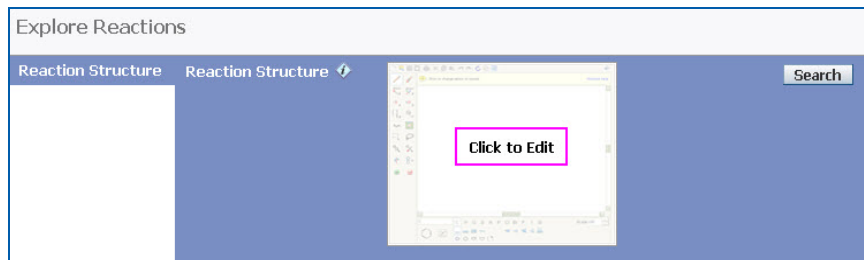


How To...

Use Explore Reactions to find reaction information with SciFinder®.

- Combine structure and functional groups
- 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 Reaction Editor.

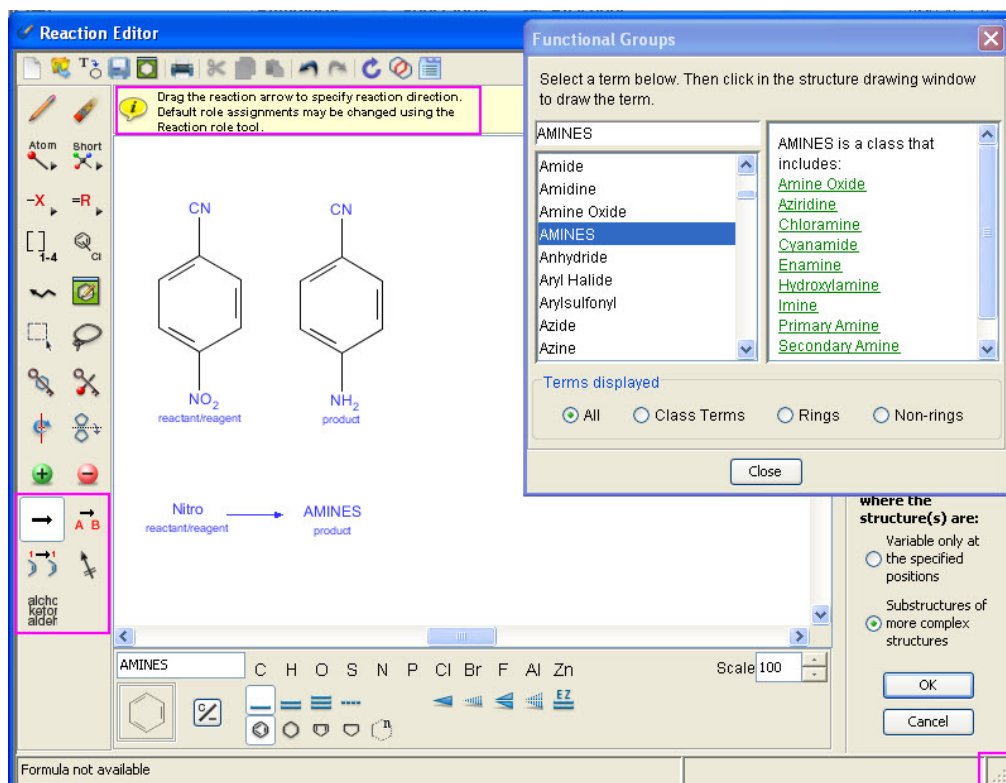


2. Use reaction-specific tools along the left side and across the bottom to:

- 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:

- You can 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 (tool tips).



Drag the reaction arrow to specify reaction direction. Default role assignments may be changed using the Reaction role tool.

Nitro reactant/reagent → AMINES product

Functional Groups

Select a term below. Then click in the structure drawing window to draw the term.

