

A background image of a molecular model with spheres and connecting rods, overlaid on a blue gradient.

# An Introduction to SciFinder®

## The Chemical Research Tool for Scientists

Yvonne Pope

Regional Marketing Manager

CAS



A division of the American Chemical Society

[www.cas.org](http://www.cas.org)

# Today's discussion

## SciFinder

- provides access to the world's authority for chemical information
- offers synthetic researchers answers to their reaction questions
- speeds discovery by providing a sophisticated suite of analysis and research tools

# CAS is a division of the American Chemical Society

## ACS Vision

Improving people's  
lives through the  
transforming power  
of chemistry



# CAS supports the mission of the ACS

## ACS Mission

To advance the broader chemistry enterprise and its practitioners for the benefit of Earth and its people.

## CAS Commitment

To support the ACS mission by providing secure access to high-quality, comprehensive chemical information.



# CAS Databases

“Being able to rapidly search for important chemical information while an idea is fresh in your mind is almost priceless. CAS databases streamline the investigative process – allowing you to take an idea and rapidly find the important and necessary information before you forget about the idea or it loses its excitement. That really is invaluable.”

Dr. Robert H. Grubbs  
Nobel Laureate  
Victor and Elizabeth Atkins Professor of Chemistry  
California Institute of Technology

# CAS is the world leader in providing chemical information...

## CAS REGISTRY<sup>SM</sup>

>53M organic and inorganic substances

>61M sequences

Updated daily with thousands of new substances

Substances reported comprehensively in literature back to 1957

Information pertaining to these substances has been enriched with experimental and predicted property data with more than 2.8 billion property values, data tags, and spectra

## CASREACT<sup>®</sup>

>24M single- and multi-step reactions

>13.6M synthetic preparations

Extracted from patents and journal articles

Updated weekly (30K-50K per week)

Reactions back to 1840

Reaction conditions starting in 2003

## CAS Databases

## CAplus<sup>SM</sup>

>32M patent and journal article references

>10K major scientific journals covered

Patents from 60 patent offices

Updated daily (~3K daily)

Links to more than 360 publishers and 3 patent offices

Literature back to early 1800s

Cited articles from 1997 onward, currently more than 259M citations

## CHEMCATS<sup>®</sup>

>39M commercially available compounds

>1,000 suppliers

>1,100 chemical catalogs

Updated when new or revised catalogs are available

Contact/ordering information including quantity and pricing (when available)

## Types of reactions in CASREACT

- **Single-step reactions**
  - Single-step multi-stage reactions
- **Multi-step reactions**
- **Stereo-specific syntheses**
- **Biologically mediated reactions**
- **Prophetic reactions from patents**

SciFinder

Draw or change atoms or bonds.

reactant/reagent

product

alchc  
ketor  
alder

Scale 125

$C_4H_6O \cdot C_5H_8O_2$  (query)

70.09 . 100.12

**Drawing Editor:**

- Structure
- Reaction

**Get reactions where the structure(s) are:**

- Variable only at the specified positions
- Substructures of more complex structures

OK

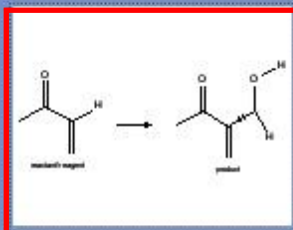
Cancel

## Explore Reactions

Reaction Structure

Reaction Structure ⓘ

Search



Click image to change structure or view detail

Search type: ⓘ  Allow variability only as specified  
 Substructure

Solvents ⓘ

Select Solvents **NEW**

Number of Steps ⓘ

Examples: 1, 1-3, 1-, -3

Classification(s) ⓘ

- |  |  |  |
|--|--|--|
| <input type="checkbox"/> Biotransformation | <input type="checkbox"/> Electrochemical | <input type="checkbox"/> Radiochemical   |
| <input type="checkbox"/> Catalyzed         | <input type="checkbox"/> Gas-phase       | <input type="checkbox"/> Regioselective  |
| <input type="checkbox"/> Chemoselective    | <input type="checkbox"/> Non-catalyzed   | <input type="checkbox"/> Stereoselective |
| <input type="checkbox"/> Combinatorial     | <input type="checkbox"/> Photochemical   |  |

Source(s)

