

**SciFinder<sup>®</sup> ...**  
Part of the Chemical Synthesis Process

Revised December 2009



## ***Introduction***

SciFinder allows researchers to tap into a wealth of chemical synthesis information. The combination of SciFinder's rich database content and its powerful and sophisticated search and analysis tools lets you easily explore synthetic pathways as well as link to patents, journal articles, substance information, and commercial sources with just one click.

SciFinder lets you explore for chemical synthesis information in a variety of ways, depending on your precise need. You can begin your explorations by searching:

- Research topics
- Chemical names or structures
- Reaction structure drawings
- Functional group transformations

You quickly access relevant references, substances, reactions, and supplier information, which can help you determine what is patented in a particular area, find alternative preparation methods, or decide between purchasing and preparing a substance. Trying a combination of exploration pathways within SciFinder is often very effective and can generate ideas that you might not have considered beforehand.

This paper discusses some of the essential needs that SciFinder addresses and provides an overview of SciFinder's database content and tools. Four examples illustrate the power and convenience of using SciFinder to spark and energize your search and discovery process.

Because there are many additional features and exploration pathways available in SciFinder, please visit [www.cas.org](http://www.cas.org) for more information or contact [CAS Customer Care](#) to be put in touch with a sales representative in your area.

## ***Today's challenges***

Chemists have many reasons for studying reactions, whether it is for preparing compounds or discovering more efficient synthetic pathways. Chemists might wish to:

- Prepare compounds that are useful in everyday life, e.g., pharmaceuticals, polymers, semiconductor materials
- Prove structures of natural compounds via assembly of smaller structural components
- Study reaction mechanisms or biological metabolisms through use of labeled compounds
- Solve problems that require new synthetic approaches and potentially lead to new reactions, reagents, methods, and catalysts

Research and development is rarely straightforward, and competitive pressures make it critical to have an accurate and current knowledge of approaches that have worked, or perhaps not worked, as reported in the published literature. Organizations need to act quickly and confidently to gain a competitive edge.

Likewise in an academic setting, it is important to have quick and easy access to chemical synthesis information for teaching and research.




This is where SciFinder can help.

## Exploring the world's largest database of synthetic information

SciFinder provides multiple points of access to the CAS databases, the most authoritative, comprehensive, and reliable source for chemical and related information. These databases cover biomedical sciences, chemistry, engineering, materials science, agricultural science, and more.

To build the databases, CAS monitors, indexes, and abstracts the world's chemistry-related patents and literature, updates this information daily, and makes it accessible through state-of-the-art information services like SciFinder.

### Overview of the information and search starting points in SciFinder\*

Type of information	Content and coverage	Starting points for locating chemical synthesis information
 <b>References</b>	<ul style="list-style-type: none"><li>&gt;31 million references from 59 patent authorities worldwide and &gt;10,000 major scientific journals</li><li>&gt;18 million references from MEDLINE®</li><li>1907 to present, plus selected pre-1907 articles and patents</li></ul>	<ul style="list-style-type: none"><li>Research topic</li></ul>
 <b>Substances</b>	<ul style="list-style-type: none"><li>&gt;51 million organic and inorganic substances</li><li>&gt;61 million sequences</li><li>&gt;2.6 billion predicted and experimental properties, spectra, and data tags, plus &gt;29.6 million proton NMR spectra and 29.7 million predicted <sup>13</sup>C-NMR spectra</li><li>1957 to present, plus selected substances back to the early 1900s</li><li>Commercial source information from &gt;1,000 suppliers for &gt;38 million substances</li><li>Regulatory information for &gt; 270,000 substances</li></ul>	<ul style="list-style-type: none"><li>Chemical name or CAS Registry Number®</li><li>Molecular formula</li><li>Chemical structure drawing</li></ul>
 <b>Reactions</b>	<ul style="list-style-type: none"><li>&gt;29 million preparations, including &gt;21 million single- and multi-step reactions</li><li>1840 to present</li></ul>	<ul style="list-style-type: none"><li>Reaction structure drawing</li><li>Functional group transformation</li></ul>

\* For details about CAS database content and SciFinder features, visit [www.cas.org](http://www.cas.org).

SciFinder lets you approach your exploration in a variety of ways. For example, you can develop a very precise structure-based query and use SciFinder's synthetic pathway features to make connections to related research.

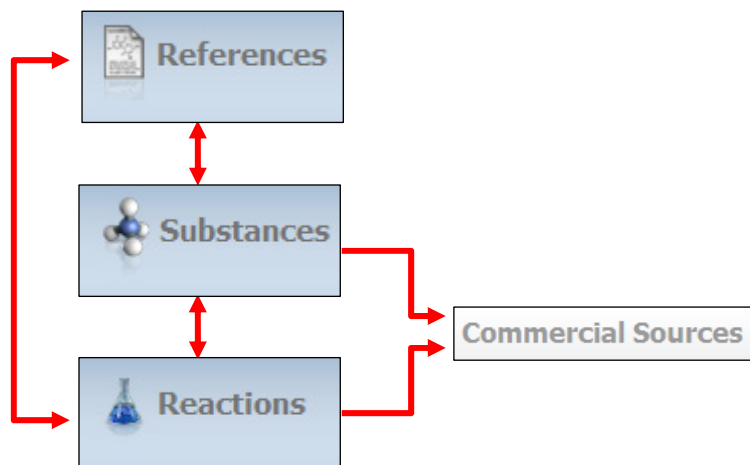
Alternatively, you might start with a broad research topic and then use SciFinder's powerful and sophisticated analysis tools to focus in on exactly what you need.

