

# SciFinder中的物质详情界面（续：文献角色分类）

## ▼ CAS REFERENCE ROLES

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

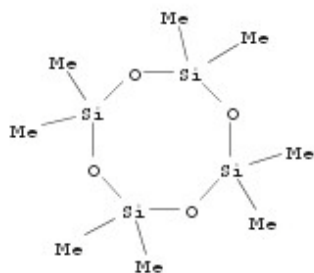
### 检索Tips:

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


C<sub>8</sub> H<sub>24</sub> O<sub>4</sub> Si<sub>4</sub>

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

### Get Reactions ⓘ

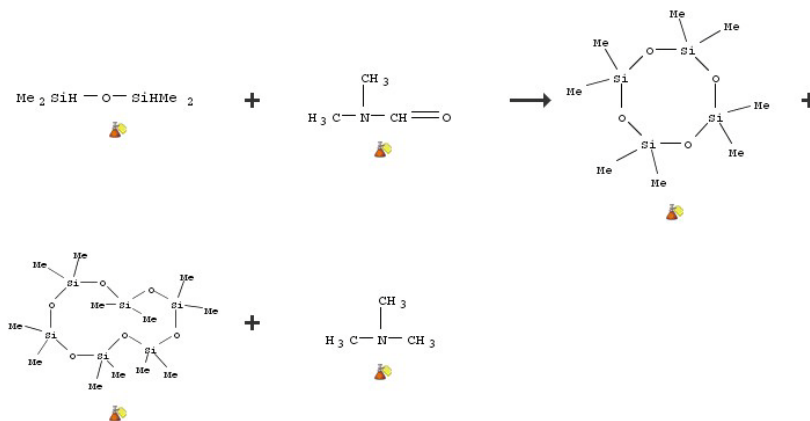
Limit results by reaction role:

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

Get Cancel

## 1. View Reaction Detail ⓘ Link

2 Steps Hover over any structure for more options.



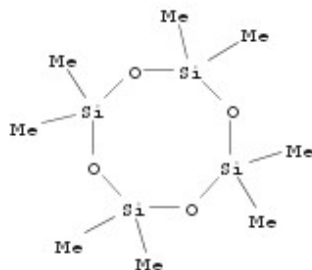
## 检索Tips:

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



C8 H24 O4 Si4

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"/> Prophetics 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:

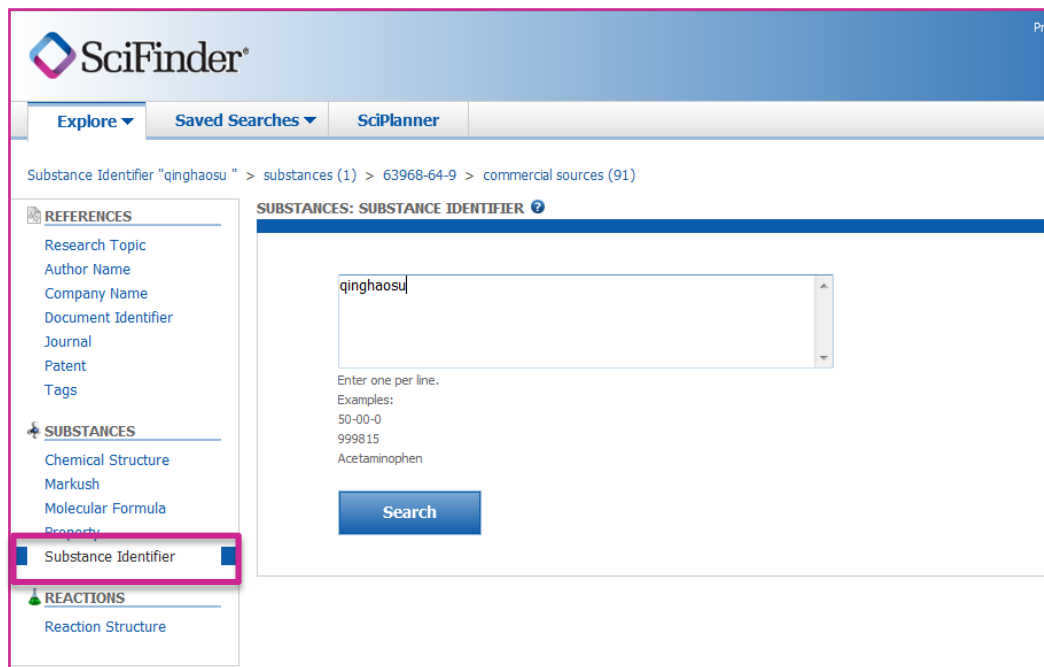
- ☐ Additional related references, e.g., activity studies, disease studies.

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)

**REFERENCES**

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

**SUBSTANCES**

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

**REACTIONS**

- Reaction Structure

**SUBSTANCES: SUBSTANCE IDENTIFIER**

qinghaosu


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

**Search**

## 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



Explore ▼
 Saved Searches ▼
 SciPlanner

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

**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: PROPERTY ?**

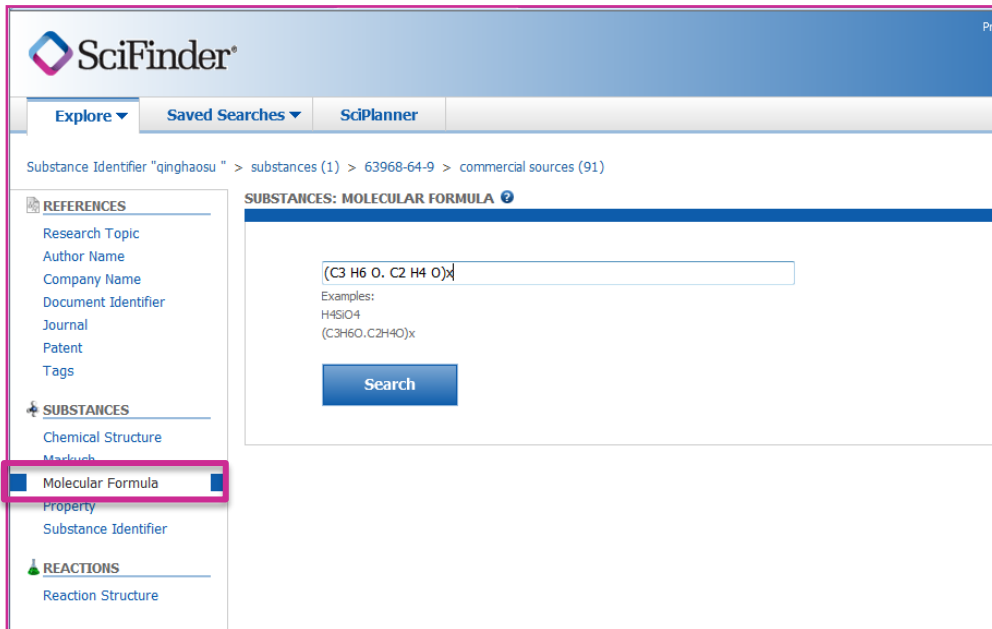
Select the category and enter an appropriate value or range.

