

SciFinder中的物质详情界面（续：文献角色分类）

▼CAS REFERENCE ROLES

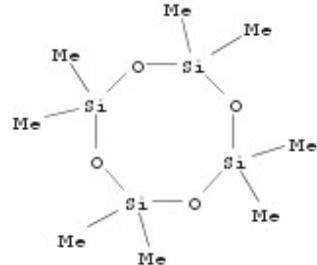
| Roles | Patents | Nonpatents | Nonspecific Derivatives from Patents | Nonspecific Derivatives from Nonpatents |
|---------------------------|---------|------------|--------------------------------------|---|
| Analytical Study | ✓ | ✓ | | ✓ |
| Biological Study | ✓ | ✓ | ✓ | ✓ |
| Formation, Nonpreparative | ✓ | ✓ | | |
| Miscellaneous | ✓ | ✓ | | |
| Occurrence | ✓ | ✓ | | ✓ |
| Preparation | ✓ | ✓ | ✓ | ✓ |
| Process | ✓ | ✓ | ✓ | ✓ |
| Properties | ✓ | ✓ | ✓ | ✓ |
| Prophetic in Patents | ✓ | | | |
| Reactant or Reagent | ✓ | ✓ | ✓ | ✓ |
| Uses | ✓ | ✓ | ✓ | ✓ |

检索Tips:

1. 这是根据CAS Role做的一张文献分类表
2. 可以快速的通过这个表，获得物质在专利和非专利文献中在特定领域的文献报道

物质有关的反应

1. Substance Detail
556-67-2



~4816



C₈ H₂₄ O₄ Si₄
Cyclotetrasiloxane, 2,2,4,4,6,6,8,8-octamethyl-

Get Reactions 

Limit results by reaction role:

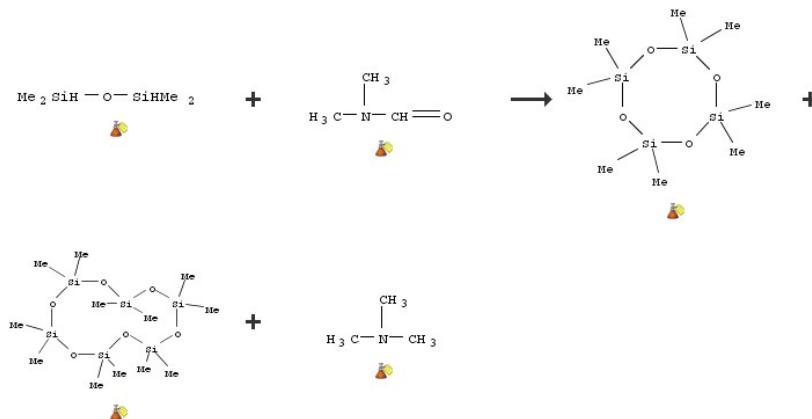


Get

Cancel

1. View Reaction Detail 

2 Steps Hover over any structure for more options.

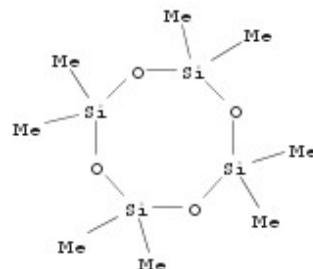


检索Tips:

1. 检索到物质后，可以通过绿色三角瓶，直接获得该物质的反
2. 需要选取物质在反应中的角色
3. 有绿色三角瓶，表示SciFinder中一定可以找到该物质的反应，但是不一定是作为产物的反应

物质有关的文献信息

1. Substance Detail
556-67-2



4816



C₈H₂₄O₄Si₄

Cyclotetrasiloxane, 2,2,4,4,6,6,8,8-octamethyl-

Experimental P

检索Tips:

1. 一键获得文献，可以获得全部，也可以勾选特别感兴趣的内容
2. 不勾选，默认获得全部

Get References

Limit results to:

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

For each sequence, retrieve:

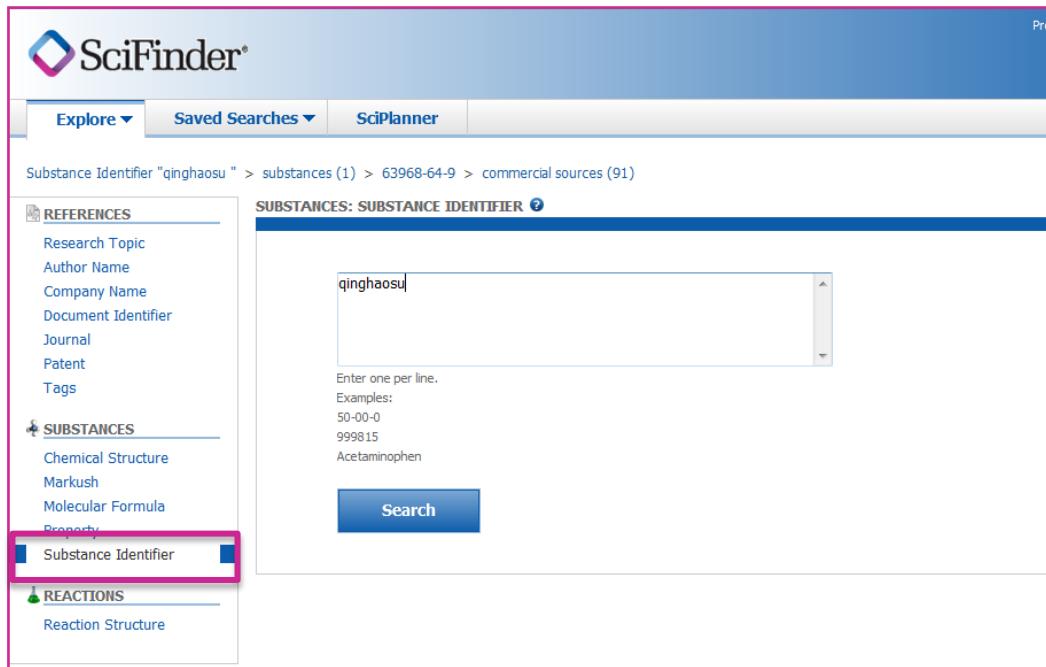
- Additional related references, e.g., activity studies, disease studies.

Get **Cancel**

SciFinder中的物质检索方法

- 功能方面
 - 物质名称, CAS No
 - 分子式
 - 结构式
 - 理化性质
- 推荐的物质检索功能
 - 有机物, 天然产物及衍生物 ---结构比较方便
 - 无机物 ---分子式比较方便
 - 高分子化合物 ---首先分子式, 其次结构

物质名称检索



Substance Identifier "qinghaosu" > substances (1) > 63968-64-9 > commercial sources (91)

