

朱传娴

客户顾问

hzhu@acs-i.org

如何使用SciFinder获取医药信息

----反应部分

中国药科大学

2018.06.07



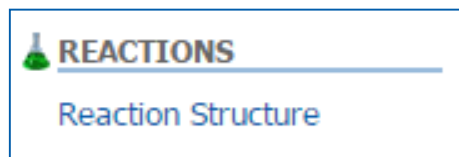
提纲

- SciFinder中的反应检索
- 反应检索疑难分析
- 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



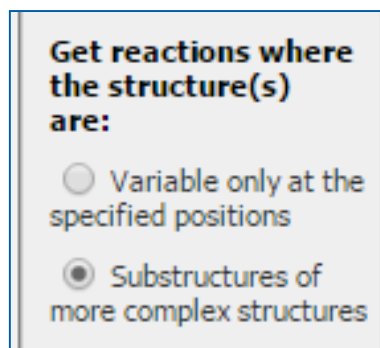
- 常用获取方法

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 window with various toolbars and a central canvas. The interface includes a top toolbar with icons for file operations, a left toolbar with drawing tools, a right sidebar with 'Drawing Editor' options, and a bottom toolbar with element selection and bond types. A yellow status bar at the top of the canvas reads 'Draw or change atoms or bonds.' and 'Shortcut Keys'. The 'Drawing Editor' sidebar has radio buttons for 'Structure', 'Reaction' (selected), and 'Markush'. Below it, there are options for 'Get reactions where the structure(s) are:' with radio buttons for 'Variable only at the specified positions' and 'Substructures of more complex structures'. The bottom status bar shows 'CH₄' on the left and '16.04' on the right.

Reaction Arrow (反应箭头)

Reaction Role Tools (反应角色工具)

Reaction Atom Marking Tools (反应原子标记工具)

Functional Group List (官能团列表)

Reaction Position Marking Tools (反应位置标记工具)

SciFinder反应检索——精确反应检索

The screenshot displays the SciFinder Structure Editor interface. The central workspace shows a chemical reaction: nitrobenzene (reactant) is converted to aniline (product). The reactant is a benzene ring with a nitro group (NO_2) at the bottom position, and the product is a benzene ring with an amino group (NH_2) at the bottom position. An arrow points from the reactant to the product.

The interface includes a drawing toolbar on the left with various tools for creating and editing chemical structures. A yellow banner at the top of the workspace reads "Draw or change atoms or bonds." and "Shortcut Keys".

On the right side, the "Drawing Editor" panel is visible, with the "Reaction" option selected. Below this, the "Get reactions where the structure(s) are:" section contains two radio button options:

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

A callout box with a purple border and the text "精确反应检索" (Precise Reaction Search) points to the "Variable only at the specified positions" option.

At the bottom of the interface, there is a search bar containing "NH2", a list of elements (C, H, O, S, N, P, Cl, Br, F, I, Si), and a molecular formula display showing $\text{C}_7\text{H}_7\text{NO}_2 \cdot \text{C}_7\text{H}_7\text{N}$ and a numerical range "137.14 . 107.16".

反应检索结果

浏览记录，发现很多反应来自同一篇文章，
通过Group by Document合并。

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

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

Cc1ccc([N+](=O)[O-])cc1 → Cc1ccc(N)cc1

~102 100% ~122

Overview

Steps/Stages

1.1 R:NaBH₄, C:1832616-28-0, S:THF, 45 min, 25°C

Notes

solid-supported catalyst, ruthenium supported on porous organic polymer used, reusable catalyst, sealed tube used, scalable, Reactants: 1, Reagents: 1, Catalysts: 2, Solvents: 2, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Fabrication of Ruthenium Nanoparticles in Porous Organic Polymers: Towards Advanced Heterogeneous Catalytic Nanoreactors

获取相似反应

选择相似反应的相似限制：

Broad：仅反应中心相似

Medium：反应中心及附属原子和键

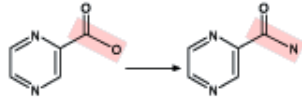
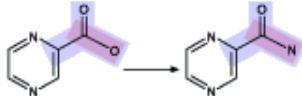
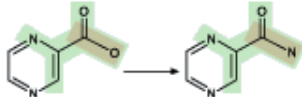
Narrow：反应中心及扩展的原子和键

Get Similar Reactions ?

Retrieve similar reactions from:

- All reactions
- Current answer set

Include this level of similarity:

- Broad - Reaction centers only (2934)

- Medium - Reaction centers plus adjacent atoms and bonds (109)

- Narrow - Reaction centers plus extended atoms and bonds (95)


按照反应类型排序

Group by: Transformation ▼ Sort by: Frequency ▼ ↓

0 of 560 Reactions Selected

1. Reduction of Nitro Compounds to Amines
538 Reactions

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

2. Reduction of Nitro to Azo Compounds
11 Reactions

$$\text{Ar-NO}_2 \longrightarrow \text{Ar-N=N-Ar}$$

3. Reduction of Nitro to Azoxy Compounds
11 Reactions

$$\text{Ar-NO}_2 \longrightarrow \text{Ar-N}^+\text{=N-Ar} \text{O}^-$$

更精确的查找需要的反应

反应检索结果的筛选

获得特定物质做还原剂的反应

REACTIONS

Analyze Refine

Analyze by: Reagent

H ₂	148
NaBH ₄	51
N ₂ H ₄ -H ₂ O	43
KOH	17
CO	16
HCO ₂ H	16
NH ₄ ⁺ •HCO ₂ ⁻	16
H ₂ O	14
N ₂ H ₄	14
NaOH	14

Show More

Get References Tools

Group by: No Grouping Sort by: Relevance

0 of 512 Reactions Selected

1. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.

Cc1ccc(cc1[N+](=O)[O-]) → Cc1ccc(cc1)N

~102 ~122

100%

Overview

Steps/Stages

1.1 R:NaBH₄, C:1832616-28-0, C:Ru, S:H₂O, S:THF, 45 min, 25°C

Notes

solid-supported catalyst, ruthenium supported on porous organic polymer used, reusable catalyst, sealed tube used, scalable, Reactants: 1, Reagents: 1, Catalysts: 2, Solvents: 2, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Fabrication of Ruthenium Nanoparticles in Porous Organic Polymers: Towards Advanced Heterogeneous Catalytic Nanoreactors

SciFinder囊括最大的反应实验过程合集

Single Step Hover over any structure for more options.



▼ Overview

Steps/Stages

1.1 R:H₂, R:Cs₂CO₃, C:1610424-70-8, C:1034343-98-0 (oxide), S:PhMe, 2 h, 100°C, 1 atm

Notes

solid-supported catalyst, palladium catalyst supported on graphene oxide prepared and used, reusable catalyst, Reactants: 1, Reagents: 2, Catalysts: 2, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Catalyst Enhancement and Recyclability by Immobilization of Metal Complexes onto Graphene Surface by Noncovalent Interactions

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

By Sabater, Sara et al

From ACS Catalysis, 4(6), 2038-2047; 2014

▼ Experimental Procedure



General/Typical Procedure: **General Procedure for Nitroarene Reductions.** Molecular hydrogen was added with a balloon filled with 1 atm of H₂ to a mixture of nitroarene (0.3 mmol), Cs₂CO₃ (0.3 mmol), anisole as internal standard (0.3 mmol), and NHC-Pd-rGO (6 × 10⁻³ mmol, based on metal) in toluene (5 mL). The system was then evacuated and backfilled with H₂ in cycles for three times before putting the reaction vessel in an oil bath at 100°C for 2h. Yields were determined by GC analyses using anisole (0.3 mmol) as internal standard. Products were identified according to spectroscopic data of the commercially available compounds. Entry: 4; Yield 100%.

不用阅读全文，直接获得包含实验过程的反应记录

亚结构反应检索

通过C-H活化对苯并噁唑或者恶唑进行烷基化

The screenshot displays the Structure Editor interface. On the left, a toolbar includes an atom selection tool labeled "=R". A purple arrow points from this tool to the R-group Definitions dialog box on the right. The dialog box shows "R1 = O, S" and a periodic table where the element Sulfur (S) is highlighted. The Structure Editor shows a benzimidazole-like structure with an R1 group attached to the C2 position. The status bar at the bottom left indicates "Formula is not available".

亚结构反应检索

The screenshot displays the SCIFINDER Structure Editor interface. The main workspace shows a chemical reaction scheme where a reactant (a benzimidazole-like structure with an R1 group and a hydrogen atom) is converted to a product (the same structure with an Ak group). A purple arrow points from the Ak variable in the product to the 'Variables' dialog box.

Structure Editor

Drag the reaction arrow to specify reaction direction.

