renqiang; Tian, Renyu; Yan, Jingai; Zhang, Yong; Yang, Jian; Hou, Qiong; Yang, Wei; Zhang, Chi; Cao, Yong
From Macromolecules (2005), 38(2), 244-253. | Language: English, Database: CAPLUS ~226

Categorize系统分类功能，基于Index Term，对文献依学科方向进行分类

SciFinder中的Categorize

一级目录

二级目录

和二级目录相关的
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	Catalysts (8251)	Page: 1 of 83 Select All Deselect All <input type="checkbox"/> Palladium <input type="checkbox"/> Palladium diacetate <input type="checkbox"/> Tetrakis(triphenylphosphine)p <input type="checkbox"/> Tris(dibenzylideneacetone)dip <input type="checkbox"/> Dichlorobis(triphenylphosphin <input type="checkbox"/> Palladium dichloride <input type="checkbox"/> Carbene complexes <input type="checkbox"/> Ligands <input type="checkbox"/> Transition metal complexes <input type="checkbox"/> Triphenylphosphine <input type="checkbox"/> Phosphines <input checked="" type="checkbox"/> PdCl ₂ (dppf) <input type="checkbox"/> Silica <input type="checkbox"/> Tricyclohexylphosphine <input type="checkbox"/> Tri-tert-butylphosphine	Click 'x' to remove the category from 'Selected Terms' * Catalysis > Catalysts (1 Terms)
General chemistry	Catalysis (122)		
Synthetic chemistry			
Catalysis			
Physical chemistry			
Technology			
Biotechnology			
Polymer chemistry			
Environmental chemistry			
Genetics & protein chemistry			
Biology			
Analytical chemistry			

Catalysis > Catalysts > 1 Index Term(s) Selected

OK Cancel

提纲

- 介绍
 - SciFinder Web中的新界面及内容
- **SciFinder Web中的检索举例**
 - SciFinder中的基础检索
 - SciFinder中的结构面板使用技巧
 - SciFinder中的反应筛选
 - SciFinder中的反应设计
- **SciFinder Web网络资源**

SciFinder结构绘制工具

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)
- 结构和反应切换功能 (Structure and reaction switching function)
- 元素周期表 (Periodic table)
- 常用基团 (Common groups)
- 可变基团 (Variable groups)
- R基团定义工具 (R-group definition tool)
- 重复基团工具 (Repeat group tool)
- 可变位置连接工具 (Variable position connection tool)
- 碳链工具 (Carbon chain tool)
- 模版工具 (Template tool)
- 选择工具 (Selection tool)
- 索套选择工具 (Lasso selection tool)
- 环锁定工具 (Ring locking tool)
- 原子锁定工具 (Atom locking tool)
- 旋转工具 (Rotation tool)
- 镜面旋转工具 (Mirror rotation tool)
- 正电子 (Positron)
- C原子和单键恢复工具 (C-atom and single bond recovery tool)
- 负电子 (Electron)
- 常见环, 多元环工具 (Common rings, multi-ring tool)
- 结构检索选择 (Structure search selection)
- 单双键, RS构型, 不确定键定义工具 (Single/double bond, RS configuration, uncertain bond definition tool)

The interface includes a toolbar with icons for drawing and editing, a central workspace for drawing structures, and a right-hand panel for search options (Exact search, Substructure search, Similarity search) and drawing editor settings (Structure, Reaction, Markush). The bottom of the interface shows a chemical formula input field (C H O S N P Cl Br F I Si) and a scale control (Scale 100).

SciFinder中的反应定义工具

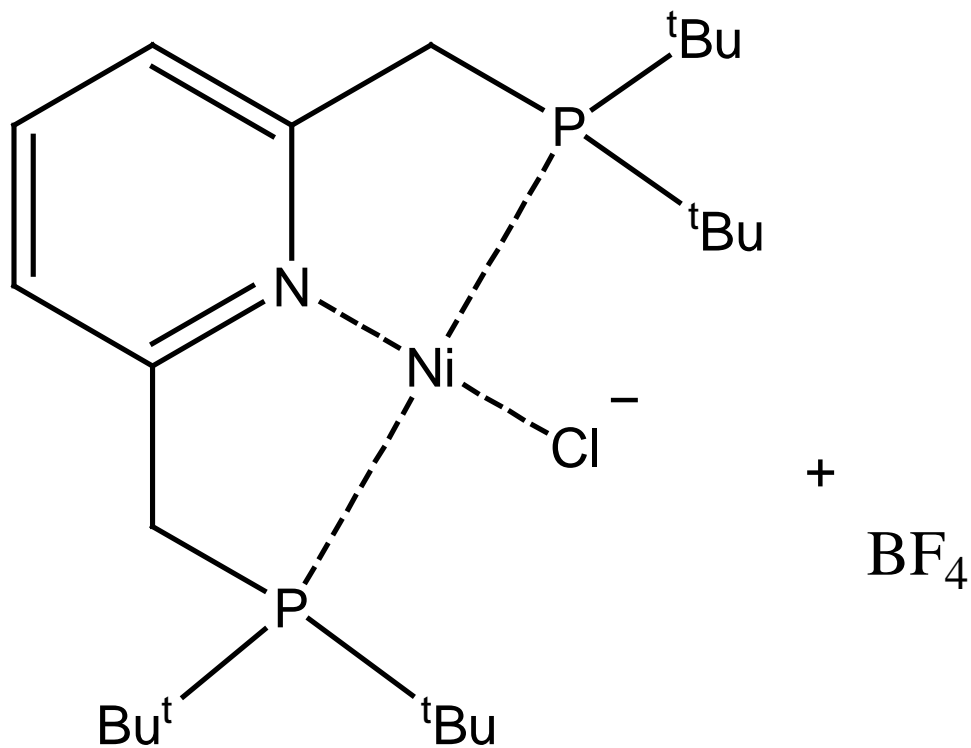
The image shows the Reaction Editor window in SciFinder. The interface includes a toolbar on the left, a central workspace, and a right-hand panel. Red boxes with lines pointing to specific tools are annotated with Chinese text:

- 反应箭头** (Reaction Arrow): Points to the arrow icon in the toolbar.
- 反应原子标记工具** (Reaction Atom Marking Tool): Points to the 'A' and 'B' atom marking icons.
- 反应官能团列表** (Reaction Functional Group List): Points to the 'alicyclic ketone aldol' list in the toolbar.
- 反应角色工具** (Reaction Role Tool): Points to the scissors icon in the toolbar.
- 反应位置标记工具** (Reaction Position Marking Tool): Points to the arrow with a dot icon in the toolbar.

The right-hand panel contains the **Drawing Editor** section with radio buttons for **Structure**, **Reaction** (selected), and **Markush**. Below this is a section titled **Get reactions where the structure(s) are:** with options for **Variable** (radio button) and **Substructures of more complex structures** (radio button).

At the bottom of the window, there is a **Scale** set to 100 and a **(query)** input field.

精确结构检索—检索金属配合物



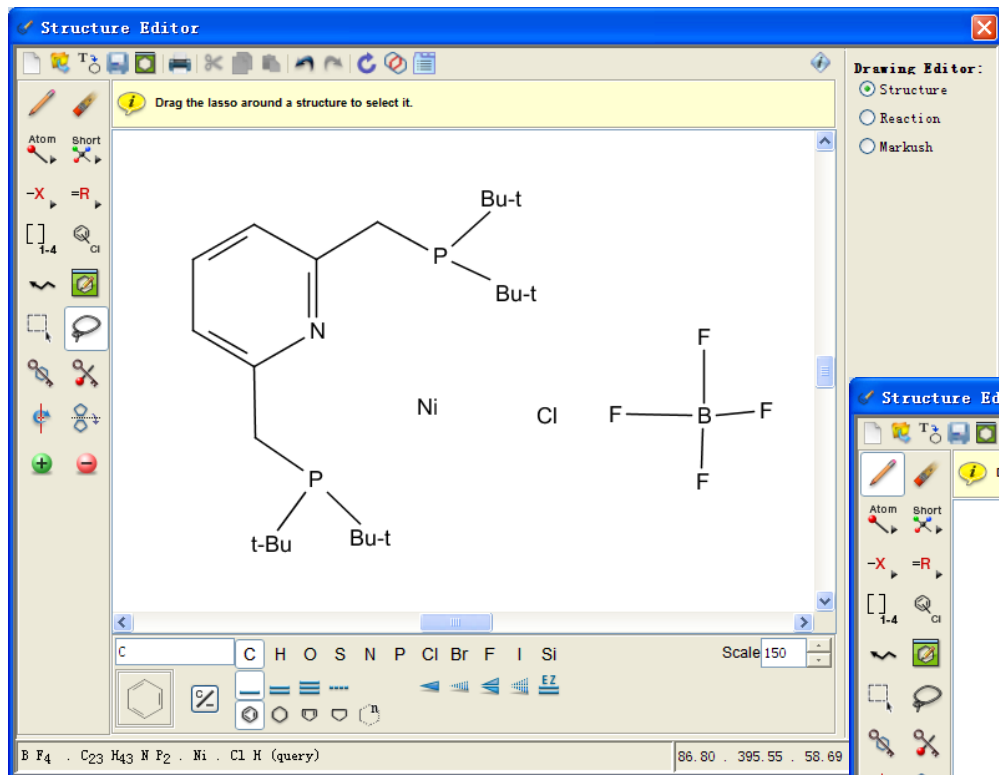
该结构中包含:

配体
金属
阳离子
阴离子

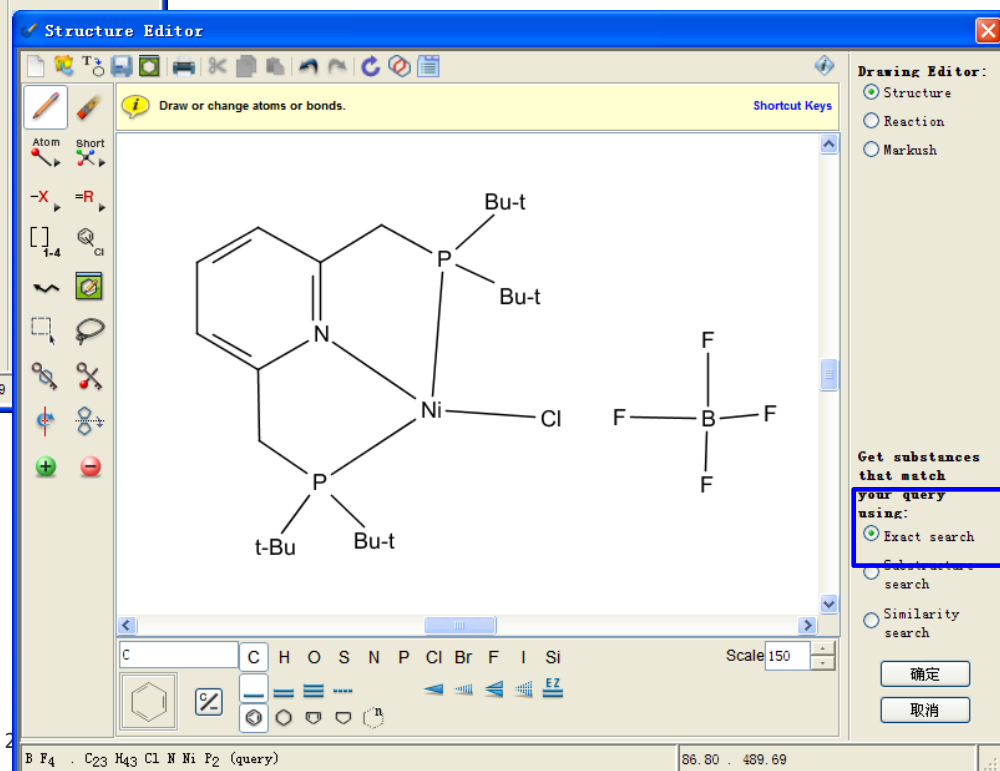
结构式检索—精确检索

The screenshot displays the SciFinder web interface. At the top left is the SciFinder logo. Below it are navigation tabs: 'Explore', 'Saved Searches', and 'SciPlanner'. The breadcrumb trail reads: 'Substance Identifier "qinghaosu" > substances (1) > 63968-64-9 > commercial sources (91)'. On the left sidebar, there are three main sections: '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). The 'SUBSTANCES' section is currently active. The main content area is titled 'SUBSTANCES: CHEMICAL STRUCTURE'. It features a central window with a chemical structure editor and the text 'Click to Edit'. To the right of this window, under 'Search Type:', there are three radio buttons: 'Exact Structure' (selected), 'Substructure', and 'Similarity'. Below these is a checkbox for 'Show precision analysis'. At the bottom of the main area, there is an 'Import CXF' label, a blue 'Search' button, and a link for 'Advanced Search'.

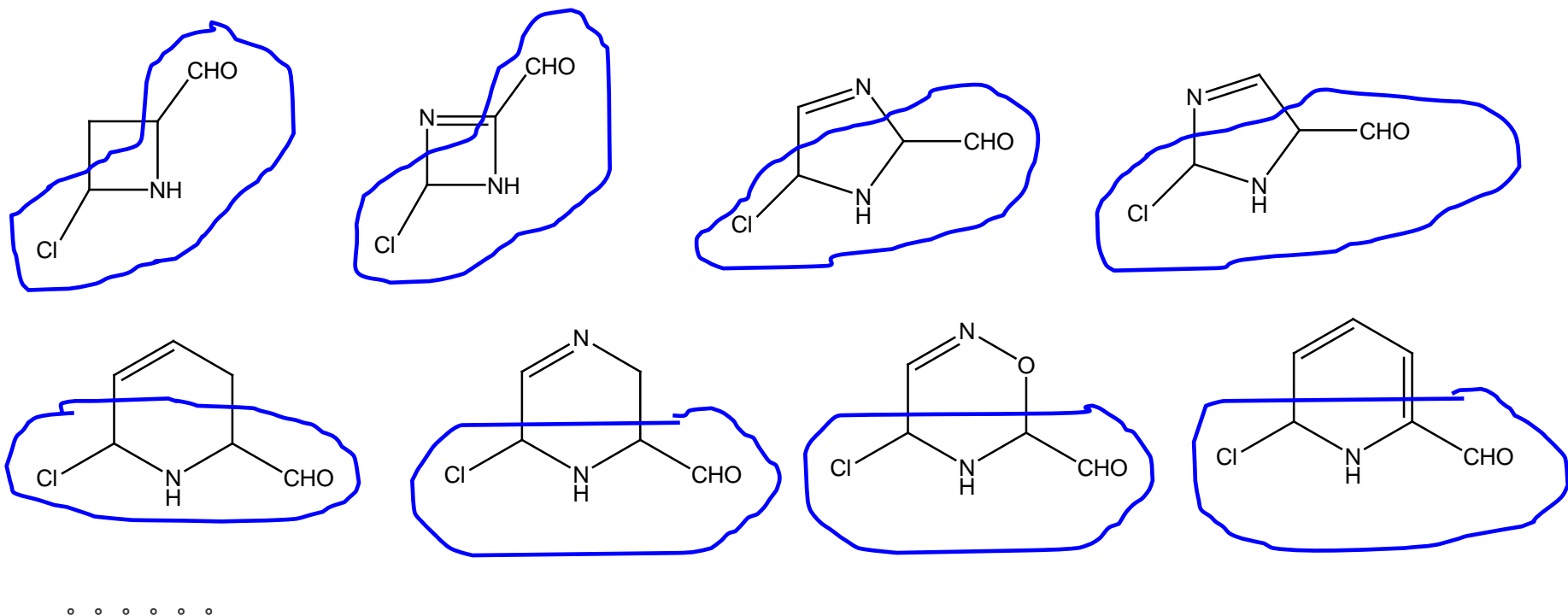
检索界面



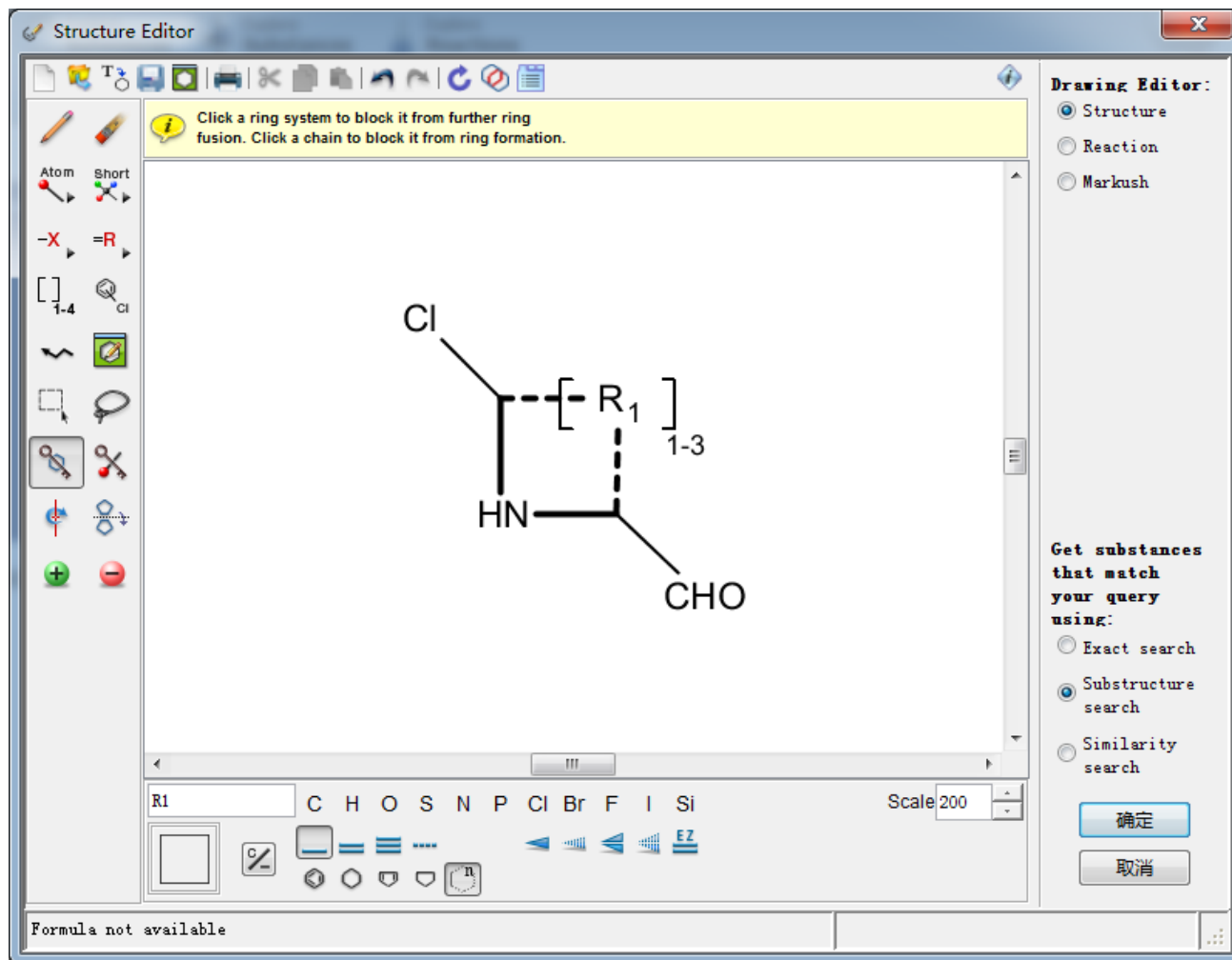
任何一种结构,使用精确结构都可以检索到



我想获得以下的一系列物质



结构定义



用亚结构检索获得所有的物质

亚结构检索结果

SciFinder® Preferences | SciFinder Help | Sign Out

Welcome Sam Yu

Explore ▾ Saved Searches ▾ SciPlanner Save Print Export

Chemical Structure substructure > substances (469)

SUBSTANCES ? Get References Get Reactions Get Commercial Sources Tools ▾ Create Keep Me Posted Alert Send to SciPlanner