- Any source  
 Patents only  
 Sources other than patents

Publication Year(s) ⓘ

Examples: 1995, 1995 - 1999, 1995-, -1995

## Reactions

Get  
References

970 Reactions

0 Selected

Keep Selected

Remove Selected

Save

Print

Export

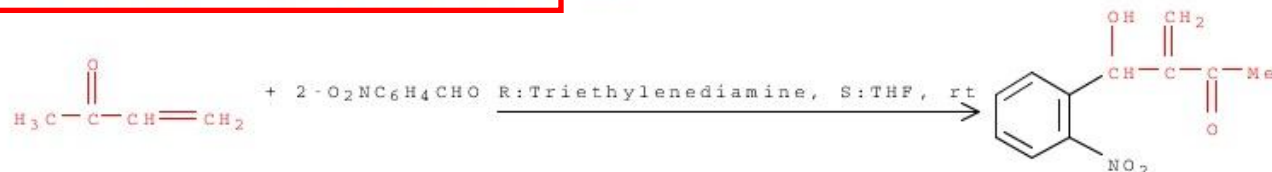
Select All Deselect All

Sort by: Accession Number

Answers per Page [15]

1 2 3 4 5 6 ... 65

Display:

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

Novel synthesis of indolylquinoline derivatives via the C-alkylation of Baylis-Hillman adducts

By Ramesh, Chintakunta et al  
From Tetrahedron Letters, 50(28), 4037-4041; 2009 2. Reaction Detail [Link](#) [Similar Reactions](#) **NEW**

Analysis

Refine

Analyze by:

Catalyst

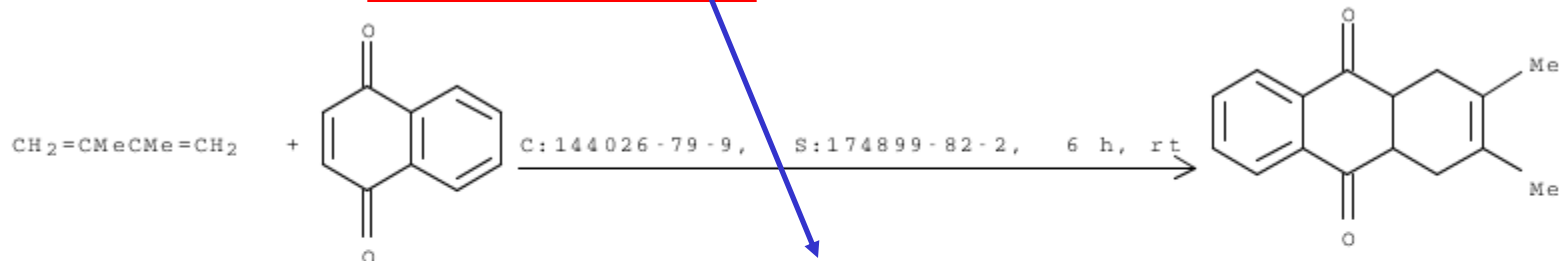
Click bar to view only those reactions within the current answer set

(S)-Proline	121
Triethylenediamine	80
1H-Imidazole	58
19529-00-1	33
4-PyNMe <sub>2</sub>	33
18284-36-1	30
PPh <sub>3</sub>	26
93675-38-8	21
51-35-4	19
618436-75-2	19

Show More

# Get similar reactions to create a new answer set

3. Reaction Detail [Link](#) **Similar Reactions** NEW



NOTE: stereoselective, Diels-Alder  
 lower yield, green chem.-rec  
 Reactants: 2, Catalysts: 1,  
 Steps: 1, Stages: 1

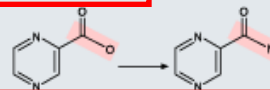
## Get Similar Reactions

### Retrieve similar reactions from:

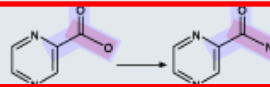
- All reactions
- Current answer set

### Include this level of similarity:

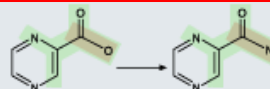
- Broad - Reaction centers only (20411)



- Medium - Reaction centers plus adjacent atoms and bonds (754)



- Narrow - Reaction centers plus extended atoms and bonds (97)



