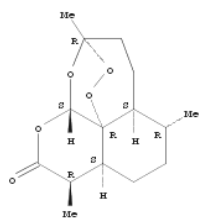


物质有关的反应

1. Substance Detail
63968-64-9

~3242



Absolute stereochemistry.

C₁₅ H₂₂ O₅
3,12-Epoxy-12H-pyrano[4,3-j]-1,2-benzodioxepin-10(3H)-one, octahydro-3,6,9-trimethyl-, (3R,5aS,6R,8aS,9R,12S,12aR)-

Get Reactions

Limit results by reaction role:

☒ Product

☐ Reactant

☐ Reagent

☐ Reactant or reagent

☐ Catalyst

☐ Solvent

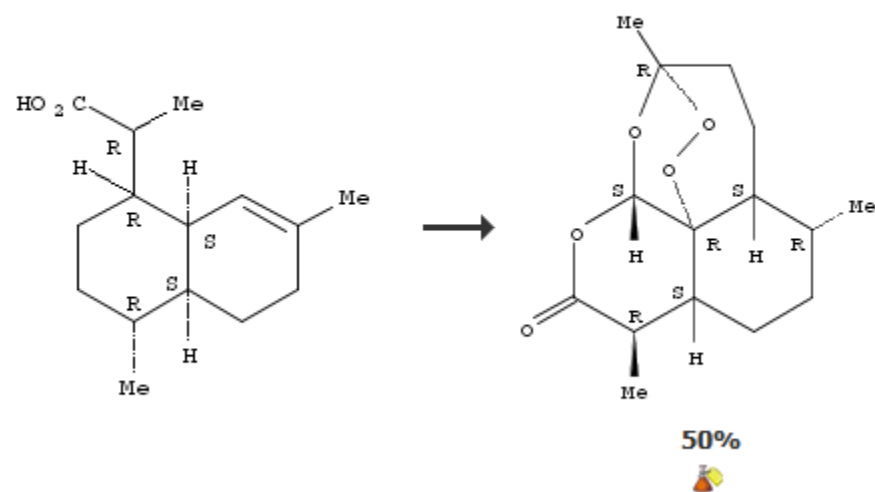
☐ Any role

Get

Cancel

1. View Reaction Detail

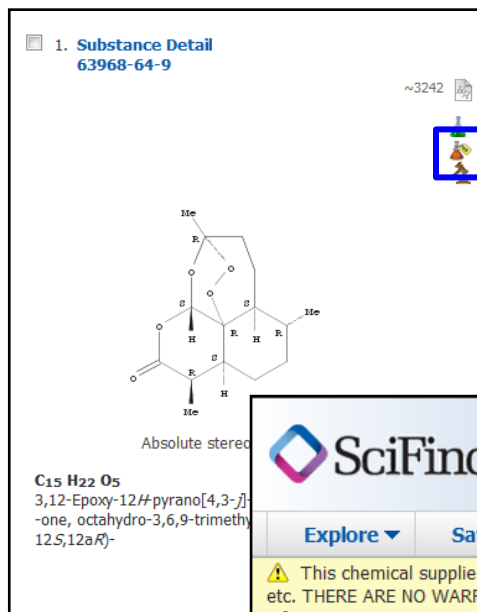
Single Step *Hover over any structure for more options.*



Overview

物质有关的商业来源

可以直接Export到Excel中，又或者使用分析工具，对商业信息进行处理



SciFinder®

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⚠ This chemical supplier information is provided on an "as is" basis. Please consult the suppliers for current information regarding pricing, regional availability, available quantities, purities, etc. THERE ARE NO WARRANTIES OF ANY KIND, EITHER EXPRESSED OR IMPLIED. ACS is not liable for any loss of profit, goodwill or any other damages arising out of the use of this information.

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

COMMERCIAL SOURCES ?

Analyze

Sort by: Catalog Name ↑

0 of 91 Commercial Sources Selected

Answers per Page [20]

Analyze by: ?

Catalog Name

Accel Pharmtech
Product List 2

AK Scientific Product
Catalog 2

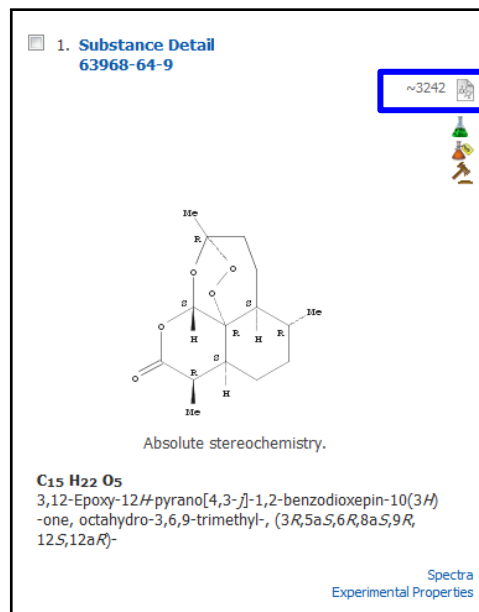
Chemieliva
Pharmaceutical
Product List 2

ChemPacific Product


1. **3B Scientific Corporation Product List**
 Supplier Name: 3B Scientific Corporation, Catalog Publication Date: 12 Jul 2012
 Order Number: 382-3802
 Quantity: 1g
 63968-64-9 Artemisinin
[Link](#)

2. **A Chemtek Product List**
 Supplier Name: A Chemtek, Catalog Publication Date: 13 Mar 2013
 Order Number: 031-18967
 Quantity: N/A
 63968-64-9 Artemisinin

物质有关的文献信息



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，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:

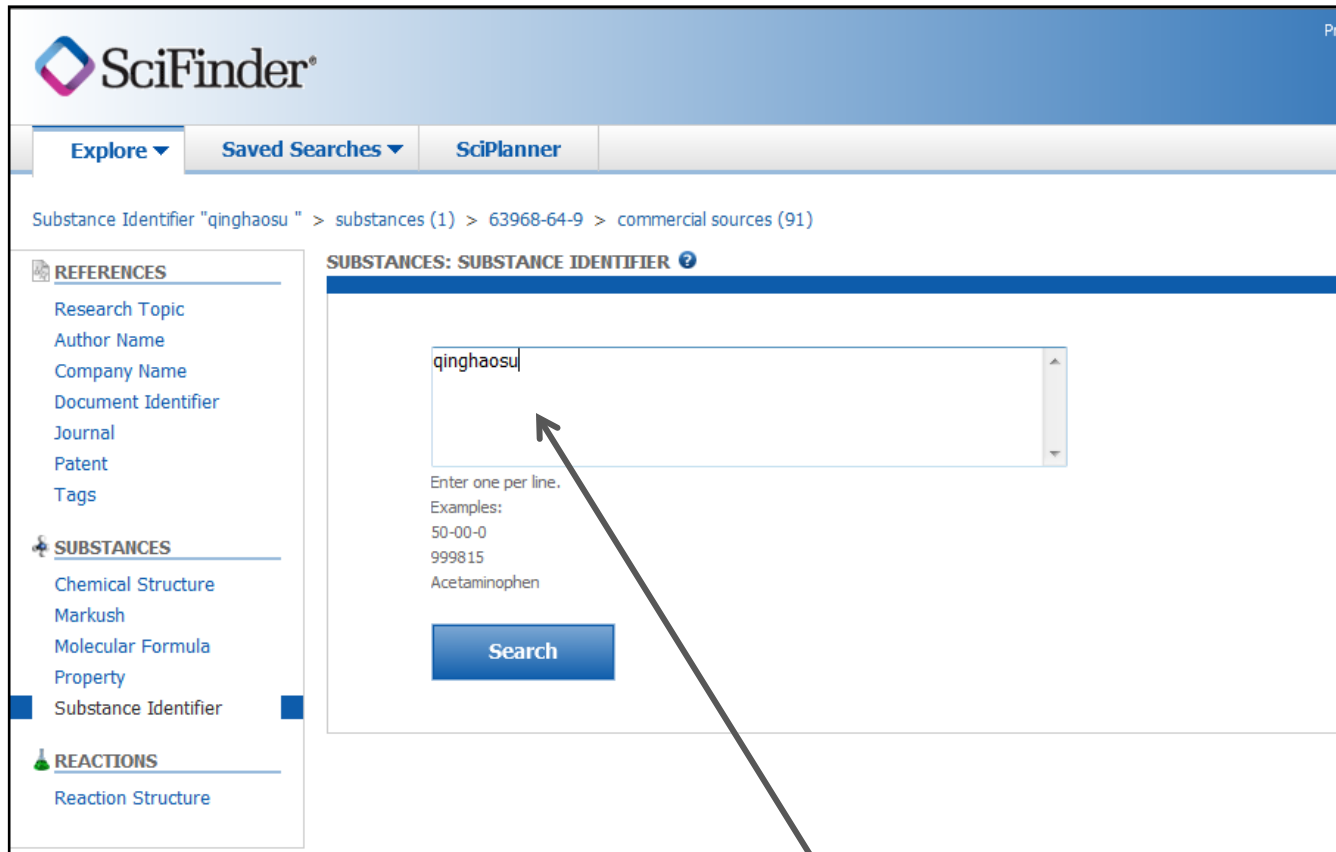
☐ Additional related references, e.g., activity studies, disease studies.

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

直接输入物质的名称, CAS No, 俗名, 都能检索, 一次最多检索25个物质, 用换行换开

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

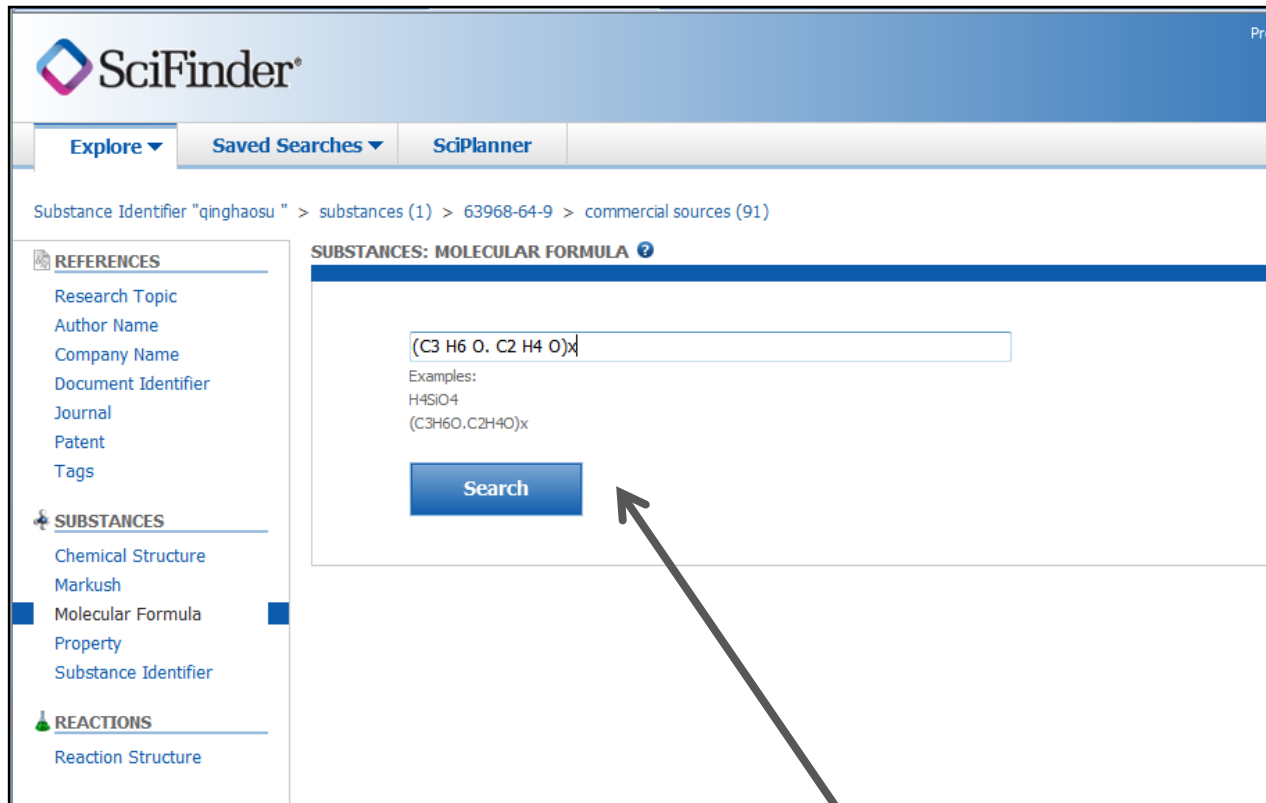
Examples: Individual value as 44,
range as 25-35, or open ended range
as >125 or <125

