

钱欣博士
Application Specialist

cqian@acs-i.org

如何使用SciFinder检索反应信息

反应检索

- 反应检索绘制工具及反应信息详情
- 如何通过**Analyze**、**Refine**来精选反应
- 巧用原子标记工具和位置标记工具提高检索精度
- 通过**PatentPak**节省反应信息检索时间
- 高级反应案例分享
 - 片段反应
 - 按照化合物类型查找反应
- 手性反应专题
 - 手性分子合成反应
 - 手性构型翻转反应
 - 手性分子拆分反应

反应检索：精确结构反应检索



反应箭头



反应角色定义工具



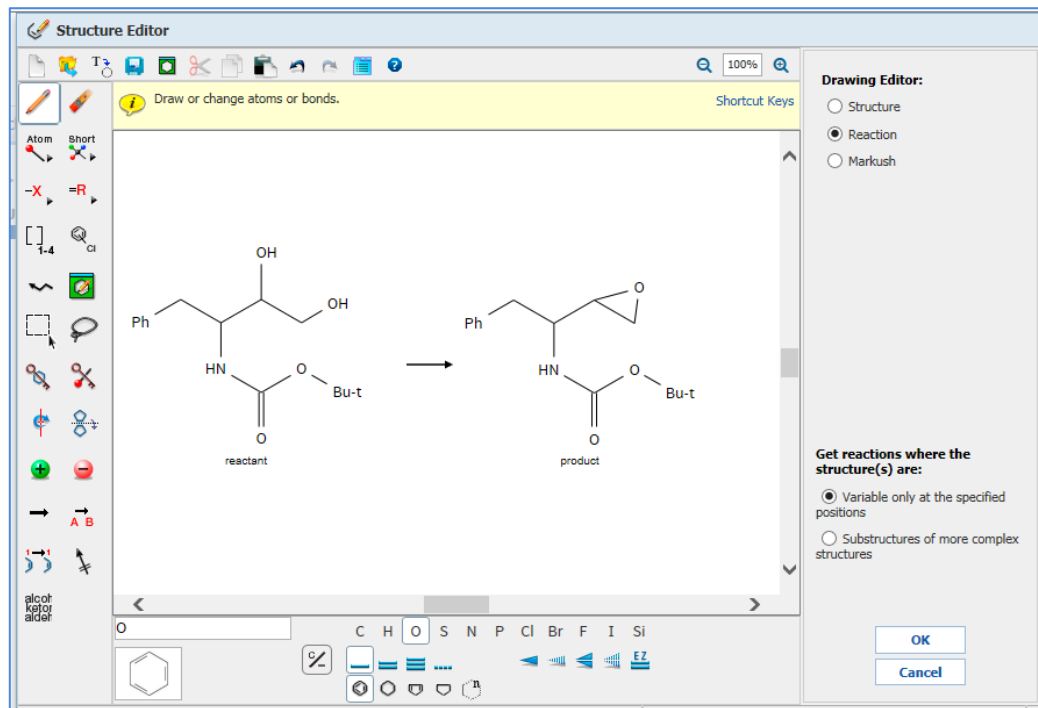
反应原子标记工具



反应位置标记工具



官能团列表



反应结果集

点击Transformation,
获得反应类型的分类

Group by: Transformation Sort by: Frequency

0 of 18 Reactions Selected

☐ 1. Conversion of Alcohols to Ether/ Mitsunobu Etherification
12 Reactions

$$R-OH + R^1-OH \longrightarrow R-O-R^1$$

☐ 2. Multi-Step Reactions
6 Reactions

REACTIONS

Analyze Refine

Analyze by: Reagent

Et ₃ N	6
PPh ₃	6
EtO ₂ CN=NCO ₂ Et	4
MeSO ₂ Cl	4
1H-Imidazole	3
Bu ₄ N ⁺ •F ⁻	3
K ₂ CO ₃	3
NaOMe	3
<i>t</i> -BuSiMe ₂ Cl	3
C ₃ H ₅ N	2

Show More

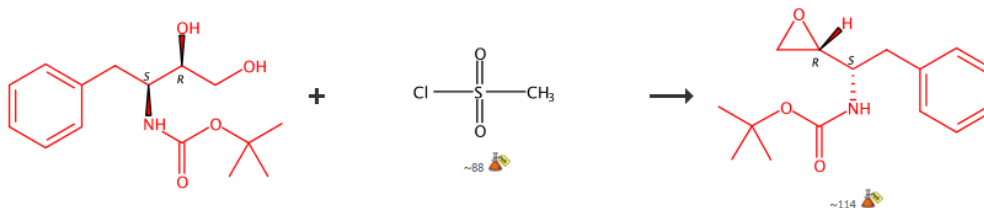
Get References Tools

Group by: No Grouping Document Transformation

Sort by: Relevance

16. View Reaction Detail Link

2 Steps Hover over any structure for more options.



Overview

Steps/Stages

- 1.1 R:Et₃N, S:(*t*-Pr)₂O
2.1 R:NaOMe, S:AcOEt, S:MeOH

Notes

1) ice-cooling for 1 h, 2) ice-cooling for 10 min, Reactants: 2, Reagents: 2, Solvents: 3, Steps: 2, Stages: 2, Most stages in any one step: 1

References

Process for producing optically active threo-3-amino-1,2-epoxy compounds

Quick View

By Sagawa, Yukihiro et al.

From PCT Int. Appl., 9938855, 05 Aug 1999



SciFinder
A CAS SOLUTION

反应结果处理：分析

13种分析选项

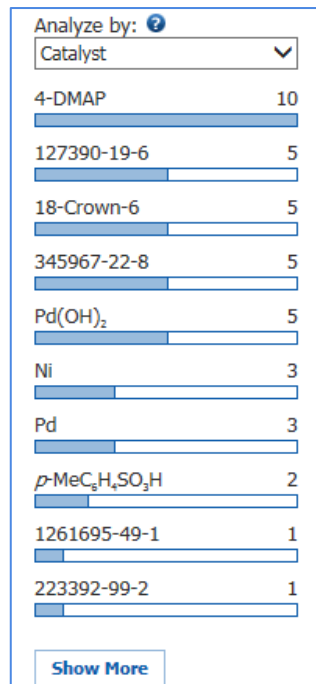
Analyze Refine

Analyze by: ?

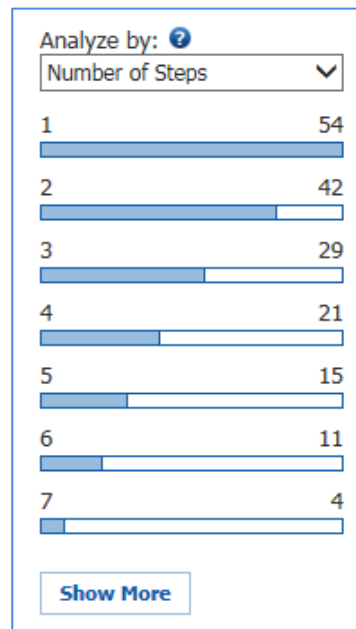
- Author Name
- Catalyst
- Company-Organization
- Document Type
- Experimental Procedure
- Journal Name
- Language
- MethodsNow
- Number of Steps
- Product Yield
- Publication Year
- Reagent
- Solvent



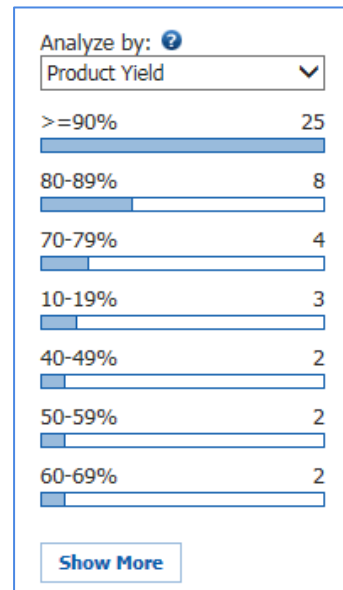
催化剂



反应步数



产率



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针对感兴趣的反应查看实验详情

☐ 0 of 3 Reactions Selected

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

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

Overview

Steps/Stages

1.1 R:Et₃N, R:4-DMAP, S:PhMe

1.2

2.1 R:(NH₄)F, R:AcOH, S:MeOH

3.1 R:^tBuOK, S:Me₂CHOH, S:THF

Notes

3) key step, stereoselective, Reactants: 3, Reagents: 5, Solvents: 4, Steps: 3, Stages: 4, Most stages in any one step: 2

References

Process Research and Development for an Efficient Synthesis of the HIV Protease Inhibitor BMS-232632

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

By Xu, Zhongmin et al

From Organic Process Research & Development, 6(3), 323-328; 2002

Experimental Procedure

METHODSNOW™

Experimental Procedure

数字标记

Experimental Procedure

OPR&D

Step 1

冗长的化学名称

[3-tert-butyl-dimethylsilyloxy-2(S)-[(methylsulfonyl)-oxy]-1(S)-(phenylmethyl)propyl]-carbamic Acid, 1,1-Dimethylethyl Ester (12). A solution of diol 10 (544 g, 1.034 mol) in 1.2 L of toluene was heated to 88 °C, and a clear solution was obtained. The solution was then cooled to 50 °C. Dimethylamino pyridine (23.6 g, 0.195 mol) and triethylamine (325 mL, 2.32 mol) were charged followed by the slow addition of tert-butyl-dimethylsilyl chloride (350 g, 2.32 mol) while keeping the internal temperature around 50 °C. The reaction mixture was cooled to 0 °C over 3 h. Triethylamine (417 mL) was added followed by the slow addition of trifluoromethanesulfonyl chloride (198 mL), keeping the internal temperature under 5 °C. The resulting mixture was stirred at 0 °C for about 3 h. The solid was filtered through Celite and washed with toluene (2 × 700 mL). The filtrate was washed with water (4 L), 1 N HCl (4 L), and brine (4 L), in that order, and then concentrated in a vacuum to afford 1.04 kg of product 12 as a yellow oil. This product was subjected to the next step without further purification.

Step 2

数字标记

[3-Hydroxy-2(S)-[(methylsulfonyl)oxy]-1(S)-(phenyl-methyl)propyl]-carbamic Acid, 1,1-Dimethylethyl Ester (13). Into a reactor was charged ammonium fluoride (358 g, 9.67 mol), a solution of the crude mesylate 12 (1.04 kg, 1.034 mol) in methanol (5.6 L), and acetic acid (550 mL). The mixture was stirred at ambient temperature for 11 h. The reaction mixture was concentrated to dryness to afford a solid, which was dissolved in 11 L of methyl tert-butyl ether. The resulting solution was washed with water (5 L), 5% sodium bicarbonate (3 × 4 L), and brine (4 L) and then dried over MgSO₄ (300 g). Filtration and partial concentration afforded 5 L of solution. The concentrated solution was then cooled to 4 °C and stirred at this temperature for 18 h to give a slurry. The solid was filtered, washed with cold MTBE (200 mL) and dried under partial pressure to afford 489.1 g of 13. The filtrate was concentrated to 1 L, cooled to 4 °C, and stirred at this temperature for 18 h to give a slurry. Another 61.7 g of solid was obtained after filtration and drying. Thus, a total of 550.8 g of product 13 was obtained as a white solid (80% yield, AP 98).

