

朱传娴

客户顾问

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SciFinder反应检索难点解析

中国药科大学



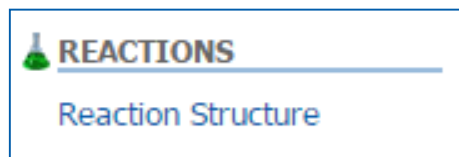
提纲

- SciFinder反应检索难点解析
 - 反应的精准定义
 - 巧妙获得有实验步骤的相关反应
 - 如何获得最全面的合成信息
 - 反应信息太少时如何获得更多的反应信息
 - 结果集庞大时如何限定反应
 - 直接检索反应受限时如何处理
 - 如何排除不要的反应
 - 新化合物的合成路线设计
 - 案例分析
 - 反应检索上机练习

SciFinder检索选项——反应检索

- 反应检索方法

结构式



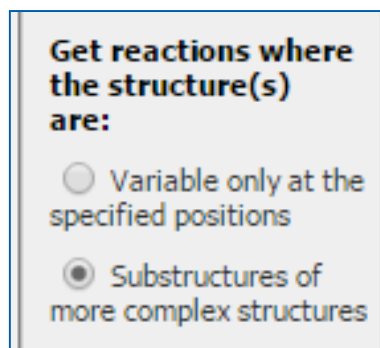
- 常用获取方法

已知物质：由物质获取反应

已知文献：从文献中获取反应

精确结构反应检索

亚结构反应检索



反应绘制工具

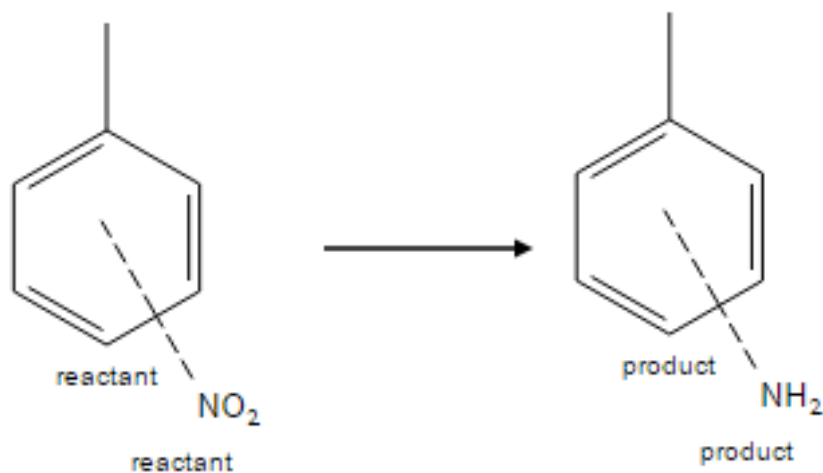
The screenshot shows the Structure Editor interface with the following components and annotations:

- Reaction Arrow:** A green arrow icon in the left toolbar, labeled "反应箭头".
- Reaction Role Tools:** A red circle with a plus sign and a red circle with a minus sign in the left toolbar, labeled "反应角色工具".
- Reaction Atom Marking Tools:** A black arrow pointing to the right and a black arrow pointing to the right with "A" and "B" labels in the left toolbar, labeled "反应原子标记工具".
- Functional Group List:** A list of functional groups including "alcohol" and "ketone" in the left toolbar, labeled "官能团列表".
- Reaction Position Marking Tools:** A blue circle with "1" and "2" and a black arrow pointing to a bond in the left toolbar, labeled "反应位置标记工具".

The interface includes a top toolbar with icons for file operations, a central drawing area with a yellow status bar "Draw or change atoms or bonds.", a right sidebar with "Drawing Editor" options (Structure, Reaction, Markush) and search filters, and a bottom toolbar with element selection (C, H, O, S, N, P, Cl, Br, F, I, Si) and bond types. The status bar at the bottom shows "CH₄" and "16.04".

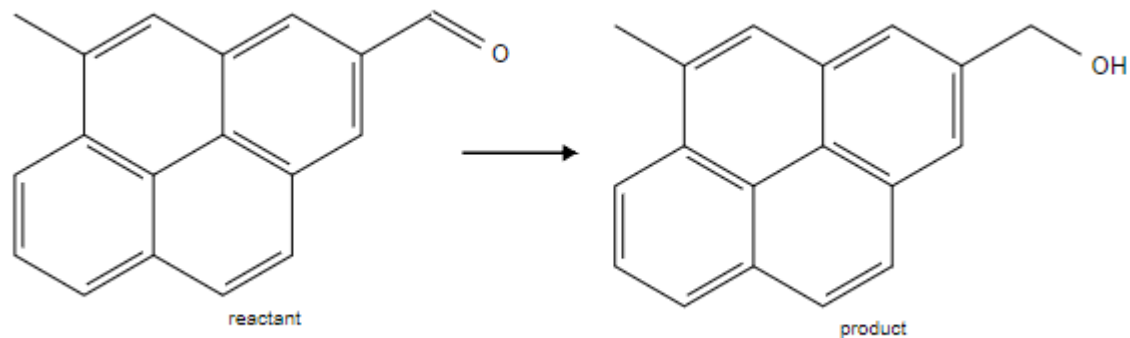
反应的精准定义

检索符合以下要求的反应，硝基还原



巧妙获得有实验步骤的相关反应

该还原反应如何操作？



Structure Editor

Draw or change atoms or bonds. Shortcut Keys

100%

Atom Short

-X =R

Cl

Get reactions where the structure(s) are:

Variable only at the specified positions

Substructures of more complex structures

OK

Cancel

C₁₈H₂₀O . C₁₈H₂₀O

244.29 . 246.31

CAS Solutions

SciFinder[®]
A CAS SOLUTION

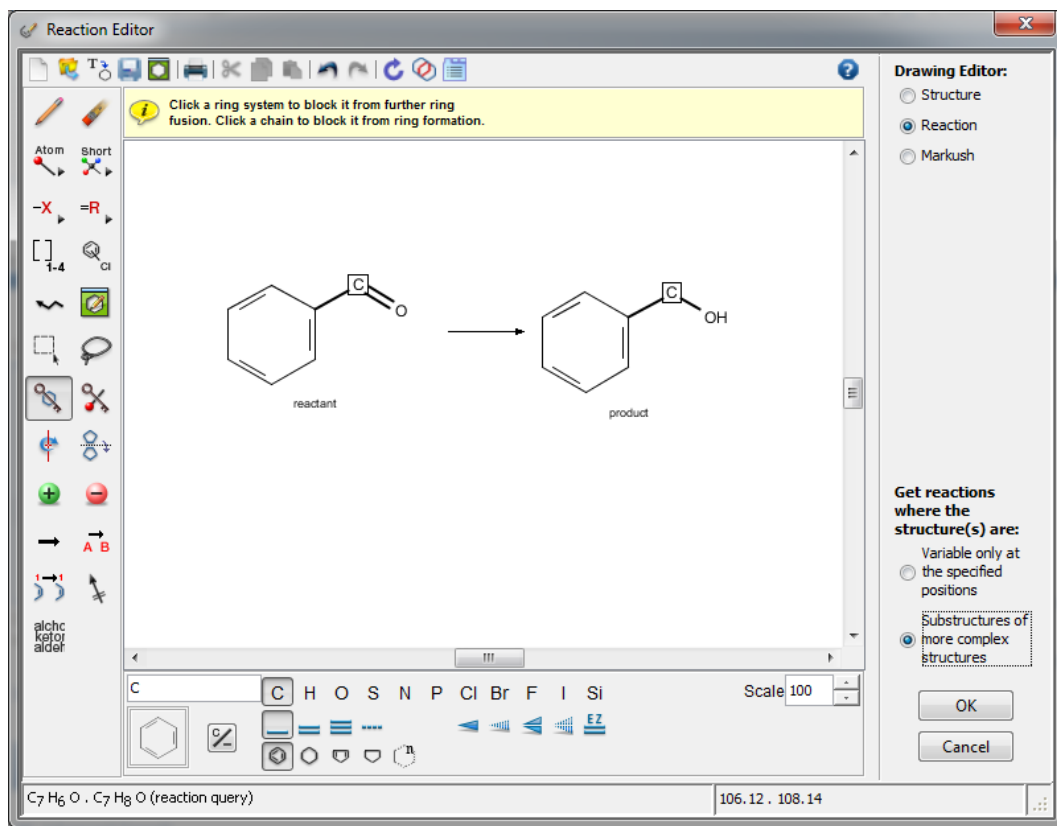
Explore Saved Searches SciPlanner

⚠ Explore Reactions resulted in 0 reactions [Return](#) [Find Additional Reactions](#)

Reaction Structure structure variable only at spe... > reactions (0)

REACTIONS [Find Additional Reactions](#)

巧妙获得有反应步骤的相关反应



聚焦反应关键部位，查找类似反应

巧妙获得有反应步骤的相关反应

Reaction Structure variable only at spe... > reactions (1930)

REACTIONS Get References Tools

Analyze Refine

Group by: No Grouping Sort by: Relevance

0 of 1930 Reactions Selected

1. View Reaction Detail Similar Reactions

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

100%
~123

1862
40
7
6
6
4
4
1

Show More

REACTIONS Get References Tools

Analyze Refine

Group by: No Grouping Sort by: Relevance

0 of 496 Reactions Selected

1. View Reaction Detail Similar Reactions

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

100%
~123

MethodsNow Available 496

Show More

REACTIONS Get References Tools

Analyze Refine

Group by: No Grouping Sort by: Relevance

0 of 496 Reactions Selected

1. View Reaction Detail Similar Reactions

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

100%
~123

Overview

METHODSNOW™

Procedure

1. Prepare a solution of tris(4-fluorophenyl)phosphine (0.01 mmol) and tBuOK (5.6 mg, 0.05 mmol) in dry 2-propanol (5 mL) under argon in a 25 mL Schlenk flask.
2. Heat the solution to 80 °C for 15 minutes in a thermostated oil bath.

View more...

View with MethodsNow

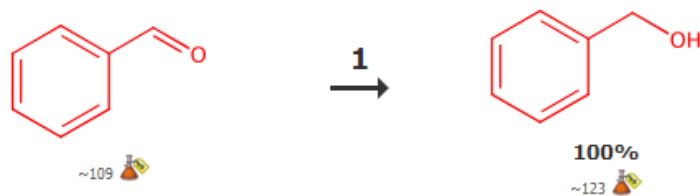
通过Refine获得单步反应后选取有实验步骤的反应

巧妙获得有反应步骤的相关反应

MethodsNow

N-Heterocyclic olefins as ancillary ligands in catalysis: a study of their behaviour in transfer hydrogenation reactions

By Iturmendi, Amaia; Garcia, Nestor; Jaseer, E. A.; Munarriz, Julen; Sanz Miguel, Pablo J.; Polo, Victor; Iglesias, Manuel; Oro, Luis A.
From Dalton Transactions, 45(32), 12835-12845; 2016
Published by Royal Society of Chemistry



Products	Benzyl alcohol, 100%, CAS RN: 100-51-6
Reactants	Benzaldehyde, CAS RN: 100-52-7
Reagents	Isopropanol, CAS RN: 67-63-0 Potassium <i>tert</i> -butoxide, CAS RN: 865-47-4
Catalysts	CAS RN: 1801329-25-8 Tris(4-fluorophenyl)phosphine, CAS RN: 18437-78-0
Solvents	Tetrahydrofuran, CAS RN: 109-99-9
Procedure	<ol style="list-style-type: none">1. Prepare a solution of tris(4-fluorophenyl)phosphine (0.01 mmol) and tBuOK (5.6 mg, 0.05 mmol) in dry 2-propanol (5 mL) under argon in a 25 mL Schlenk flask.2. Heat the solution to 80 °C for 15 minutes in a thermostated oil bath.3. Add benzaldehyde (1 mmol) and mesitylene (140 μL, 1 mmol) to the mixture.4. Stir the resulting mixture at 80 °C.5. Monitor the reaction by gas chromatography.

Print/Export

Close

获得全面的合成信息

查找合成Daclatasvir的反应

The screenshot displays the SciFinder web interface. At the top, the navigation bar includes 'Explore', 'Saved Searches', and 'SciPlanner'. The breadcrumb trail reads: 'Reaction Structure substructure > reactions (60953) > refine "1 step" (14724)'. The left sidebar contains a 'REFERENCES' section with fields like 'Research Topic', 'Author Name', and 'Company Name', and a 'SUBSTANCES' section with options like 'Chemical Structure', 'Markush', and 'Molecular Formula'. The main content area shows the search results for 'Daclatasvir', with 'get reactions (50)' selected. A 'Get References' button is highlighted with a red box. Below this, there are filters for 'Group by: No Grouping' and 'Sort by: Accession Number'. A table of reagents is shown on the left, and the main area displays a reaction scheme for the synthesis of Daclatasvir, including reagents like EtN(Pr-)₂, HCl, NH₄OAc, H₂O, EtN=C=N(CH₂)₃NMe₂·HCl, 1-Benzotriazolol, 148893-10-1, F₃CCO₂H, Disodium carbonate, and K₂CO₃. The reaction scheme shows the synthesis of Daclatasvir from four starting materials: dichloroacetyl chloride, biphenyl, a cyclic amide, and a chiral auxiliary. The reaction is labeled '4 Steps' and 'View Reaction Detail'. The SciFinder logo and 'A CAS SOLUTION' are visible at the bottom right.

Reagent	Count
EtN(Pr-) ₂	31
HCl	27
NH ₄ OAc	20
H ₂ O	19
EtN=C=N(CH ₂) ₃ NMe ₂ ·HCl	17
1-Benzotriazolol	16
148893-10-1	13
F ₃ CCO ₂ H	11
Disodium carbonate	10
K ₂ CO ₃	10

获得全面的合成信息

CAS Solutions | Preferences | SciFinder Help | Sign Out

WELCOME Helen Zhu

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

Substance Identifier "Daclatasvir" > substances (1) > **get reactions (50)** > get references (11)

REFERENCES

Get Substances | Get Reactions | Get Related Citations | Tools

This functionality is not available for this answer set. | Create Keep Me Posted Alert | Send to SciPlanner

Analyze | Refine | Categorize

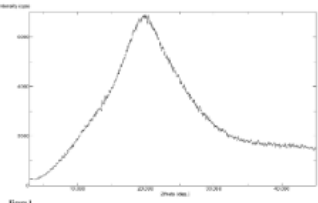
Sort by: Accession Number

0 of 11 References Selected

Analyze by: Author Name

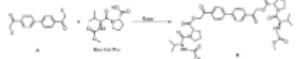
Feng Zhiyong	2
Zhou Shengfeng	2
Bai Shunqiang	1
Cai Jin	1
Chava Satyanarayana	1
Chen Bo	1
Chen Hui	1
Chen Junqing	1
Chen Long	1

1. **Process for the preparation of daclatasvir, its oxalate and dihydrochloride salts**
PATENTPAK
By Swargam, Sathyanarayana; Medikonduri, Sreekanth; Salla, Rammohan; Indukuri, Venkata Sunil Kumar; Kalidindi, Srihari Raju; Chava, Satyanarayana
From PCT Int. Appl. (2017), WO 2017021904 A1 20170209. | Language: English, Database: CAPLUS



The invention is related to a process for the prepn. of daclatasvir (I) and its pharmaceutically acceptable salts by: (a) reacting biphenyl with XCOCH₂X in the presence of a suitable Lewis acid; (b) reacting XCH₂CO-p-C₆H₄-p-C₆H₄-COCH₂X (II) [X = halogen] with III [PG = protecting group] in the presence of a base in an org. solvent; (c) cyclization of IV; (d) deprotecting the PG of IV; converting V to I or one of its pharmaceutically acceptable salts. The invention is also relates to a process for the prepn. and purifn. of daclatasvir dihydrochloride. Thus, acylation of biphenyl with chloroac...

2. **A synthetic method of daclatasvir**
PATENTPAK
By Yan, Qing; Xie, Hai; Chen, Wenrui; Bai, Shunqiang; Zhang, Li
From Faming Zhuanli Shenqing (2016), CN 106256825 A 20161228. | Language: Chinese, Database: CAPLUS



The present invention provides a synthetic method of daclatasvir, which comprises: taking 4,4'-bis(2-halogenated acetyl)biphenyl as raw material, carrying out esterification reaction with N-(methoxycarbonyl)-L-valine-L-proline in the presence of org. solvent and alkali to obtain intermediate B; then, carrying out cyclodehydration reaction on intermediate B with ammonium acetate to obtain

还有其他文献描述了目标化合物的合成吗？

获得全面的合成信息

Get References **Tools** Select to view available menu items. Send to SciPlanner

Group by: No Group Number 0 of 50 Reactions Selected Display Options

- Find Additional Reactions
- Combine Answer Sets

1. View Reaction Detail [Link](#)

4 Steps Hover over any structure for more options.

Analyze Refine

Analyze by: Answer Type

Reactions 18

Additional Reactions 1

Show More

51. View Reaction Detail [Link](#)

Hover over any structure for more options.

~24 references

获得的附加反应不是完整反应

获得全面的合成信息

CAS Solutions | Preferences | SciFinder Help | Sign Out

WELCOME Helen Zhu

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

0 duplicates were automatically removed.

Substance Identifier "Daclatasvir" > substances (1) > get reactions (50) > get references (11) > **Combine Reference Answer Sets "24 (24)" (32)**

REFERENCES | Get Substances | Get Reactions | Get Related Citations | Tools | Create Keep Me Posted Alert | Send to SciPlanner

Analyze | Refine | Categorize | Sort by: Accession Number | Display Options

0 of 32 References Selected | Page: 1 of 2

Analyze by: Author Name

Yang Fukang	6
Belema Makonen	5
Nguyen Van N	5
Lopez Omar D	4
Meanwell Nicholas A	4
Snyder Lawrence B	4
St Laurent Denis R	4
Bachand Carol	3
Good Andrew C	3
Hamann Lawrence	

1. **A process for preparing daclatasvir and its intermediates**
Quick View PATENTPAK
By Ying, Shuhuan; Pi, Hongjun; Wang, Liang; Chen, Jian
From Faming Zhuanli Shenqing (2017), CN 106496199 A 20170315. | Language: Chinese, Database: CAPLUS
The invention relates to a process for the prepn. of daclatasvir and its intermediates. For instance, daclatasvir was prepd. via substitution of 4,4'-bis(2-bromoacetyl)biphenyl with N-Boc-L-proline in the presence of DIPEA/CH₃CN followed by intramol. heterocyclization in the presence of NH₄OAc, deprotection, and amidation with N-(methoxycarbonyl)-L-valine.

2. **Process for the preparation of daclatasvir, its oxalate and dihydrochloride salts**
Quick View PATENTPAK
By Swargam, Sathyanarayana; Medikonduri, Sreekanth; Salla, Rammohan; Indukuri, Venkata Sunil Kumar; Kalidindi, Srihari Raju; Chava, Satyanarayana
From PCT Int. Appl. (2017), WO 2017021904 A1 20170209. | Language: English, Database: CAPLUS

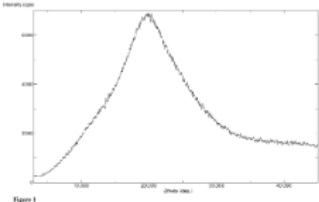


Figure 1

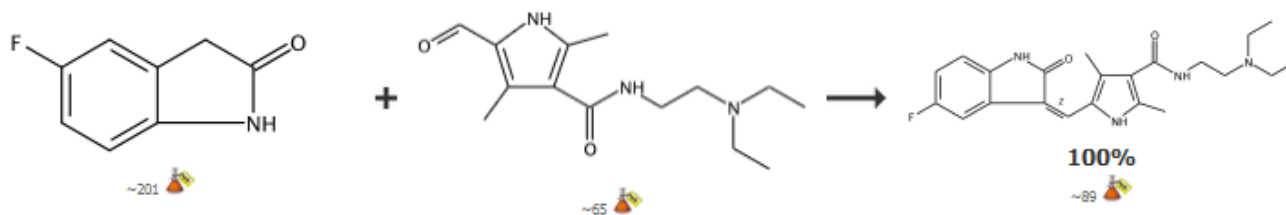
The invention is related to a process for the prepn. of daclatasvir (I) and its pharmaceutically acceptable salts by: (a) reacting biphenyl with XCOCH₂X in the presence of a suitable Lewis acid; (b) reacting XCH₂CO-p-C₆H₄-p-C₆H₄-COCH₂X (II) [X = halogen] with III [PG = protecting group] in the presence of a base in an org. solvent; (c) cyclization of IV; (d) deprotecting the PG of IV; converting V to I or one of its pharmaceutically acceptable salts. The invention is also relates to a process for the prepn. and purifn. of daclatasvir dihydrochloride. Thus, acylation of biphenyl with chloroac...

合并后的文献结果集

获得相关的反应信息

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

Single Step Hover over any structure for more options.



Overview

Steps/Stages

1.1

Get Similar Reactions

Notes

no exp

Refer

Novel s

Quick

By Sang

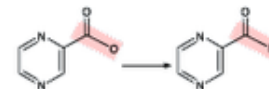
From In

Retrieve similar reactions from:

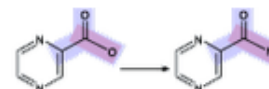
- All reactions
- Current answer set

Include this level of similarity:

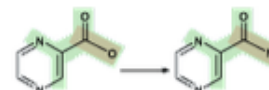
- Broad - Reaction centers only (157156)



- Medium - Reaction centers plus adjacent atoms and bonds (8506)



- Narrow - Reaction centers plus extended atoms and bonds (2994)



Get Reactions

Cancel

反应信息太少，通过Similar Reaction
获得更多反应信息

反应结果集庞大时如何限定—反应试剂的限定

The screenshot displays the Structure Editor interface with the following components:

- Structure Editor:** The main workspace shows a reaction scheme with "Aldehyde reactant" and "Carboxylic Acid product". A yellow tooltip reads: "Click a reaction participant. A list of roles appears. Click a reaction role and click OK."
- Drawing Editor:** Includes radio buttons for "Structure", "Reaction" (selected), and "Markush".
- Get reactions where the structure(s) are:** Includes radio buttons for "Variable only at the specified positions" and "Substructures of more complex structures" (selected).
- Search Filters (Right Panel):**
 - Solvents:** Select Solvents
 - Non-participating Functional Groups:** Select Groups
 - Number of Steps:** Input field with "1" and examples: 1, 1-3, 1-, -3
 - Classifications:** Biotransformation, Catalyzed, Chemoselective, Combinatorial, Electrochemical, Gas-phase, Non-catalyzed, Photochemical, Radiochemical, Regioselective, Stereoselective.
 - Sources:** Any source (selected), Patents only, Sources other than patents.
 - Publication Years:** Input field with examples: 1995, 1995-1999, 1995-, -1995
- Bottom Panel:** A search bar containing "Carboxylic Acid" and a list of elements: C, H, O, S, N, P, Cl, Br, F, I, Si.

反应结果集庞大时如何限定—反应试剂的限定

CAS Solutions

Preferences | SciFinder Help | Sign Out

WELCOME SCIFINDER[®]
A CAS SOLUTION

Welcome Helen Zhu

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

Reaction Structure substructure with limiters > reactions (20364)

REACTIONS

Get References | Tools

Analyze | Refine

Group by: No Grouping | Sort by: Accession Number

0 of 20364 Reactions Selected

Display Options

Page: 1 of 408

Sample Analysis: Reagent

NaOClO	≥ 6548
NaH ₂ PO ₄	≥ 4447
HCl	≥ 3406
Me ₂ C=CHMe	≥ 3348
O ₂	≥ 2382
H ₂ O ₂	≥ 2275
NaOH	≥ 2067
KMnO ₄	≥ 1644
H ₂ NSO ₃ H	≥ 875
KH ₂ PO ₄	≥ 767

1. View Reaction Detail Similar Reactions

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

2. View Reaction Detail Similar Reactions

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

Overview

反应结果集庞大时如何限定—反应试剂的限定

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

Aldehyde reactant Carboxylic Acid product

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

Refine

Structure Editor

Click a reaction participant. A list of roles appears.
Click a reaction role and click OK.

Aldehyde reactant Carboxylic Acid product

reagent

Get reactions where the structure(s) are:

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

OK Cancel

Formula is not available

反应结果集庞大时如何限定—反应试剂的限定

CAS Solutions

SCIFINDER[®]
A CAS SOLUTION

Preferences | SciFinder Help | Sign Out

Welcome Helen Zhu

Explore | Saved Searches | SciPlanner

Save | Print | Export

Reaction Structure substructure with limiters > reactions (20364) > refine "substructure" (20364) > refine "substructure" (1743)

REACTIONS ?

Get References | Tools

Send to SciPlanner

Analyze | Refine

Group by: No Grouping | Sort by: Accession Number

0 of 1743 Reactions Selected

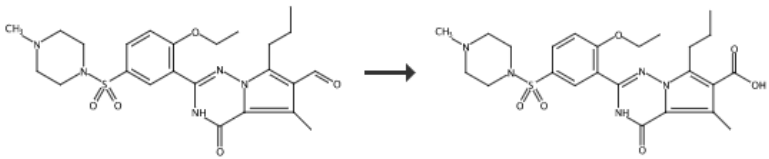
Display Options

Analyze by: Reagent

KMnO ₄	1657
HCl	580
NaOH	224
KOH	134
NaHSO ₃	96
Na ₂ SO ₃	81
10101-50-5	56
Disodium carbonate	54
H ₂ SO ₄	51
NaH ₂ PO ₄	51

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

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



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

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

Overview

Waiting for scifinder.cas.org...

反应结果集庞大时如何限定—催化剂的限定

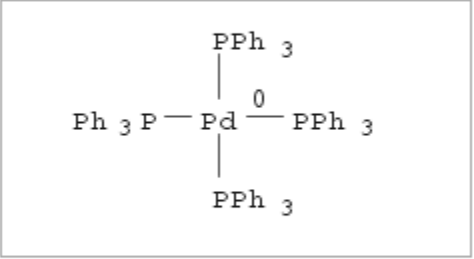
获得四三苯基磷钯作为催化剂的反应

1. 先获得四三苯基磷钯这个化合物
2. 获得催化剂的反应

0 of 1 Substance Selected

1. **14221-01-3** 🔍

~9425 📄 ~185 🧪



C₇₂H₆₀P₄Pd
Palladium, tetrakis(triphenylphosphine)-,
(T-4)-

[Regulatory Information](#)
[Experimental Properties](#)

CAS Registry Number: 14221-01-3

- View Substance Detail
- Explore by Structure ▶
- Synthesize this...
- Get Reactions where Substance is a ▶**
 - Product
 - Reactant
 - Reagent
 - Reactant/Reagent
 - Catalyst**
 - Solvent
 - Any Role
- Get Commercial Sources
- Get Regulatory Information
- Get References
- Export as Image
- Export as molfile
- Send to SciPlanner

反应结果集庞大时如何限定—催化剂的限定

REACTIONS

Get References Tools

Analyze Refine

Group by: No Grouping Sort by: Accession Number

0 of 7122582 Reactions Selected

Page: 1 of 142452

Refine by:

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

Structure Editor: Java Non-Java

Click to Edit

Search type: Substructure

Refine

1. View Reaction Detail Link

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

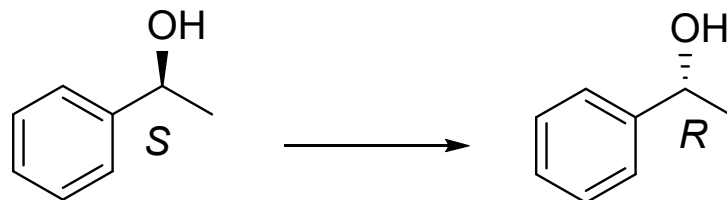
Substance Image Cannot Be Displayed 2133401-30-4

Overview

如有结构，再通过Refine做结构限定

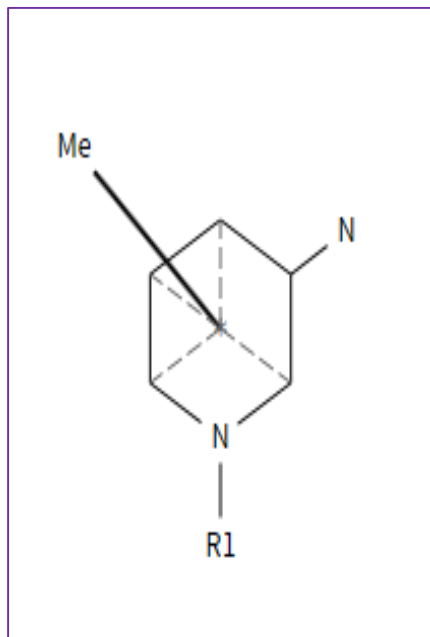
直接检索反应受限的处理

检索如下构型翻转的反应

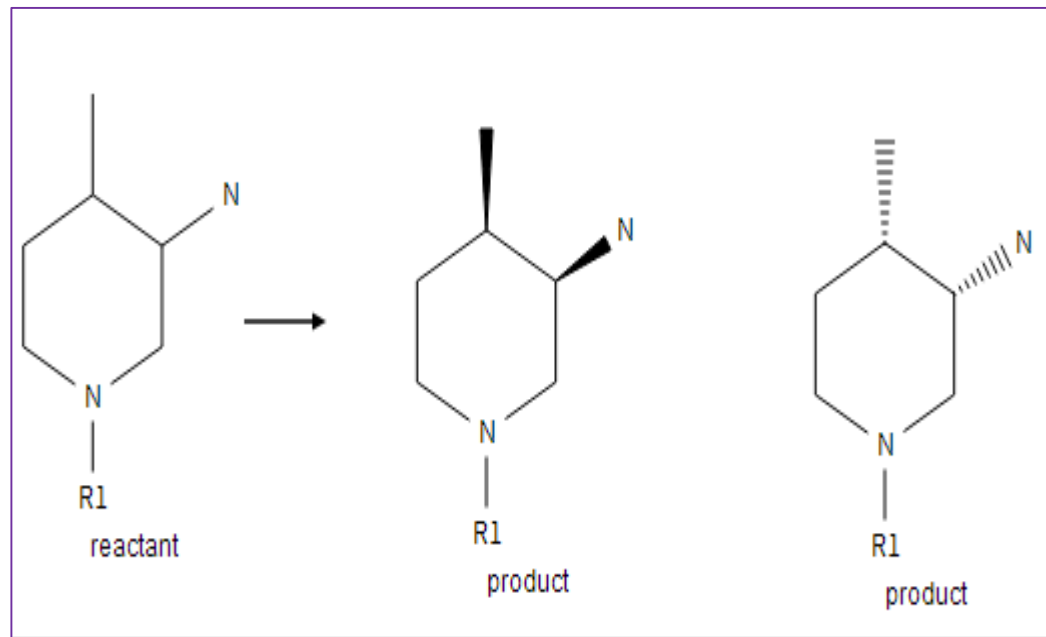


手性拆分反应

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：不考虑物质的手性，快速检索
- 检索思路2：考虑物质的手性，精准检索
- 都是从物质检索出发，然后获取反应，再限定反应物和产物结构

手性拆分反应：检索思路1

- 从产物的反应检索出发

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：从产物的反应检索出发

Structure Editor

Draw or change atoms or bonds. Shortcut Keys

Me N product

Me N product

product

product

OK

Cancel

$C_{11}H_{22}N_2O_2 \cdot C_{11}H_{22}N_2O_2$ 214.31 . 214.31

反应

绘制无立体键的产物,并标明角色为“产物”

亚结构反应检索

手性拆分反应：限定反应物

Explore ▾ Saved Searches ▾ SciPlanner Save Print Export

Reaction Structure substructure > **reactions (681)**

REACTIONS ⓘ Get References Tools ▾

Analyze Refine

Refine by: ⓘ

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

Group by: No Grouping Sort by: Accession Number

0 of 681 Reactions Selected

1. View Reaction Detail ⓘ Link

9 Steps (Converging) Hover over any structure for more

Structure Editor: Java Non-Java

Click image to change

Structure Editor

Click a reaction participant. A list of roles appears. Click a reaction role and click OK.

Get reactions where the structure(s) are:

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

OK Cancel

绘制没有立体构型的反应物

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

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

REACTIONS ? Get References Tools ▼ Send to SciPlanner

Analyze Refine

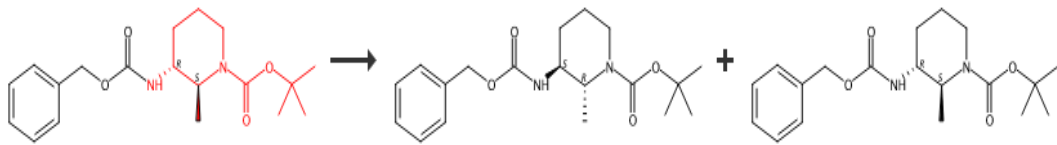
Analyze by: ? Reagent NaOD 1 Show More

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	对映异构体的分离	Notes
1.1		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

检索思路2

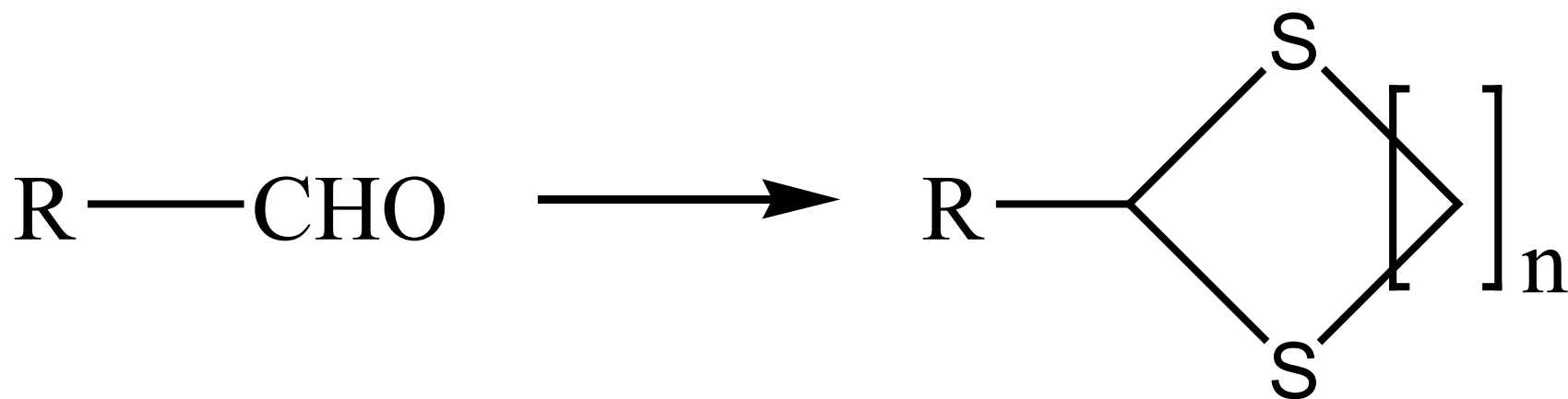
- 从物质检索出发，获取反应
 - 反应物的反应：从物质检索出发，获取反应物（挑选没有立体构型的物质结果集）结果集，点击**Get Reaction**获得反应结果集1
 - 产物的反应：与1采取相同策略（挑选具有绝对立体构型的物质结果集），获得产物的反应结果集2。
- 反应结果集处理
 - 合并反应结果集1与2，取交集获得结果集3
 - 在3的结果集中，用**Reaction Structure**进行**Refine**处理：同时绘制两个产物结构（无需画立体构型），并标明角色都为产物
 - 查看反应结果集，可根据需求（如反应步数，产率，反应类型等）限定结果

手性拆分反应：

- 检索思路1：不考虑物质的手性，有噪音，但快速获得结果；
- 检索思路2：考虑物质的手性，步骤稍多，但无噪音，精准获得结果；
- 可根据检索要求的复杂程度，灵活地选择检索策略，进行快速或精准的检索。

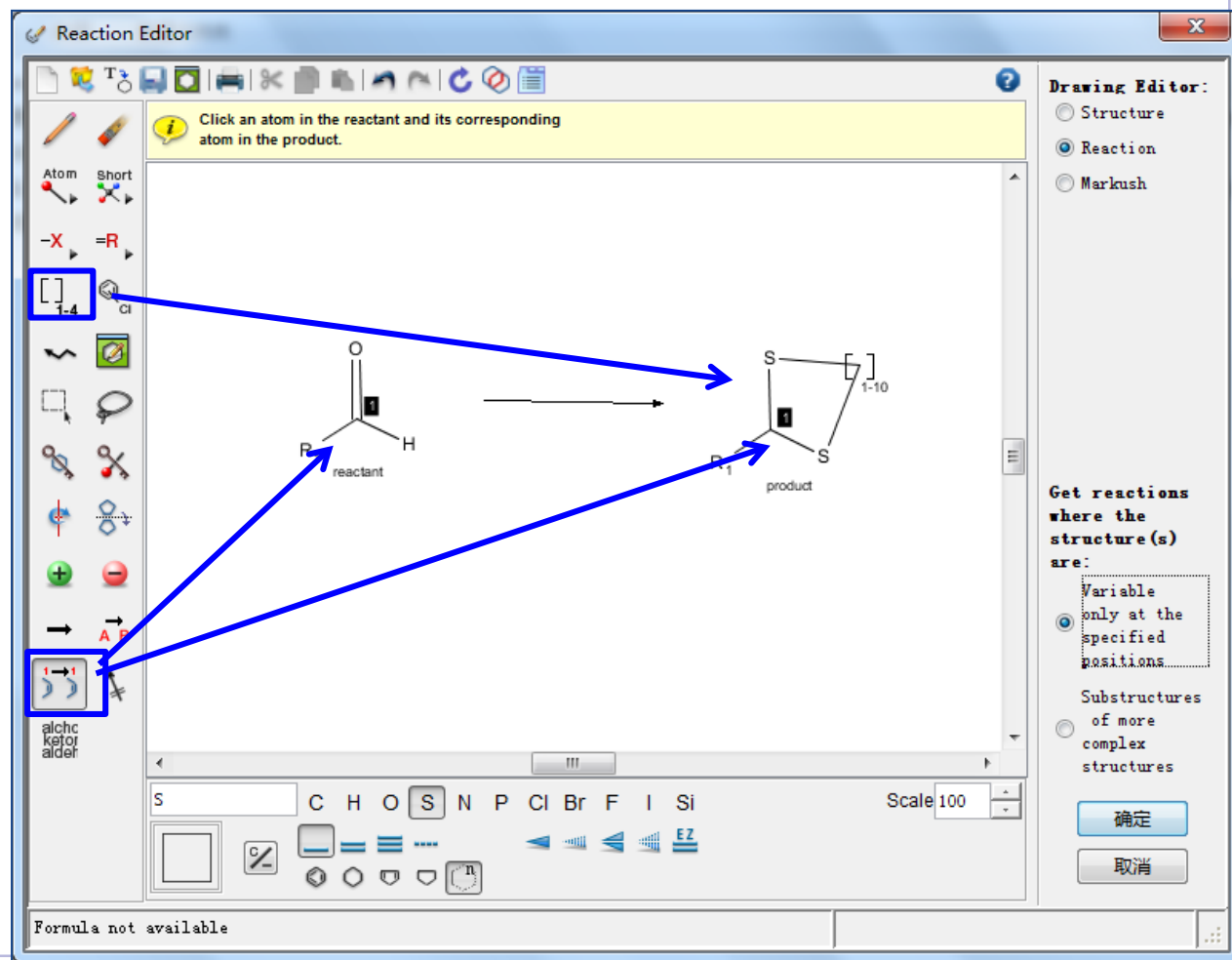
SciFinder中的反应排除策略

在做以下反应的过程中，不允许使用硫醇作为反应物



获得全部符合反应变化要求的反应

- 使用R基团定义
R1=Ak,Cy
- 使用重复基团定义，
定义产物C原子的
重复阈值
- 使用原子标记工具，
标记成环位置。



获得全部符合反应变化要求的反应

SciFinder®

Explore | Saved Searches | SciPlanner

REFERENCES

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

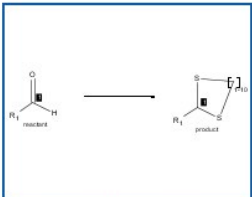
SUBSTANCES

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

REACTIONS

- Reaction Structure

REACTIONS: REACTION STRUCTURE



Search Type:

- Allow variability only as specified
- Substructure

Click image to change structure or view detail.

Import CXF

Search

Advanced Search

SciFinder®

Preferences | SciFinder Help | Sign Out

Welcome Sam Yu

Explore | Saved Searches | SciPlanner

Save | Print | Export

Reaction Structure structure variable only at spe... > reactions (817)

REACTIONS

Get References | Tools

Send to SciPlanner

Analyze | Refine

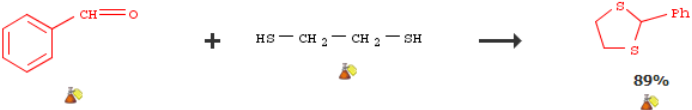
Group by: No Grouping | Sort by: Accession Number

Answers per Page [20] Display: []

0 of 817 Reactions Selected

1. View Reaction Detail | Link | Similar Reactions

Single Step Hover over any structure for more options.



89%

Overview

2. View Reaction Detail | Link | Similar Reactions

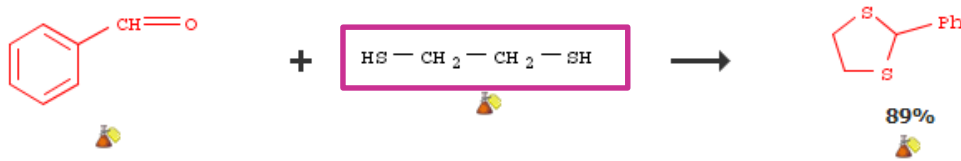
Single Step Hover over any structure for more options.

Analyze by:	Count
Catalyst	
SiO2	41
P2O5	19
H2SO4	17
262297-13-2	15
5952-71-6	15
63295-47-6	15
I2	15
RuCl3	15

获得全部符合反应变化要求的反应

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

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

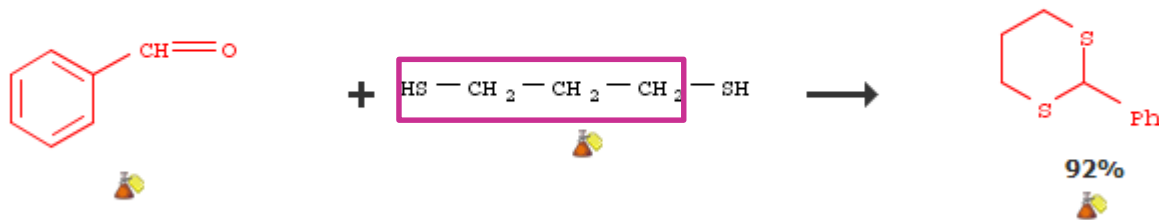


► Overview

大部分反应都是用硫醇

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

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



► Overview

获得全部符合反应变化要求的反应

The screenshot displays the SciFinder web interface. At the top, there are navigation links for 'Preferences', 'SciFinder Help', and 'Sign Out'. Below this, a 'Welcome Sam Yu' message is visible. The main navigation bar includes 'Explore', 'Saved Searches', 'SciPlanner', and a 'Save' button highlighted with a red box. The search results page shows 'Reaction Structure structure variable only at spe... > reactions (817)'. On the left, there is an 'Analyze' section with a 'Catalyst' dropdown menu and a list of catalysts with their respective counts: SiO2 (41), P2O5 (19), H2SO4 (17), 262297-13-2 (15), 5952-71-6 (15), and 63295-47-6 (15). The main content area shows a reaction scheme: a benzaldehyde molecule (C6H5CHO) reacting with ethane-1,2-dithiol (HS-CH2-CH2-SH) to form a cyclic thiolane derivative. The reaction is labeled 'Single Step' and '89%'. A 'Save This Answer Set' dialog box is overlaid on the right side of the screen. It contains a 'Save:' section with two radio buttons: 'All answers' (selected) and 'Only selected answers'. Below this is a 'Title: *' field with the text 'total reaction' and a 'Description:' field. At the bottom right of the dialog are 'OK' and 'Cancel' buttons.

先将结果集保存


获得需要排除的反应

Analyze Refine

Refine by: ?

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

Reaction Structure:



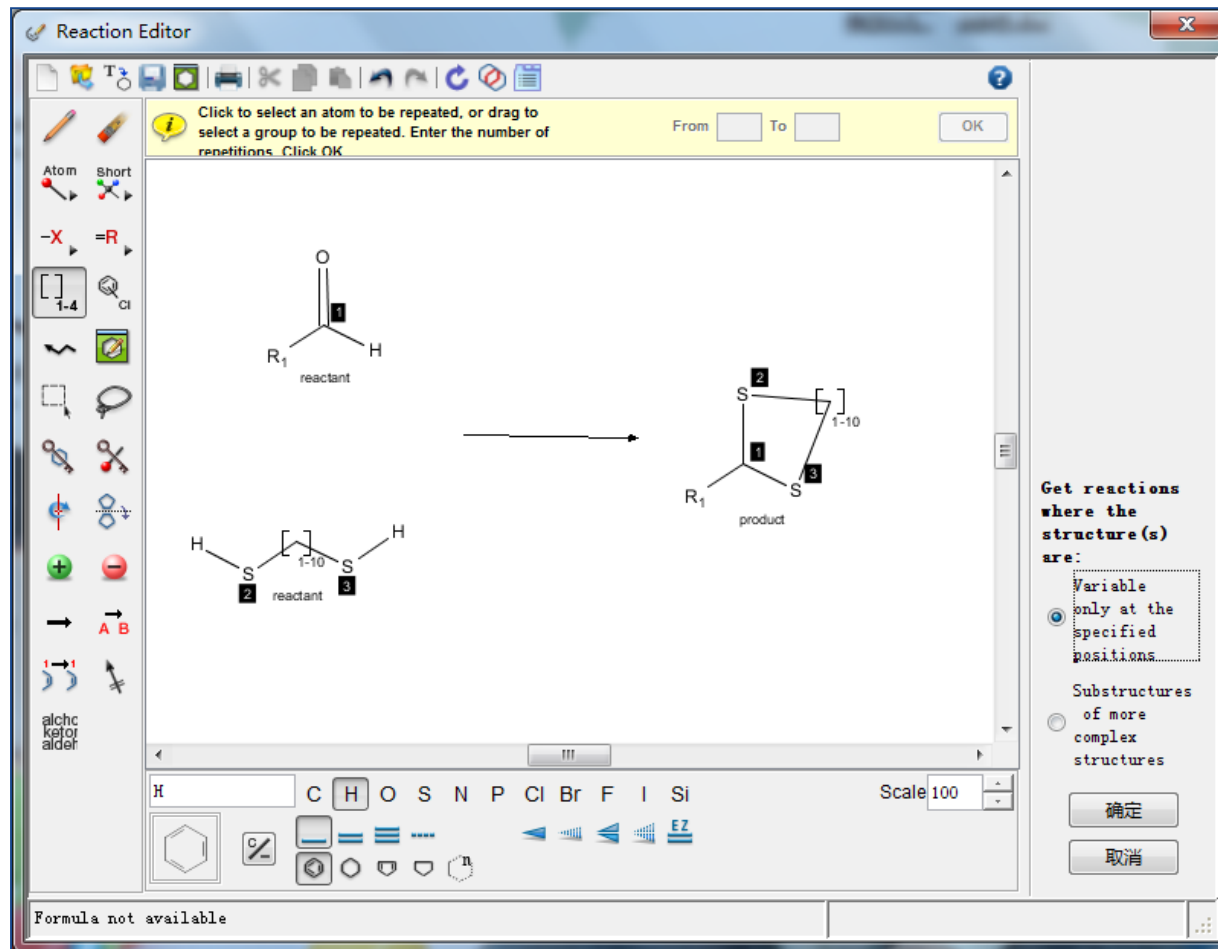
Click image to change structure or view detail
Search type: **Substructure**

Refine

Reaction Editor

Click to select an atom to be repeated, or drag to select a group to be repeated. Enter the number of repetitions. Click OK

From To OK



Get reactions where the structure(s) are:

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

确定 取消

Formula not available

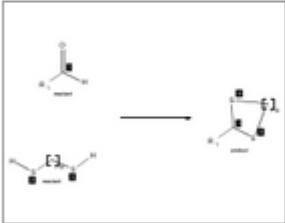
获得需要排除的反应

Analyze Refine

Refine by: ?

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

Reaction Structure:



Click image to change structure or view detail
Search type: **Allow variability only as specified**

Refine

SciFinder® Preferences | SciFinder Help ▾ Sign Out

Welcome Sam Yu

Explore ▾ Saved Searches ▾ SciPlanner Save Print Export

Reaction Structure structure variable only at spe... > reactions (817) > refine "structure variable only at spe..." (754)

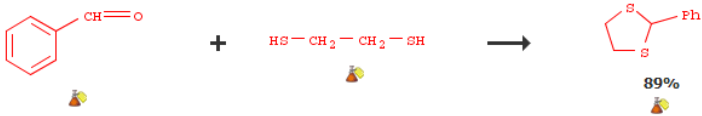
REACTIONS ⓘ Get References Tools ▾ Send to SciPlanner

Analyze Refine Group by: No Grouping ▾ Sort by: Accession Number ▾ ↓ Answers per Page [20] Display: ⓘ ⓘ

0 of 754 Reactions Selected Page: 1 of 38

1. View Reaction Detail ⓘ Link ⓘ Similar Reactions

Single Step Hover over any structure for more options.



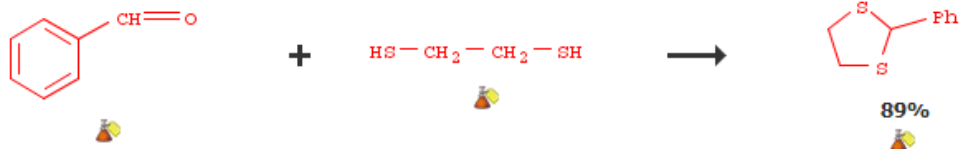
Overview

这里限定出来的都是我们不需要的反应

获得需要排除的反应

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

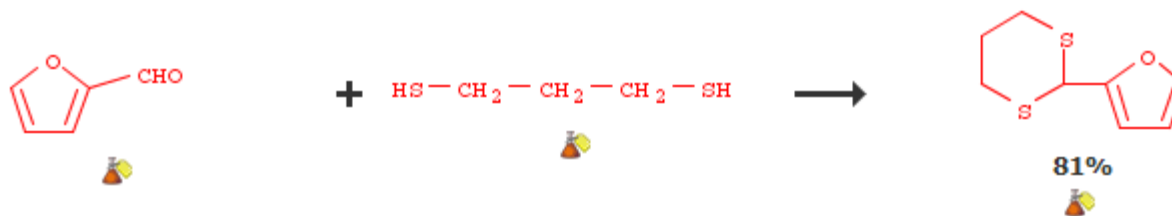
Single Step *Hover over any structure for more options.*



► Overview

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

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



► Overview

去除不要的反应—Combine

SciFinder® Preferences | SciFinder Help ▾ **Sign Out**

Welcome Sam Yu

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

Reaction Structure structure variable only at spe... > reactions (817) > **refine "structure variable only at spe..." (754)**

REACTIONS ⓘ Get References **Tools ▾** Send to SciPlanner

Analyze **Refine** Group by: No Group **Combine Answer Sets** on Number ▾ Answers per Page [20] Display: ⚙

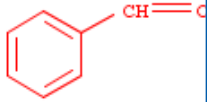
Analyze by: ⓘ
Catalyst ▾

SiO2	39
P2O5	19
H2SO4	17
262297-13-2	15
5952-71-6	15
I2	15

0 of 754 Reactions Selected

1. **View Reaction Detail**

Single Step *Hover over an*



Overview

Combine Answer Sets

Select saved answer set(s) to combine with your current answer set (754):

24 Answer Sets 1 Selected	
Reaction Answer Set Details	Date Saved
<input checked="" type="checkbox"/> total reaction (817) Reaction Structure structure variable only at specified positions > reactions (817)	Sep 24, 2013
<input type="checkbox"/> Autosaved Reaction Set (53) An answer set was automatically saved because the session ended due to inactivity on Thu Aug 29 00:30:02 EDT 2013. Reaction Structure substructure > reactions (83) > refine "2-4 steps" (55) > remove 1 reaction (54) > remove 1 reaction (53)	Aug 29, 2013
<input type="checkbox"/> pyridine (1942) Reaction Structure substructure > reactions (5455) > refine "substructure" (1942)	Jul 8, 2013

Select an option for combining the answer sets:

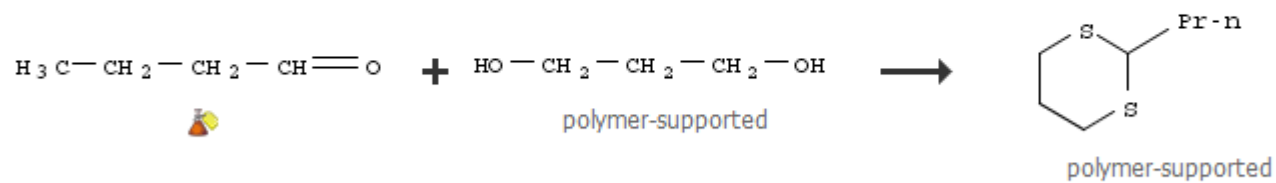
- Combine** Include all answers from both sets
- Intersect** Include only answers that appear in both sets
- Exclude** Include only answers from **current answer set (754)** that are not in **total reaction (817)**
- Exclude** Include only answers from **total reaction (817)** that are not in **current answer set (754)**

Combine Answer Sets **Cancel**

最后的结果

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

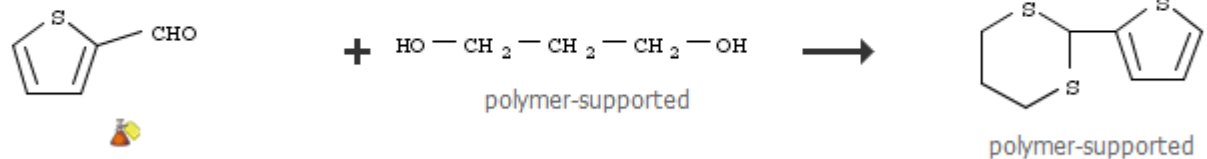
Single Step *Hover over any structure for more options.*



[Overview](#)

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

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



[Overview](#)

新化合物合成路线设计

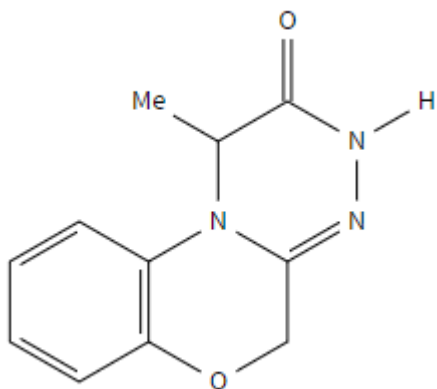
检索思路1: 检索结构相似的物质, 获得有参考价值的合成路线;

检索思路2: 检索通式结构, 获得有参考价值的合成路线;

检索思路3: 先自行做逆合成反应分析, 然后验证相关的反应。

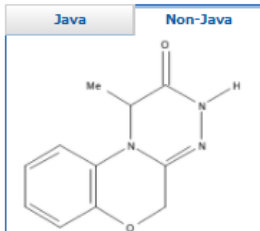
新化合物合成路线设计

检索思路1: 检索相似结构, 获得有参考价值的合成路线



The screenshot displays the SciFinder interface. At the top, it says "CAS Solutions" and "SCIFINDER A CAS SOLUTION". Below this are navigation tabs: "Explore", "Saved Searches", and "SciPlanner". A yellow warning banner indicates "Explore Substances resulted in 0 substances" with a "Return" link. Below the banner, it shows "Chemical Structure exact > substances (0)". A table with the header "SUBSTANCES" is shown, but it is empty. At the bottom, there are "Analyze" and "Refine" buttons. Under "Analyze", it says "Analyze by: No substances available".

Structure Editor:



Click image to change structure or view detail.

Import CXF

Search

Advanced Search Always Show

Search Type:

- Exact Structure
- Substructure
- Similarity

Show precision

ChemDraw
Launch a SciFinder

Select All Deselect All

1 of 7 Similarity Candidates Selected

	Substances
<input type="checkbox"/> ≥ 99 (most similar)	0
<input type="checkbox"/> 95-98	0
<input checked="" type="checkbox"/> 90-94	6
<input type="checkbox"/> 85-89	6
<input type="checkbox"/> 80-84	16
<input type="checkbox"/> 75-79	26
<input type="checkbox"/> 70-74	57
<input type="checkbox"/> 65-69	103
<input type="checkbox"/> 0-64 (least similar)	309

Get Substances

Characteristics

Similarity
 Chemical
 In

Classes

Absolute stereochemistry
 Chemical
 In
 M
 P
 O

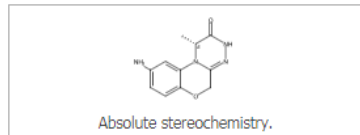
Studies

A
 B
 P
 R

0 of 6 Substances Selected

Score: 91

1. 1613721-07-5



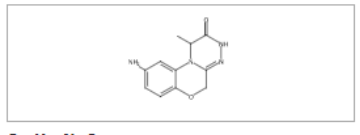
C₁₁H₁₂N₄O₂

[1,2,4]Triazino[3,4-c][1,4]benzoxazin-2(1H)-one, 9-amino-3,5-dihydro-1-methyl-, (1R)-

Key Physical Properties

Score: 91

2. 1613722-60-3



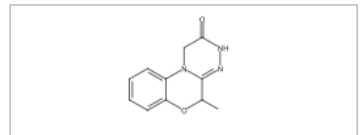
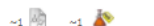
C₁₁H₁₂N₄O₂

[1,2,4]Triazino[3,4-c][1,4]benzoxazin-2(1H)-one, 9-amino-3,5-dihydro-1-methyl-

Key Physical Properties

Score: 90

3. 139605-55-3



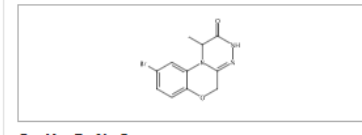
C₁₁H₁₁N₃O₂

[1,2,4]Triazino[3,4-c][1,4]benzoxazin-2(1H)-one, 3,5-dihydro-5-methyl-

Key Physical Properties

Score: 90

4. 1613721-69-9



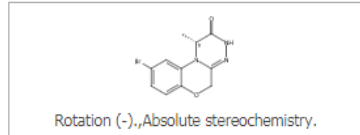
C₁₁H₁₀BrN₃O₂

[1,2,4]Triazino[3,4-c][1,4]benzoxazin-2(1H)-one, 9-bromo-3,5-dihydro-1-methyl-

Key Physical Properties

Score: 90

5. 1613721-93-9



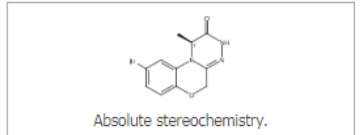
C₁₁H₁₀BrN₃O₂

[1,2,4]Triazino[3,4-c][1,4]benzoxazin-2(1H)-one, 9-bromo-3,5-dihydro-1-methyl-, (1R)-

Key Physical Properties

Score: 90

6. 1613722-23-8



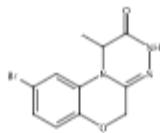
C₁₁H₁₀BrN₃O₂

[1,2,4]Triazino[3,4-c][1,4]benzoxazin-2(1H)-one, 9-bromo-3,5-dihydro-1-methyl-, (1S)-

Key Physical Properties

Score: 90

4. 1613721-69-9



CAS Registry Number: 1613721-69-9

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

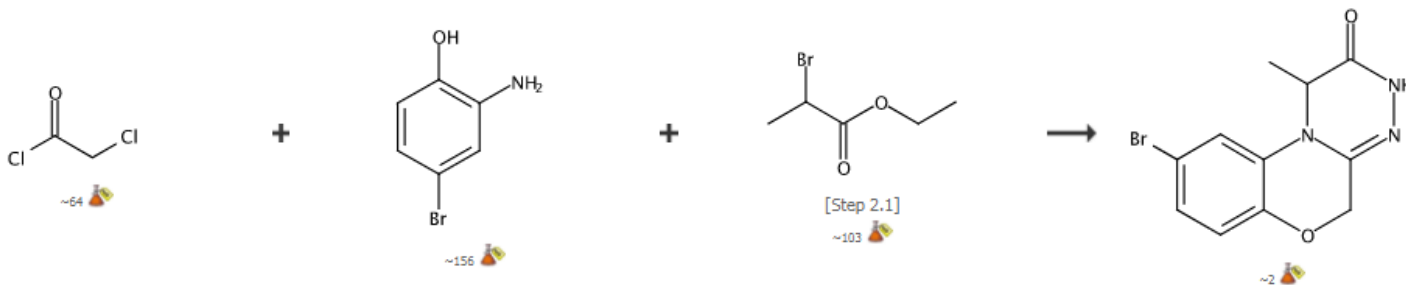
Send to SciPlanner

C₁₁H₁₀BrN₃O₂
[1,2,4]Triazino[3,4-c][1,4]benzoxazin-2(1H)-one,
9-bromo-3,5-dihydro-1-methyl-

Key Physical Properties

1. View Reaction Detail Link

4 Steps Hover over any structure for more options.



Overview

Steps/Stages

- 1.1 R:NaHCO₃, S:H₂O, S:(CH₂OMe)₂, 0°C; 0.5 h, 15°C; overnight, 80°C; 80°C → rt
- 1.2 R:H₂O
- 2.1 R:K₂CO₃, S:Me₂CO, 5 h, 70°C
- 3.1 R:Lawesson's reagent, S:PhMe, 3 h, 120°C
- 4.1 R:N₂H₄-H₂O, S:EtOH, overnight, rt

Notes

1) alternate reaction conditions gave lower yield, Reactants: 3, Reagents: 5, Solvents: 5, Steps: 4, Stages: 5, Most stages in any one step: 2

References

Triazinone compounds as PKC kinase inhibitors and their preparation

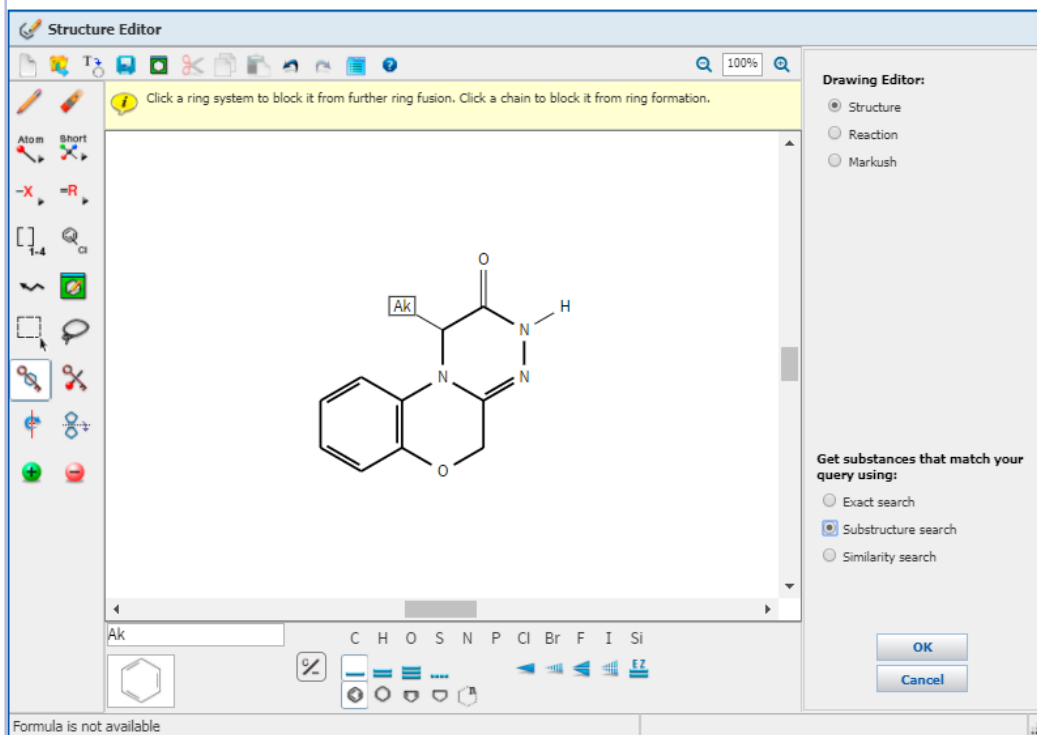
Quick View PATENTPAK

By George, Dawn M. et al

From PCT Int. Appl., 2014089904, 19 Jun 2014

新化合物合成路线设计

检索思路2：检索通式结构，获得有参考价值的合成路线



- | | |
|-----------------|---|
| Characteristics | <input checked="" type="checkbox"/> Single component |
| | <input type="checkbox"/> Commercially available |
| | <input type="checkbox"/> Included in references |
| Classes | <input type="checkbox"/> Alloys |
| | <input type="checkbox"/> Coordination compounds |
| | <input type="checkbox"/> Incompletely defined |
| | <input type="checkbox"/> Mixtures |
| | <input type="checkbox"/> Polymers |
| | <input checked="" type="checkbox"/> Organics, and others not listed |
| Studies | <input type="checkbox"/> Analytical |
| | <input type="checkbox"/> Biological |
| | <input checked="" type="checkbox"/> Preparation |
| | <input type="checkbox"/> Reactant or reagent |

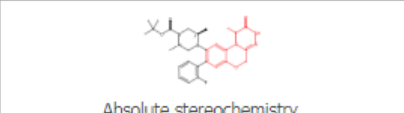
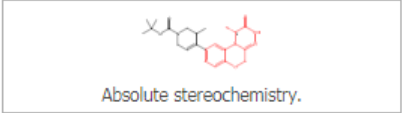
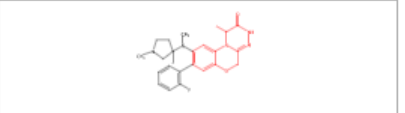
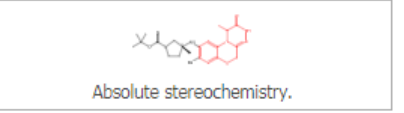
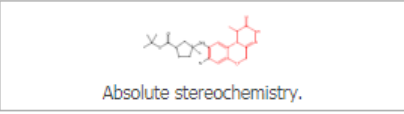
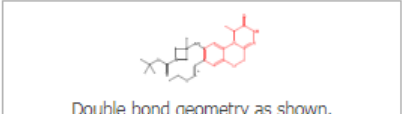
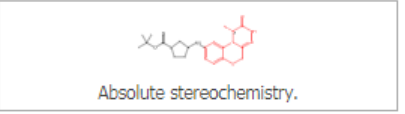
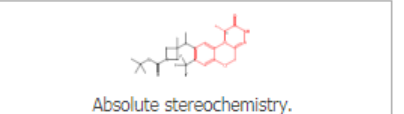
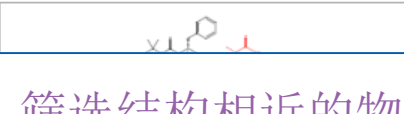
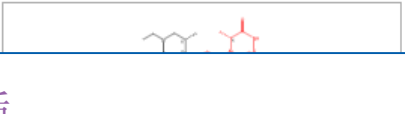
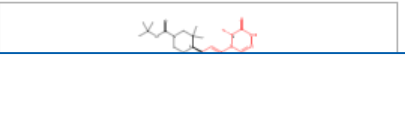
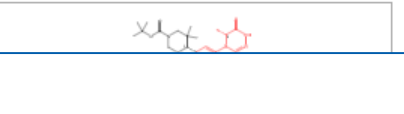
新化合物合成路线设计

Sort by: CAS Registry Number

0 of 424 Substances Selected

Display Options

Page: 1 of 9

<p>1. 1654735-60-0</p>  <p>Absolute stereochemistry.</p> <p>C₂₈H₃₄F N₅O₄ 1-Piperazinecarboxylic acid, 4-[8-(2-fluorophenyl)-1,2,3,5-tetrahydro-1-methyl-2-oxo[1,2,4]triazino[3,4-c][1,4]benzoxazin-9-yl]-2,5-dimethyl-, 1,1-dimethylethyl ester, (2S,5R)-</p> <p>▶ Key Physical Properties</p>	<p>2. 1654735-59-7</p>  <p>Absolute stereochemistry.</p> <p>C₂₂H₂₈N₄O₄ 1(2H)-Pyridinecarboxylic acid, 3,6-dihydro-3-methyl-4-[(1R)-1,2,3,5-tetrahydro-1-methyl-2-oxo[1,2,4]triazino[3,4-c][1,4]benzoxazin-9-yl]-, 1,1-dimethylethyl ester</p> <p>▶ Key Physical Properties</p>	<p>3. 1654735-57-5</p>  <p>Absolute stereochemistry.</p> <p>C₂₄H₂₈F N₅O₂ 1-Pyrrolidinecarboxylic acid, 3-[[1,2,4]triazino[3,4-c][1,4]benzoxazin-2(1H)-one, 9-[[1,3-dimethyl-3-pyrrolidinyl)methylamino]-8-(2-fluorophenyl)]-3,5-dihydro-1-methyl-</p> <p>▶ Key Physical Properties</p>	<p>4. 1654735-48-4</p>  <p>Absolute stereochemistry.</p> <p>C₂₁H₂₈Br N₅O₄ 1-Pyrrolidinecarboxylic acid, 3-[[8-bromo-1,2,3,5-tetrahydro-1-methyl-2-oxo[1,2,4]triazino[3,4-c][1,4]benzoxazin-9-yl]amino]-3-methyl-, 1,1-dimethylethyl ester, (3R)-</p> <p>▶ Key Physical Properties</p>
<p>5. 1654732-77-0</p>  <p>Absolute stereochemistry.</p> <p>C₂₁H₂₈Br N₅O₄ 1-Pyrrolidinecarboxylic acid, 3-[[8-bromo-1,2,3,5-tetrahydro-1-methyl-2-oxo[1,2,4]triazino[3,4-c][1,4]benzoxazin-9-yl]amino]-3-methyl-, 1,1-dimethylethyl ester, (3S)-</p> <p>▶ Key Physical Properties</p>	<p>6. 1654732-76-9</p>  <p>Double bond geometry as shown.</p> <p>C₂₄H₃₃N₅O₅ 1-Azetidinecarboxylic acid, 3-[[8-[[1,2,3,5-tetrahydro-1-methyl-2-oxo[1,2,4]triazino[3,4-c][1,4]benzoxazin-9-yl]amino]-3-methyl-, 1,1-dimethylethyl ester</p> <p>▶ Key Physical Properties</p>	<p>7. 1654728-88-7</p>  <p>Absolute stereochemistry.</p> <p>C₂₀H₂₇N₅O₄ 1-Pyrrolidinecarboxylic acid, 3-[[1,2,3,5-tetrahydro-1-methyl-2-oxo[1,2,4]triazino[3,4-c][1,4]benzoxazin-9-yl]amino]-, 1,1-dimethylethyl ester</p> <p>▶ Key Physical Properties</p>	<p>8. 1654728-63-8</p>  <p>Absolute stereochemistry.</p> <p>C₂₃H₂₉F₃N₄O₄ 1-Azetidinecarboxylic acid, 3-methyl-3-[[1,2,3,5-tetrahydro-1-methyl-2-oxo-8-(trifluoromethyl)[1,2,4]triazino[3,4-c][1,4]benzoxazin-9-yl]ethyl]-, 1,1-dimethylethyl ester</p> <p>▶ Key Physical Properties</p>
<p>9. 1654725-00-4</p>  <p>Absolute stereochemistry.</p> <p>C₂₈H₃₄F N₅O₄ 1-Piperazinecarboxylic acid, 4-[8-(2-fluorophenyl)-1,2,3,5-tetrahydro-1-methyl-2-oxo[1,2,4]triazino[3,4-c][1,4]benzoxazin-9-yl]-2,5-dimethyl-, 1,1-dimethylethyl ester, (2S,5R)-</p> <p>▶ Key Physical Properties</p>	<p>10. 1632329-18-0</p>  <p>Absolute stereochemistry.</p> <p>C₂₈H₃₄F N₅O₄ 1-Piperazinecarboxylic acid, 4-[8-(2-fluorophenyl)-1,2,3,5-tetrahydro-1-methyl-2-oxo[1,2,4]triazino[3,4-c][1,4]benzoxazin-9-yl]-2,5-dimethyl-, 1,1-dimethylethyl ester, (2S,5R)-</p> <p>▶ Key Physical Properties</p>	<p>11. 1632329-17-9</p>  <p>Absolute stereochemistry.</p> <p>C₂₈H₃₄F N₅O₄ 1-Piperazinecarboxylic acid, 4-[8-(2-fluorophenyl)-1,2,3,5-tetrahydro-1-methyl-2-oxo[1,2,4]triazino[3,4-c][1,4]benzoxazin-9-yl]-2,5-dimethyl-, 1,1-dimethylethyl ester, (2S,5R)-</p> <p>▶ Key Physical Properties</p>	<p>12. 1632329-16-8</p>  <p>Absolute stereochemistry.</p> <p>C₂₈H₃₄F N₅O₄ 1-Piperazinecarboxylic acid, 4-[8-(2-fluorophenyl)-1,2,3,5-tetrahydro-1-methyl-2-oxo[1,2,4]triazino[3,4-c][1,4]benzoxazin-9-yl]-2,5-dimethyl-, 1,1-dimethylethyl ester, (2S,5R)-</p> <p>▶ Key Physical Properties</p>

筛选结构相近的物质

新化合物合成路线设计

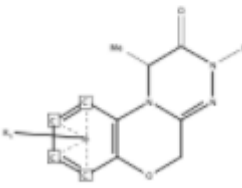
Analyze Refine

Refine by: ?

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

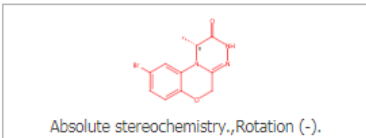
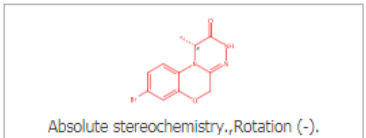
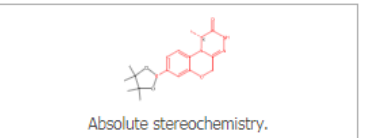
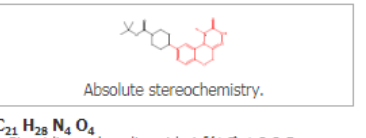
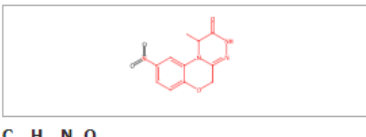
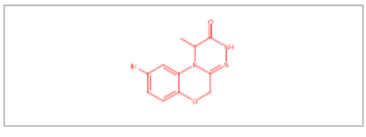
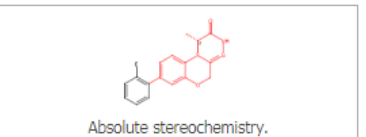
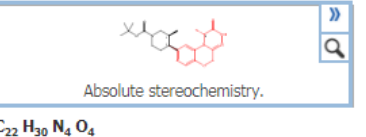
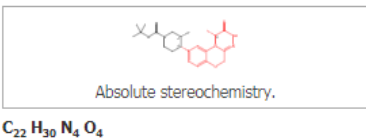
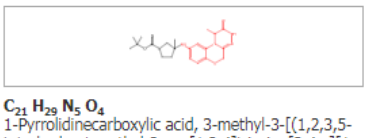
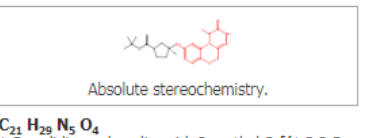
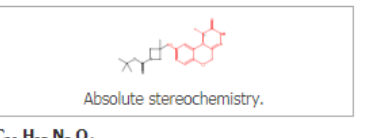
Structure Editor:

Java Non-Java



Click image to change structure or view detail.