SUBSTANCES: SUBSTANCE IDENTIFIER 

qinghaosu

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

Search

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

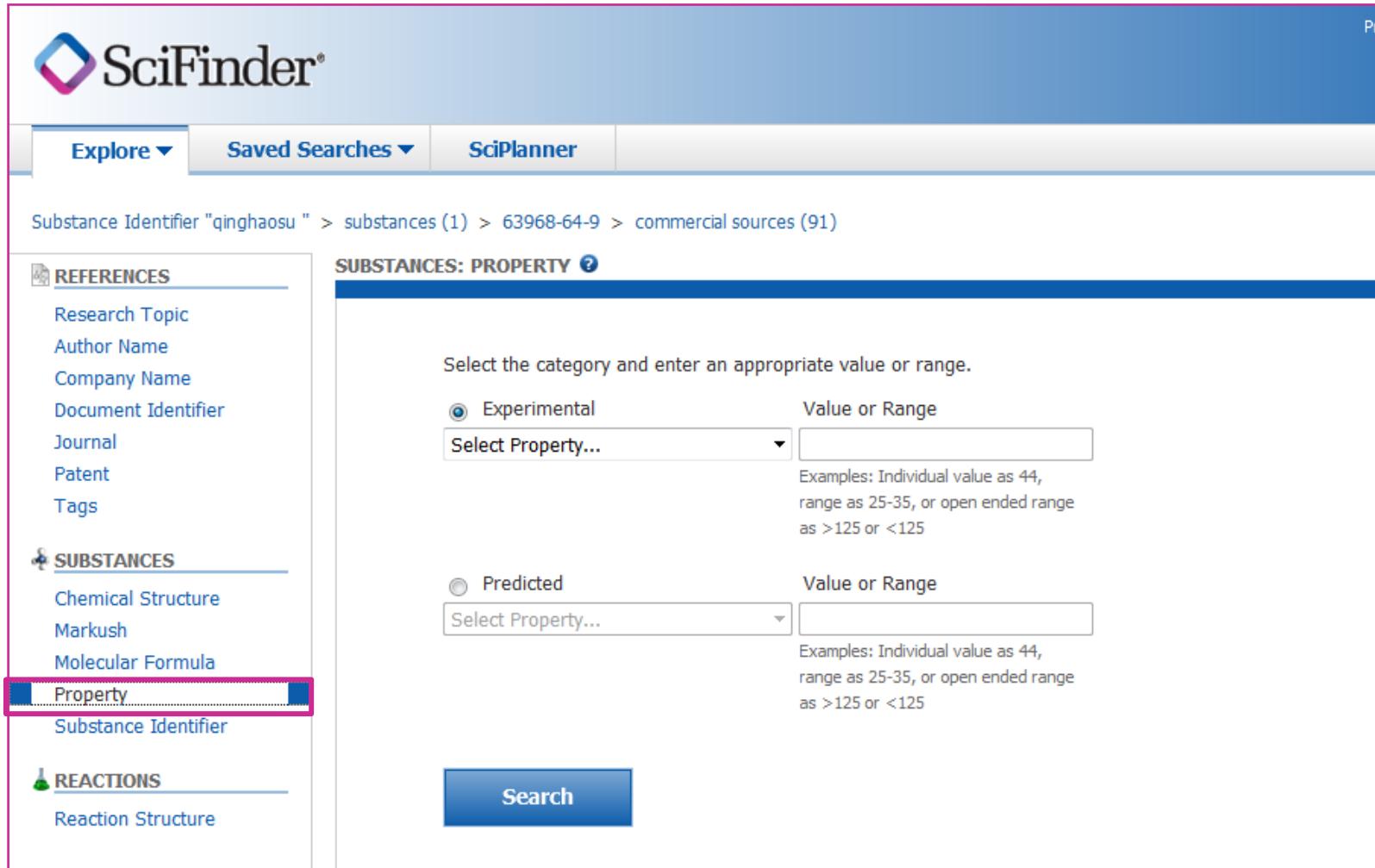
SUBSTANCES
Chemical Structure
Markush
Molecular Formula
Property
Substance Identifier

REACTIONS
Reaction Structure

检索Tips:

1. 直接输入物质的名称, CAS No, 俗名, 都能检索
2. 一次最多检索25个物质, 用换行换开
3. 建议一次最多检索3-5个, 因为给出结果的顺序和输入的顺序是不一样的。

理化性质检索



Substance Identifier "qinghaosu" > substances (1) > 63968-64-9 > commercial sources (91)

SUBSTANCES: PROPERTY 

Select the category and enter an appropriate value or range.

Experimental Value or Range

Examples: Individual value as 44, range as 25-35, or open ended range as >125 or <125

Predicted Value or Range

Examples: Individual value as 44, range as 25-35, or open ended range as >125 or <125

Search

REFERENCES

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

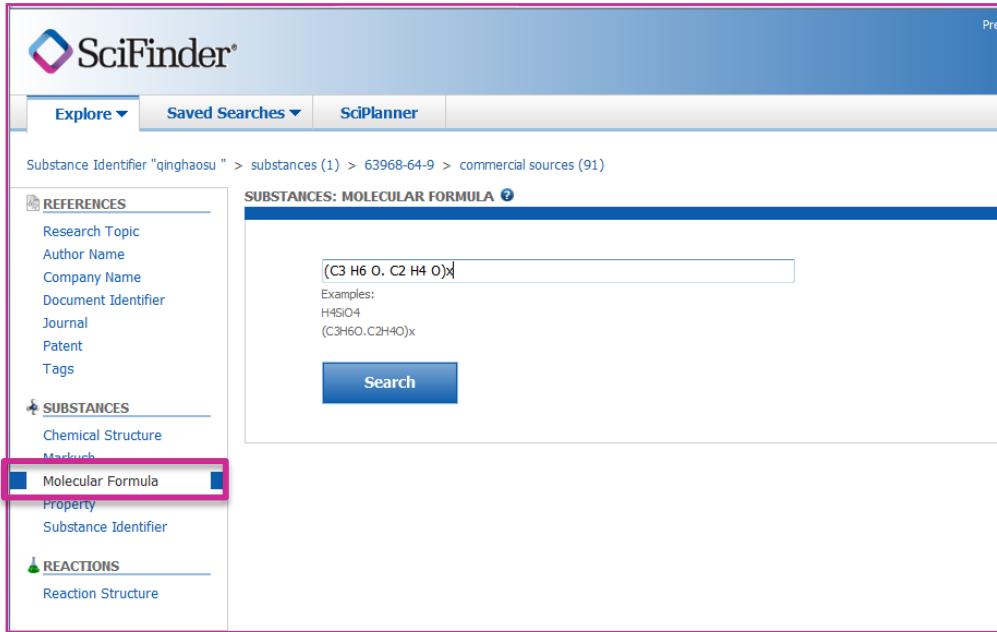
SUBSTANCES

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

REACTIONS

- Reaction Structure

分子式检索



The screenshot shows the SciFinder search interface. The top navigation bar includes 'Explore', 'Saved Searches', and 'SciPlanner'. The main search area is titled 'SUBSTANCES: MOLECULAR FORMULA'. A search input field contains the text '(C3 H6 O. C2 H4 O)x'. Below the input field are 'Examples: H4SiO4' and '(C3H6O.C2H4O)x'. A 'Search' button is located at the bottom of the input field. On the left, a sidebar menu is open under the 'SUBSTANCES' section, with 'Molecular Formula' selected and highlighted in blue. Other options in the sidebar include 'Chemical Structure', 'Molecule', 'Property', 'Substance Identifier', and 'Reaction Structure'.

