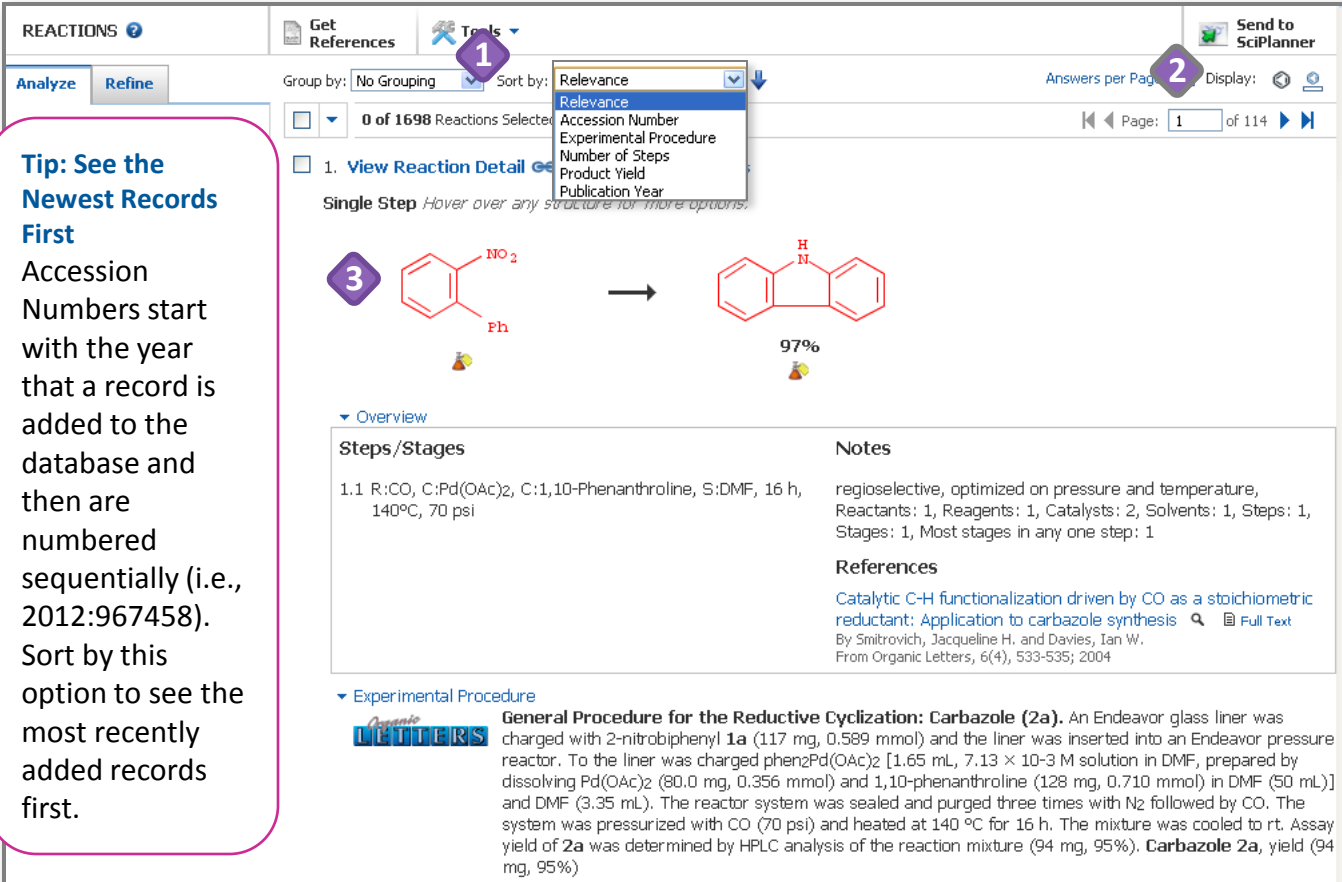


How to... Work with a Reaction Answer Set

Find all relevant reactions based on criteria you specify

Quickly retrieve relevant information from the world's largest, publicly available reaction database. This guide provides an overview of the tools in SciFinder that you can use to evaluate and narrow even a large answer set. From there, a single click retrieves references associated with your reaction(s) of interest. For more detailed information and additional training resources, consult the online Help or visit www.cas.org/training/scifinder.