Get Reactions

Cancel

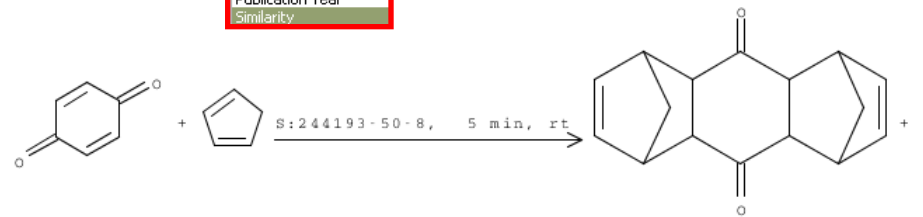
# Sort reaction answer sets to display relevant reactions

Reactions [Get References](#)

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

Select All Deselect All | Sort by: **Similarity** [Accession Number](#) [Number of Steps](#) [Percent Yield](#) [Publication Year](#) [Similarity](#) [Answers per Page \[15\]](#) [1](#) [2](#) [3](#) [4](#) [5](#) [6](#) ... [12](#) ▶

1. Reaction Detail [Go](#) [L](#) [Reactions](#) **NEW** [Display:](#) [▲](#) [▼](#)



S:244193-50-8, 5 min, rt

98% (7:93)

Relative stereochemistry.  
98% (7:93)

NOTE: stereoselective, ultrasound, 40 kHz, alternative preparation shown, without sonication lower yields,  
Reactants: 2, Solvents: 1,  
Steps: 1, Stages: 1

Sonochemical cycloadditions in ionic liquids. Lessons from model cases involving common dienes and carbonyl dienophiles  
By Bravo, Jose Luis et al  
From Ultrasonics Sonochemistry, 13(5), 408-414; 2006

# Limit a solvent before a search

Explore Reactions

Reaction Structure Reaction Structure Search

CC(=C)C O=C1C=CC(=O)C=C1  
Click image to change structure or view detail

Search type:  Allow variability only as specified  
 Substructure

Solvents Select Solvents NEW

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

Classification(s)

<input type="checkbox"/> Biotransformation	<input type="checkbox"/> Electrochemical	<input type="checkbox"/> Radiochemical
<input type="checkbox"/> Catalyzed	<input type="checkbox"/> Gas-phase	<input type="checkbox"/> Regioselective
<input type="checkbox"/> Chemoselective	<input type="checkbox"/> Non-catalyzed	<input type="checkbox"/> Stereoselective
<input type="checkbox"/> Combinatorial	<input type="checkbox"/> Photochemical	

Source(s)

Any source  
 Patents only  
 Sources other than patents

Publication Year(s)   
Examples: 1995, 1995 - 1999, 1995 -, - 1995

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## Limit by solvents using the Solvent Hierarchy

The screenshot shows a software interface titled "Solvent Hierarchy". At the top left, there is a "Close" button with a "NEW" badge. Below the title, there is a link "[View solvent list]" which is highlighted with a red rectangle. Underneath, there are three buttons: "0 Selected", "Select All", and "Deselect All". The main area contains a hierarchical list of solvent categories, each with a checkbox and a collapse/expand icon:

- Ionic liquids
  - Imidazolium derivatives
  - Nonimidazolium derivatives
- Nonpolar solvents
  - Aliphatic compounds
  - Aromatic compounds
  - Silanes
- Polar solvents
  - Polar solvents, aprotic
  - Polar solvents, protic
- Supercritical fluids

At the bottom, there is a "Find:" search box, a "Next" button with a downward arrow, and a "Previous" button with an upward arrow.

## Limit by solvents using the Solvent List

**Solvent List** Display:  all solvents  
 selected solvents

[\[View solvent hierarchy\]](#)

0 Selected [Select All](#) [Deselect All](#)

- 4H-1,2,4-Triazolium, 1-heptyl-4-(4-sulfobutyl)-, 1,1,1-trifluoromethanesulfonate (1:1)
- 4H-1,2,4-Triazolium, 4-butyl-1-[(1-butyl-1H-imidazolium-3-yl)methyl]-, iodide (1:2)
- 5-Ethyl-2-methylpyridine
- 5-Nonanone
- 5-tert-Butyl-m-xylene
- 6-Amino-1-hexanol
- 8-Ethyl-1,8-diazabicyclo[5.4.0]-7-undecenium trifluoromethanesulfonate
- Acetaldehyde
- Acetamide
- Acetic acid
- Acetic acid-d
- Acetic acid-d4
- Acetic anhydride
- Acetic-d3 acid
- Acetic-d3 acid, methyl-d3 ester

Find:  [↓Next](#) [↑Previous](#)



