

HOW TO

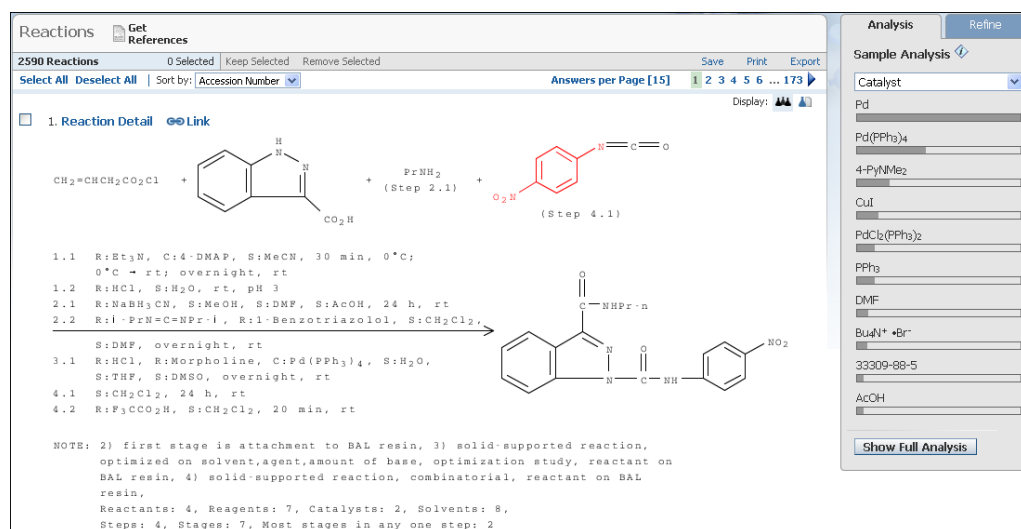
Analyze Reaction Answer Sets



Analyze is one of the many SciFinder[®] tools that allow you to explore, evaluate, and review your reaction answer sets. Analyzing helps you get different views of your answer set based on, for example, author or organization, catalyst or solvent, or other reaction characteristics.

1. When reactions are displayed, an analysis of the answer set automatically appears at the right.

Analyze by Catalyst is the default, and the first 10 analysis bars are displayed. Each bar represents a subset of the answer set.



Reactions Get References

2590 Reactions 0 Selected Keep Selected Remove Selected Save Print Export

Select All Deselect All Sort by: Accession Number Answers per Page [15] 1 2 3 4 5 6 ... 173 Display:

1. Reaction Detail [Link](#)

CH2=CHCH2CO2Cl + C1=CC=C2C(=C1)N(C2)C(=O)O + PrNH2 + O=Cc1ccc([N+](=O)[O-])cc1 (Step 4.1)

1.1 R:Et3N, C:4-DMAP, S:MeCN, 30 min, 0°C, 0°C - rt; overnight, rt
 1.2 R:HCl, S:H2O, rt, pH 3
 2.1 R:NaBH3CN, S:MeOH, S:DMF, S:AcOH, 24 h, rt
 2.2 R:PrH=C-NPr-i, R:1-Benzotriazolol, S:CH2Cl2, S:DMF, overnight, rt
 3.1 R:HCl, R:Morpholine, C:Pd(PPh3)4, S:H2O, S:THF, S:DMSO, overnight, rt
 4.1 S:CH2Cl2, 24 h, rt
 4.2 R:F3CCO2H, S:CH2Cl2, 20 min, rt

NOTE: 2) first stage is attachment to BAL resin, 3) solid-supported reaction, optimized on solvent,agent,amount of base, optimization study, reactant on BAL resin, 4) solid-supported reaction, combinatorial, reactant on BAL resin.
 Reactants: 4, Reagents: 7, Catalysts: 2, Solvents: 8, Steps: 4, Stages: 7, Most stages in any one step: 2

Analysis

Sample Analysis

Catalyst

Pd

Pd(PPh3)4

4-PyNMe2

CuI

PdCl2(PPh3)2

PPh3

DMF

Bu4N⁺ Br⁻

33309-88-5

AcOH

Note: For answer sets with more than 1,000 substances, a sample analysis is initially displayed. To conduct the full analysis, click **Show Full Analysis**.

2. (Optional) To change the analysis category, select another option from the drop-down menu.

Analysis Refine

Sample Analysis ⓘ

Catalyst

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

PPh₃

DMF

Bu₄N⁺ •Br⁻

33309-88-5

AcOH

Show Full Analysis

In a full analysis, the number to the right is the number of reactions in that subset. To view a full analysis, click **Show Full Analysis**.