☐ Predicted

Value or Range

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

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

REACTIONS

- Reaction Structure

SUBSTANCES: MOLECULAR FORMULA

(C3 H6 O. C2 H4 O)x

Examples:
 H4SiO4
 (C3H6O.C2H4O)x

Search

SciFinder中的分子式的检索，需要按照HILL排序方式输入，简单来说，CH写前面，其他的按照字母顺序写

结构式检索



Explore ▼

Saved Searches ▼

SciPlanner

REFERENCES

Research Topic
Author Name
Company Name
Document Identifier
Journal
Patent
Tags

SUBSTANCES

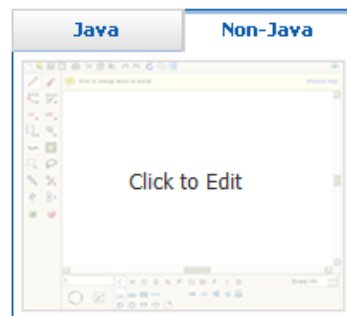
Chemical Structure
Markush
Molecular Formula
Property
Substance Identifier

REACTIONS

Reaction Structure

SUBSTANCES: CHEMICAL STRUCTURE ?

Structure Editor:



Import CXF

Search

Search Type:

- ☐ Exact Structure
☒ Substructure
☐ Similarity

☐ Show precision analysis



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

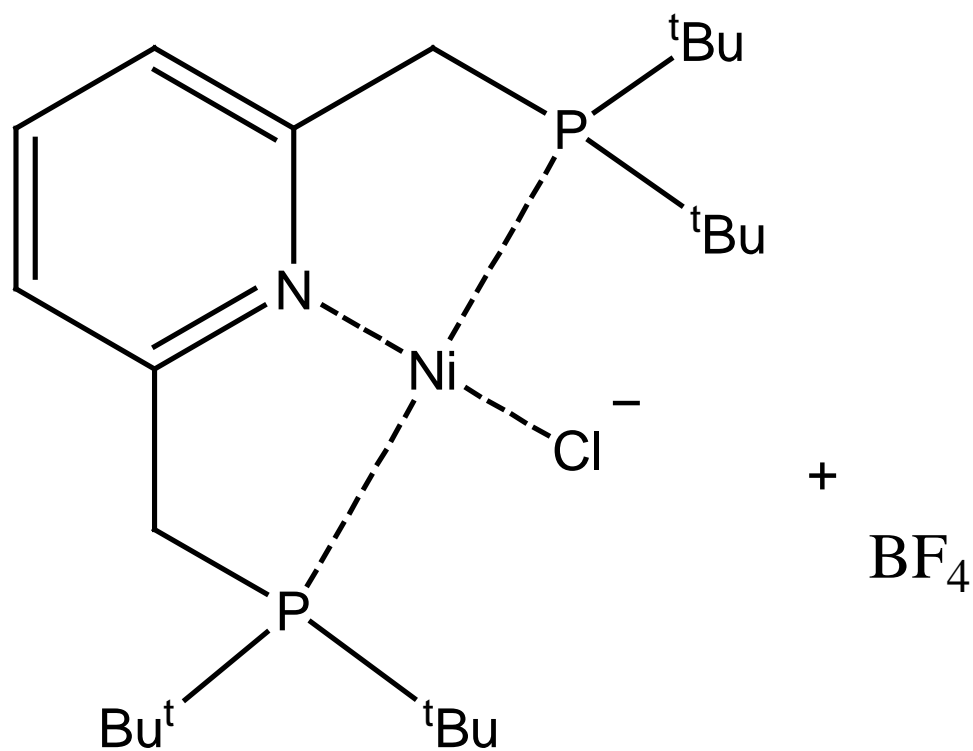
SciFinder结构绘制工具

The image shows the SciFinder Structure Editor window with various tools and options labeled in Chinese. The labels are as follows:

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

The interface includes a toolbar with icons for drawing and editing, a central workspace for the chemical structure, and a right-hand panel with search options (Exact search, Substructure search, Similarity search) and buttons for '确定' (OK) and '取消' (Cancel).