检索Tips:

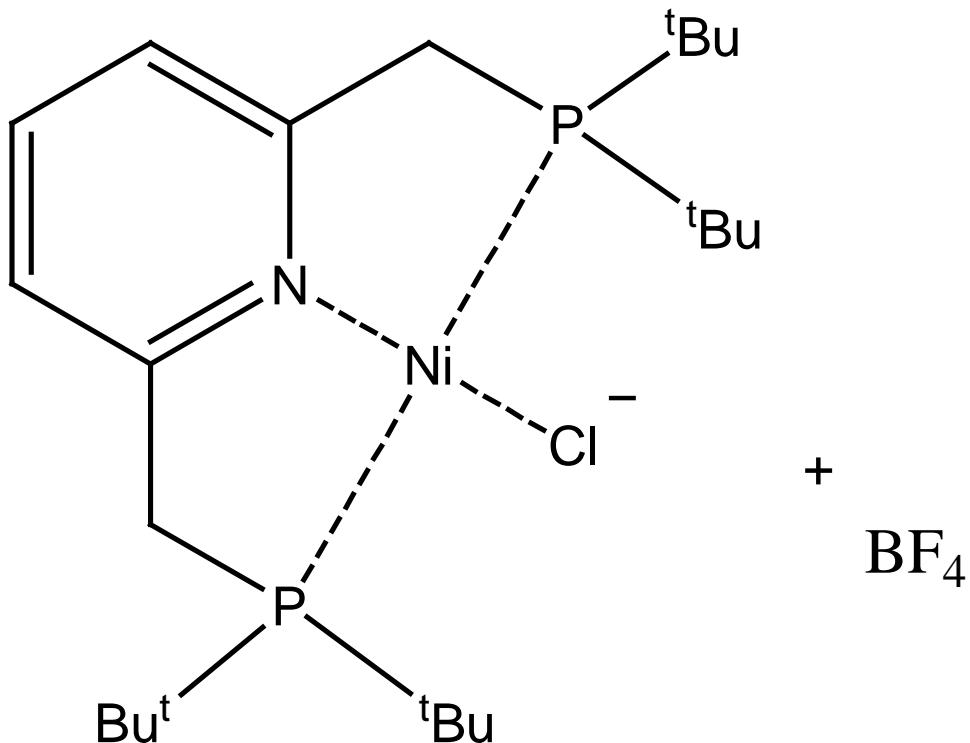
1. 分子式的检索，需要按照HILL排序进行，简单的说CH写前面，其他的按照字母顺序排序
2. 多组分物质，需要用“.”分开

结构式检索—精确检索

检索Tips:

1. 启动Java面板，电脑中需要安装Java
2. 建议将Java升级到最高版本后，停止Java自动更新
3. 初次使用Java会有插件弹出，选择允许即可
4. 不用使用360浏览器或开着360安全卫士，因为他们会禁止Java的启动

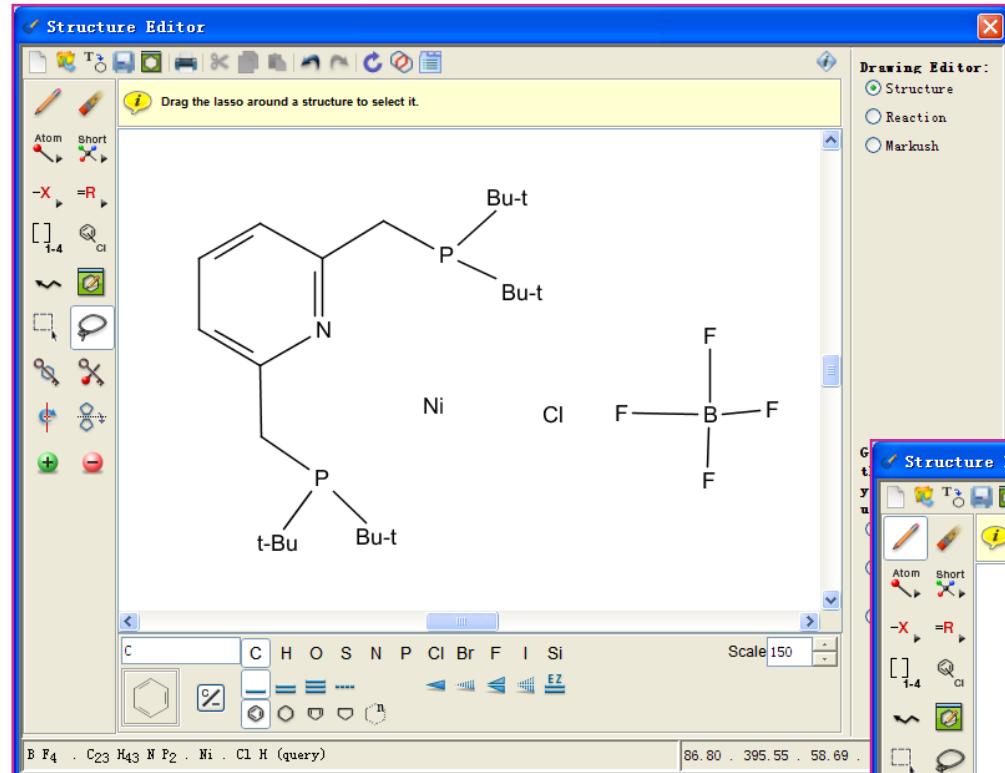
精确结构检索—检索金属配合物



该结构中包含：

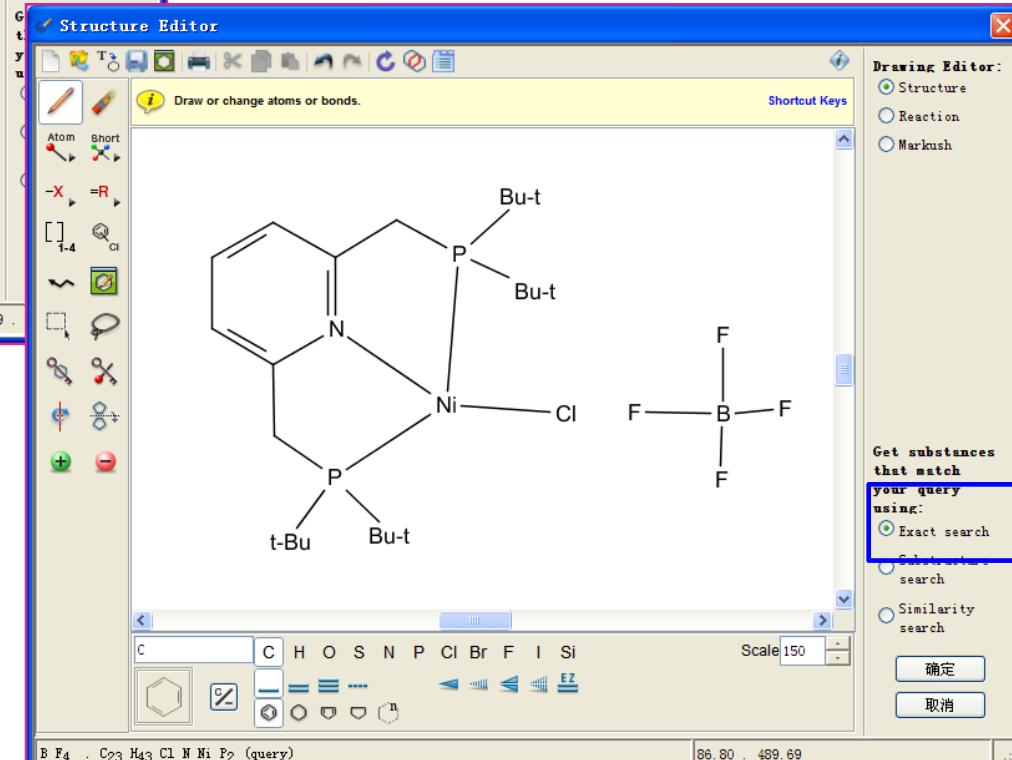
配体
金属
阳离子
阴离子

检索界面



检索Tips:

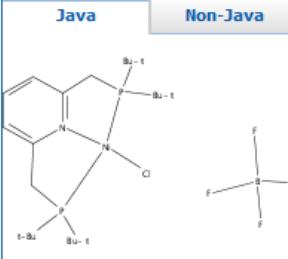
1. 精确结构检索检索到结构本身，聚合物，配合物，盐等



进行检索时的选项

Structure Editor:

Java Non-Java



Click image to change structure or view detail.