☒ Experimental
 Value or Range  
 Select Property...   
 Examples: Individual value as 44,  
 range as 25-35, or open ended range  
 as >125 or <125

☐ Predicted
 Value or Range  
 Select Property...   
 Examples: Individual value as 44,  
 range as 25-35, or open ended range  
 as >125 or <125

Search

# 分子式检索



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

**REFERENCES**

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

**SUBSTANCES**

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

**REACTIONS**

- Reaction Structure

**SUBSTANCES: MOLECULAR FORMULA**

(C3 H6 O. C2 H4 O)x

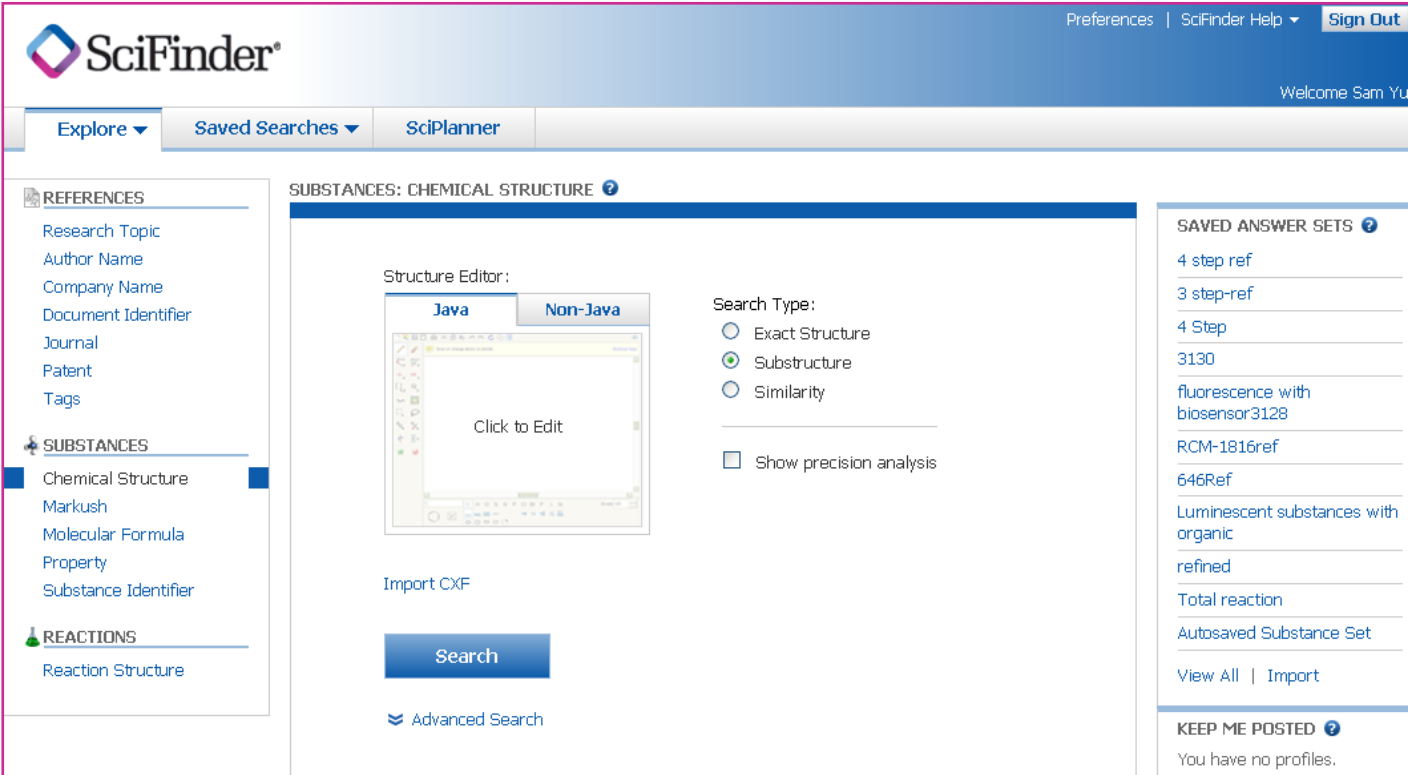
Examples:  
 H4SiO4  
 (C3H6O.C2H4O)x

Search

## 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



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**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

Import CXF

**Search**

Advanced Search

**SAVED ANSWER SETS**

- 4 step ref
- 3 step-ref
- 4 Step
- 3130
- fluorescence with biosensor3128
- RCM-1816ref
- 646Ref
- Luminescent substances with organic
- refined
- Total reaction
- Autosaved Substance Set

View All | Import

**KEEP ME POSTED**

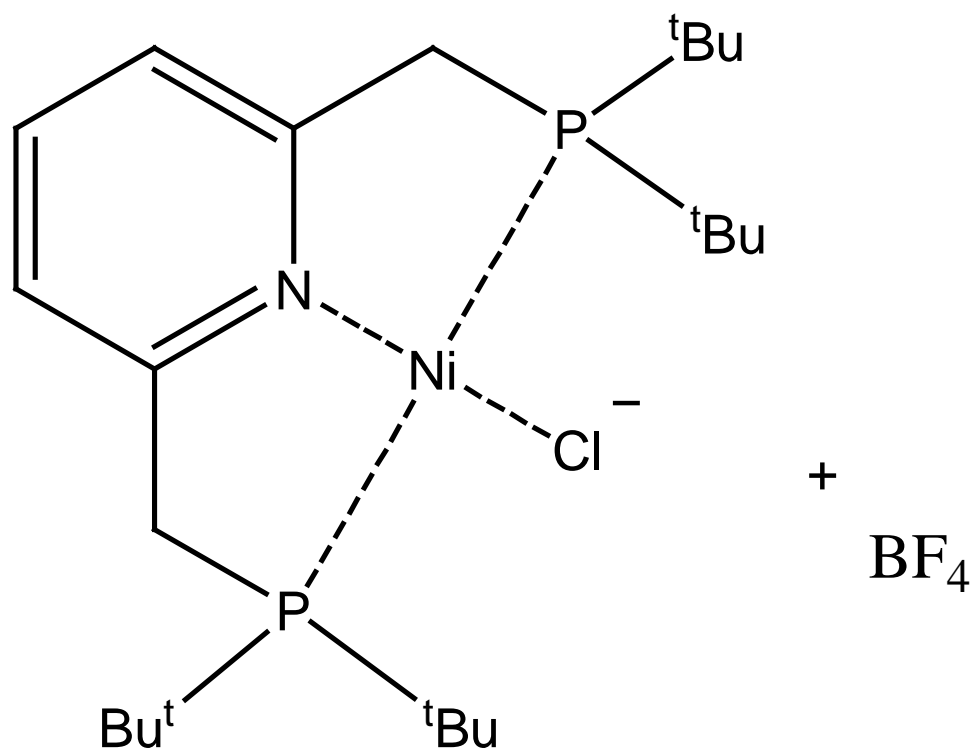
You have no profiles.