Analyze **Refine** Sort by: Number of References ▾ Answers per Page [50] View:

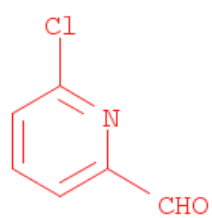
Analyze by: ?
Substance Role ▾

Preparation 155
Reactant or Reagent 123
Biological Study 15
Uses 11
Prophetic in Patents 8
Properties 6
Formation, Nonpreparative 2
Analytical Study 1

0 of 469 Substances Selected Page: 1 of 10

1. Substance Detail
54087-03-5

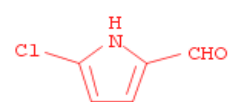
~33



C₆ H₄ Cl N O

2. Substance Detail
1757-28-4

~19

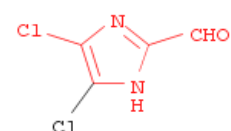


C₅ H₄ Cl N O
1#Pyrrole-2-carboxaldehyde, 5-chloro-

[Experimental Properties](#)

3. Substance Detail
81293-97-2

~11



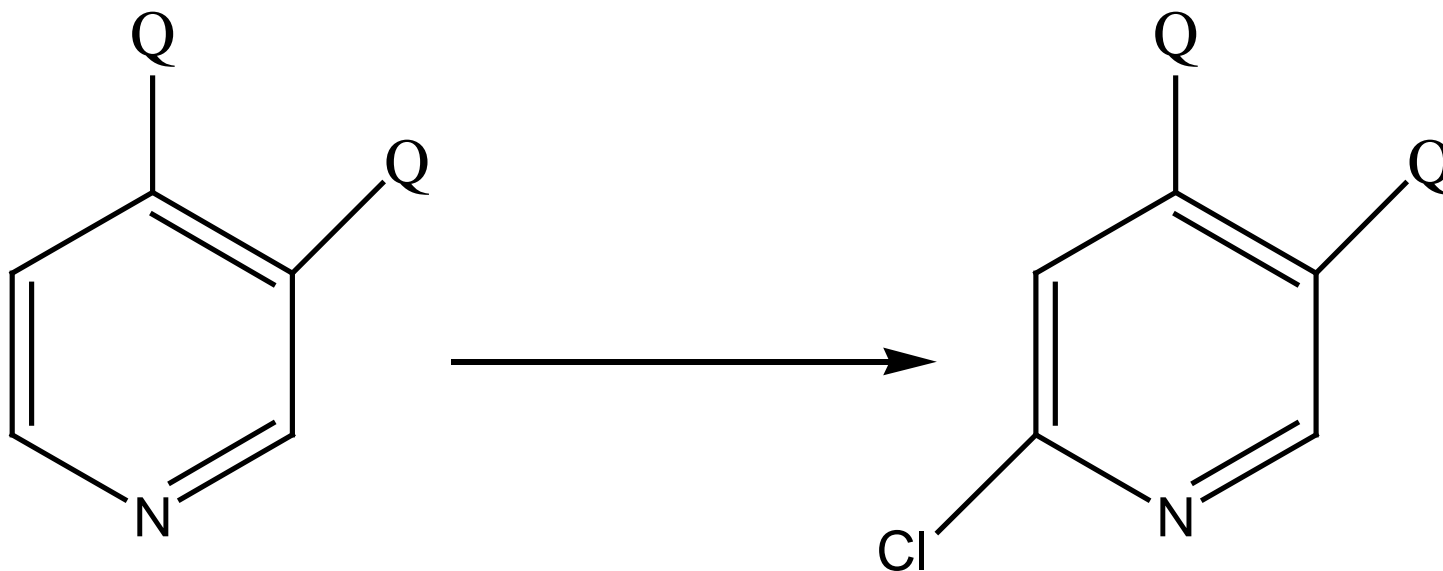
C₄ H₂ Cl₂ N₂ O
1#Imidazole-2-carboxaldehyde, 4,5-dichloro-

提纲

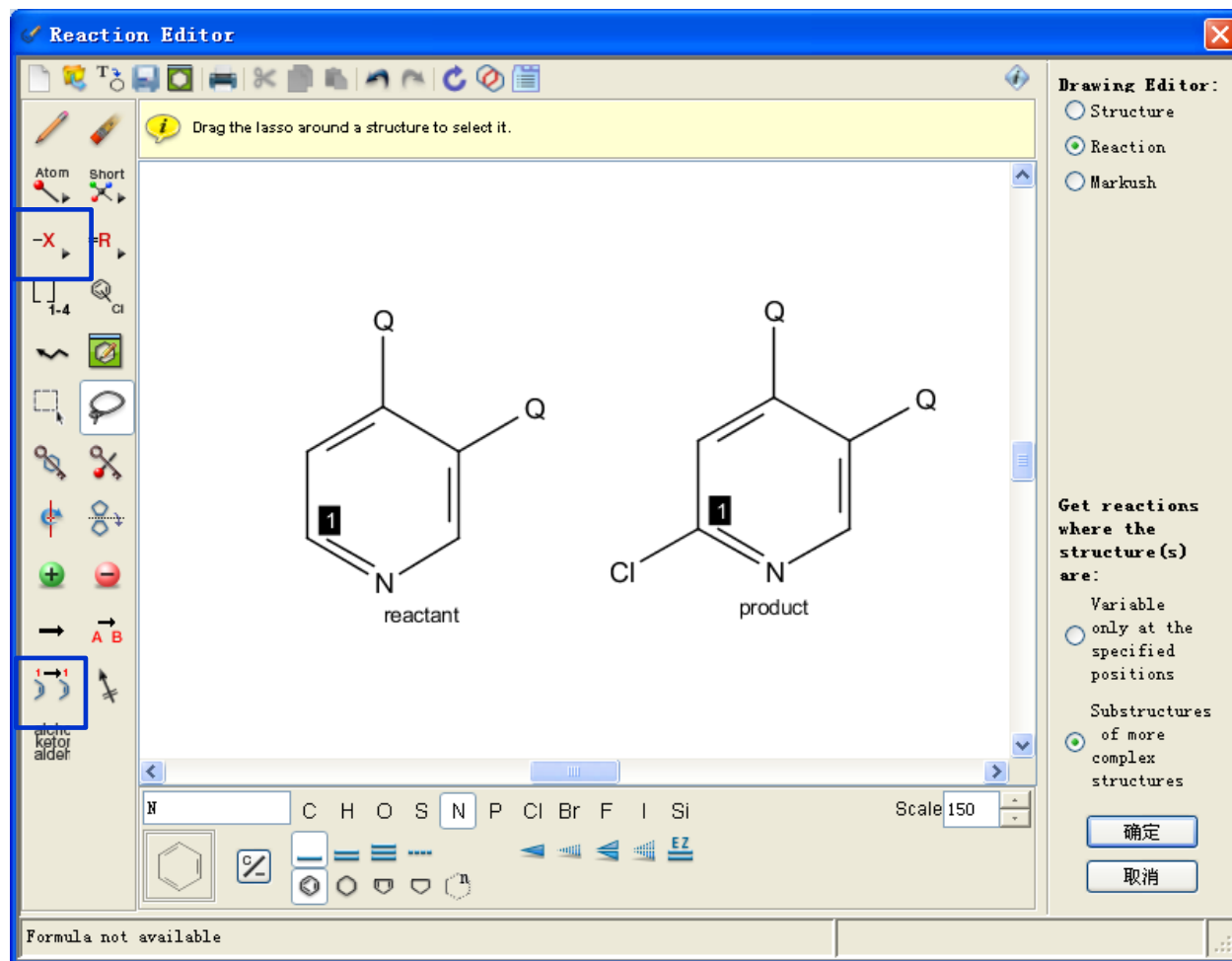
- 介绍
 - SciFinder Web中的新界面及内容
- **SciFinder Web中的检索举例**
 - SciFinder中的基础检索
 - SciFinder中的结构面板使用技巧
 - SciFinder中的反应筛选
 - SciFinder中的反应设计
- **SciFinder Web网络资源**

SciFinder反应检索—检索中的筛选

- 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



定义反应结构



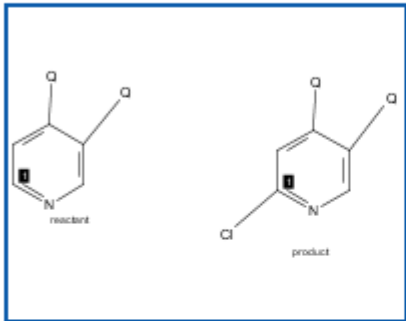
大多数科研工作者，刚开始都会画成这样。

但是，这样足够吗？

尝试SciFinder中的初步检索。

亚结构检索，帮助获得所有的相关反应

REACTIONS: REACTION STRUCTURE ?



reactant

product

Search Type:

- Allow variability only as specified
- Substructure

Click image to change structure or view detail.

Import CXF

Search

Advanced Search

亚结构检索反应，帮助在最大范围内获得刚兴趣的内容

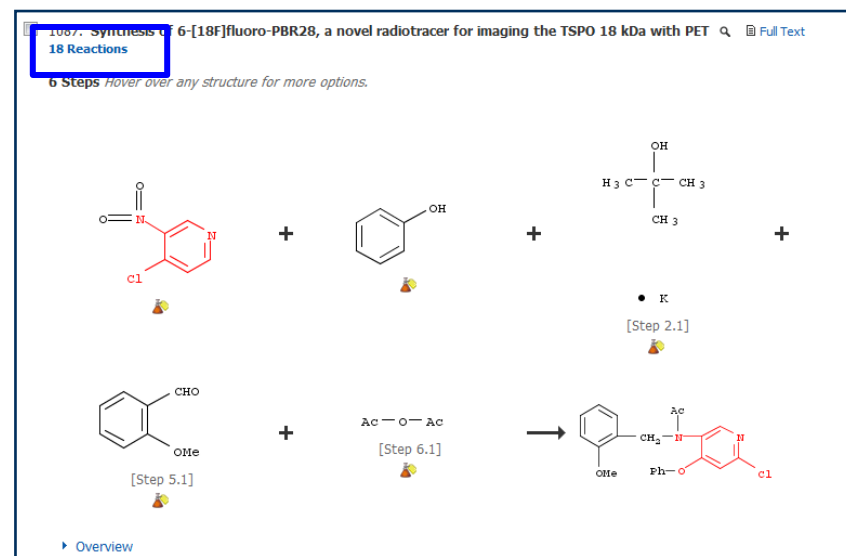
SciFinder中的反应筛选

The screenshot shows the SciFinder search results page. The search term "reactions (5455)" is highlighted in a blue box. The interface includes navigation tabs for "Explore", "Saved Searches", and "SciPlanner". Below the search bar, there are options for "REACTIONS", "Get References", and "Tools". The "Analyze" section shows "Group by: No Grouping" and "Sort by: Accession Number". The "Refine" section shows "Analyze by: Catalyst". The results section indicates "0 of 5455 Reactions Selected" and provides a link to "View Reaction Detail".