When discussing the value of CAS information for synthetic chemistry, research chemist Steven Furyk of DuPont said the following in the 2007 American Chemical Society annual report:

"When I'm in the lab trying to come up with a synthesis of a molecule, the first thing I do is search through SciFinder and within minutes I have a prep for a new compound. It saves me time because somebody else has done the work so I can move on and do the novel chemistry that I want to do."

Whether you take a specific or general approach to looking for answers to your questions, you can easily move among reference, substance, reaction, and commercial source information. Once you identify a substance of interest, you can quickly review options for obtaining the substance or investigate potential ways of making it.

**Pathways for moving among reference, substance, reaction, and commercial availability information.**



**Pathways for exploring substance information from a reaction diagram.**

Reaction Detail Get Reference Detail Get Full Text Get Similar Reactions

91.

Click on any structure, reagent, solvent, or catalyst to obtain reaction, reference, substance, or commercial source information.

NOTE: Reaction Step

Reactions	Product
References	Reactant
Substance Detail	Reagent
Commercial Sources	Reactant or Reagent
Regulatory Information	Catalyst
Explore by Chemical Structure	Solvent
Explore Reactions	Any role

The examples that follow illustrate some of the many ways to utilize the power, convenience, and flexibility of SciFinder when looking for chemical synthesis information. Many SciFinder searchers try a combination of these approaches to spark ideas for their research.

### Example 1. Starting with a research topic

Use this approach when you have a general topic or a named reaction to “cast a wide net” for references. Focus your answer set appropriately, and then investigate reactions associated with the references.

#### Locate patents involving Suzuki coupling chemistry in the synthesis of substituted biphenyls.

**Background:** Suzuki coupling is the reaction of an aryl or vinyl boronic acid with an aryl or vinyl halide catalyzed by Pd complexes. It is widely used in the synthesis of polyolefins, styrenes, and other commercially important compounds, including substituted biphenyls, which have a variety of uses in the chemical and pharmaceutical industries.

Conduct a broad reference search on “suzuki reaction,” but limit retrievals to only patents.

The screenshot shows the SciFinder search interface with the following details:

- Search Bar:** "suzuki reaction" is entered in the "Research Topic" field. A red box highlights the text, and a red arrow points to the "Search" button.
- Document Type(s):** The "Patent" checkbox is checked and highlighted with a red box. Other options include Biography, Book, Clinical Trial, Commentary, Conference, Dissertation, Editorial, Historical, Journal, Letter, Preprint, Report, and Review.
- Language(s):** Options include Chinese, English, French, German, Italian, Japanese, Polish, Russian, and Spanish.
- Author Name:** Fields for Last \*, First, and Middle.
- Company Name:** A field with examples: "Minnesota Mining and Manufacturing", "DuPont".

Because SciFinder retrieves more than 500 references, use Refine by Research Topic to limit to only references related to "substituted biphenyls." You can refine as many times as needed to make your answer set a reasonable size.

Review and select references of interest.

Then "Get Reactions" to retrieve and investigate information on reactions identified in the references.

Save or print the references and reactions of interest, or request the full text for a patent or journal article.

Note: This example shows how you can easily obtain some good, general results, but it's just one possible approach to this research question. For example, you may wish to use SciFinder's substance and reaction features to perform more precise searches. Examples 2-4 highlight some of these features.

Research Topic: "suzuki reaction" with limiters > references (520) > refine "substituted biphenyls" (27)

References

27 References | 0 Selected | Keep Selected | Remove Selected | Remove Duplicates | Add Tags

Select All | Deselect All | Sort by: Accession Number

1. Process for preparation of substituted biphenylanilides  
By Dockner, Michael; Rieck, Heiko  
From PCT Int. Appl. (2009), WO 2009106234 A1 20090903. Language: English, Database: CAPLUS  
Substances Reactions Citing Full Text Link Comments Tags

2. Polycyclic/heterocyclic aromatic group-substituted triphenylamine as high-performance and its application in organic light-emitting device  
By Ma, Yuguang; Yang, Bing; Shen, Fangzhong; Tang, Shi; Lu, Ping; Xu, Hai; Gu, Cheng; Liu, Dandan; Li, Weijun  
From Faming Zhuanli Shengqing Gongkai Shuomingshu (2009), CN 101423757 A 20090506. Language: Chinese, Database: CAPLUS  
Substances Reactions Citing Full Text Link Comments Tags