AMINES is a class that includes:

- [Amine Oxide](#)
- [Aziridine](#)
- [Chloramine](#)
- [Cyanamide](#)
- [Enamine](#)
- [Hydroxylamine](#)
- [Imine](#)
- [Primary Amine](#)
- [Secondary Amine](#)

Terms displayed

All Class Terms Rings Non-rings

Close

where the structure(s) are:

Variable only at the specified positions

Substructures of more complex structures

OK

Cancel

For details about drawing reactions and using each of the drawing tools, see SciFinder Help or review the SciFinder Drawing interactive tutorials in the [Learning Solutions](#) resource center.

- After drawing all the reaction participants, use the **Reaction Arrow** or **Reaction Role** tool to assign a role to each participant.
- Select a search type and click **OK**.

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.
Substructure of more complex structures	Allow additional substitution and ring fusion.

Reaction Editor

Draw or change atoms or bonds. Shortcut Keys

Atom Short

-X =R

[] 1-4 Cl

+

-

→ A B

alc hc ketor alder

CN

NO₂
reactant/reagent

CN

NH₂
product

Nitro
reactant/reagent

→

AMINES
product

AMINES C H O S N P Cl Br F Al Zn Scale 100

Drawing Editor:

Structure

Reaction

Markush

Get reactions where the structure(s) are:

Variable only at the specified positions

Substructures of more complex structures

OK

Cancel

Formula not available

SciFinder provides options to further define the types of reactions you want to find.

SPECIFY THIS FILTER...	TO IDENTIFY REACTIONS THAT...
Solvents	Are limited to the selected solvents or solvent groups.
Non-participating Functional Group(s)	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.

If necessary, change the search type (variable or substructure) that you already specified with the drawing editor.

5. 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

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

6. Review your answers.

Reaction answer sets are displayed in order of relevance, by default (as determined by Tanimoto similarity).

Tips:

- Use the **Sort by** list to sort your answers in a variety of ways, e.g., by Relevance (default), Accession Number, Experimental Procedure, Number of Steps, Product Yield, or Publication Year.
- Use the **Display** icons to display only one reaction per reference or all reactions, reaction schema, or schema and overview.
- Click **Overview** and/or **Experimental Procedure** to view detail or to minimize the amount of information displayed.

The screenshot shows a web interface for viewing chemical reactions. At the top, there are navigation buttons: "Reactions", "Get References", "Tools", and "Send to SciPlanner". Below this, a status bar indicates "220 Reactions" and "0 Selected". On the right, there are "Save", "Print", and "Export" options, along with a pagination control showing "Answers per Page [15]" and a list of page numbers "1 2 3 4 5 6 ... 15".

The main content area displays two reaction entries, each with a checkbox on the left. The first entry is selected and shows a chemical reaction: 4-nitrobenzonitrile (a benzene ring with a nitro group O_2N and a cyano group CN in para positions) reacting to form 4-aminobenzonitrile (a benzene ring with an amino group H_2N and a cyano group CN in para positions). The yield for this reaction is 86%. Below the reaction, there are two expandable options: "Overview" and "Experimental Procedure".

The second entry is also selected and shows the same reaction, but with a yield of 91%. It also has "Overview" and "Experimental Procedure" options.

Key UI elements are highlighted with pink boxes:

- A dropdown menu for "Sort by:" is open, showing options: "Relevance", "Accession Number", "Experimental Procedure", "Number of Steps", "Product Yield", and "Publication Year".
- A "Display:" control on the right shows icons for different view modes: a person icon (one reaction per reference), a flask icon (all reactions), a hexagon icon (reaction schema), and a document icon (schema and overview).
- The "Overview" and "Experimental Procedure" links for the first reaction are highlighted.