我们获得5400+ 反应

反应筛选第一步是Group By Document, 这样可以来来自同一篇文章的反应合并掉

This screenshot shows the "Group by" dropdown menu in the SciFinder interface. The "Document" option is highlighted in a blue box, indicating the selection of reactions grouped by document.

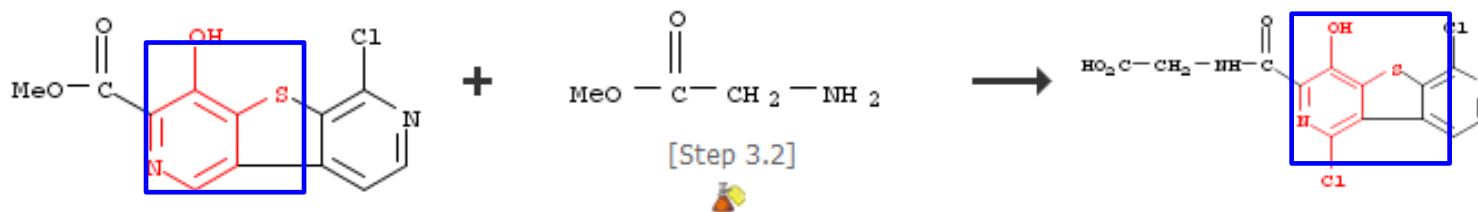


简单的看一下这些反应

120. **Pyridine derivatives for treating HIF-related disorders** 🔍 [Full Text](#)

15 Reactions

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



▶ Overview

▶ Experimental Procedure

吡啶环系发生破坏，不是我们想要的

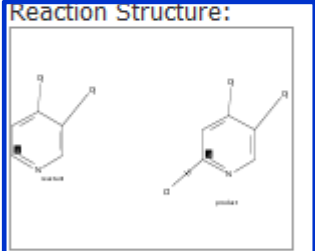
反应中的Refine工具，添加环锁定

Analyze Refine

Refine by: ?

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

Reaction Structure:



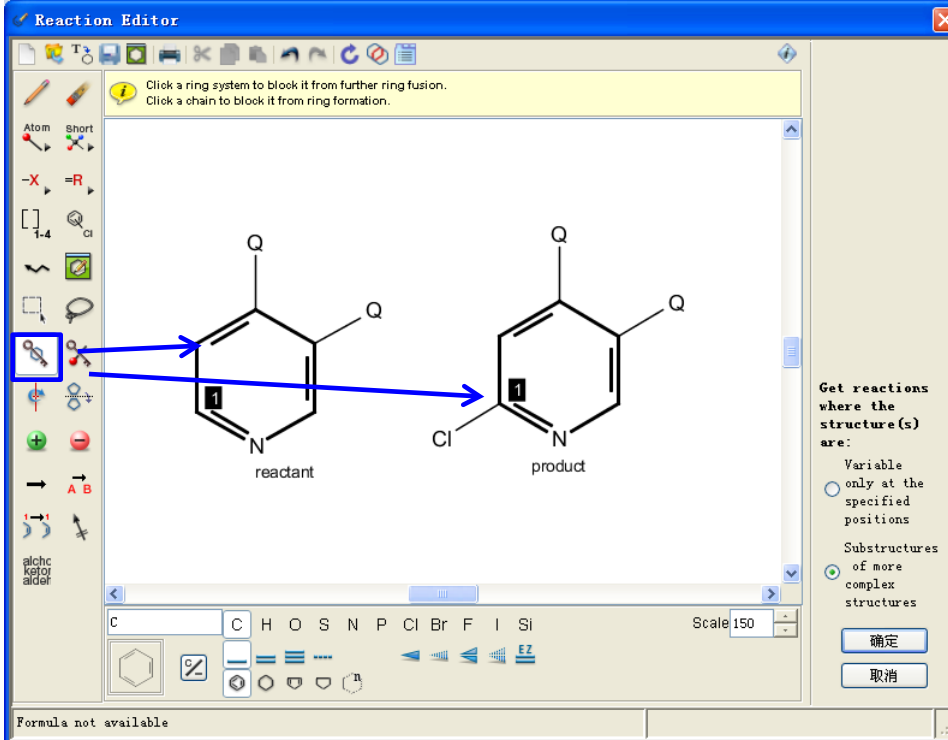
Click image to change structure or view detail

Search type: **Substructure**

Refine

Reaction Editor

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



Get reactions where the structure(s) are:

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



确定 取消

Formula not available



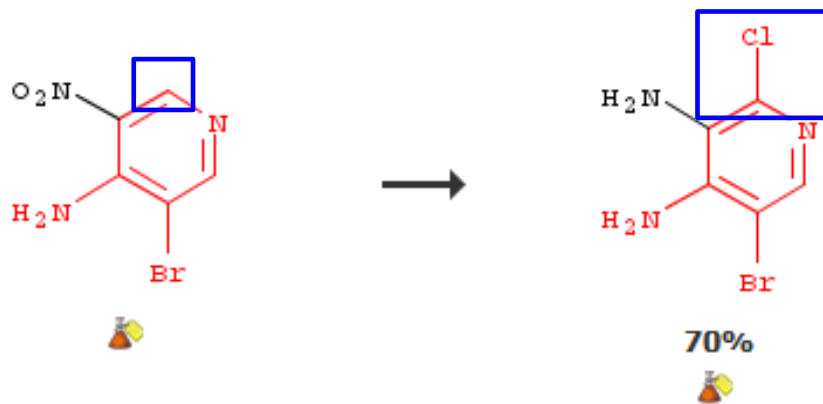
环锁定工具，当使用亚结构检索时，不允许发生稠环。

锁定环后的结果—继续浏览

33. Preparation of novel 2,3,8-trisubstituted pyrido[3,4-b]pyrazines and pyrido[2,3-b]pyrazines   Full Text

1 Reaction  Similar Reactions

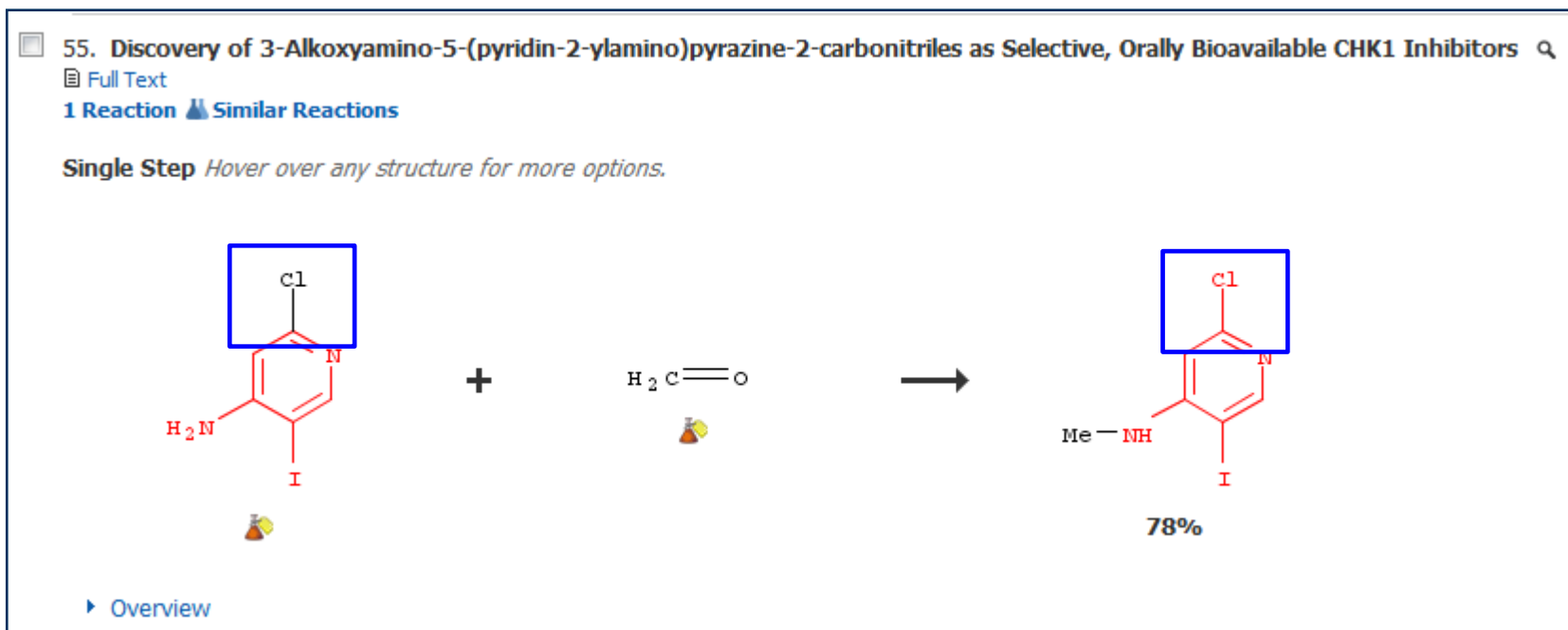
Single Step *Hover over any structure for more options.*