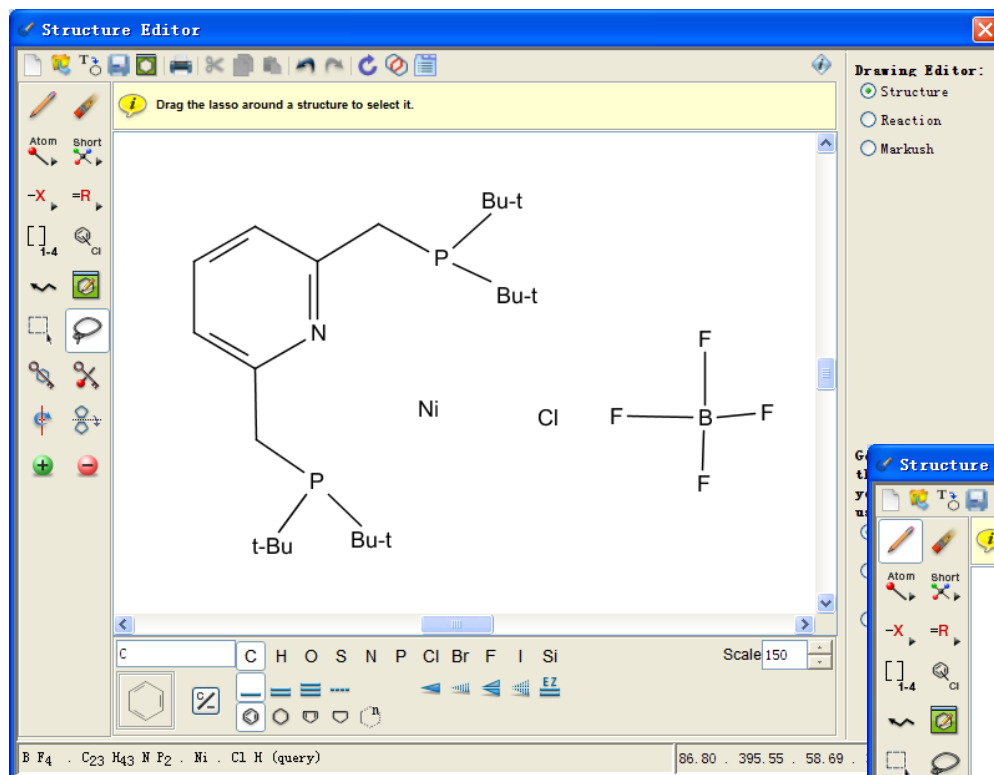
精确结构检索—检索金属配合物



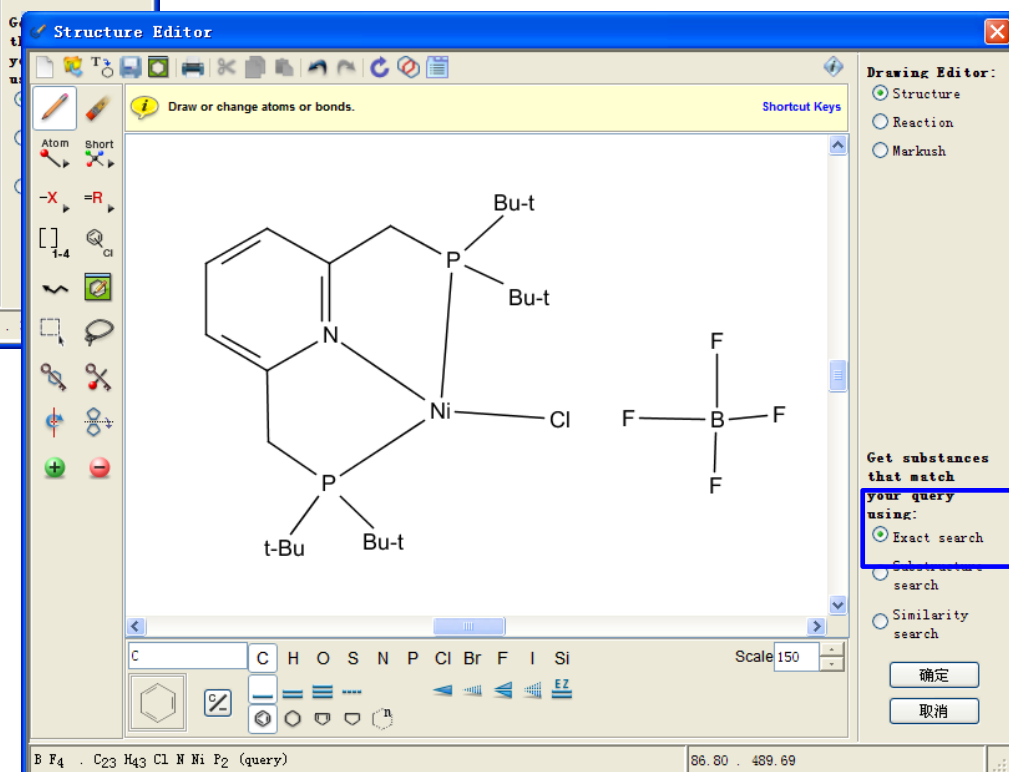
该结构中包含:

配体
金属
阳离子
阴离子

检索界面



任何一种结构, 使用精确结构都可以检索到



精确查到该物质

Chemical Structure exact > substances (1)

SUBSTANCES ?

Get References Get Reactions Get Comp Sources

Analyze Refine

Sort by: CAS Registry Number

Analyze by: ?
Substance Role

Preparation 1

Properties 1

Reactant or Reagent 1


Show More

0 of 1 Substance Selected


1. 1136166-99-8

~1

1136166-98-7
C₂₃ H₄₃ Cl N Ni P₂

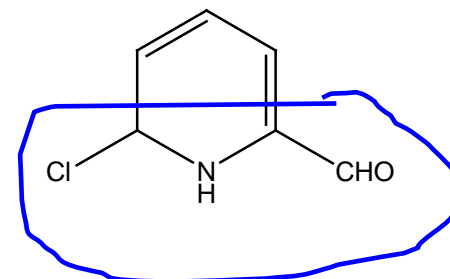
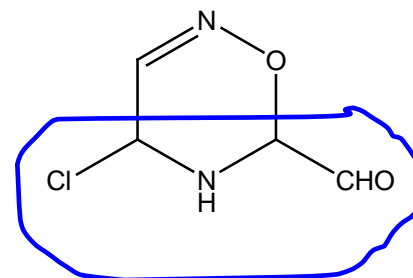
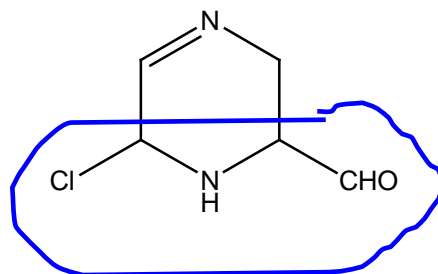
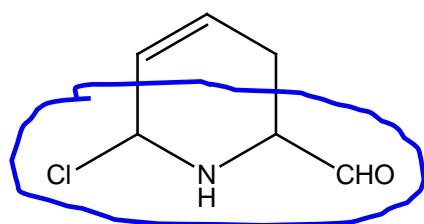
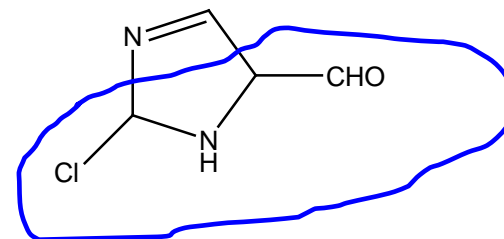
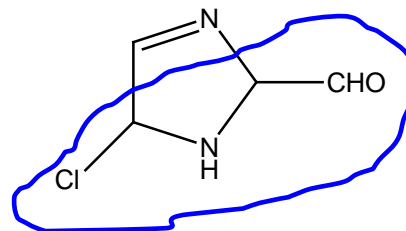
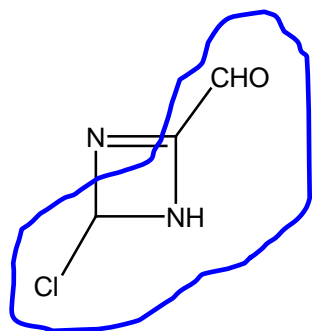
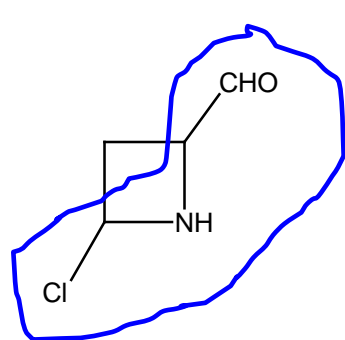