Step 3

N-(tert-butyloxycarbonyl)-2(S)-amino-1-phenyl-3(R)-3,4-epoxy-butane (6). To a clear solution of hydroxy mesylate 13 (629.9 g, 1.75 mol) in a mixture of IPA (6.3 L) and THF (1.8 L) at 17 °C, was added KO^tBu (207 g, 95%, 1.75 mol) over 20 min. The mixture was stirred for 1.5 h followed by addition of 30 mL of acetic acid over 15 min. The resulting solution was concentrated under vacuum to dryness to afford a white solid. The solid was dissolved in MTBE (9.0 L), and the resulting solution was washed with water (4.5 L), saturated sodium bicarbonate solution (4.5 L), and brine (4.5 L), dried over anhydrous Na₂SO₄, filtered, and concentrated to give an oil (455.2 g). The oil was diluted with hexane (1.3 L) followed by addition of water (200 mL). The mixture was cooled to -4 °C, and solid was observed. The solid was collected by filtration, washed with 700 mL of cold hexane (0 °C), and dried under vacuum for 18 h to give epoxide 6 as a white solid (400.5 g, 88% yield, AP 97).

字母简写

整段文字描述实验步骤



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窗口

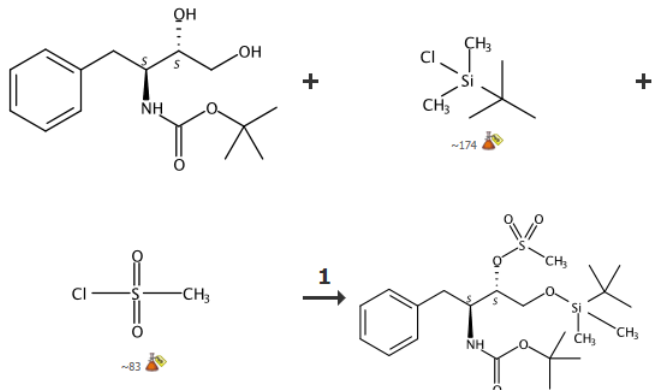
MethodsNow

Process Research and Development for an Efficient Synthesis of the HIV Protease Inhibitor BMS-232632

By Xu, Zhongmin; Singh, Janak; Schwinden, Mark D.; Zheng, Bin; Kissick, Thomas P.; Patel, Bharat; Humora, Michael J.; Quiroz, Fernando; Dong, Lin; Hsieh, Dau-Ming et al.
From Organic Process Research & Development, 6(3), 323-328; 2002
Published by American Chemical Society

Reaction Steps

1 2 3



产物，反应物，试剂，溶剂，步骤，
反应类型，规模，CAS方法号

CAS RN即时查看物质

MethodsNow

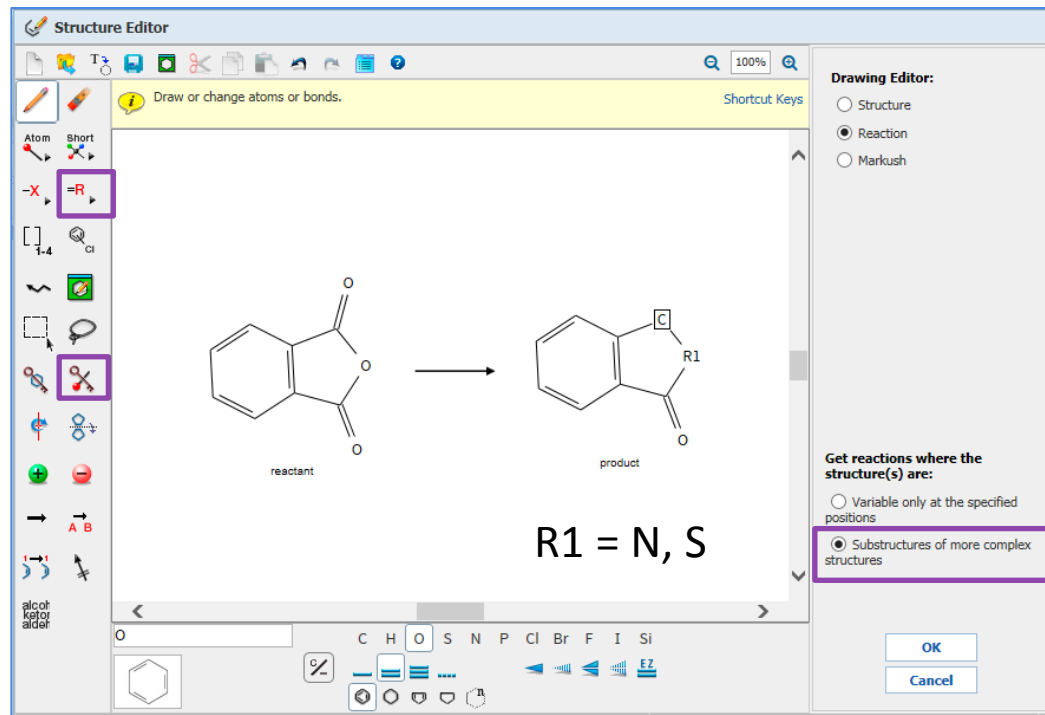
Products	Carbamic acid, [(1 <i>S</i> ,2 <i>S</i>)-3-[[[(1,1-dimethylethyl)dimethylsilyloxy]-2-[(methylsulfonyl)oxy]-1-(phenylmethyl)propyl]-, 1,1-dimethylethyl ester, CAS RN: 437713-03-6
Reactants	Carbamic acid, <i>N</i> -[(1 <i>S</i> ,2 <i>S</i>)-2,3-dihydroxy-1-(phenylmethyl)propyl]-, 1,1-dimethylethyl ester, CAS RN: 149451-80-9 <i>tert</i> -Butyl(dimethylsilyl) chloride, CAS RN: 18162-48-6 Methanesulfonyl chloride, CAS RN: 124-63-0
Reagents	Triethylamine, CAS RN: 121-44-8 4-(Dimethylamino)pyridine, CAS RN: 1122-58-3
Solvents	Toluene, CAS RN: 108-88-3
Procedure	<ol style="list-style-type: none"> 1. Heat the solution of chiral diol (544 g) in 1.2 L of toluene to 88 °C. 2. Cool the solution to 50 °C. 3. Charge the dimethylamino pyridine (23.6 g, 0.195 mol) and triethylamine (325 mL, 2.32 mol) followed by the slow addition of <i>tert</i>-butyl-dimethylsilyl chloride (350 g, 2.32 mol) while keeping the internal temperature around 50 °C. 4. Cool the reaction mixture to 0 °C over 3 hours. 5. Add triethylamine (417 mL) followed by the slow addition of trifluoromethanesulfonyl chloride (198 mL) while keeping the internal temperature under 5 °C. 6. Stir the resulting mixture at 0 °C for about 3 hours. 7. Filter the solid through Celite. 8. Wash the solid with toluene (2 x 700 mL). 9. Wash the filtrate with water (4 L), 1 N HCl (4 L) and brine (4 L). 10. Concentrate the filtrate in a vacuum.
Scale	gram
CAS Method Number	3-008-CAS-1545731

PDF或XLS格式

Print/Export

Close

反应检索：亚结构反应检索



输入的反应物和产物的结构会被修饰，但母体结构不变

反应结果集

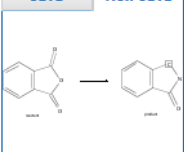
REACTIONS ?

Analyze Refine

Refine by: ?
☒ Reaction Structure
☐ Product Yield
☐ Number of Steps
☐ Reaction Classification
☐ Excluding Reaction Classification
☐ Non-participating functional groups

Structure Editor:

Java Non-Java



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

Refine

Get References

Tools

Group by: No Grouping

Sort by: Relevance

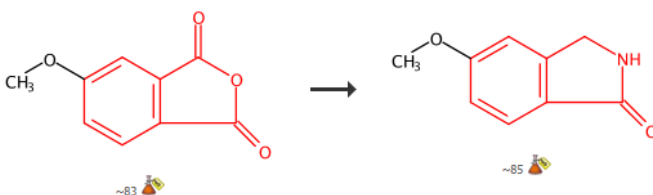
↓

0 of 1208 Reactions Selected

Page: 1 of 81

1. View Reaction Detail Link

2 Steps Hover over any structure for more options.



Overview

Steps/Stages

1.1 R:H₂NCHO
 2.1 R:HCl, R:Sn, S:H₂O, 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

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11

反应结果处理：筛选

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)、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



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反应类型筛选

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

REACTIONS ? Get References Tools

Analyze Refine

Group by: No Grouping Sort by: Relevance

0 of 1154 Reactions Selected

Page: 1 of 77

Refine by: ?