Import CXF

Search

Advanced Search Always Show

Search Type:

- Exact Structure
- Substructure
- Similarity

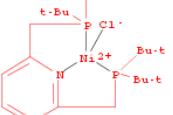
Show precision analysis

 ChemDraw®

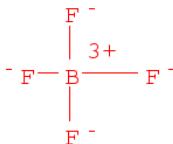
Launch a SciFinder substance or reaction search directly from ChemBioDraw Ultra 14. [Learn More](#)

1. 1136166-99-8 

1136166-98-7
 $C_{23} H_{43} Cl N Ni P_2$



14874-70-5
 $B F_4$



$C_{23} H_{43} Cl N Ni P_2 \cdot B F_4$
 Nickel(1+), [2,6-bis[[bis(1,1-dimethylethyl)phosphino-κP]methyl]pyridine-κN]chloro-, ($S^2P-4-3-$) \cdot , tetrafluoroborate(1-)
 (1:1)

Characteristics

Classes Alloys Coordination compounds Incompletely defined Mixtures Polymers Organics, and others not listed

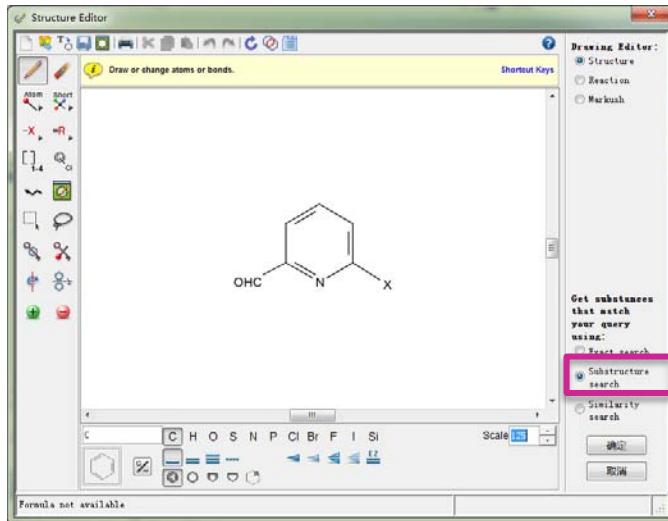
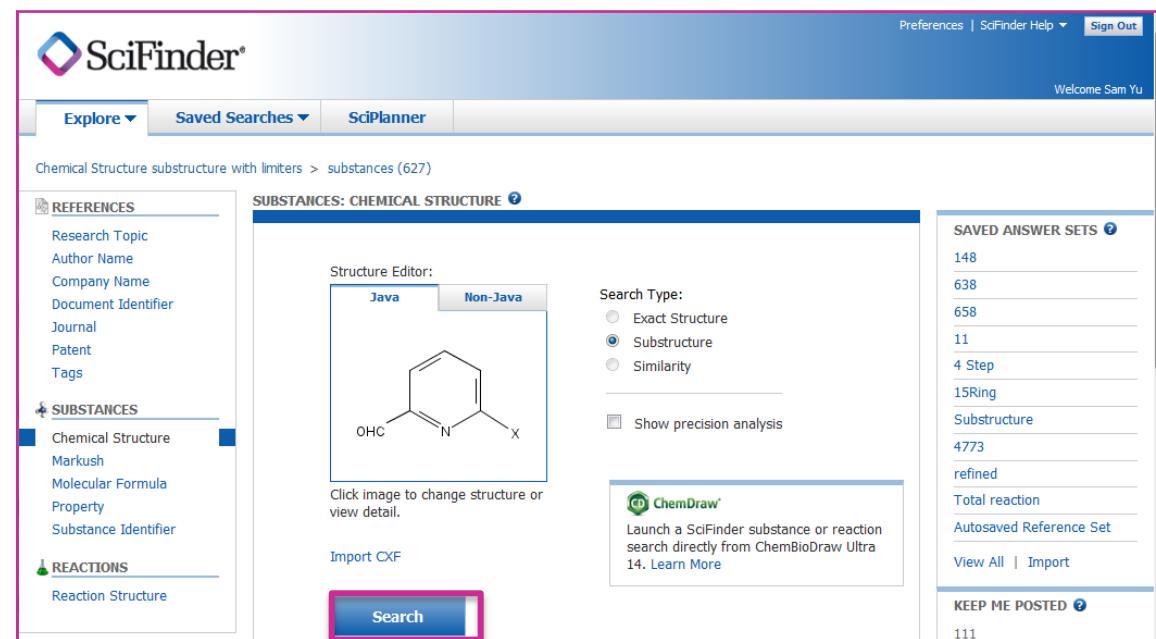
Studies Analytical Biological Preparation Reactant or reagent

检索Tips:

1. 可以通过Advanced Search提前做出一些设置
2. 对于配位化合物, 聚合物, 有特定的种类选项, 建议勾选
3. Single Component, 帮助将多组分物质去除

亚结构检索—检索包含核心结构的物质

- 检索包含以下核心结构的所有物质

SciFinder

Explore Saved Searches SciPlanner

Chemical Structure substructure with limiters > substances (627)

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

Structure Editor: Java Non-Java

Search Type:

- Exact Structure
- Substructure** (selected)
- Similarity

Show precision analysis

Click image to change structure or view detail.

Import CXF

ChemDraw

Launch a SciFinder substance or reaction search directly from ChemBioDraw Ultra 14. [Learn More](#)

Search

SAVED ANSWER SETS

- 148
- 638
- 658
- 11
- 4 Step
- 15Ring
- Substructure
- 4773
- refined
- Total reaction
- Autosaved Reference Set
- [View All](#) | Import

KEEP ME POSTED

111

SciFinder中的检索结果

SciFinder®

Explore ▾ Saved Searches ▾ SciPlanner Preferences | SciFinder Help ▾ Sign Out

Welcome Sam Yu

Chemical Structure substructure with limiters > substances (627)

SUBSTANCES ?

Get References | Get Reactions | Get Commercial Sources | Tools ▾

Create Keep Me Posted Alert | Send to SciPlanner

Analyze Refine

Analyze by: Substance Role

Preparation 73

Reactant or Reagent 69

Prophetic in Patents 8

Biological Study 6

Uses 5

Combinatorial Study 1

Formation, Nonpreparative 1

Process 1

Properties 1

Sort by: CAS Registry Number

Display Options

0 of 627 Substances Selected

Page: 1 of 13

1. 1639023-88-3

Absolute stereochemistry.,Rotation (-).

2. 1639023-49-6

Relative stereochemistry.