Drawing Editor:

- Structure
- Reaction
- Markush

Variables

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

Get reactions where the structure(s) are:

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

Buttons: OK, Cancel, Close

Bottom status bar: Formula is not available

通过后处理工具筛选反应--Analyze

通过催化剂筛选反应

Analyze Refine

Analyze by: ?
Catalyst

CuI	28
312696-09-6	17
AgNO ₃	17
(MeOCH ₂ CH ₂) ₂ O	16
NaI	15
1905414-33-6	14
CoBr ₂	11
Me ₃ SiCH ₂ MgCl	10
Ph ₂ P(CH ₂) ₃ PPh ₂	10
658062-48-7	9

Group by: No Grouping
Sort by: Accession Number

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

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

Overview

Steps/Stages

- 1.1 R:LiO-Bu-*t*, C:1905414-33-6, S:Dioxane, 16 h, 100°C
- 1.2 S:H₂O, rt
- 1.3 R:HCl, S:H₂O, neutralized

Notes

catalyst prepared and used, screw cap tube used, Reactants: 2, Reagents: 2, Catalysts: 1, Solvents: one step: 3

References

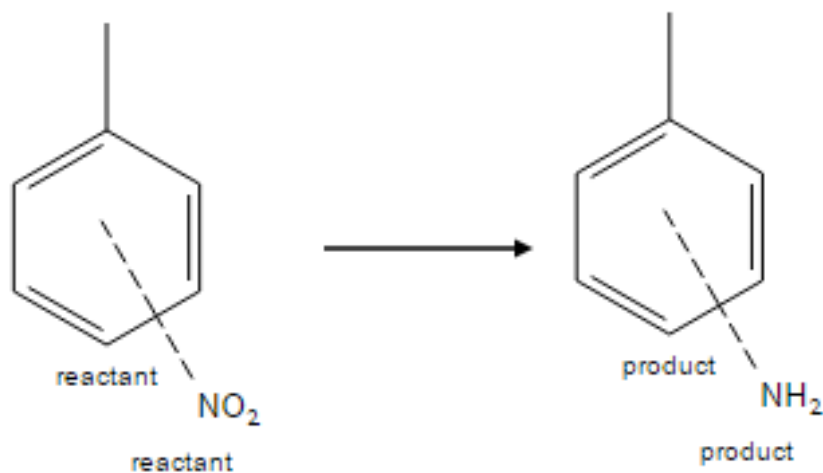
ACS / Proprietary and Confidential / Do Not Distribute

提纲

- SciFinder中的反应检索
- 反应检索疑难分析
- 反应检索上机练习

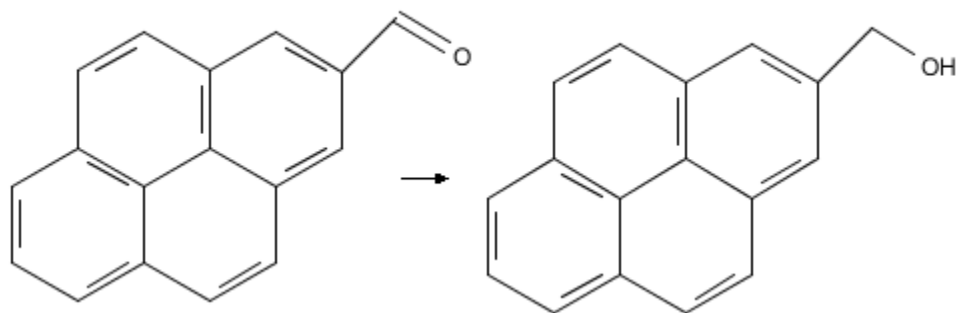
反应的精准定义

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

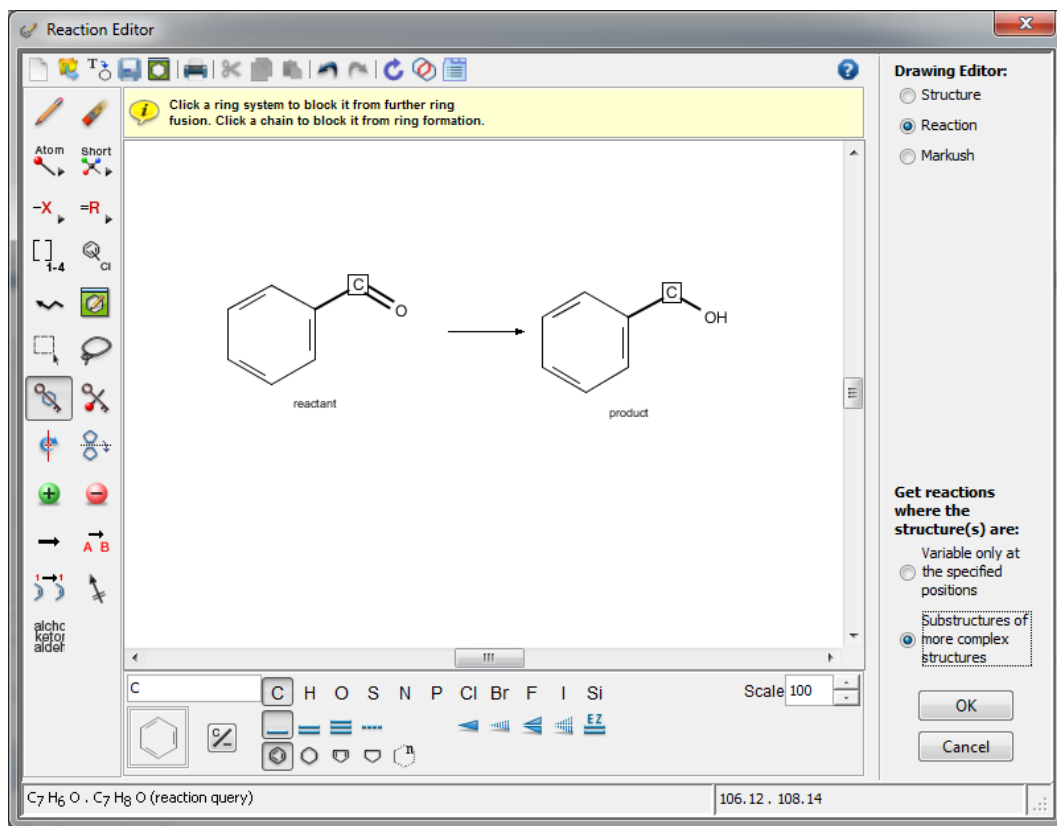
该还原反应如何操作？



The screenshot shows the 'Reaction Editor' window. The main canvas displays the reaction between the aldehyde and the alcohol. The interface includes a toolbar on the left with various drawing tools, a 'Drawing Editor' panel on the right with radio buttons for 'Structure', 'Reaction', and 'Markush', and a bottom status bar showing the reaction query C17H10O.C17H12O and the scale set to 100.

The screenshot shows the SciFinder search results page. The SciFinder logo is at the top. Below it are buttons for 'Explore', 'Saved Searches', and 'SciPlanner'. A yellow warning banner at the bottom states: 'Explore Reactions resulted in 0 reactions' with links for 'Return' and '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

CAS Solutions | SciFinder®

Preferences | SciFinder Help | Sign Out

Welcome Helen Zhu

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

Reaction Structure substructure > reactions (60953) > refine "1 step" (14724)

REACTIONS 0

Get References | Tools | Send to SciPlanner

Analyze | Refine

Group by: No Grouping

0 of 60953 Reactions Selected

1. View Reaction Detail

Single Step

Click to view detail

Sample Analysis: Reagent

NaBH ₄	≥ 9683
HCl	≥ 7777
K ₂ CO ₃	≥ 6658
Et ₃ N	≥ 4779
H ₂ O	≥ 4266
NaOH	≥ 3980
NH ₄ Cl	≥ 3438
LiAlH ₄	≥ 3182
H ₂	≥ 2661
NaHCO ₃	≥ 2580

Overview

Steps/Stages

1.1 R:KOH, C:1820757-77-4, S:Me₂CHOH, S:MeCN, 3 h, 80°C

Experimental Procedures Not Available 9504

Experimental Procedures Available 5220

Show More

Group by: No Grouping | Sort by: Relevance

0 of 14724 Reactions Selected

1. View Reaction Detail | Link | Similar Reactions

Single Step

100%

Notes

optimization study, optimized on catalysts, Reactants: 1, Reagents: 1, Catalysts: 1, Solvents: 2, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Complexes of (η⁶-benzene)ruthenium(II) with 1,4-bis(phenylthio/seleno-methyl)-1,2,3-

通过Refine获得单步反应后选取有实验步骤的反应



获得全面的合成信息

查找合成Daclatasvir的反应

The screenshot displays the SciFinder web interface. The top navigation bar includes 'Explore', 'Saved Searches', and 'SciPlanner'. The main content area shows the search results for 'Daclatasvir', with a 'Get References' button highlighted in a pink box. The interface is divided into several sections:

- Left Sidebar:** Contains navigation options like 'REFERENCES' (Research Topic, Author Name, etc.) and 'SUBSTANCES' (Chemical Structure, Markush, etc.).
- Top Navigation:** 'Explore', 'Saved Searches', 'SciPlanner', 'Save', 'Print', 'Export'.
- Search Path:** 'Substance Identifier "Daclatasvir" > substances (1) > get reactions (50)'. The 'Get References' button is highlighted.
- Reactions Section:** Shows '0 of 50 Reactions Selected'. A 'View Reaction Detail' button is visible.
- Reaction List:** A table of reagents used in the synthesis, sorted by frequency.
- Chemical Structures:** Four chemical structures are shown, representing the starting materials and intermediates in the synthesis of Daclatasvir. The structures are labeled with their respective step numbers: [Step 2.1] and [Step 4.1].

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

SCIFINDER
A CAS SOLUTION

Explore | Saved Searches | SciPlanner Save | Print | Export

Welcome Helen Zhu

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

0 duplicates were automatically removed.

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

Get Substances | Get Reactions | Get Related Citations | Tools

Analyze | Refine | Categorize

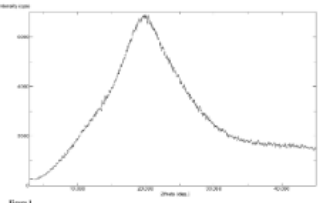
Sort by: Accession Number

0 of 11 References Selected

Analyze by: Author Name

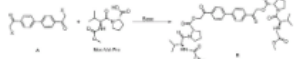
Feng Zhiyong	2
Zhou Shengfeng	2
Bai Shunqiang	1
Cai Jin	1
Chava Satyanarayana	1
Chen Bo	1
Chen Hui	1
Chen Junqing	1
Chen Long	1

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 | Display Options

0 of 50 Reactions Selected

- 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.