3. Method for synthesizing  $\alpha$ -biphenylnitrone carbocyclic carbene-Pd complexes as catalytic coupling reaction  
By Wu, Jinlong; Dai, Jing; Dai, Weimin  
From Faming Zhuanli Shengqing Gongkai Shuomingshu (2008), CN 101250202 A 20080827. Language: Chinese, Database: CAPLUS  
Substances Reactions Citing Full Text Link Comments Tags

4. Method to prepare cross coupling products via carbon-carbon bond-forming reactions  
By Subhash, Nandurkar Nitin; Mahadeo, Bhanage Bhalchandra  
From Indian Pat. Appl. (2008), IN 2008MU00237 A 20080704. Language: English, Database: CAPLUS  
Substances Reactions Citing Full Text Link Comments Tags

Refine by:

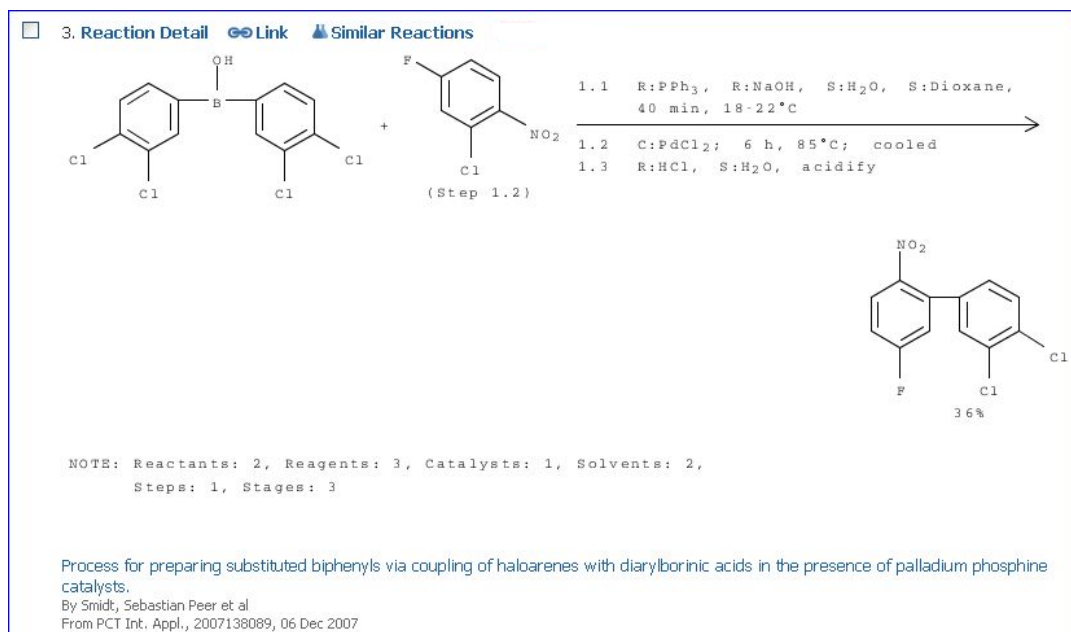
- Research Topic
- Author Name
- Company Name
- Document Type
- Publication Year
- Language
- Database

Research Topic:  
substituted biphenyls

Examples:  
The effect of antibiotic residues on dairy products  
Photocyanation of aromatic compounds

Refine

### Sample reaction:



**SciFinder provides integrated access to chemical synthesis information in patents and chemical literature.**

## Example 2. Starting with a specific substance

Use this approach when you have a specific reactant, reagent, or product in mind. You can search its name, CAS Registry Number, or chemical structure, and then get reactions associated with the substance. With chemical structure, you can request exact, similarity, or substructure (core structure) matches.

### Locate information about the preparation of 1,3-propanediol by biological methods.

**Background:** 1,3-propanediol is an aliphatic diol that is a key starting material in the manufacture of polyesters and/or co-polyesters used in fibers, composites, adhesives, coatings, moldings, etc. This starting material has historically been prepared by using petroleum-based methods such as hydroformylation of ethylene oxide or hydration of acrolein followed by reduction. Many organizations are now looking at alternative methods to prepare these kinds of building block chemicals, where the processes are more economically and environmentally friendly.

Conduct a chemical name search to locate the substance record for "1,3-propanediol."

Explore Substances

Chemical Structure  
Molecular Formula  
Substance Identifier

Substance Identifier(s) 1,3-propanediol

Search

Enter one per line.  
Examples:  
50-00-0  
999815  
Acetaminophen

Get reactions in which the substance is a product.

Note: Alternatively, you could get references in which the substance is prepared. Then get reactions.

