

HOW TO

Explore Reactions



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

With Explore Reactions, you can:

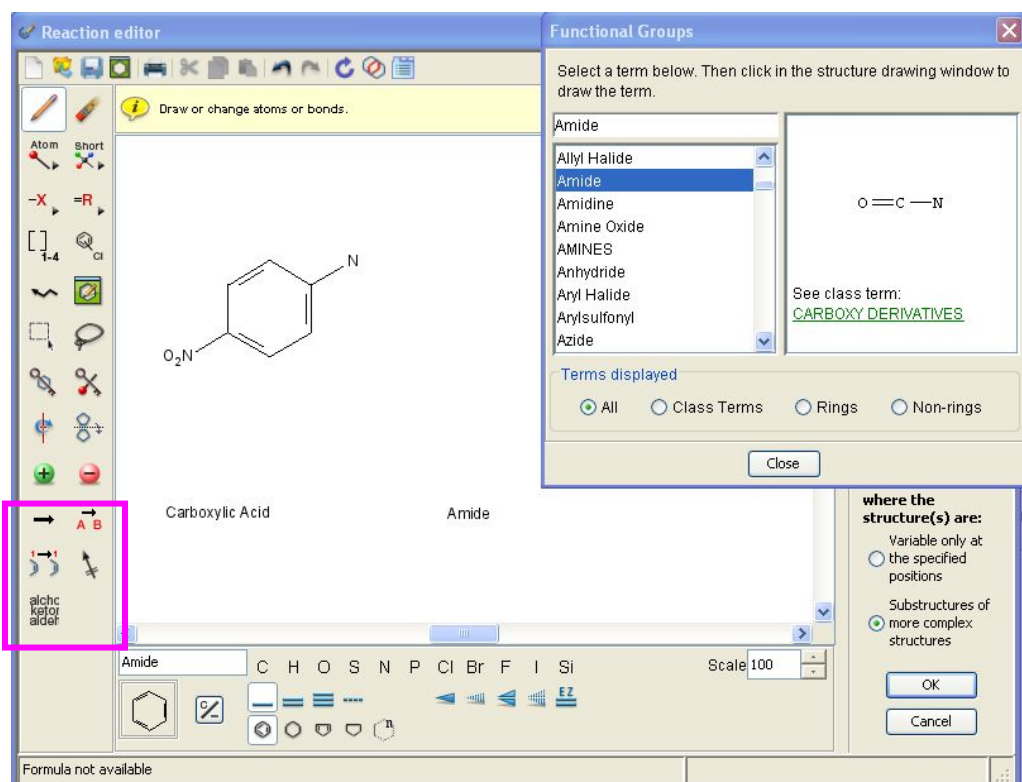
- Indicate the role of each participant
- Use all the substructure drawing features
- Allow or prohibit additional substitution and/or ring fusion
- Filter your results by solvents, number of steps, and other attributes