Tips:

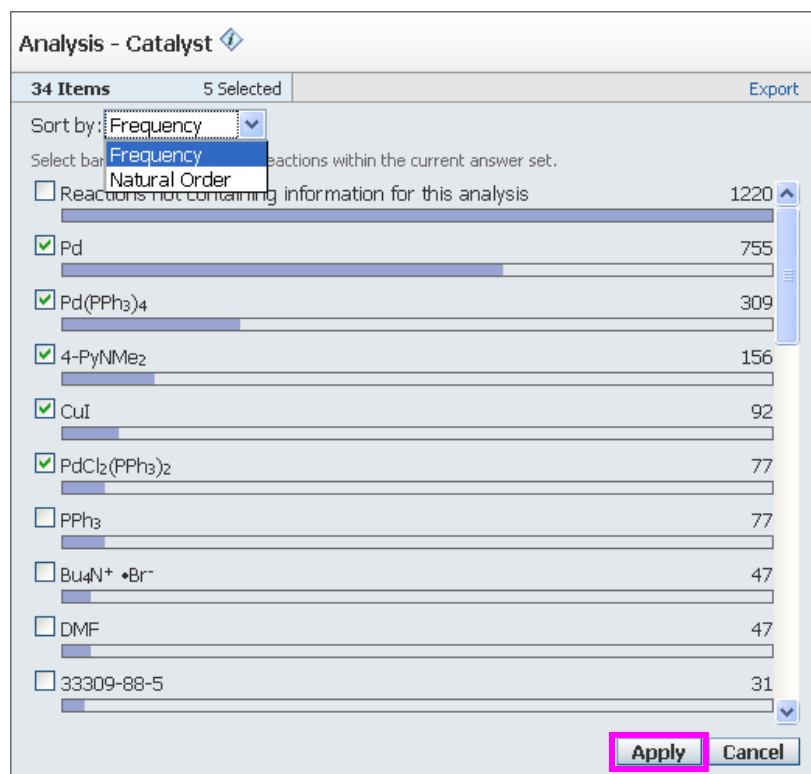
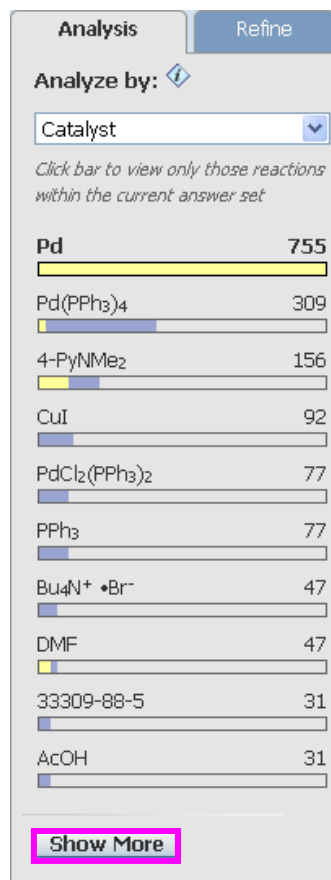
Select this option...	To identify...
Author Name	Authors reporting the reactions
Catalyst	Catalysts used in the reactions
Company-Organization	Companies or organizations reporting the reactions
Document Type	Type of document in which the reactions were reported
Journal Name	Journals in which the reactions were published
Language	Languages in which the reactions were reported
Number of Steps	Number of steps in the reactions
Product Yield	Percent yields of the reactions
Publication Year	Years in which the reactions were published
Solvent	Solvents used in the reactions

3. To display just one subset, click on an analysis bar.

The bar that was clicked turns yellow, as well as portions of other bars that represent the reactions within the subset. In this example, 755 reactions involve Pd as a catalyst. Some of those reactions also involve Pd(PPh₃)₄, PyNMe₂, DMF, etc.

Although the answer set is unchanged, only the references in the subset display.

To select multiple subsets at once, click **Show More**. Then select the subsets of interest, and click **Apply**.



Tip: Select the way in which you want the bars sorted

- **Frequency** displays only the top 500 bars.
- **Natural Order** displays all the bars in alphanumeric order.

4. The filtered answer set displays. This is indicated by the message displayed in yellow.

To create a new answer set containing only the reactions in the analyzed set, click **Keep Analysis**.

To return to the full answer set (without the analysis applied), click **Clear Analysis**.

Reactions Get References

2590 Reactions 0 Selected Keep Selected Remove Selected Save Print Export

755 reactions with Catalyst Pd are displayed Keep Analysis Clear Analysis

Select All Deselect All Sort by: Accession Number Answers per Page [15] 1 2 3 4 5 6 ... 51

3. Reaction Detail Link

$(\text{CO}_2\text{Me})_2$ + C1=CC=C2C(=C1)C(=O)N2 + CC(C)C=O + KCN + CC(C)(C)OC(=O)OC(=O)OC(C)(C)C + CCN(C)C(=O)O + CN(C)C(=O)O + COC(=O)C1=CC=C2C(=C1)C(=O)N2

converging, R:NaOBu-t, R:NH3, R:POCl3, R:HNO3, R:MnO2, R:H2, R:LiOH, R:HCl, R:4-DMAP, R:EDAP, C:Pd, S:DMF, S:H2O, S:AcOH, S:MeOH, S:Dioxane, S:EtOH, S:AcOEt

CCN(C)C(=O)Nc1ccc2c(c1)c(c3ccc(NC(=O)C4=CC=CC=C4)cc32)C(=O)Nc5ccc6c(c5)c(c7ccc(NC(=O)C8=CC=CC=C8)cc7)nc6

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:

- Working with Reaction Answer Sets: Overview
- Refine Reaction Answer Sets
- Combine Answer Sets
- Print, Save, and Export Results