220 Reactions 0 Selected Save Print Export

Select All Deselect All Sort by: Relevance Answers per Page [15] 1 2 3 4 5 6 ... 15

Display:

1. View Reaction Detail [Link](#) [Similar Reactions](#)
Single Step *Hover over any structure for more options.*

86%

▼ Overview

Steps/Stages	Notes
1.1 R:Cu, R:NH ₄ ⁺ •HCO ₂ ⁻ , S:(CH ₂ OH) ₂ , 9 h, 120°C	chemoselective, Cu nanoparticles used, scalable, Reactants: 1, Reagents: 2, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1


References

[Highly Chemoselective Reduction of Aromatic Nitro Compounds by Copper Nanoparticles/Ammonium Formate](#)
[Full Text](#)
 By Saha, Amit and Ranu, Brindaban
 From Journal of Organic Chemistry, 73(17), 6867-6870; 2008

▼ Experimental Procedure

The Journal of Organic Chemistry General/Typical Procedure: **Representative Experimental Procedure for Reduction of Aromatic Nitro Compound (entry 2, Table 1).** A mixture of 3-nitrotoluene (137 mg, 1 mmol), Cu nanoparticles (191 mg, 3 mmol) in ethylene glycol (10 mL), and ammonium formate (315 mg, 5 mmol) was heated at 120 °C with stirring for 12 h (TLC) under argon. Copper particles were filtered off through a short plug of silica gel. The filtrate was extracted with ethyl acetate. Evaporation of solvent followed by column chromatography over basic alumina furnished 3-nitroaniline (86 mg, 80%) as a pale yellow oil. The spectroscopic data (IR, ¹H NMR, ¹³C NMR) of this compound are in good agreement with those reported.⁴⁹

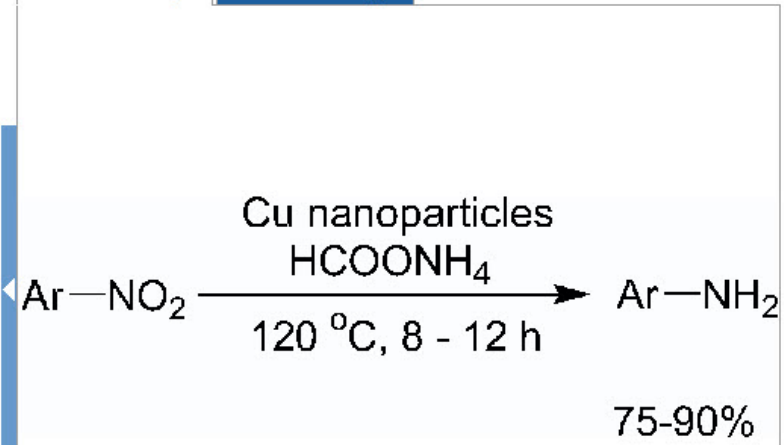
7. Click the Quick View icon  to preview the reference information (without leaving your answer set).

Quick View 

Highly Chemoselective Reduction of Aromatic Nitro Compounds by Copper Nanoparticles/Ammonium Formate
Full Text
By Saha, Amit; Ranu, Brindaban
From Journal of Organic Chemistry (2008), 73(17), 6867-6870. | Language: English, Database: CAPLUS

A highly chemoselective redn. of arom. nitro compds. to the corresponding amino compds. was achieved by a combination of copper nanoparticles and ammonium formate in ethylene glycol at 120°. The redns. are successfully carried out in presence of a wide variety of other reducible functional groups in the mol., such as Cl, I, OCH₂Ph, NHCH₂Ph, COR, COOR, and CN. The reactions are very clean and high yielding.

Reference Images **Substance Images**



$$\text{Ar-NO}_2 \xrightarrow[120\text{ }^\circ\text{C, 8-12 h}]{\text{Cu nanoparticles, HCOONH}_4} \text{Ar-NH}_2$$

75-90%

Additional resources

To learn more about working with reaction answer sets, refer to

- SciFinder online help files
- How To Guides for:
 - Analyze Reaction Answers
 - Refine Reference Answers
 - Combine Answer Sets
 - Print, Save, and Export
- Self-directed learning options in the [Learning Solutions](#) resource center



A division of the American Chemical Society

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