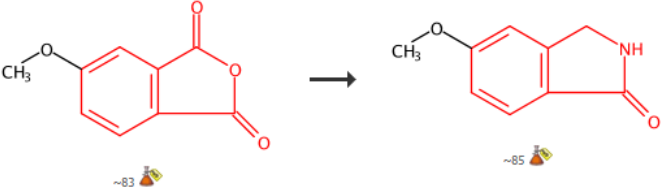
- ☐ Reaction Structure
- ☐ Product Yield
- ☐ Number of Steps
- ☐ Reaction Classification
- ☒ Excluding Reaction Classification
- ☐ Non-participating functional groups

Excluding Reaction Classification(s):

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

1. View Reaction Detail Link

2 Steps Hover over any structure for more options.



~83 ~85

Overview

Steps/Stages

1.1 R:H₂NCHO
2.1 R:HCl, R:Sn, S:H₂O, 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.



限定某官能团参与反应

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

REACTIONS

Analyze **Refine**

Group by: Sort by:

☐ 0 of 435 Reactions Selected Display Options Page: 1 of 29

Refine by:

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

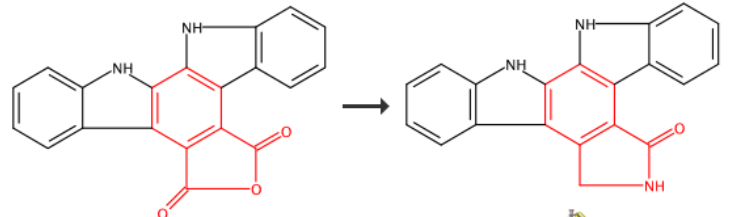
Non-participating Functional Group(s)
View:

2 Selected [Clear Selections](#)

- ☐ AMINES
- ☐ CARBONATE DERIVAT
- ☐ CARBOXY DERIVATIVE
- ☐ HALIDES
- ☒ **HETEROCYCLES**
- ☒ **KETONES**
- ☐ ORGANOMETALLICS

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

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



Overview

Steps/Stages

1.1 R: NH₄OAc, 3 h, 140°C
2.1

Notes

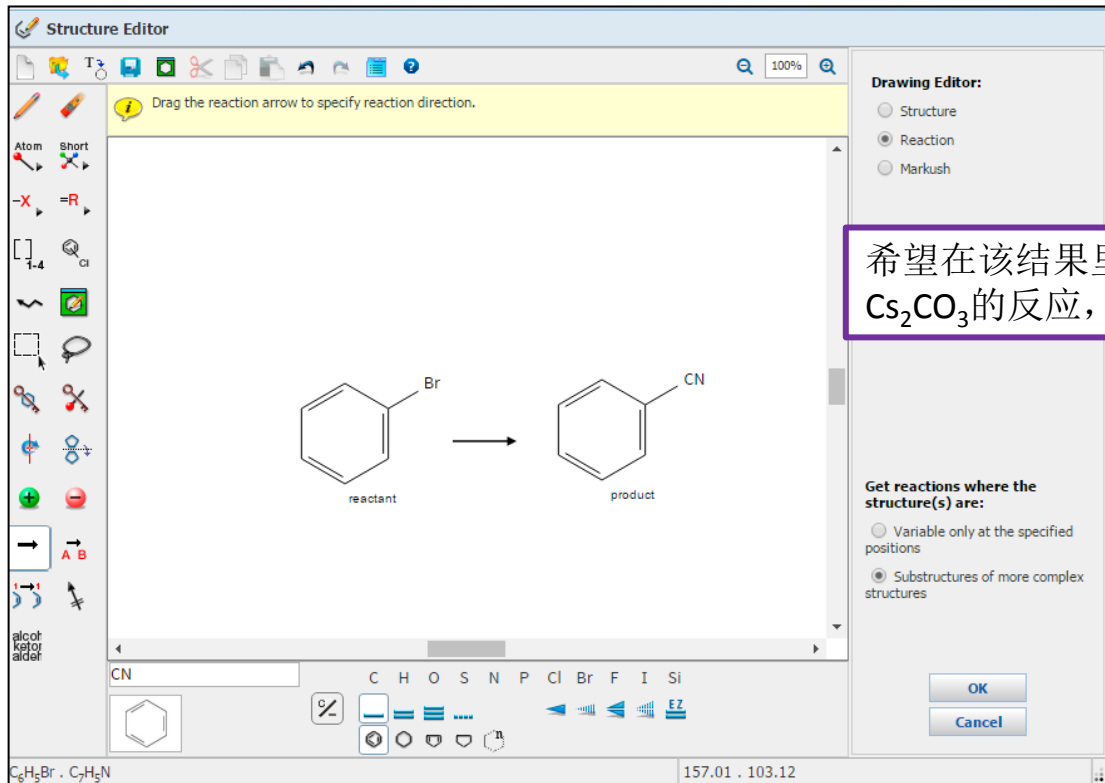
1) thermal, 2) literature preparation, no experimental detail, Reactants: 1, Reagents: 1, Steps: 2, Stages: 2, Most stages in any one step: 1

References

反应检索

- 反应检索绘制工具及反应信息详情
- 如何通过Analyze、Refine来精选反应
- 巧用原子标记工具和位置标记工具提高检索精度
- 通过PatentPak节省反应信息检索时间
- 高级反应案例分享
 - 片段反应
 - 按照化合物类型查找反应
- 手性反应专题
 - 手性分子合成反应
 - 手性构型翻转反应
 - 手性分子拆分反应

案例一：检索由溴苯转化为苯腈的反应



希望在该结果里进一步限定:溶剂为DMF, 试剂为 Cs_2CO_3 的反应, 应如何操作?

获得34万多条反应，噪音较大

Reaction Structure substructure > reactions (343247)

REACTIONS

Get References Tools

Analyze Refine

Sample Analysis:
Reagent

HCl ≥ 8898

K_2CO_3 ≥ 5988

Et_3N ≥ 5774

H_2O ≥ 4430

NaOH ≥ 4293

$EtH(Pr)_2$ ≥ 3928

$NaHCO_3$ ≥ 3884

Disodium carbonate ≥ 3711

CS_2CO_3 ≥ 3314

F_3CCO_2H ≥ 3183

Show More

Group by: No Grouping Sort by: Relevance

0 of 343247 reactions Selected

1. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.

• 4 K⁺
~24

~113

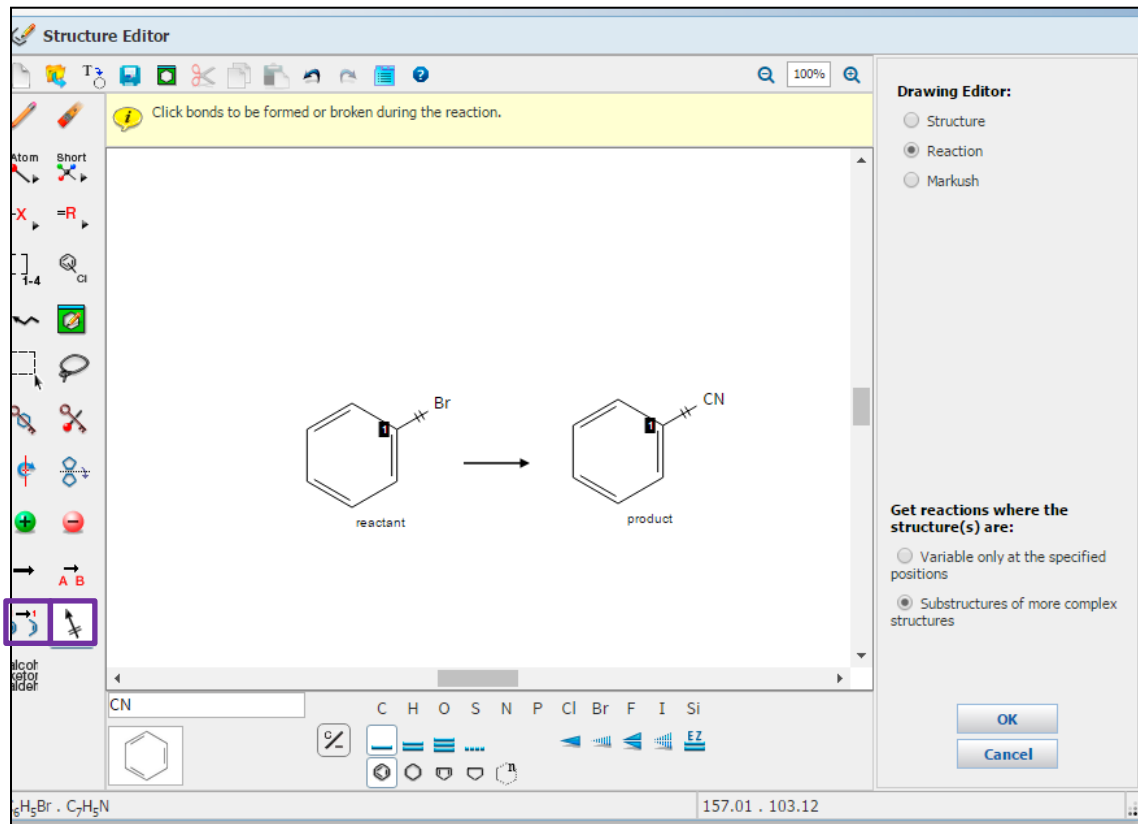
99%
~87

Overview
Steps/Stages

1.1 C:1863984-13-7 (inclusion complexes with palladium nanopar), S:DMF, 15 h, 140°C

Notes
alternative reaction conditions shown, nanoparticle cat.
Cubator 1, Stage 1, Stage 1, Most Reaction...

可以通过反应原子标记工具和反应位置标记工具提高反应检索精度



获得反应97188条

Explore ▾ Saved Searches ▾ SciPlanner Save Print Export

Reaction Structure substructure > reactions (97188)

REACTIONS ⓘ Get References Tools ▾ Send to SciPlanner

Analyze Refine

Sample Analysis: ⓘ
Reagent ▾

HCl	≥ 9324
Et ₃ N	≥ 5595
H ₂ O	≥ 5573
NaHCO ₃	≥ 5064
NaOH	≥ 4585
K ₂ CO ₃	≥ 4516
EtN(Pr- <i>i</i>) ₂	≥ 3777
NH ₄ Cl	≥ 3625
F ₃ CCO ₂ H	≥ 3264

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

0 of 97188 reactions Selected

1. View Reaction Detail ⓘ Link ⓘ Similar Reactions

Single Step Hover over any structure for more options.

• 4 K⁺ ~25 ⓘ

~116 ⓘ

99% ~93 ⓘ

使用反应结果集中的Analyze功能，需要将结果集压缩到20000以下

将反应限定为1步反应

Explore ▾ Saved Searches ▾ SciPlanner Save Print Export

Reaction Structure substructure > reactions (97188) > refine "1 step" (9551)

REACTIONS ⓘ Get References Tools ▾ Send to SciPlanner

Analyze Refine

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

0 of 9551 Reactions Selected

1. View Reaction Detail ⓘ Link ⓘ Similar Reactions

Single Step Hover over any structure for more options.

Refine by: ⓘ

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

Number of Steps:

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

Refine

The reaction scheme shows an iron complex (Fe²⁺) with four cyanide (C≡N) ligands reacting with bromobenzene (a benzene ring with a bromine atom) to form a nitrile product (a benzene ring with a cyano group). The product is labeled with a 99% yield. Below the reaction, there are two small icons: one labeled '~116' and another labeled '~93'.

• 4 K⁺
~25

通过Analyze by Solvent选择在DMF溶剂中进行的反应

Explore ▾ Saved Searches ▾ SciPlanner

Save Print Export

4,977 reactions with the Solvent **DMF** are displayed [Keep Analysis](#) [Clear Analysis](#)

Reaction Structure substructure > reactions (97188) > refine "1 step" (9551) > refine "1 step" (9551)

REACTIONS ⓘ Get References Tools ▾ Send to SciPlanner

Analyze Refine

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

0 of 9551 Reactions Selected

1. View Reaction Detail Link Similar Reactions

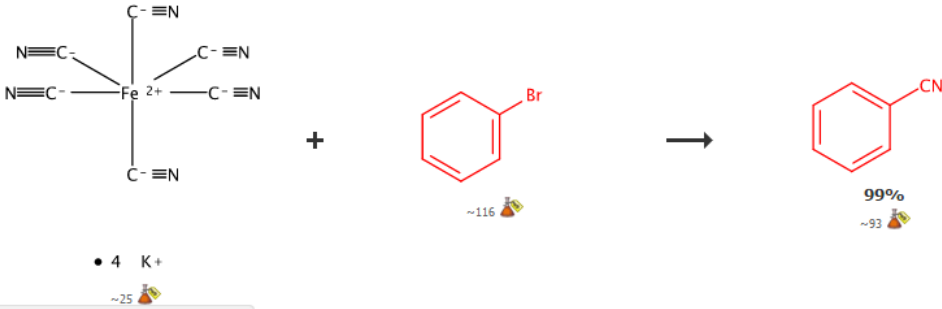
Single Step Hover over any structure for more options.