► Overview

这条反应，完全
符合我们的要求

锁定环后的结果—继续浏览



这条反应，原来的6位上就有Cl，不符合我们的要求

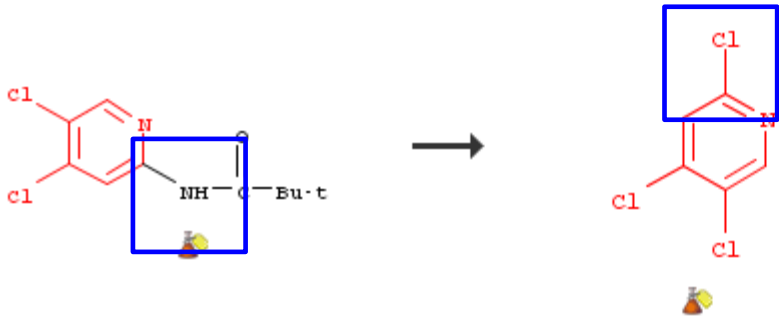
锁定环后的结果—继续浏览

6. Preparation of 3-azabicyclo[4.1.0]heptanes used as orexin antagonists for treating mood disorders, sleep disorders, and other diseases

🔍 📄 Full Text

2 Reactions

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



▶ Overview

▶ Experimental Procedure

这条反应，或许
符合我们的要求

思考：什么样的反应是我们想要的

第一条反应：6位H变成6位Cl—肯定是我们想要的

第二条反应：6位Cl变成6位Cl—肯定不是我们想要的

第三条反应：6位非H非Cl变成6位Cl—有可能是我们想要的

不同的人在这里的选择不一样，我们先假设只想获得第一类的反应。

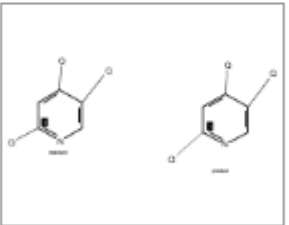
继续使用Refine

Analyze **Refine**

Refine by: ?

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

Reaction Structure:



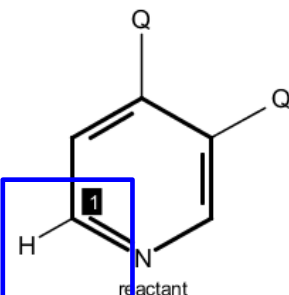
Click image to change structure or view detail

Search type: **Substructure**

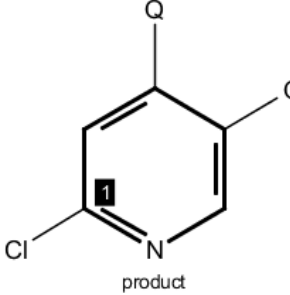
Refine

Reaction Editor

Draw or change atoms or bonds. Shortcut Keys





reactant




product

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

Scale 150



Formula not available

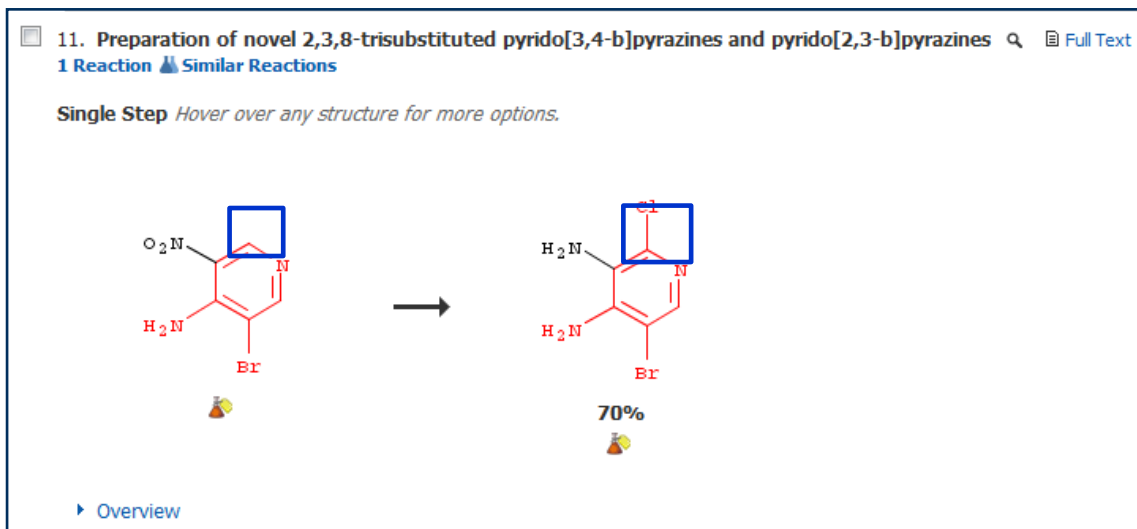
Get reactions where the structure(s) are:

Variable only at the specified positions

Substructures of more complex structures

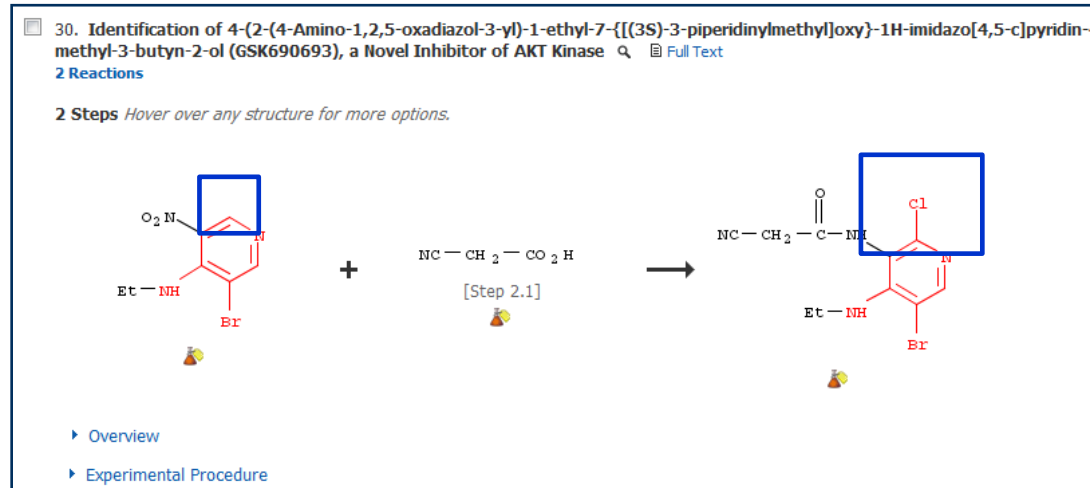
确定 取消

这是我们要的反应



所有的反应都符合我们的结构要求

在吡啶环的6位存在H到Cl的变化



一些值得思考的问题

- 并不是所有的科研工作者，一开始就能准确的定义反应结构。
- 建议先大致浏览下反应结果集，然后去思考如何去掉我们不想要的反应。
- 使用**Analyze/Refine**工具，或其他的检索策略，去除不想要的反应。

案例的衍生

在刚才的检索过程中，我们认为以下的反应不是我们想要的反应。

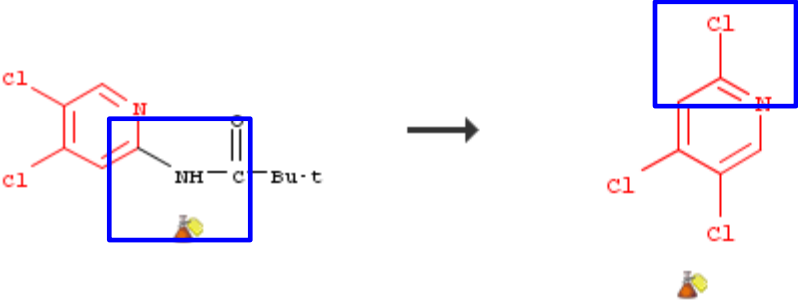
但是，如果我们认为，符合要求，那该如何处理？

6. Preparation of 3-azabicyclo[4.1.0]heptanes used as orexin antagonists for treating mood disorders, sleep disorders, and other diseases

🔍 [Full Text](#)

2 Reactions

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



▶ [Overview](#)

▶ [Experimental Procedure](#)

将结果保存在网络上

SciFinder®

Preferences | SciFinder Help | Sign Out

Welcome Sam Yu

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

Reaction Structure substructure > reactions (5455) > refine "substructure" (1942) > refine "substructure" (83)

REACTIONS

Get References | Tools | Send to SciPlanner

Analyze | Refine

Group by: Document | Sort by: Accession Number | Answers per Page [20] | Display: [Icons]

0 of 1942 Reactions Selected

1. Preparation of substituted oxazopyridine derivatives as EDG-1 receptor activators | Full Text

1 Reaction | Similar Reactions

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

Chemical reaction scheme showing the synthesis of a substituted oxazopyridine derivative from a pyridine derivative and a substituted benzamide derivative.

100%

Overview

Analyze by: Catalyst

Pd(OAc) ₂	83
Pd	77
Ni	57
C ₅ H ₅ N	49
161265-03-8	34
H ₂ SO ₄	28
CuCl	27
8-Quinolinol	24
PdCl ₂ (PPh ₃) ₂	22

使用导航条返回曾经检索过的界面。

保存结果到网络上。

Save This Answer Set ⓘ

* Required

Save:

All answers

Only selected answers

Title: *

pyridine

Description:

OK Cancel

Refine工具来获取不需要的反应

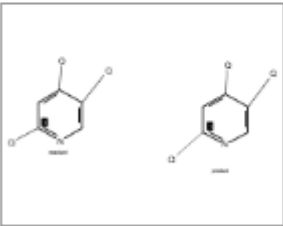
Analyze

Refine

Refine by: ?