3. 1622218-78-3

C12H13BrClFN2O2
2-Pyridinecarboxaldehyde, 6-bromo-4-chloro-3-[(2R,6S)-2,6-dimethyl-4-morpholinyl]-5-fluoro-, *rel*-

C13H8BrFeNNO3
INDEX NAME NOT YET ASSIGNED

检索Tips:

1. SciFinder中的亚结构检索，获得的是包含所绘制结构片段的所有化合物
2. 与所绘制结构不同的可能是原子上面的取代会不同，又或者环系发生稠环等
3. 可以使用结构的Analyze/Refine功能对检索到的结果进行处理

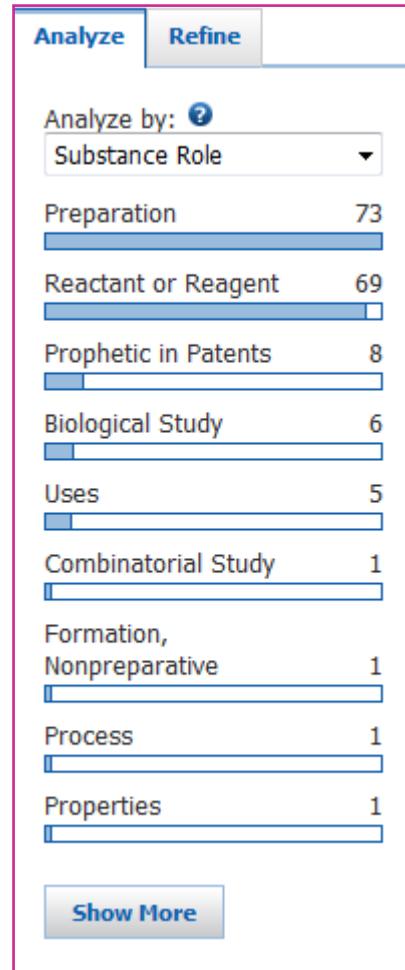
SciFinder中的结构结果后处理—Analyze

Analyze Refine

Analyze by: ?

Substance Role

Bioactivity Indicators
Commercial Availability
Elements
Reaction Availability
Substance Role
Target Indicators



检索Tips:

1. 分析方面，提供6种分析手段
2. 提供**靶点标记，生物活性分析**，帮助快速对检索到的物质进行筛选
3. Substance Role分析，帮助获得物质研究角色的文献

SciFinder中的结构结果后处理—Refine

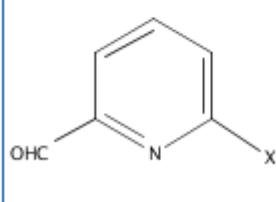
Analyze Refine

Refine by: ②

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

Structure Editor:

Java Non-Java



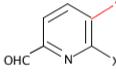
Click image to change structure or view detail.

Search type: Substructure

Refine by Atom Attachment ②

1. Click an atom to display the attachments present at that site.

Substructure



2. Select attachment(s) of interest.

Atom Attachments

Select All Deselect All

| | |
|--|-----|
| <input type="checkbox"/> H or None | 385 |
| <input type="checkbox"/> C | 114 |
| <input type="checkbox"/> O | 63 |
| <input type="checkbox"/> N | 29 |
| <input type="checkbox"/> S | 9 |
| <input type="checkbox"/> F | 9 |
| <input type="checkbox"/> I | 6 |
| <input type="checkbox"/> Br | 4 |
| <input type="checkbox"/> B | 4 |
| <input type="checkbox"/> A - Any (not H) | 242 |
| <input type="checkbox"/> Q - Any (not C,H) | 128 |
| <input type="checkbox"/> Ak - Alkyl chain | 58 |
| <input type="checkbox"/> Cb - Carbocycle | 50 |
| <input type="checkbox"/> X - Halogen | 23 |
| <input type="checkbox"/> Hy - Heterocycle | 10 |

? =

Refine Cancel

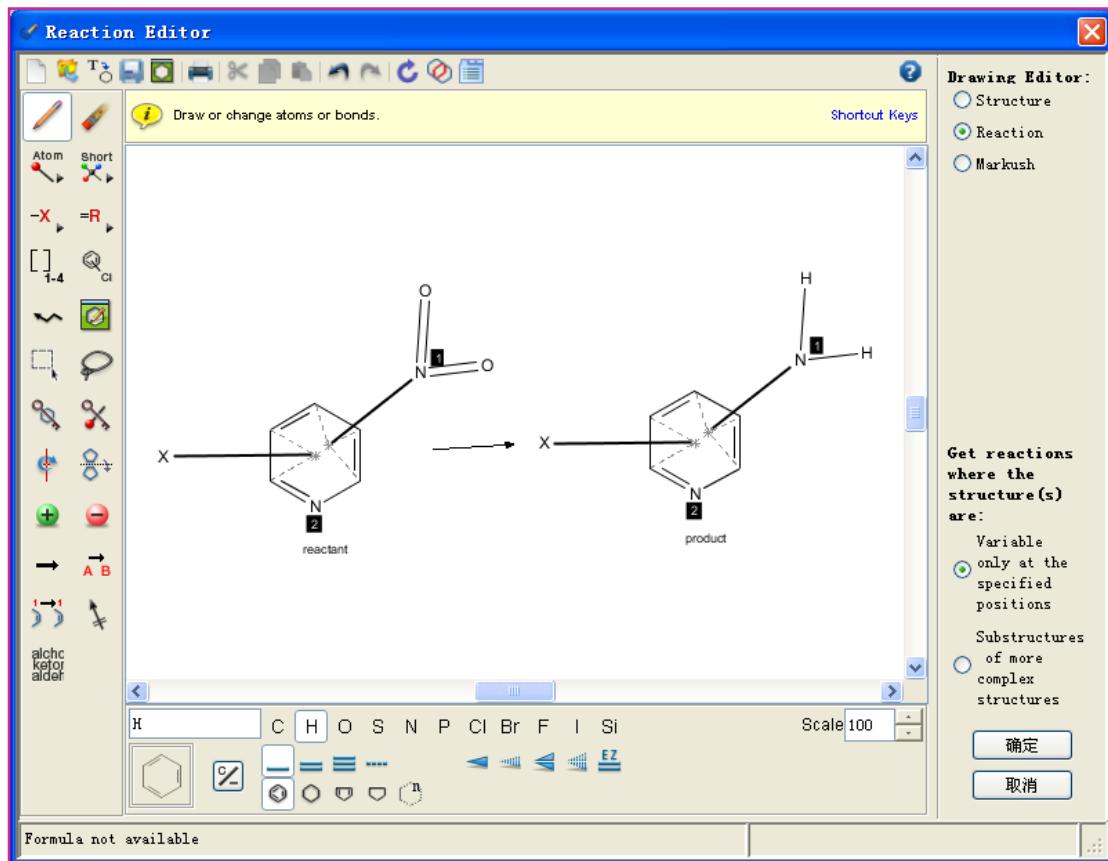
检索Tips:

1. 限定方面，提供7种限定手段
2. Isotope-Containing，用于获得是否包含同位素的物质
3. Property Value，用于通过理化性质的数值对物质进行限定
4. Atom Attachment，用于通过对结构取代的限定，帮助获得某位点的不同取代基团分布。

提纲

- 介绍
 - SciFinder Web中的内容
- **SciFinder Web中的检索和后处理**
 - SciFinder Web中的文献记录及主题检索
 - SciFinder Web中的物质结果及物质检索方法
 - SciFinder Web中的反应记录及反应检索
- **SciFinder Web的注册**

SciFinder反应检索



检索要求:

1: 吡啶环2, 3, 4位上存在一个硝基还原成氨基

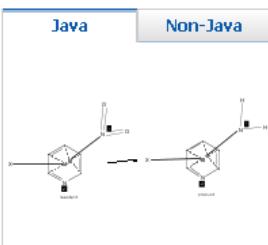
2: 吡啶环5, 6位上存在一个卤素

SciFinder Web中的检索

REACTIONS: REACTION STRUCTURE

Structure Editor:

Java Non-Java



Search Type:

Allow variability only as specified
 Substructure

Click image to change structure or view detail.