Search type: **Substructure**

<p><input type="checkbox"/> 25. 1613721-93-9 </p> <p> </p>  <p>Absolute stereochemistry.,Rotation (-).</p> <p>C₁₁H₁₀BrN₃O₂ [1,2,4]Triazino[3,4-c][1,4]benzoxazin-2(1<i>H</i>)-one, 9-bromo-3,5-dihydro-1-methyl-, (1<i>R</i>)- ▶ Key Physical Properties</p>	<p><input type="checkbox"/> 26. 1613721-90-6 </p> <p> </p>  <p>Absolute stereochemistry.,Rotation (-).</p> <p>C₁₁H₁₀BrN₃O₂ [1,2,4]Triazino[3,4-c][1,4]benzoxazin-2(1<i>H</i>)-one, 8-bromo-3,5-dihydro-1-methyl-, (1<i>R</i>)- ▶ Key Physical Properties</p>	<p><input type="checkbox"/> 27. 1613721-87-1 </p> <p> </p>  <p>Absolute stereochemistry.</p> <p>C₁₇H₂₂BN₃O₄ [1,2,4]Triazino[3,4-c][1,4]benzoxazin-2(1<i>H</i>)-one, 3,5-dihydro-1-methyl-8-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-, (1<i>R</i>)- ▶ Key Physical Properties</p>	<p><input type="checkbox"/> 28. 1613721-85-9 </p> <p> </p>  <p>Absolute stereochemistry.</p> <p>C₂₁H₂₈N₄O₄ 1-Piperidinecarboxylic acid, 4-[(1<i>R</i>)-1,2,3,5-tetrahydro-1-methyl-2-oxo[1,2,4]triazino[3,4-c][1,4]benzoxazin-9-yl]-, 1,1-dimethylethyl ester ▶ Key Physical Properties</p>
<p><input type="checkbox"/> 29. 1613721-72-4 </p> <p> </p>  <p>C₁₁H₁₀N₄O₄ [1,2,4]Triazino[3,4-c][1,4]benzoxazin-2(1<i>H</i>)-one, 3,5-dihydro-1-methyl-9-nitro- ▶ Key Physical Properties</p>	<p><input type="checkbox"/> 30. 1613721-69-9 </p> <p> </p>  <p>C₁₁H₁₀BrN₃O₂ [1,2,4]Triazino[3,4-c][1,4]benzoxazin-2(1<i>H</i>)-one, 9-bromo-3,5-dihydro-1-methyl- ▶ Key Physical Properties</p>	<p><input type="checkbox"/> 31. 1613721-49-5 </p> <p> </p>  <p>Absolute stereochemistry.</p> <p>C₁₇H₁₄FN₃O₂ [1,2,4]Triazino[3,4-c][1,4]benzoxazin-2(1<i>H</i>)-one, 8-(2-fluorophenyl)-3,5-dihydro-1-methyl-, (1<i>R</i>)- ▶ Key Physical Properties</p>	<p><input type="checkbox"/> 32. 1613721-44-0 </p> <p> </p>  <p>Absolute stereochemistry.</p> <p>C₂₂H₃₀N₄O₄ 1-Piperidinecarboxylic acid, 3-methyl-4-[(1<i>R</i>)-1,2,3,5-tetrahydro-1-methyl-2-oxo[1,2,4]triazino[3,4-c][1,4]benzoxazin-9-yl]-, 1,1-dimethylethyl ester, (3<i>S</i>,4<i>S</i>)- ▶ Key Physical Properties</p>
<p><input type="checkbox"/> 33. 1613721-38-2 </p> <p> </p>  <p>Absolute stereochemistry.</p> <p>C₂₂H₃₀N₄O₄ 1-Piperidinecarboxylic acid, 3-methyl-4-[(1<i>R</i>)-1,2,3,5-tetrahydro-1-methyl-2-oxo[1,2,4]triazino[3,4-c][1,4]benzoxazin-9-yl]-, 1,1-dimethylethyl ester, (3<i>S</i>,4<i>S</i>)- ▶ Key Physical Properties</p>	<p><input type="checkbox"/> 34. 1613721-34-8 </p> <p> </p>  <p>C₂₁H₂₉N₅O₄ 1-Pyrrolidinecarboxylic acid, 3-methyl-3-[(1,2,3,5-tetrahydro-1-methyl-2-oxo[1,2,4]triazino[3,4-c][1,4]benzoxazin-9-yl)]-, 1,1-dimethylethyl ester, (3<i>S</i>,4<i>S</i>)- ▶ Key Physical Properties</p>	<p><input type="checkbox"/> 35. 1613721-25-7 </p> <p> </p>  <p>Absolute stereochemistry.</p> <p>C₂₁H₂₉N₅O₄ 1-Piperidinecarboxylic acid, 2-methyl-2-[(1,2,3,5-tetrahydro-1-methyl-2-oxo[1,2,4]triazino[3,4-c][1,4]benzoxazin-9-yl)]-, 1,1-dimethylethyl ester, (3<i>S</i>,4<i>S</i>)- ▶ Key Physical Properties</p>	<p><input type="checkbox"/> 36. 1613721-09-7 </p> <p> </p>  <p>Absolute stereochemistry.</p> <p>C₂₀H₂₇N₅O₄ 1-Piperidinecarboxylic acid, 2-methyl-2-[(1,2,3,5-tetrahydro-1-methyl-2-oxo[1,2,4]triazino[3,4-c][1,4]benzoxazin-9-yl)]-, 1,1-dimethylethyl ester, (3<i>S</i>,4<i>S</i>)- ▶ Key Physical Properties</p>

新化合物合成路线设计

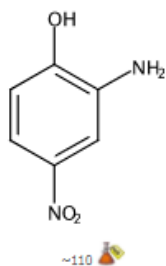
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Display Options

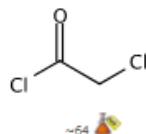
0 of 8 Reactions Selected

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

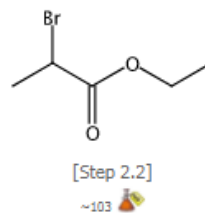
4 Steps *Hover over any structure for more options.*



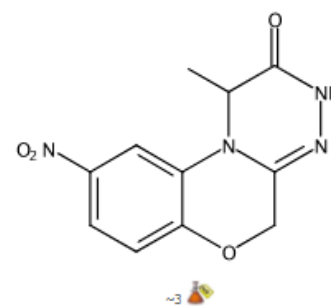
+



+



→



Overview

Experimental Procedure

METHODSNow™

Procedure

1. Add 2-chloroacetyl chloride (83.6 mL, 1110 mmol) dropwise to a solution of 2-amino-4-nitrophenol (114.0 g, 740 mmol) , K_2CO_3 (306.2 g, 2220 mmol) and tetrabutyl ammonium bromide (23.8 g, 74 mmol) in acetonitrile (1.50 L) at 0 °C.
2. Heat the reaction mixture at 80 °C for 1 h.

[View more...](#)

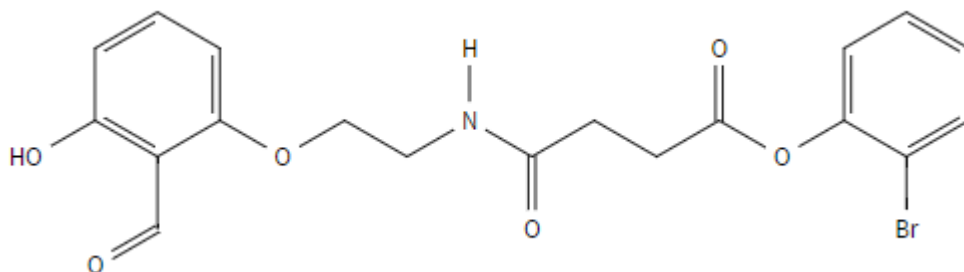
Available Experimental Data

1H NMR, R_f , State

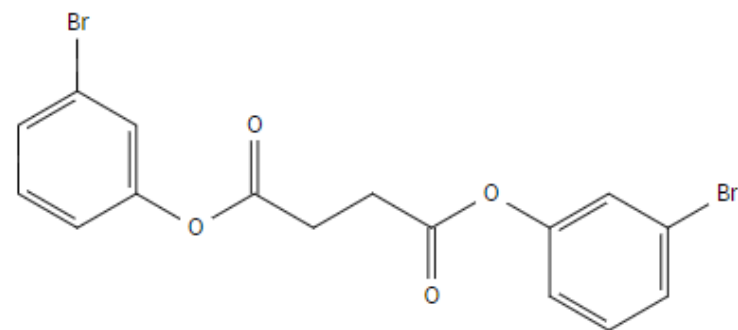
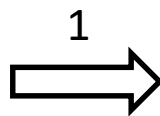
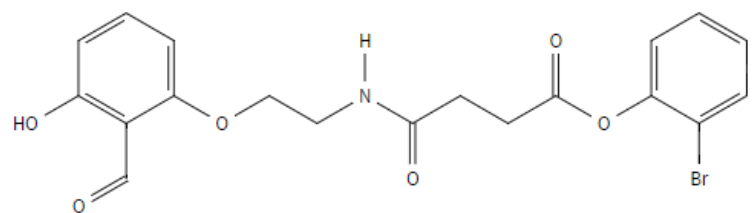
[View with MethodsNow](#)

新化合物合成路线设计

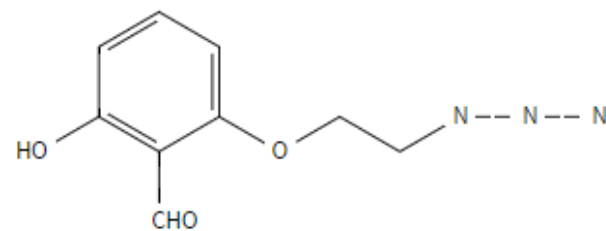
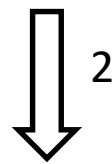
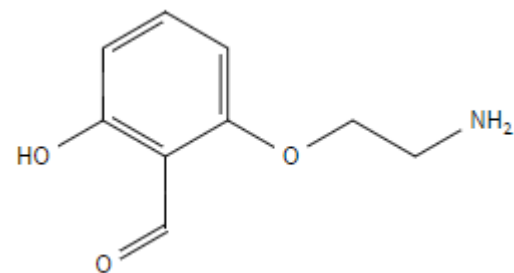
检索思路3：先自行做逆合成反应分析，然后检索相关的反应



逆合成反应分析



+



新化合物合成路线设计

反应1

Structure Editor

Click a reaction participant. A list of roles appears.
Click a reaction role and click OK.

Atom Short
-X =R
1.4
Aldehyde

Primary Amine reactant
Amide product
Phenol non-reacting

Aldehyde

Get References
Retrieve references for selected reactions.

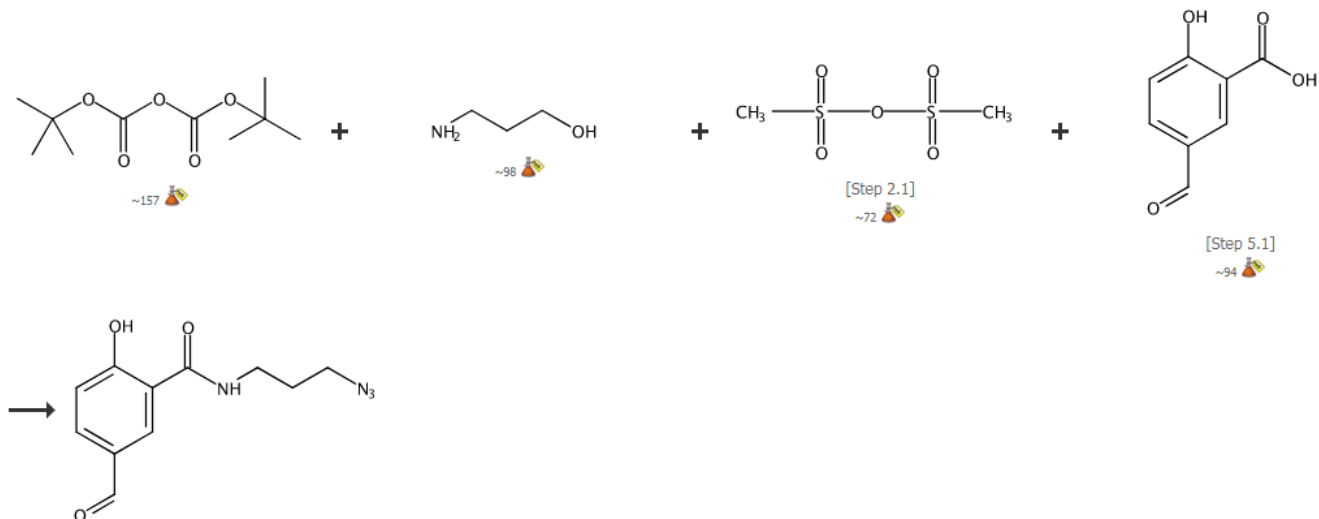
Group by: No Grouping Sort by: Accession Number

0 of 1538 Reactions Selected

1. View Reaction Detail Link

5 Steps Hover over any structure for more options.

Formula is not available



新化合物合成路线设计

问题：反应底物太多，不理想

Analyze Refine

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

Get References Tools

Group by: No Grouping Sort by: Accession Number

0 of 855 Reactions Selected

1. View Reaction Detail [Link](#)

22 Steps (Converging) *Hover over any structure for more options.*

Structure Editor:
Java
Carboxylate Ester
Click image to change structure or view details
Search type: **Substructure**

Refine

Chemical structures shown in the reaction scheme:

- 4-nitrobenzoic acid (~121)
- allyl bromide (~93)
- 3,4-dihydroxybenzaldehyde (~108)
- isobutyl bromide (~83)
- acetyl chloride (~83)
- methyl acrylate (~53)
- iodomethane (~96)

SciFinder A CAS SOLUTION

新化合物合成路线设计

进一步筛选

Analyze Refine

Refine by: ?