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

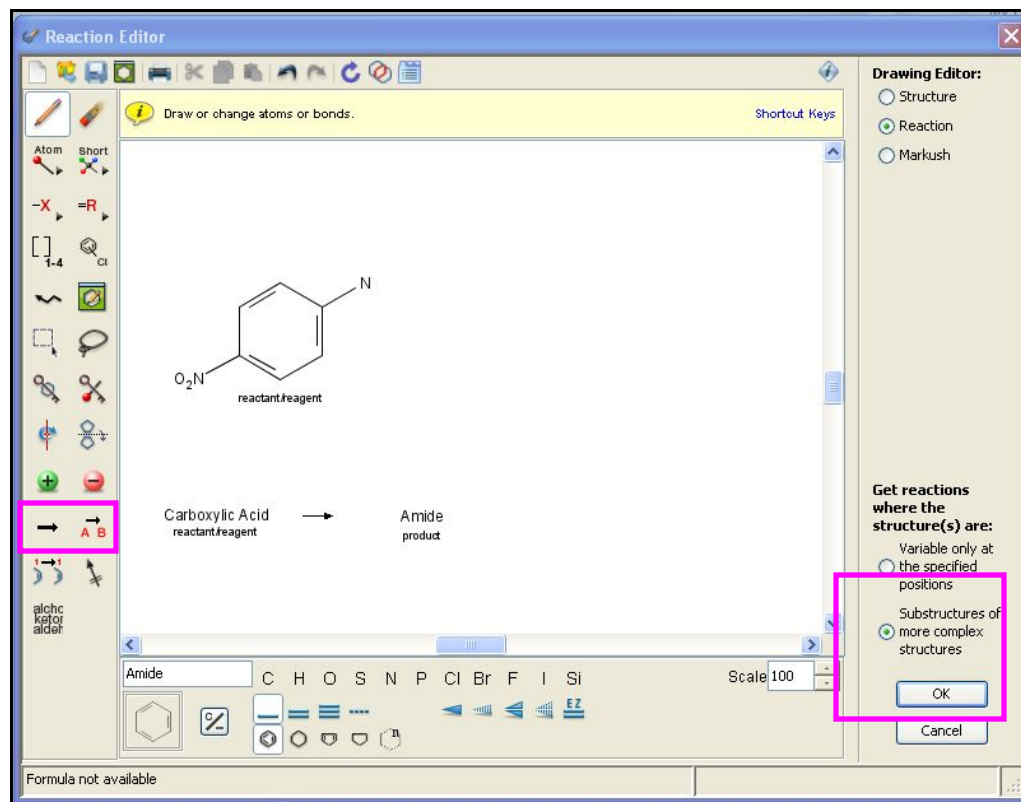


Tips:

- 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.

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**.

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 | Are limited to the selected solvents or solvent groups. |
| Non-participating Functional Groups | Contain a functional group in a reactant that is mapped to the same functional group in a product and which survives the reaction unchanged. |
| 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 non-patent reference. |
| Publication Year(s) | Were published in a particular year or range of years. |

4. Review your answers. The default display for reaction answer sets is Relevance (as determined by Tanimoto similarity).

The screenshot shows the SciFinder Reactions interface. At the top, there are buttons for 'Get References' and 'Combine Answer Sets'. Below that, a search bar shows '128 Reactions' and '0 Selected'. A dropdown menu is open, showing 'Sort by:' with options: 'Relevance (New)', 'Relevance (New)', 'Accession Number', 'Experimental Procedure', 'Number of Steps', 'Product Yield', and 'Publication Year'. The 'Relevance (New)' option is selected. To the right, there are buttons for 'Save', 'Print', and 'Export', and a 'Display:' section with icons for 'List', 'Schema', 'Overview', and 'Full Text'. The main reaction is shown as a chemical equation: 4-aminobenzonitrile + formaldehyde → N-(4-cyanophenyl)formamide, with a 77% yield. Below the reaction, there are sections for 'Overview', 'Steps/Stages', 'Notes', 'References', and 'Experimental Procedure'. The 'Steps/Stages' section shows '1.1 C:ZnO, 720 min, 70°C'. The 'Notes' section contains 'green chem. - catalyst, no solvent, Reactants: 2, Catalysts: 1, Steps: 1, Stages: 1, Most stages in any one step: 1'. The 'References' section lists 'Zinc oxide as a new catalyst for N-formylation of amines under solvent-free conditions' by Hosseini-Sarvari, Mona and Sharghi, Hashem, from the Journal of Organic Chemistry, 71(17), 6652-6654; 2006. The 'Experimental Procedure' section provides a detailed procedure: 'General/Typical Procedure: General Procedure: To a mixture of HCO₂H (3 mmol, 0.11 mL) and ZnO (0.5 mmol, 0.04 g) an amine (1 mmol) was added and then the reaction mixture was heated in an oil bath at 70 °C and stirred with a magnetic stirrer. The progress of the reaction was monitored by TLC. After the reaction was complete, CH₂Cl₂ or EtOAc was added to the reaction mixture and ZnO was removed by filtration. The organic solvent was then washed with H₂O (2x10 mL), saturated solution of NaHCO₃, and dried over anhydrous Na₂SO₄. After removal of the solvent, the pure product was obtained. This was further purified by recrystallization with suitable solvent (ether or CHCl₃). The structure of the products was confirmed by ¹H NMR, IR and comparison with authentic samples obtained commercially or prepared by reported methods. ¹H NMR (250 MHz, CDCl₃) δ 10.43 (brs, 1H), 8.31 (s, 1H), 7.97 (d, 2H, J= 8.75, Ar-H), 7.57 (d, 2H, J= 8.72, Ar-H); ¹³C NMR (62.9 MHz, CDCl₃) δ 112.1, 117.1, 129.7, 130.4, 132.9, 133.4, 141.5, 141.7, 159.8, 162.3.

Tips:

- Use the **Sort by** list to sort your answers in a variety of ways, e.g., by Relevance (default), Experimental Procedure availability, Product Yield, Number of Steps, etc.
- Use the **Display** icons to display only one reaction per reference or all reactions, reaction schema, or schema and overview

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



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CAS Customer Center
Phone: 800-753-4227 (North America)
614-447-3700 (worldwide)
Fax: 614-447-3751
E-mail: help@cas.org
Internet: www.cas.org