Analyze by: Solvent

DMF 4977

H ₂ O	2088
NMP	1510
THF	752
AcNMe ₂	586
CH ₂ Cl ₂	470
C ₆ H ₅ N	432
PhMe	284
MeCN	266

Waiting for scifinder.cas.org...



在反应结果集中继续通过Analyze by Reagent选择Cs₂CO₃作为试剂的反应

Reaction Structure substructure > reactions (97188) > refine "1 step" (9551) > refine "1 step" (9551) > keep analysis "Solvent" (4977)

REACTIONS

Get References Tools

Analyze Refine

Analyze by: Reagent

H ₂ O	345
HCl	300
K ₂ CO ₃	190
NH ₃	181
NH ₄ OH	164
FeCl ₃	155
Zn	134
Disodium carbonate	121
NaHCO ₃	115
NH ₄ Cl	100

Show More

Group by: [No Grouping] Sort by: [No Grouping]

0 of 4977 Reactions Selected

1. View Reaction Detail

Single Step Hover over any structure

• 4 K⁺
~25

Overview
Steps/Stages

1.1 C:1863984-13-7 (incl...)

Analyze - Reagent

261 Items 1 Selected Export

Sort by: Frequency Page: 1 of 6

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

<input type="checkbox"/> O ₂	60
<input type="checkbox"/> EtN=C=N(CH ₂) ₃ NMe ₂ • HCl	59
<input type="checkbox"/> LiOH	57
<input type="checkbox"/> CuCN	56
<input type="checkbox"/> H ₂ SO ₄	54
<input type="checkbox"/> TMEDA	52
<input type="checkbox"/> (NO)H(SO ₄)	51
<input type="checkbox"/> AcOH	49
<input checked="" type="checkbox"/> Cs ₂ CO ₃	48
<input type="checkbox"/> NaH	45

Apply Cancel

获得以 DMF为溶剂, Cs_2CO_3 为试剂的一步反应, 保存结果集

Analyze by: Reagent

Cs_2CO_3	48
KI	24
1427296-27-2	11
HCl	6
Et_3N	4
H_2O	4
CuCl_2	3
EtOH	3
$\text{F}_3\text{CCO}_2\text{H}$	3
Fe	3

[Show More](#)

0 of 48 Reactions Selected
1. [View Reaction Detail](#) [Link](#) [Similar Reactions](#)

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

• 3 K⁺

Overview

Steps/Stages

1.1 R:

R: KI, R: Cs_2CO_3 , C: CuI, S: DMF, 8 h, 130°C

Notes

alternative preparation shown, pressure tube used, Reactants: 2, Reagents: 3, Catalysts: 1, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

A new oxazole ligand for the copper-catalyzed cyanation of aryl halides with $\text{K}_4[\text{Fe}(\text{CN})_6]$

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

By Sajadi, S. Mohammad and Maham, Mehdi

From Letters in Organic Chemistry, 11(2), 136-140; 2014

ACS / Proprietary and Confidential / Do Not Distribute

SciFinder®
A CAS SOLUTION

23

在初始反应结果集中限定2步反应，重复刚才的步骤

Explore ▼ Saved Searches ▼ SciPlanner

Reaction Structure substructure > reactions (97188)

REACTIONS ?

Get References Tools ▼

Analyze Refine

Group by: No Grouping Sort by: Relevance

0 of 97188 Reactions Selected

1. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.

Refine by: ?

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

Number of Steps: 2

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

Refine

The reaction scheme shows an iron complex reacting with bromobenzene to form a nitrile. The iron complex is a central Fe²⁺ ion coordinated by six cyanide (C≡N) groups. The bromobenzene molecule is shown in red, with a benzene ring and a bromine atom. The product is a nitrile, also shown in red, with a benzene ring and a cyano group (CN). The reaction is labeled with a yield of 99% and a reference number of ~116.

获得以 DMF 为溶剂, Cs_2CO_3 为试剂的 2 步反应, 保存结果集

Reaction Structure substructure > reactions (97188) > refine "2 steps" (13339) > keep analysis "Solvent" (5734) > keep analysis "Reagent" (249)

REACTIONS ?

Get References Tools

Analyze Refine

Analyze by: Reagent

Cs_2CO_3	249
HCl	26
$\text{F}_3\text{CCO}_2\text{H}$	15
NH_4Cl	14
Zn	14
NaI	12
NMP	12
NaCl	11
H_2O	10

Group by: No Grouping Sort by: Relevance

0 of 249 Reactions Selected

1. View Reaction Detail Link

2 Steps Hover over any structure for more options.

Chemical reaction scheme showing the conversion of 1-iodo-4-bromobenzene (left, ~144) to 1,4-dicyanobenzene (right, ~106) using a ferrocene-based catalyst (middle, ~111). The catalyst is a ferrocene complex with three cyanide ligands and a 3+ iron center. The reaction is shown with reagents Cs_2CO_3 and solvent DMF.

在Saved Searches中的反应结果集中找到刚保存过的结果集

Explore ▾ Saved Searches ▾ SciPlanner

Reaction Structure: [Saved Answer Sets](#)
[Keep Me Posted](#)
[History](#)

REACTIONS ⓘ [Tools ▾](#)

Group by: No Grouping ▾ Sort by: Relevance ▾

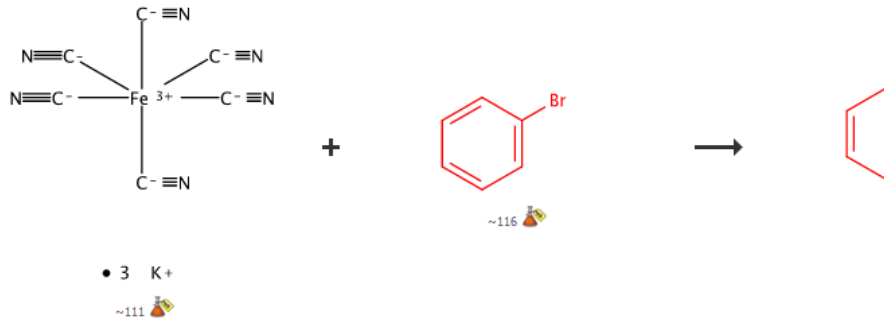
0 of 48 Reactions Selected

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

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

Analyze by: [?](#)
Reagent ▾

Cs ₂ CO ₃	48
KI	24
1427296-27-2	11
HCl	6
Et ₃ N	4
H ₂ O	4
CuCl ₂	3
EtOH	3
F ₃ CCO ₂ H	3


• 3 K+
~111

合并结果集

Explore Saved Searches SciPlanner

Reaction Structure substructure > reactions (97188) > refine "1 step" (9551) > keep analysis "Solvent" (4977) > keep analysis "Reagent" (48)

SAVED ANSWER SETS Combine selected saved answer sets and view combined set.

SAVED SEARCHES

- ☒ Saved Answer Sets
- ☐ Keep Me Posted
- ☐ History

2 of 49 Reaction Answer Sets Selected **References (38)** **Substances (8)** **Reactions (49)**

Selection	Search Name	Count	Path	Actions	Created
<input checked="" type="checkbox"/>	1010dmf1step (48)		Reaction Structure substructure > reactions (97188) > refine "1 step" (9551) > keep analysis "Solvent" (4977) > keep analysis "Reagent" (48)	Edit Link	Saved Oct 10, 2016
<input checked="" type="checkbox"/>	1010dmf2step (249)		Reaction Structure substructure > reactions (97188) > refine "2 steps" (13339) > keep analysis "Reagent" (249)		
<input type="checkbox"/>	DMF-cyanation (4977)		Reaction Structure substructure > reactions (97188) > refine "1 step" (9551) > keep analysis "Solvent" (4977)		
<input type="checkbox"/>	1010reaction2 (813)		Chemical Structure substructure > substances (164) > get reactions (813)		
<input type="checkbox"/>	1010reaction1 (780)		Chemical Structure substructure > substances (3920) > get reactions (780)		
<input type="checkbox"/>	a2 (3728)		Chemical Structure exact with limiters > substances (11) > 1517-69-7 > get reactions (3728)		
<input type="checkbox"/>	a1 (697)				

Combine Answer Sets

Select an option for combining the two selected saved answer sets:

- Combine** Include all reactions from both sets
- Intersect** Include only reactions that appear in both sets
- Exclude** Include only answers from 1010dmf1step that are not in 1010dmf2step
- Exclude** Include only answers from 1010dmf2step that are not in 1010dmf1step

Combine Answer Sets **Cancel**

反应检索

- 反应检索绘制工具及反应信息详情
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 - 片段反应
 - 按照化合物类型查找反应
- 手性反应专题
 - 手性分子合成反应
 - 手性构型翻转反应
 - 手性分子拆分反应

通过物质检索获得香根酮的制备的专利文献

Substance Identifier "solavetivone" > substances (1) > get references (43) > refine "Patents only" (5)

SUBSTANCES **Get References** Retrieve references for selected substances. **Tools** ▾

Analyze **Refine**

Analyze by: Substance Role ▾

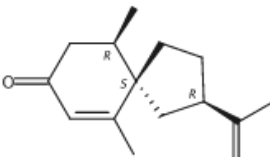
Analytical Study 1
Biological Study 1
Formation, Nonpreparative 1
Occurrence 1
Preparation 1
Process 1
Properties 1
Reactant or Reagent 1

Sort by: CAS Registry Number ▾

0 of 1 Substance Selected

1. 54878-25-0 🔍

~211



Rotation (-), Absolute stereochemistry.