Reaction Search Results



Tip: See the Newest Records First
Accession Numbers start with the year that a record is added to the database and then are numbered sequentially (i.e., 2012:967458). Sort by this option to see the most recently added records first.

1 Sort by: Relevance

2 Answers per Page: 1 of 114

3 Hit structures are red.

3 Click the red flask below a structure to see supplier catalog information for that substance.

1 By default, answers are sorted from most to least relevant.

- Click the drop-down arrow to select other sorting criteria.
- Click the blue arrow to reverse the sort order.

2 Here, the reaction schema and the **Overview** are displayed, as indicated by the benzene ring with the rectangle under it.

- Click the benzene ring to see only the reaction schema.

3 Hit structures are red.

- Click the red flask below a structure to see supplier catalog information for that substance.

Overview

Steps/Stages	Notes
1.1 R:CO, C:Pd(OAc) ₂ , C:1,10-Phenanthroline, S:DMF, 16 h, 140°C, 70 psi	regioselective, optimized on pressure and temperature, Reactants: 1, Reagents: 1, Catalysts: 2, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Catalytic C-H functionalization driven by CO as a stoichiometric reductant: Application to carbazole synthesis [Full Text](#)
By Smitrovich, Jacqueline H. and Davies, Ian W.
From Organic Letters, 6(4), 533-535; 2004

Experimental Procedure

General Procedure for the Reductive Cyclization: Carbazole (2a). An Endeavor glass liner was charged with 2-nitrophenyl **1a** (117 mg, 0.589 mmol) and the liner was inserted into an Endeavor pressure reactor. To the liner was charged phen₂Pd(OAc)₂ [1.65 mL, 7.13 × 10⁻³ M solution in DMF, prepared by dissolving Pd(OAc)₂ (80.0 mg, 0.356 mmol) and 1,10-phenanthroline (128 mg, 0.710 mmol) in DMF (50 mL)] and DMF (3.35 mL). The reactor system was sealed and purged three times with N₂ followed by CO. The system was pressurized with CO (70 psi) and heated at 140 °C for 16 h. The mixture was cooled to rt. Assay yield of **2a** was determined by HPLC analysis of the reaction mixture (94 mg, 95%). **Carbazole 2a**, yield (94 mg, 95%)

Continued

Tip

Click the **Similar Reactions** link to search for reactions based on the same reaction centers and similar structural characteristics. See the online help for more information.

4 1. [View Reaction Detail](#) [Link](#) [Similar Reactions](#)

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

5

6

Overview

Steps/Stages

1.1 R:CO, C:Pd(OAc)₂, C:1,10-Phenanthroline, S:DMF, 16 h, 140°C, 70 psi

Notes

regioselective
Reactant
Stages: 1

Reference

6 Catalytic C-H functionalization driven by CO as a stoichiometric reductant: Application to carbazole synthesis [Full Text](#)
By Smitrovich, Jacqueline H. and Davies, Ian W.
From Organic Letters, 6(4), 533-535; 2004

4 Click the box beside an answer number to select it. You can work with selected items several ways, such as saving them or getting references for them.

5 Mouse over a structure to access additional substance information and search options.

- Click the blue arrows to see related search options.
- Click the magnifying glass to see the **Substance Details** in a separate window (called a **Quick View**).

6 Click the reference title to go to the **Reference Detail** page, or click the magnifying glass to open the reference information in a **Quick View** window.

Refine to Narrow the Answer Set

1 On the **Refine** tab, click a radio button to select a **Refine by:** option.

2 Below the radio buttons, further define the criteria by which you want to refine.

3 Click **Refine**.

4 The answer set is narrowed according to the criteria you specified.

Tip: Steps vs. Stages
In many cases, a single step can have different stages. Stages occur when reagents are added sequentially, causing different reactions, but often without purification of intermediates.