Substances Get References Get Reactions Get Commercial Sources

1 Substance 0 Selected Keep Selected Remove Selected Save Print Export

Select All Deselect All Sort by: CAS Registry Number Answers per Page [15]

View: [Icons]

1. Substance Detail  
504-63-2

OCCCO

C<sub>3</sub>H<sub>8</sub>O<sub>2</sub>  
1,3-Propanediol

~7,133 References  
Reactions  
Commercial Sources  
Regulatory Information  
Link

Get Reactions

Retrieve reactions for:  
 All substances  Selected substances

Select a reaction role:  
 Product  
 Reactant  
 Reagent  
 Reactant or reagent  
 Catalyst  
 Solvent  
 Any role

Get Reactions Cancel

Limit your answers to only biotransformation reactions.

Reactions [Get References](#)

43 Reactions 43 Selected Keep Selected Remove Selected Save Print Export

Select All Deselect All | Sort by: Accession Number | Answers per Page [15] 1 2 3 | Display: [Icons]

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

OCC(O)CO  $\xrightarrow{R:K_2HPO_4, R:KH_2PO_4, C:81611-70-3, S:H_2O}$  OCCO

EtOH + CC(O)C(=O)O + AcOH +

NOTE: regioselective, enzymic, biotransformation, resting cell system used (micro-aerobic conditions), 60% conversion to 1,3-propanediol, NADH-1 1,3-propanediol oxidoreductase overexpressed in Klebsiella pneumoniae cells, Reactants: 1, Reagents: 2, Catalysts: 1, Solvents: 1, Steps: 1, Stages: 1

Over-expression of glycerol dehydrogenase and 1,3-propanediol oxidoreductase in Klebsiella pneumoniae and glycerol into 1,3-propanediol in resting cell system  
By Zhao, Li et al  
From Journal of Chemical Technology and Biotechnology, 84(4), 626-632; 2009

2. Reaction Detail [Link](#) [Similar Reactions](#)

OCC(O)CO  $\xrightarrow{S:H_2O, 24 h, 30^\circ C, pH 7}$  OCCO

**Refine**

Analysis Refine

Refine by:

- Reaction Structure
- Product Yield
- Number of Steps
- Reaction Classification
- Excluding Reaction Classification

**Reaction Classification(s):**

- Biotransformation
- Catalyzed
- Chemoselective
- Combinatorial
- Electrochemical
- Gas-phase
- Non-catalyzed
- Photochemical
- Radiochemical
- Regioselective
- Stereoselective

**Refine**

View the Reaction Detail to investigate possible preparation methods. For example, review details and notes for each step and the patent or journal article from which the reaction originated.

Save or print the reactions and references of interest.

Create Keep Me Posted Substance Identifier "1,3-propanediol" > substances (1) > get reactions (194) > refine "Biotransformation" (43) > reaction

Reaction Detail [Get Reference Detail](#) [Get Full Text](#) [Get Similar Reactions](#) [Link](#) [Save](#) [Print](#) [Export](#)

22.

OCC(O)CO + C1=CC=C(C=C1)C(=O)O + C1=CC=C(C=C1)N

Absolute stereochemistry.  
Rotation (+).  
Reagent

$\xrightarrow{R:AcOH, R:K_2HPO_4, R:CoCl_2, R:FeSO_4 \cdot 7H_2O, R:NH_4OH, R:MgSO_4, R:KH_2PO_4, S:H_2O, rt, pH 6.5}$  OCCO

NOTE: biotransformation, Clostridium butyricum VPI 3266 used, buffered soln., fermn., optimization study, optimized on concentration, Reactants: 1, Reagents: 9, Solvents: 1, Steps: 1, Stages: 1

[Previous](#) [Next](#)

**SciFinder makes it quick and easy to find a substance of interest and specify reaction roles and classifications.**

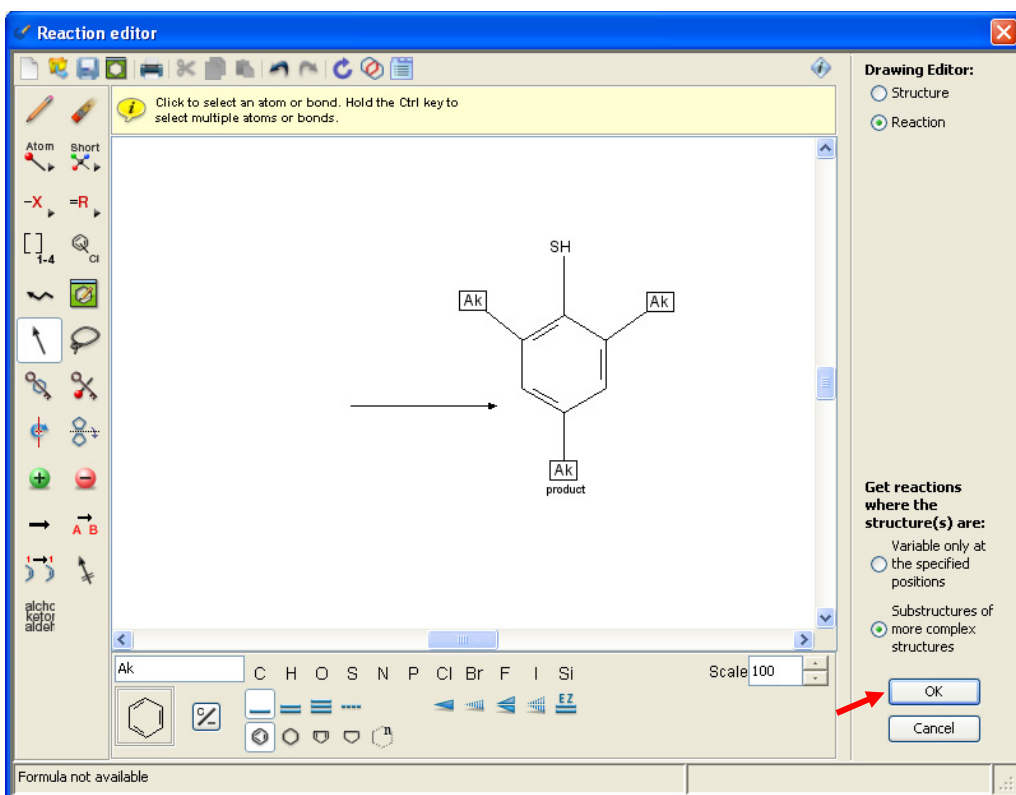
### Example 3. Starting with a reaction structure drawing