14874-70-5
B F₄



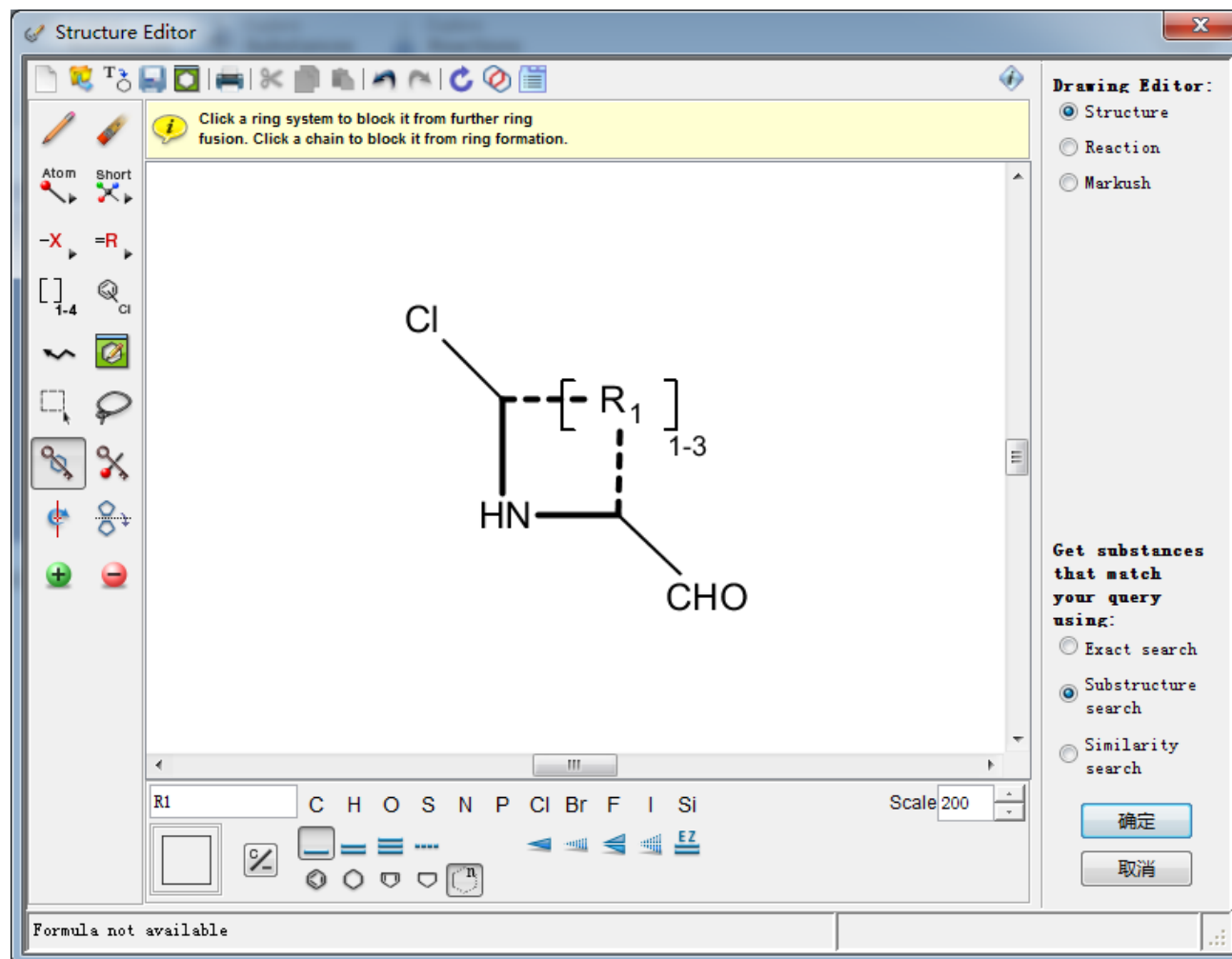
C₂₃ H₄₃ Cl N Ni P₂ . B F₄
Nickel(1+), [2,6-bis[[bis(1,1-dimethylethyl)phosphino-κP]methyl]pyridine-κN]chloro-, (SP-4-3)-, tetrafluoroborate(1-) (1:1)

我想获得以下的一系列物质




○ ○ ○ ○ ○ ○

结构定义



用亚结构检索获得所有的物质

亚结构检索结果



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Chemical Structure substructure > **substances (469)**

SUBSTANCES

[Get References](#) | [Get Reactions](#) | [Get Commercial Sources](#) | [Tools](#)

[Create Keep Me Posted Alert](#) | [Send to SciPlanner](#)