Import CXF

Search

Advanced Search

检索Tips:

1. Allow Variability only as specified表示，只在你所绘制的位点上发生变化
2. Substructure表示，除了在所绘制的位点上发生变化外，还能在结构中没有绘制出来的H上做随意的取代
3. Advanced Search，可以设置反应的溶剂，产率，步数等等
4. 不建议一开始就设置反应的溶剂，产率，步数，或许会遗漏掉很多重要信息

SciFinder中的检索结果

SciFinder®

Preferences | SciFinder Help ▾ | Sign Out

Welcome Sam Yu

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

Reaction Structure structure variable only at spe... > reactions (56)

REACTIONS | Get References | Tools ▾ | Send to SciPlanner

Analyze Refine

Group by: No Grouping Sort by: Accession Number

NEW! Display Options

Analyze by: Reagent (New)

0 of 56 Reactions Selected

Page: 1 of 3

1. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.

H₂ 26

Fe 9

KF 6

Mg 5

NH₃ 5

TiCl₄ 5

HCl 4



96%

▶ Overview

Group By Document

Get References Tools ▾

Group by: **Document** Sort

No Grouping
 Document Selected
 Transformation

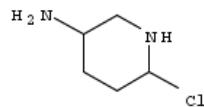
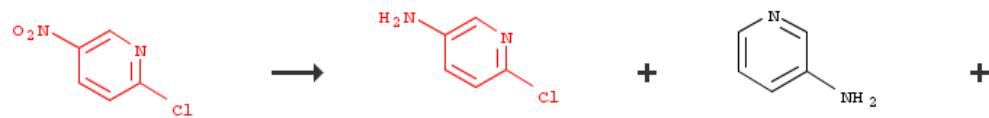
1. **View Reaction Detail**

检索Tips:

1. Group By Document将来自同篇文献的反应合并

6. Selective catalytic hydrogenation of nitro groups in the presence of activated heteroaryl halides [Quick View](#) [Full Text](#)
[4 Reactions](#) [Similar Reactions](#)

Single Step Hover over any structure for more options.

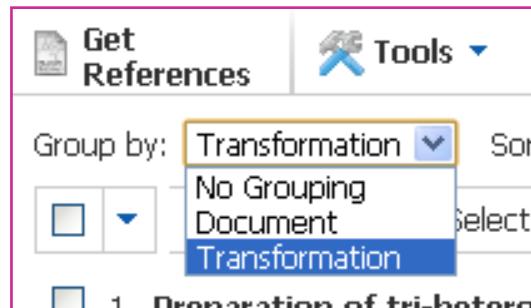


▶ Overview

▶ Experimental Procedure

10. N-Pyridyl and Pyrimidine Benzamides as KCNQ2/Q3 Potassium Channel Openers for the Treatment of Epilepsy [Quick View](#)
[Full Text](#)
[3 Reactions](#)

Group By Transformation



检索Tips:

1. **Group By Transformation**
针对检索结果中的单步反应，将具备同样反应变化的反应合并
2. 多步反应会全部集中在最后的选项

0 of 56 Reactions Selected

1. Reduction of Nitro Compounds to Amines
49 Reactions

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

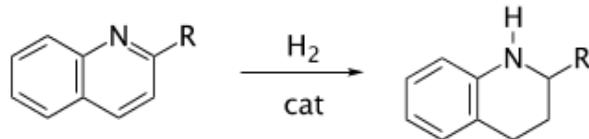
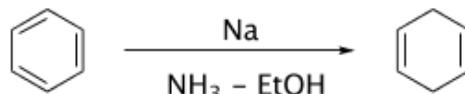
2. Dehalogenation of Aromatic Compounds
2 Reactions

$$\text{Ar}-\text{X} \xrightarrow{\text{cat.}} \text{Ar}-\text{H}$$

3. Reduction of Alkyl Halides/ Dehalogenation
2 Reactions

$$\text{R}-\text{X} \longrightarrow \text{R}-\text{H}$$

4. Reduction of Aromatic Rings/ Birch or Benkeser Reduction
1 Reaction

Similary Reaction

1. Preparation of tri-heterocyclic derivatives as Flt3 kinase inhibitors
[1 Reaction](#) [Similar Reactions](#)

[Quick View](#)

[Full Text](#)

Single Step Hover over any structure for more options.



[▶ Overview](#)

检索Tips:

1. 只有单步反应后才有相似反应的链接
2. 根据设置的相似级别, 寻找和该反应在反应中心上完全一样的反应
3. 相似级别的设定:
 - a. **Broad:** 仅反应中心相同
 - b. **Medium:** 反应中心和附属原子相同
 - c. **Narrow:** 反应中心及扩展原子和键相同

Get Similar Reactions

Retrieve similar reactions from:

- All reactions
 Current answer set

Include this level of similarity:

- Broad - Reaction centers only (96991) 
- Medium - Reaction centers plus adjacent atoms and bonds (92590) 
- Narrow - Reaction centers plus extended atoms and bonds (88722) 

[Get Reactions](#)

[Cancel](#)

相似反应结果

1. Preparation of tri-heterocyclic derivatives as Flt3 kinase inhibitors

[Quick View](#)

[Full Text](#)

1 Reaction [Similar Reactions](#)

Single Step Hover over any structure for more options.

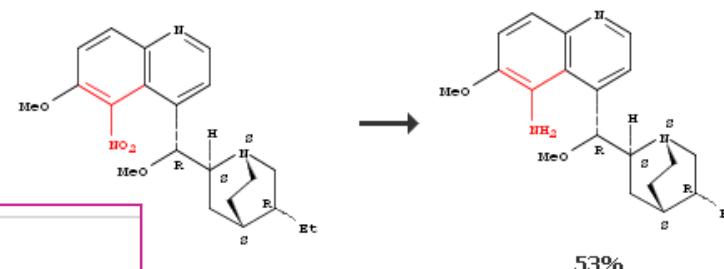


[Overview](#)

0 of 88722 Reactions Selected

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

Single Step Hover over any structure for more options.