Use this approach when you want to utilize SciFinder's reaction drawing and searching features, such as specifying multiple participants, substitution, variability (R groups), reaction sites, and atom mapping. Also use this approach when you want to import structures in molfile format. As with all SciFinder reaction displays, you can get commercial source, synthetic pathway, and other related information for any reaction participant.

**Identify candidate thiol ligands with desired structural characteristics, and investigate whether to purchase or prepare the thiol.**

**Background:** Metal-sulfur bonds, e.g., in metal thiolate salts, are of interest in both inorganic and bioinorganic chemistry as models in various catalytic processes and as biological active sites. An inorganic chemist will likely have distinct preferences on the chemical, electronic, and structural characteristics of the desired thiol ligand or salt. Furthermore, it may be desirable or more cost effective to purchase rather than prepare the thiol(s) of interest.

Draw a sterically hindered aromatic thiol with alkyl groups at the 2, 4, and 6 positions, and assign the role of product.



SciFinder retrieves 42 reaction answers.

Review the answers. If desired, use Refine by Product Yield or Number of Steps to narrow in on effective preparations.

Reactions [Get References](#)

42 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

1. Reaction Detail [Link](#)

Cc1c(C)c(C)c(S)cc1  $\xrightarrow{\text{R: Pb(OAc)}_2, \text{S: MeOH}, 2 \text{ h, rt}}$  Cc1c(C)c(C)c(S)cc1

• 1/2 Pb(II)  
78%

NOTE: Reactants: 1, Reagents: 1, Solvents: 1, Steps: 1, Stages: 1

Synthesis and Characterization of Chalcogenolato-Bridged Allyl Palladium Complexes: Versatile Precursors for...  
By Ghavale, Ninad et al  
From Organometallics, 27(13), 3297-3302; 2008

2. Reaction Detail [Link](#)

Cc1c(C)c(C)c(S)cc1  $\xrightarrow[2. \text{ R: Pb(OAc)}_2, \text{ S: MeOH}, \text{ S: Benzene}, 4 \text{ h, rt}]{1. \text{ R: NaBH}_4, \text{ S: MeOH}, 4 \text{ h, rt}}$  Cc1c(C)c(C)c(S)cc1

**Refine**

Analysis **Refine**

Refine by:

- Reaction Structure
- Product Yield
- Number of Steps
- Reaction Classification
- Excluding Reaction Classification

**Product Yield:**

%

Upper Limit  
Example: 80

Lower Limit  
Example: 20

Include answers that have no product yield

**Refine**

View the Reaction Detail for reactions of interest.

Click on any reaction participant to access further exploration options.

Choose "Commercial Sources" for detailed catalog information. You can see if there is a supplier in your area and check the price.

Create Keep Me Posted | [Reaction Structure substructure](#) > [reactions \(42\)](#) > [reaction 12 \(of 42\)](#) [Link](#) [Save](#) [Print](#) [Export](#)

Reaction Detail [Get Reference Detail](#) [Get Full Text](#) [Get Similar Reactions](#)

12.

Cc1c(C)c(C)c(S(=O)(=O)Cl)cc1  $\xrightarrow[1.2. \text{ S: EtOH}, \text{ S: Benzene}]{1.1. \text{ R: LiAlH}_4, \text{ S: THF}, 3 \text{ h, reflux}}$  Cc1c(C)c(C)c(S)cc1

79%

NOTE: analogs prep'd. similarly,  
Reactants: 1, Reagents: 1, Solvents: 3,  
Steps: 1, Stages: 2

Reactions

- References
- Substance Detail
- Commercial Sources**
- Regulatory Information
- Explore by Chemical Structure
- Explore Reactions

Print catalog information, or export it to Microsoft<sup>®</sup> Excel<sup>®</sup>.

