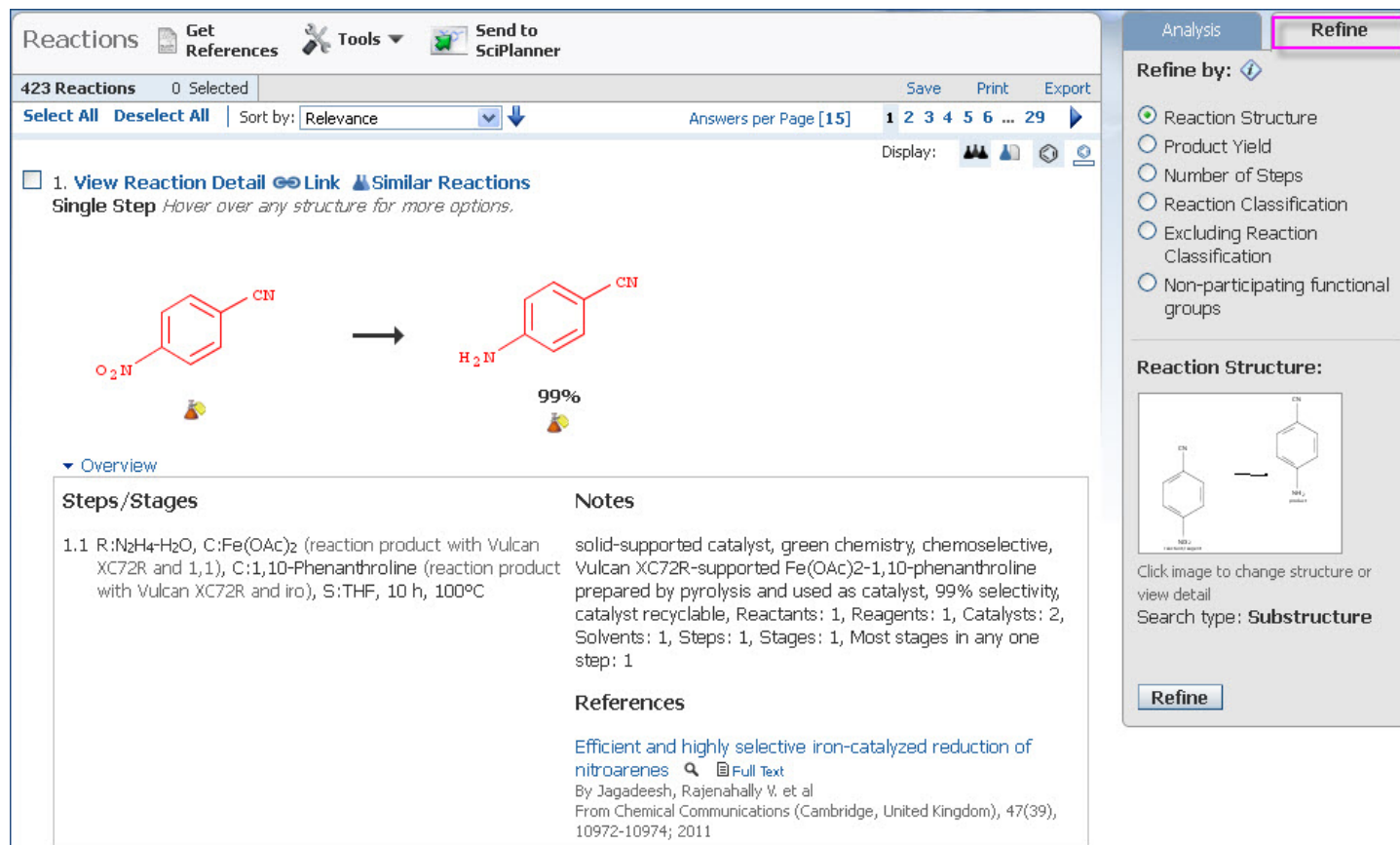


# How To...

## Refine Reaction Answers

Use Refine to explore, evaluate, and review a reaction answer set. Refining can help you extract the most relevant reactions from your answer set based on the criteria you specify.

1. Click the **Refine** tab at the right of the displayed reactions to select criteria for narrowing your answer set.



The screenshot displays the SciFinder interface. On the left, a reaction is shown: 4-nitrobenzonitrile is reduced to 4-aminobenzonitrile with a 99% yield. Below the reaction, the 'Overview' section lists the reaction conditions: 1.1 R:N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O, C:Fe(OAc)<sub>2</sub> (reaction product with Vulcan XC72R and 1,1), C:1,10-Phenanthroline (reaction product with Vulcan XC72R and iro), S:THF, 10 h, 100°C. The 'Notes' section describes the catalyst as a solid-supported catalyst, green chemistry, chemoselective, Vulcan XC72R-supported Fe(OAc)<sub>2</sub>-1,10-phenanthroline prepared by pyrolysis and used as catalyst, 99% selectivity, catalyst recyclable, Reactants: 1, Reagents: 1, Catalysts: 2, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1. The 'References' section includes a link to 'Efficient and highly selective iron-catalyzed reduction of nitroarenes' by Jagadeesh, Rajenahally V. et al. On the right, the 'Refine' panel is active, showing 'Refine by:' options: Reaction Structure (selected), Product Yield, Number of Steps, Reaction Classification, Excluding Reaction Classification, and Non-participating functional groups. Below these is a 'Reaction Structure:' section with a thumbnail of the reaction and a 'Refine' button.

You may refine multiple times with any combination of the options.

SELECT THIS OPTION...	TO IDENTIFY REACTIONS THAT...
Reaction Structure	Contain an additional or particular structural component in a specific reaction role
Product Yield	Are reported to give a specific yield or range of yields
Number of Steps	Include a particular number or range of reaction steps
Reaction Classification	Are categorized as a specific type of reaction (e.g., catalyzed, stereochemical)
Excluding Reaction Classification	Are not associated with the reaction classification that you specify
Non-participating functional groups	Include one or more functional groups and/or functional group classes in a non-participating role

2. Select an option for refining your answer set. Then specify the required information.

For example, if you choose Product Yield, specify the yield or range of yields. (Note: Not all reactions have yield data available, so you can choose to retain all reactions that do not include yield data.)

Analysis **Refine**

Refine by:

- Reaction Structure
- Product Yield
- Number of Steps
- Reaction Classification
- Excluding Reaction Classification
- Non-participating functional groups

**Product Yield:**

%  
Upper Limit  
Example: 80

%  
Lower Limit  
Example: 20

Include answers that have no product yield

**Refine**

3. Click **Refine**.

The new answer set includes only reactions that meet the specified criteria. All reactions that did not meet the specified criteria are eliminated. To return to the previous answer set, use the breadcrumb trail.

Select the criteria for sorting your answer set from the Sort by drop-down menu. In the example shown below, **Product Yield** has been selected.

Add KMP Alert Reaction Structure substructure > reactions (423) > **refine "80 - 100% yield" (351)**

Reactions Get References Tools **Send to SciPlanner**

**351 Reactions** 0 Selected Save Print Export

Select All Deselect All Sort by: Relevance Answers per Page [15] 1 2 3 4 5 6 ... 24 Display:

1. **View Reaction Detail** **Single Step** Hover over any s...

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

► Overview

## SciPlanner

SciPlanner lets you organize and manage your search results. Select the reaction(s) of interest and click **Send to SciPlanner** where you can easily combine and visualize reaction schemes. For information on using SciPlanner, see the interactive tutorial: Plan a Synthesis Project in [Learning Solutions](#) resource center.

## Additional resources

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

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



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