

# How to... Work with a Reaction Answer Set

## Find all relevant reactions based on criteria you specify

Quickly retrieve relevant information from the world's largest, publicly available reaction collection. This guide provides an overview of the tools in SciFinder® that you can use to evaluate and narrow even a large answer set. From there, a single click retrieves references associated with your reaction(s) of interest. For more detailed information and additional training resources, consult the online Help or visit [www.cas.org/training/scifinder](http://www.cas.org/training/scifinder).

## Reaction Search Results

**REACTIONS** Get References Tools Send to SciPlanner

Analyze Refine

Analyze by: Reagent

Me-morpholineoxide 195

NaIO<sub>4</sub> 195

Na<sub>2</sub>SO<sub>3</sub> 163

Group by: No Grouping Sort by: Relevance

0 of 220 Reactions Selected

1. View Reaction Detail Link Similar Reactions

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

100%  
~2

**Overview**

**Steps/Stages**

1.1 R:Me-morpholineoxide, C:OsO<sub>4</sub>, S:#BuOH, S:THF, overnight, rt

1.2 R:Na<sub>2</sub>SO<sub>3</sub>, S:H<sub>2</sub>O, 30 min, rt

1.3 R:NaIO<sub>4</sub>, S:H<sub>2</sub>O, S:MeOH, overnight, rt

**Notes**

Reactants: 1, Reagents: 3, Catalysts: 1, Solvents: 4, Steps: 1, Stages: 3, Most stages in any one step: 3

**References**

Preparation of pyrazole derivatives as S1P1 agonists

Quick View **PATENTPAK**

By Erra Sola, Montserrat et al

From PCT Int. Appl., 2011144338, 24 Nov 2011

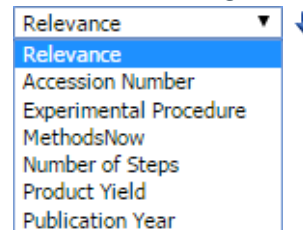
Experimental Procedure

### Tip: See the Newest Records First

Accession Numbers start with the year when a record becomes available followed by sequential numbering (i.e., 2015:967458). Sort by this option to see the most recent records first.

1 By default, answers are sorted from most to least relevant.

- Click the blue drop-down arrow to select other sorting criteria.



- Click the blue arrow to reverse the sort order.

2 Click **Display Options** to specify the number of answers displayed per page (15, 20, 25 or 50) and to select whether the **Overview** is opened or closed by default.

3 Hit structures are red.

- Click the flask below a structure to see commercial source information for the substance.

*Continued*

4

Get References Tools

Send to SciPlanner

Group by: No Grouping Sort by: Relevance

0 of 220 Reactions Selected Page: 1 of 11

1. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.

5

6

CAS Registry Number: 1233500-63-4

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

Note

Reaction stages: 4, Steps: 1, Stages: 3, Most

References

Preparation of pyrazole derivatives as S1P1 agonists

Quick View PATENTPAK

By Erra Sola, Montserrat et al

From PCT Int. Appl., 2011144338, 24 Nov 2011

Tip

**PATENTPAK™** offers immediate access to full text PDFs for indexed patents and their patent families for major patent offices and includes page numbers for substances from covered patents. Learn more about this add-on product at <http://www.cas.org/products/scifinder/patentpak>.

Experimental Procedure

General/Typical Procedure: Preparation 42 To a solution of Preparation 4 (0.59 g, 1.59 mmol) in a mixture of THF/*tert*-butanol (13 mL/2 mL) 4-methylmorpholine 4-oxide (0.373 g, 3.28 mmol) and osmium(VIII) oxide (0.194 mL, 0.03 mmol) were added. The reaction mixture was stirred overnight at r.t. Then 40% solution of Na<sub>2</sub>SO<sub>3</sub> was added and the mixture stirred for 30 min. Ethyl acetate was added and the organic layer separated, washed twice with water, dried over magnesium sulphate and concentrated to give the title compound. (85% yield). To a suspension of Example 1 (505 mg, 1.25 mmol) in methanol (14 mL) and water (1.6 mL) NaIO<sub>4</sub> (401 mg, 1.87 mmol) was added and the mixture stirred overnight at r.t. Methanol was concentrated and the residue dissolved in ethyl acetate and water. Organic layer was separated, washed with water and brine, dried over magnesium sulphate and concentrated to give the title compound. (100% yield). Preparation 42 Preparation 42 2-(4-(5-(1-ethyl-5-phenyl-1H-pyrazol-3-yl)-1,2,4-oxadiazol-3-yl)-2,6-dimethylphenyl)acetaldehyde Obtained from Preparation 41 following the procedure described in Example 1 followed by procedure described in Preparation 5. Preparation 107 3,5-Dimethyl-4-(2-oxoethyl)benzotrile Obtained from Preparation 2 following the procedure described in Preparation 42. (100%). LRMS: m/z 174 (M+1)+ Retention time: 5.23 min (Method B).