~96

~100

~24 references

[Step 4.1] ~71

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

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**
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**
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

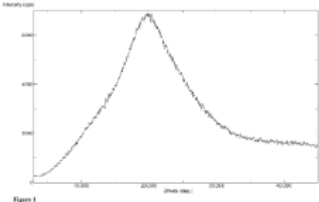


Figure 1

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

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:** Contains 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:** Includes a chemical structure input field (containing "Carboxylic Acid"), a periodic table (C, H, O, S, N, P, Cl, Br, F, I, Si), and a "Formula is not available" status bar.

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 HELLEN 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

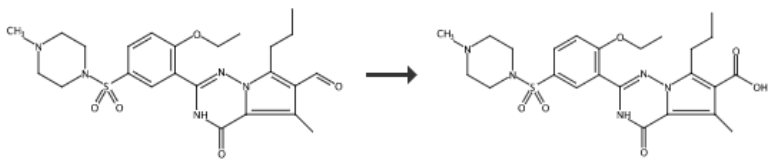
Page: 1 of 408

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 | 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

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

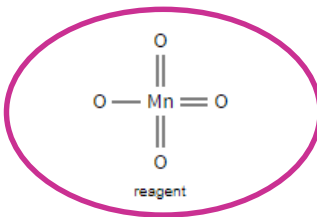
Click image to change structure or view detail.
Search type: **Substructure**

Refine

Structure Editor

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

Aldehyde reactant Carboxylic Acid product



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

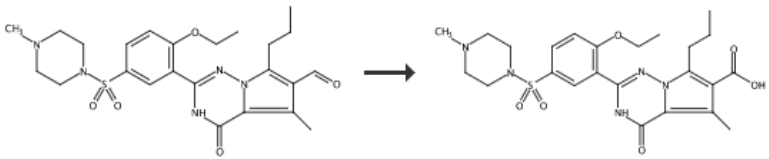
Display Options

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.

Waiting for scifinder.cas.org...

反应结果集庞大时如何限定—催化剂的限定

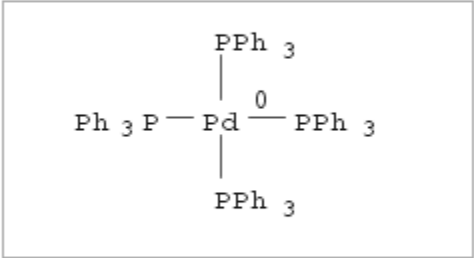
获得四三苯基磷钯作为催化剂的反应

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

Display Options

Refine by:

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

Structure Editor:

Click to Edit

Search type: **Substructure**

1. View Reaction Detail Link

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

+ + + +

[Step 2.1] ~56

[Step 3.1] ~5

[Step 4.1] ~99

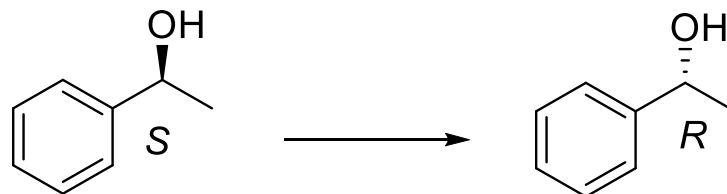
Substance Image Cannot Be Displayed 2133401-30-4

[Overview](#)

如有结构，再通过Refine做结构限定

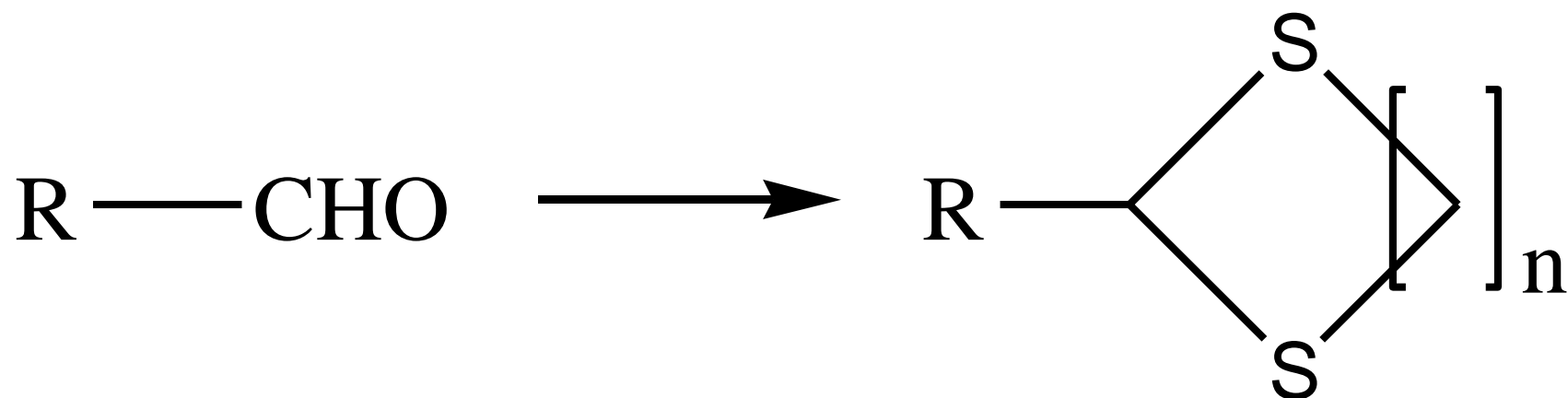
直接检索反应受限的处理

检索如下构型翻转的反应



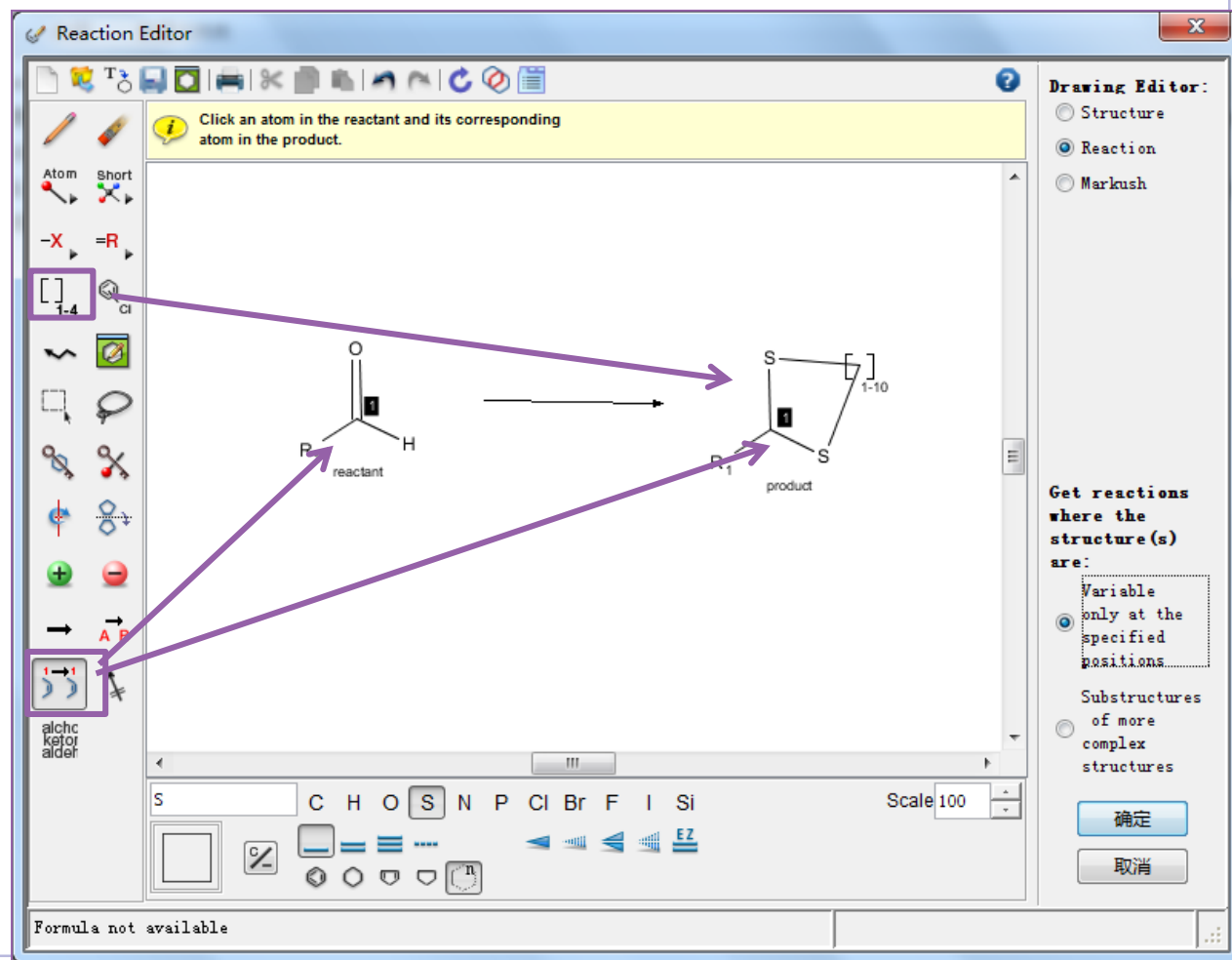
SciFinder中的反应排除策略

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

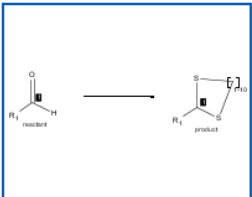
SUBSTANCES

- 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

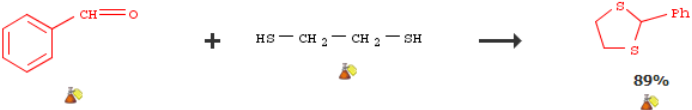
Group by: No Grouping | Sort by: Accession Number

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.