## Case Study: Patents involving Suzuki Cross-coupling Chemistry

- I am interested in intellectual property pertaining to Suzuki Cross-Coupling Chemistry
- “Difficult” to solve through structure query in any reaction database!
- Coverage of patents in reaction database is important
- One solution is to search text information in a database that is directly linked to a reaction database

## SciFinder's Explore by Research Topic is a good solution to the problem

The image shows a screenshot of the SciFinder web interface. The top navigation bar includes the SciFinder logo and three main explore options: 'Explore References', 'Explore Substances', and 'Explore Reactions'. Below this, a user is logged in as 'William A Weida'. The main content area is titled 'Explore References' and features a search bar with the text 'SUZUKI'. A dropdown menu on the left lists various search criteria: 'Research Topic', 'Author Name', 'Company Name', 'Document Identifier', 'Journal', 'Patent', and 'Tags'. The 'Research Topic' dropdown is selected, showing a list of examples including 'The effect of antibiotic residues on dairy products' and 'Photocyanation of aromatic compounds'. Below the search bar, there are buttons for 'Get Substances', 'Get Reactions', 'Get Cited', 'Get Citing', 'Get Full Text', and 'Combine Answer Sets'. The results section shows '12340 References' and includes a table with columns for '0 Selected', 'Keep Selected', 'Remove Selected', 'Remove Duplicates', 'Add Tags', 'Save', 'Print', and 'Export'. The first result is titled '1. Synthesis of antimicrotubule dibenzoxepines' and includes a brief abstract and a list of authors and journal information.

SciFinder®

Welcome | Sign Out

Explore References Explore Substances Explore Reactions

Explore References

Research Topic Research Topic  Search

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

Company Name

Document Identifier

Journal

Patent

Tags

SciFinder®

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Create Keep Me Posted Research Topic "SUZUKI" > references (12340)

References Get Substances Get Reactions Get Cited Get Citing Get Full Text Combine Answer Sets

12340 References 0 Selected Keep Selected Remove Selected Remove Duplicates Add Tags Save Print Export

Select All Deselect All Sort by: Accession Number Answers per Page [20] 1 2 3 4 5 6 ... 617 Display: [icon]

1. **Synthesis of antimicrotubule dibenzoxepines**  
By Colombel, Virginie; Joncour, Agnes; Thoret, Sylviane; Dubois, Joelle; Bignon, Jerome; Wdzieczak-Bakala, Joanna; Baudoin, Olivier  
From Tetrahedron Letters (2010), 51(23), 3127-3129. Language: English, Database: CAPLUS  
New dibenzoxepines 5a-i bearing various substituents on B- and C-rings were synthesized in a straightforward manner using a **Suzuki**-Miyaura coupling, a Grignard addn., and a cyclodehydration as key steps. The antimicrotubule activity of all analogs was evaluated and compared to ref. compds. Compds. 5d-f displayed the highest activity for this type of allocolchicinoids to date.  
Substances Reactions Citing Full Text Link 0 Comments 0 Tags

2. **Total synthesis of graphis lactone G**

## References for patents are analyzed to focus on IP in this area

References Get Substances Get Reactions Get Cited Get Citing Get Full Text Combine Answer Sets

12340 References 0 Selected Keep Selected Remove Selected Remove Duplicates Add Tags Save Print Export

851 references with the Document Types **Patent** are displayed Keep Analysis Clear Analysis

Select All Deselect All Sort by: Accession Number Answers per Page [20] 1 2 3 4 5 6 ... 43 Display:

34. **Preparation of pentafluorothiobenzenes**  
 By Nishino, Shigeyoshi; Shima, Hidetaka; Oda, Hiroyuki; Omata, Yoji  
 From Ger. Offen. (2010) DE 102009045366 A1 20100422. Language: German, Database: CAPLUS  
 Title compds. I [R1, R2, R3, R4 = H, F; R5 = alkyl with provisios; Z = CO, CS, CH2, CF2] were prepd. For example, Pd(II) mediated **Suzuki** coupling of II and III afforded pentafluorothiobenzene IV.  
 Substances Reactions Citing Full Text Link 0 Comments 0 Tags