4 Click the box beside an answer number to select it. You can work with selected items several ways, such as saving them or getting references for them.

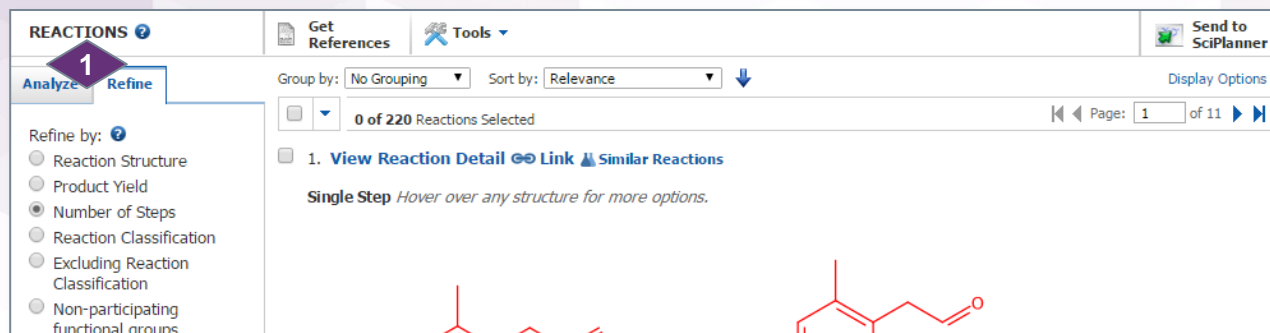
5 Mouse over a structure to access additional substance information and search options.

- Click the blue arrows to see related search options.
- Click the magnifying glass to see the **Substance Detail** in a separate window (called a **Quick View**).

6 Click the reference title to go to the **Reference Detail** page, or click the magnifying glass to open the reference information in a **Quick View** window.

# Refine to Narrow the Answer Set

**1** On the **Refine** tab, click a radio button to select a **Refine by:** option.



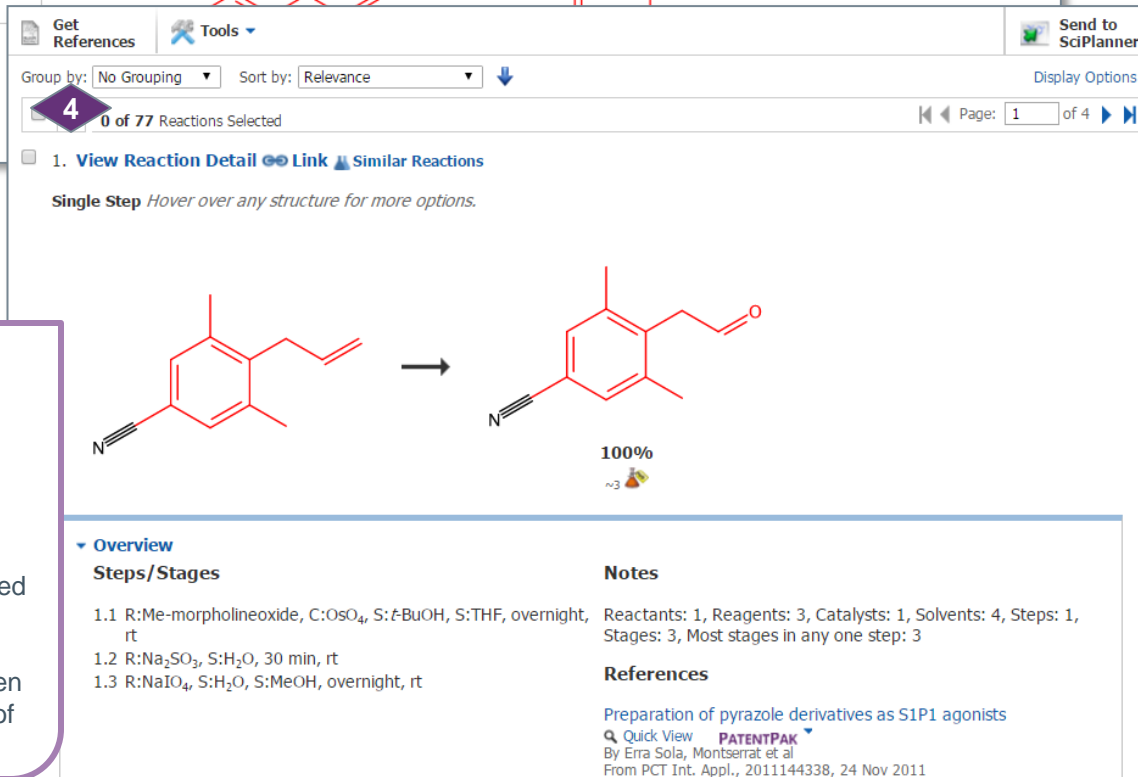
**2** Below the radio buttons, further define the refine criteria.