Overview

2. View Reaction Detail | Link | Similar Reactions

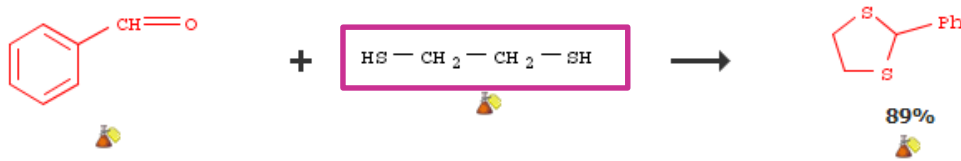
Single Step Hover over any structure for more options.

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.*

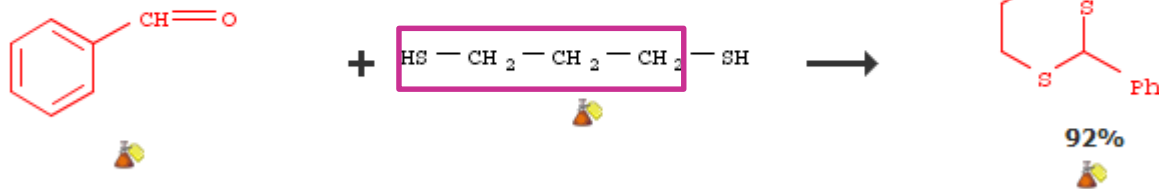


► Overview

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 section shows 'Reaction Structure structure variable only at spe... > reactions (817)'. A 'REACTIONS' section includes 'Get References' and 'Tools' buttons. The 'Analyze' and 'Refine' tabs are active. The 'Analyze by:' dropdown is set to 'Catalyst'. A table lists catalysts and their counts: SiO2 (41), P2O5 (19), H2SO4 (17), 262297-13-2 (15), 5952-71-6 (15), and 63295-47-6 (15). The main reaction view shows a benzaldehyde molecule 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, with the 'Save:' section set to 'All answers' and the 'Title:' field containing 'total reaction'. The 'Description:' field is empty. 'OK' and 'Cancel' buttons are at the bottom of the dialog.

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:



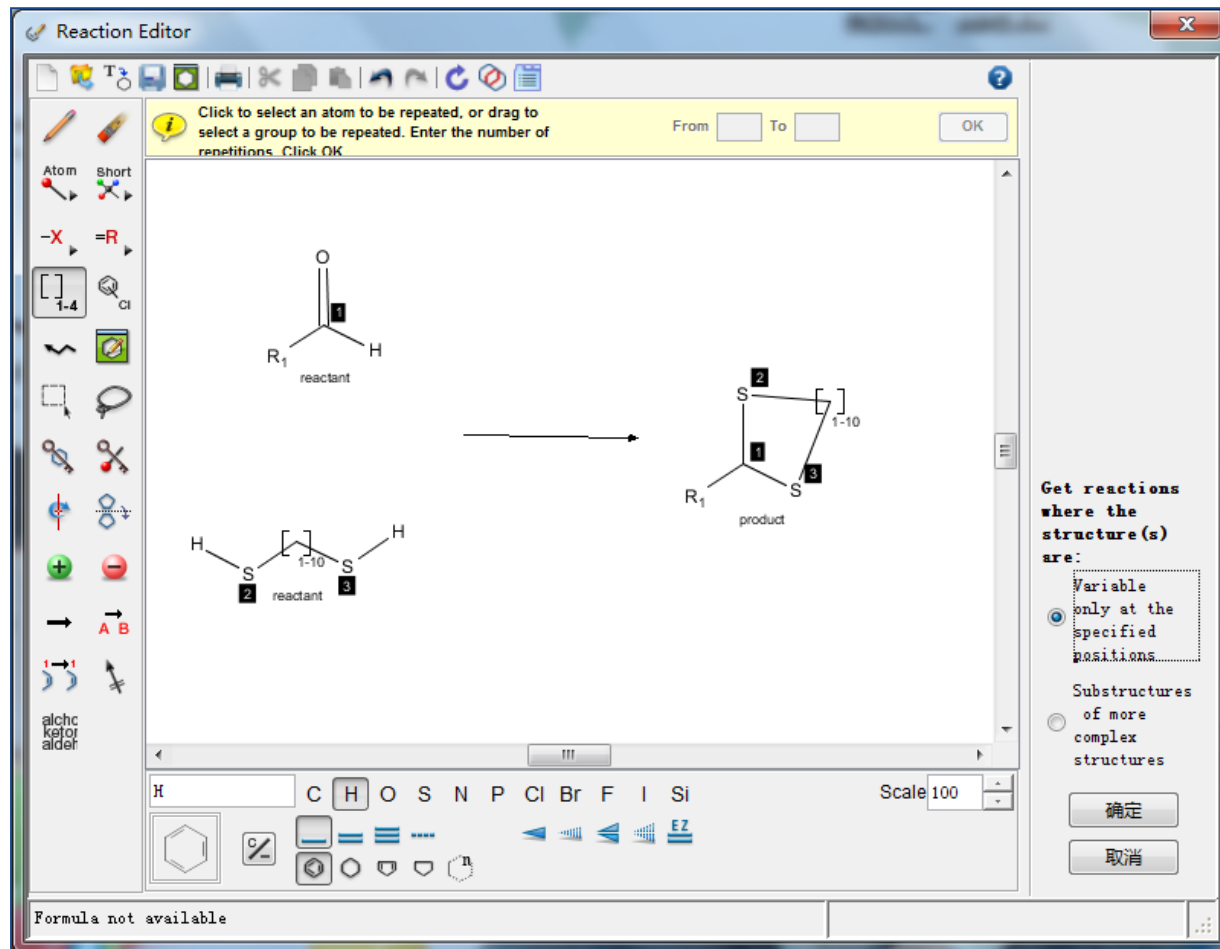
Click image to change structure or view detail
Search type: **Substructure**

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

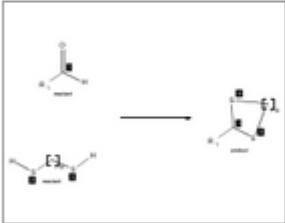
获得需要排除的反应

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)

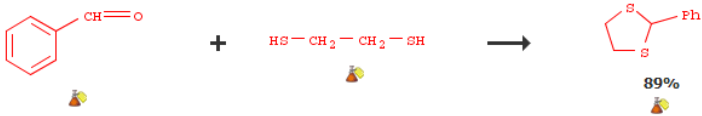
REACTIONS ⓘ Get References Tools ▾ Send to SciPlanner

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

0 of 754 Reactions Selected

1. View Reaction Detail ⓘ Link ⓘ Similar Reactions

Single Step Hover over any structure for more options.



Overview

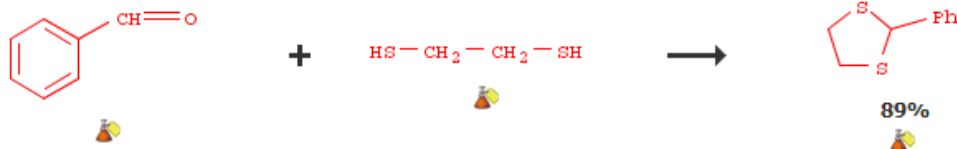
Analyze by: ?	
Catalyst	
SiO2	39
P2O5	19
H2SO4	17
262297-13-2	15
5952-71-6	15
I2	15

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](#)

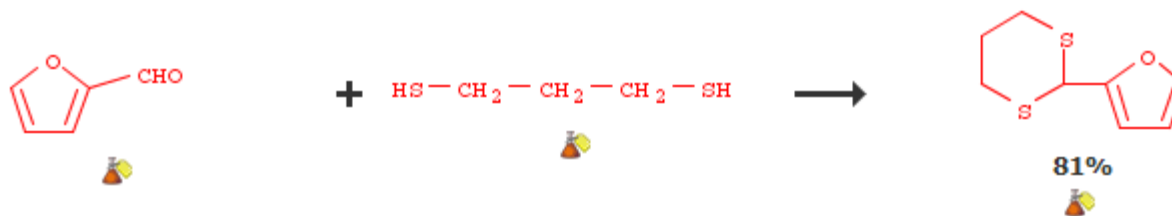
Single Step *Hover over any structure for more options.*



► 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 Grouping Combine Answer Sets Reaction Number Answers per Page [20] Display:

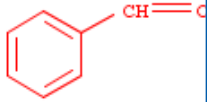
Analyze by: Catalyst

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 answer to view details*



Overview

Combine Answer Sets

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

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:

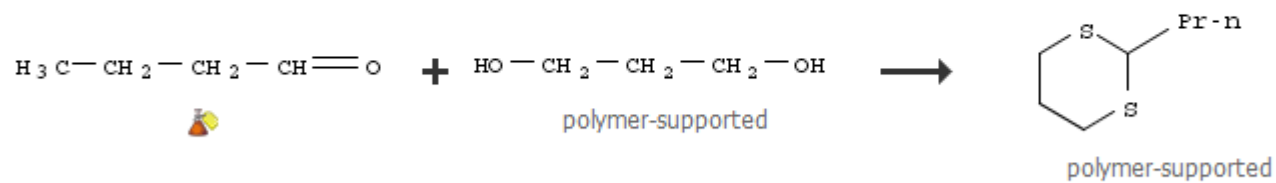
- Combine** Include all answers from both sets
- Intersect** Include only answers that appear in both sets
- Exclude** Include only answers from **current answer set (754)** that are not in **total reaction (817)**
- Exclude** Include only answers from **total reaction (817)** that are not in **current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

Combine Answer Sets Cancel

最后的结果

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

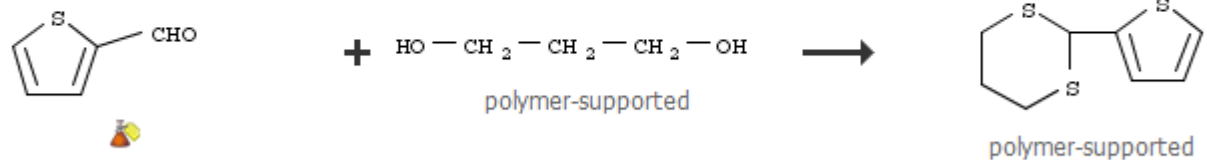
Single Step *Hover over any structure for more options.*



[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

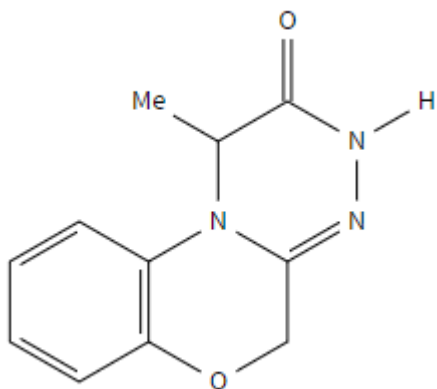
检索思路1: 检索结构相似的物质, 获得有参考价值的合成路线;

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。

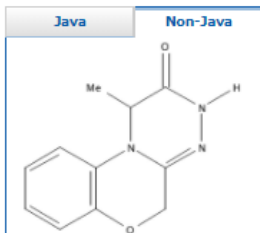
新化合物合成路线设计

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. The search criteria are "Chemical Structure exact" and the results are "substances (0)". There are tabs for "Analyze" and "Refine". 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

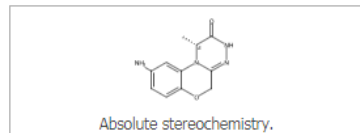
0 of 6 Substances Selected

Classes

Studies

Score: 91

1. 1613721-07-5



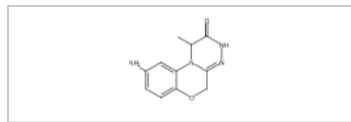
C₁₁H₁₂N₄O₂

[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



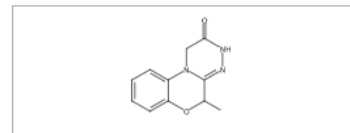
C₁₁H₁₂N₄O₂

[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



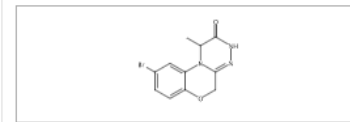
C₁₁H₁₁N₃O₂

[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



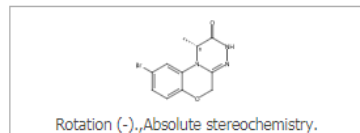
C₁₁H₁₀BrN₃O₂

[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



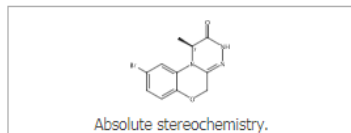
C₁₁H₁₀BrN₃O₂

[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



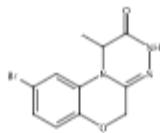
C₁₁H₁₀BrN₃O₂

[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

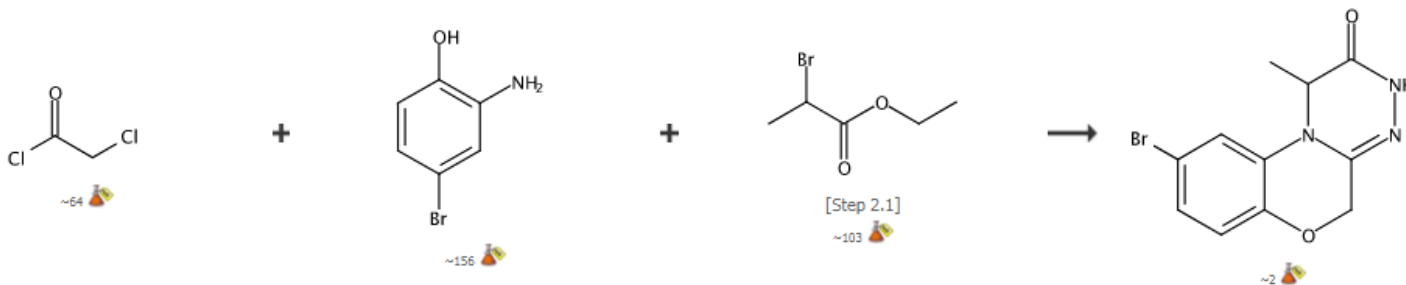
$C_{11}H_{10}BrN_3O_2$

[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

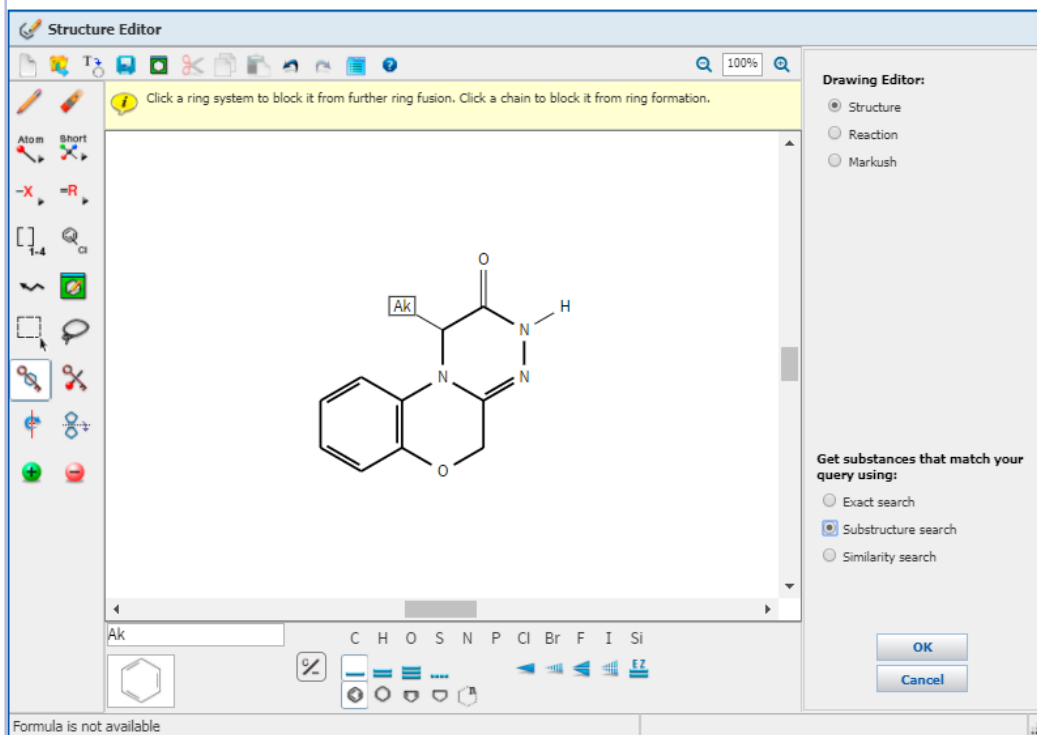
Quick View PATENTPAK

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 Display Options

0 of 424 Substances Selected 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, (2<i>S</i>,5<i>R</i>)-</p> <p>▶ Key Physical Properties</p>	<p>2. 1654735-59-7</p> <p>Absolute stereochemistry.</p> <p>C₂₂H₂₈N₄O₄ 1-(2<i>H</i>)-Pyrrolidinecarboxylic acid, 3,6-dihydro-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</p> <p>▶ Key Physical Properties</p>	<p>3. 1654735-57-5</p> <p>Absolute stereochemistry.</p> <p>C₂₄H₂₈F N₅O₂ [1,2,4]Triazino[3,4-c][1,4]benzoxazin-2(1<i>H</i>)-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, (3<i>R</i>)-</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, (3<i>S</i>)-</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<i>E</i>]-2-ethoxyethenyl]-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<i>R</i>]-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-[[1<i>R</i>]-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>10. 1632329-18-0</p>	<p>11. 1632329-17-9</p>	<p>12. 1632329-16-8</p>

筛选结构相近的物质

新化合物合成路线设计

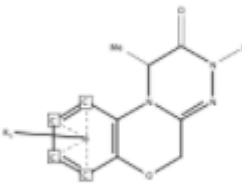
Analyze Refine

Refine by: ?

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

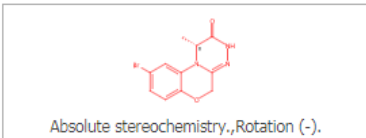
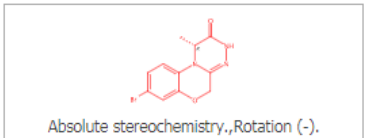
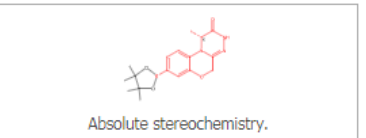
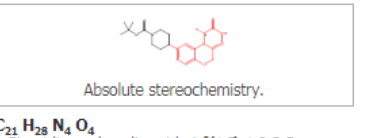
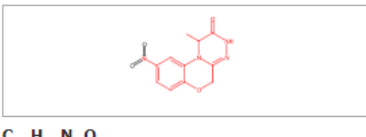
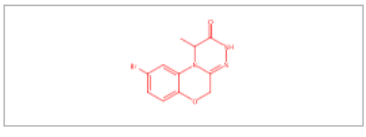
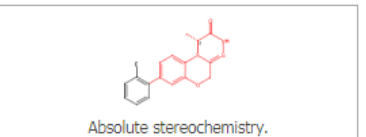
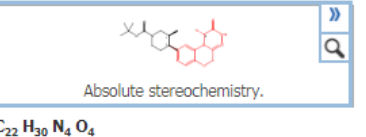
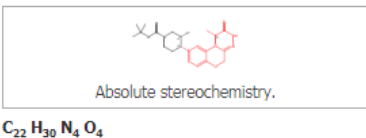
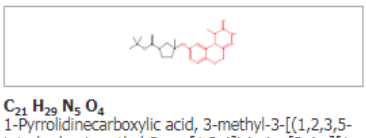
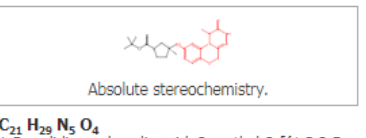
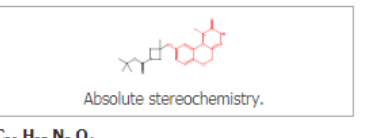
Structure Editor:

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>C₂₁H₂₈N₅O₄ 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>C₂₁H₂₈N₅O₄ 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

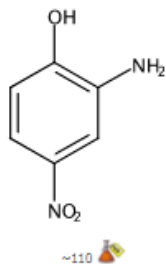
Group by: **No Grouping** Sort by: **Accession Number**

Display Options

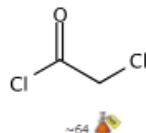
0 of 8 Reactions Selected

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

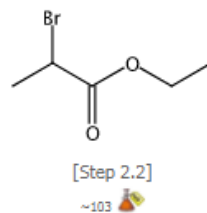
4 Steps *Hover over any structure for more options.*



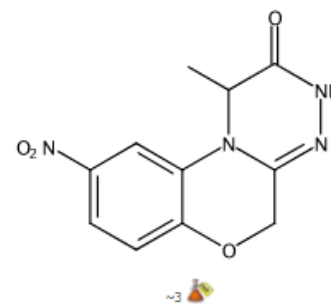
+



+



→



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...](#)

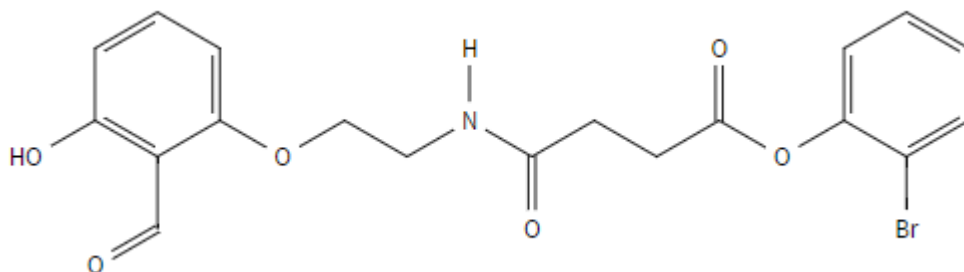
Available Experimental Data

1H NMR, R_f , State

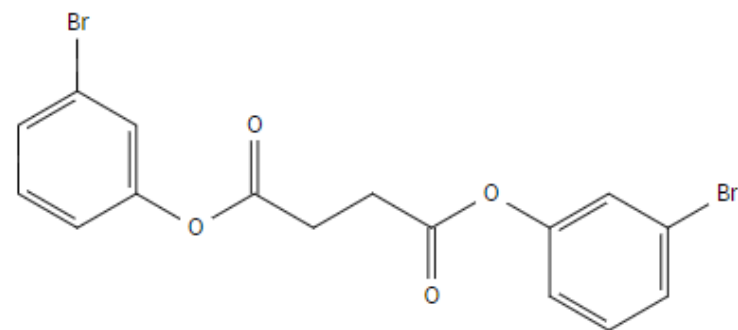
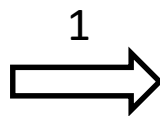
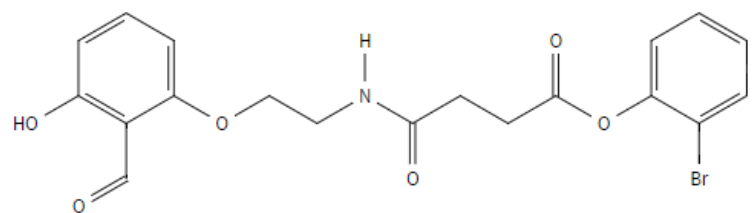
[View with MethodsNow](#)

新化合物合成路线设计

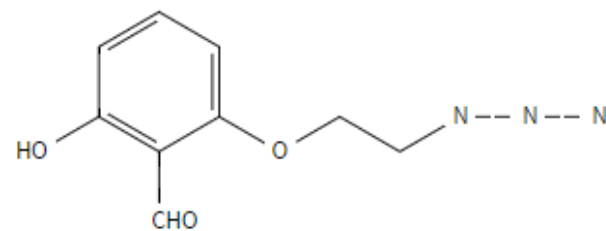
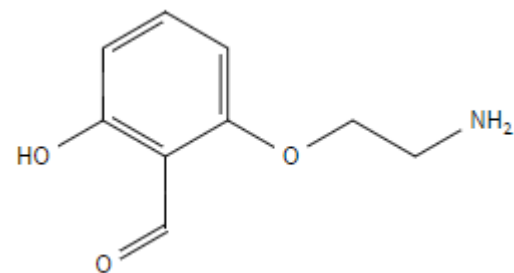
检索思路3：先自行做逆合成反应分析，然后检索相关的反应



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

Primary Amine reactant

Amide product

Phenol non-reacting

Aldehyde

Get References Retrieve references for selected reactions.

Group by: No Grouping Sort by: Accession Number

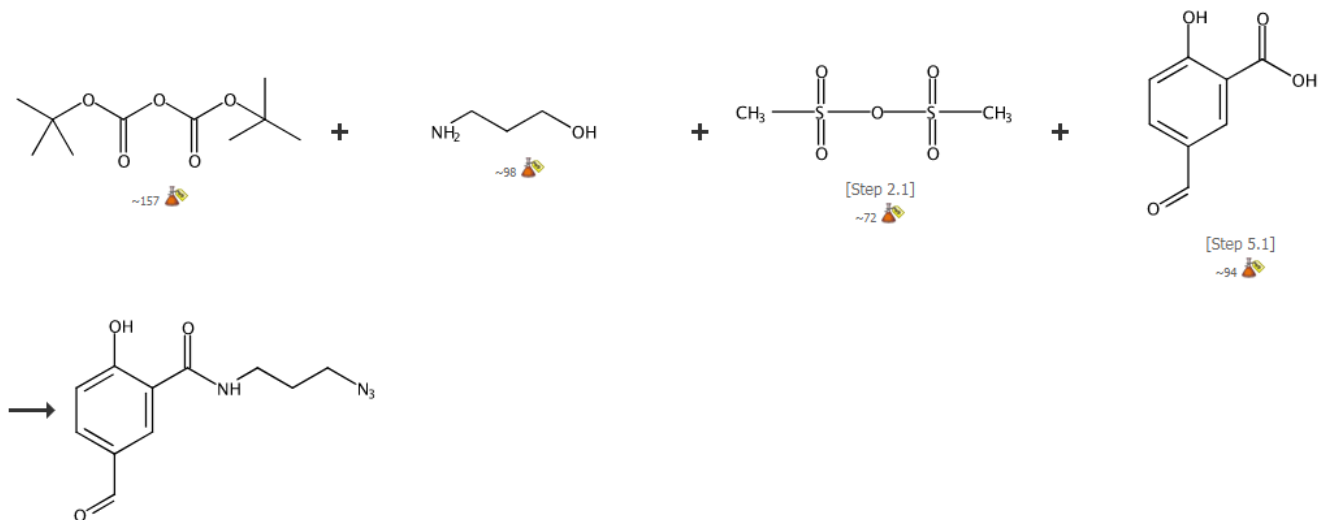
0 of 1538 Reactions Selected

1. View Reaction Detail Link

5 Steps Hover over any structure for more options.

Aldehyde

Formula is not available



新化合物合成路线设计

问题：反应太乱

Analyze Refine

Refine by:
 Reaction Structure
 Product Yield
 Number of S
 Reaction Clas
 Excluding Re
 Classification
 Non-particip
 functional gr

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 No
 Carboxylate Ester

 Click image to change structure or view details
 Search type: Su
 Refine

Send to SciPlanner
 Display Options
 Page: 1 of 18

Chemical reaction scheme showing the synthesis of a complex molecule from multiple starting materials. The scheme includes: 4-nitrobenzoic acid (~121), allyl bromide (~93), 3,4-dihydroxybenzaldehyde (~108), isobutyl bromide (~83), acetyl chloride (~83), methyl 3-oxo-3-phenylprop-2-enoate (~53), and methyl iodide (~96). The reaction proceeds through several steps, including the formation of an enone intermediate and a final product with a complex side chain.