## 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



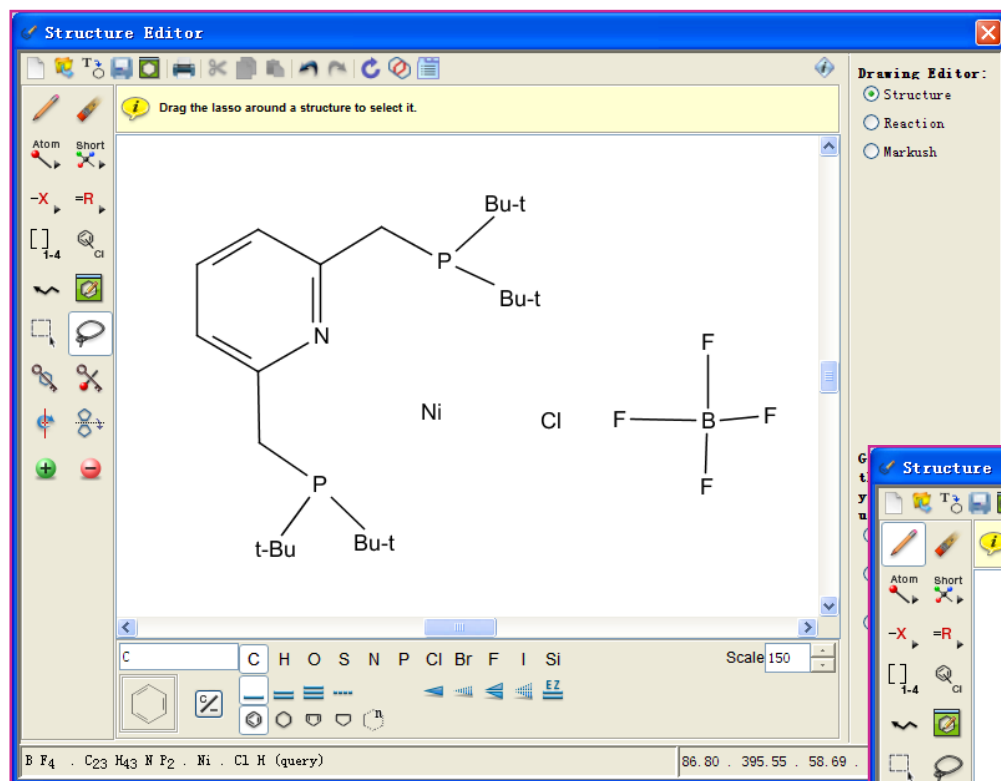
# 精确结构检索—检索金属配合物



该结构中包含:

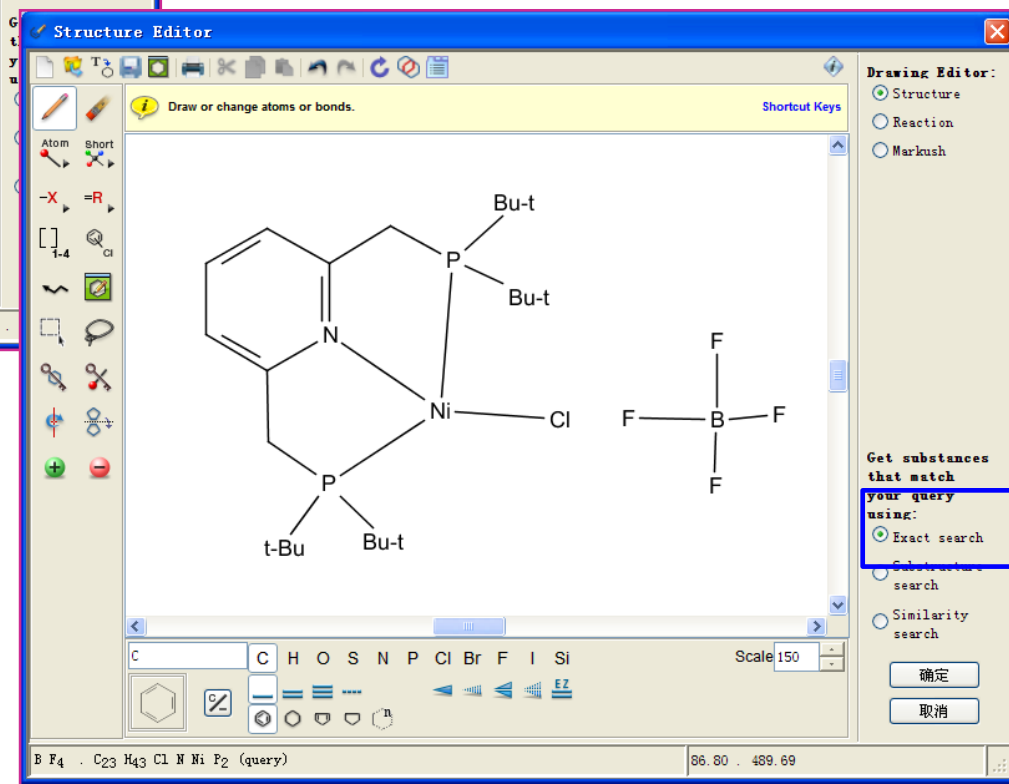
配体  
金属  
阳离子  
阴离子

# 检索界面



## 检索Tips:

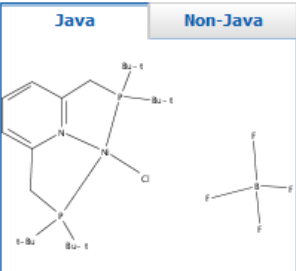
1. 精确结构检索检索到结构本身，聚合物，配合物，盐等



# 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

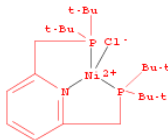
**ChemDraw**

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

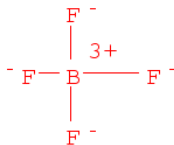
1. 1136166-99-8

~1

1136166-98-7  
C<sub>23</sub> H<sub>43</sub> Cl N Ni P<sub>2</sub>



14874-70-5  
B F<sub>4</sub>



**C<sub>23</sub> H<sub>43</sub> Cl N Ni P<sub>2</sub> · B F<sub>4</sub>**  
Nickel(1+), [2,6-bis[[bis(1,1-dimethylethyl)phosphino-κP]methyl]pyridine-κN]chloro-, (SP-4-3)-, tetrafluoroborate(1-)  
(1:1)