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

Number of Steps:

1-2

Examples: 1, 1-3, 1-7

Refine

Get References

Tools

Group by: No Grouping Sort by: Accession Number

0 of 66 Reactions Selected

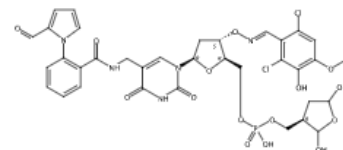
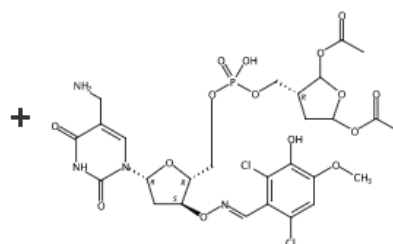
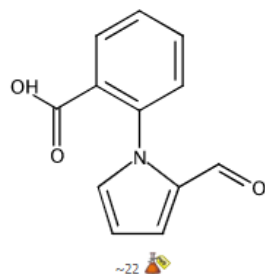
Send to SciPlanner

Display Options

Page: 1 of 2

1. View Reaction Detail Link

2 Steps Hover over any structure for more options.

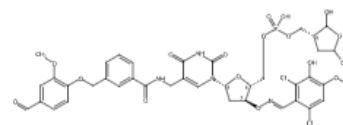
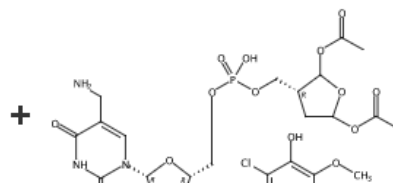
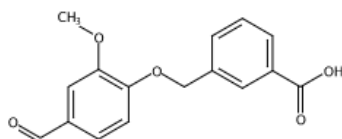


酰化剂为羧酸，不符合要求

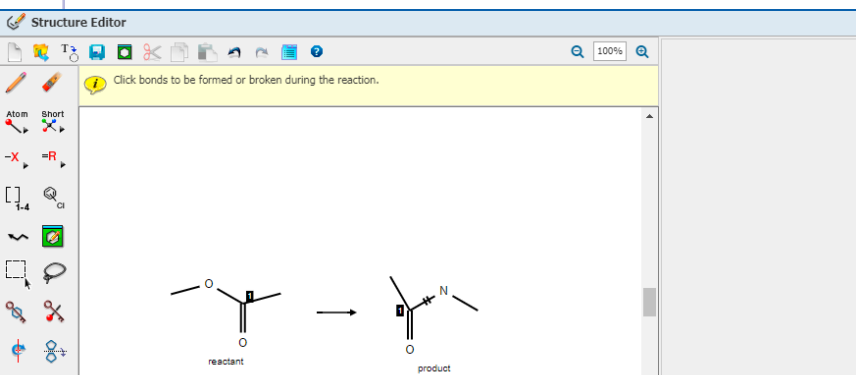
Overview

2. View Reaction Detail Link

2 Steps Hover over any structure for more options.



新化合物合成路线设计



进一步限定用酯做酰化剂的反应

Get References Tools

Send selected records to SciPlanner. Send to SciPlanner

Group by: No Grouping Sort by: Relevance

0 of 59 Reactions Selected

1. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.

~74 ~120

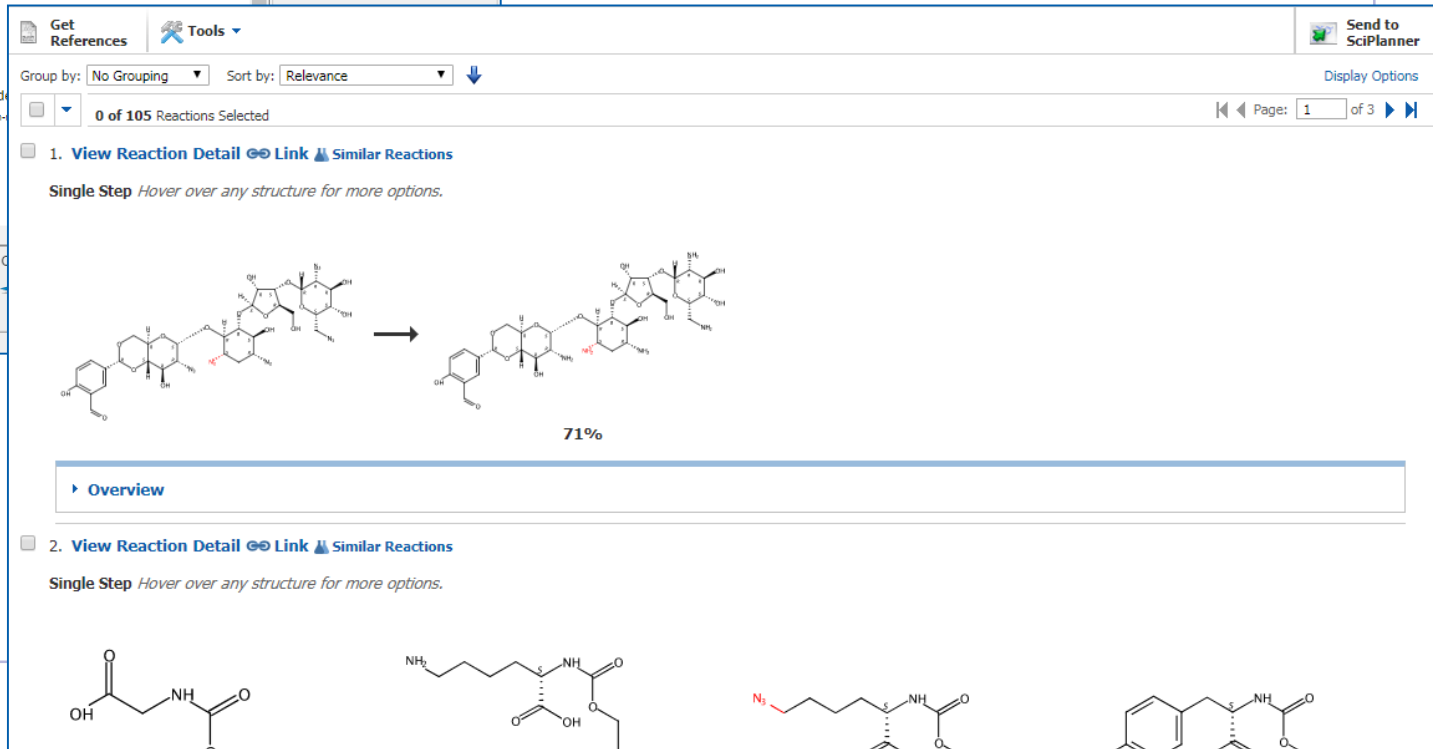
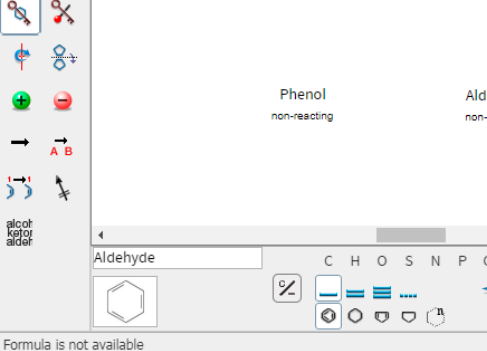
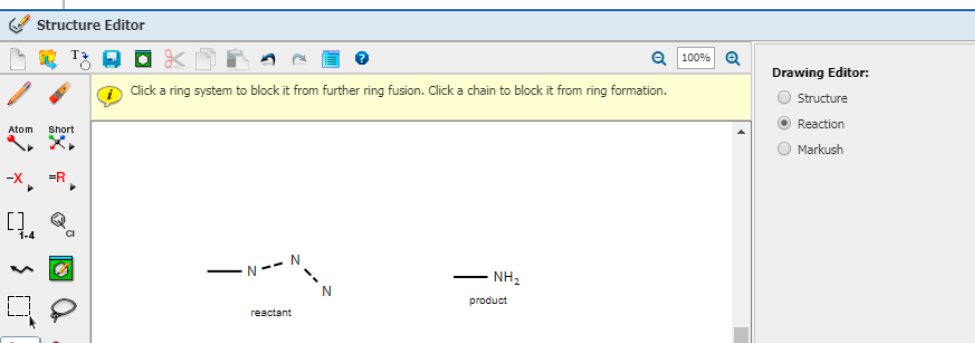
Overview

2. View Reaction Detail Link

2 Steps Hover over any structure for more options.

新化合物合成路线设计

反应2



案例分析

检索要求:

- 某个结构中包含环和Cbz，环上存在Br或者I
- 寻找脱Cbz的一步反应，而环上卤素不脱掉

定义困难:

如何定义这个环系，杂环？C环？

Cbz和环的连接方法

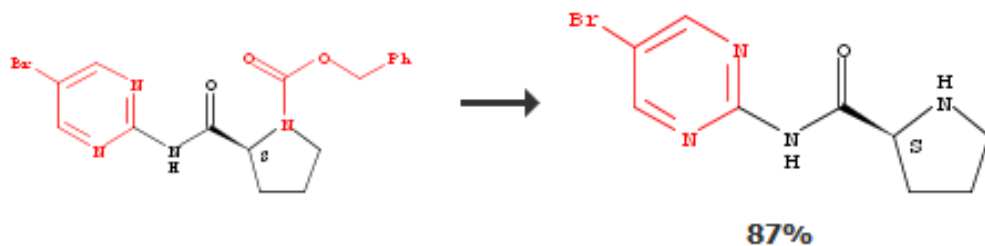
案例分析

The screenshot displays the Reaction Editor software interface. At the top, a yellow banner reads "Click bonds to be formed or broken during the reaction." The main workspace contains three chemical structures: a reactant with a dashed triangle labeled R_1 and R_2 , a product with a similar dashed triangle, and a reactant with a six-membered ring and a carbonyl group. The left sidebar contains various tool icons for atom selection, bond creation, and reaction types. The bottom panel shows a list of elements (A, C, H, O, S, N, P, Cl, Br, F, I, Si) and a scale of 100. The status bar at the bottom left indicates "Formula not available". On the right side, there are two radio button options: "Variable only at the specified positions" (unselected) and "Substructures of more complex structures" (selected). Below these are buttons for "确定" (OK) and "取消" (Cancel).

案例分析

32. 1 Hits in this Reference Similar Reactions

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



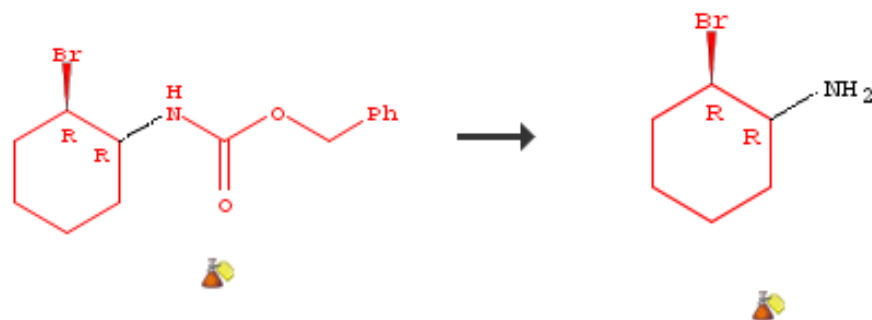
► Overview

► Experimental Procedure

存在我们想要的结果集

33. 1 Hits in this Reference Similar Reactions

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

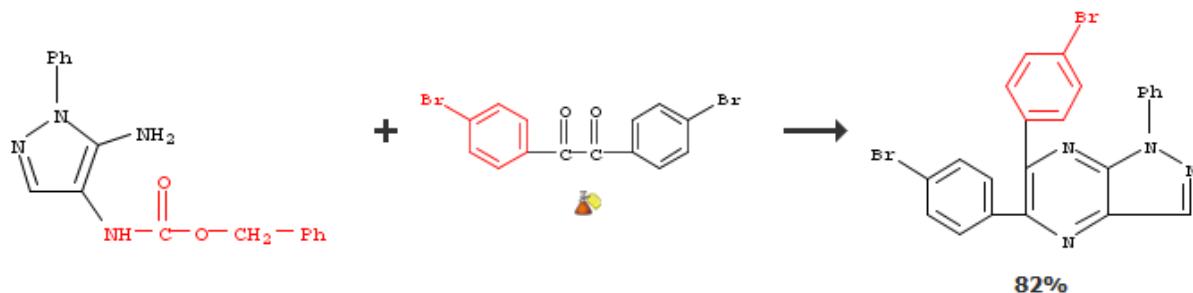


► Overview

► Experimental Procedure

案例分析

36. 1 Hits in this Reference Similar Reactions
Single Step Hover over any structure for more options.

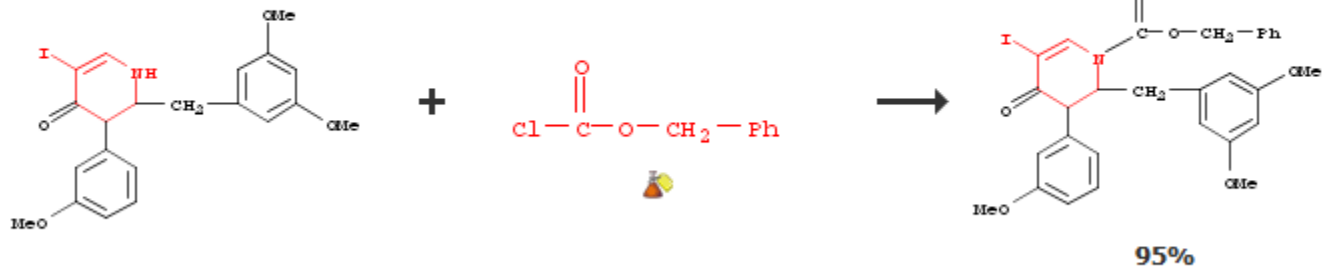


- ▶ Overview
- ▶ Experimental Procedure

存在大量的环与Cbz不在一个结构上的反应

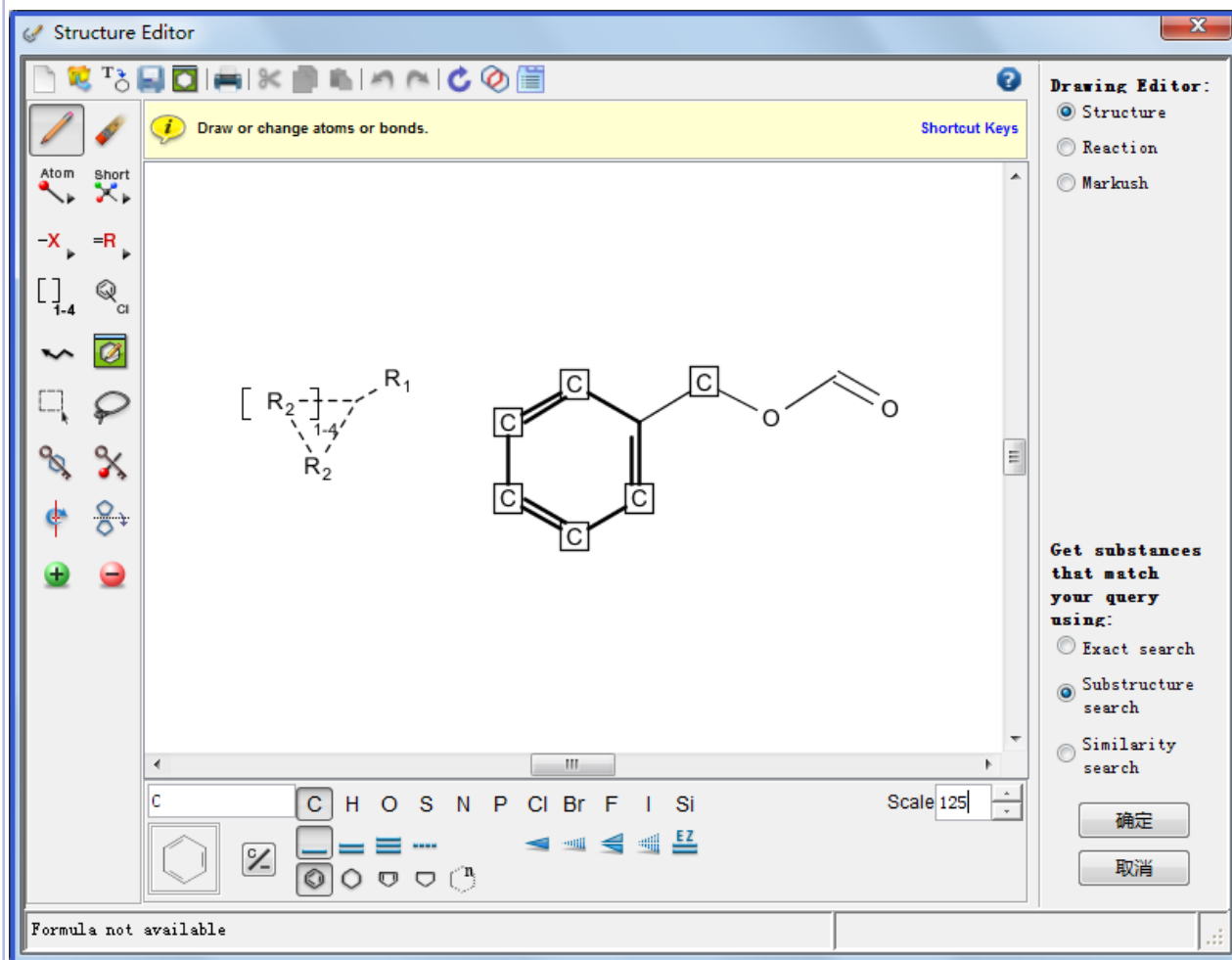
如何去除？

38. 1 Hits in this Reference Similar Reactions
Single Step Hover over any structure for more options.