C₁₅ H₂₂ O
Spiro[4.5]dec-6-en-8-one, 6,10-dimethyl-2-(1-methyl-2-propenyl)-, (2*R*,5*S*,10*R*)-
▶ **Key Physical Properties**
Spectra

Get References

Retrieve references for:

☒ All substances
☐ Selected substances

Limit results to:

<input type="checkbox"/> Adverse Effect, including toxicity	<input checked="" type="checkbox"/> Preparation
<input type="checkbox"/> Analytical Study	<input type="checkbox"/> Process
<input type="checkbox"/> Biological Study	<input type="checkbox"/> Properties
<input type="checkbox"/> Combinatorial Study	<input type="checkbox"/> Prophetic in Patents
<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**

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REFERENCES	Get Substances	Get Reactions	Get Related Citations	Tools
Analyze Refine Categorize				
Sort by: Accession Number ▼				
Refine by: <ul style="list-style-type: none"> <input type="radio"/> Research Topic <input type="radio"/> Author <input type="radio"/> Company Name <input checked="" type="radio"/> Document Type <input type="radio"/> Publication Year <input type="radio"/> Language <input type="radio"/> Database 	0 of 43 References Selected			
Document Type(s)	<ol style="list-style-type: none"> Solavetivone and 5-epi-beta-vetivone as pest repellents and pesticides Quick View PATENTPAK By Goldblum, Seth; Warren, Craig B. From PCT Int. Appl. (2014), WO 2014099821 A2 20140626. Language: English The claimed pest (mostly insect) repellent and pesticidal (mostly alone or in combinations with one or more addnl. biol. active formers, antioxidants, preservatives, aerosol propellants, colorants) wide variety of application forms for animal, human, and tech. uses... Isolation and identification of chemical constituents of Przewalskia tangutica Maxim. Quick View Other Sources By Shao, Jun-jie; Peng, Yong; He, Chun-nian; Xu, Li-jia; Xiao, Xuan; Li, Yu-shan From Shenyang Yaokexue Xuebao (2013), 30(11), 840-845. Language: Chinese The chem. constituents of Przewalskia tangutica Maxim. were separated by HPLC, and structures were established by ESI-MS, ¹H-NMR, IR, MS ext. and EtOAc ext. of the aerial parts of P. tangutica Maxim., are phenylpropionate (4), tropine (5), thymine (6), cytidine (7), inositol (8). Effect of different preprocessing methods on determination of aroma constituents in aging tobacco Quick View Other Sources By Shen, Jin; Xiao, Zuo-bing; Tian, Huai-xiang; Xu, Ying-bo; Xu, Zhi-qiang; Feng, Yanyan From Shipin Gongye (Shanghai, China) (2013), 34(9), 209-214. Language: Chinese In order to compare the different preprocessing methods combination of aroma constituents in aging tobacco, simultaneous distillation-extraction and these three pretreatment methods were adopted for comparison of SDE detected 105 kinds of aroma compounds; the method of HS-SPME was used for sample preparation. 			
	0 of 5 References Selected			
	<ol style="list-style-type: none"> Solavetivone and 5-epi-beta-vetivone as pest repellents and pesticides Quick View PATENTPAK By Goldblum, Seth; Warren, Craig B. From PCT Int. Appl. (2014), WO 2014099821 A2 20140626. Language: English, Database: CAPLUS The claimed pest (mostly insect) repellent and pesticidal (mostly insecticidal) formulations contain at least one or more active ingredients selected based on their prodn. qualities, suitable auxiliary components (antioxidants, preservatives, aerosol propellants, colorants) are selected based on the product quality requirements. A wide variety of application forms for animal, human, and tech. uses... Novel fragrance and methods for production of 5-epi-β-vetivone, 2-isopropyl-6,10-dimethyl-spiro[4.5]undecane-8-one Quick View PATENTPAK By Julien, Bryan N.; Wallace, David M. From U.S. Pat. Appl. Publ. (2010), US 20100129306 A1 20100527. Language: English, Database: CAPLUS The present invention relates to 5-epi-β-vetivone, 2-isopropyl-6,10-dimethyl-spiro[4.5]undecane-2,6-dien-8-one for their fragrant qualities, and to novel methods for their prodn. using (-)-premnaspirodienone as starting material, such as farnesyl diphosphate, in host cells transformed or transfected with a vector comprising nucleic acid sequences described. Use of the fragrant components or any compn. contg. the component c... Novel methods for production of 5-epi-β-vetivone, 2-isopropyl-6,10-dimethyl-spiro[4.5]deca-2,6-dien-8-one Quick View PATENTPAK By Julien, Bryan N.; Wallace, David M. From PCT Int. Appl. (2008), WO 2008116056 A2 20080925. Language: English, Database: CAPLUS The present invention is directed to novel methods for prodn. of 5-epi-β-vetivone (I), 2-isopropyl-6,10-dimethyl-spiro[4.5]deca-2,6-dien-8-one (II), which are useful for their fragrant qualities, in one embodiment... 			

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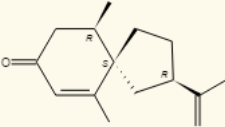
PAGE 21 / 25

ZOOM - +

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Key Substances in Patent

CAS RN 54878-25-0



Search in SciFinder | View Detail

Analyst Markup Location

page 21

CAS RN 7758-19-2

O=C1C=CC(=O)N1

Na

Search in SciFinder | View Detail

Analyst Markup Location

page 21

medium was prepared by inoculating 50 mL of SDE-ura medium with CAL1-5 or ALX7-95 containing YEp-HPS-ura. This culture was grown until early stationary phase (24-48 hr). One mL of this culture was inoculated into 500 mL of SDE-ura medium and grown for 24 hr. A 400-mL aliquot (5% inoculum) was used to inoculate the 8 L of medium.

[0188] The fermentor was maintained at 26°C. The air flow was 4.5 L/min and the dO₂ was maintained above 30% by adjusting the rpm. Furthermore, the pH was maintained at 4.5 using acetic acid and NaOH.

[0189] Once the glucose concentration was below 1 g/L, a feeding regimen was initiated such that the glucose in the fermentor was kept between 0 and 1 g/L. The glucose feed was made by mixing 1400 mL of 60% glucose and 328 mL of 12.5% yeast extract.

[0190] After 5 days, the air and agitation were turned off, and the oil was allowed to rise to the top of the tank and decanted.

Example 3

Preparation of 2-Isopropyl-6,10-dimethyl-spiro[4.5]dec-6-en-8-one (the “(-)-solavetivone”) (5)

[0191] 3,5-Dimethylpyrazole (47 g, 0.49 mol) was dissolved in a mixture of CH₂Cl₂ (650 mL) and t-butyl alcohol (31 mL). The solution was then cooled to ±78°C. Chromyl chloride (CrO₂Cl₂) (13.3 mL) was added over 15 min and stirred for another 15 min before it was allowed to warm to room temperature. Premnaspirodiene (6.69 g, 32.7 mmol) was dissolved in CH₂Cl₂ (650 mL) and added rapidly to the reaction. The dark red solution was stirred for 48 hours. The

Example 5

Preparation of 2-Isopropyl-6,10-dimethyl-spiro[4.5]deca-2,6-dien-8-one (3) & 2-Isopropyl-6,10-dimethyl-spiro[4.5]deca-1,6-dien-8-one (4).

[0193] To a solution of (-)-solavetivone (5) (100 mg, 0.46 mmol) dissolved in ethanol (2 mL) was added Amberlyst® IR-15 (150 mg). The suspension was then heated at 105°C. in a sealed reaction flask for 96 hours. The suspension was then filtered through Celite and evaporated under vacuum. The residue was purified on a silica gel column (hexane:ether, 85:15) to afford the mixture as a colorless oil (67 mg, 67%). ESIMS m/z 219 (M+H), 78.7% at 14.71 min; 219 (M+H), 17.1% at 14.89 min.

Example 6

Oxidation of (+)-Valencene to (+)-Nootkatone

[0194] In order to test various reaction conditions for the oxidation of premnaspirodiene to solavetivone, reactions were carried out on commercially available valencene, a compound that is chemically similar to premnaspirodiene and would be expected to oxidized under similar reaction conditions. Reactions were carried out using 250 mg of starting material in a single reaction, using combinations of sodium chlorite and either t-butylhydroperoxide (t-BuOOH) or N-hydroxyphthalimide (NHPI) as described (S. M. Silvestre & I.

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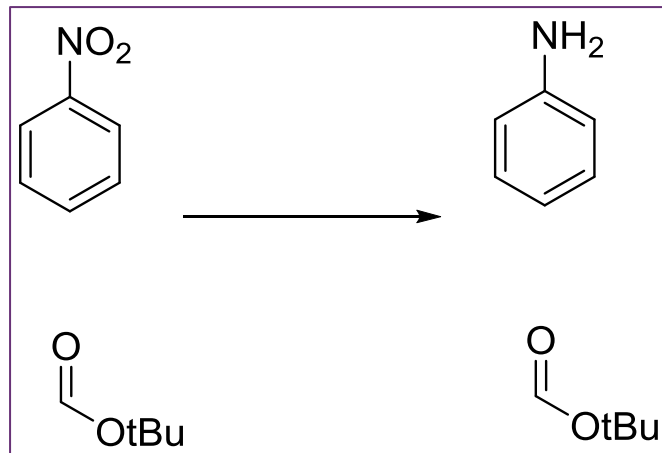


反应检索

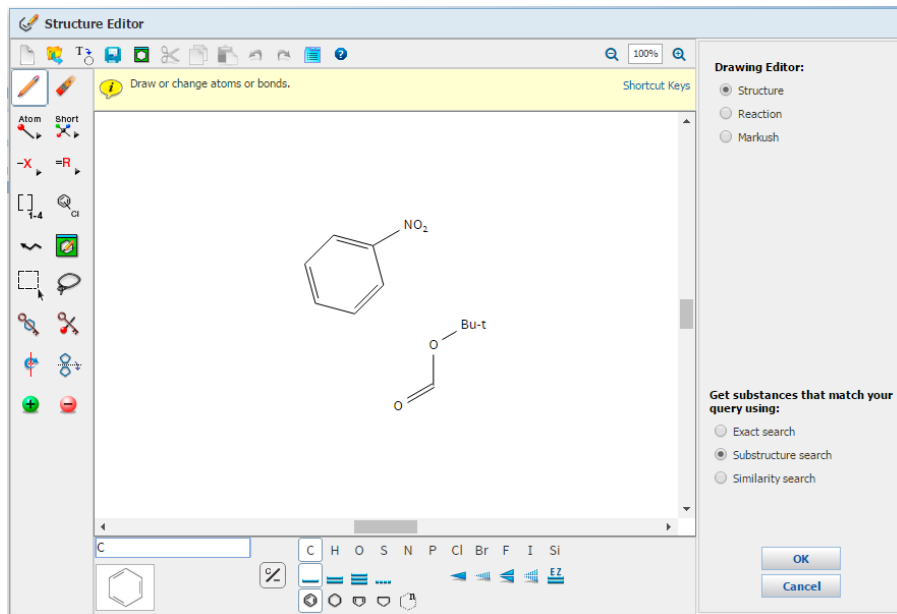
- 反应检索绘制工具及反应信息详情
- 如何通过**Analyze**、**Refine**来精选反应
- 巧用原子标记工具和位置标记工具提高检索精度
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- 手性反应专题
 - 手性分子合成反应
 - 手性构型翻转反应
 - 手性分子拆分反应

片段反应检索

- 检索要求：
 - 起始物上带有**BOC**基团
 - 苯环上的硝基还原为氨基
 - BOC**基团不变
- 检索思路：
 - 要保证苯环和**BOC**基团在同一个结构上，
需要从物质结构检索开始，通过物质获得
反应，再对反应进行限定。



绘制片段结构，选择亚结构反应检索，并定义为单一组分



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 More

Characteristics

- ☒ Single component
- ☐ Commercially available
- ☐ Included in references


获得亚结构检索结果，并获得这些物质作为反应物的反应

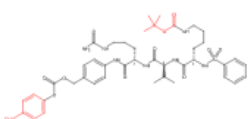
Get References | **Get Reactions** | Retrieve reactions for selected substances.

Sort by: CAS Registry Number ▾

0 of 35896 Substances Selected

1. **1884208-13-2** 🔍


~1 

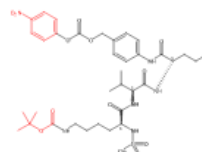


Absolute stereochemistry.

C₄₂ H₅₆ N₈ O₁₃ S
INDEX NAME NOT YET ASSIGNED
▶ **Key Physical Properties**

2. **1884208-09-6** 🔍

~1 



Absolute stereochemistry.

C₃₇ H₅₄ N₈ O₁₃ S
INDEX NAME NOT YET ASSIGNED
▶ **Key Physical Properties**

Get Reactions

Retrieve reactions for:

☒ All substances
☐ Selected substances

Limit results by reaction role:

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

Get **Cancel**

限定反应步数为一步反应

Explore ▼ Saved Searches ▼ SciPlanner Save Print Export

Chemical Structure substructure with limiters > substances (35896) > **get reactions (374800)** > get reactions (374800)

REACTIONS ⓘ Get References Tools ▼ Send to SciPlanner

Analyze Refine

Group by: No Grouping Sort by: Accession Number ↓

0 of 374800 Reactions Selected

1. View Reaction Detail ⓘ Link

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

Refine by: ⓘ

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

Number of Steps:
Examples: 1, 1 - 3, 1 - 3

Refine

[Step 2.1] ~38

[Step 3.1] ~74

[Step 4.1]

反应结构限定

Analyze

Refine

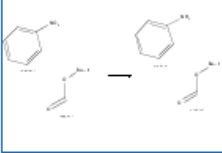
Refine by: ?

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

Structure Editor:

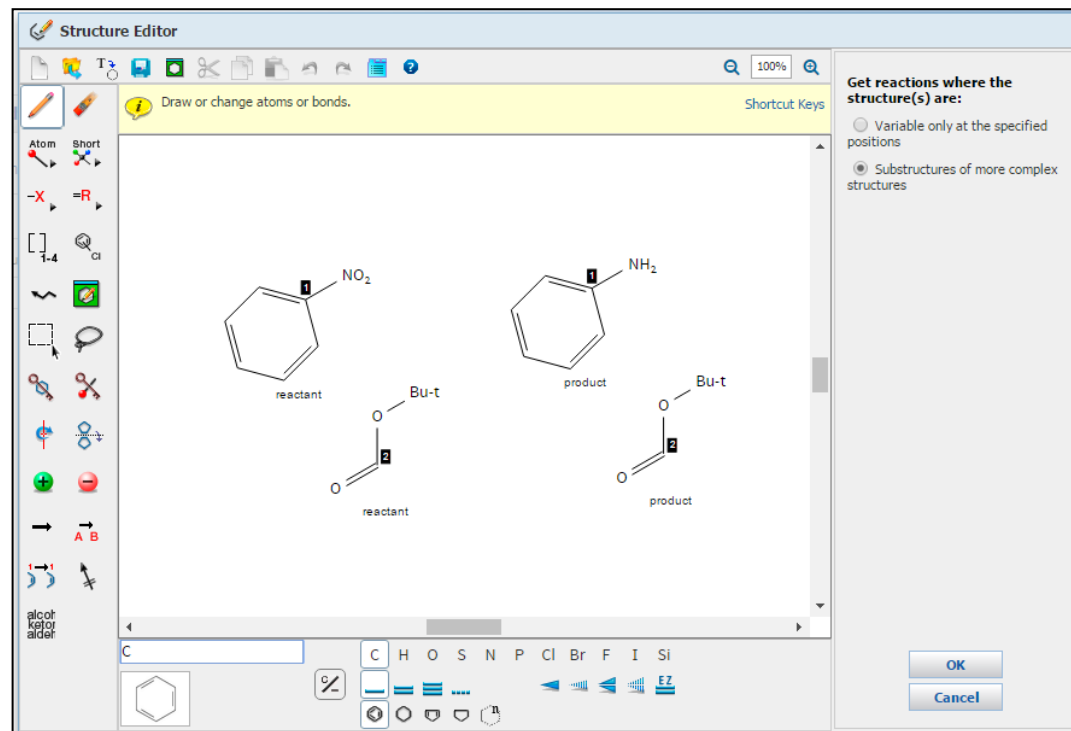
Java

Non-Java



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

Refine



符合检索要求的反应

0 of 6545 Reactions Selected

Page: 1 of 131

1. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.

~31

100%

~112

Overview

Steps/Stages

1.1 R:H₂, C: Pd, S: MeOH, rt

Notes

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

References

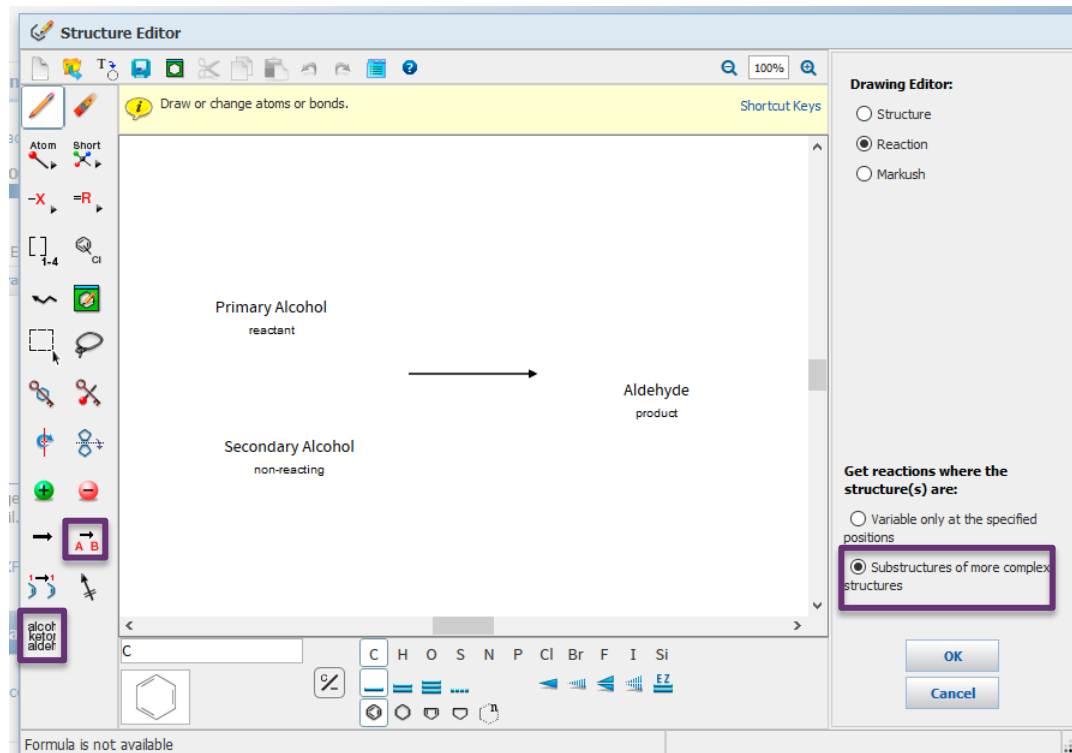
Rational Design of Substituted Diarylureas: A Scaffold for Binding to G-Quadruplex Motifs

Quick View Other Sources

By Drewe, William C. et al

From Journal of Medicinal Chemistry, 51(24), 7751-7767; 2008

案例：在非反应仲醇存在的条件下，将伯醇转换为乙醛



使用反应角色定义工具和官能团列表

案例：在非反应仲醇存在的条件下，将伯醇转换为乙醛

REACTIONS

Get References Tools

Analyze Refine

Analyze by:
Reagent

NaHCO ₃	1891
Et ₃ N	1836
1H-Imidazole	1222
Bu ₄ N ⁺ • F ⁻	1154
NH ₄ 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

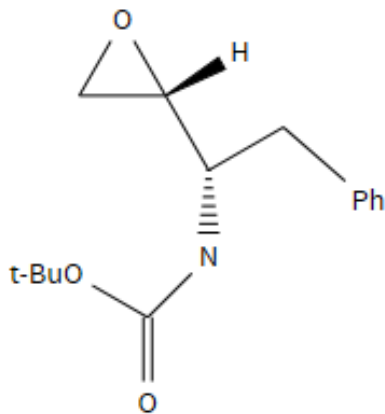
$$\text{R}-\text{CH}(\text{OH})-\text{R}^1 \longrightarrow \text{R}-\text{C}(=\text{O})-\text{R}^1$$

反应检索

- 反应检索绘制工具及反应信息详情
- 如何通过**Analyze**、**Refine**来精选反应
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 - 手性分子合成反应
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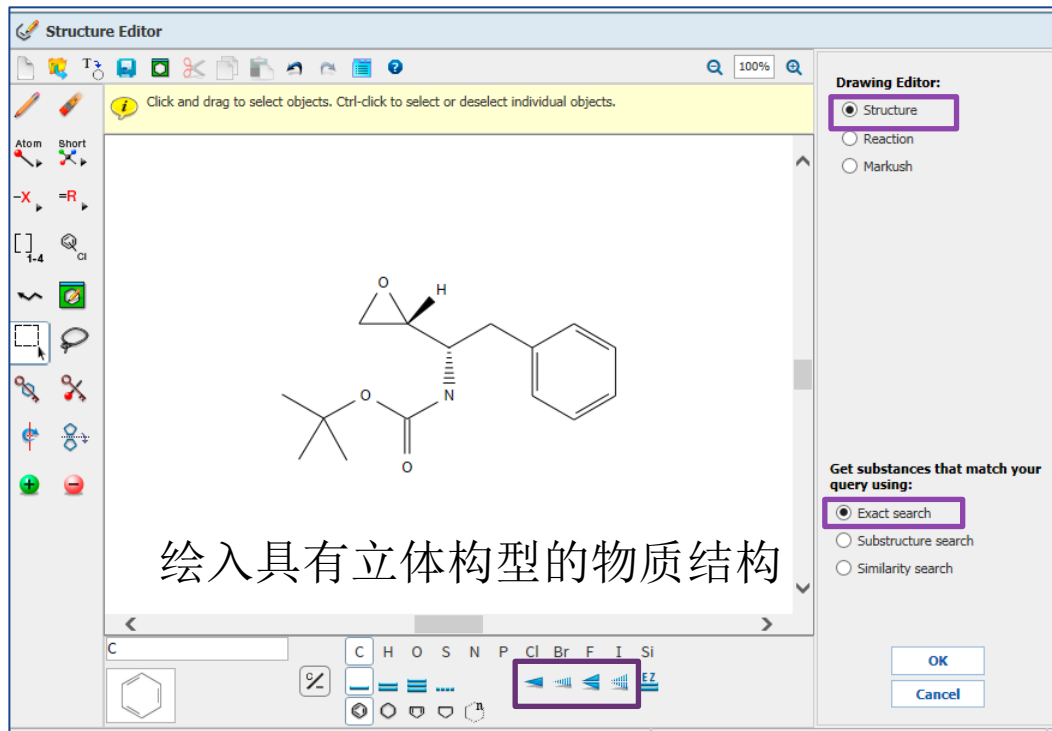
不对称合成反应