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

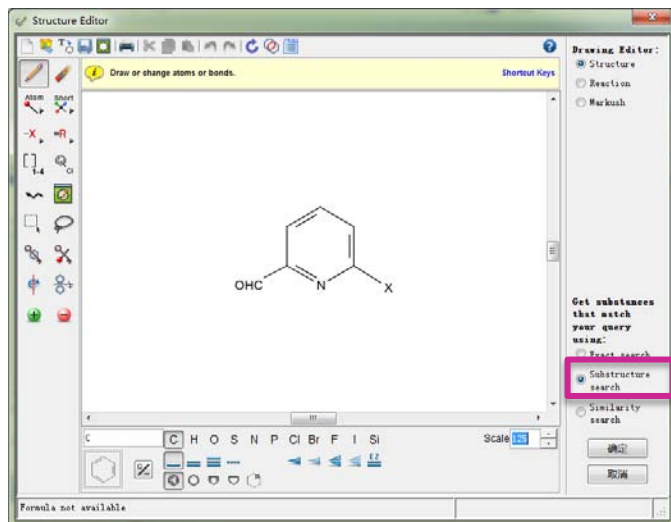
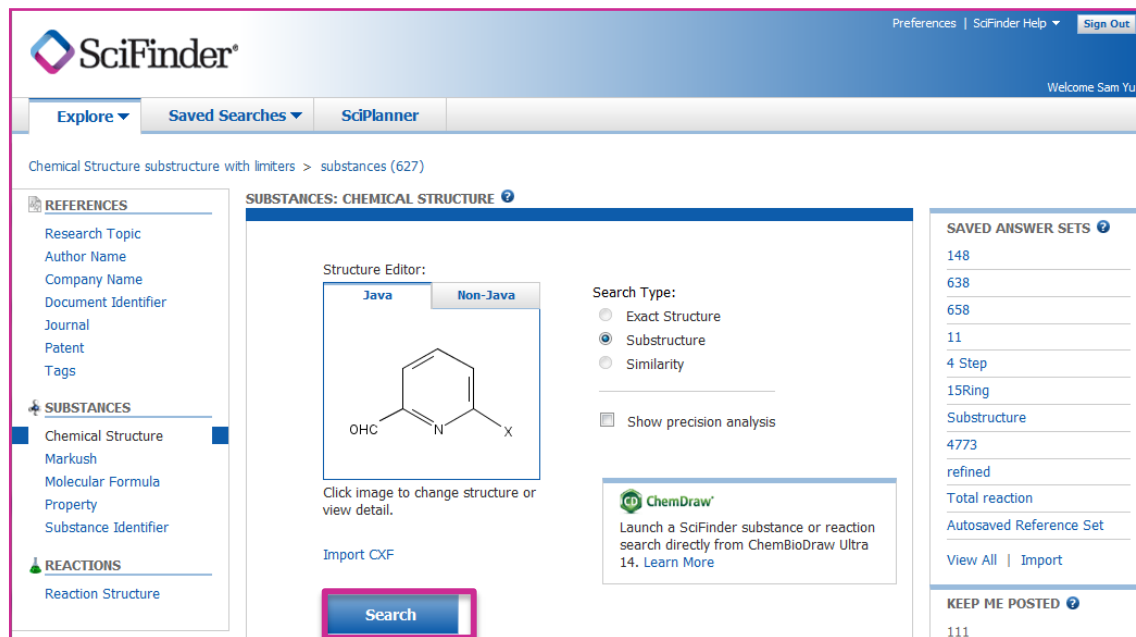
☐ Reactant or reagent

## 检索Tips:

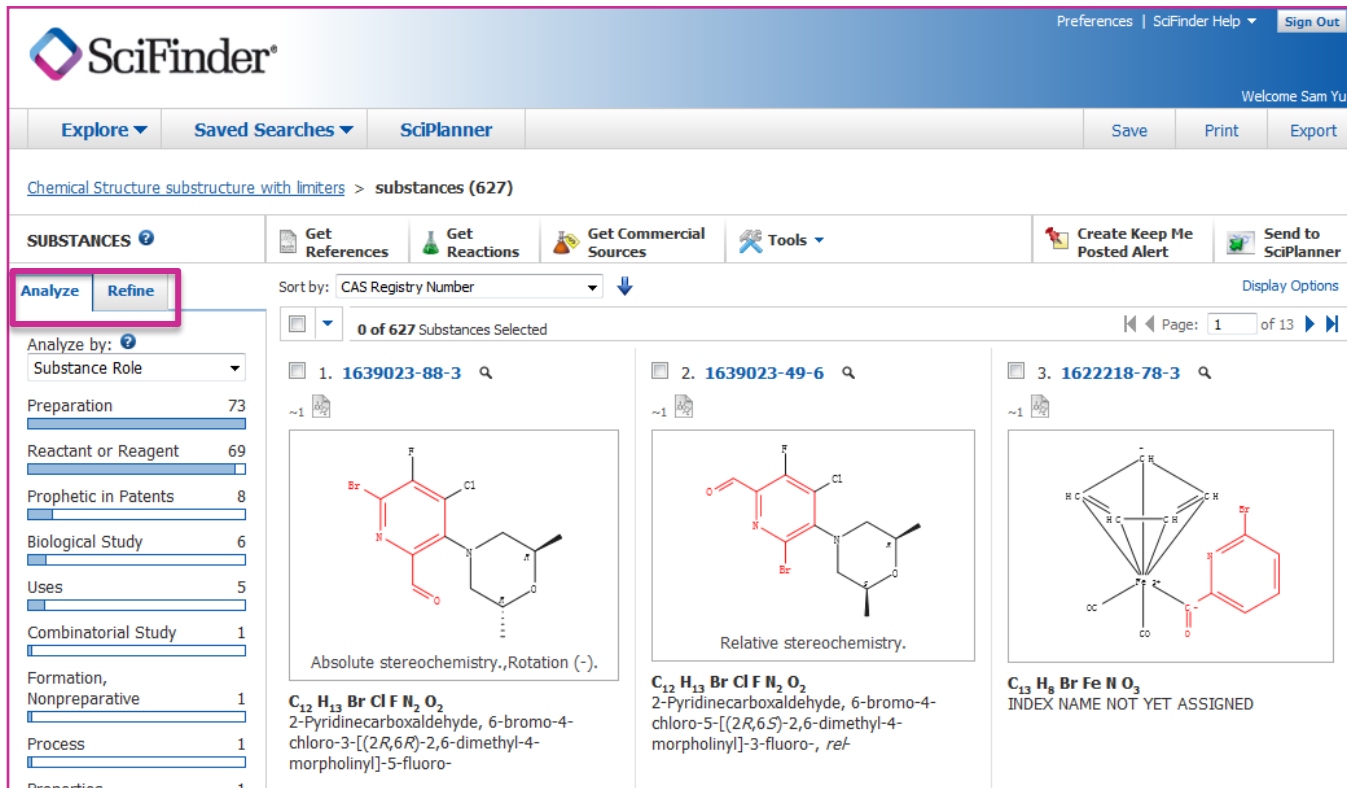
1. 可以通过Advanced Search提前做出一些设置
2. 对于配位化合物，聚合物，有特定的种类选项，建议勾选
3. Single Component，帮助将多组分物质去除