35. **Diaryl and heteroaryl butadiynes, substituted with boronate and trifluoroborate functional groups as reagents for Suzuki coupling reaction in preparation of electrooptical materials**  
 By Richter, Andreas M.; Herm, Marc; Schoenewerk, Jens  
 From Ger. Offen. (2010) DE 102008052315 A1 20100422. Language: German, Database: CAPLUS  
 Diarylbutadiynes, substituted by boronate, boronamide or trifluoroborate groups, (GR1)nAr1(G)C≡CC≡Ar2(G) (R2G)m [5, Ar1, Ar2 = (hetero)arylene; R1, R2 = H, C1-40 alkylene, oxyalkylene, C5-40 arylene, halo, CN, NO2, sulfonyl; G = borono, (cyclic) boronic ester, boronamide, oxa-, azaborolanyl, borate, preferably, G = B(OH)2, dialkoxyboryl, substituted 1,3,2-dioxaborolan-2-yl, 1,3,2-dioxaborinan-2-yl, catecholboryl, 1,3,2-benzoxazaborolan-2-yl, 1,3,2-benzodiazaborolan-2-yl, BF3-M+, where M = alkali metal cation, tetraalkylammonium, tetraalkylphosphonium], useful as reagents for **Suzuki** coupling re...  
 Substances Reactions Citing Full Text Link 0 Comments 0 Tags

36. **Aromatic and heteroaromatic poly(trifluoroborate) Suzuki coupling synthons for production of**

**Analysis** Refine

Analyze by:

Document Type

*Click bar to view only those references within the current answer set*

Journal	10471
Article	2187
JOURNAL ARTICLE	2187
RESEARCH SUPPORT NONUS GOVT	1003
Conference	920
<b>Patent</b>	<b>851</b>
Meeting Abstract	799
General Review	539
Computer Optical Disk	404

# Patented Suzuki chemistry technology areas are analyzed

SciFinder®

Welcome William A Weida | Sign Out

Explore References | Explore Substances | Explore Reactions

Saved Answer Sets | Help  
Keep Me Posted Results | History  
My Connections | Preferences

Create Keep Me Posted | Research Topic "suzuki" > references (12340) > keep analysis "Document Type" (851)

References | Get Substances | Get Reactions | Get Cited | Get Citing | Get Full Text | Combine Answer Sets

851 References | 0 Selected | Keep Selected | Remove Selected | Remove Duplicates | Add Tags | Save | Print | Export

351 references with the Index Terms **Suzuki coupling reaction** are displayed | Keep Analysis | Clear Analysis

Select All | Deselect All | Sort by: Accession Number | Answers per Page [20] | 1 2 3 4 5 6 ... 18 | Display: [Icons]

1. Preparation of pentafluorothiobenzenes  
By Nishino, Shigeyoshi; Shima, Hidetaka; Oda, Hiroyuki; Omata, Yoji  
From Ger. Offen. (2010), DE 102009045366 A1 20100422. Language: German, Database: CAPLUS  
Title compds. I [R1, R2, R3, R4 = H, F; R5 = alkyl with provisos; Z = CO, CS, CH2, CF2] were prepd. For example, Pd (II) mediated **Suzuki** coupling of II and III afforded pentafluorothiobenzene IV.  
Substances Reactions Citing Full Text Link 0 Comments 0 Tags

2. Diaryl and heteroaryl butadiynes, substituted with boronate and trifluoroborate functional groups as reagents for **Suzuki** coupling reaction in preparation of electrooptical materials  
By Richter, Andreas M.; Herm, Marc; Schoenewerk, Jens  
From Ger. Offen. (2010), DE 102008052315 A1 20100422. Language: German, Database: CAPLUS  
Diarylbutadiynes, substituted by boronate, boronamide or trifluoroborate groups, (GR1)nAr1(G)C≡CC=CAr2(G)(R2G)m [5, Ar1, Ar2 = (hetero)arylene; R1, R2 = H, C1-40 alkylene, oxyalkylene, C5-40 arylene, halo, CN, NO2, sulfonyl; G = borono, (cyclic) boronic ester, boronamide, oxa-, azaborolanyl, borate, preferably, G = B(OH)2, dialkoxyboryl, substituted 1,3,2-dioxaborolan-2-yl, 1,3,2-dioxaborinan-2-yl, catecholboryl, 1,3,2-benzoxazaborolan-2-yl, 1,3,2-benzodiazaborolan-2-yl, BF3-M+, where M = alkali metal cation, tetraalkylammonium, tetraalkylphosphonium], useful as reagents for **Suzuki** coupling re...  
Substances Reactions Citing Full Text Link 0 Comments 0 Tags

**Analysis** | