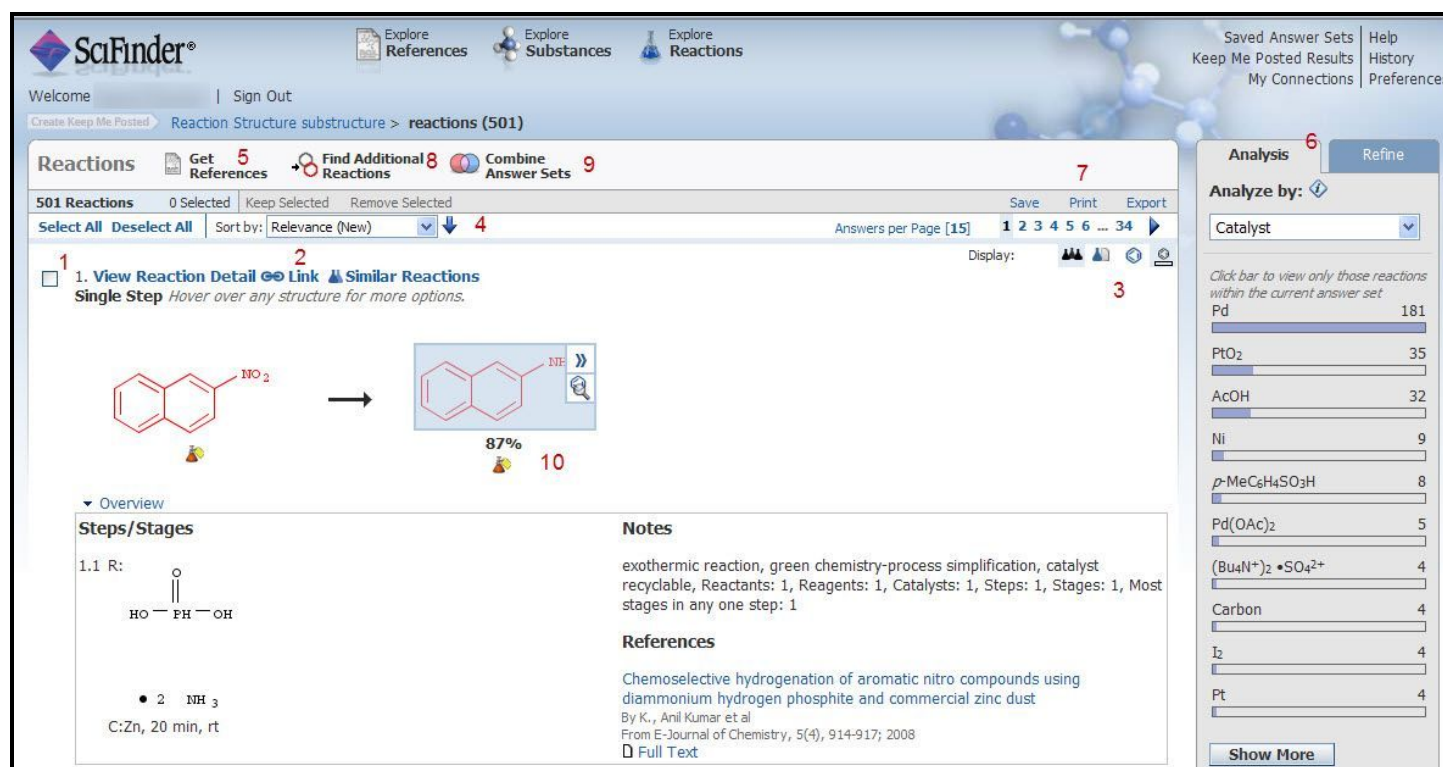


HOW TO

Work with Reactions



SciFinder® offers many options that allow you to explore, evaluate, and review your reaction answer sets. The following screen highlights those options.






The screenshot shows the SciFinder interface with the following elements:

- Navigation:** Explore References, Explore Substances, Explore Reactions.
- Search Results:** 501 Reactions, 0 Selected, Keep Selected, Remove Selected. Sort by: Relevance (New). Display: 1 2 3 4 5 6 ... 34.
- Reaction 1:**
 - 1. View Reaction Detail:** Click on the reaction structure to view details.
 - 2. Similar Reactions:** Click on the 'Similar Reactions' link.
 - Reaction Structure:** c1ccc(cc1)[N+](=O)[O-] → c1ccc(cc1)N (87% yield).
 - Overview:**
 - Steps/Stages:** 1.1 R: HO-C(=O)-NH2 → HO-CH2-NH2.
 - Reagents:** 2 NH₃, C:Zn, 20 min, rt.
 - Notes:** exothermic reaction, green chemistry-process simplification, catalyst recyclable, Reactants: 1, Reagents: 1, Catalysts: 1, Steps: 1, Stages: 1, Most stages in any one step: 1.
 - References:** Chemoselective hydrogenation of aromatic nitro compounds using diammonium hydrogen phosphite and commercial zinc dust. By K., Anil Kumar et al. From E-Journal of Chemistry, 5(4), 914-917; 2008. Full Text.
- Analysis Panel (Right):** Analyze by: Catalyst. List of catalysts and their counts: Pd (181), PtO₂ (35), AcOH (32), Ni (9), p-MeC₆H₄SO₃H (8), Pd(OAc)₂ (5), (Bu₄N⁺)₂ •SO₄²⁻ (4), Carbon (4), I₂ (4), Pt (4).

