

# HOW TO

## Explore Reactions



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

With Explore Reaction, you can:

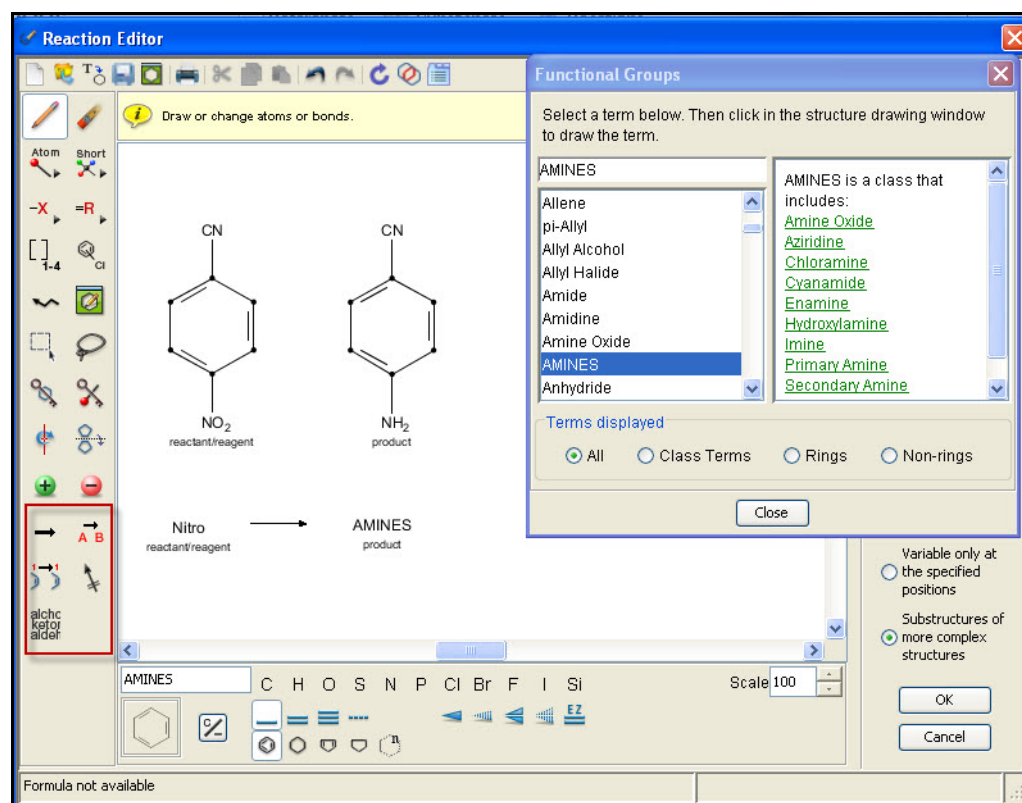
- Assign roles for reaction participants
- Use all the substructure drawing features, such as allow/prohibit additional substitution and/or ring fusion
- Filter your results by solvent, number of steps, and other attributes

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

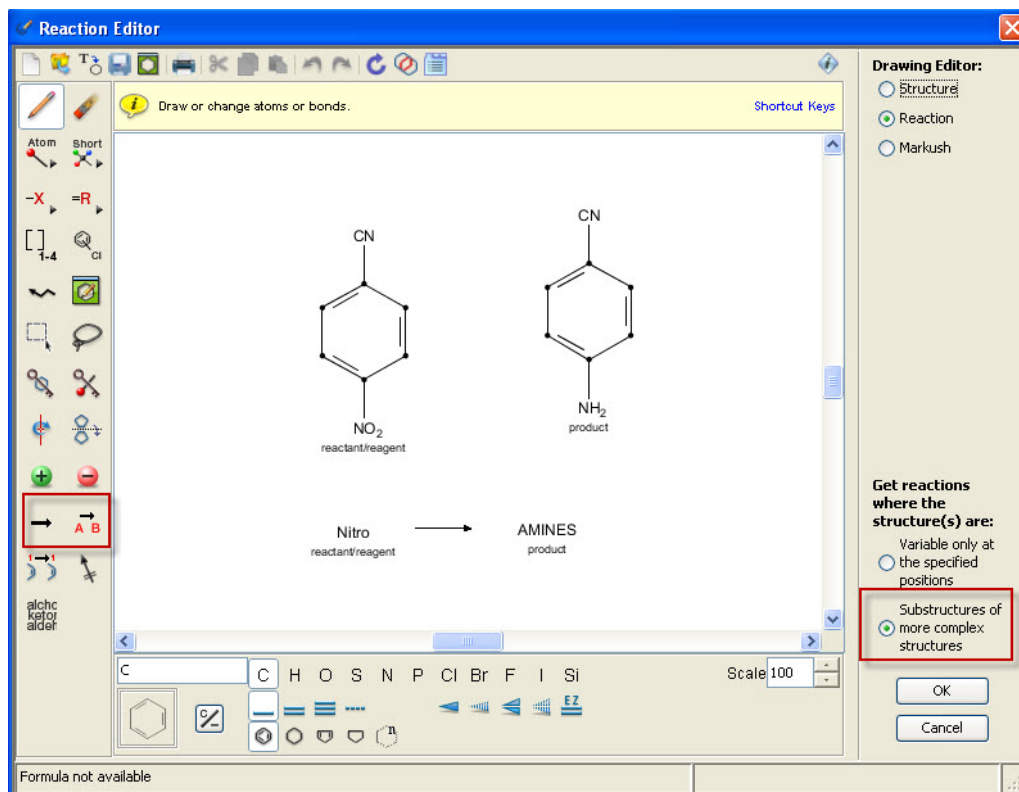


### Tips:

- 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**.

Explore Reactions

Reaction Structure
Reaction Structure

Click image to change structure or view detail

Search

Search type:  Allow variability only as specified  
 Substructure

Solvent(s)

Non-participating Functional Group(s)

Number of Steps

Classification(s)

Source(s)

Publication Year(s)

[Select Solvents](#)

[Select Groups](#)

Examples: 1, 1 - 3, 1 -, - 3

Biotransformation

Electrochemical

Radiochemical

Catalyzed

Gas-phase

Regioselective

Chemoselective

Non-catalyzed

Stereoselective

Combinatorial

Photochemical

Any source  
 Patents only  
 Sources other than patents

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	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).

380 Reactions 0 Selected Save Print Export  
Select All Deselect All Sort by: Relevance  
Answers per Page [15] 1 2 3 4 5 6 ... 26  
Display: [Icons]

1. View Reaction Detail  
Single Step Hover over any

O=[N+]([O-])c1ccc(C#N)cc1 → Nc1ccc(C#N)cc1  
99%

Overview

Steps/Stages	Notes
1.1 R:N(CH <sub>2</sub> CH <sub>2</sub> OH) <sub>3</sub> , C:12513-95-0, S:MeCN, 20 h, rt	photochem., green chem., selective photocatalytic reduction, 440nm LED used, Reactants: 1, Reagents: 1, Catalysts: 1, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Selective photocatalytic reductions of nitrobenzene derivatives using PbBiO<sub>2</sub>X and blue light  
By Fueldner, Stefan et al  
From Green Chemistry, 13(3), 640-643; 2011  
[Full Text](#)

**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:

- Analyze Reaction Answer Sets
- Refine Reaction Answer Sets
- Combine Answer Sets
- Print, Save, and Export Results