[Analyze](#) | [Refine](#)

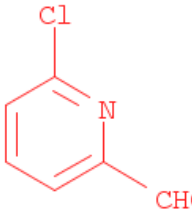
Sort by: Number of References

Answers per Page [50] View:

0 of 469 Substances Selected

1. **Substance Detail**
54087-03-5

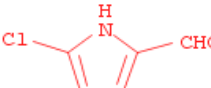
~33



C₆ H₄ Cl N O

2. **Substance Detail**
1757-28-4

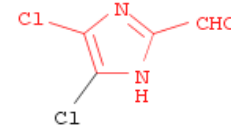
~19



C₅ H₄ Cl N O
 1H-Pyrrole-2-carboxaldehyde, 5-chloro-
[Experimental Properties](#)

3. **Substance Detail**
81293-97-2

~11



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

Analyze by:

Substance Role

Preparation

155

Reactant or Reagent

123

Biological Study

15

Uses

11

Prophetic in Patents

8

Properties

6

Formation, Nonpreparative

2

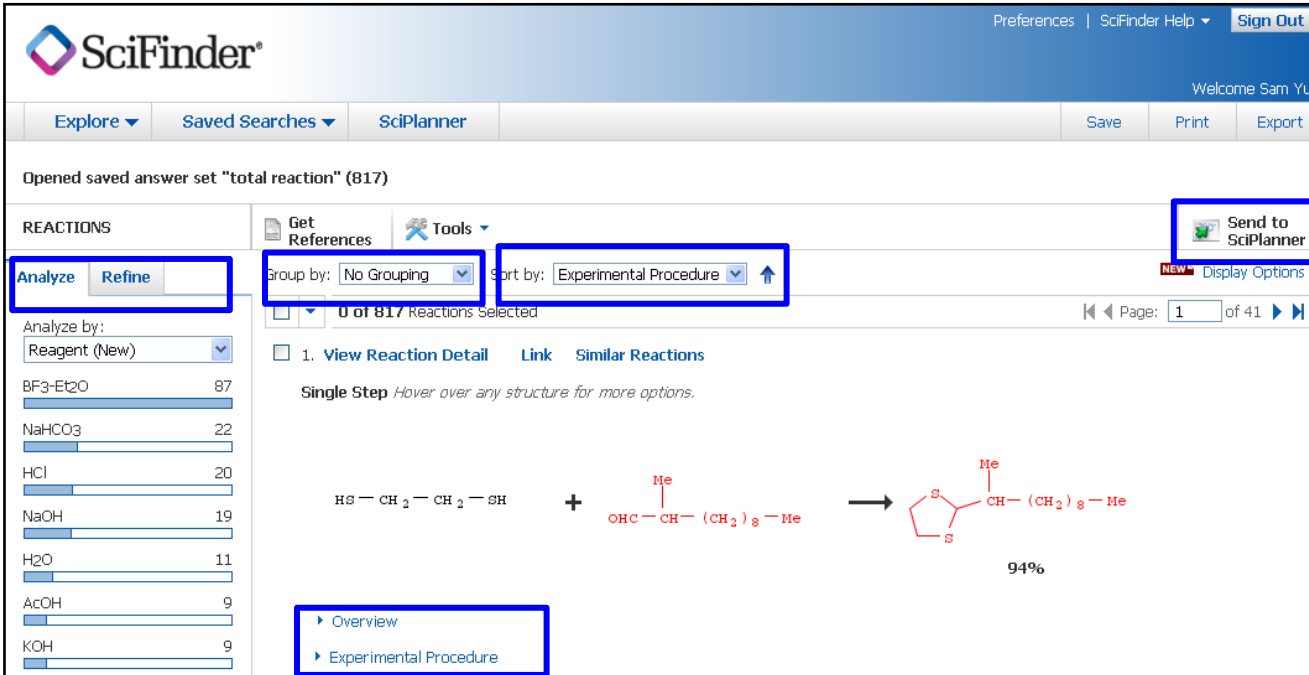
Analytical Study

1

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使用常见问题**

SciFinder Web中的反应记录



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Opened saved answer set "total reaction" (817)

REACTIONS

Analyze Refine

Get References Tools

Group by: No Grouping Sort by: Experimental Procedure

Send to SciPlanner

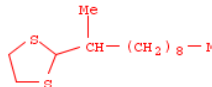
Analyze by: Reagent (New)

BF ₃ -Et ₂ O	87
NaHCO ₃	22
HCl	20
NaOH	19
H ₂ O	11
AcOH	9
KOH	9

0 of 817 Reactions Selected

1. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.