# 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中的检索结果



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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

Property 1

Sort by: CAS Registry Number

0 of 627 Substances Selected

Page: 1 of 13

1. 1639023-88-3

Absolute stereochemistry., Rotation (-).

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

2. 1639023-49-6

Relative stereochemistry.

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

3. 1622218-78-3

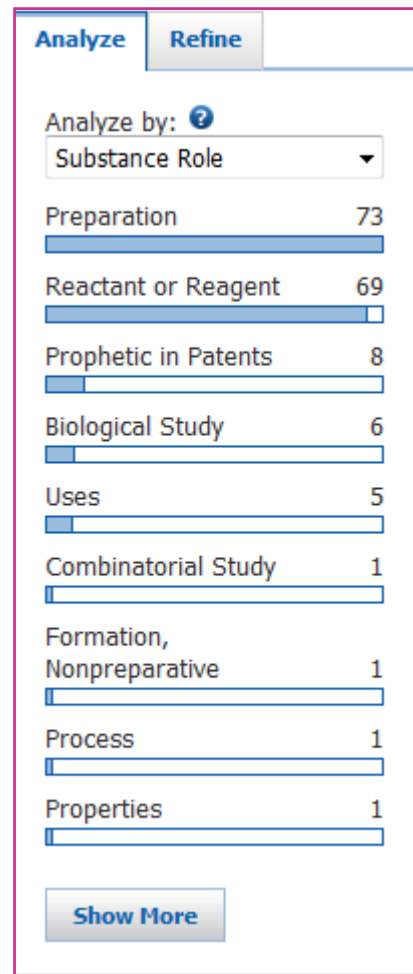
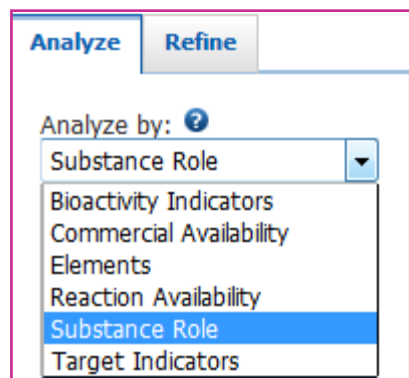
INDEX NAME NOT YET ASSIGNED

C13H9BrFeN3O3

## 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基不同，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



## 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

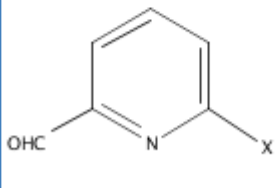
Refine by: ?

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

Structure Editor:

Java

Non-Java



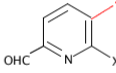
Click image to change structure or view detail.

Search type: **Substructure**

Refine by Atom Attachment ?

1. Click an atom to display the attachments present at that site.      2. Select attachment(s) of interest.

Substructure



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"/> Cl	6
<input type="checkbox"/> I	4
<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"/> Alk - Alkyl chain	58
<input type="checkbox"/> Cb - Carbocycle	50
<input type="checkbox"/> X - Halogen	23
<input type="checkbox"/> Hy - Heterocycle	10

? =

Refine

Cancel

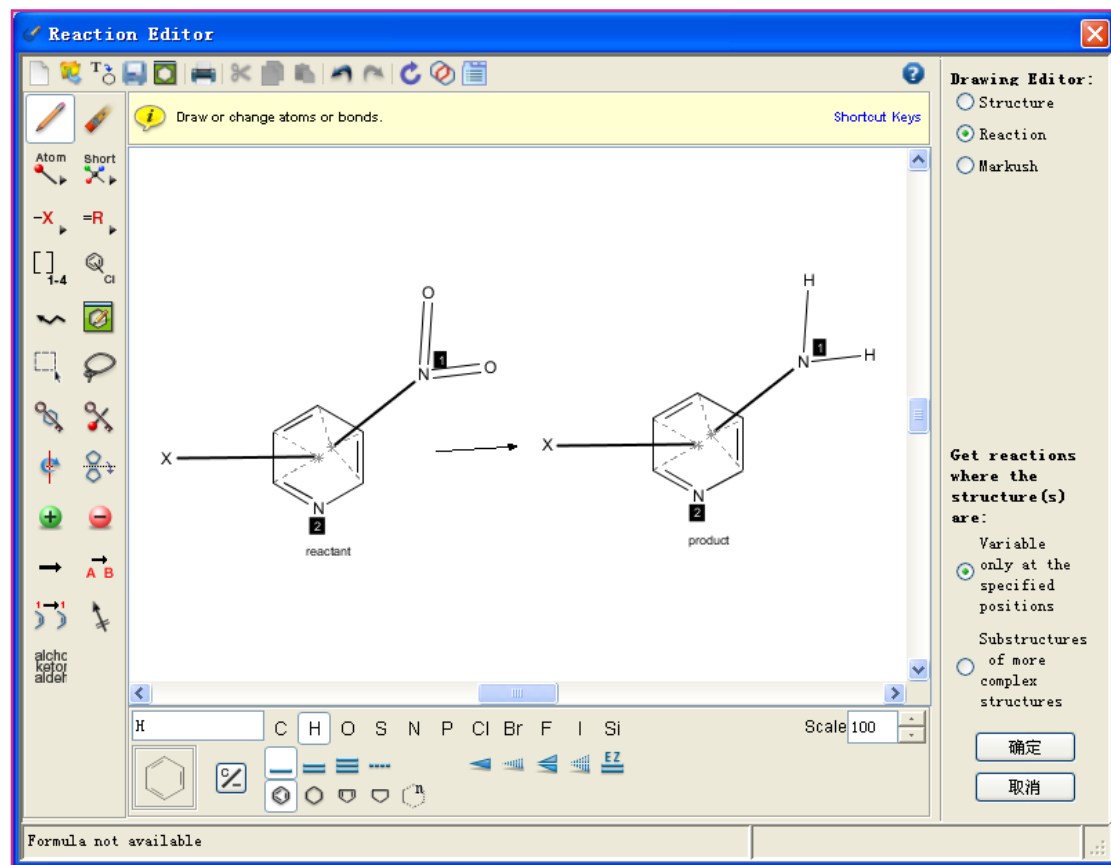
## 检索Tips:

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**





检索要求:

1: 吡啶环2, 3, 4位上存在一个硝基还原成氨基

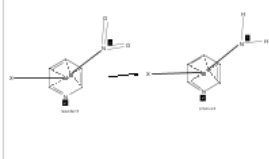
2: 吡啶环5, 6位上存在一个卤素

# SciFinder Web中的检索

REACTIONS: REACTION STRUCTURE

Structure Editor:

**Java** **Non-Java**



Click image to change structure or view detail.

Import CXF

**Search**

[Advanced Search](#)

Search Type:


☒ Allow variability only as specified

☐ Substructure

## 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



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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](#)

☐ 0 of 56 Reactions Selected

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

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




96%


[Overview](#)

Analyze by: [Reagent \(New\)](#)

H <sub>2</sub>	26
Fe	9
KF	6
Mg	5
NH <sub>3</sub>	5
TiCl <sub>4</sub>	5
HCl	4

# Group By Document


**Get References**


**Tools** ▼

Group by: Document ▼

☐ ▼

No Grouping  
**Document**  
 Transformation

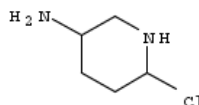
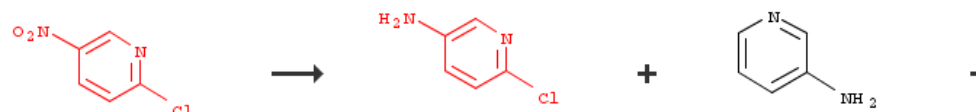
☐ 1. **View Reaction Detail**

## 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](#)

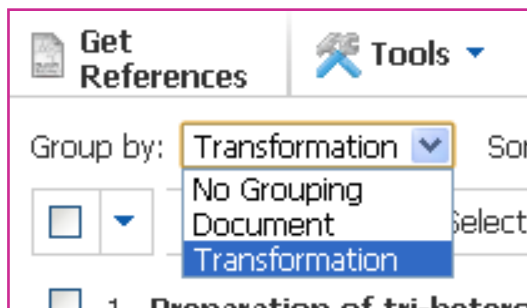
**Single Step** *Hover over any structure for more options.*



- 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

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

☐ 2. Dehalogenation of Aromatic Compounds  
2 Reactions

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

☐ 3. Reduction of Alkyl Halides/ Dehalogenation  
2 Reactions

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

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

# Similary Reaction

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](#)

## 检索Tips:

- 只有单步反应后才有相似反应的链接
- 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
- 相似级别的设定：
  - Broad:** 仅反应中心相同
  - Medium:** 反应中心和附属原子相同
  - Narrow:** 反应中心及扩展原子和键相同

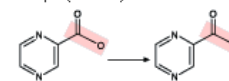
## Get Similar Reactions

Retrieve similar reactions from:

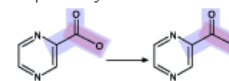
- ☒ All reactions
- ☐ Current answer set

Include this level of similarity:

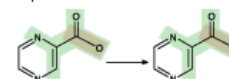
- ☐ Broad - Reaction centers only (96991)



- ☐ 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.*

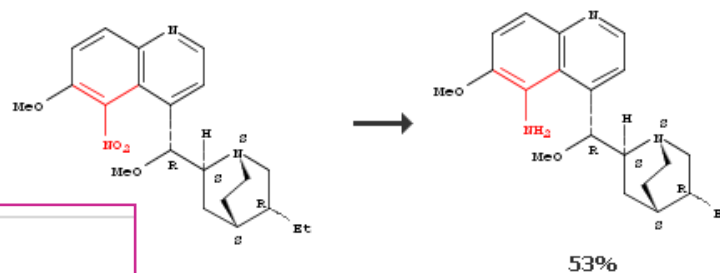


[Overview](#)

0 of 88722 Reactions Selected

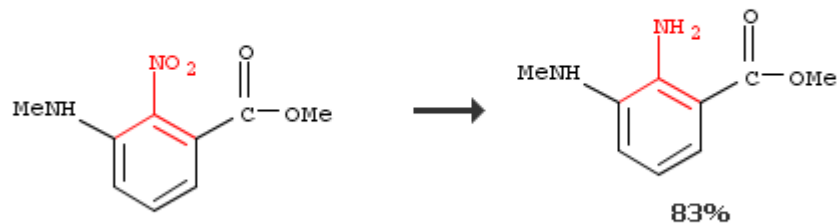
1. [View Reaction Detail](#) [Link](#) [Similar Reactions](#)