Get References **Tools** **Send to SciPlanner**

Group by: No Grouping Sort by: Relevance Answers per Page [15] Display: [icon]

1 of 1698 Reactions Selected

1. [View Reaction Detail](#) [Link](#) [Similar Reactions](#)

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

Get References **Tools** **Send to SciPlanner**

Group by: No Grouping Sort by: Accession Number Answers per Page [15] Display: [icon]

0 of 673 Reactions Selected

1. [View Reaction Detail](#) [Link](#)

2 Steps *Hover over any structure for more options.*

Overview

Steps/Stages	Notes
1.1 R: PPh ₃ , S: o-Dichlorobenzene, 8 h, 180°C	2) Suzuki coupling, Reactants: 2, Reagents: 2, Catalysts: 1, Solvents: 4, Steps: 2, Stages: 2, Most stages in any one step: 1
2.1 R: Disodium carbonate, C: Pd(PPh ₃) ₄ , S: H ₂ O, S: (CH ₂ OMe) ₂ , S: PhMe, 8 h, 80°C	

References

[Biscarbazole derivatives and organic electroluminescent devices using them](#) [Full Text](#)

By Inoue, Tetsuya et al
From PCT Int. Appl., 2013024872, 21 Feb 2013

1

Get References Tools

Group by: Transformation Sort by: Frequency

0 of 673 Reactions Selected

1. Formation of Nitrogen Heterocycles
251 Reactions

Z = Electron withdrawing group

2. Reduction of Nitro Compounds to Amines
29 Reactions

$$\text{R-NO}_2 \longrightarrow \text{R-NH}_2$$

3. Hydrolysis or Hydrogenolysis of Amides/ Imides/ Carbamates
7 Reactions

Tip

By default, answers are sorted by frequency. Click the drop-down arrow for other sort options.

1

Group by: Transformation groups single-step reactions based on transformation types so you can quickly evaluate synthesis options and preferred pathways.

- Reactions can fall into more than one category.
- Unclassified single- and multi-step reactions (if any) appear at the end of the answer set.

2

Group by: Document shows all the reference titles for the answer set, and the total number of reactions associated with each title.

2

Get References Tools

Group by: Document Sort by: Relevance

Answers per Page [15] Display: []

1 of 1698 Reactions Selected

1. Catalytic C-H functionalization driven by CD as a stoichiometric reductant: Application to carbazole synthesis

Full Text

5 Reactions (1 Selected) Similar Reactions

Single Step Hover over any structure for more options.

Overview

Experimental Procedure

2. Triphenylphosphine-Mediated Reductive Cyclization of 2-Nitrophenyls: A Practical and Convenient Synthesis of Carbazoles

Full Text

13 Reactions Similar Reactions

Single Step Hover over any structure for more options.

Overview

Experimental Procedure

Tip

Click the number of reactions to see just those reactions.

1 Click the **Analysis** tab.

2 Click the drop-down arrow to select an **Analyze by:** option.

REACTIONS ? Get References Tools Send to SciPlanner

Analyze Refine

Group by: Document Sort by: Relevance Answers per Page [15] Display: ⌂ ⌕

1 of 1698 Reactions Selected Page: 1 of 9

Analyze by: ? **2**

- Catalyst
- Author Name
- Catalyst
- Company-Organization
- Document Type
- Experimental Procedure**
- Journal Name
- Language
- Number of Steps
- Product Yield
- Publication Year
- Solvent

PdCl₂(PPh₃)₂ 88

PPh₃ 71

Pd(dba)₂ 64

Bu₄N⁺ HSO₄⁻ 53

72287-26-4 47

Show More

1. Catalytic C-H functionalization driven by CD as a stoichiometric reductant: Application to carbazole synthesis Full Text

5 Reactions (1 Selected) Similar Reactions

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

O=[N+]([O-])c1ccccc1 + c1ccccc1 → c1ccc2c(c1)c3ccccc3[nH]2 (97%)

