

# HOW TO

Explore Reactions



SciFinder® lets you combine chemical structures and functional groups to locate reaction information.

With Explore Reactions, you can:

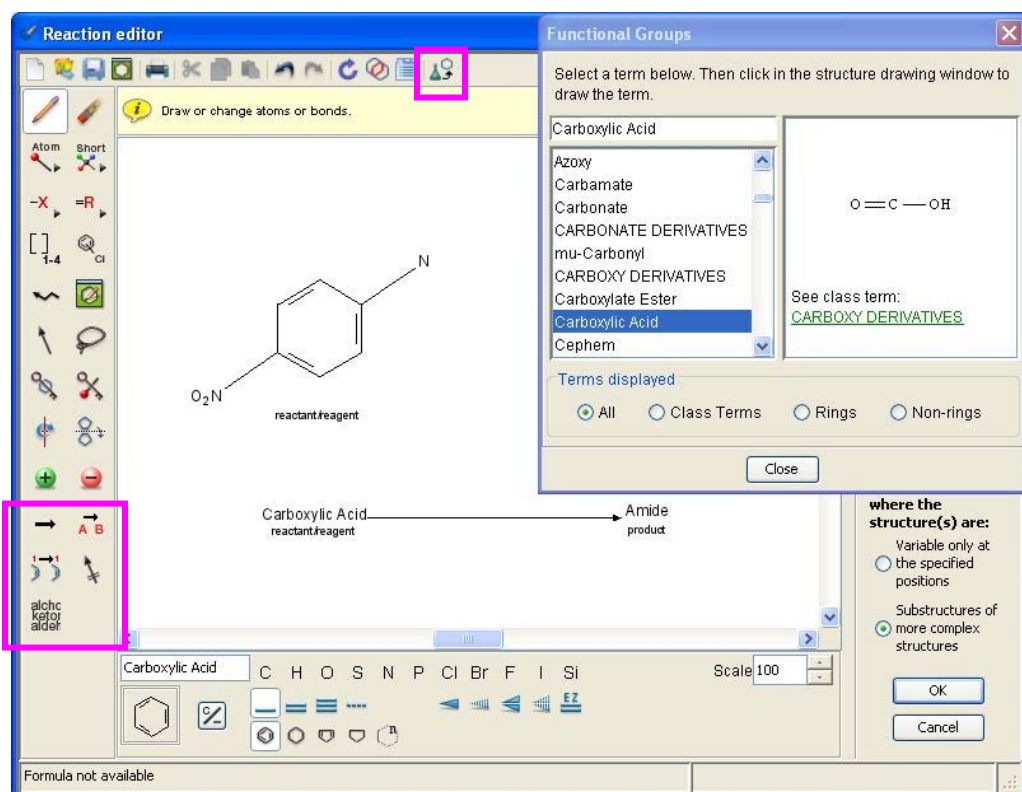
- Indicate the role of each participant
- Use all the substructure drawing features
- Allow or prohibit additional substitution and/or ring fusion
- Filter your results by solvents or other attributes

1. Click the reaction drawing thumbnail to open the editor.



Use tools along the left side and across the bottom to draw your reaction.

Reaction-specific tools let you:

- Specify reaction roles for participants
- Map atoms from a reactant to a product
- Specify sites where bonds are changed
- Include functional groups in your query

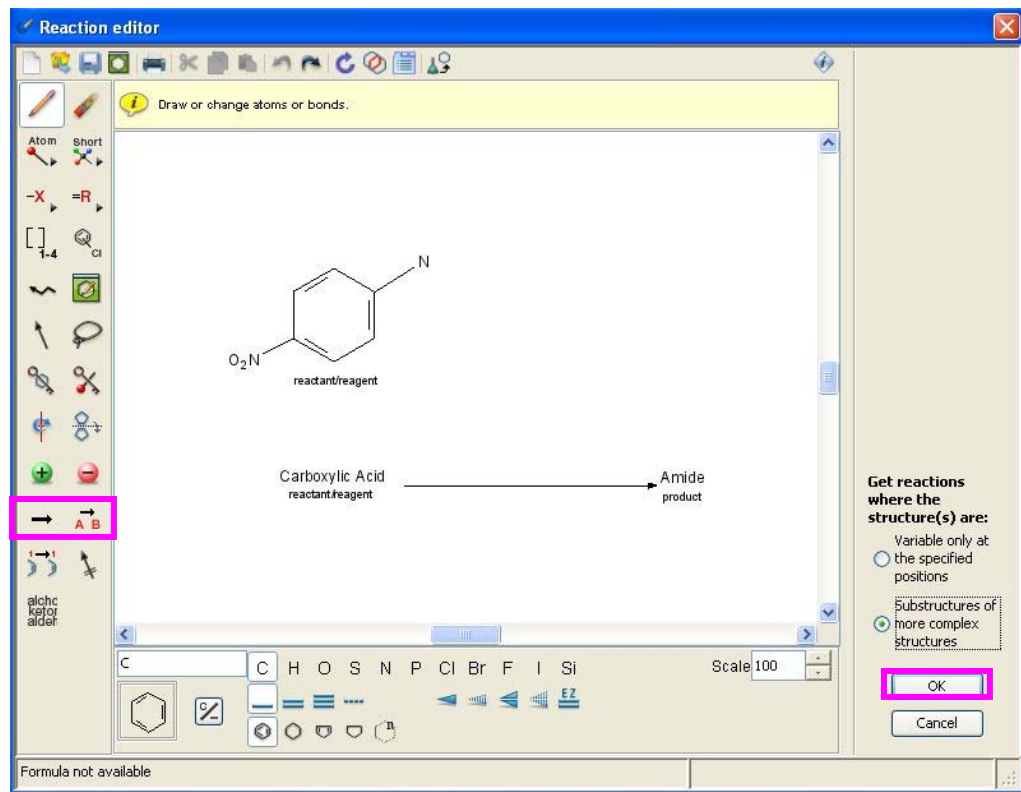


### Tips:

- It may be helpful to set your browser to full screen when using the Reaction Editor. You can also resize the window by dragging its lower-right corner .
- Mouse over the tool buttons to see names or descriptions for the tools.
- Once you select a tool, information also displays above the drawing area.
- For details about drawing reactions and using each of the tools, see the SciFinder Help files.
- If you want to switch to the Structure Editor for any reason, click .

2. Once you have drawn all the reaction participants, use the **Reaction Arrow** or **Reaction Role** tool to ensure each participant has been assigned a role.

Select a search type, and click **OK**.



**Tip:** Choose the type of search that best fits your needs:

Select...	If you want to...
Variable only at the specified positions	Prohibit substitution at all atoms (except variables and R-groups) and prohibit additional ring fusion.
Substructures of more complex structures	Allow additional substitution and ring fusion.

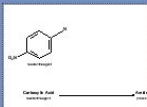
**Note:** You can selectively prohibit substitution and ring fusion by using the **Lock Out** tools. See the SciFinder Help files for more information.

3. SciFinder provides you with options to further define your search.

Click **Search**.

Explore Reactions

Reaction Structure Reaction Structure Search



Click image to change structure or view detail

Search type:  Allow variability only as specified  
 Substructure

**Solvents** Select Solvents

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

**Classification(s)**

<input type="checkbox"/> Biotransformation	<input type="checkbox"/> Electrochemical	<input type="checkbox"/> Radiochemical
<input type="checkbox"/> Catalyzed	<input type="checkbox"/> Gas-phase	<input type="checkbox"/> Regioselective
<input type="checkbox"/> Chemoselective	<input type="checkbox"/> Non-catalyzed	<input type="checkbox"/> Stereoselective
<input type="checkbox"/> Combinatorial	<input type="checkbox"/> Photochemical	

**Source(s)**

Any source  
 Patents only  
 Sources other than patents

**Publication Year(s)**   
Examples: 1995, 1995 - 1999, 1995 -, - 1995

**Tips:**

- If necessary, change the search type (variable or substructure) that you already specified within the drawing editor.
- Use these options to include particular types of reactions:

Specify this filter...	To identify reactions that...
Solvents	Include the selected solvents or solvent groups.
Number of Steps	Have the specified number of reaction steps
Classification(s)	Have been categorized as a particular type of reaction, e.g., catalyzed, stereoselective.
Source(s)	Were discussed in a patent or nonpatent reference.
Publication Year(s)	Were published in a particular year or range of years.

#### 4. Review your answers.

Reactions Get References

17459 Reactions 0 Selected | Keep Selected | Remove Selected Save Print Export

Select All Deselect All | Sort by: Number of Steps | Answers per Page [15] 1 2 3 4 5 6 ... 1164

Display:

1. Reaction Detail Link Similar Reactions

CCCC(=O)N1CCSC1C(=O)O + Cc1c(N)cc(C)c1[N+](=O)[O-] → CCCC(=O)N1CCSC1C(=O)Nc2c(C)c(C)cc2[N+](=O)[O-]

Absolute stereochemistry.  
Rotation (-).

(Step 1.3)

1.1 R:Et<sub>3</sub>N, S:THF, rt → 0°C  
1.2 R:ClCO<sub>2</sub>Et, 30 min, 0°C; 1 h, rt  
1.3 1 h, 0°C; 2 h, rt; 6-48 h, reflux  
1.4 R:F<sub>3</sub>CCO<sub>2</sub>H, S:CH<sub>2</sub>Cl<sub>2</sub>, 0°C; 3 h, rt  
1.5 R:NH<sub>4</sub>OH, S:H<sub>2</sub>O, rt

Absolute stereochemistry.  
Rotation (-).  
60%

#### Tips:

- Use the **Sort by** list to sort your answers in a variety of ways.
- Use the **Display** icons to display only one reaction per reference or all reactions.

#### 5. Work with reactions....

SciFinder allows you to work with reaction answer sets in a variety of ways. For hints and tips, see the How To Guides for:

- Working with Reaction Answer Sets: Overview
- Analyze Reaction Answer Sets
- Refine Reaction Answer Sets
- Combine Answer Sets
- Print, Save, and Export Results