Reaction Structure substructure > reactions (42) > reaction 12 (of 42) > commercial sources (29)

### Commercial Sources

29 Commercial Sources 0 Selected Keep Selected Remove Selected [Print](#) [Export](#)

This chemical supplier information is provided on an "as is" basis. Please consult the suppliers for current information regarding pricing, regional availability, available quantities, purities, etc. THERE ARE NO WARRANTIES OF ANY KIND, EITHER EXPRESSED OR IMPLIED. ACS is not liable for any loss of profit, goodwill or any other damages arising out of the use of this information.

Select All Deselect All Sort by: Catalog Name [Answers per Page \[20\]](#) 1 2

- 1. **3B Scientific Corporation Product List**  
Company Name: 3B Scientific Corporation  
Order Number: 3B3-019959, Quantity: 25g  
1541-10-2 2,4,6-Trimethylthiophenol  
[Link](#)
- 2. **ABCR Product List**  
Company Name: ABCR GmbH KG  
Order Number: AB147301, Quantity: 25g  
1541-10-2 2,4,6-Trimethylthiophenol  
[Link](#)
- 3. **ACC Corp. Chemical Comp**  
Company Name: American Cust  
Order Number: CHMOD19509, Quantity: 25g  
1541-10-2 2,4,6-Trimethylbenzene  
[Link](#)
- 4. **AKos Screening Library**  
Company Name: Akos Consulting  
Order Number: AKE-PB5710899, Quantity: 25g  
1541-10-2 Benzenethiol, 2,4,6-trimethyl-  
[Link](#)

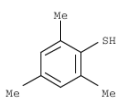
#### Commercial Source Detail

1. **3B Scientific Corporation Product List**

8 Sep 2009

Order Number: 3B3-019959	CAS Registry Number: 1541-10-2
Quantity: 25g	Price: \$570
2,4,6-Trimethylthiophenol	

**3B Scientific Corporation**  
1840 Industrial Drive, Suite 160  
Libertyville, IL, 60048  
USA  
Phone: 847-281-9822  
Fax: 847-281-9855  
Email: sales@3bsc.com  
Web: http://www.3bsc.com



If purchasing the final product is not an option, you can investigate purchasing the starting material. Or, you can locate potentially better or shorter pathways for synthesizing it.

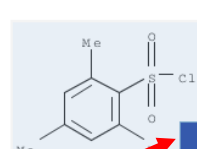
Note: You can repeat these steps until you find starting materials that can be easily obtained or made.

Reaction Structure substructure > reactions (42) > reaction 12 (of 42)

### Reaction Detail

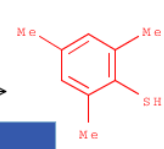
[Get Reference Detail](#) [Get Full Text](#) [Get Similar Reactions](#) [Link](#) [Save](#) [Print](#) [Export](#)

12.



1.1 R: LiAlH<sub>4</sub>, S: THF, 3 h, reflux

1.2 S: EtOH, S: Benzene



7.9 %

Reactions	Product
References	Reactant
Substance Detail	Reagent
Commercial Sources	Reactant or Reagent
Regulatory Information	Catalyst
Explore by Chemical Structure	Solvent
Explore Reactions	Any role

NOTE: analogs p  
Reactants  
Steps: 1,

For the starting material above, SciFinder locates six synthesis reactions.

Review the reactions, and save or print reactions of interest.

Reactions [Get References](#)

6 Reactions 0 Selected Keep Selected Remove Selected [Save](#) [Print](#) [Export](#)

Select All Deselect All Sort by: Accession Number [Answers per Page \[15\]](#)

Display:

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

NOTE: ClSO<sub>3</sub>H, -10 C to 0 C, 60 C to r.t., Condensation, Sulphonation, Reactants: 1, Reagents: 1, Steps: 1, Stages: 1

Mesitylenesulfonylhydrazine, and (1a,2a,6b)-2,6-Dimethylcyclohexanecarbonitrile and (1a,2b,6a)-2,6-Dimethylcyclohexanecarbonitrile as a Racemic Mixture  
By Reid, Jack R., et al  
From Organic Syntheses, 74, No pp. given; 1997

2. [Reaction Detail](#) [Link](#) [Similar Reactions](#)

R: Cyanuric trichloride, C: 18-Crown-6, S: Me<sub>2</sub>CO, 20 h, reflux

94%

**SciFinder helps you quickly and effectively identify candidates, find commercial suppliers, and explore synthetic pathways.**

## Example 4. Starting with a functional group transformation

Functional group searching offers an effective way to quickly explore a single broadly defined reaction type and then compare and evaluate retrieved reactions for criteria such as yields, conditions and types, characteristics, and convenience of the reagents used. You can even combine functional groups and structures in the same reaction search.

Use this approach when the key requirement is to assess the reactivity of a particular functional group. Apply the appropriate search limits and use SciFinder's automatic analysis to focus the reaction answer set.