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

Reaction Structure:

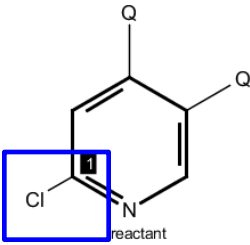


Click image to change structure or view detail
Search type: **Substructure**

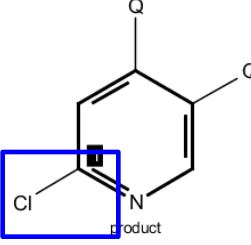
Refine

Reaction Editor
✕

Draw or change atoms or bonds.
Shortcut Keys



reactant





product


Cl


C H O S N P Cl Br F I Si


Scale 150














Formula not available

Get reactions where the structure(s) are:

Variable

only at the specified positions

Substructures of more complex structures

确定

取消

因为我们很明确的知道，我们不需要这类反应。所以可以先获得这些反应，然后去除他们既可。

使用Combine去除不想要的反应

SciFinder®

Preferences | SciFinder Help | Sign Out

Welcome Sam Yu

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

Reaction Structure substructure > reactions (5455) > refine "substructure" (1942) > refine "substructure" (1794)

REACTIONS

Get References | Tools | Send to SciPlanner

Analyze Refine

Analyze by: Catalyst

Pd(OAc)₂ 83

Pd 77

Ni 57

C₅H₅N 49

161265-03-8 34

H₂SO₄ 28

CuCl 27

8-Quinolinol 24

PdCl₂(PPh₃)₂ 23

Group by: Document

0 of 1

Combine Answer Sets

Answers per Page [20] Display: [Full Text]

Page: 1 of 14

1. Preparation of substituted oxazopyridine derivatives as EDG-1 receptor activators

1 Reaction Similar Reactions

Single Step Hover over any structure for more options.

Chemical reaction showing the synthesis of a substituted oxazopyridine derivative.

这些是我们不想要的

如果将这些反应去除掉，那么剩下的就是我们的目标反应

Combine Answer Sets

Select saved answer set(s) to combine with your current answer set (1794):

23 Answer Sets 1 Selected

Reaction Answer Set Details	Date Saved
<input checked="" type="checkbox"/> pyridine (1942) Reaction Structure substructure > reactions (5455) > refine "substructure" (1942)	Jul 8, 2013
<input type="checkbox"/> Autosaved Reaction Set (47) An answer set was automatically saved because the session ended due to inactivity on Wed Jun 19 05:34:34 EDT 2013. Author Name "zhang, J" > references (20525) > refine "2010-" (6377) > refine "100069" (8) > get reactions (47)	Jun 19, 2013
<input type="checkbox"/> Lock Ring (1956) Reaction Structure substructure > reactions (5457) > refine "substructure" (1956)	May 14, 2013

Select an option for combining the answer sets:

Combine Include all answers from both sets

Intersect Include only answers that appear in both sets

Exclude Include only answers from **current answer set (1794)** that are not in **pyridine (1942)**

Exclude Include only answers from **pyridine (1942)** that are not in **current answer set (1794)**

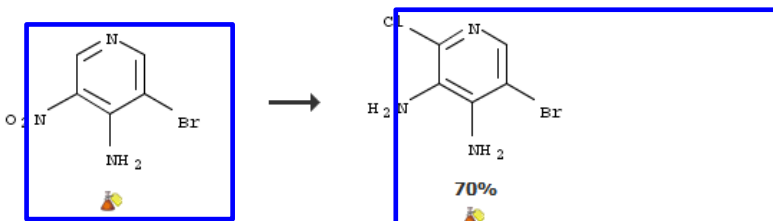
Combine Answer Sets | Cancel

需要的反应结果集

31. Preparation of novel 2,3,8-trisubstituted pyrido[3,4-b]pyrazines and pyrido[2,3-b]pyrazines [Full Text](#)

1 Reaction [Similar Reactions](#)

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

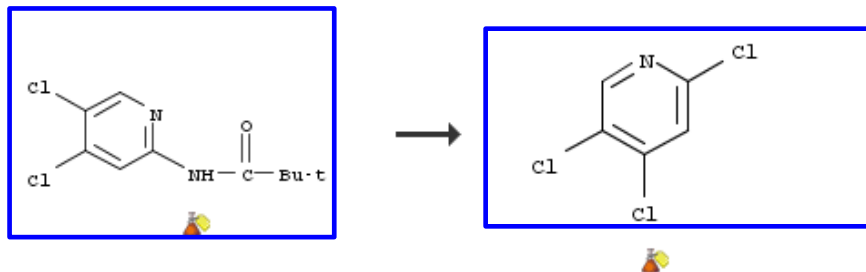


[Overview](#)

34. Preparation of 3-azabicyclo[4.1.0]heptanes used as orexin antagonists for treating mood disorders, sleep disorders, and other diseases [Full Text](#)

2 Reactions

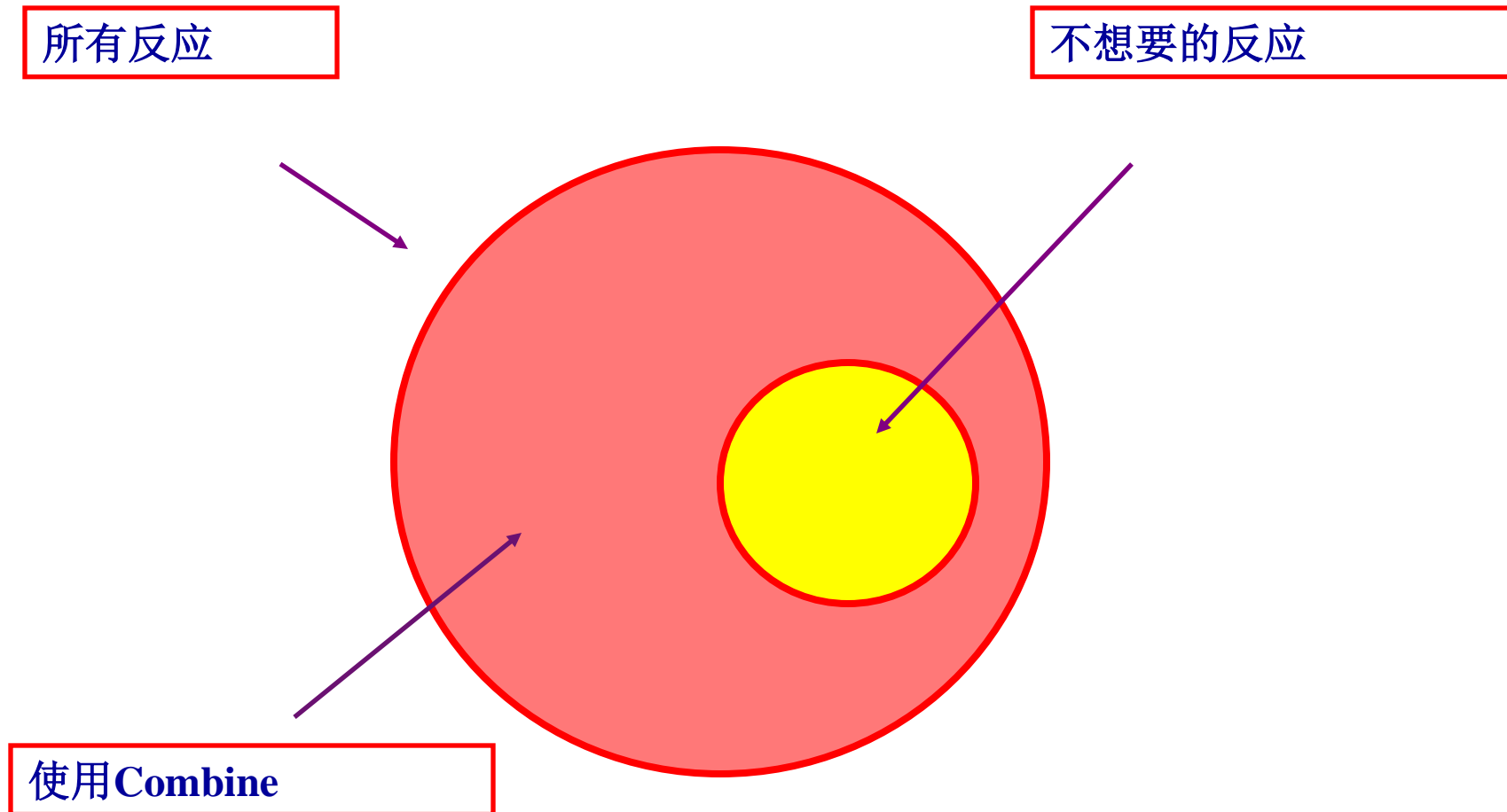
2 Steps *Hover over any structure for more options.*



[Overview](#)

[Experimental Procedure](#)

检索策略



提纲

- 介绍
 - SciFinder Web中的新界面及内容
- **SciFinder Web中的检索举例**
 - SciFinder中的基础检索
 - SciFinder中的结构面板使用技巧
 - SciFinder中的反应筛选
 - SciFinder中的反应设计
- **SciFinder Web网络资源**

