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# 通过SciFinder高效获取合成制备信息

# 提纲

- SciFinder中获取化合物制备信息的方法
- 反应相关信息获取方法
  - 结构编辑器的使用（绘图、限定反应的工具）
  - 如何通过反应式检索反应，精炼结果并获得实验详情
  - 利用SciPlanner实现反应路线设计
  - 反应检索案例分享
- 通过文献主题检索合成制备相关信息的方法

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# 在SciFinder中，检索化合物制备信息主要有4种方式：

方法1：在文献检索Research Topic中输入preparation of 50-78-2或者synthesis of aspirin进行检索

The screenshot displays the SciFinder REFERENCES page. At the top, there are navigation buttons: 'Get Substances', 'Get Reactions', 'Get Related Citations', and 'Tools'. On the right, there are 'Create Keep Me Posted Alert' and 'Send to SciPlan' buttons. Below the navigation bar, there are tabs for 'Analyze', 'Refine', and 'Categorize'. The 'Analyze' tab is active, showing an 'Analyze by:' dropdown menu set to 'Author Name'. A list of authors and their corresponding number of references is shown on the left side of the 'Analyze' panel.

Author Name	Count
Patrono C	4
Valles Juana	4
Dineen Annie E	3
Fahey Jodie T	3
Moscardo Antonio	3
Nizankowska E	3
Pulliam Curtis R	3
Wennmalm A	3

The main content area shows search results sorted by 'Accession Number'. It indicates '0 of 227 References Selected'. Two results are visible:

- 1. A kind of method for catalyzed synthesis of aspirin by using choline eutectic solvent [Machine Translation].**  
Quick View PATENTPAK  
By Wang, Yinglei; Li, Wenhuan; Liu, Xueguo; Du, Chaojun; Li, Jin  
From Faming Zhuanli Shenqing (2017), CN 106928055 A 20170707. | Language: Chinese, Database: CAPLUS  
[Machine Translation of Descriptors]. The present invention belongs to environment-friendly org. **synthesis** chem. tech. field, particularly relates to a kind of method for catalyzed **synthesis of aspirin** by using choline eutectic solvent. The method comprises: adding choline eutectic solvent, salicylic acid, acetic anhydride into reaction vessel, after heating reaction 15 ~ 40min at 70 ~ 80 DEG C; purifying the crude products obtained by reaction, obtaining the **aspirin**. The method catalyzed **synthesis of aspirin** by using choline eutectic solvent of the present invention has simple operation, gent...
- 2. Synthesis of novel aspirin analogs for medicinal testing**  
Quick View Other Sources  
By Albasrawi, Hadeel K.; Timmons, Shannon C.  
From Abstracts, 48th Central Regional Meeting of the American Chemical Society, Dearborn, MI, United States, June 6-9 (2017), CERM-66. | Language: English, Database: CAPLUS  
**Aspirin** is a common nonsteroidal anti-inflammatory drug used to treat pain, fever, and inflammation. It is one of the most widely used medications in the world with an estd. 40,000 tons produced and consumed annually. Recent research has shown that this inexpensive age-old drug holds promise as an anticancer agent. Studies have shown that **aspirin** has a remarkable ability to inhibit the proliferation of colorectal cancer cells in vitro, for example. Although the mechanism of action has not yet been established, it is clear that the **synthesis of aspirin** analogs to further probe this finding ...

## 方法2：检索物质后，在物质信息详情页面，可以由此物质获得制备 (preparation) 相关文献或者产物为此物质的反应。

The screenshot displays the SciFinder interface for a substance. On the left, the 'SUBSTANCE DETAIL' page shows the following information:

- CAS Registry Number:** 50-36-2
- Chemical Formula:**  $C_{17}H_{21}NO_4$
- Structure:** 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(benzoyloxy)-8-methyl ester, (1*R*,2*R*,3*S*,5*S*)-
- Molecular Weight:** 303.35
- Melting Point (Experimental):** Value: 98 °C
- Boiling Point (Experimental):** Value: 187 °C | Condition: Press: 0.1 Torr
- Density (Predicted):** Value: 1.22±0.1 g/cm<sup>3</sup> | Condition: Temp: 20 °C Press: 760 Torr
- pKa (Predicted):** Value: 8.97±0.60 | Condition: Most Basic Temp: 25 °C

On the right, the 'Get References' dialog box is open, with the following settings:





- Limit results to:**
  - Preparation
  - Process
  - Properties
- For each sequence, retrieve:**
  - Additional related references, e.g., a

Below this, the 'Get Reactions' dialog box is open, with the following settings:

- Retrieve reactions for:**
  - All substances
  - Selected substances
- Limit results by reaction role:**
  - Product
  - Reactant
  - Reagent
  - Reactant or reagent
  - Catalyst
  - Solvent
  - Any role




The background interface shows a search result for '50-78-2' with a chemical structure of Benzoic acid, 2-(acetyloxy)- ( $C_9H_8O_4$ ).

## 方法3：也可以点击物质结构右上角的蓝色双箭头，点击Synthesis this，获得相关反应

**SUBSTANCE DETAIL**   **Get References**  **Get Reactions**  **Get Commercial Sources**

[Return](#)

**CAS Registry Number** 50-78-2

~39,113   ~106 

**C<sub>9</sub> H<sub>8</sub> O<sub>4</sub>**  
Benzoic acid, 2-(acetyloxy)-

**Molecular Weight**  
180.16

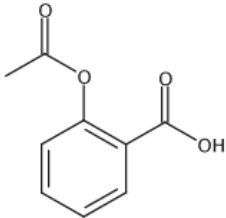
**Melting Point (Experimental)**  
Value: 135 °C

**Boiling Point (Experimental)**  
Value: 197-200 °C | Condition: Press: 7 Torr

**Density (Experimental)**  
Value: 1.40 g/cm<sup>3</sup>

**pKa (Predicted)**  
Value: 3.48±0.10 | Condition: Most Acidic Temp: 25 °C

**Other Names**  
Rhodine (7CI)  
Salicylic acid acetate (8CI)  
2-(Acetyloxy)benzoic acid  
2-Acetoxybenzoic acid



**CAS Registry Number:** 50-78-2

- [View Substance Detail](#)
- [Explore by Structure](#)
- [Synthesize this...](#)**
- [Get Reactions where Substance is a](#)
- [Get Commercial Sources](#)
- [Get Regulatory Information](#)
- [Get References](#)
- [Export as Image](#)
- [Export as molfile](#)
- [Send to SciPlanner](#)

## 方法4：在SciFinder反应检索编辑器中绘制结构，获得反应。

The screenshot displays the SciFinder Structure Editor interface. The main workspace shows a chemical structure of a benzene ring with an acetate group (-O-C(=O)-CH<sub>3</sub>) at the 1-position and a carboxylate group (-C(=O)-O-) at the 3-position, labeled "product". A reaction arrow points to the left of the structure. The left sidebar contains various drawing tools, with the reaction arrow tool (A → B) highlighted by a red box. The top toolbar includes standard editing functions like copy, paste, and zoom. The right sidebar, titled "Drawing Editor:", has the "Reaction" option selected and highlighted with a red box. Below it, the "Get reactions where the structure(s) are:" section has the "Variable only at the specified positions" option selected and highlighted with a red box. The bottom status bar shows the molecular formula C<sub>9</sub>H<sub>8</sub>O<sub>4</sub> and the CAS number 180.16.

## 小结：获取化合物制备信息的方法

**方法1：** 基于物质名称和主题词获取到合成制备信息；

**方法2：** 基于物质的CAS号检索合成制备信息；

**方法3：** 在CAS REACT中获取到该结构的精确合成信息；

**方法4：** 在CAS REACT中获取到该结构的精确反应信息、该结构的盐、同位素、立体构型等合成信息。



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# 结构编辑器

直接导入已保存的.cxf或者.mol文件

画笔/橡皮

画图工具

选中工具  
锁定工具

旋转/翻转  
阴阳离子

The screenshot shows the Structure Editor interface. At the top, there is an "Add to Editor" dialog box with a text input field for "Enter CAS Registry Number, SMILES, or InChI:" and examples: "50-00-0", "CCCO", and "InChI=1S/C3H8O/c1-2-3-4/h4H,2-3H2,1H3". Below this is the main editor window with a toolbar containing icons for file operations, drawing, and editing. A yellow banner below the toolbar says "Click and drag to select objects. Ctrl-click to select or deselect individual objects." On the left, there are four vertical toolbars: the first contains drawing tools (pencil, eraser), the second contains atom and bond tools (Atom, Short, -X, =R, [ ], 1-4, Cl), the third contains selection and locking tools (select, lasso, lock, unlock), and the fourth contains rotation and charge tools (rotate, flip, +, -). On the right, there is a "Drawing Editor" panel with radio buttons for "Structure" (selected), "Reaction", and "Markush". Below it is a search panel titled "Get substances that match your query using:" with radio buttons for "Exact search", "Substructure search" (selected), and "Similarity search". At the bottom, there is a "Common atoms/bonds/rings" panel with buttons for C, H, O, S, N, P, Cl, Br, F, I, Si, and various bond types. A purple box highlights this panel with the text "常用的原子/键/环".

结构  
反应  
马库什

常用的原子/键/环

# 结构编辑器

元素周期表

可变基团

重复单元

碳链

Structure Editor

Click and drag to select objects. Ctrl-click

Atom Short

-X =R

取代位点不确定

结构模板

环/原子锁定

C H

苯环结构

常用官能团

自定义取代基

取代位点不确定

结构模板

环/原子锁定

Atoms

H																	He				
Li	Be															B	C	N	O	F	Ne
Na	Mg															Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr				
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe				
Cs	Ba		Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn				
Fr	Ra																				
		La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu					
		Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr					

Close

Shortcuts

CH	CH <sub>2</sub>	Me	OMe	Et	OEt	Pr-n	Pr-i	OPr-n
OPr-i	Bu-n	Bu-i	Bu-s	Bu-t	OBU-n	OBU-i		
OBU-s	OBU-t	Ph	OPh	o-C <sub>6</sub> H <sub>4</sub>	m-C <sub>6</sub> H <sub>4</sub>			
p-C <sub>6</sub> H <sub>4</sub>	CF <sub>2</sub>	CF <sub>3</sub>	CCl <sub>2</sub>	CCl <sub>3</sub>	CBR <sub>2</sub>	CBR <sub>3</sub>	CI <sub>2</sub>	
CI <sub>3</sub>	CHO	CN	C(O)CH <sub>3</sub>	CO <sub>2</sub> H	COOH	COSH		
CS <sub>2</sub> H	CSSH	NH	NH <sub>2</sub>	NH <sub>3</sub>	NO <sub>2</sub>	OH	OPO <sub>3</sub> H <sub>2</sub>	
OSO <sub>3</sub> H	PO <sub>3</sub> H <sub>2</sub>	SH	SO <sub>2</sub>	SO <sub>3</sub> H				