如何合成如下绝对立体构型的手性分子？ 或检索此分子参与的所有反应？



思路：从物质检索出发，然后从具有绝对构型的物质获取反应

不对称合成反应：从物质检索出发



物质检索

精确结构检索

不对称合成反应：获得物质结果集，再从物质获取反应

1 of 5 Stereo Candidates Selected

选择立体构型完全匹配的结果

<input checked="" type="checkbox"/>	Absolute stereo match	2
<input type="checkbox"/>	Absolute stereo mirror image	1
<input type="checkbox"/>	Relative stereo match	1
<input type="checkbox"/>	Stereo that doesn't match query	9
<input type="checkbox"/>	No stereo in answer structure	1

Get Substances

获得物质结果集

0 of 2 Substances Selected

1. 98760-08-8

~162 94

Absolute stereochemistry., Rotation (+).

2. 1026616-57-8

~0

Absolute stereochemistry.

C₁₅ H₂₁ N O₃
Carbamic acid, *M*-[(1*S*)-1-(2*R*)-2-oxiranyl-2-phenylethyl]-, 1, 1-dimethylethyl ester
INDEX NAME NOT YET ASSIGNED

Key Physical Properties
Regulatory Information
Experimental Properties

Get Reactions

Limit results by reaction role:

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

Get Cancel

不对称合成反应：获得作为产物的反应结果

Chemical Structure exact > substances (2) > **get reactions (176)**

REACTIONS ?

Get References Tools

Send to SciPlanner

Analyze Refine

Group by: No Grouping Sort by: Accession Number

Display Options

0 of 176 Reactions Selected

1. View Reaction Detail Link

6 Steps Hover over any structure for more options.

Analyze by: Reagent

NaOH	57
Et ₃ N	56
mCPBA	46
KOH	37
NaBH ₄	36
NaHCO ₃	29
HCl	23
H ₂ O	21
BuLi	20
K ₂ CO ₃	19

Chem More

~184

~59

~94

2. View Reaction Detail Link

5 Steps Hover over any structure for more options.

~59

~94

不对称合成反应：获得作为任意角色的反应结果

Chemical Structure exact > substances (2) > **get reactions (6803)**

REACTIONS ?

Get References Tools

Send to SciPlanner

Analyze Refine

Group by: No Grouping Sort by: Accession Number

0 of 6803 Reactions Selected

Page: 454 of 454

Analyze by: Reagent

HCl	5391
NaOH	3633
H ₂	3506
1-Benzotriazolol	3033
N-Methylmorpholine	2718
EtN=C=N(CH ₂) ₃ NMe ₂ • HCl	2578
Et ₃ N	2568
EtN(Pr- <i>i</i>) ₂	1714
NaHCO ₃	1562
F ₃ CCO ₂ H	1297

6796. [View Reaction Detail](#) [Link](#)

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

[Step 2.1]

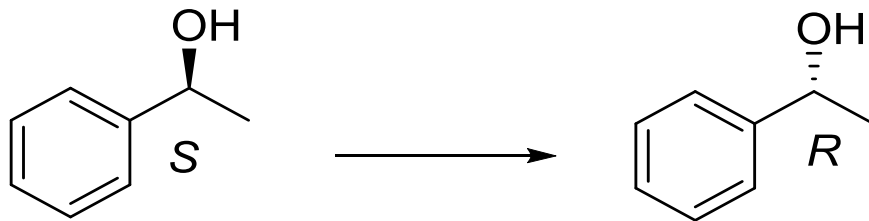
~94

提纲

- 手性反应专题
 - 手性分子合成反应
 - 手性构型翻转反应
 - 手性分子拆分反应
 - 手性分子分离的分析方法

手性翻转反应

如何通过精确反应检索如下的一步手性翻转反应？

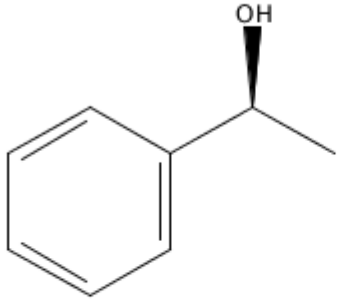


思路：通过物质检索，分别获得起始物和产物的一步反应，再对结果集进行交集。

手性翻转反应：通过精确结构检索S构型起始物

Structure Editor:

Java Non-Java



Click image to change structure or view detail.


Import CXF

Search

Search Type:

- ☒ Exact Structure
- ☐ Substructure
- ☐ Similarity

☐ Show precision analysis

 ChemDraw[®]

Launch a SciFinder substance
More

Select All Deselect All

1 of 4 Stereo Candidates Selected

- ☒ Absolute stereo match
- ☐ Absolute stereo mirror image
- ☐ Relative stereo match
- ☐ Stereo that doesn't match query
- ☐ No stereo in answer structure

Get Substances

手性翻转反应：得到S构型物质，并通过Get Reaction获取其为“反应物”的反应

SUBSTANCE DETAIL ?

Get References **Get Reactions** Retrieve reaction information for this record.

[Return](#)

1. CAS Registry Number 1445-91-6

~3,350 ~99

C₈H₁₀O
Benzenemethanol, α-methyl-, (αS)-

Molecular Weight
122.16

Boiling Point (Experimental)
Value: 93 °C | Condition: Press: 14 Torr

Density (Predicted)
Value: 1.013±0.06 g/cm3 | Condition: Temp: 20 °C Press: 760 Torr

pKa (Predicted)
Value: 14.43±0.20 | Condition: Most Acidic Temp: 25 °C

Absolute stereochemistry, Rotation (-).

Get Reactions

Limit results by reaction role:

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

Get **Cancel**

手性翻转反应：将反应结果集限定为一步反应，并保存为answer1

REACTIONS ?

Get References Tools

Analyze Refine

Refine by: ?

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

Number of Steps:

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

Refine

Group by: No Grouping Sort by: Accession Number

0 of 7373 Reactions Selected

1. View Reaction Detail Link

6 Steps Hover over any structure for more options.

O=[N+]([O-])c1ccccc1C(=O)O + OC=O

~114

将所得结果集保存为“answer1”

Save This Answer Set

* Required

Save:

- ☒ All answers
- ☐ Only selected answers

Title: *

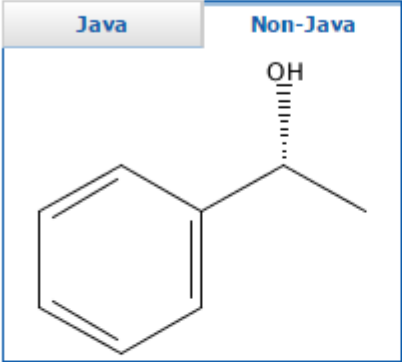
Description:

OK Cancel

手性翻转反应：通过精确结构检索R构型产物

Structure Editor:

Java Non-Java



Click image to change structure or view detail.


Import CXF

Search

Search Type:

- ☒ Exact Structure
- ☐ Substructure
- ☐ Similarity

☐ Show precision analysis

 ChemDraw[®]

Launch a SciFinder substance
More

Select All Deselect All

1 of 4 Stereo Candidates Selected

- ☒ Absolute stereo match
- ☐ Absolute stereo mirror image
- ☐ Relative stereo match
- ☐ Stereo that doesn't match query
- ☐ No stereo in answer structure

Get Substances

手性翻转反应：得到R构型物质，并通过Get Reaction获得其为“产物”的反应

1. CAS Registry Number 1517-69-7

~3,242   ~104 

C₈ H₁₀ O

Benzenemethanol, α -methyl-, (a*R*)-

Molecular Weight

122.16

Melting Point (Experimental)

Value: 9-11 °C

Boiling Point (Experimental)

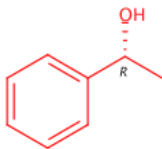
Value: 98 °C

Density (Predicted)

Value: 1.013±0.06 g/cm³ | Condition: Temp: 20 °C Press: 760 Torr

pKa (Predicted)

Value: 14.43±0.20 | Condition: Most Acidic Temp: 25 °C



Absolute stereochemistry., Rotation (+).

Get Reactions

Limit results by reaction role:

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

Get

Cancel



手性翻转反应：将反应结果集限定为一步反应，并存储为answer2

REACTIONS ?

Get References Tools

Analyze Refine

Group by: No Grouping Sort by: Accession Number

0 of 3991 Reactions Selected

1. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.