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

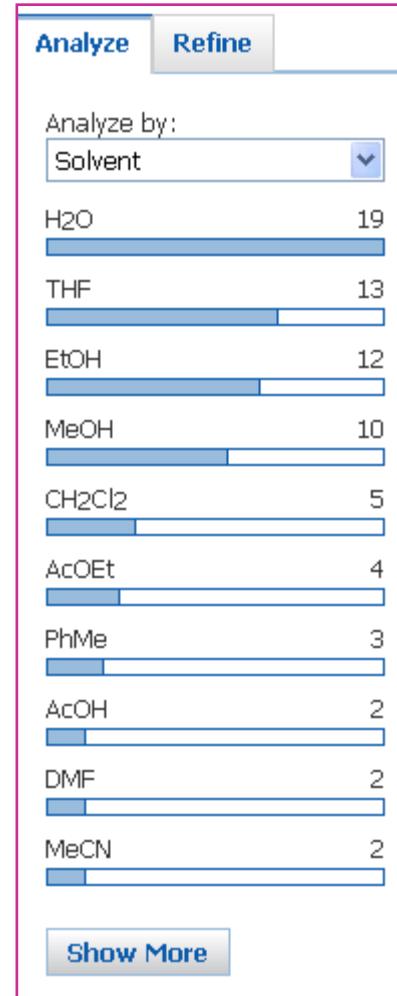
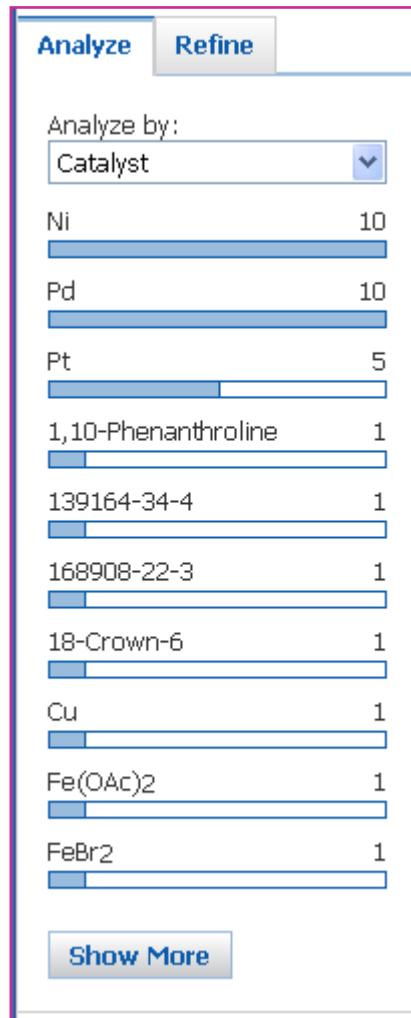
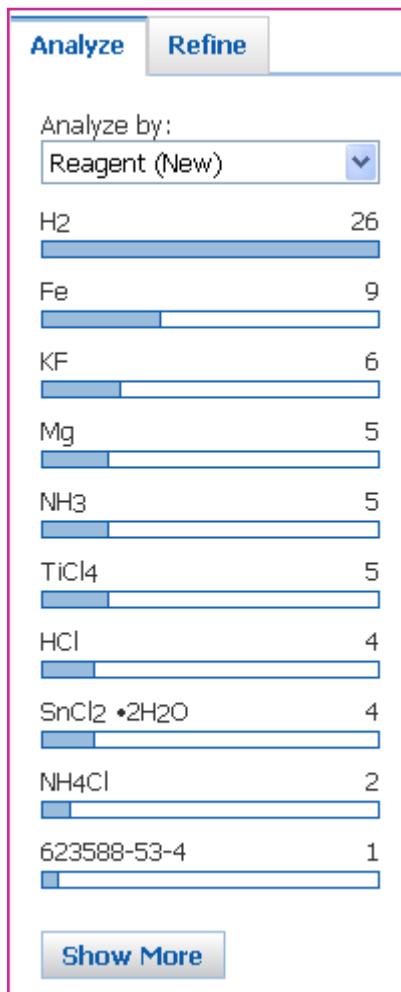
Single Step Hover over any structure for more options.



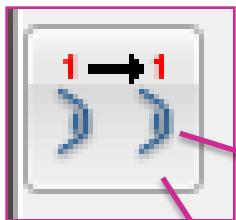
[Overview](#)