Close

Variables

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

Close

R-group Definitions

R1 R2 R3 R4 R5 R6 R7 R8 R9 R10

R1 =

Atoms

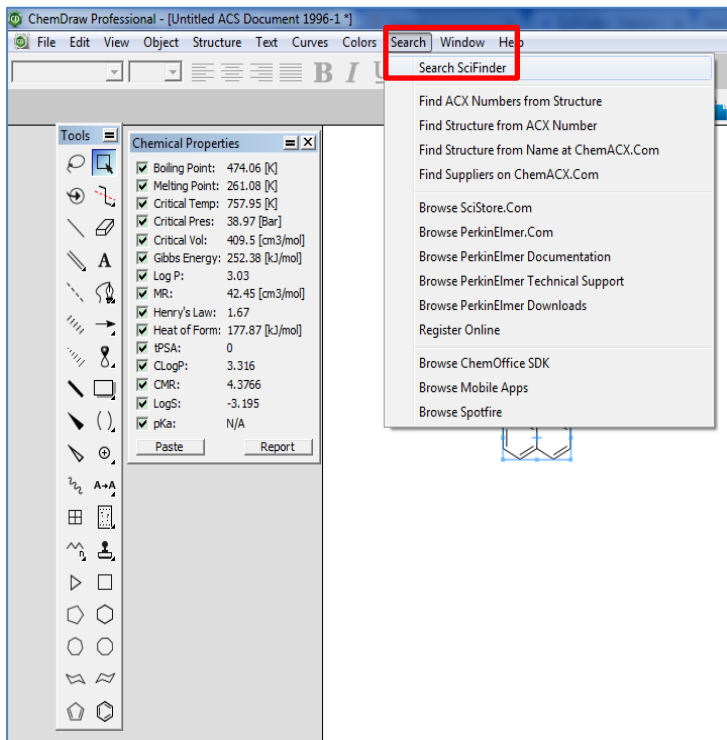
H																	He				
Li	Be															B	C	N	O	F	Ne
Na	Mg															Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr				
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe				
Cs	Ba		Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn				
Fr	Ra																				
		La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu					
		Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr					

Variables

Shortcuts

Close

# Chemdraw 14.0以上正版用户可以直接在chemdraw里边画结构然后在SF中检索



如果想用复制/粘贴功能，请在java条件下运行结构编辑器，并且保证Java及时更新

Chemical Structure exact with limiters > substances (200) > refine "include isotope-con

**REFERENCES**

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

**SUBSTANCES**

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

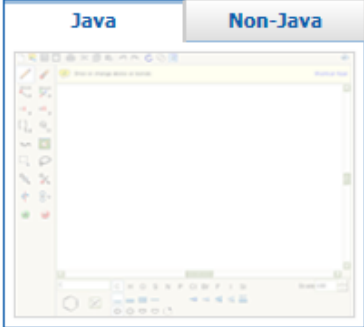
**REACTIONS**

- Reaction Structure

**SUBSTANCES: CHEMICAL STRUCTURE**

Structure Editor:

Java Non-Java



Import CXF

**Search**

# 结构编辑器：绘制反应工具

The screenshot shows the Structure Editor software interface. On the left, a 'Functional Groups' panel lists categories like Alcohols (13), Alkenes (11), Alkynes (4), Amines (11), Carbonate Derivatives (7), Carboxy Derivatives (17), Halides (16), Heterocycles (54), Ketones (6), Organometallics (19), Non-Rings (136), and Rings (71). The main workspace contains a toolbar with various drawing tools, a central canvas with a benzene ring and a CH<sub>4</sub> label, and a 'Drawing Editor' panel on the right with options for Structure, Reaction, and Markush. A yellow banner at the top of the canvas reads 'Draw or change atoms or bonds.' and 'Shortcut Keys'. Four purple callout boxes with white text and arrows point to specific features: '角色定义' (Role Definition) points to the 'C' label; '反应箭头' (Reaction Arrow) points to the arrow icon in the toolbar; '化学键变化' (Chemical Bond Change) points to the 'A B' icon; and '原子标记' (Atom Label) points to the 'alcohol ketone aldehyde' icon.

Functional Groups

Enter 3 or more characters...

- ▶ Alcohols (13)
- ▶ Alkenes (11)
- ▶ Alkynes (4)
- ▶ Amines (11)
- ▶ Carbonate Derivatives (7)
- ▶ Carboxy Derivatives (17)
- ▶ Halides (16)
- ▶ Heterocycles (54)
- ▶ Ketones (6)
- ▶ Organometallics (19)
- ▶ Non-Rings (136)
- ▶ Rings (71)

Close

Structure Editor

Draw or change atoms or bonds. Shortcut Keys

Atom Short

-X =R

1-4 Cl

角色定义

反应箭头

化学键变化

原子标记

官能团列表

Drawing Editor:

- Structure
- Reaction
- Markush

Get reactions where the structure(s) are:

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

OK Cancel

CH<sub>4</sub> 16.04

# 例：反应前后物质中的原子标记

Structure Editor

Click an atom in the reactant and its corresponding atom in the product.

reactant/reagent

product

标记反应原料和产物中相同的原子

Structure Editor

Drawing Editor:

- Structure
- Reaction
- Markush

Get reactions where the structure(s) are:

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

OK

Cancel

$C_4H_6O \cdot C_4H_6OSi$

70.09 . 98.18

# 例：发生变化的化学键标记

The screenshot shows the Structure Editor interface. The main workspace displays a chemical reaction between a reactant and a product. The reactant is a five-membered ring with a double bond and an oxygen atom. The product is a five-membered ring with a double bond, an oxygen atom, and a silicon atom. The silicon atom is bonded to two other atoms, and the bonds to these atoms are marked with a lightning bolt symbol, indicating they are the bonds that change during the reaction. A yellow banner at the top of the workspace says "Click bonds to be formed or broken during the reaction." The left sidebar contains various drawing tools, and the right sidebar contains the Drawing Editor options. The bottom status bar shows the chemical formula  $C_4H_6O \cdot C_4H_6OSi$  and the date 70.09.98.18.

Structure Editor

Click bonds to be formed or broken during the reaction.

reactant/reagent

product

标记发生变化的化学键

Get reactions where the structure(s) are:

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

OK

Cancel

$C_4H_6O \cdot C_4H_6OSi$  70.09.98.18



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  - 如何通过反应式检索反应，精炼结果并获得实验详情
  - 利用SciPlanner实现反应路线设计
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# 精确结构反应检索：绘制反应式

The screenshot shows the 'Structure Editor' window. The main canvas displays a chemical reaction: a benzothiazole ring (labeled 'reactant') reacts to form a benzothiazole ring with a methyl carbonyl group attached (labeled 'product'). The 'Drawing Editor' panel on the right has the 'Reaction' radio button selected, highlighted with a purple box. Below it, the 'Get reactions where the structure(s) are:' section has the 'Variable only at the specified positions' radio button selected, also highlighted with a purple box. A callout bubble points to this option with the text '执行的是锁环锁原子的检索'. The 'OK' and 'Cancel' buttons are at the bottom of the panel.

反应

执行的是锁环  
锁原子的检索

# 精确结构反应检索：查看反应结果集

Explore ▾ Saved Searches ▾ SciPlanner Save Print Export

Reaction Structure structure variable only at spe... > reactions (8)

## 分组, 排序

REACTIONS ⓘ

Get References Tools

Send to SciPlanner

Analyze Refine

Group by: No Grouping Sort by: Number of Steps ↑

0 of 8 Reactions Selected

1. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.

~85 ~102 58% ~79

▼ Overview

Steps/Stages

Notes

1.1 R:BuLi, S:THF, S:Me(CH<sub>2</sub>)<sub>2</sub>, -78°C; 1 h, -78°C

ice-bath removed after stirring at -78°C for 1 hour (stage 2), Reactants: 2, Reagents: 2, Solvents: 2, Steps: 1, Stages: 2. Most stages is any one step.

# 精确结构反应检索：查看反应结果集

点击Document，合并来自同一篇文献的反应；  
点击Transformation，获得反应类型的分类。

Reaction Structure structure variable only at spe... > reactions (8)

**REACTIONS** Get References Tools

Analyze Refine

Analyze by: Reagent

BuLi	4
t-BuOOH	3
HCl	2
19468-88-3	1
H <sub>2</sub> O	1
H <sub>2</sub> SO <sub>4</sub>	1

Show More

Group by: No Grouping Document Transformation 0 of 8 Reactions Selected

Sort by: Relevance

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

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

**Overview**

**Steps/Stages**

1.1 R: t-BuOOH, S: Me(CH<sub>2</sub>)<sub>2</sub>Me, 24 h, 80°C  
1.2 R: H<sub>2</sub>O

**Notes**

optimized on amount of TBHP, amount of phosphate, temperature and solvent, using hydrogen peroxide in MeCN resulted in lower yield, optimization study, Reactants: 2, Reagents: 2, Solvents: 1, Steps: 1, Stages: 2, Most stages in any one step: 2

**References**

[Peroxides as "Switches" of Dialkyl H-Phosphonate: Two Mild and Metal-Free Methods for](#)

**Get References** Tools

Group by: Transformation Sort by: Frequency

0 of 8 Reactions Selected

1. [Decarboxylative Alkylation, Acylation and Carboxylation of Nitrogen Heterocycle](#)  
5 Reactions

R<sup>4</sup> = R, COR<sup>1</sup>, OCOR<sup>3</sup>

2. [Uncategorized Single-Step Reactions](#)  
2 Reactions

3. [Multi-Step Reactions](#)  
1 Reaction

# 精确结构反应检索：查看反应结果集

Explore ▾ Saved Searches ▾ SciPlanner Save Print Export

Reaction Structure structure variable only at spe... > reactions (8)

REACTIONS ⓘ

Get References Tools

Sort by: **Number of Steps**

0 of 8 Reactions Selected

1. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.

Analyze by: Reagent

BuLi	4
t-BuOOH	3
HCl	2
19468-88-3	1
H <sub>2</sub> O	1
H <sub>2</sub> SO <sub>4</sub>	1

Show More

~85

~102

58% ~79

Overview

Steps/Stages

Notes

1.1 R:BuLi, S:THF, S:Me(CH<sub>2</sub>)<sub>2</sub>Me, -78°C; 1 h, -78°C

ice-bath removed after stirring at -78°C for 1 hour (stage 2), Reactants: 2, Reagents: 2,

排序：相关度，入库号，实验步骤，MethodsNow，步数，产率，发表年份

# 精确结构反应检索：查看反应结果集

Reaction Structure structure variable only at spe... > reactions (8)

REACTIONS Get References Tools Send to SciPlanner

Analyze Refine

Analyze by: Reagent

BuLi 4  
t-BuOOH 3  
HCl 2  
19468-88-3 1  
H<sub>2</sub>O 1  
H<sub>2</sub>SO<sub>4</sub> 1

Show More

Group by: No Grouping Document Transformation Selected Sort by: Relevance

1. View Reaction Detail Link Similar Reactions

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

对于一步反应，可以点击 similar Reaction, 获取相似反应

~101 ~93 90% ~83

**Overview**

**Steps/Stages**

1.1 R: t-BuOOH, S: Me(CH<sub>2</sub>)<sub>3</sub>Me, 24 h, 80°C  
1.2 R: H<sub>2</sub>O

**Notes**

optimized on amount of TBHP, amount of phosphate, temperature and solvent, using hydrogen peroxide in MeCN resulted in lower yield, optimization study, Reactants: 2, Reagents: 2, Solvents: 1, Steps: 1, Stages: 2, Most stages in any one step: 2

**References**

[Peroxides as "Switches" of Dialkyl H-Phosphonate: Two Mild and Metal-Free Methods for](#)

# 精确结构反应检索：获取相似反应

### Get Similar Reactions ?

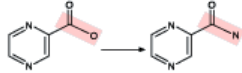
**Retrieve similar reactions from:**

All reactions

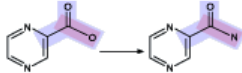
Current answer set

**Include this level of similarity:**

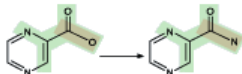
Broad - Reaction centers only



Medium - Reaction centers plus adjacent atoms and bonds



Narrow - Reaction centers plus extended atoms and bonds



相似度限制：

Broad：仅反应中心相似

Medium：反应中心及附属原子和键

Narrow：反应中心及扩展的原子和键

# 精确结构反应检索：查看感兴趣的反应信息

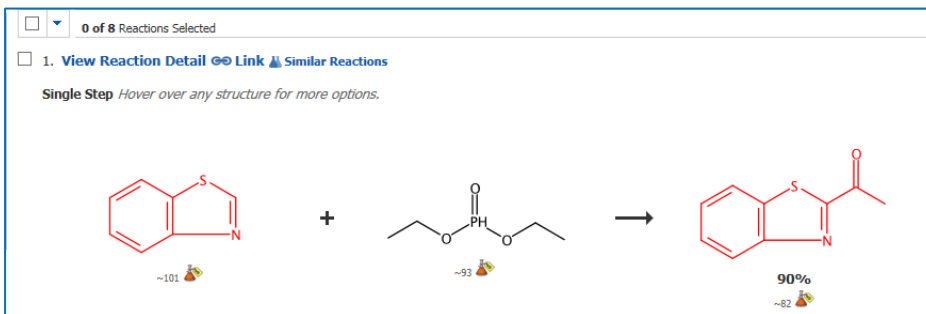
**REACTIONS** ?

Analyze Refine

Analyze by: ?

- Reagent
- Author Name
- Catalyst
- Company-Organization
- Document Type
- Experimental Procedure**
- Journal Name
- Language
- MethodsNow
- Number of Steps
- Product Yield
- Publication Year
- Reagent
- Solvent

## 实验步骤



### Overview

#### Steps/Stages

- 1.1 R: t-BuOOH, S: Me(CH<sub>2</sub>)<sub>2</sub>Me, 24 h, 80°C
- 1.2 R: H<sub>2</sub>O

#### Notes

optimized on amount of TBHP, amount of phosphate, temperature and solvent, using hydrogen peroxide in MeCN resulted in lower yield, optimization study, Reactants: 2, Reagents: 2, Solvents: 1, Steps: 1, Stages: 2, Most stages in any one step: 2

#### References

Peroxides as "Switches" of Dialkyl H-Phosphonate: Two Mild and Metal-Free Methods for Preparation of 2-Acylbenzothiazoles and Dialkyl Benzothiazol-2-ylphosphonates

[Quick View](#) [If Other Sources](#)

By Chen, Xiao-Lan et al  
From Journal of Organic Chemistry, 79(17), 8407-8416; 2014

### Experimental Procedure

JOC  
The Journal of Organic Chemistry

**Experimental Procedures for the Synthesis of 2-Acylbenzothiazoles (3a-3ab).** A mixture of benzothiazole (135.0 mg, 1.0 mmol), phosphonate (5.0 mmol), and TBHP (10.0 mmol) in CH<sub>2</sub>CN (2.0 mL) was stirred at 80 °C for 24 h. The reaction mixture was quenched with water (5.0 mL) and extracted with ethyl acetate (3 x 5.0 mL). The combined organic layers were washed with brine (15.0 mL) and dried over anhydrous MgSO<sub>4</sub>. After filtration, the solvent was evaporated in vacuo. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 20/1) to give the desired product. *1-(Benzo[d]thiazol-2-yl)ethanone (3a)*: yield 90%. mp 107-110 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 2.83 (s, 3H), 7.53 (td, *J* = 7.6, 1.3 Hz, 1H), 7.58 (td, *J* = 8.0, 1.3 Hz, 1H), 7.98 (d, *J* = 8.0 Hz, 1H), 8.18 (d, *J* = 7.8 Hz, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 26.2, 122.5, 125.5, 127.0, 127.7, 137.5, 153.6, 166.5, 193.2; HRMS (ESI) calcd for C<sub>8</sub>H<sub>7</sub>NOS [M + H]<sup>+</sup>, 178.0321, found 178.0320.



## MethodsNow Synthesis——人工标引的反应信息，节省您宝贵的时间

- 详细、明确的物质信息
- 全面、有条理的实验过程信息
- 更好的阅读体验——表格形式
- 无需查看原文直接获取实验详情——反应物，反应条件，步骤，产物性质，谱图等

# MethodsNow Synthesis: 通过Analyze, 选择有MethodsNow标引的反应, 点击MethodsNow查看实验详情

**REACTIONS** ?

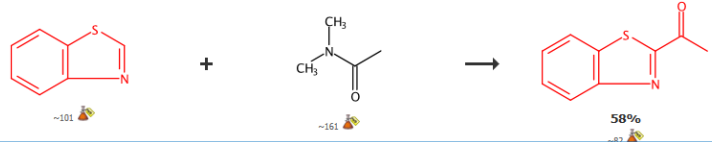
Analyze Refine

Analyze by: ?

- Reagent
- Author Name
- Catalyst
- Company-Organization
- Document Type
- Experimental Procedure
- Journal Name
- Language
- MethodsNow**
- Number of Steps
- Product Yield
- Publication Year
- Reagent
- Solvent

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

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



**Overview**

**Steps/Stages**

- 1.1 R:BuLi, S:THF, S:Me(CH<sub>2</sub>)<sub>2</sub>Me, -78°C; 1 h, -78°C
- 1.2 1 h, -78°C; 10 min
- 1.3 R:HCl, S:H<sub>2</sub>O, rt, acidify

**Notes**

ice-bath removed after stirring at -78°C for 1 hour (stage 2), Reactants: 2, Reagents: 2, Solvents: 3, Steps: 1, Stages: 3, Most stages in any one step: 3

**References**

Rhodium Catalyzed Asymmetric Hydrogenation of 2-Pyridine Ketones  
[Quick View](#) [Other Sources](#)  
By Yang, Hailong et al  
From Organic Letters, 17(17), 4144-4147; 2015

**METHODSNOW™**

**Procedure**

1. Cool the solution (0.5 M) of benzothiazole in dry THF under nitrogen to -78 °C.
2. Add dropwise nBuLi (1.1 equiv, 5.5 mmol, 2.3M in hexane).

[View more...](#)

**Available Experimental Data**

<sup>1</sup>H NMR, <sup>13</sup>C NMR, State

[View with MethodsNow](#)

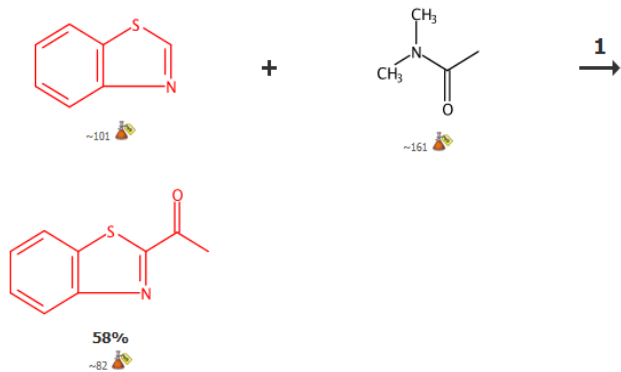
点击查看MethodsNow窗口

# MethodsNow Synthesis: 实验详情展示窗口

## MethodsNow

### Rhodium Catalyzed Asymmetric Hydrogenation of 2-Pyridine Ketones

By Yang, Hailong; Huo, Ningning; Yang, Ping; Pei, Hao; Lv, Hui; Zhang, Xumu  
From Organic Letters, 17(17), 4144-4147; 2015  
Published by American Chemical Society



产物, 反应物, 试剂, 溶剂, 步骤,  
反应类型, 规模, 核磁氢谱, 核磁碳谱,  
产物状态, CAS方法号

Products	Ethanone, 1-(2-benzothiazolyl)-, 58%, CAS RN: 1629-78-3
Reactants	Benzothiazole, CAS RN: 95-16-9 Dimethylacetamide, CAS RN: 127-19-5
Reagents	Butyllithium, CAS RN: 109-72-8 Hydrochloric acid, CAS RN: 7647-01-0
Solvents	Tetrahydrofuran, CAS RN: 109-99-9 Hexane, CAS RN: 110-54-3 Water, CAS RN: 7732-18-5
Procedure	<ol style="list-style-type: none"> <li>Cool the solution (0.5 M) of benzothiazole in dry THF under nitrogen to -78 °C.</li> <li>Add dropwise nBuLi (1.1 equiv, 5.5 mmol, 2.3M in hexane).</li> <li>Keep the resulted mixture for 1 h under -78 °C.</li> <li>Add N,N-dimethylacetamide (1 equiv, 5 mmol) to the stirred solution at -78 °C.</li> <li>Stir the mixture was continuously for 1 h.</li> <li>Remove the cold bath and stir the mixture for additional 10 min.</li> <li>Hydrolyze with concd hydrochloric acid (1 mL).</li> <li>Stir the acidic solution continuously until the temperature reach to room temperature.</li> <li>Pour the mixture into same amount of water.</li> <li>Extract the aqueous mixture with ethyl acetate 3 times.</li> <li>Dry the combined organic solution with Na<sub>2</sub>SO<sub>4</sub>.</li> <li>Purify by flash column chromatography to afford product.</li> </ol>
Transformation	Decarboxylative Alkylation, Acylation and Carbalkoxylation of Nitrogen Heterocycle
<sup>1</sup> H NMR	(400 MHz, CDCl <sub>3</sub> )δ8.22 (d, J = 8.0Hz, 1H), 8.01 (d, J = 7.6Hz, H), 7.55-7.63 (m, 2H), 2.87 (s, 3H);
<sup>13</sup> C NMR	(101MHz, CDCl <sub>3</sub> )δ193.2, 166.5, 153.6, 137.4, 127.7, 127.0, 125.5, 122.5, 26.2.
State	white solid
CAS Method Number	3-219-CAS-1662290

点击CAS RN,  
即时查看物质

PDF or XLS格式

Print/Export

Close



SCIFINDER®  
A CAS SOLUTION

# 亚结构反应检索: 绘制反应式

Structure Editor

Draw or change atoms or bonds. Shortcut Keys

Atom Short

-X -R

reactant

product

R1 = N, S

Drawing Editor:

- Structure
- Reaction
- Markush

Get reactions where the structure(s) are:

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

OK

Cancel

输入的反应物和产物结构可以被修饰，但母体结构不变

# 亚结构反应检索：获得反应结果集

REACTIONS ⓘ

Get References | Tools ▾

Send to SciPlanner

Analyze Refine

Group by: No Grouping ▾ Sort by: Relevance ▾ ↓

0 of 1208 Reactions Selected

1. View Reaction Detail 🔗 Link

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

~83

~85

▼ Overview

**Steps/Stages**

1.1 R:H<sub>2</sub>NCHO  
2.1 R:HCl, R:Sn, S:H<sub>2</sub>O, S:EtOH

**Notes**

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

**References**

Studies on the chemistry of isoindoles and isoindolenines. XXVII. 3-Alkoxy-1H-isoindoles: syntheses and properties  
Quick View Other Sources  
By Hennige, Hans et al  
From *Chemische Berichte*, 121(2), 243-52; 1988

Structure Editor:  
Java Non-Java

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

Refine



# 亚结构反应检索：分析处理

## 13种分析选项

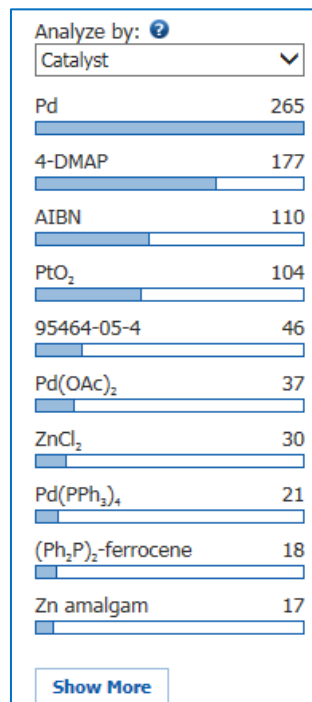
Analyze Refine

Analyze by: ?

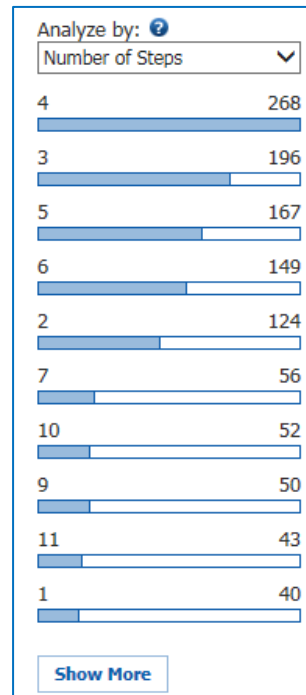
- Author Name
- Catalyst
- Company-Organization
- Document Type
- Experimental Procedure
- Journal Name
- Language
- MethodsNow
- Number of Steps
- Product Yield
- Publication Year
- Reagent
- Solvent



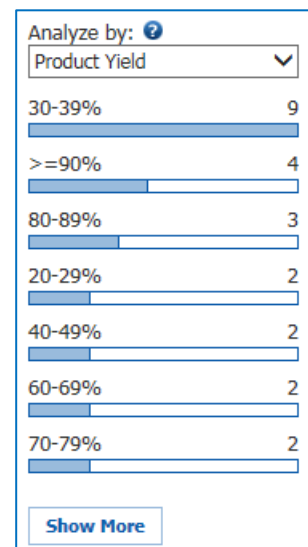
## 催化剂



## 反应步数



## 产率



## 亚结构反应检索：筛选处理

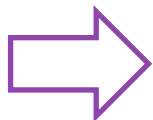
**6种筛选选项：** 反应结构、产率、反应步数、包含/排除的反应类型(11种)、不参与反应官能团(217种)

**REACTIONS ?**

Analyze Refine

Refine by: ?

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



Reaction Classification(s):

- Biotransformation
- Catalyzed
- Chemoselective
- Combinatorial
- Electrochemical
- Gas-phase
- Non-catalyzed
- Photochemical
- Radiochemical
- Regioselective
- Stereoselective

Refine

- 生物转化
- 催化反应
- 化学选择性
- 组合化学
- 电子化学
- 气相反应
- 非催化反应
- 光化学
- 放射化学
- 区域选择反应
- 立体选择反应

# 亚结构反应检索：勾选反应类型

REACTIONS ? Get References Tools Send to SciPlanner

Analyze Refine

Group by: No Grouping Sort by: Relevance

0 of 1217 Reactions Selected

1. View Reaction Detail [Link](#)

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

Reaction Classification(s):

- Biotransformation
- Catalyzed
- Chemoselective
- Combinatorial
- Electrochemical
- Gas-phase
- Non-catalyzed
- Photochemical
- Radiochemical
- Regioselective
- Stereoselective

Refine

**Overview**

**Steps/Stages**

- 1.1
- 2.1

**Notes**

1) no experimental details, prophetic reaction, 2) literature preparation, prophetic reaction, no experimental details, Reactants: 1, Steps: 2, Stages: 2, Most stages in any one step: 1

**References**

Lenalidomide isotopologues and their preparation and use for the treatment of diseases

Quick View **PATENTPAK**

By Muller, George W. and Man, Hon-Wah

From PCT Int. Appl., 2010093434, 19 Aug 2010



# 亚结构反应检索：排除反应类型

Reaction Structure substructure > reactions (1208) > refine "Electrochemical Gas-phase Phot..." (1154)

REACTIONS ? Get References Tools Send to SciPlanner

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

0 of 1154 Reactions Selected Page: 1 of 77

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

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

~83 ~85

**Excluding Reaction Classification**

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

**Excluding Reaction Classification(s):**

- Biotransformation
- Catalyzed
- Chemoselective
- Combinatorial
- Electrochemical
- Gas-phase
- Non-catalyzed
- Photochemical
- Radiochemical
- Regioselective
- Stereoselective

**Overview**

**Steps/Stages**

1.1 R:H<sub>2</sub>NCHO  
2.1 R:HCl, R:Sn, S:H<sub>2</sub>O, S:EtOH

**Notes**

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

**References**

Studies on the chemistry of isoindoles and isoindolenines. XXVII. 3-Alkoxy-1H-isoindoles: syntheses and properties  
[Quick View](#) [Other Sources](#)  
By Hennig, Hans et al.



# 亚结构反应检索：筛选官能团

Reaction Structure substructure > reactions (1208) > refine "Electrochemical Gas-phase Phot..." (1154) > **refine "any HETEROCYCLES KETONES" (435)**

REACTIONS ? Get References Tools Send to SciPlanner

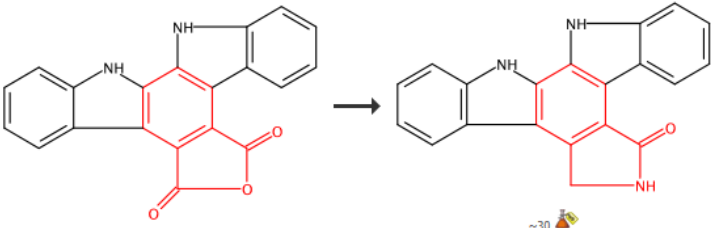
Analyze Refine

Group by: No Grouping Sort by: Relevance

0 of 435 Reactions Selected

1. View Reaction Detail [Link](#)

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



**Overview**

Steps/Stages	Notes
1.1 R: NH <sub>2</sub> OAc, 3 h, 140°C	1) thermal, 2) literature preparation, no experimental detail, Reactants: 1, Reagents: 1, Steps: 2, Stages: 2, Most stages in any one step: 1
2.1	

**References**

**Non-participating functional groups**

Non-participating Functional Group(s)  
View: Classes 10

- AMINES
- CARBONATE DERIVAT
- CARBOXY DERIVATIV
- HALIDES
- HETEROCYCLES
- KETONES
- ORGANOMETALLICS

# 提纲

- SciFinder中获取化合物制备信息的方法
- 反应相关信息获取方法
  - 结构编辑器的使用（绘图、限定反应的工具）
  - 如何通过反应式检索反应，精炼结果并获得实验详情
  - 利用SciPlanner实现反应路线设计
  - 反应检索案例分享
- 通过文献主题检索合成制备相关信息的方法

# 利用SciPlanner设计拟合成反应路线

点击打开SciPlanner工作界面

Reaction Structure substructure > reactions (1208) > refine "Catalyzed" (535)

REACTIONS ⓘ

Get References Tools ▾

Analyze Refine

Analyze by: ⓘ  
Catalyst ▾  
No reactions available

Group by: No Grouping ▾ Sort by: Number of Steps ▾ ↑

1 of 535 Reactions Selected

1. View Reaction Detail ⓘ Link Similar Reactions

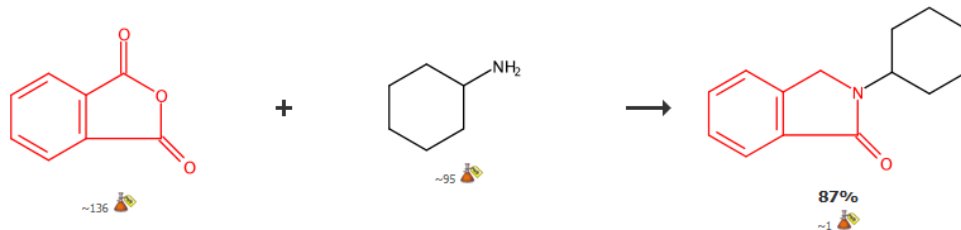
Single Step Hover over any structure for more options.

Send to SciPlanner

Display Options

Page: 1 of 36

选择感兴趣的反应，点击send to SciPlanner



# SciPlanner工作界面

SciPlanner 09\_01\_2016\_172400

Workspace Edit View GoTo

Click and drag to workspace

SciPlanner 09\_01\_2016\_172400

Workspace Edit View GoTo

The image displays two screenshots of the SciPlanner software interface. The top screenshot shows a sidebar on the right containing a reaction scheme. A purple arrow points from the text '点击拖拽至工作区' (Click and drag to workspace) to this reaction scheme. The bottom screenshot shows the same reaction scheme in the main workspace area. The reaction scheme depicts the synthesis of a cyclic amide derivative from a cyclic amine and a cyclic imide.

SciPlanner SciPlanner\_09\_01\_2016\_172400

Workspace Edit View GoTo

CAS Registry Number: 85-44-9

- View Substance Detail
- Explore by Structure
- Synthesize this...
- Get Reactions where Substance is a
- Get Commercial Sources
- Get Regulatory Information

点击物质右上角的双箭头，检索其合成方法

Get References Tools

Group by: No Grouping Sort by: Accession Number

1 of 382 Reactions Selected

4. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.

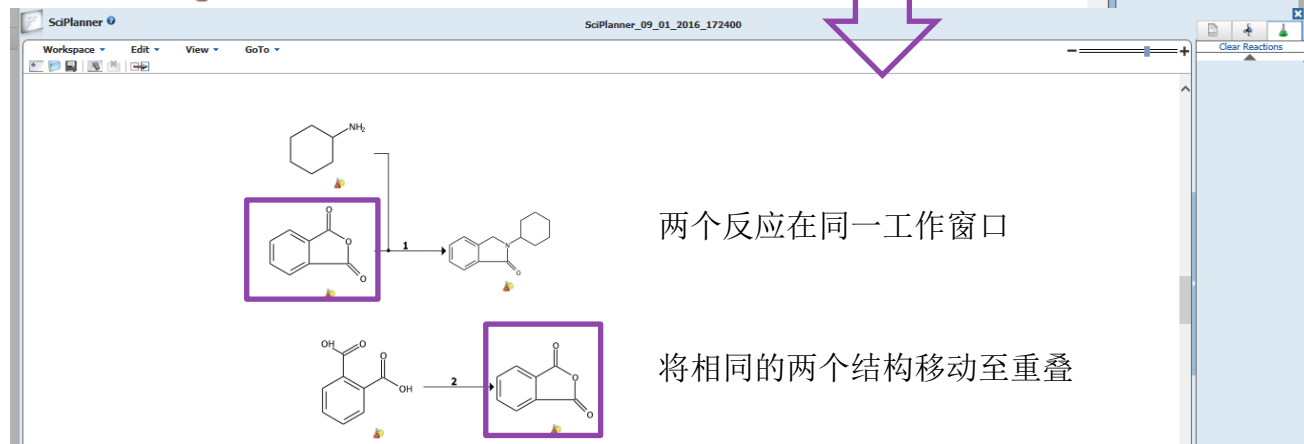
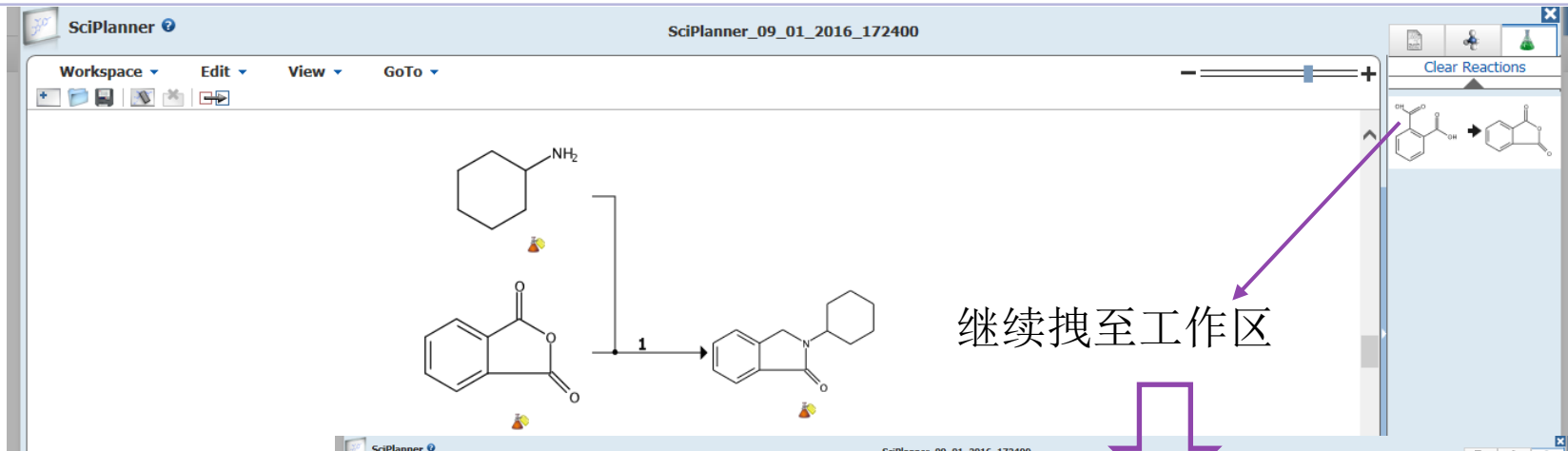
OH

97%

~132 ~136

Send to SciPlanner

从结果中选择感兴趣的反应，继续推送至SciPlanner



# SciPlanner——设计拟合成的反应路线

The screenshot displays the SciPlanner software interface. The main workspace shows a chemical synthesis route starting from salicylic acid (2-hydroxybenzoic acid) on the left. An arrow labeled '2' points to an intermediate bicyclic structure. A second arrow labeled '1' points to the final product, a bicyclic amide with a cyclohexyl group. Above the intermediate structure is a cyclohexylamine molecule. A context menu is open on the left side of the workspace, with 'Export' highlighted. On the right side, an 'Export' dialog box is open, showing options for file format (Portable Document Format selected), file name (SciPlanner\_09\_01\_2016\_172400), and inclusion of reaction details and substance details. The text '导出设计的路线' (Export the designed route) is overlaid on the right side of the workspace. Below the reaction scheme, the text '合二为一的合成路线' (A synthesis route combined into one) is displayed.

SciPlanner\_09\_01\_2016\_172400

Workspace Edit View GoTo

New  
Open  
Save  
Duplicate  
Import  
Export  
Print  
Close

导出设计的路线

合二为一的合成路线

Export

For:

Offline Review

Portable Document Format (\*.pdf)

Citations (\*.ris)

Image (\*.png)

Saving Locally

SciPlanner eXchange (\*.plx)

Details: \*

File Name: \*  
SciPlanner\_09\_01\_2016\_172400

Title

Include:

SciPlanner Image

Reaction Details

Substance Details

Reference Details

Export Cancel



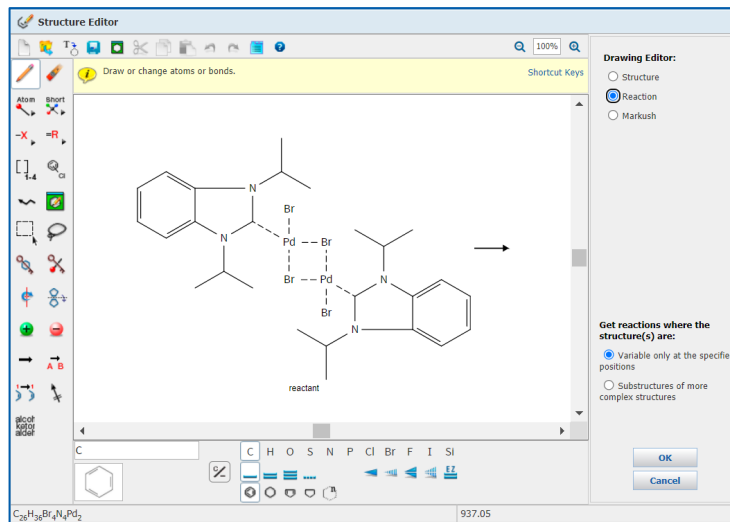
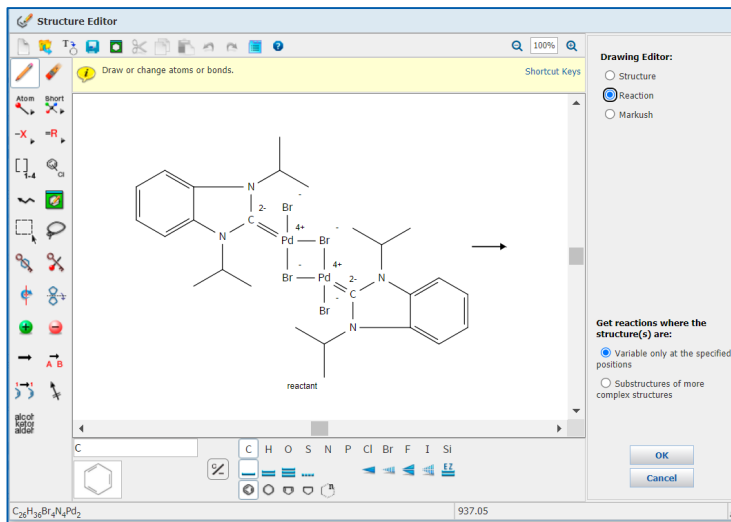
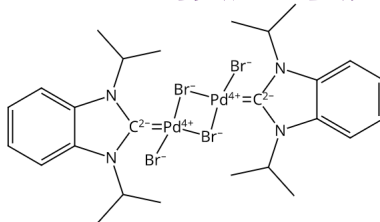
# 提纲

- SciFinder中获取化合物制备信息的方法
- 反应相关信息获取方法
  - 结构编辑器的使用（绘图、限定反应的工具）
  - 如何通过反应式检索反应，精炼结果并获得实验详情
  - 利用SciPlanner实现反应路线设计
  - 反应检索案例分享
- 通过文献主题检索合成制备相关信息的方法

# 提纲

- 反应检索案例：
  - 金属有机物质的反应
  - 溴代杂芳环与炔烃的 Sonogashira偶联反应检索
  - 片段结构的化学选择性反应
  - 检索某物质作为试剂的反应
  - 系列化合物的反应

# 例1：金属有机化合物的反应——直接进行反应检索



# 通过MethodsNow Synthesis获取合成实验详情

Reaction Structure structure variable only at spe... > reactions (347)

REACTIONS

Get References Tools

Analyze Refine

Analyze by:

Reagent

Ag <sub>2</sub> O	126
KPF <sub>6</sub>	28
Bu <sub>4</sub> N <sup>+</sup> Br <sup>-</sup>	21
Et <sub>3</sub> N	16
BuLi	15
EtN(Pr-) <sub>2</sub>	15
KOH	13
NaOH	13
NaH	9
NaN <sub>3</sub>	8

Show More

Group by: No Grouping Sort by: Relevance

0 of 347 Reactions Selected

1. View Reaction Detail Similar Reactions

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

Overview

Experimental Procedure

METHODSNow™

Procedure

1. Stir a suspension of di-μ-bromobis(1,3-diisopropylbenzimidazol-2-ylidene)di-bromodipalladium(II) (47 mg, 0.05 mmol) in CH<sub>3</sub>CN (5 mL) at ambient temperature for 6 hours.
2. Reflux the mixture for 2 hours.

View more...

Available Experimental Data

<sup>1</sup>H NMR, <sup>13</sup>C NMR, Elemental Analysis, Mass Spec, State

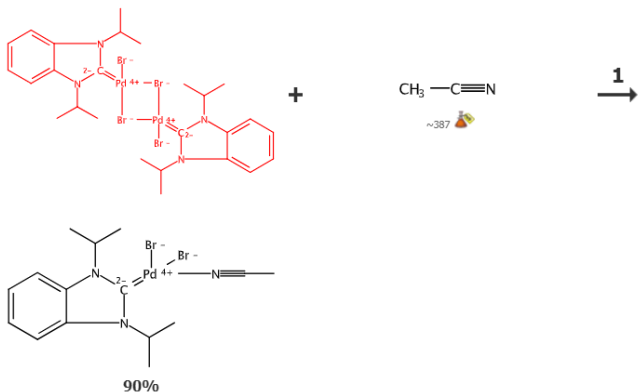
View with MethodsNow

# MethodsNow Synthesis 合成实验详情

## MethodsNow

### Palladium(II) complexes of a sterically bulky, benzannulated N-heterocyclic carbene with unusual intramolecular C-H...Pd and Carben...

By Huynh, Han Vinh; Han, Yuan; Ho, Joanne Hui Hui; Tan, Geok Kheng  
 From Organometallics, 25(13), 3267-3274; 2006  
 Published by American Chemical Society



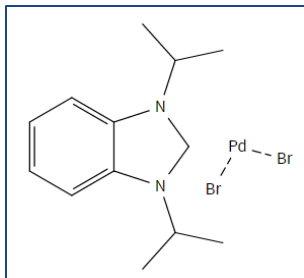
<b>Products</b>	(SPA-4-1)-(Acetonitrile)dibromo[1,3-dihydro-1,3-bis(1-methylethyl)-2H-benzimidazol-2-ylidene]palladium, 90%, CAS RN: 895632-20-9
<b>Reactants</b>	Stereoisomer of di-μ-bromodibromobis[1,3-dihydro-1,3-bis(1-methylethyl)-2H-benzimidazol-2-ylidene]dipalladium, CAS RN: 895632-19-6 Acetonitrile, CAS RN: 75-05-8
<b>Solvents</b>	Acetonitrile, CAS RN: 75-05-8

<b>Procedure</b>	<ol style="list-style-type: none"> <li>1. Stir a suspension of di-μ-bromobis[1,3-diiisopropylbenzimidazolin-2-ylidene]di-bromodipalladium(II) (47 mg, 0.05 mmol) in CH<sub>3</sub>CN (5 mL) at ambient temperature for 6 hours.</li> <li>2. Reflux the mixture for 2 hours.</li> <li>3. Filter the reaction mixture over Celite.</li> <li>4. Remove the solvent in vacuo to afford trans-dibromo(acetonitrile)(1,3-diiisopropylbenzimidazolin-2-ylidene)palladium(II).</li> </ol>
<b>Transformation</b>	Coordination of a Metal to Carbon and Heteroatom Ligand Substitution
<b>Scale</b>	milligram
<b><sup>1</sup>H NMR</b>	(300 MHz, CD <sub>3</sub> CN): δ 7.73 (dd, 2 H, Ar-H), 7.29 (dd, 2 H, Ar-H), 6.14 (m, <sup>3</sup> J(H,H) = 7.1 Hz, 2 H, NCH(CH <sub>3</sub> ) <sub>2</sub> ), 1.96 (s, CH <sub>3</sub> CN, correct integration is not possible due to ligand exchange with the solvent), 1.70 (d, <sup>3</sup> J(H,H) = 7.1Hz, 12 H, CH <sub>3</sub> ).
<b><sup>13</sup>C NMR</b>	(75.47 MHz, CD <sub>3</sub> CN): 158.4 (s, NCN), 133.8, 123.9 (s, Ar-C), 118.3 (s, CN), 113.9 (s, Ar-C), 55.8 (s, NCH(CH <sub>3</sub> ) <sub>2</sub> ), 20.5 (s, CH <sub>3</sub> ), 1.32 (m, CH <sub>3</sub> CN, assignment is tentative due to overlap with solvent signals).
<b>Elemental Analysis</b>	Anal. Calc for C <sub>15</sub> H <sub>21</sub> Br <sub>2</sub> N <sub>2</sub> Pd: C, 35.36; H, 4.15; N, 8.25. Found: C, 35.64; H, 4.08; N, 8.06.
<b>Mass Spec</b>	MS (ESI): = 471 [M - Br + CH <sub>3</sub> CN] <sup>+</sup> .
<b>State</b>	yellow powder
<b>CAS Method Number</b>	3-562-CAS-8549846

[Print/Export](#)

[Close](#)

# 根据物质获取反应——金属有机化合物的检索



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 image to change structure or view detail.

Search Type:

- Exact Structure
- Substructure
- Similarity

Show precision analysis

ChemDraw  
Launch a SciFinder/SciFind  
ChemDraw. [Learn More](#)

Import CXF

**Search**

Advanced Search  Always Show

Characteristics

- Single component
- Commercially available
- Included in references

Classes

- Alloys
- Coordination compounds



ters > substances (7)

Get References

Get Reactions

Get Commercial Sources

Tools

Create Keep Me Posted Alert

Send to SciPlanner

Sort by: CAS Registry Number

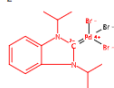
Display Options

0 of 7 Substances Selected

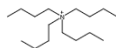
1. 2095501-02-1



895632-21-0  
C<sub>13</sub> H<sub>18</sub> Br<sub>3</sub> N<sub>2</sub> Pd

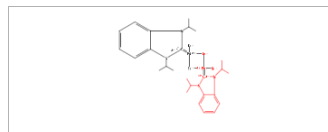


10549-76-5  
C<sub>16</sub> H<sub>36</sub> N



C<sub>16</sub> H<sub>36</sub> N . C<sub>13</sub> H<sub>18</sub> Br<sub>3</sub> N<sub>2</sub> Pd  
INDEX NAME NOT YET ASSIGNED

2. 1189146-19-7

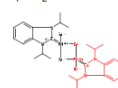


C<sub>26</sub> H<sub>36</sub> Br<sub>4</sub> N<sub>4</sub> Pd<sub>2</sub>  
Palladium, di-μ-bromodibromobis[1,3-dihydro-1,3-bis(1-methylethyl)-2H-benzimidazol-2-ylidene-2<sup>13</sup>C]di-, stereoisomer

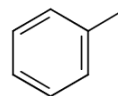
3. 896142-63-5



895632-19-6  
C<sub>26</sub> H<sub>36</sub> Br<sub>4</sub> N<sub>4</sub> Pd<sub>2</sub>



108-88-3  
C<sub>7</sub> H<sub>8</sub>



C<sub>26</sub> H<sub>36</sub> Br<sub>4</sub> N<sub>4</sub> Pd<sub>2</sub> . C<sub>7</sub> H<sub>8</sub>  
Palladium, di-μ-bromodibromobis[1,3-dihydro-1,3-bis(1-methylethyl)-2H-benzimidazol-2-ylidene]di-, stereoisomer, compd. with methylbenzene (1:1) (9CI)

4. 895632-25-4

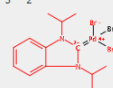


67-66-3  
C H Cl<sub>3</sub>

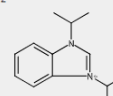


895632-22-1  
C<sub>13</sub> H<sub>19</sub> N<sub>2</sub> . C<sub>13</sub> H<sub>18</sub> Br<sub>3</sub> N<sub>2</sub> Pd

895632-21-0  
C<sub>13</sub> H<sub>18</sub> Br<sub>3</sub> N<sub>2</sub> Pd



736926-78-6  
C<sub>13</sub> H<sub>19</sub> N<sub>2</sub>



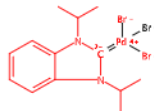
SCIFINDER®

A CAS SOLUTION

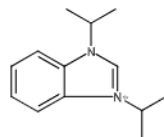
5. **895632-22-1** 🔍



895632-21-0  
 $C_{13} H_{18} Br_3 N_2 Pd$

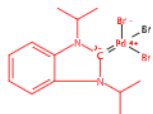


736926-78-6  
 $C_{13} H_{19} N_2$



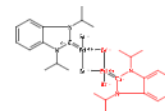
$C_{13} H_{19} N_2 \cdot C_{13} H_{18} Br_3 N_2 Pd$   
1*H*-Benzimidazolium, 1,3-bis(1-methylethyl)-,  
(*SP*-4-2)-tribromo[1,3-dihydro-1,3-bis(1-  
methylethyl)-2*H*-benzimidazol-2-ylidene]  
palladate(1-) (9CI)

6. **895632-21-0** 🔍



$C_{13} H_{18} Br_3 N_2 Pd$   
Palladate(1-), tribromo[1,3-dihydro-1,3-bis(1-  
methylethyl)-2*H*-benzimidazol-2-ylidene]-, (*SP*-  
4-2)-

7. **895632-19-6** 🔍



$C_{26} H_{36} Br_4 N_4 Pd_2$   
Palladium, di- $\mu$ -bromodibromobis[1,3-dihydro-  
1,3-bis(1-methylethyl)-2*H*-benzimidazol-2-  
ylidene]di-, stereoisomer



## 例2：溴代杂芳环与炔烃的 Sonogashira 偶联反应检索

Structure Editor

Draw or change atoms or bonds.

Shortcut Keys

Drawing Editor:

- Structure
- Reaction
- Markush

Get reactions where the structure(s) are:

- Variable only at the specified position(s)

Variables

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

Close

OK

Cancel

reactant

reactant

product

Hy

Br

Hy

H

C H O S N P Cl Br F I Si

alcohol aldehyde

检索过程：（1）绘制反应结构式，杂环用-x中的Hy表示即可

# 在反应结果集中选择group by transformation

SCIFINDER<sup>®</sup>  
A CAS SOLUTION

Explore ▾ Saved Searches ▾ SciPlanner

Reaction Structure substructure > reactions (19314)

REACTIONS ?

Get References Tools ▾

Analyze Refine

Analyze by: ?  
Reagent ▾

Et <sub>3</sub> N	11209
NaOH	5179
K <sub>2</sub> CO <sub>3</sub>	4147
NaH	3945
F <sub>2</sub> CCO <sub>2</sub> H	3615
HCl	3151
EtN(Pr- <i>i</i> ) <sub>2</sub>	2808

Group by: No Grouping ▾ Sort by: Relevance ▾ ↓

- No Grouping
- Document
- Transformation

1. View Reaction Detail Link Similar Reactions

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

~19 ~53 20%

Overview

Steps/Stages

Notes

1.1. R:Et<sub>3</sub>N, C: PdCl<sub>2</sub>(PPh<sub>3</sub>)<sub>2</sub>, S:DME, 24 h, rt

Sonogashira coupling reaction, alternative preparation s

# 根据需求，选择相应的反应类型（如，aryl-alkyne sonogashira偶联）

Explore ▾ Saved Searches ▾ SciPlanner

Reaction Structure substructure > reactions (19314)

REACTIONS ?

Get References Tools ▾

Group by: Transformation ▾ Sort by: Frequency ▾ ↓

3910 of 19314 Reactions Selected

Analyze Refine

Analyze by: ?

Reagent ▾

Et <sub>3</sub> N	11209
NaOH	5179
K <sub>2</sub> CO <sub>3</sub>	4147
NaH	3945
F <sub>3</sub> CCO <sub>2</sub> H	3615
HCl	3151
EtN(Pr- <i>i</i> ) <sub>2</sub>	2808
NaHCO <sub>3</sub>	2639

1. Aryl-Alkyne Coupling/ Stephens-Castro Coupling/ Sonogashira Coupling  
3910 Reactions (3910 Selected)

$$\text{Ar-X} + \text{HC}\equiv\text{CR} \xrightarrow{\text{cat.}} \text{Ar-C}\equiv\text{CR}$$

2. Alkylation/ Silylation at an Alkynyl Carbon  
230 Reactions

$$\text{R}\equiv\text{CH} \begin{cases} \xrightarrow{\text{X-SiR}^1_3} \text{R}\equiv\text{SiR}^1_3 \\ \xrightarrow{\text{X-R}^2} \text{R}\equiv\text{R}^2 \end{cases}$$

3. Acylation of Nitrogen Nucleophiles with Carboxylic Esters and Analogs  
126 Reactions (126 Selected)

# 获得全面、准确的反应

Explore ▾ Saved Searches ▾ SciPlanner

Reaction Structure substructure > reactions (19314) > reactions with transformation "Aryl-Alkyne Coupling/ Stephens..." (3910)

REACTIONS ⓘ

Get References Tools ▾

Analyze Refine

Group by: No Grouping ▾ Sort by: Relevance ▾ ↓

0 of 3910 Reactions Selected

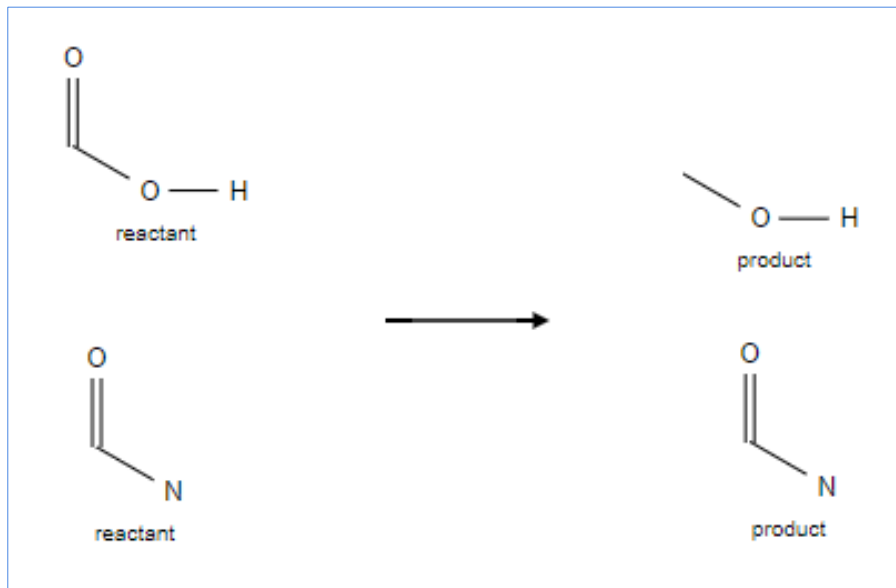
1. [View Reaction Detail](#) [Link](#) [Similar Reactions](#)

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

**Overview**

Steps/Stages	Notes
1.1 R:Et <sub>3</sub> N, C: PdCl <sub>2</sub> (PPh <sub>3</sub> ) <sub>2</sub> , S: DMF, 24 h, rt	Sonogashira coupling reaction, alternative preparation Catalysts: 1, Solvents: 1, Steps: 1, Stages: 1, Most sta

### 例3：片段结构的化学选择性反应



检索要求：

1. 反应物中含有羧基和酰胺基团；
2. 反应物种的羧基被还原为产物中的羟基；
3. 反应物中的酰胺基在反应后没有发生变化。

分析：

化学选择性反应可以使用non-participating functional groups来限定不参与反应的官能团。

# 使用标亮的工具，绘制如下反应式，进行亚结构反应检索

The screenshot shows the Structure Editor interface. The main workspace displays a chemical reaction: a reactant with a central atom 'A' bonded to a carbonyl group (C=O) and a hydroxyl group (O-H), and a product where the carbonyl carbon is highlighted with a red box and labeled 'C'. The interface includes a top toolbar, a left sidebar with various drawing tools (some highlighted with red boxes), a bottom toolbar with element buttons (C, H, O, S, N, P, Cl, Br, F, I, Si), and a right sidebar with 'Drawing Editor' and 'Get reactions where the structure(s) are:' options. The 'Get reactions where the structure(s) are:' section has two radio buttons, with the second one, 'Substructures of more complex structures', being selected and highlighted with a red box.

The Variables dialog box lists several variables with checkboxes:

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

A 'Close' button is located at the bottom of the dialog.

Author Name  
Company Name  
Document Identifier  
Journal  
Patent  
Tags

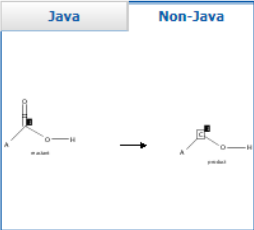
**SUBSTANCES**

Chemical Structure  
Markush  
Molecular Formula  
Property  
Substance Identifier

**REACTIONS**

Reaction Structure

Structure Editor:  
Java Non-Java



Click image to change structure or view detail.

Search Type:  
 Allow variability only as specified  
 Substructure

Import CXF

Search

Advanced Search  Always Show

Solvents  Select Solvents

Non-participating Functional Groups  Close

View: All 217

1 Selected Clear Selections

- pi-Allyl
- Allyl Alcohol
- Allyl Halide
- Amide
- Amidine

ChemDraw  
Launch a SciFinder substance or reaction  
More

1. 点击高级检索;
2. 点击不参与反应官能团;
3. 选择酰胺amide。

## REACTIONS ?

Get  
References

Tools ▾

Analyze Refine

Analyze by: ?

Reagent ▾

NaBH<sub>4</sub> 1888EtN(Pr-)<sub>2</sub> 1819

HCl 1745

Et<sub>3</sub>N 1738F<sub>3</sub>CCO<sub>2</sub>H 1345

NaOH 1345

AcOH 1261

H<sub>2</sub> 1238NaHCO<sub>3</sub> 917H<sub>2</sub>O 766

Show More

Group by: No Grouping ▾

Sort by: Accession Number ▾ ↓



No Grouping

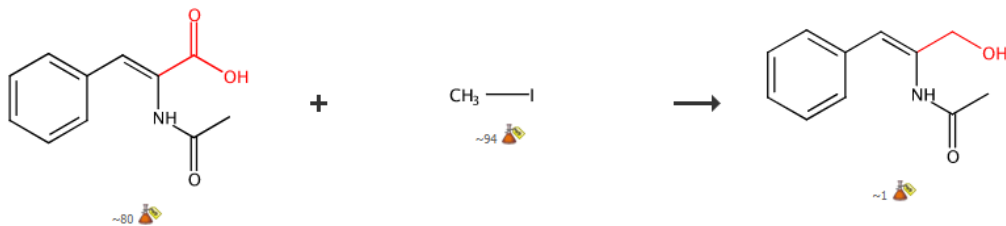
Document

Transformation

None Selected

 1. View Reaction Detail [Link](#)

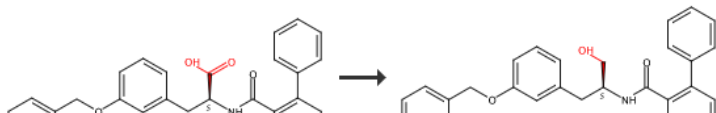
2 Steps Hover over any structure for more options.



Overview

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

Single Step Hover over any structure for more options.





Reaction Structure substructure with limiters > reactions (4522)

REACTIONS ? Get References Tools

Analyze Refine Group by: Transformation Sort by: Frequency

Analyze by: Reagent

NaBH <sub>4</sub>	1888
EtN(Pr-) <sub>2</sub>	1819
HCl	1745
Et <sub>3</sub> N	1738
F <sub>3</sub> CCO <sub>2</sub> H	1345
NaOH	1345
AcOH	1261
H <sub>2</sub>	1238
NaHCO <sub>3</sub>	917
H <sub>2</sub> O	766

Show More

673 of 4522 Reactions Selected

1. Reduction of Carboxylic Acids to Alcohols  
673 Reactions (673 Selected)

$$\text{R}-\overset{\text{O}}{\parallel}{\text{C}}-\text{OH} \longrightarrow \text{R}-\text{CH}_2-\text{OH}$$

2. Acylation of Nitrogen Nucleophiles by Carboxylic Acids  
102 Reactions (23 Selected)

$$\text{R}-\overset{\text{O}}{\parallel}{\text{C}}-\text{OH} + \text{R}^1-\text{NH}-\text{R}^1 \longrightarrow \text{R}-\overset{\text{O}}{\parallel}{\text{C}}-\text{N}(\text{R}^1)_2$$

3. Transamidation/ Zip Reaction  
75 Reactions (16 Selected)

$$\text{R}^2-\overset{\text{O}}{\parallel}{\text{C}}-\text{N}(\text{R}^1)_2 + \text{R}-\text{NH}-\text{R}^1 \longrightarrow \text{R}^2-\overset{\text{O}}{\parallel}{\text{C}}-\text{N}(\text{R})-\text{R}^1 + \text{R}^1-\text{NH}-\text{R}^1$$

4. Formation of Alkyl Halides/ Alcohols from Ethers /Silyl Ethers  
73 Reactions (5 Selected)

$$\text{R}-\text{O}-\text{R}^1 \xrightarrow{\text{HX}} \text{R}-\text{X} + \text{R}^1-\text{OH}$$

$\text{R}^1 = \text{CR}'_3, \text{SiR}'_3$

选择羧酸还原为醇的这类反应

REACTIONS ?

Get References

Tools ▾

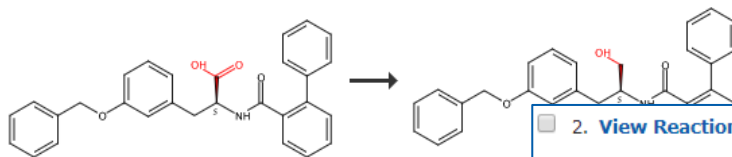
Analyze Refine

Group by: No Grouping ▾ Sort by: Accession Number ▾ ↓

0 of 673 Reactions Selected

1. View Reaction Detail Link Similar Reactions

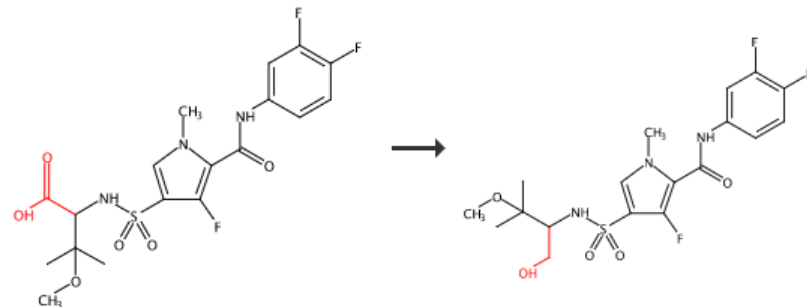
Single Step Hover over any structure for more options.



Overview

2. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.



最终，获得全面精准的片段结构的化学选择性反应结果集



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A CAS SOLUTION

## 例4：检索使用 $\text{Na}_2\text{S}_2\text{O}_4$ 作为试剂的反应

Molecular Formula "H2 O4 S2 . 2 Na" > substances (2)

### REFERENCES

Research Topic  
Author Name  
Company Name  
Document Identifier  
Journal  
Patent  
Tags

### SUBSTANCES

Chemical Structure  
Markush  
Molecular Formula  
Property  
Substance Identifier

### REACTIONS

Reaction Structure

### SUBSTANCES: MOLECULAR FORMULA ?

H2 S2 O4 . 2Na

Examples:

H4SiO4

(C3H6O.C2H4O)x

Search

思路：先检索物质，然后通过物质获取反应

- 分子式检索无机物，要按照Hill排序规则检索。具体为，不含碳化合物，按照元素符号字母顺序排序。含碳化合物，碳在前，氢紧随其后，其他元素按照字母排序。
- 无机含氧酸盐，按照多组物质检索（比如 $\text{Na}_2\text{S}_2\text{O}_4$ ，就按照相应的酸和钠的混合物标引，阳离子有多少个阳离子，阴离子部分用H补齐），所用分子式为： $\text{H}_2\text{O}_4\text{S}_2.2\text{Na}$

# 通过物质获取反应，并限制反应角色为Reagent

Molecular Formula "H2 O4 S2 . 2 Na" > substances (2)

**SUBSTANCES** ? Get References Get Reactions Get Commercial Sources Tools ▼

Analyze Refine

Sort by: CAS Registry Number ▼

▼ 0 of 2 Substances Selected

1. **37070-73-8**   
(Component: 754124-42-0)  
~2

$\text{OH}-\text{S}(\text{O})_2-\text{O}-\text{SH}$   
• 2 Na

**H<sub>2</sub> O<sub>4</sub> S<sub>2</sub> . 2 Na**  
Thioperoxymonosulfuric acid ((HO)S(O)<sub>2</sub>(OSH)), sodium salt (1:2)

2. **7775-14-6**   
(Component: 15959-26-9)  
~6888 ~53

  
 $\text{OH}-\text{S}(\text{O})-\text{S}(\text{O})-\text{OH}$   
• 2 Na

### Get Reactions

Limit results by reaction role:

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

# 获得使用Na<sub>2</sub>S<sub>2</sub>O<sub>4</sub>作为试剂的反应

Analyze by:

Reagent

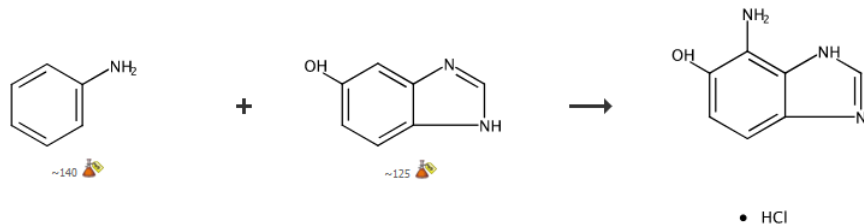
37070-73-8	2
HCl	2
NaOH	2
H <sub>2</sub> O	1
NaNO <sub>2</sub>	1

Show More

0 of 2 Reactions Selected

1. View Reaction Detail Link

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



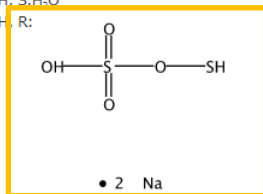
## Overview

### Steps/Stages

1.1 R:NaNO<sub>2</sub>, R:H<sub>2</sub>O, S:H<sub>2</sub>O

1.2 R:NaOH, S:H<sub>2</sub>O

2.1 R:NaOH, R:



S:H<sub>2</sub>O

2.2 R:HCl, S:EtOH

### Notes

Reactants: 2, Reagents: 5, Solvents: 2, Steps: 2, Stages: 4, Most stages in any one step: 2

### References

[Azo coupling of 5\(6\)-hydroxybenzimidazole and its derivatives](#)

[Quick View](#) [Other Sources](#)

By Kuznetsov, Yu. V. et al

From Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya, (3), 662-4; 1990

## 例5：在非反应仲醇存在的条件下，将伯醇转换为醛

Structure Editor

Draw or change atoms or bonds. Shortcut Keys

Primary Alcohol reactant

Secondary Alcohol non-reacting

Aldehyde product

Drawing Editor:

- Structure
- Reaction
- Markush

Get reactions where the structure(s) are:

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

alcohol ketone aldehyde

Formula is not available

Functional Groups

Enter 3 or more characters...

- ▶ Alcohols (13)
- ▶ Alkenes (11)
- ▶ Alkynes (4)
- ▶ Amines (11)
- ▶ Carbonate Derivatives (7)
- ▶ Carboxy Derivatives (17)
- ▶ Halides (16)
- ▶ Heterocycles (54)
- ▶ Ketones (6)
- ▶ Organometallics (19)
- ▶ Non-Rings (136)
- ▶ Rings (71)

Close

使用反应角色定义工具  
和官能团列表

# 通过Group by: Transformation, 筛选需要的反应类型

REACTIONS

Get References Tools ▾

Analyze Refine

Analyze by: Reagent ▾

NaHCO <sub>3</sub>	1891
Et <sub>3</sub> N	1836
1H-Imidazole	1222
Bu <sub>4</sub> N <sup>+</sup> • F <sup>-</sup>	1154
NH <sub>4</sub> Cl	1104
2,6-Lutidine	1005
Martin's reagent	976

Group by: No Grouping ▾ Sort by: Accession Number ▾ ↓

0 of 5067 Reactions Selected

1. View Reaction Detail Similar Reactions

Single Step *Hover over any*

> reactions (5067) > reactions with transformation "Oxidation or Dehydrogenation o..." (1448)

Get References Tools ▾

Group by: Transformation ▾ Sort by: Frequency ▾ ↓

0 of 5067 Reactions Selected

1. Oxidation or Dehydrogenation of Alcohols to Aldehydes and Ketones  
1448 Reactions

$$\begin{array}{ccc} \text{OH} & & \text{O} \\ | & \longrightarrow & || \\ \text{R}-\text{C} & & \text{R}-\text{C} \\ | & & | \\ \text{R}^1 & & \text{R}^1 \end{array}$$





# 提纲

- SciFinder中获取化合物制备信息的方法
- 反应相关信息获取方法
  - 结构编辑器的使用（绘图、限定反应的工具）
  - 如何通过反应式检索反应，精炼结果并获得实验详情
  - 利用SciPlanner实现反应路线设计
  - 反应检索案例分享
- 通过文献主题检索合成制备相关信息的方法

# 例1. 通过文献主题词检索，获取有关氯吡格雷纯化方面的文献

Explore ▾ Saved Searches ▾ SciPlanner

Research Topic "purification of clopidogrel" > references (92) > refine by categories

**REFERENCES**

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

**SUBSTANCES**

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

**REACTIONS**

- Reaction Structure

**REFERENCES: RESEARCH TOPIC**

purification of clopidogrel

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

**Search**

Advanced Search

Select All Deselect All

3 of 5 Research Topic Candidates Selected

- 3 references were found containing "purification of clopidogrel" as entered.
- 35 references were found containing the two concepts "purification" and "clopidogrel" closely associated with one another.
- 103 references were found where the two concepts "purification" and "clopidogrel" were present anywhere in the reference.
- 2539670 references were found containing the concept "purification".
- 21557 references were found containing the concept "clopidogrel".

**Get References**

concept代表对主题词中的关键词进行了同义词扩展



## 例2：去除N-甲基甲酰胺（123-39-7）

The image shows two screenshots of the SciFinder web interface. The top screenshot displays the search process: a search bar contains the text "remove of 123-39-7", and below it, example references are listed: "The effect of antibiotic residues on dairy products" and "Photocyanation of aromatic compounds". A blue "Search" button is visible. The bottom screenshot shows the search results page. It features a navigation bar with "Explore", "Saved Searches", and "SciPlanner". Below the navigation bar, the search topic "Research Topic 'remove of 123-39-7'" is displayed. A "REFERENCES" section includes "Select All" and "Deselect All" options, and a summary: "1 of 4 Research Topic Candidates Selected". A list of four candidates follows, each with a checkbox and a description of the search results:

- 49 references were found containing the two concepts "remove" and "123-39-7" closely associated with one another.
- 264 references were found where the two concepts "remove" and "123-39-7" were present anywhere in the reference.
- 2808271 references were found containing the concept "remove".
- 4512 references were found containing the concept "123-39-7".

A "Get References" button is located at the bottom of the list.

# 文献详情中的Substance标引, 指出物质在文献中的作用

## 1. Removal of gas phase dimethylamine and N,N-dimethylformamide using non-thermal plasma

By: Wang, Wenzheng; Fan, Xing; Zhu, Tianle; Wang, Haining; Ye, Daiqi; Hong, Xiaowei

Dimethylamine (DMA) and N,N-dimethylformamide (DMF) are typical N-VOCs exhausted from manufg. factories. In the present study, the behavior of non-thermal plasma (NTP) was systematically investigated for **removal** of gas-phase DMA and DMF in a link tooth wheel-cylinder plasma reactor. Exptl. results show that DMA is much easier to be decompd. by NTP than DMF. Coexisting DMF has no effect on DMA conversion while DMF conversion is significantly promoted by the addn. of DMA. Regardless of initial gas compns. as well as DMA and DMF concn., CO<sub>2</sub> selectivity increased monotonously with increasing ED. But CO<sub>2</sub> selectivity of 100% cannot be obtained even with ED higher than 70 J L<sup>-1</sup>, indicating the formation of org. intermediates during DMA and DMF decompn. Based on org. products anal. with GC-MS and mol. optimization results with d. functional theory calcn., possible mechanisms on DMA and DMF decompn. were proposed. The org. products from DMA and DMF decompn. by NTP were found to have great soly. and high biodegradability. Thus, NTP enhanced absorption/biol. method is suggested for complete **removal** of DMA and DMF.

### Indexing

Air Pollution and Industrial Hygiene (Section59-4)

### Concepts

Absorption	Air pollution control
Bond energy	Bond length
Decomposition	Decomposition catalysts
Plasma	Waste gas treatment

**removal** of gas phase dimethylamine and N,N-dimethylformamide using non-thermal plasma

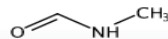
Volatile organic compounds

**removal** of gas phase dimethylamine and N,N-dimethylformamide using non-thermal plasma

Removal or disposal; Process

### Substances

56-40-6 Glycine, formation (nonpreparative) 🔍  
64-18-6 Formic acid, formation (nonpreparative) 🔍  
75-12-7 Formamide, formation (nonpreparative) 🔍  
79-20-9 Methyl acetate 🔍  
105-37-3 Ethyl propionate 🔍  
107-31-3 Methyl formate 🔍  
**123-39-7** N-Methyl formamide 🔍



144-62-7 Oxalic acid, formation (nonpreparative) 🔍

**removal** of gas phase dimethylamine and N,N-dimethylformamide using non-thermal plasma

Formation, unclassified; Formation, nonpreparative

需要的文献



# 通过Categorize, 精准获取所需文献

CAS Solutions

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Preferences | SciFinder Help | Sign Out

Welcome Helen Zhu

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

Research Topic "remove of 123-39-7" > references (49) > Removing agent containing alky...

REFERENCES

Get Substances | Get Reactions | Get Related Citations | Tools

Create Keep Me Posted Alert | Send to SciPlanner

Analyze | Refine | **Categorize**

Sort by: Accession Number

0 of 49 References Selected

Display Options

Page: 1 of 3

Analyze by: Author Name

Author Name	Count
Egbe Matthew I	4
Hara Yasushi	4
Takahashi Fumiharu	4
Bang Sun Hong	2
Hong Heon Pyo	2
Legenza Michael Walter	2
Ward Irl E	2
Albrecht Herbert	1
Alsters Paul	1
Aoba Kazuhiro	1

- Removal of gas phase dimethylamine and N,N-dimethylformamide using non-thermal plasma**  
Quick View | Other Sources  
By Wang, Wenzheng; Fan, Xing; Zhu, Tianle; Wang, Haining; Ye, Daiqi; Hong, Xiaowei  
From Chemical Engineering Journal (Amsterdam, Netherlands) (2016), 299, 184-191. | Language: English, Database: CAPLUS  
Dimethylamine (DMA) and N,N-dimethylformamide (DMF) are typical N-VOCs exhausted from manuf. factories. In the present study, the behavior of non-thermal plasma (NTP) was systematically investigated for **removal** of gas-phase DMA and DMF in a link tooth wheel-cylinder plasma reactor. Exptl. results show that DMA is much easier to be decompd. by NTP than DMF. Coexisting DMF has no effect on DMA conversion while DMF conversion is significantly promoted by the addn. of DMA. Regardless of initial gas compns. as well as DMA and DMF concn., CO<sub>2</sub> selectivity increased monotonously with increasing E...
- Stripping composition for removing photoresist and a method, for peeling photoresist, using same**  
Quick View | PATENTPAK  
By Park, Tae Moon; Jung, Dae Chul; Lee, Dong Hoon; Lee, Woo Ram; Lee, Hyun Jun; Kim, Ju Young  
From PCT Int. Appl. (2016), WO 2016027985 A1 20160225. | Language: Korean, Database: CAPLUS  
The present invention relates to a stripping compn. for **removing** a photoresist and a method, for peeling a photoresist, using same, the stripping compn. comprising: one or more amine compds.; an amide-based compd. substituted with one or two of C1-5 straight or branched alkyl groups; a polar org. solvent; a particular triazole-based compd.; and a benzimidazole-based compd.
- Removing agent containing alkylamide mixture**  
Quick View | PATENTPAK  
By Li, Bo; Yu, Ran  
From Faming Zhuanli Shenqing (2015), CN 104698775 A 20150610. | Language: Chinese, Database: CAPLUS  
The present invention relates to a kind of alkylamide **removing** agent. The **removing** agent comprises N-methylformamide 50-70 wt.%, N, N-dimethyl acetamide 30-50 wt.%,

# 通过Categorize, 精准获取所需文献

**Categorize** ?

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

Category Heading	Category	Index Terms	Selected Terms
All	Substances in technology (824)	<b>Select All</b> <b>Deselect All</b>	Click 'x' to remove the category from 'Selected Terms'
<b>Technology</b>	Materials & products (76)	<input checked="" type="checkbox"/> N-Methyl formamide 6	<b>x</b> Technology > Formed, removed, & other substances (1 Terms)
General chemistry	<b>Formed, removed, &amp; other substances (61)</b>	<input type="checkbox"/> N,N-Dimethylformamide 3	
Physical chemistry	Metallurgy (45)	<input type="checkbox"/> Copper 2	
Biotechnology	Processes & apparatus (35)	<input type="checkbox"/> Copper alloy 2	
Polymer chemistry	Imaging & recording (4)	<input type="checkbox"/> Dimethylamine 2	
Environmental chemistry	Power & fuel topics (5)	<input type="checkbox"/> Formamide 2	
Synthetic chemistry	Ceramics (2)	<input type="checkbox"/> Oxides (inorganic) 2	
Catalysis	Construction (2)	<input type="checkbox"/> Polyimides 2	
Genetics & protein chemistry		<input type="checkbox"/> 1-Fluoro-1,2,2-trichloroethane 1	
Biology		<input type="checkbox"/> 2,3-Dimethyl-1-butanol 1	
Analytical chemistry		<input type="checkbox"/> 2,4-Di-tert-butylphenol 1	
		<input type="checkbox"/> 2,6-Di-tert-butyl-1,4-benzoquinone 1	
		<input type="checkbox"/> 2-(Methyl mercapto)benzothiazole 1	

Technology > Formed, removed, & other substances > 1 Index Term(s) Selected

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