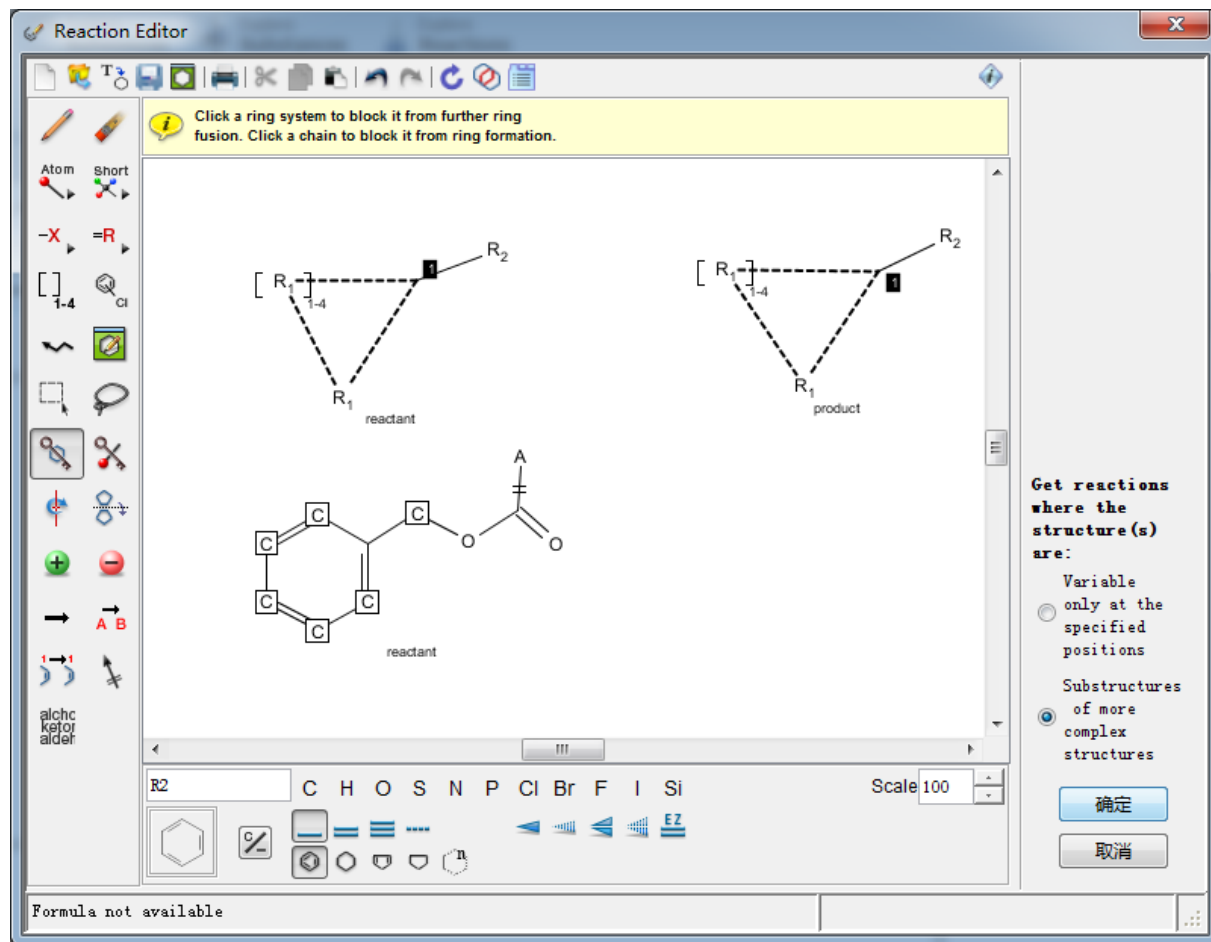
SciFinder中的反应设计

- 检索要求
 - 单一芳环上存在Br或者I
 - 寻找脱Cbz的反应条件
 - 一步反应

定义困难:

如何定义这个环系，杂环？C环？
Cbz和环的连接方法

有些人会这么定义

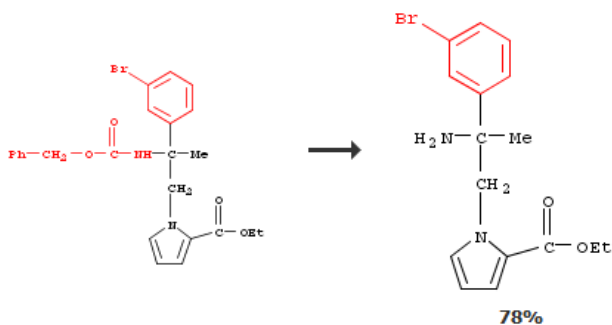


反应中心定义正确，
但是会出现问题

检索出来的结果

22. Preparation of dihydropyrrolopyrazinylamine derivatives for use as beta-secretase (BACE) inhibitors [Full Text](#)
 2 Reactions [Similar Reactions](#)

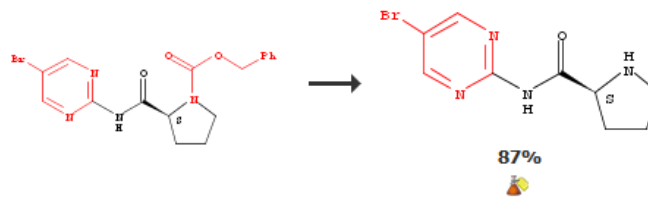
Single Step *Hover over any structure for more options.*



[Overview](#)

98. Preparation of arylenheteroarylenes, bisarylenes, and biheteroarylenes end-capped with amino acid and peptide derivatives as inhibitors of hepatitis C virus replication for treating hepatitis C infection and liver fibrosis [Full Text](#)
 1 Reaction [Similar Reactions](#)

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



[Overview](#)

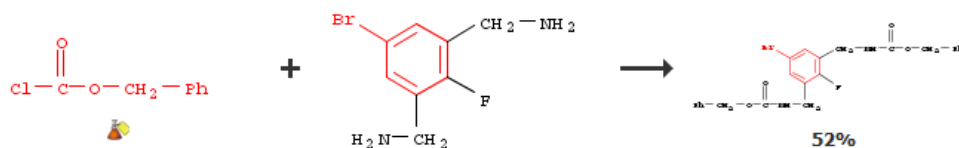
[Experimental Procedure](#)

存在我们想要的结果集

但是，更多的是.....

97. Substituent Effects in Synthetic Lectins - Exploring the Role of CH-n Interactions in Carbohydrate Recognition [Full Text](#)
 1 Reaction [Similar Reactions](#)

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



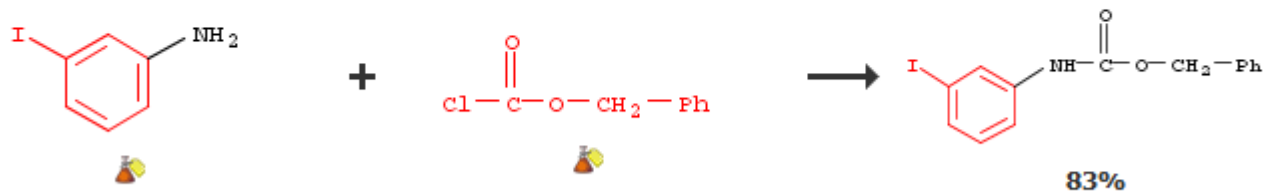
[Overview](#)

[Experimental Procedure](#)

存在大量的环与
Cbz不在一个结构
上的反应

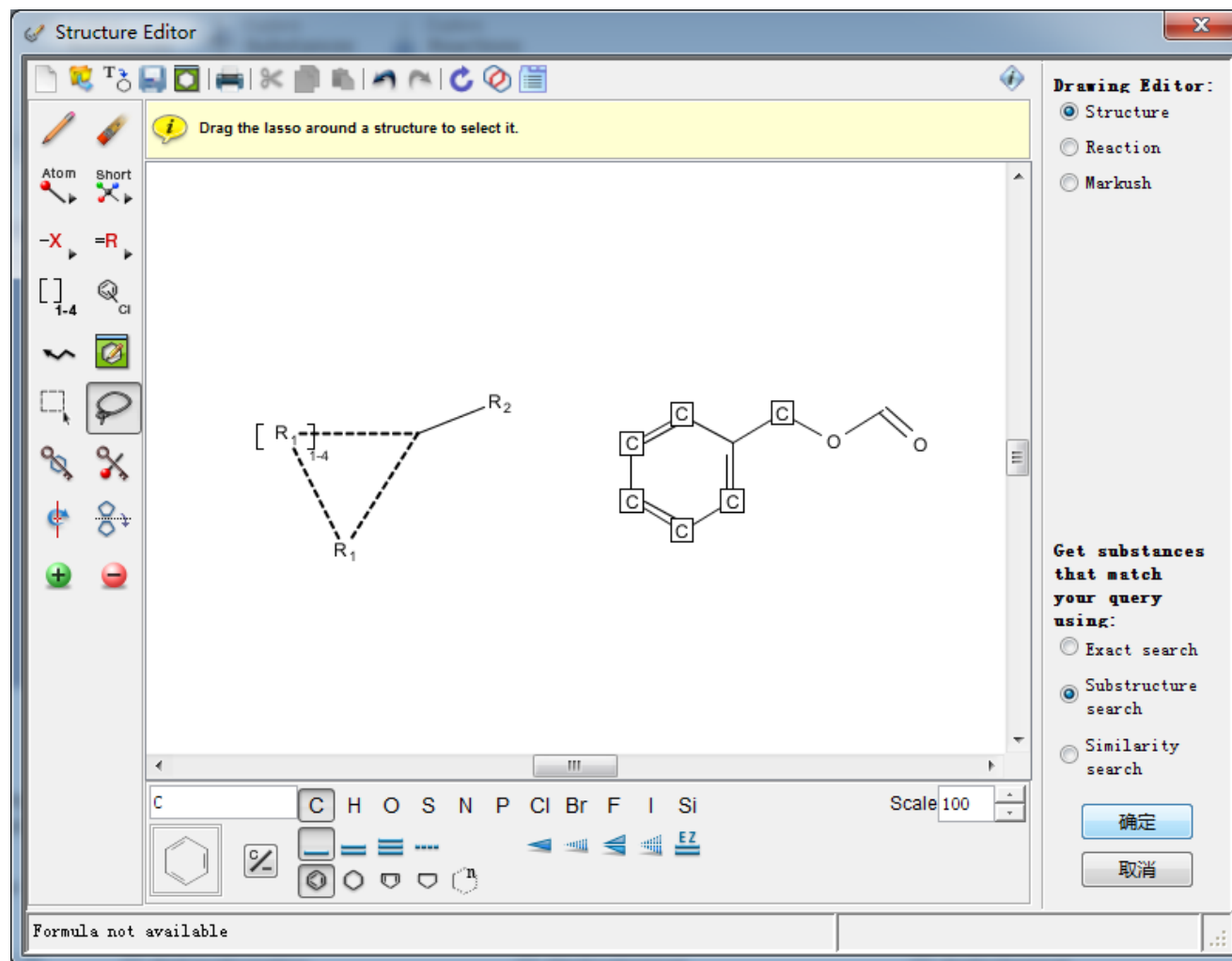
4. Synthesis of Complex ortho-Allyliodoarenes by Employing the Reductive Iodonio-Claisen Rearrangement [Full Text](#)
 1 Reaction [Similar Reactions](#)

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



[Overview](#)

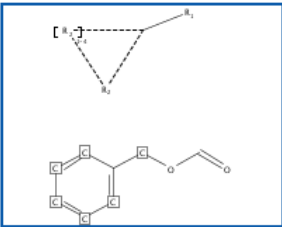
SciFinder中的碎片反应检索



这种类型的反应，
需要先去检索和
反应相关的物质

亚结构物质检索，获得所有可能的反应物

SUBSTANCES: CHEMICAL STRUCTURE ?