**3** Click **Refine**.

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

**Refine**

**4** The answer set is narrowed based on the criteria you specified.



**Overview**

Steps/Stages	Notes
1.1 R:Me-morpholineoxide, C:OsO <sub>4</sub> , S:t-BuOH, S:THF, overnight, rt	Reactants: 1, Reagents: 3, Catalysts: 1, Solvents: 4, Steps: 1, Stages: 3, Most stages in any one step: 3
1.2 R:Na <sub>2</sub> SO <sub>3</sub> , S:H <sub>2</sub> O, 30 min, rt	
1.3 R:NaIO <sub>4</sub> , S:H <sub>2</sub> O, S:MeOH, overnight, rt	

**References**

Preparation of pyrazole derivatives as S1P1 agonists  
Quick View **PATENTPAK**  
By Erra Sola, Montserrat et al  
From PCT Int. Appl., 2011144338, 24 Nov 2011

## Tip

In many cases, a single step can have different stages. For example, stages occur when reagents are added sequentially, causing different reactions, but often without isolation of intermediates.

# Group by Document or Transformation

1

Get References Tools

Group by: Transformation Sort by: Frequency

0 of 77 Reactions Selected

1. Ozonolysis  
25 Reactions

$$\begin{matrix} R^1 & & R^2 \\ & \backslash & / \\ & C=C & \\ & / & \backslash \\ R^1 & & R^2 \end{matrix} \longrightarrow R^1-C(=O)-R^1 + R^2-C(=O)-R^2$$

2. Formation of Alkyl Halides/ Alcohols from Ethers /Silyl Ethers  
4 Reactions

Send to SciPlanner Display Options

Tip

By default, answers are sorted by frequency. Click the drop-down arrow for other sort options.

1

**Group by: Transformation** groups single-step reactions based on transformation types so you can quickly evaluate synthesis options and preferred pathways.

- Reactions can fall into more than one category.
- Unclassified single- and multi-step reactions (if any) appear at the end of the answer set.

2

**Group by: Document** shows all the reference titles for the answer set, the total number of reactions associated with each title and a representative reaction for each title.

Get References Tools

Group by: Document Sort by: Relevance

0 of 77 Reactions Selected

1. Preparation of pyrazole derivatives as S1P1 agonists  
Quick View PATENTPAK  
39 Reactions Similar Reactions

Single Step Hover over any structure for more options.

$$\text{C}_6\text{H}_3(\text{Me})_3(\text{CN})-\text{CH}_2\text{CH}_2\text{CHO} \longrightarrow \text{C}_6\text{H}_3(\text{Me})_3(\text{CN})-\text{CH}_2\text{CHO}$$

100% ~3

2. Preparation of 1,2,4-oxadiazole derivatives for treating diseases susceptible to amelioration by sphingolipid receptors (S1P1) agonists  
Quick View PATENTPAK  
8 Reactions Similar Reactions

Single Step Hover over any structure for more options.

$$\text{C}_6\text{H}_3(\text{Me})_3(\text{CN})-\text{CH}_2\text{CH}_2\text{CHO} \longrightarrow \text{C}_6\text{H}_3(\text{Me})_3(\text{CN})-\text{CH}_2\text{CHO}$$

100%

Overview Experimental Procedure

Tip

Click the number of reactions to see just those reactions.