这些都和原有的反应，在反应中心，及扩展的原子和键上是一致的

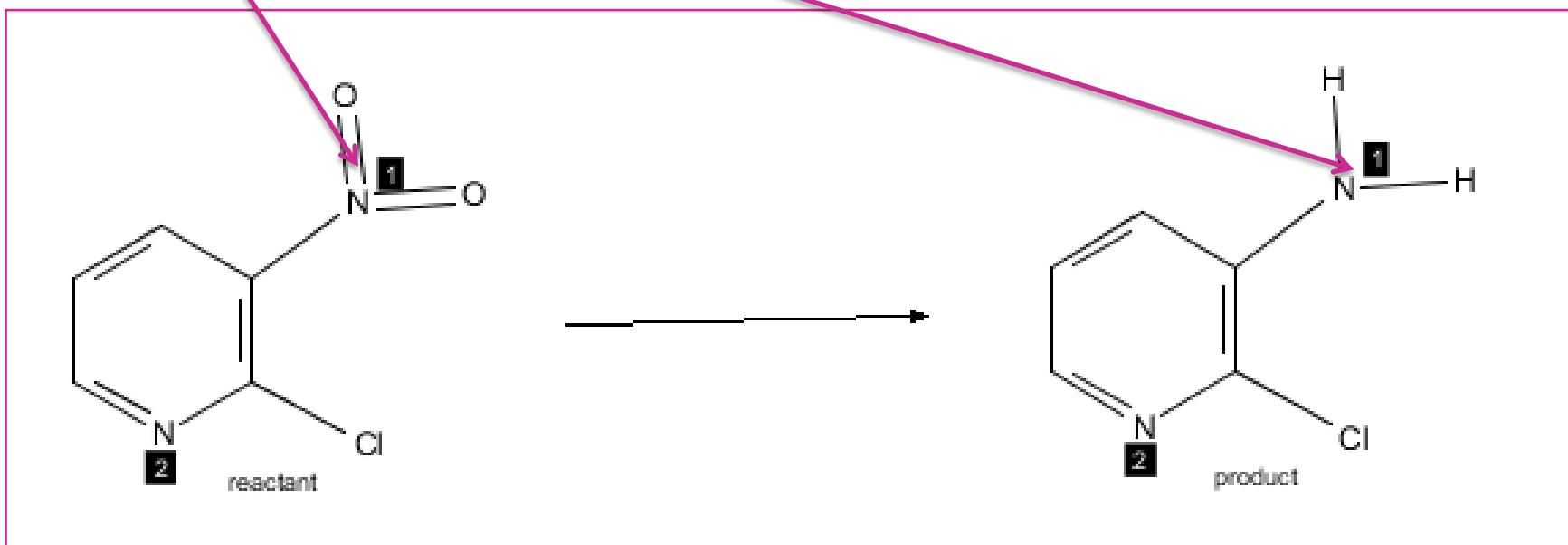
SciFinder Web中的反应后处理



反应精准性定义工具—原子标记工具



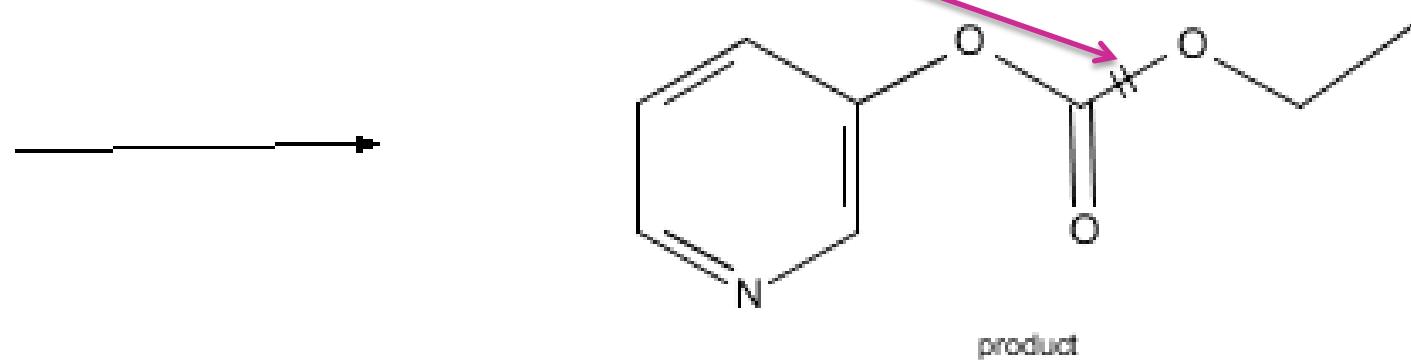
原子标记工具标记反应前后必须匹配的原子，主要用于反应中心的定义



反应精准性定义工具—键标记工具



键标记工具，用于标记反应过程中必须发生变化的键



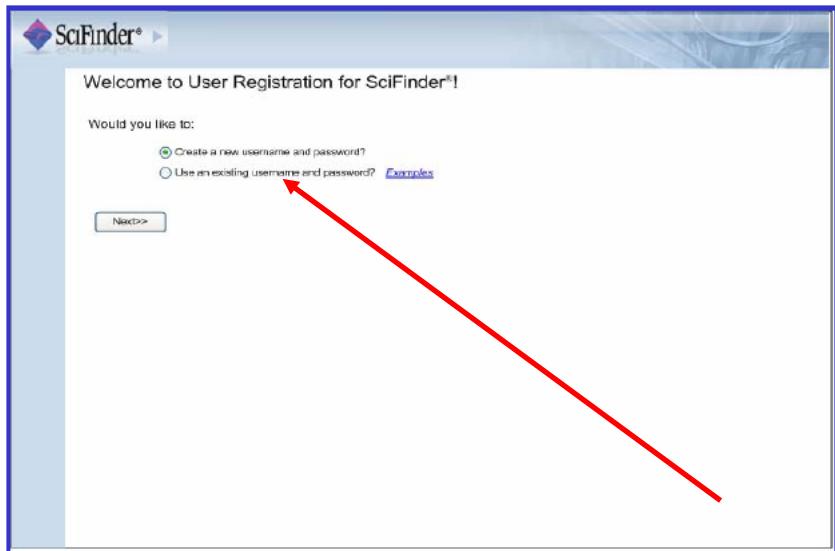
提纲

- 介绍
 - SciFinder Web中的内容
- **SciFinder Web中的检索和后处理**
 - SciFinder Web中的文献记录及主题检索
 - SciFinder Web中的物质结果及物质检索方法
 - SciFinder Web中的反应记录及反应检索
- **SciFinder Web的注册**

SciFinder Web的注册

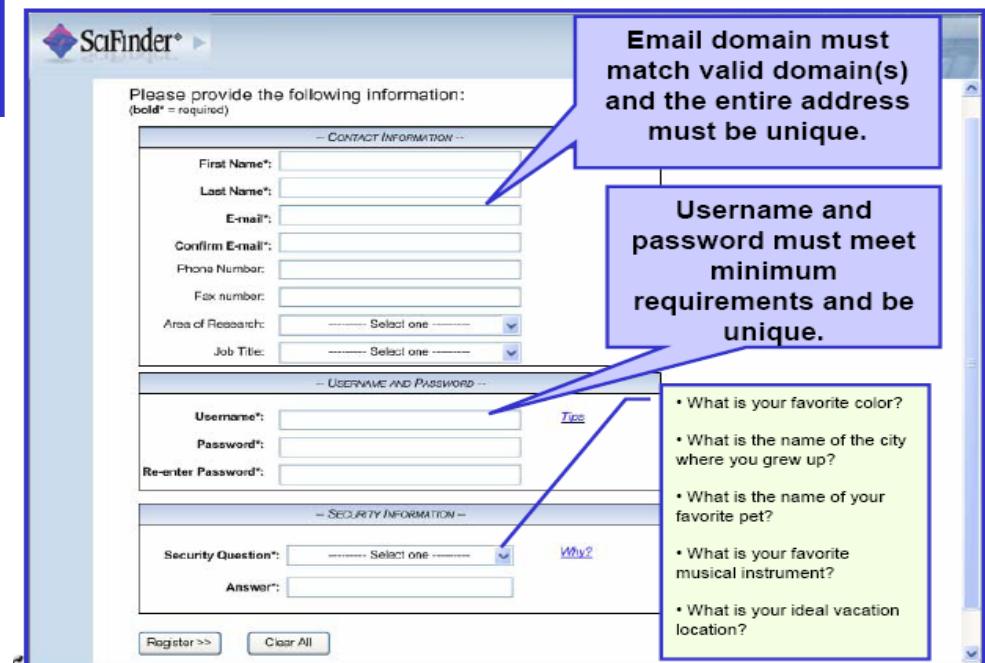
- 在图书馆相关页面上找到SciFinder Web注册用的网址
- 不要使用360浏览器登录SciFinder，即使使用Firefox等浏览器，也请关闭360安全卫士
- 欢迎加入SciFinder使用答疑QQ群：

点击URL创建SciFinder Web账号



开始创建SciFinder Web帐号

创建ID所用的IP不能是代理服务器的IP



Please provide the following information:
 (bold* = required)

CONTACT INFORMATION

First Name*:
 Last Name*:
 E-mail*:
 Confirm E-mail*:
 Phone Number:
 Fax number:
 Area of Research:
 Job Title:

USERNAME AND PASSWORD

Username*:
 Password*:
 Re-enter Password*:

SECURITY INFORMATION

Security Question*:
 Answer*:

• What is your favorite color?
 • What is the name of the city where you grew up?
 • What is the name of your favorite pet?
 • What is your favorite musical instrument?
 • What is your ideal vacation location?

Why?

Register >>

设置用户名及密码注意事项

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)

密码:

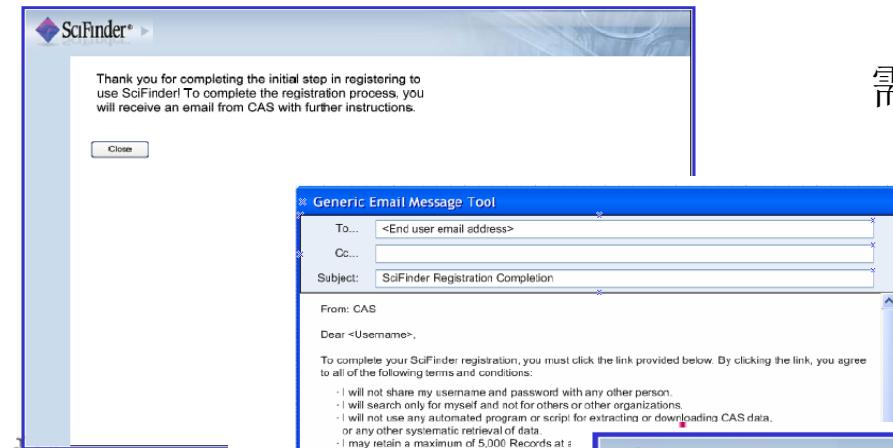
必须包含 7-15 个字符, 并且至少包含三个以下字符:

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

密码设置小技巧:

- 1: 不要和账号中有重复的字符
- 2: 密码格式最好是abc@123

对新ID的Email确认



需要点击邮件中的确认链接



Http://scifinder.cas.org

SciFinder Web 常见问题

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The choice for chemistry research.™

Username and/or password is invalid. Try again, or contact CAS for assistance.

Sign In

Username

Password

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

[Forgot Username or Password?](#)

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



News & Updates

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CAS is Collaborating with Springer to Help You Identify Preferred Synthetic Methods Faster

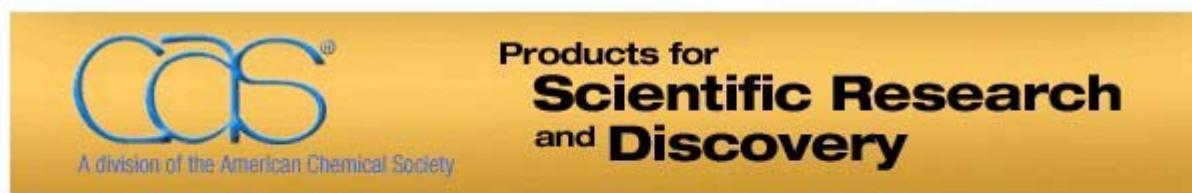
Thousands of new experimental procedures are

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SciFinder Web 常见问题

任何需要反馈给图书馆的问题，都请点击测试IP地址的链接

<http://www.cas.org/cgi-bin/casip>



将页面截图下来，一并发给图书馆

Thank You

李虹

SciFinder 培训专员

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