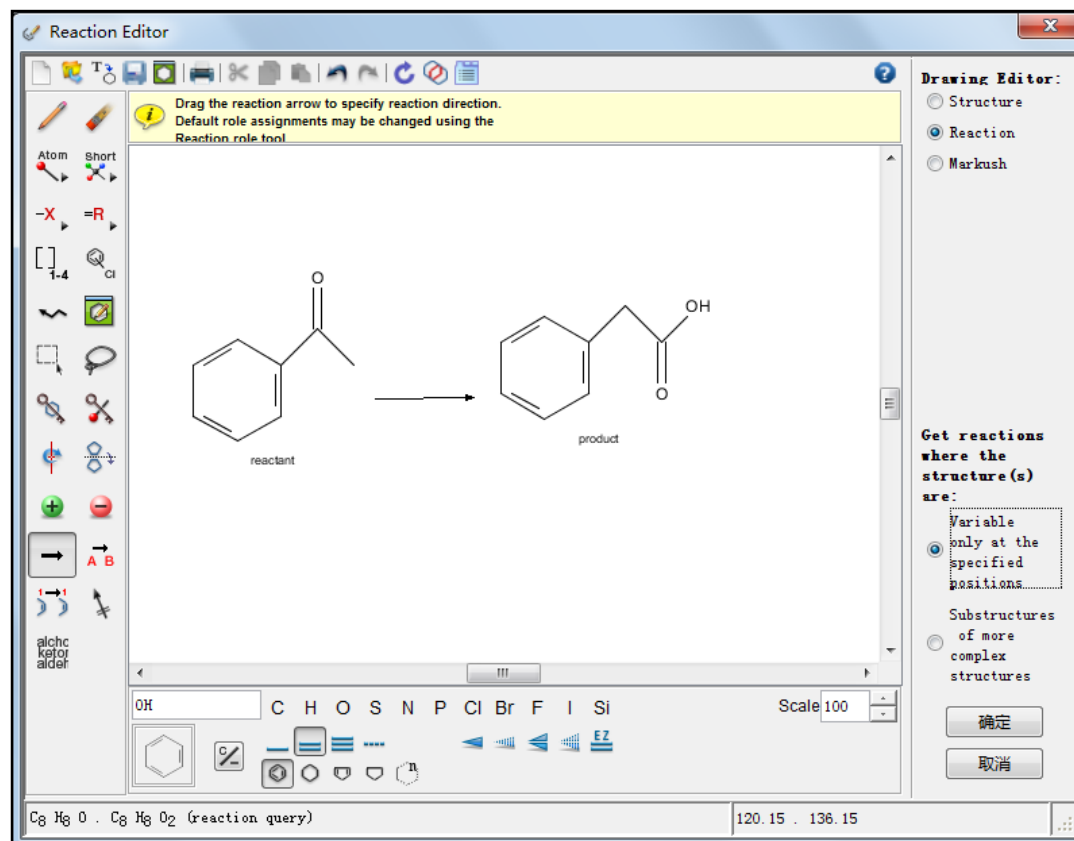
$\text{HS}-\text{CH}_2-\text{CH}_2-\text{SH}$ +
 $\text{OHC}-\overset{\text{Me}}{\text{CH}}-(\text{CH}_2)_8-\text{Me}$
 \longrightarrow


 94%

Overview
Experimental Procedure

1. 反应分组功能
2. 反应排序功能
3. 反应后处理功能
4. 反应全景及实验过程
5. SciPlanner

SciFinder反应检索



Allow variability only as specified: 仅在特定位点发生变化

Substructure: 亚结构检索, 允许有更多取代情况

反应检索界面

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Saved Searches
SciPlanner

REFERENCES

[Research Topic](#)
[Author Name](#)
[Company Name](#)
[Document Identifier](#)
[Journal](#)
[Patent](#)
[Tags](#)

SUBSTANCES

[Chemical Structure](#)
[Markush](#)
[Molecular Formula](#)
[Property](#)
[Substance Identifier](#)

REACTIONS

[Reaction Structure](#)

REACTIONS: REACTION STRUCTURE

Click image to change structure or view detail.

Import CXF

Search

[Advanced Search](#)

Search Type:

☒ Allow variability only as specified

☐ Substructure

SAVED ANSWER SETS

1

[Autosaved Reference Set](#)

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精确反应检索结果

Reaction Structure structure variable only at spe... > reactions (9)

REACTIONS ⓘ

[Get References](#)
[Tools](#)

[Send to SciPlanner](#)

Analyze **Refine**


Group by: No Grouping Sort by: Relevance

Answers per Page [15] Display:

0 of 9 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:S, R:Morpholine, R:p-MeC6H4SO3H, 8 h, 120-130°C	Reactants: 1, Reagents: 6, Catalysts: 1, Solvents: 2, Steps: 1, Stages: 7, Most stages in any one step: 7 References A facile synthesis of phenylacetic acids via Willgerodt-Kindler reaction under PTC condition By Alam, M. Mujahid and Adapa, Srinivas R. From Synthetic Communications, 33(1), 59-63; 2003
1.2 R:NaOH, C:TEBAC, S:H2O, 5 h, 100°C	
1.3 R:HCl, S:H2O, pH 6	
1.4 R:HCl, S:H2O, pH 2	
1.5 R:NaHCO3, S:H2O	
1.6 S:AcOEt	
1.7 R:HCl, S:H2O	

Group by Document 按照出处文献分类显示

Reaction Structure structure variable only at spe... > reactions (9)

REACTIIONS ?

Get References Tools

Analyze Refine

Analyze by: Catalyst

HSO₃F 2

BF₃·Et₂O 1

SeO₂ 1

TEBAC 1

Show More

Group by: Document Sort by: Relevance

No Grouping

Document

Transformation

Selected

1. A facile synthesis of phenylacetic acids via Willgerodt-Kindler reaction under PTC condition

1 Reaction Similar Reactions

Single Step Hover over any structure for more options.

Overview

Steps/Stages

1.1 R:S, R:Morpholine, R:p-MeC₆H₄SO₃H, 8 h, 120-130°C

1.2 R:NaOH, C:TEBAC, S:H₂O, 5 h, 100°C

1.3 R:HCl, S:H₂O, pH 6

1.4 R:HCl, S:H₂O, pH 2

1.5 R:NaHCO₃, S:H₂O

1.6 S:AcOEt

Notes

Reactants: 1, Reagents: 6, Catalysts: 1, Solvents: 2, Steps: 1, Stages: 7, Most stages in any one step: 7

References

A facile synthesis of phenylacetic acids via Willgerodt-Kindler reaction under PTC condition

Full Text

来自同一篇文献的反应都被整合到一起并集中显示

Group by Transformation 按照反应类型分类显示

Get References
Tools

Group by: Transformation Sort by: Frequency

0 of 9 Reactions Selected

☐ 1. Reduction of Carbonyl to Methylene in Aldehydes and Ketones/ Clemmensen Reduction/ Wolff-Kishner Reduction
4 Reactions

$$\text{R}-\overset{\text{O}}{\parallel}{\text{C}}-\text{R}^1 \longrightarrow \text{R}-\underset{\text{R}^1}{\underset{\text{H}}{\overset{\text{H}}{\text{C}}}}$$

☐ 2. Willgerodt/ Willgerodt-Kindler Reactions
4 Reactions

$$\text{R}-\overset{\text{O}}{\parallel}{\text{C}}-\text{CH}_3 \xrightarrow{(\text{NH}_4)_2\text{S}_n} \text{R}-\text{CH}_2-\overset{\text{NH}_2}{\underset{\text{Y}}{\parallel}{\text{C}}}$$