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



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

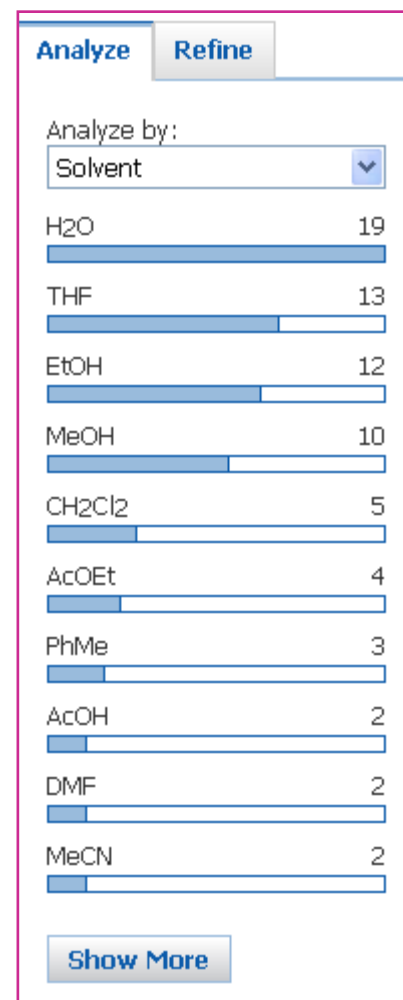
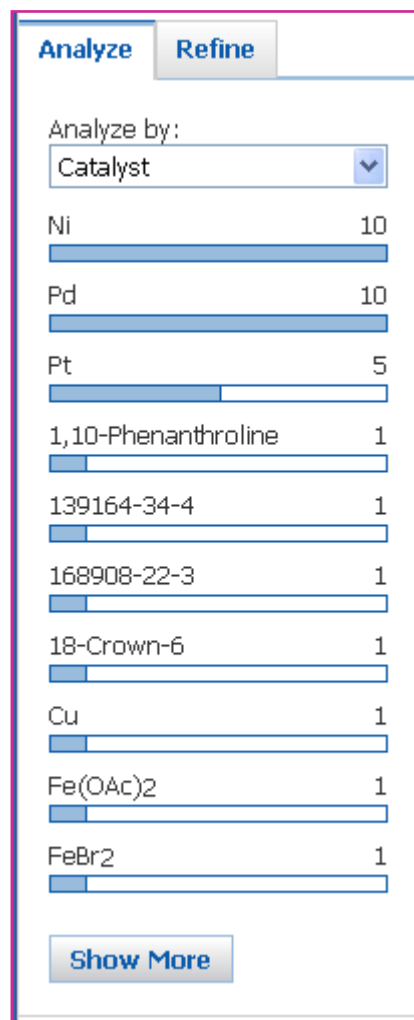
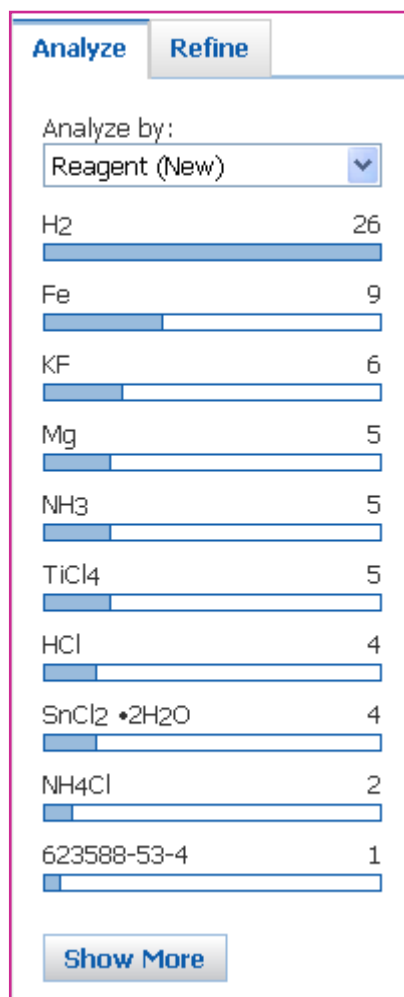
Single Step *Hover over any structure for more options.*



[Overview](#)