1. Get related information for an individual reaction.


Click...	When you want to...
1. Reaction Detail	View detailed information about the reaction
Reference title link	Display the details for the reference from which the reaction was indexed (for example, <i>Chemoselective hydrogenation of aromatic nitro compounds..</i> above)

Reaction Structure substructure > reactions (501) > reaction 1 (of 501)


Reaction Detail   

Return Link Save Print Export

1. Single Step *Hover over any structure for more options.*



Stages Yield 87%

1.1 R: 


• 2 NH₃
C:Zn, 20 min, rt






Notes: exothermic reaction, green chemistry-process simplification, catalyst recyclable, Reactants: 1, Reagents: 1, Catalysts: 1, Steps: 1, Stages: 1

Source: Chemoselective hydrogenation of aromatic nitro compounds using diammonium hydrogen phosphite and commercial zinc dust
K., Anil Kumar; K. S., Shruthi; Naik, Nagaraja; Gowda, D. Chame
E-Journal of Chemistry
Volume 5
Issue 4
Pages 914-917
Journal
2008



Company/Organization: Department of Studies in Chemistry
University of Mysore,
Manasagangothri
Mysore , India 570006

Number of Steps: 1




Click...	When you want to...
 Get Reference Detail	Retrieve reference associated with the reaction.
 Get Full Text	Access the full text or view full-text options for the reference.
 Get Similar Reactions	Retrieve reactions similar to this one. For more information, see Step 2.
 Combine Answer Sets	Combine current and saved answer sets into a new answer set. Note: only entire answer sets of a similar type may be combined. See Step 9 for more information.
	Go to the Reference Detail page for the next or previous reaction in the current answer set.

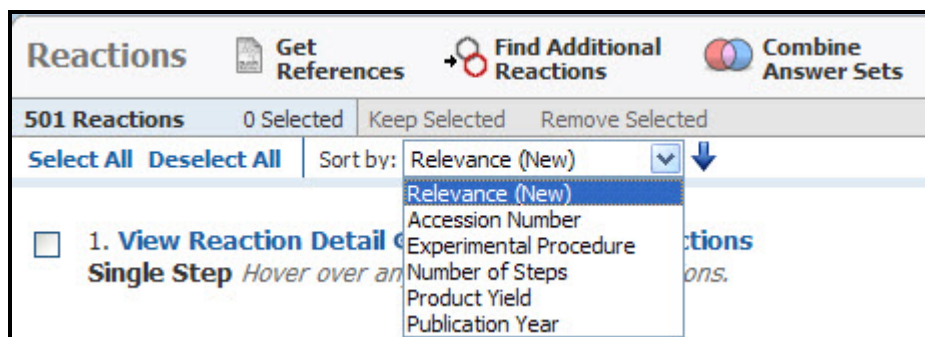
2. Create a link to this reaction, e-mail it to a colleague, or get other reactions similar to it.

Click...	When you want to...
 Link	Copy and paste a link to this reaction.
 Similar Reactions	Retrieve reactions more or less similar to the current reaction. The degree of similarity is based on "reaction centers" and related structural characteristics, which you can specify in a subsequent dialog box. Note: Only single-step reactions are eligible for similar reaction searching.

3. Control the number of answers displayed per page, and the number of reactions per reference.

Click...	When you want to...
Answers per Page [15]	Change the number of reaction answers displayed per page
Display: 	View either all reactions or only one reaction for each reference. Display Schema and Overview, or Schema only.

4. Keep reactions in or remove reactions from your answer set, or sort reactions.



Click...	When you want to...
	Retain only selected reactions. All others will be removed from the answer set.
	Eliminate the selected reactions from the answer set. Only unselected reactions will remain in the answer set.
	Sort reactions by one of these criteria: <ul style="list-style-type: none"> • Relevance (default) • Accession Number • Experimental Procedure • Number of Steps • Product Yield • Publication Year

Tip: Use **Select All** and **Deselect All** to help you quickly select or deselect many reactions at once.

5. Get references for the reactions in your answer set.

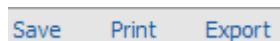
Click...	When you want to...
	Retrieve references for selected reaction(s)

Tip: To retrieve references for only a subset of the answers, select the reactions of interest before clicking **Get References**. If no reactions are selected, the entire answer set will be included.

6. Analyze or refine your answer set.

- Use the drop-down menu and bars on the **Analysis** tab to view various subsets of your answer set.
- Use the **Refine** tab to narrow your answer set using any of the listed attributes.


7. Save, print, or export your answer set.



Click...	When you want to...
	Save your answer set to the SciFinder server
	Print your answer set in PDF format
	Save your answer set to a local or shared file location


Tip: To save, print, or export only a subset of the answers, select the reactions of interest before clicking one of the above three options. If no reactions are selected, the entire answer set will be included (subject to system limits).

8. Find Additional Reactions.

Click...	When you want to...
 The icon features a red arrow pointing to the right, followed by the text "Find Additional Reactions" in black. To the right of this text is a red rectangular box with the word "NEW" in white capital letters.	Find references that contain structurally matching substances that have a Synthetic Preparation role (but different CAS Registry Numbers®) from those in the reaction answer set.

Note: The presence of the Find Additional Reactions icon does not guarantee that additional reactions will be returned. The substances and references retrieved may not include reaction details.

9. Combine Answer Sets.


Click...	When you want to...
 The icon shows two overlapping circles, one red and one blue, to the left of the text "Combine Answer Sets" in black.	Combine current and saved answer sets into a new answer set – displayed as the current answer set in the main view.

Note: Only entire answer sets can be combined. You cannot add selected answers from the current answer set to one or more saved answer sets.

Only answer sets of the same type (reference, substance, reaction, or commercial source) can be combined.

The combined answer set is not saved until you save it to the server.

10. Commercial source information.

Click...	When you want to...
 The icon depicts a laboratory flask containing a yellow liquid, with a small yellow flame or light source above it.	View commercial source or availability information for suppliers of a substance.



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Phone: 800-753-4227 (North America)
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