- ▶ Overview

案例分析

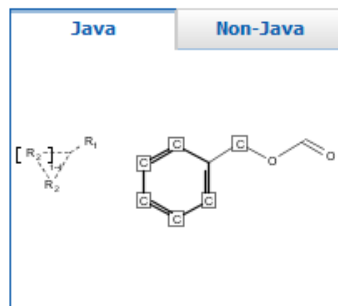


这种类型的反应，
需要先去检索和反
应相关的物质

案例分析

SUBSTANCES: CHEMICAL STRUCTURE ?

Structure Editor:



Click image to change structure or view detail.

Import CXF

Search

Advanced Search Always Show

Search Type:

- Exact Structure
 Substructure
 Similarity

Show precision analysis



Launch a SciFinder substance or [More](#)

- | | |
|-----------------|---|
| Characteristics | <input checked="" type="checkbox"/> Single component |
| | <input type="checkbox"/> Commercially available |
| | <input type="checkbox"/> Included in references |
| Classes | <input type="checkbox"/> Alloys |
| | <input type="checkbox"/> Coordination compounds |
| | <input type="checkbox"/> Incompletely defined |
| | <input type="checkbox"/> Mixtures |
| | <input type="checkbox"/> Polymers |
| | <input checked="" type="checkbox"/> Organics, and others not listed |
| Studies | <input type="checkbox"/> Analytical |
| | <input type="checkbox"/> Biological |
| | <input type="checkbox"/> Preparation |
| | <input checked="" type="checkbox"/> Reactant or reagent |

需要定义为单一组分和具备
反应物或试剂角色的物质

案例分析

SciFinder®

Preferences | SciFinder Help | Sign Out

Welcome Helen Zhu

Explore | Saved Searches | SciPlanner

Save | Print | Export

Chemical Structure substructure with limiters > substances (4727) > get reactions (77364) > refine "1 step" (5909) > refine "substructure" (414)

SUBSTANCES **Get References** **Get Reactions** **Get Commercial Sources** **Tools** **Create Keep Me Posted Alert** **Send to SciPlanner**

Analyze **Refine** Sort by: CAS Registry Number **Display Options**

0 of 4727 Substances Selected Page: 1 of 316

Analyze by: Substance Role

Reactant or Reagent 4727

Preparation 4348

Prophetic in Patents 556

Biological Study 512

Uses 470

Properties 75

Process 26

Combinatorial Study 13

Analytical Study 2

Formation, Nonpreparative 2

1. **1687759-75-6**

C₂₈H₂₈BrN₅O₃
1-Piperidinecarboxylic acid, 4-[[4-[(3-bromophenyl)amino]-7-methoxy-6-quinazolinyl]amino]-, phenylmethyl ester

2. **1687759-73-4**

C₂₆H₂₄BrN₅O₃
1-Azetidinecarboxylic acid, 3-[[4-[(3-bromophenyl)amino]-7-methoxy-6-quinazolinyl]amino]-, phenylmethyl ester

3. **1687758-88-8**

4. **1687758-80-0**

获得所有可能的反应物，并获得这些物质作为反应物的反应

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

案例分析

SciFinder®

Preferences | SciFinder Help | Sign Out

Welcome Helen Zhu

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

Chemical Structure substructure with limiters > substances (4727) > **get reactions (77364)** > refine "1 step" (5909) > refine "substructure" (414)

REACTIONS **?** | Get References | Tools

Send to SciPlanner

Analyze | Refine

Group by: No Grouping | Sort by: Accession Number

0 of 77364 Reactions Selected

Page: 1 of 1548

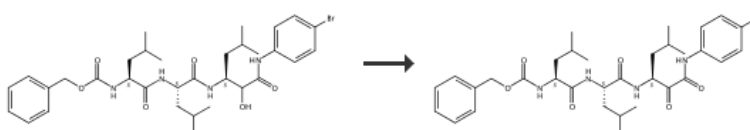
Sample Analysis: **?**

Reagent

H ₂	≥ 10560
HCl	≥ 9264
Et ₃ N	≥ 8636
K ₂ CO ₃	≥ 7682
EtN(Pr-) ₂	≥ 6769
NaHCO ₃	≥ 6634
AcOK	≥ 5176
F ₃ CCO ₂ H	≥ 4608
EtN=C(N(CH ₂) ₃ NMe ₂)	≥ 4311
•HCl	≥ 4311
148893-10-1	≥ 4280

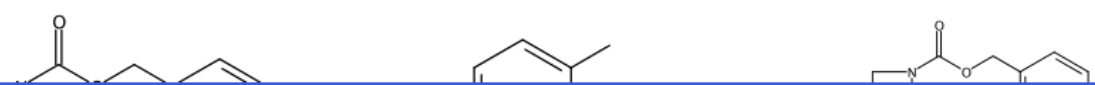
1. **View Reaction Detail** | Link | Similar Reactions

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



2. **View Reaction Detail** | Link | Similar Reactions

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



这些反应中的反应物都包含要求的结构，
需进一步把产物限定进去。

案例分析

Analyze Refine

Refine by: ?

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

Number of Steps:

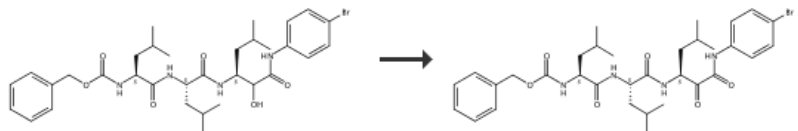
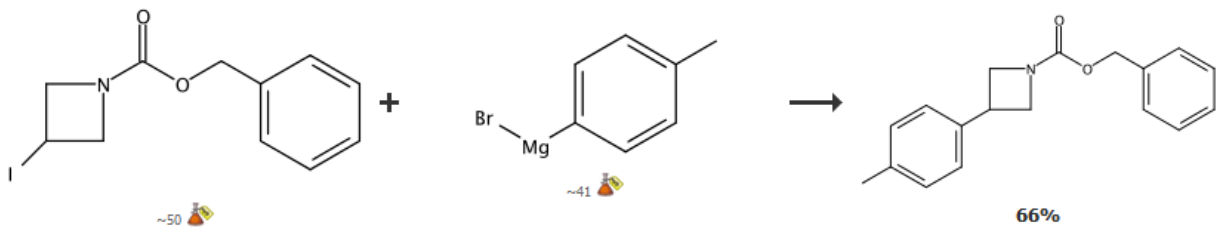
1

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

Refine

先限定反应步数为一步反应

0 of 5909 Reactions Selected

- 1. View Reaction Detail** [Link](#) [Similar Reactions](#)
Single Step *Hover over any structure for more options.*

[Click to view detail](#)
[Overview](#)
- 2. View Reaction Detail** [Link](#) [Similar Reactions](#)
Single Step *Hover over any structure for more options.*

[Overview](#)
- 3. View Reaction Detail** [Link](#) [Similar Reactions](#)
Single Step *Hover over any structure for more options.*

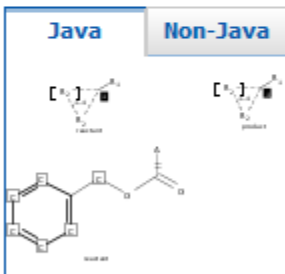
案例分析

Analyze Refine

Refine by: ?

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

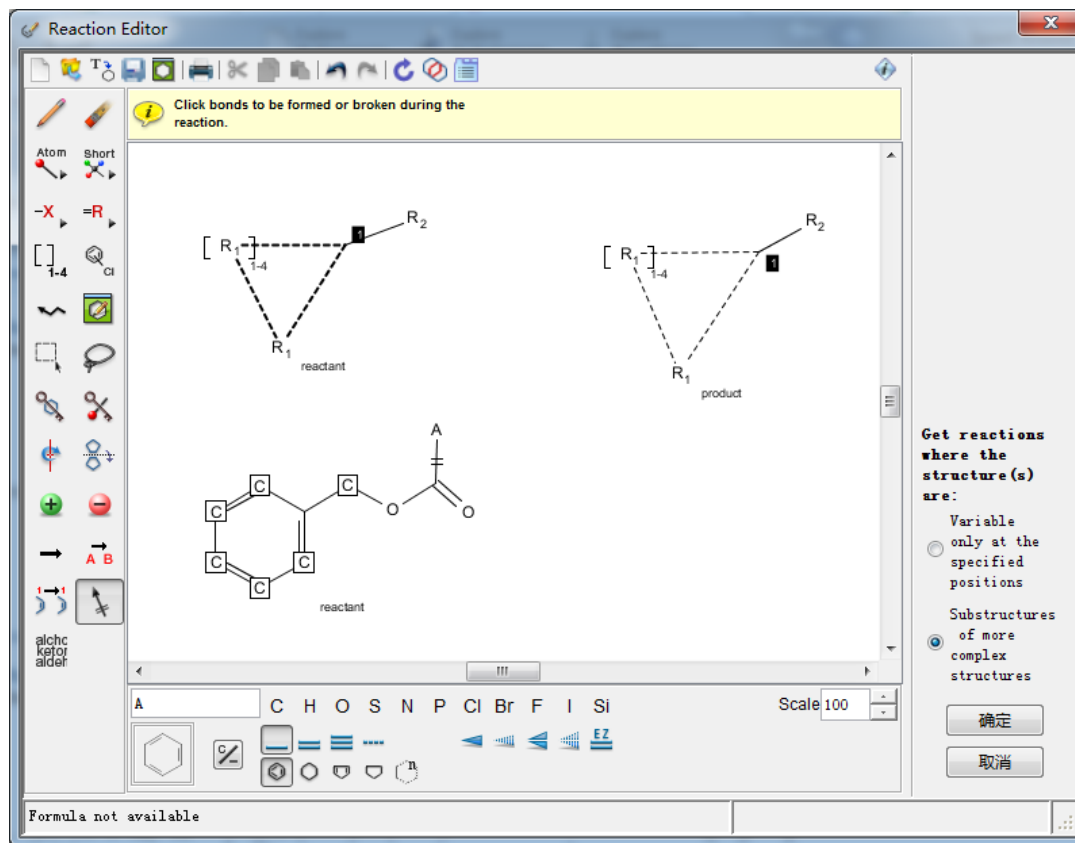
Structure Editor:



Click image to change structure or view detail.

Search type: **Substructure**

Refine



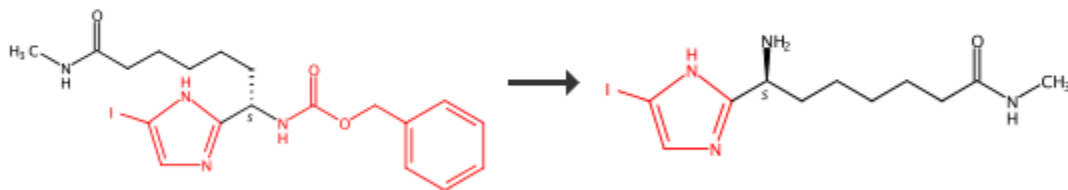
再做反应中心限定，沿用之前的定义

案例分析

0 of 414 Reactions Selected

1. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.

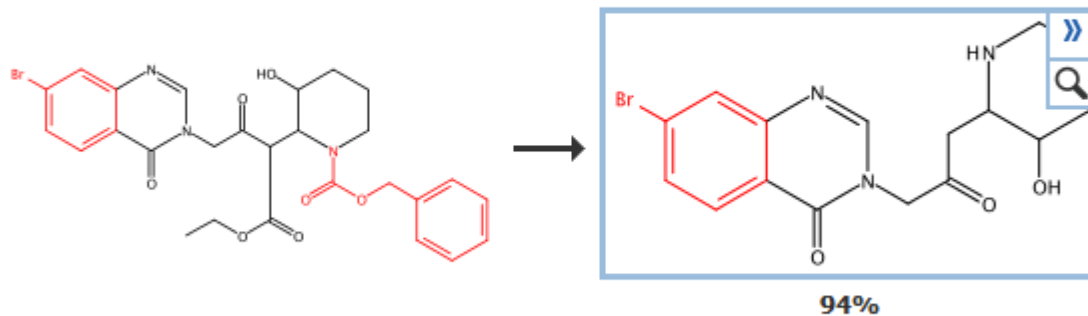


Overview

都是我们想要的反应结果

7. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.



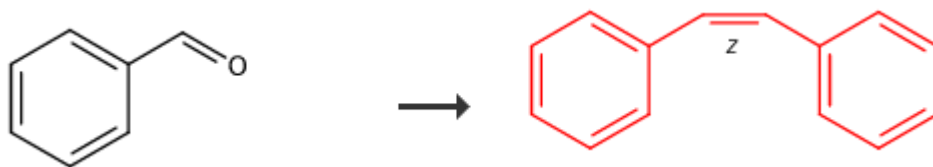
Overview

SciFinder中的检索思路

- 初步检索
- 浏览结果集，判断是否符合要求，利用系统工具限定结果
- 修正检索式，再次检索
- 浏览结果集，判断

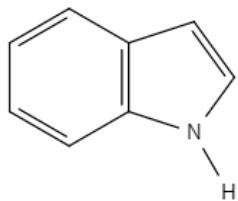
上机练习

1. 检索以下反应:



2. 底物上有伯羟基和仲羟基，能否找到合适的氧化剂使伯羟基氧化成醛而仲羟基不受影响？

3. 检索保护吲哚环上N原子而环上的羟基不受影响的反应？



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010-62508026

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