Y = O, S

☐ 3. Arylation at a Carbon Containing an Active Hydrogen/ Hurtley Reaction
1 Reaction

$$\text{Ar}-\text{Y} + \text{Z}-\text{CH}_2-\text{R} \longrightarrow \text{Ar}-\underset{\text{Z}}{\underset{\text{R}}{\text{CH}}}-\text{CH}_2-\text{R}$$

Y = OSO₂R', Halogen
Z = Electron withdrawing group

☐ 4. Multi-Step Reactions
4 Reactions

同一类反应被整合到一起并以通式结构集中显示；
仅适用于单步反应，未被分类的反应显示在结果集最后

获得有实验步骤的反应结果集

REACTIONS

Get References Tools

Send to SciPlanner

Analyze Refine

Analyze by:

Author Name

Khosrowshahi, Jaffar S. 2

Moriarty, Robert M. 2

Prakash, Om 2

Adapa, Srinivas R. 1

Alam, M. Mujahid 1

Andersch, Joerg 1

Chandalia, Sampatraj B. 1

Ghaffarzadeh, Mohammad 1

Haiss, Peter 1

Li, Jin-lian 1

Show More

Group by: No Grouping Sort by: Experimental Procedure

0 of 9 Reactions Selected

Experimental Procedure

1. View Reaction Details

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

Overview

Steps/Stages

1.1 R:S, R:Morpholine, R:*p*-MeC₆H₄SO₃H, 8 h, 120-130°C
 1.2 R:NaOH, C:TEBAC, S:H₂O, 5 h, 100°C
 1.3 R:HCl, S:H₂O, pH 6
 1.4 R:HCl, S:H₂O, pH 2
 1.5 R:NaHCO₃, S:H₂O
 1.6 S:AcOEt
 1.7 R:HCl, S:H₂O

Notes

Reactants: 1, Reagents: 6, Catalysts: 1, Solvents: 2, Steps: 1, Stages: 7, Most stages in any one step: 7

References

A facile synthesis of phenylacetic acids via Willgerdt-Kindler reaction under PTC condition
 Full Text
 By Alam, M. Mujahid and Adapa, Srinivas R.
 From Synthetic Communications, 33(1), 59-63; 2003

Experimental Procedure

Overview

Steps/Stages

1.1 R:S, R:Morpholine, R:*p*-MeC₆H₄SO₃H, 8 h, 120-130°C
 1.2 R:NaOH, C:TEBAC, S:H₂O, 5 h, 100°C
 1.3 R:HCl, S:H₂O, pH 6
 1.4 R:HCl, S:H₂O, pH 2
 1.5 R:NaHCO₃, S:H₂O
 1.6 S:AcOEt
 1.7 R:HCl, S:H₂O

Notes

Reactants: 1, Reagents: 6, Catalysts: 1, Solvents: 2, Steps: 1, Stages: 7, Most stages in any one step: 7

References

A facile synthesis of phenylacetic acids via Willgerdt-Kindler reaction under PTC condition
 Full Text
 By Alam, M. Mujahid and Adapa, Srinivas R.
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Experimental Procedure

Typical procedure for the preparation of phenylacetic acid: Acetophenone (1.20 g, 10 mmol), sulfur (0.64 g, 20 mmol), morpholine (3 mL, 30 mmol), *p*-toluene sulphonic acid (0.06 g, 0.35 mmol) were added and held at reflux under constant stirring in an oil bath at 120-130°C for 8 h. After completion of the reaction as indicated by TLC, the reaction mixture was allowed to cool and 20% NaOH and triethyl benzyl ammonium chloride (TEBA) (114 mg, 0.05 mmol) were added to the reaction mixture and continued hydrolysis for further 8 h at 100°C. After completion of the reaction as indicated by TLC; the reaction mixture was cooled and filtered, the filtrate was acidified with HCl to pH 6 and then filtered off. The filtrate was further acidified to pH 2 and thus crude phenylacetic acid was obtained. The acid was then taken into 10% NaHCO₃ solution and was washed with ethyl acetate (3 x 30 mL), separated the organic layer, and the aqueous layer was acidified with dilute HCl, to yield the pure phenylacetic acid as solid. In case of products from hydroxy acetophenones, the products were extracted into ethyl acetate. The dried organic layer was evaporated under reduced pressure to yield pure phenylacetic acid. Phenylacetic acid, yield 80%.

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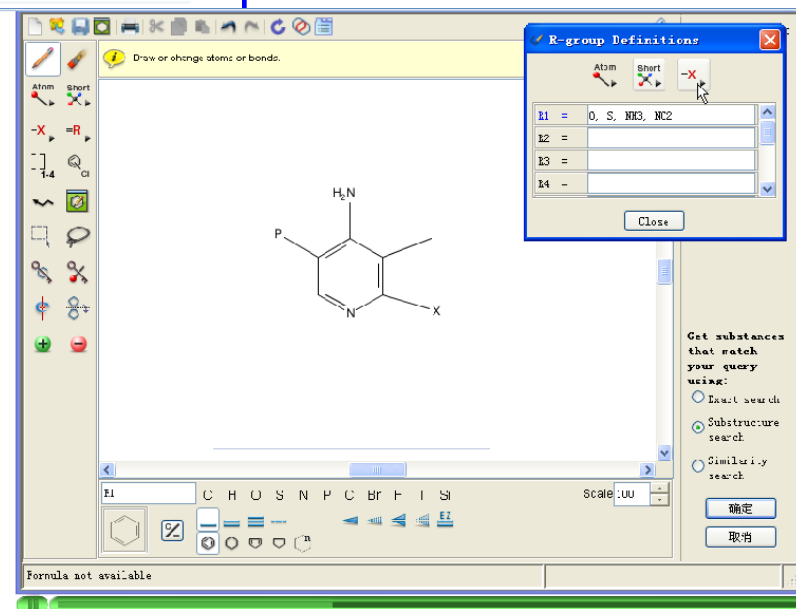
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