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 Step
- Reaction Classification
- Excluding Reactant Classification
- Non-participating functional group

Number of Steps:

1-2

Examples: 1, 1 - 3, 1 -

Refine

Get References

Tools

Group by: No Grouping Sort by: Accession Number

0 of 66 Reactions Selected

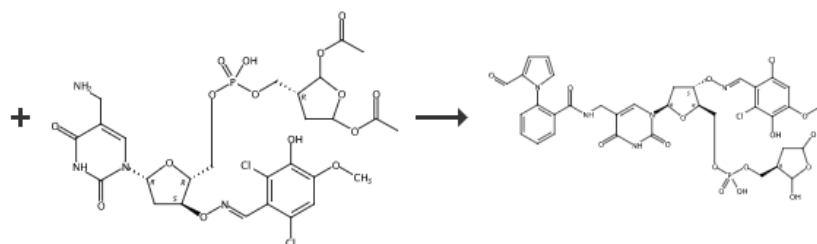
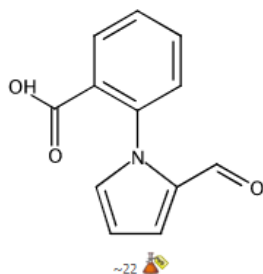
Send to SciPlanner

Display Options

Page: 1 of 2

1. View Reaction Detail Link

2 Steps Hover over any structure for more options.

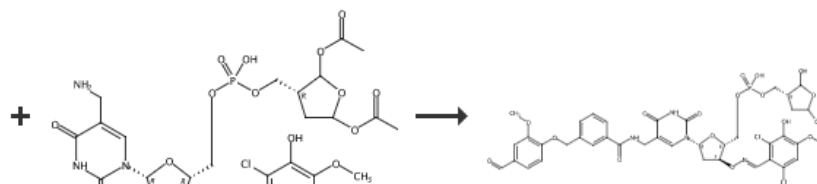
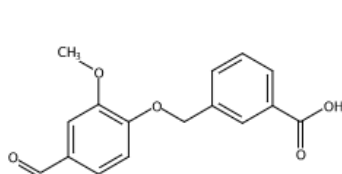


酰化剂为羧酸，不符合要求

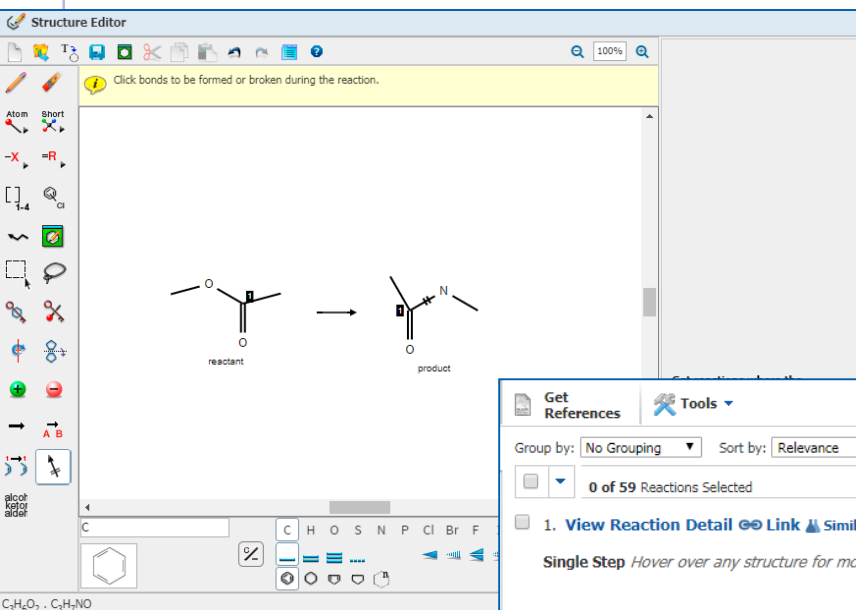
Overview

2. View Reaction Detail Link

2 Steps Hover over any structure for more options.



新化合物合成路线设计

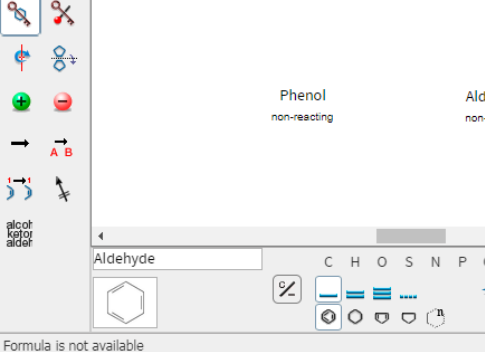
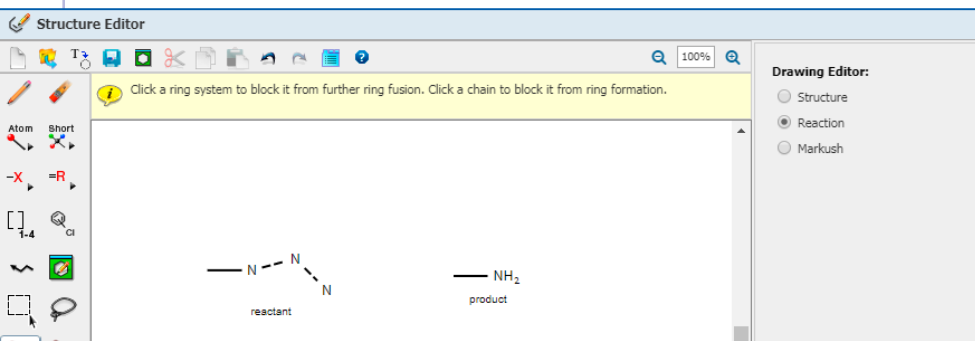


进一步限定用酯做酰化剂的反应

$C_3H_6O_2 \cdot C_3H_7NO$

新化合物合成路线设计

反应2



Get References Tools

Group by: No Grouping Sort by: Relevance

0 of 105 Reactions Selected

Page: 1 of 3

Send to SciPlanner

Display Options

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

71%
- 2. View Reaction Detail** [Link](#) [Similar Reactions](#)
Single Step *Hover over any structure for more options.*

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

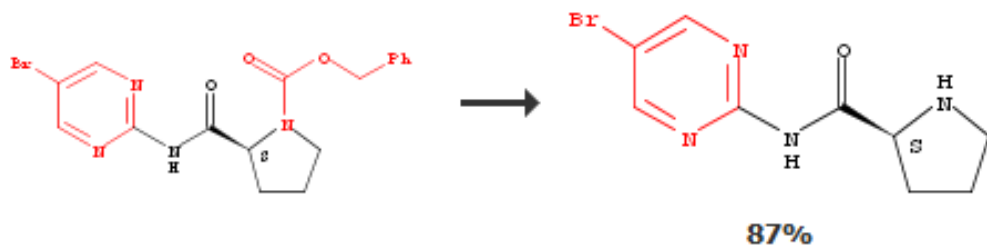
案例分析

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 and labels R₁, R₂, and "reactant"; a product with a similar dashed triangle and labels R₁, R₂, and "product"; and a reactant with a six-membered ring and a carbonyl group labeled "reactant". The interface includes a toolbar on the left with icons for Atom, Short, bond types, and other functions. A bottom toolbar shows element selection (A, C, H, O, S, N, P, Cl, Br, F, I, Si) and scale settings (Scale 100). On the right, a panel titled "Get reactions where the structure(s) are:" offers options for "Variable only at the specified positions" and "Substructures of more complex structures". Buttons for "确定" (OK) and "取消" (Cancel) are visible. The status bar at the bottom left indicates "Formula not available".

案例分析

32. 1 Hits in this Reference Similar Reactions

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



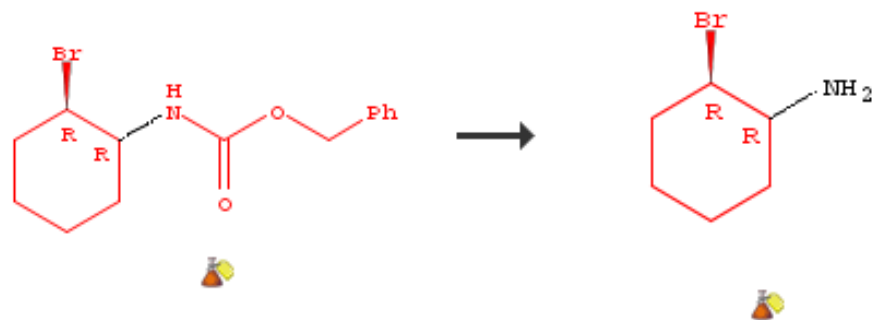
► Overview

► 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.*

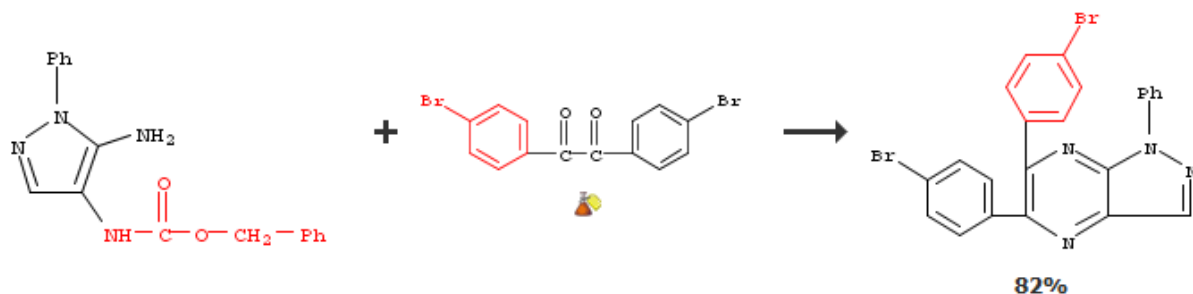


► Overview

► Experimental Procedure

案例分析

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

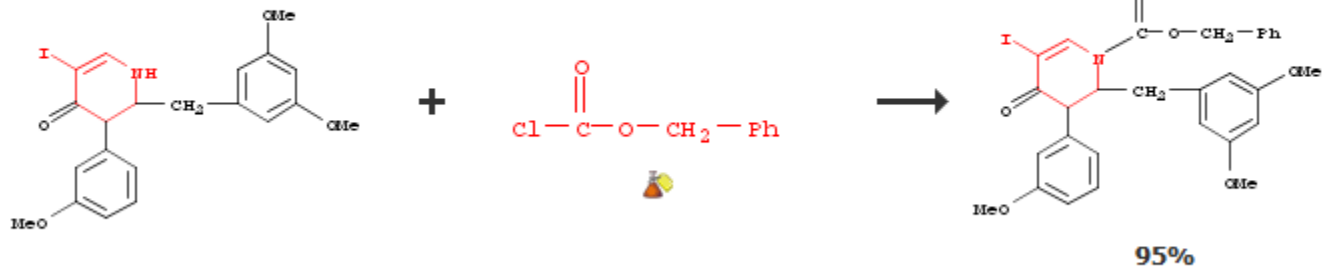


- ▶ Overview
- ▶ Experimental Procedure

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

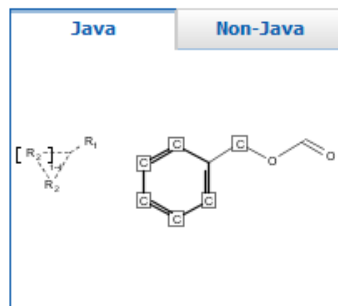
The screenshot displays the 'Structure Editor' window. The main canvas contains two chemical structures: a fragment with a dashed triangle representing a ring closure between atoms R1 and R2, and a bicyclic system consisting of a six-membered ring fused to a five-membered ring, with an aldehyde group (-CHO) attached to the five-membered ring. The interface includes a toolbar on the left with various drawing tools, a 'Drawing Editor' panel on the right with radio buttons for 'Structure', 'Reaction', and 'Markush', and a search panel at the bottom right with radio buttons for 'Exact search', 'Substructure search', and 'Similarity search'. The status bar at the bottom left shows 'Formula not available'.

