

检索片段结构的化学选择性反应

举例：如何检索右侧的反应？

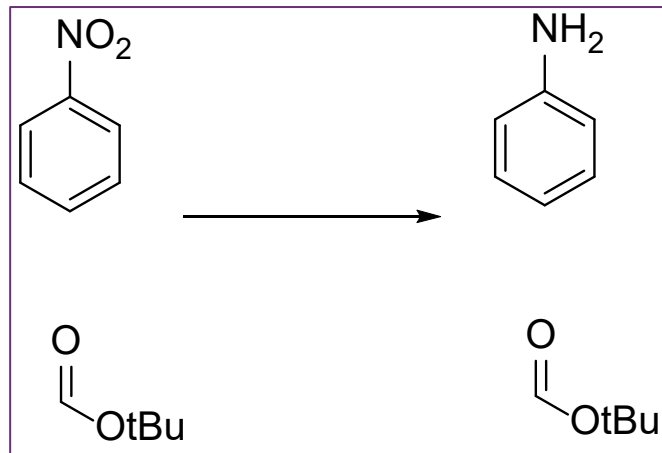
起始物上带有BOC基团；

苯环上的硝基还原为氨基；

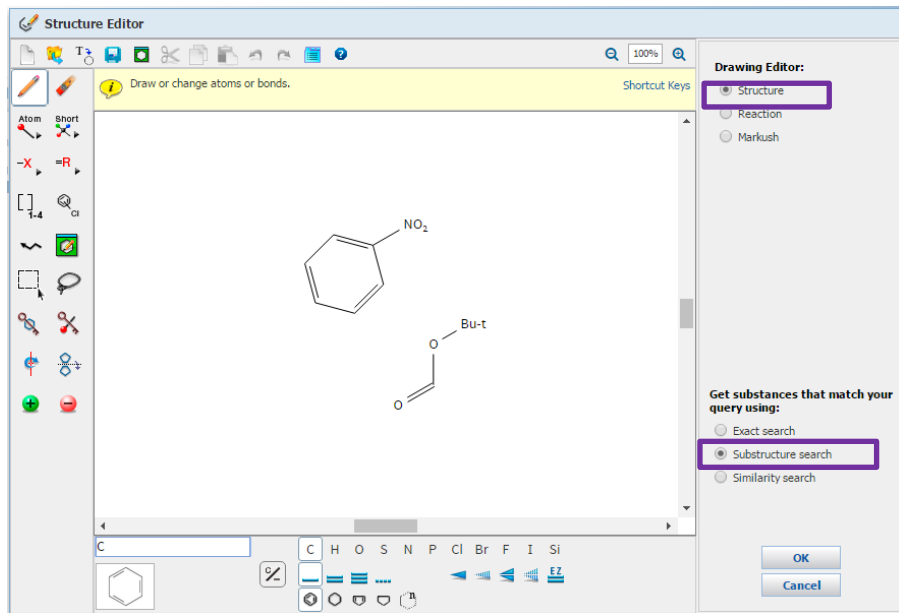
BOC基团不变。

检索思路：

要保证苯环和BOC基团在同一个结构上，需要从物质结构检索开始，通过物质获得反应，再对反应进行限定。



检索片段结构的化学选择性反应：物质的片段检索



Structure Editor

Draw or change atoms or bonds.

Shortcut Keys

Drawing Editor:

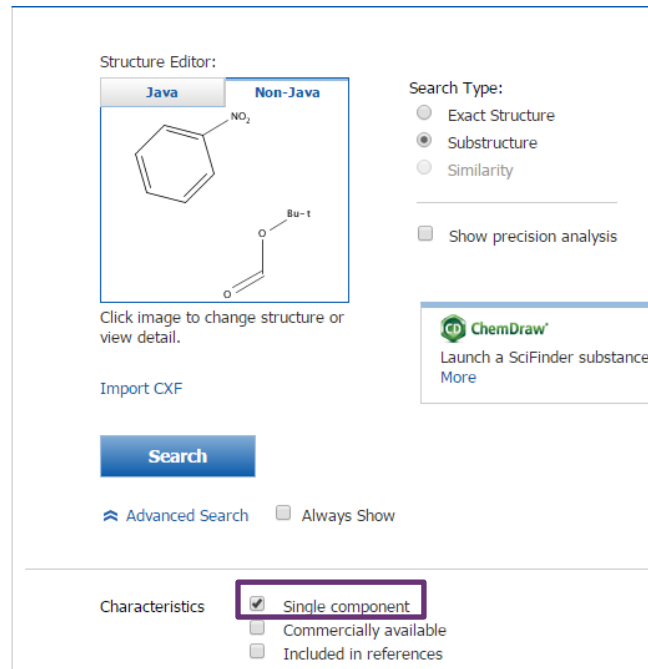
- Structure
- Reaction
- Markush

Get substances that match your query using:

- Exact search
- Substructure search
- Similarity search

OK

Cancel



Structure Editor:

Java Non-Java

Click image to change structure or view detail.

Import CXF

Search

Advanced Search Always Show

Search Type:

- Exact Structure
- Substructure
- Similarity

Show precision analysis

ChemDraw

Launch a SciFinder substance

More

Characteristics

- Single component
- Commercially available
- Included in references

绘制片段结构，选择亚结构检索，并定义为单一组分

检索片段结构的化学选择性反应：从物质获取反应

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

Sort by: CAS Registry Number

0 of 35896 Substances Selected

1. 1884208-13-2

2. 1884208-09-6

Absolute stereochemistry.

$C_{42}H_{56}N_8O_{13}S$
INDEX NAME NOT YET ASSIGNED
Key Physical Properties

Absolute stereochemistry.

$C_{37}H_{54}N_8O_{13}S$
INDEX NAME NOT YET ASSIGNED
Key Physical Properties

Get Reactions

Retrieve reactions for:

- All substances
- Selected substances

Limit results by reaction role:

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

Get Cancel

获得亚结构检索结果，并获得这些物质作为Reactant的反应

检索片段结构的化学选择性反应：限定反应步数

The screenshot shows the SciPlanner interface with the following details:

- Navigation: Explore, Saved Searches, SciPlanner, Save, Print, Export
- Breadcrumbs: Chemical Structure substructure with limiters > substances (35896) > get reactions (374800) > get reactions (374800)
- REACTIONS: Get References, Tools, Send to SciPlanner
- Group by: No Grouping, Sort by: Accession Number
- 0 of 374800 Reactions Selected
- 1. View Reaction Detail Link
- 4 Steps (highlighted in a purple box) / Hover over any structure for more options.
- Chemical structures shown: A complex molecule, a nitro-substituted benzene ring, a chloroacetyl group, a nitrile, and a complex heterocyclic molecule.
- Annotations: [Step 2.1] ~38, [Step 3.1] ~74, [Step 4.1]
- Refine by: Reaction Structure, Product Yield, Number of Steps (selected), Reaction Classification, Excluding Reaction Classification, Non-participating functional groups
- Number of Steps: 1 (highlighted in a purple box)
- Examples: 1, 1 - 3, 1 -, - 3
- Refine button

点击Refine, 限定反应步数为一步

检索片段结构的化学选择性反应：限定产物结构，并标记同一原子

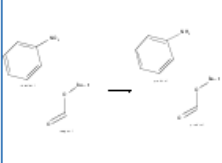
Analyze Refine

Refine by: ?

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

Structure Editor:

Java Non-Java

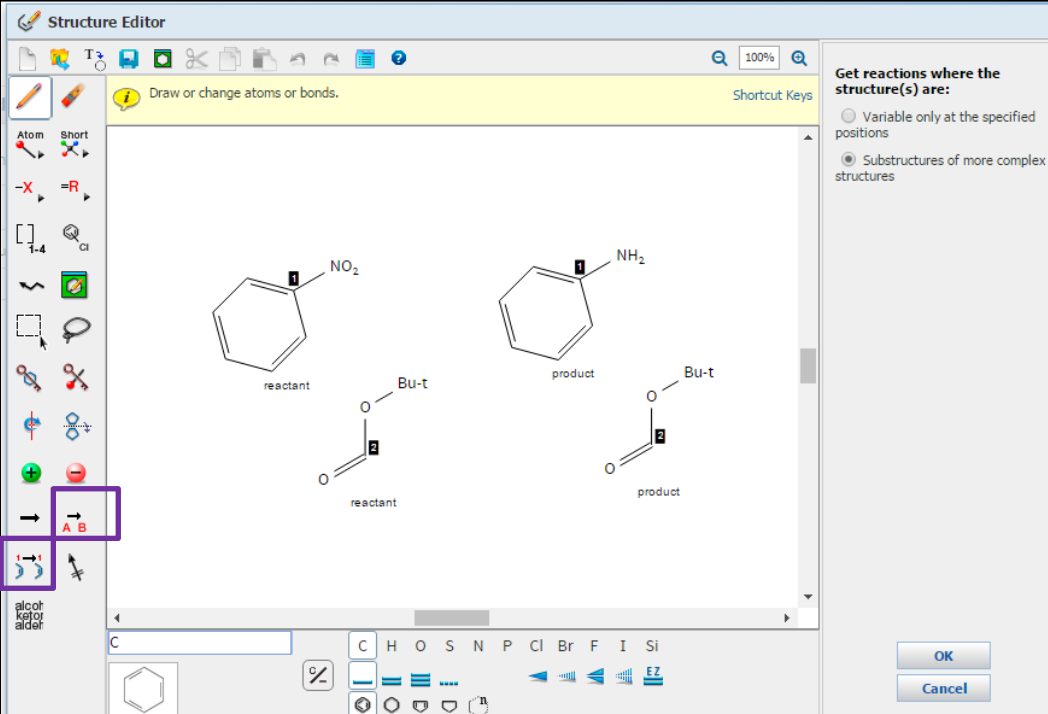


Click image to change structure or view detail.
Search type: **Substructure**

Refine

Structure Editor

Draw or change atoms or bonds.



reactant product

reactant product

Get reactions where the structure(s) are:

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

OK Cancel

绘制产物结构片段，并标明角色为product。
并利用原子标记工具同时标记反应物和产物中同一个原子。

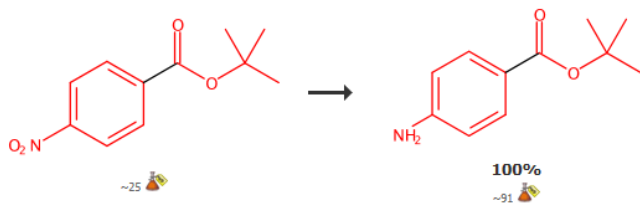
检索片段结构的化学选择性反应：获得反应结果集

0 of 7016 Reactions Selected

Page: 1 of 46

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

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



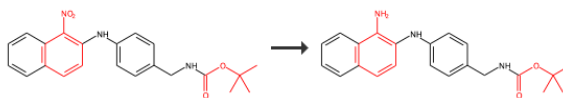
Overview

Steps/Stages

1.1 R:H₂, C:12642-25-0, C:Pd, S:BuOH, 5-300 min, 40°C, 1 atm

2986. View Reaction Detail [Link](#) [Similar Reactions](#)

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



Overview

Steps/Stages

1.1 R:H₂, C:PtO₂, S:MeOH, S:THF, 2 h, rt

Notes

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

References

Preparation of benzodiazepine derivatives P2x4 receptor antagonists

Quick View [PATENTPAK](#)

By Ushioda, Masatoshi et al

From PCT Int. Appl., 2013105608, 18 Jul 2013

检索片段结构的化学选择性反应：操作步骤推荐

1. 从物质检索出发

- 绘制出片段结构，并在Advanced Search中选中“single component”，确保片段结构出现在一个分子中
- 进行物质的亚结构检索，并获得物质结果集

2. 从物质获取反应

- 在1的物质结果集中，点击Get Reactions获得其作为Reactant的反应

3. 在反应结果集中限定产物结构

- 在2的反应结果集中，通过Refine中的“Reaction Structure”来限定产物结构
- 在结构编辑器中绘制产物的结构片段，并标明角色为“product”

4. 标记片段中相同的原子

- 利用原子标记工具，同时标记反应物和产物片段中的同一个原子，确保产物中的NH₂是由反应物中的NO₂还原得到的，并且确保产物中的BOC就是反应物中没有发生变化的BOC。

5. 查看反应结果

- 如有必要，限定步数为一步