Overview

Experimental Procedure

2. Triphenylphosphine-Mediated Reductive Cyclization of 2-Nitrobiphenyls: A Practical and Convenient Synthesis of Carbazoles Full Text

13 Reactions Similar Reactions

1 Click the **Analysis** tab.

2 Click the drop-down arrow to select an **Analyze by:** option.

- Narrow results with bibliographic data using:
 - Accession Number
 - Company-Organization
 - Document Type
 - Journal Name
 - Language
 - Publication Year
- Narrow results with reaction data using:
 - Catalyst
 - Number of Steps
 - Product Yield
 - Solvent
- Narrow results based on the availability of actual experimental details using:
 - Experimental Procedure

Tip

The top ten subsets appear on the **Analysis** tab. When additional subsets are available, click the **Show More** button at the bottom of the tab to see a complete list or to select more than one subset.

Continued

4 **Explore** **Saved Searches** **SciPlanner** 5 **Save** **Print** **Export**

⚠ 313 reactions with the Experimental Procedure **Experimental Procedures Available** are displayed [Keep Analysis](#) [Clear Analysis](#)

Reaction Structure substructure > reactions (1699) > refine "1-2 steps" (673)

REACTIONS ⓘ [Get References](#) [Tools](#) [Send to SciPlanner](#)

Analyze **Refine** Group by: No Grouping Sort by: Product Yield Answers per Page [15] Display:

0 of 673 Reactions Selected Page: 1 of 21

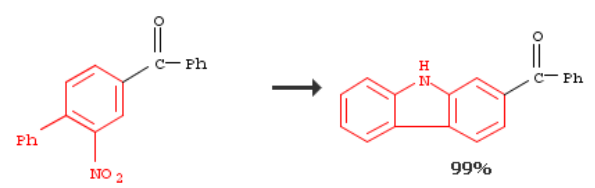
Analyze by: Experimental Procedure

Experimental Procedures Not Available 360

Experimental Procedures Available 313 [Show More](#)

13. [View Reaction Detail](#) [Link](#) [Similar Reactions](#)

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



► Overview

► Experimental Procedure

JOC The Journal of Organic Chemistry

General/Typical Procedure: *General Synthesis 1: 2-nitrophenyl derivatives via Suzuki-Miyaura cross coupling: A mixture of the desired 2-halogenitrobenzene, phenylboronic acid (1.1 equiv.), and 2 M (aq) K₂CO₃ (2 equiv.) was taken up in toluene (1.4 mL per mmol of halogen) and sparged with bubbling N₂ for 5 min. At that time, Pd(PPh₃)₄ (0.01 equiv.) was added and sparging continued for an additional 10 min before the flask was closed and the contents heated to reflux. Upon complete consumption of the halogen starting material (4-24 h), the reaction was cooled, filtered, and washed with Et₂O (~150 mL). The organic mixture was washed with H₂O (2 x 50 mL) and brine, dried over MgSO₄, and concentrated in vacuo. Chromatography of the residue gave the pure product. Chromatography (gradient of 0:100 to 10:90 EtOAc:CH₂Cl₂) gave 2-Benzoylcarbazole, yield 0.89 g, 99% as a tan-colored solid. ¹H NMR(CDCl₃) δ 7.27-7.32 (m, 1H), 7.45-7.55 (m, 4H), 7.58-7.65 (m, 1H), 7.71 (dd, J = 1.4 Hz, 8.1 Hz, 1H), 7.84-7.87 (m, 2H), 7.96 (s, 1H), 8.15 (d, J = 8.1 Hz, 2H), 8.27 (bs, 1H).*

Your answer set is divided into subsets based on the analysis criteria.