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

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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 | Display Options

0 of 77364 Reactions Selected | Page: 1 of 1548

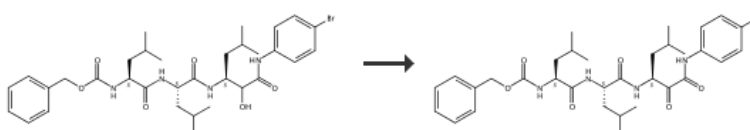
Sample Analysis: **?**

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

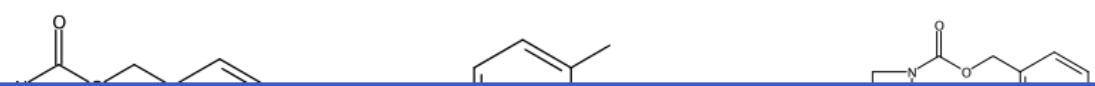
1. View Reaction Detail **?** Link **?** Similar Reactions

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:

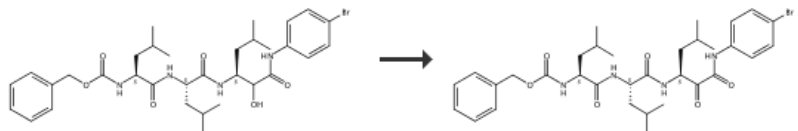
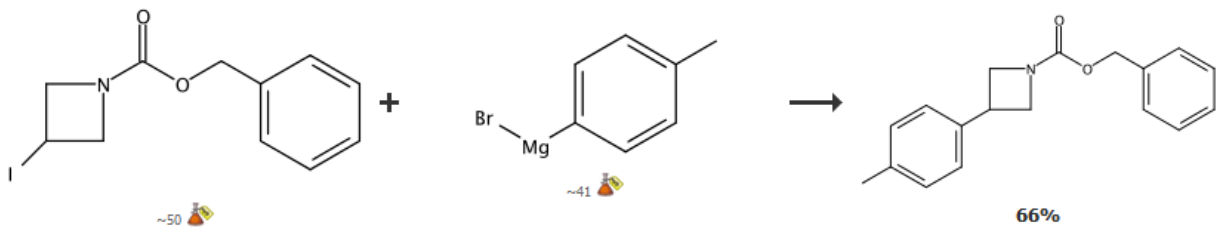
1

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

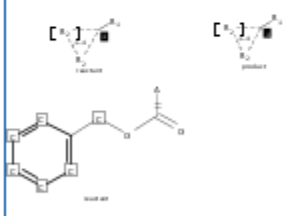
Refine by: ?

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

Structure Editor:

Java

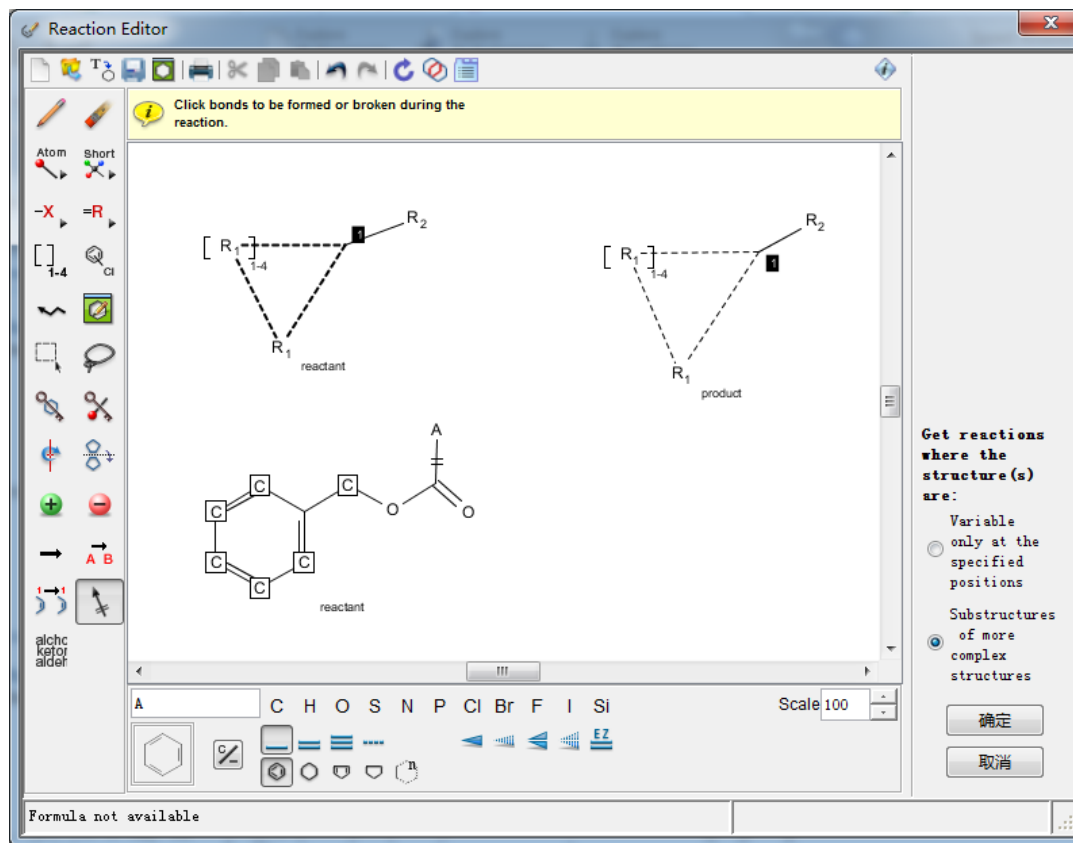
Non-Java



Click image to change structure or view detail.

Search type: **Substructure**

Refine



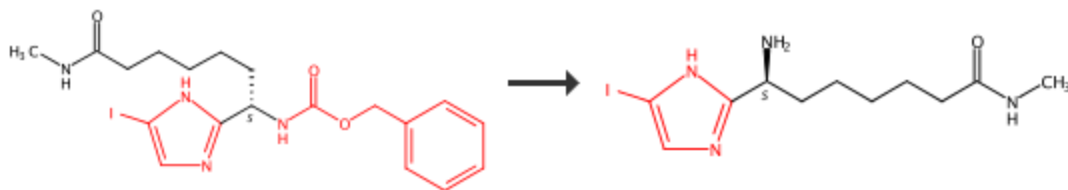
再做反应中心限定，沿用之前的定义

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.*

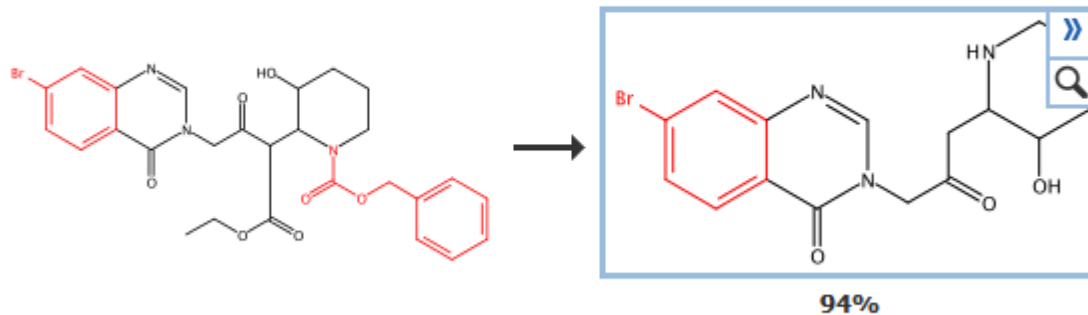


Overview

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

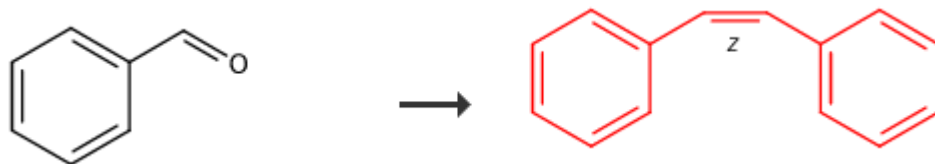
- 初步检索
- 浏览结果集，判断是否符合要求，利用系统工具限定结果
- 修正检索式，再次检索
- 浏览结果集，判断

提纲

- SciFinder中的反应检索
- 反应检索疑难分析
- 反应检索上机练习

上机练习

1. 检索以下反应:



2. 检索保护吡啶环上N原子而环上的羟基不受影响的反应?

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