Refine by:

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

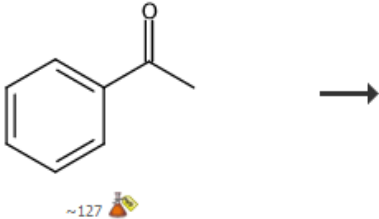
Number of Steps:

1

Examples: 1, 1-3, 1-3

Refine

Overview



将所得结果集保存为“answer2”

Save This Answer Set

* Required

Save:

- ☒ All answers
- ☐ Only selected answers

Title: *

answer2

Description:

OK Cancel

手性翻转反应：点击Tools，将answer1和answer2合并取交集

Combine Answer Sets

2 of 30 Reaction Answer Sets Selected **References (13)** **Substances (1)** **Reactions (30)**

- ☒ answer2 (3629)
Chemical Structure exact > substances (54) > 151
- ☒ answer1 (678)
Chemical Structure exact > substances (52) > 144

Combine Answer Sets

Select an option for combining the two selected saved answer sets:

- ☐ **Combine** Include all reactions from both sets
- ☒ **Intersect** Include only reactions that appear in both sets
- ☐ **Exclude** Include only answers from answer2 that are not in answer1
- ☐ **Exclude** Include only answers from answer1 that are not in answer2

Combine Answer Sets **Cancel**

手性翻转反应：获得准确的反应结果

Combine Reaction Answer Sets "Intersect: Include only answer..." (16)

REACTIONS [?](#) [Get References](#) [Tools](#) [v](#)

Analyze [Refine](#)

Analyze by: [?](#)
Reagent [v](#)

AcOEt	1
Et ₃ N	1
H ₂	1
NaOH	1
O ₂	1
<i>t</i> -BuOK	1

[Show More](#)

Group by: [No Grouping](#) [v](#) Sort by: [Accession Number](#) [v](#) [↓](#)

[0 of 16 Reactions Selected](#)

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

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

[v Overview](#)

Steps/Stages

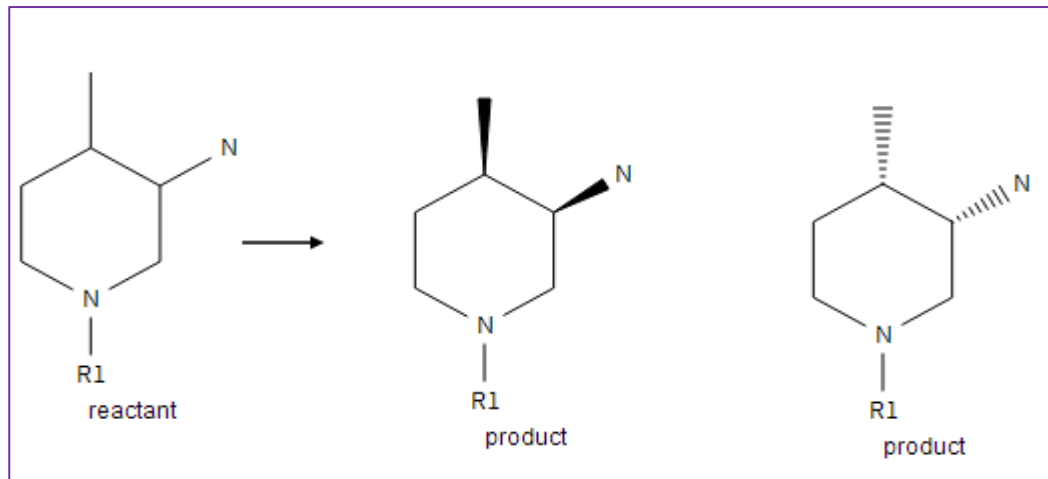
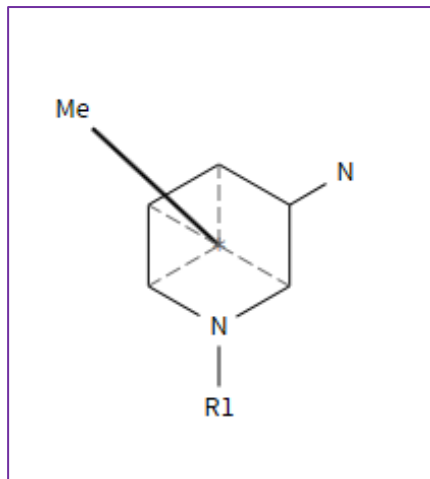
Notes

提纲

- 手性反应专题
 - 手性分子合成反应
 - 手性构型翻转反应
 - 手性分子拆分反应

手性拆分反应

如何检索如下消旋体拆分获得绝对构型的反应？



N-保护的3-氨基-甲基哌啶

举例：R1可以是一些保护基，比如Boc、Cbz等，
甲基可以在吡啶环的2,4,5或6位的任意位置。

手性拆分反应：检索思路1

- 从产物检索出发

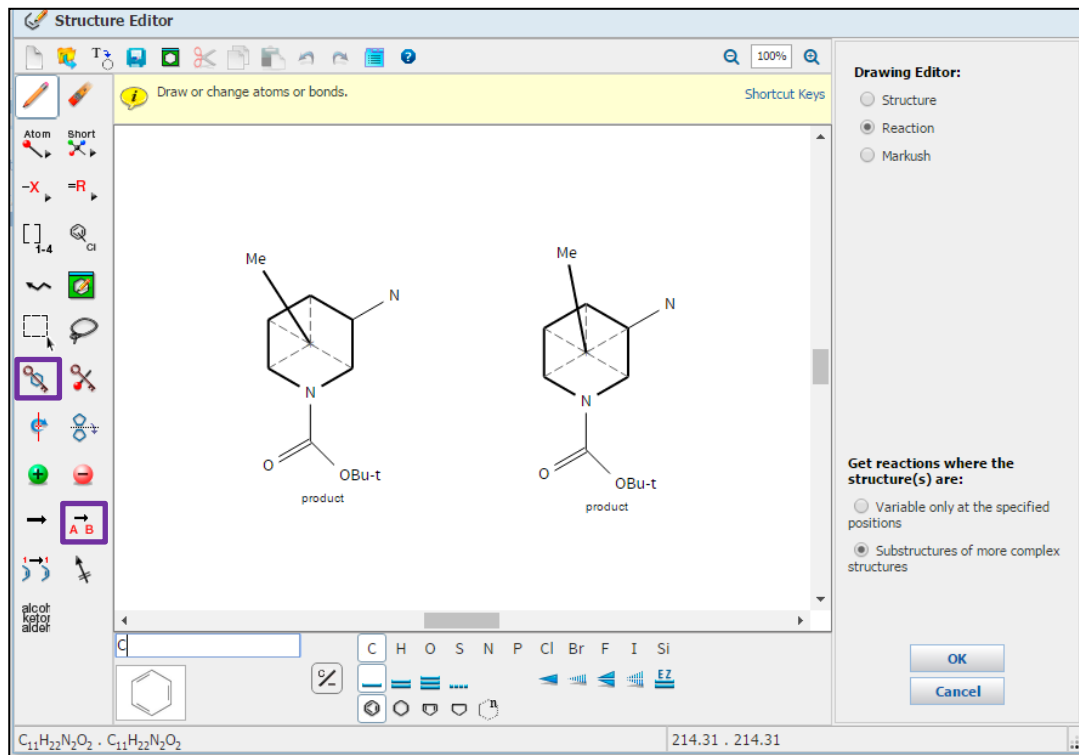
在反应结构编辑器中，同时绘制两个产物结构（无需画立体构型），选择亚结构反应检索

- 限定反应物

在反应结果集中，通过**Refine: Reaction structure**对反应进行限定，所画结构为没有立体构型的反应物

- 获得结果集

手性拆分反应：从产物检索出发



在反应结构编辑器中绘制
产物结构，无需绘制立体键，
选择亚结构反应检索

手性拆分反应：限定反应物

The screenshot displays the SciFinder web interface. At the top, navigation tabs include 'Explore', 'Saved Searches', 'SciPlanner', 'Save', 'Print', and 'Export'. The main content area is titled 'Reaction Structure substructure > reactions (681)'. On the left, a 'REACTIONS' sidebar has 'Analyze' and 'Refine' tabs. Under 'Refine by', 'Reaction Structure' is selected and highlighted with a red box. Below this, a list of refinement options includes 'Product Yield', 'Number of Steps', 'Reaction Classification', 'Excluding Reaction Classification', and 'Non-participating functional groups'. The main reaction list shows '0 of 681 Reactions Selected' and a 'View Reaction Detail' link. Below the link, a chemical reaction is shown with a reactant (a pyridine ring with a methyl ester group) and a product (a complex molecule with a benzene ring and a chiral center). A 'Structure Editor' window is open on the right, showing a chemical structure of a reactant (a pyridine ring with a methyl ester group) and a product (a complex molecule with a benzene ring and a chiral center). The editor includes a toolbar with various drawing tools and a 'Send to SciPlanner' button. A text overlay in the editor reads '绘制没有立体构型的反应物' (Draw reactants without stereochemistry). The bottom of the interface shows a 'Click image to change' prompt.

在反应结果集中通过Reaction Structure限定反应物

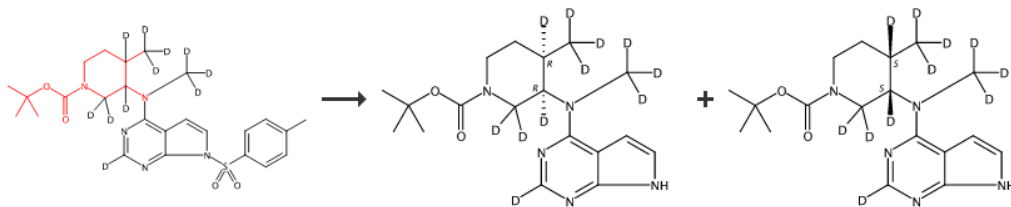
手性拆分反应：获得反应结果集

2. Deuterated tasocitinib derivatives as Janus kinase 3 inhibitors and their preparation and use for the treatment and prevention of Janus kinase 3-mediated diseases

[Quick View](#) [PATENTPAK](#)

8 Reactions

2 Steps Hover over any structure for more options.



Overview

Steps/Stages

1.1 S:NaOD, 2 h, 100°C
2.1

消旋体的拆分

Notes

2) sepn. by column chromatog. on Chiralpak IC, Reactants: 1, Solvents: 1, Steps: 2, Stages: 2, Most stages in any one step: 1

References

Deuterated tasocitinib derivatives as Janus kinase 3 inhibitors and their preparation and use for the treatment and prevention of Janus kinase 3-mediated diseases

[Quick View](#) [PATENTPAK](#)
By Rao, Tadimet S, and Zhang, Chengzhi
From PCT Int. Appl., 2010123919, 28 Oct 2010

Experimental Procedure

手性拆分反应：获得反应结果集

Reaction Structure substructure > reactions (681) > refine "substructure" (9)

REACTIONS ? Get References Tools

Analyze Refine

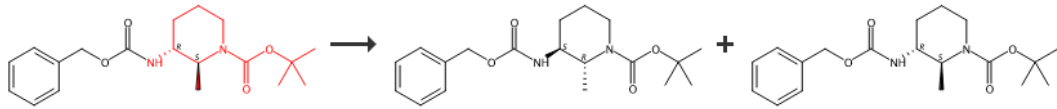
Analyze by: ?
Reagent
NaOD 1
Show More

Group by: No Grouping Sort by: Accession Number

0 of 9 Reactions Selected

1. View Reaction Detail Link

Single Step Hover over any structure for more options.



▼ Overview
Steps/Stages
1.1

对映异构体的分离

Notes
enantiomers separated by AD-H chiral SFC column. Reactants: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References
Preparation of substituted piperidine compounds as orexin receptor modulators
Quick View PATENTPAK
By Dvorak, Curt A. and Shireman, Brock T.
From U.S. Pat. Appl. Publ., 20140275095, 18 Sep 2014

谢谢关注！

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