Search Type:

Exact Structure

Substructure

Similarity

Show precision analysis

Click image to change structure or view detail.

Import CXF

Search

Advanced Search

Characteristics

Single component

Commercially available

Included in references

Studies

Analytical

Biological

Preparation

Reactant or reagent

需要定义为单一组分
和具备反应物或者试剂
角色的物质

所有可能的反应物

The screenshot shows the SciFinder web interface. At the top, there are navigation tabs: 'Explore', 'Saved Searches', and 'SciPlanner'. Below these, the search results are displayed for 'substances (2977)'. A 'Get Reactions' button is highlighted with a red box. A dialog box titled 'Get Reactions' is open, showing options to retrieve reactions for 'All substances' or 'Selected substances'. Under 'Limit results by reaction role:', 'Reactant' is selected. The dialog also includes 'Get' and 'Cancel' buttons.

Chemical Structure substructure with limiters > substances (2977)

Substances (2977) | Get References | **Get Reactions** | Get Commercial Sources | Tools | Create Keep Me Posted Alert | Send to SciPlanner

Analyze | Refine | Sort by: CAS Registry Number | Answers per Page [50] | View: [Icons] | Page: 1 of 60

0 of 2977 Substances Selected

1. Substance Detail 1443150-70-6
 Absolute stereochemistry.,Rotation (-).
 $C_{18}H_{28}BrN O_3Si$
 1-Pyrrolidinecarboxylic acid, 3-bromo-4-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-, phenylmethyl ester, (3*R*,4*R*)-

2. Substance Detail 1443150-68-2
 Absolute stereochemistry.,Rot
 $C_{12}H_{14}BrN O_3$
 1-Pyrrolidinecarboxylic acid, 3-

3. Substance Detail 1443150-60-4

Get Reactions

Retrieve reactions for:

- All substances
- Selected substances

Limit results by reaction role:

- Product
- Reactant
- Reagent
- Reactant or reagent
- Catalyst
- Solvent
- Any role

Get Cancel

获得所有的可能的反应物，并获得这些物质作为反应物的反应

可能反应物所参与的反应

SciFinder®

Preferences | SciFinder Help | Sign Out

Welcome Sam Yu

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

Chemical Structure substructure with limiters > substances (2977) > get reactions (45656)

REACTIONS | Get References | Tools | Send to SciPlanner

Analyze | Refine

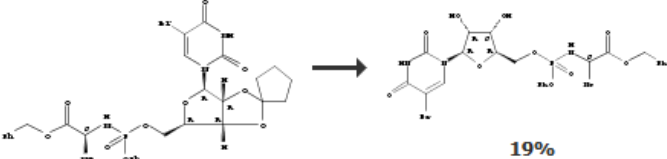
Group by: No Grouping | Sort by: Accession Number

Answers per Page [20] Display: [Icons]

0 of 45656 Reactions Selected

1. View Reaction Detail | Link | Similar Reactions

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



19%

Overview

Sample Analysis: Catalyst

Pd

Pd(PPh₃)₄

72287-26-4

CuI

Pd(OAc)₂

95464-05-4

4-DMAP

这里的反应中的反应物都包含我们要求的结构，
但是还缺少反应中心的定义

第一次限定，获得单步反应

Analyze Refine

Refine by: ?

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

Number of Steps:

Examples: 1, 1-3, 1-, -3

[Refine](#)

限定反应步数为一步反应

SciFinder®

Explore Saved Searches SciPlanner

Chemical Structure substructure with limiters > substances (2977) > get reactions (45656) > refine "1 step" (3268)

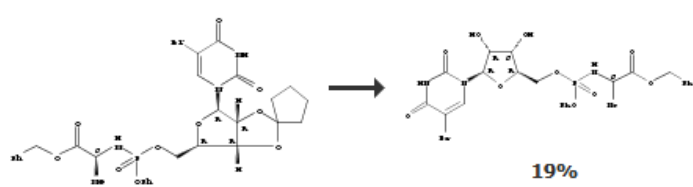
REACTIONS ? Get References Tools

Analyze Refine Group by: No Grouping Sort by: Accession Number

0 of 3268 Reactions Selected

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

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



19%

[Overview](#)

Analyze by: ?	
Catalyst	
Pd(PPh ₃) ₄	611
Pd(OAc) ₂	270
Pd	239
CuI	218
PdCl ₂ (PPh ₃) ₂	197
72287-26-4	152
4-DMAP	115

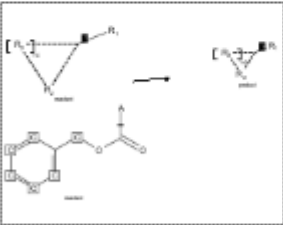
第二次限定，限定反应中心

Analyze Refine

Refine by: ?

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

Reaction Structure:



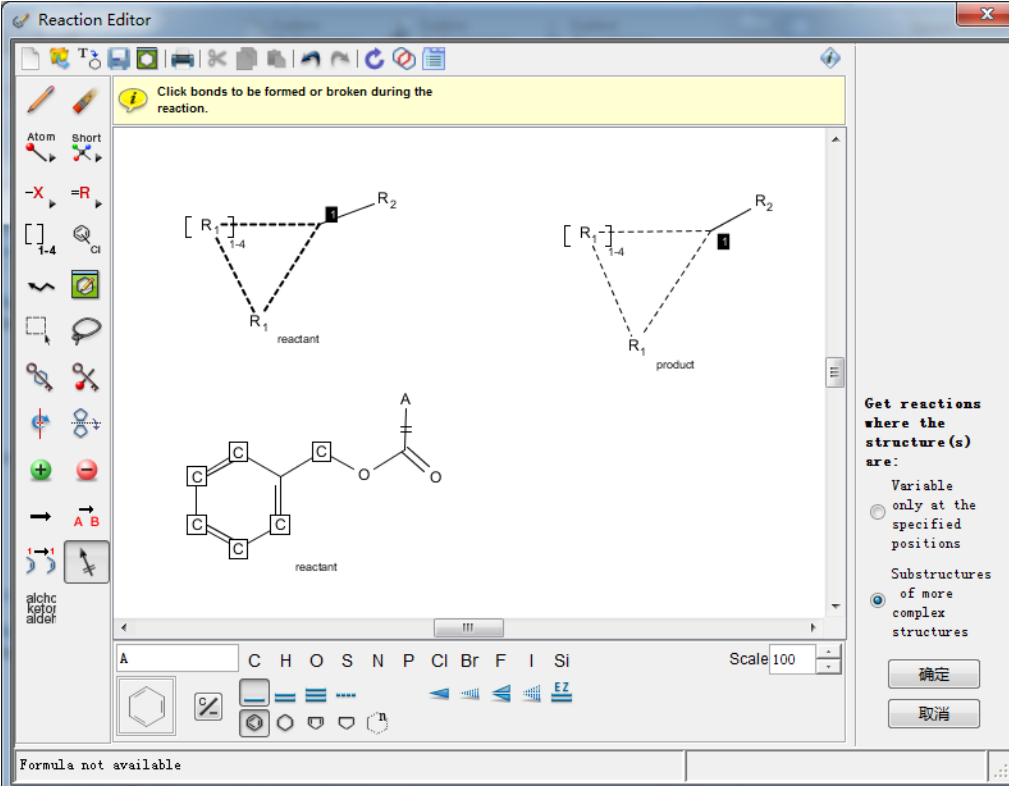
Click image to change structure or view detail

Search type: **Substructure**

Refine

Reaction Editor

Click bonds to be formed or broken during the reaction.



Get reactions where the structure(s) are:

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

确定

取消

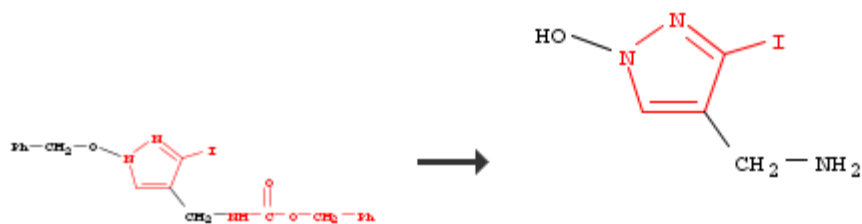
Formula not available

反应中心沿用之前的定义

限定后的结果

1. **Synthesis and Biological Evaluation of 4-(Aminomethyl)-1-hydroxypyrazole Analogues of Muscimol as Agonists** Full Text
 2 Reactions Similar Reactions

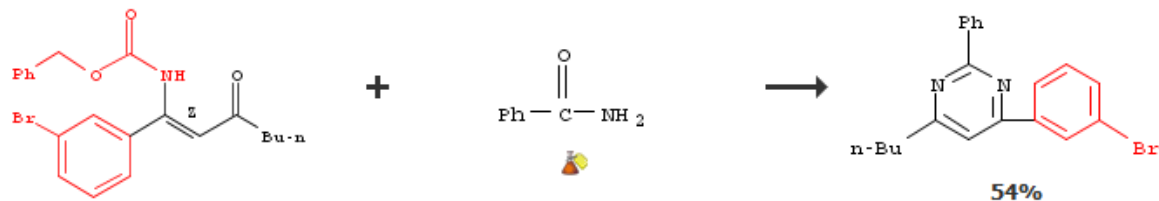
Single Step *Hover over any structure for more options.*



► Overview

5. **Stereoselective and Catalytic Access to β -Enaminones: An Entry to Pyrimidines** Full Text
 1 Reaction Similar Reactions

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



► Overview

都是我们想要的
反应结果

提纲

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Unprecedented Results



Thank You

俞靛

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