Tip

You can run a **Similar Reactions** search when the link is available. This search uses the same reaction center and similar structural characteristics as your initial search. You select how narrow or broad you want the new search to be.

Get Similar Reactions

Retrieve similar reactions from:

- All reactions
- Current answer set

Include this level of similarity:

- Broad - Reaction centers only (20926)
- Medium - Reaction centers plus adjacent atoms and bonds (6065)
- Narrow - Reaction centers plus extended atoms and bonds (529)

Get Reactions Cancel

# Analyze to See Subsets of Information

1 **REACTIONS** Get References Tools Send to SciPlanner

Analyze Refine

Group by: Document Sort by: Relevance Display Options

0 of 77 Reactions Selected

Analyze by: 2

- Reagent
- Author Name
- Catalyst
- Company-Organization
- Document Type
- Experimental Procedure**
- Journal Name
- Language
- MethodsNow
- Number of Steps
- Product Yield
- Publication Year
- Reagent
- Solvent
- PDC 5
- LiAlH<sub>4</sub> 4
- NaHCO<sub>3</sub> 4
- (PhCO<sub>2</sub>)<sub>2</sub> 3
- BCl<sub>3</sub> 3

Show More

1. Preparation of pyrazole derivatives as S1P1 agonists  
Quick View PATENTPAK  
39 Reactions Similar Reactions

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

C=CC1=CC=C(C=C1)C#N → C=CC1=CC=C(C=C1)C#N  
100%  
~3

2. Preparation of 1,2,4-oxadiazole derivatives for treating diseases susceptible to amelioration by sphingosine-1-phosphate receptors (S1P1) agonists

1 Click the **Analyze** tab.

2 Click the drop-down arrow to select an **Analyze by:** option.

Narrow results with bibliographic data using:

- **Author Name**
- **Company-Organization**
- **Document Type**
- **Journal Name**
- **Language**
- **Publication Year**

Narrow results with reaction data using:

- **Catalyst**
- **Number of Steps**
- **Product Yield**
- **Reagent**
- **Solvent**

Narrow results based on the availability of actual experimental details using:

- **Experimental Procedure**
- **MethodsNow**

## Tip

The top ten subsets appear on the **Analysis** tab. When additional subsets are available, click the **Show More** button at the bottom of the tab to see a complete list or to select more than one subset.

## Tip

MethodsNow™ features step-by-step instructions for analytical and synthetic methods. This add-on product displays experimental details in easy-to-read table format and includes materials, instrumentation, conditions and more.

*Continued*

Explore ▾ Saved Searches ▾ SciPlanner Save Print Export

⚠ 103 reactions with the Experimental Procedure **Experimental Procedures Available** are displayed 4 Keep Analysis Clear Analysis

Reaction Structure substructure > reactions (220) > refine "1-3 steps" (119)

REACTIONS ⓘ Get References Tools ▾ Send to SciPlanner

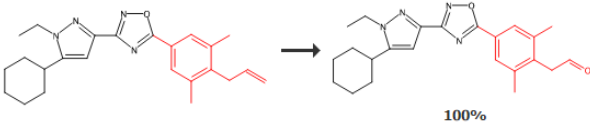
Analyze Refine Display Options

Group by: No Grouping Sort by: Product Yield ↓

0 of 119 Reactions Selected Page: 1 of 6

1. View Reaction Detail ⓘ Link Similar Reactions

Single Step Hover over any structure for more options.



100%

▼ Overview

**Steps/Stages**

1.1 R: Me-morpholineoxide, C: OsO<sub>4</sub>, S: t-BuOH, S: THF, overnight, rt  
 1.2 R: Na<sub>2</sub>SO<sub>3</sub>, S: H<sub>2</sub>O, 30 min, rt  
 1.3 R: NaIO<sub>4</sub>, S: H<sub>2</sub>O, S: MeOH, overnight, rt

**Notes**

Reactants: 1, Reagents: 3, Catalysts: 1, Solvents: 4, Steps: 1, Stages: 3, Most stages in any one step: 3

**References**

Preparation of pyrazole derivatives as S1P1 agonists  
 Quick View **PATENTPAK** ▼  
 By Erra Sola, Montserrat et al  
 From PCT Int. Appl., 2011144338, 24 Nov 2011