### Find “greener” approaches for reducing amides to amines.

**Background:** In the pharmaceutical industry, many drugs and drug candidates contain basic nitrogen atoms. A common approach to synthesizing amines is the reduction of amides with hydride reagents such as lithium aluminum hydride and diisobutylaluminum hydride (DIBAL). However, in an industrial setting, use of these types of reagents may pose problems of scalability and disposal. Functional group searching can help you locate potentially greener approaches for converting amides to amines, possibly through use of catalysts with acceptable conditions of temperature and pressure or via biotransformations.

Draw the functional group transformation.

The screenshot displays the 'Reaction editor' window. The main drawing area shows a reaction scheme: 'Amide reactant/reagent' on the left, an arrow pointing to 'AMINES product' on the right. A 'Functional Groups' dialog box is open, with 'amide' entered in the search field. The list of results includes 'Alkyl Halide', 'pi-Alkyne', 'Alkyne', 'ALKYNES', 'Allene', 'pi-Allyl', 'Allyl Alcohol', 'Allyl Halide', and 'Amide'. The 'Amide' entry is selected, and its structure is shown as  $O=C-N$ . Below the structure, it says 'See class term: CARBOXY DERIVATIVES'. The 'Drawing Editor' panel on the right has 'Reaction' selected. The 'Get reactions where the structure(s) are:' panel has 'Substructures of more complex structures' selected. A red arrow points to the 'Amide' entry in the 'Functional Groups' list, and another red arrow points to the 'Cancel' button in the 'Drawing Editor' panel.

Limit the retrievals to a maximum of two steps and selected reaction classifications.

Explore Reactions

Reaction Structure Reaction Structure

Amide reactant → AMINES product

Click image to change structure or view detail

Search type:  Allow variability only as specified  Substructure

Solvents  Select Solvents

Number of Steps: 1-2  
Examples: 1, 1-2, 1-, -2

Classification(s):  Biotransformation  Electrochemical  Radiochemical  
 Catalyzed  Gas-phase  Regioselective  
 Chemoselective  Non-catalyzed  Stereoselective  
 Combinatorial  Photochemical

Use SciFinder's analysis of the reactions by catalyst to view only reactions that involve aminoacylase in the conversion of an amide to an amine.

3862. Reaction Detail [Link](#)

Reaction scheme showing the conversion of an amide to an amine.

1.1 R:Ac<sub>2</sub>O, S:H<sub>2</sub>O, 6 h, 60°C; 16 h, 60°C; 60°C → rt  
 1.2 R:HCl, S:H<sub>2</sub>O, pH 3  
 2.1 R:NaOH, C:Aminoacylase, C:CoCl<sub>2</sub>, S:H<sub>2</sub>O, rt, pH 7.8; rt → 38.5°C; 7 h, 38.5°C;  
 38.5°C → rt  
 2.2 R:Ac<sub>2</sub>O, S:H<sub>2</sub>O, 6 h, 60°C; 16 h, 60°C; 60°C → rt  
 2.3 R:HCl, S:H<sub>2</sub>O, pH 3

Aminoacylase 316

Efficient Synthesis of (S)-2-(Cyclopentylloxycarbonyl)-amino-8-nonenic Acid: Key Building Block for BILN 2061, an HCV NS3 Protease Inhibitor  
 By Wang, Xiao-Jun et al  
 From Organic Process Research & Development, 11(1), 60-63; 2007

When you find reactions of interest, view the Reaction Detail to investigate synthetic pathways and substance and commercial information.

Review references and request full text for interesting patents and journals.

Finally, save or print the relevant reference, substance, reaction, and commercial information.

Reaction Detail [Get Reference Detail](#) [Get Full Text](#)

3862.

Multi-Step Reaction: Step 1 (of 2)

Reaction scheme showing the conversion of an amide to an amine.

1.1 R:Ac<sub>2</sub>O, S:H<sub>2</sub>O, 6 h, 60°C; 16 h, 60°C; 60°C → rt  
 1.2 R:HCl, S:H<sub>2</sub>O, pH 3

Aminoacylase 316

Efficient Synthesis of (S)-2-(Cyclopentylloxycarbonyl)-amino-8-nonenic Acid: Key Building Block for BILN 2061, an HCV NS3 Protease Inhibitor  
 Wang, Xiao-Jun; Zhang, Li; Smith-Keenan, Lana L.; Houpis, Ioannis N.; Farina, Vittorio  
 Organic Process Research & Development  
 Volume 11  
 Issue 1  
 Pages 60-63  
 Journal  
 2007

Company/Organization  
 Department of Chemical Development  
 Boehringer Ingelheim Pharmaceuticals Inc.  
 Ridgefield, USA 06877

Number of Steps  
 2

**Functional group searching in SciFinder is a convenient and powerful way to access chemical synthesis information.**

## Example 5. Limiting by solvents, and getting similar reactions

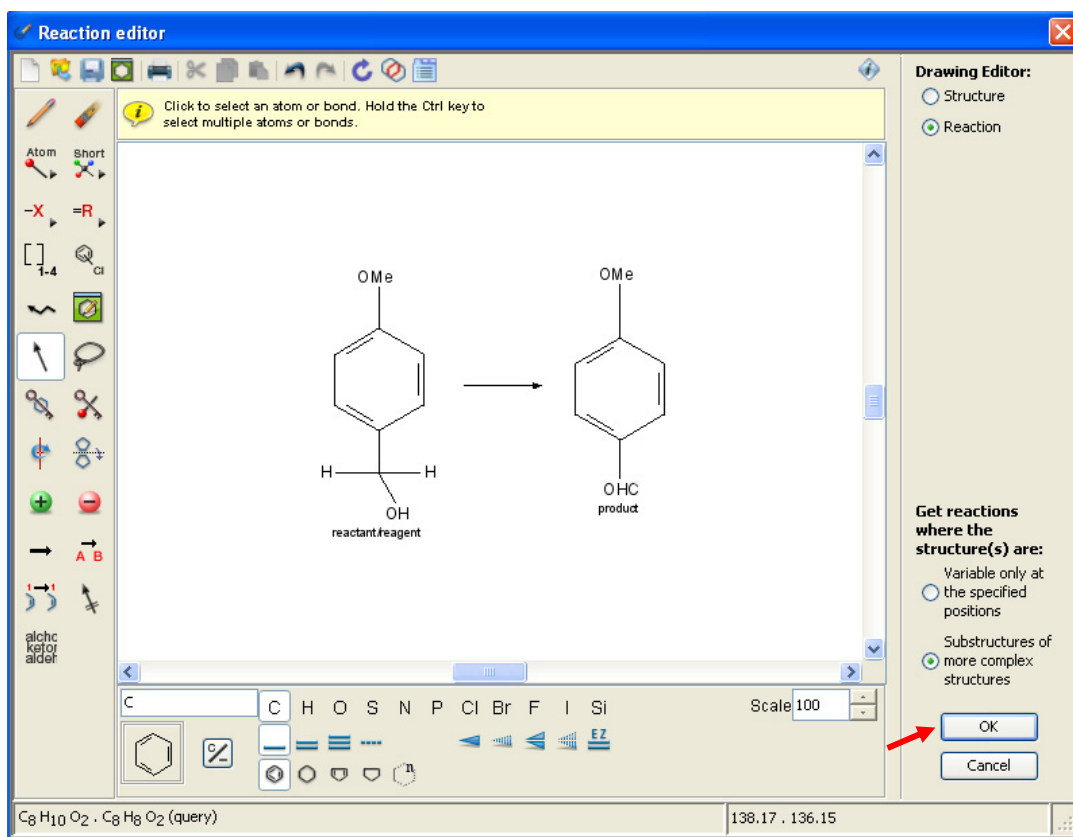
Use these approaches when you want to:

- Limit your reaction search by one or more solvents
- Find reactions similar to those within your focused search

Find “greener” approaches for oxidizing alcohols.

**Background:** Oxidation of alcohols to aldehydes or acids is an important laboratory and industrial process. However, the conversion is often carried out using stoichiometric amounts of oxidizing agents which can lead to problems of unwanted side products and other environmental concerns. Recent research has indicated that solvents such as ionic liquids show promise in enabling more environmentally friendly catalytic oxidations.

Draw your reaction search.



Limit the retrievals to catalyzed reactions using ionic liquids as solvents.

**Note:** Click the double chevron in the Solvents area to access the Solvent Hierarchy list and select your solvents.

To find reactions with structural characteristics similar to those of a particular reaction, click **Similar Reactions** (on the answer set list) or **Get Similar Reactions** (on the Reaction Detail).

Review references and request full text for interesting patents and journals.

Finally, save or print the relevant reference, substance, reaction, and commercial information.

**Limiting by solvents is an effective way to focus your SciFinder search on the appropriate solvents for your reaction. Getting similar reactions allows you to expand within your focused search.**

## **Conclusion**

SciFinder makes it easy to locate chemical synthesis information in a variety of ways, depending on your needs. It then lets you explore synthetic pathways as well as quickly and easily navigate among reference, substance, reaction, and commercial source information. This paper offers some insights into the large and comprehensive collection of chemical synthesis information and the powerful and sophisticated search and retrieval tools available in SciFinder.

SciFinder can help increase the overall effectiveness of your searching, as well as your accuracy, efficiency, and productivity. It helps organizations overcome today's challenges to gain a competitive edge, and it is an effective tool for accessing important information for teaching and academic research.

SciFinder is an essential part of the chemical synthesis research process.

## **Additional resources**

For more information about SciFinder, visit [www.cas.org](http://www.cas.org) or contact [CAS Customer Care](#) for a SciFinder brochure.

### **Acknowledgement**

CAS thanks members of the CAS Academic Advisory Committee for assistance and review of this special focus on chemical synthesis information in SciFinder.



For more information, contact **CAS Customer Care**:

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614-447-3700 (worldwide)  
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Internet: [www.cas.org](http://www.cas.org)

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