3 Click an analysis bar to display only the answers in a subset. The selected bar turns yellow.

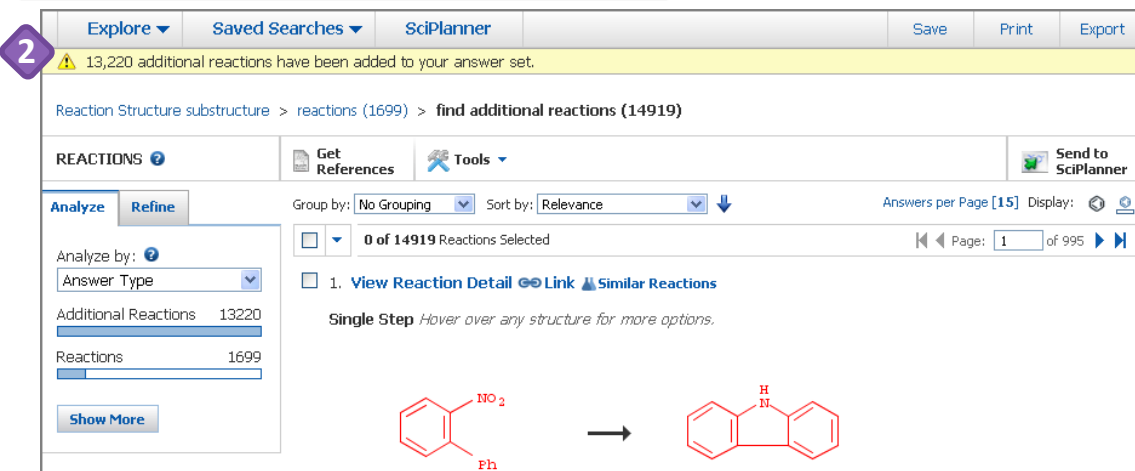
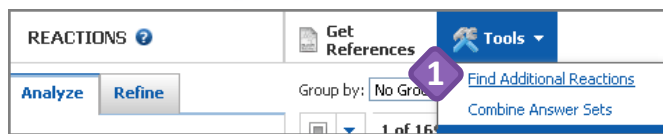
4 The yellow status message indicates the new display.

5 To replace the original answer set with the selected subset, click **Keep Analysis**.

- To return to the original answer set, click **Clear Analysis**.

Tip
Click ⓘ to see context-specific, online help.

Find Additional Reactions



Reaction Structure substructure > reactions (1699) > find additional reactions (14919)

REACTONS Get References Tools

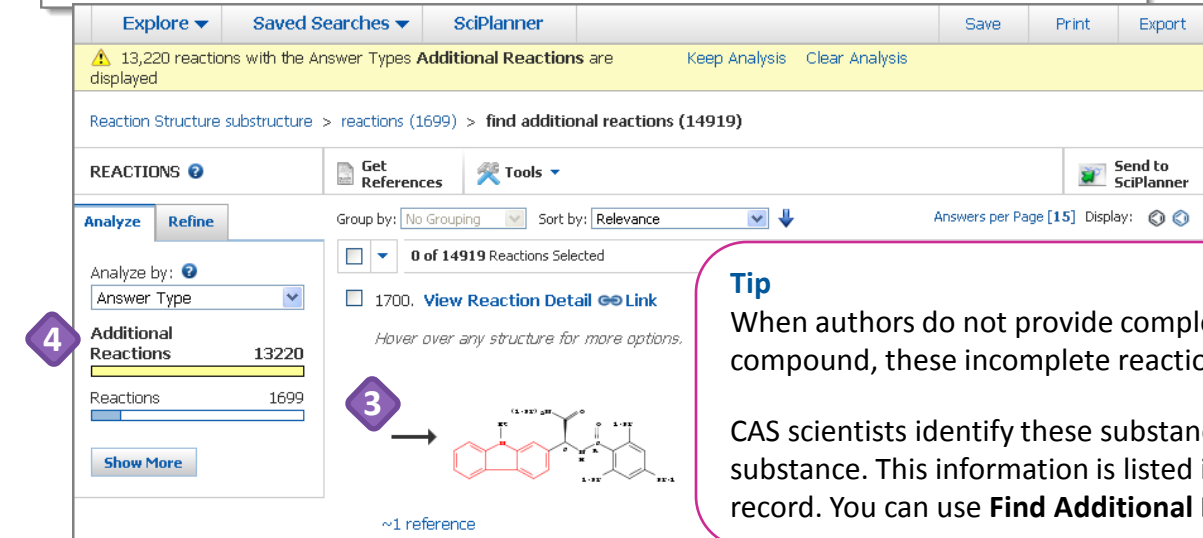

Analyze Refine

Group by: No Grouping Sort by: Relevance Answers per Page [15] Display:

0 of 14919 Reactions Selected

1. View Reaction Detail

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



13,220 reactions with the Answer Types **Additional Reactions** are displayed [Keep Analysis](#) [Clear Analysis](#)

Reaction Structure substructure > reactions (1699) > find additional reactions (14919)

REACTONS Get References Tools

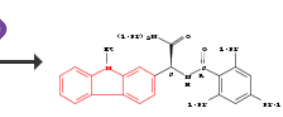
Analyze Refine

Group by: No Grouping Sort by: Relevance Answers per Page [15] Display:

0 of 14919 Reactions Selected

1700. View Reaction Detail

Hover over any structure for more options.



~1 reference

Tip

When authors do not provide complete reaction information for synthesizing a compound, these incomplete reactions cannot be put into the CASREACT® database.

CAS scientists identify these substances and apply the Preparation CAS Role to the substance. This information is listed in the indexing of the CPlus bibliographic record. You can use **Find Additional Reactions** to see these synthesized substances.

Find Additional Reactions takes advantage of the deep indexing in the CPlusSM bibliographic database. This feature identifies synthetically prepared substances in which the complete reaction information is not available but the reference indicates that the compound was synthesized. See the **Tip** for more details.

- 1 Click the **Tools** drop-down arrow and then click **Find Additional Reactions**.
- 2 The message in the yellow status bar shows the number of additional reactions that SciFinder found.
 - These reactions appear at the end of the answer set.
- 3 The synthesized compound is a product and appears to the right of the reaction arrow.
- 4 The default **Analyze** of the new answer set is **Answer Type**.
 - Select **Additional Reactions** to see only the newly added reactions.



The screenshot shows the SciFinder web interface. At the top right, there are links for 'Preferences', 'SciFinder Help', and 'Sign Out'. Below this is a navigation bar with 'Explore', 'Saved Searches', and 'SciPlanner' menus. On the right side of the navigation bar are 'Save', 'Print', and 'Export' buttons. A breadcrumb trail shows the current search path: 'Reaction Structure substructure > reactions (1635) > refine "1-2 steps" (655) > keep analysis "Experimental Procedure" (307)'. Below the breadcrumb trail are buttons for 'REACTIONS', 'Get References', 'Tools', and 'Send to SciPlanner'. Numbered callouts (1-9) point to these specific elements.

1 Access **Preferences** and **SciFinder Help** options: **Help, Training, What's New** and **Contact Us**.

2 Click the **Explore** drop-down arrow to start a new references, substances or reactions search.

3 Click the **Saved Searches** drop-down arrow to access **Saved Answer Sets, Keep Me Posted** answer sets, and your search **History**.

4 Click **SciPlanner** to open the SciPlanner workspace.

- **SciPlanner** is an interactive window where you can store and organize reference, substance, and reaction search results. Use it to gather information for a project, create a report, or export research to share with colleagues.
- Three short videos about using **SciPlanner** are available the first time you open it and also in the online Help.

5 Click **Save, Print** or **Export** to open a dialog window and initiate each of these processes. See "How to... Print, Save and Export" for more information.

6 The breadcrumb trail shows each step in your current search history. Mouse over a step to see more information about it. Click a step to return to that part of the search.

7 Click **Get References** to retrieve references for part or all of your answer set.

8 Click the Tools drop down arrow to access **Find Additional Reactions** and **Combine Answer Sets**.

9 Click **Send to SciPlanner** to send selected answers to the SciPlanner workspace.