▼ Experimental Procedure

General/Typical Procedure: Preparation 42 To a solution of Preparation 4 (0.59 g, 1.59 mmol) in a mixture of THF/*tert*-butanol (13 mL/2 mL) 4-methylmorpholine 4-oxide (0.373 g, 3.28 mmol) and osmium(VIII) oxide (0.194 mL, 0.03 mmol) were added. The reaction mixture was stirred overnight at r.t. Then 40% solution of Na<sub>2</sub>SO<sub>3</sub> was added and the mixture stirred for 30 min. Ethyl acetate was added and the organic layer separated, washed twice with water, dried over magnesium sulphate and concentrated to give the title compound. **(85% yield)**. To a suspension of Example 1 (505 mg, 1.25 mmol) in methanol (14 mL) and water (1.6 mL) NaIO<sub>4</sub> (401 mg, 1.87 mmol) was added and the mixture stirred overnight at r.t. Methanol was concentrated and the residue dissolved in ethyl acetate and water. Organic layer was separated, washed with water and brine, dried over magnesium sulphate and concentrated to give the title compound. (100% yield). Preparation 42 Preparation 42 **2-(4-(5-(1-ethyl-5-phenyl-1H-pyrazol-3-yl)-1,2,4-oxadiazol-3-yl)-2,6-dimethylphenyl)acetaldehyde** Obtained from Preparation 41 following the procedure described in Example 1 followed by procedure described in Preparation 5. Preparation 171 **2-(4-(3-(5-Cyclohexyl-1-ethyl-1H-pyrazol-3-yl)-1,2,4-oxadiazol-5-yl)-2,6-dimethylphenyl)acetaldehyde** Obtained from Preparation 170 following the procedure described in Preparation 42. (100%). LRMS: m/z 393 (M+1)<sup>+</sup> Retention time: 7.45 min (Method B).

Your answer set is divided into subsets based on the analysis criteria.

3 Click an analysis bar to display only the answers in a subset. The selected bar turns yellow.

4 The yellow status message indicates the new display.

- To replace the original answer set with the selected subset, click **Keep Analysis**.
- To return to the original answer set, click **Clear Analysis**.

**Tip**  
Click ⓘ to access context-specific online help.

# Manage Your Searching

The screenshot shows the SciFinder web interface. At the top right, there are links for 'Preferences', 'SciFinder Help', and 'Sign Out' (callout 1). Below the header is a navigation bar with 'Explore', 'Saved Searches', and 'SciPlanner' (callouts 2, 3, and 4). To the right of this bar are 'Save', 'Print', and 'Export' buttons (callout 5). The main content area features a breadcrumb trail: 'Reaction Structure substructure > reactions (220) > refine "1-2 steps" (77) > keep analysis "Experimental Procedure" (61)' (callout 6). Below the breadcrumb are 'REACTIONS', 'Get References', and 'Tools' buttons (callouts 7 and 8). At the bottom right, there is a 'Send to SciPlanner' button (callout 9).

1 Access **Preferences** and **SciFinder Help** options: **Help**, **Training**, **What's New** and **Contact Us**.

2 Click the **Explore** drop-down arrow to start a new references, substances or reactions search.

3 Click the **Saved Searches** drop-down arrow to access **Saved Answer Sets**, **Keep Me Posted** answer sets and your search **History**.

4 Click **SciPlanner™** to open the SciPlanner workspace.

- SciPlanner is an interactive window where you can store and organize reference, substance, and reaction search results. Use it to gather information for a project, create a report or export research to share with colleagues.
- Three short videos about using **SciPlanner** are available the first time you open it and also in the online Help.

5 Click **Save**, **Print** or **Export** to open a dialog window and initiate each of these processes. See "How to... Print, Save and Export" for more information.

6 The breadcrumb navigation trail shows each step in your current search history. Mouse over a step to see more information about it. Click a step to return to that part of the search.

7 Click **Get References** to retrieve references for part or all of your answer set.

8 Click the **Tools** drop down arrow to access **Combine Answer Sets**.

9 Click **Send to SciPlanner** to send selected answers to the SciPlanner workspace.

## CAS Customer Center

E-mail: [help@cas.org](mailto:help@cas.org)

Phone numbers: <http://www.cas.org/contact-us/cas-customer-center>