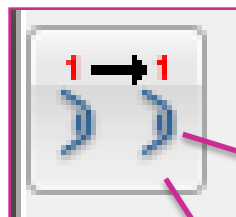
这些都和原有的反应，在反应中心，及扩展的原子和键上是一致的

# SciFinder Web中的反应后处理

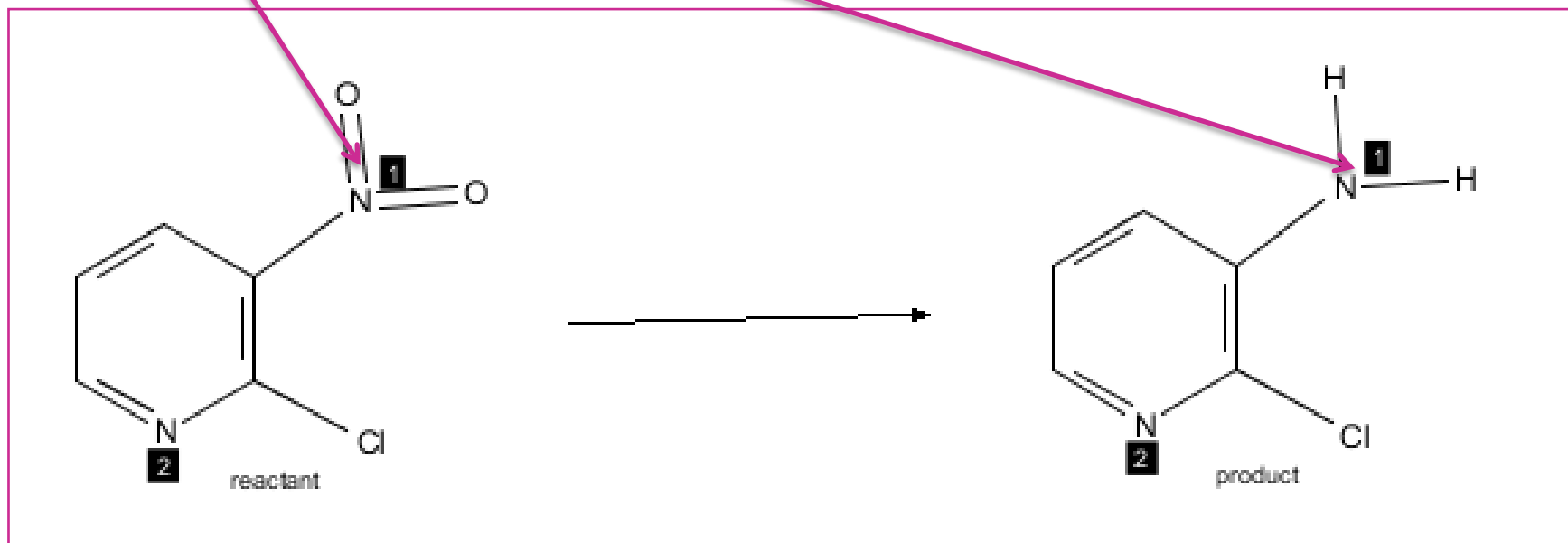




# 反应精准性定义工具—原子标记工具



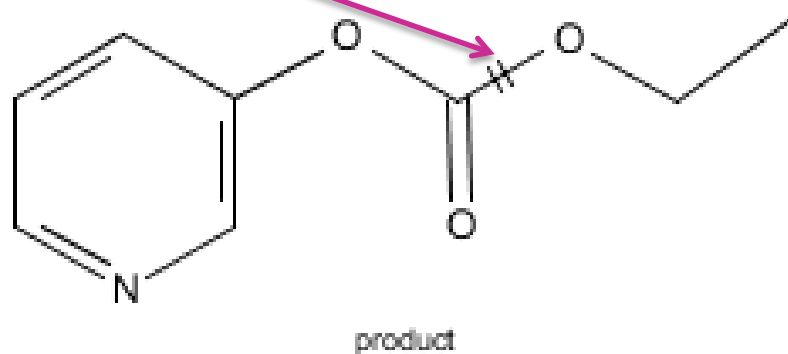
原子标记工具标记反应前后必须匹配的原子，主要用于反应中心的定义



# 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



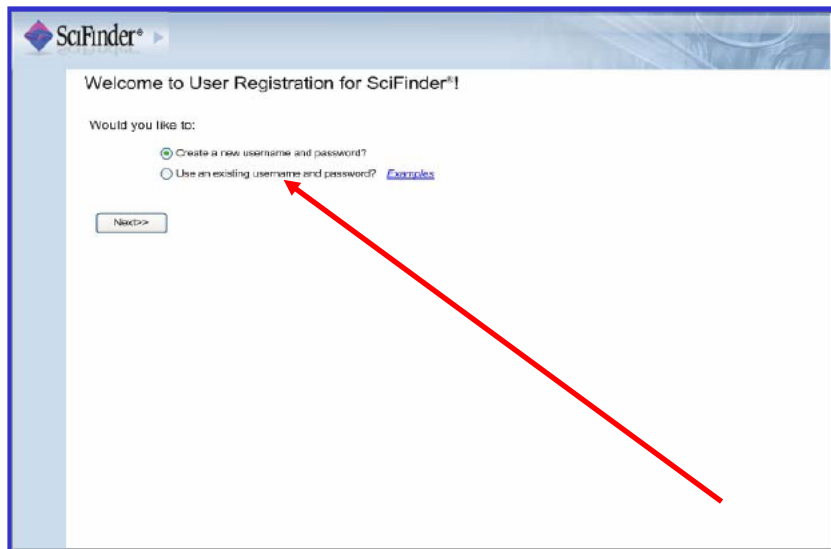
# 提纲

- 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



Welcome to User Registration for SciFinder®!

Would you like to:

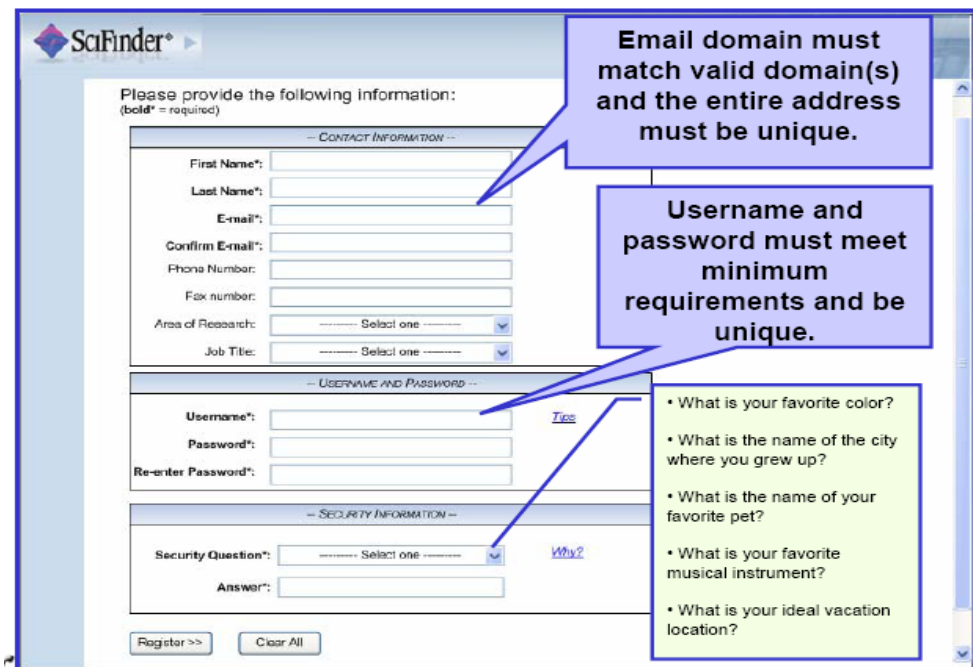
☒ Create a new username and password?

☐ Use an existing username and password? [Examples](#)

[Next >>](#)

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:  Select one

Job Title:  Select one

**USERNAME AND PASSWORD**

Username\*:

Password\*:

Re-enter Password\*:

**SECURITY INFORMATION**

Security Question\*:  Select one

Answer:

[Why?](#)

[Register >>](#) [Clear All](#)

**Email domain must match valid domain(s) and the entire address must be unique.**

**Username and password must meet minimum requirements and be unique.**

- 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?

# 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：

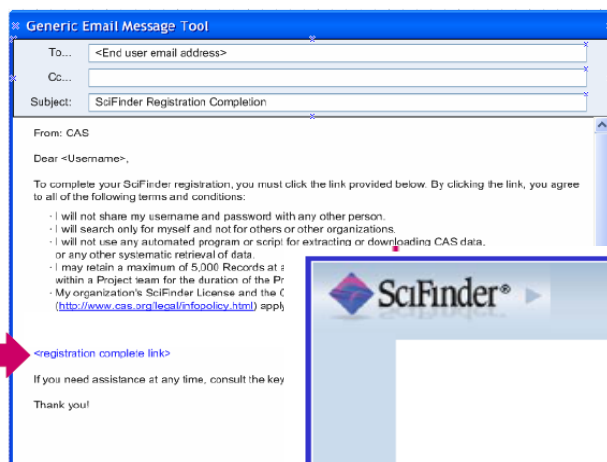
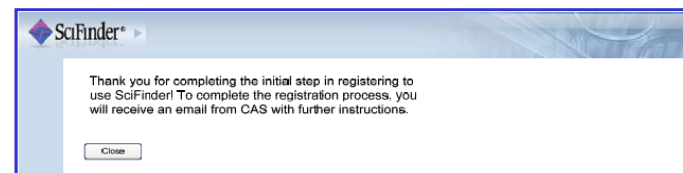
- 字母
- 混合的大小写字母
- 数字
- 非字母数字的字符（例如 @、#、%、&、\*）

## 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



# SciFinder Web 常见问题


**SciFinder®**  
 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

### Welcome to SciFinder

#### The New SciFinder is Here!

What do you think of our new look? See [What's New in SciFinder](#) to learn about our sleek new design and capabilities, and start exploring today!

#### Collaboration Helps Integrate SciFinder to Streamline Research Workflows

See how our collaboration with several customers, including Vertex Pharmaceuticals, helped them better integrate SciFinder to streamline research workflows.

#### Expanded Coverage of Chemical Reaction Information in SciFinder

Learn how our [collaboration with Thieme Publishing Group](#) will add hundreds of thousands of new experimental procedures to SciFinder for chemical reactions reported in SYNLETT and SYNTHESIS.

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

Thousands of new experimental procedures are being added to SciFinder for chemical reactions.

账号或密码错误，请在username处填写，截图，并与图书馆联系



# 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>



Your IP address comes across to CAS as: 210.32.9.45

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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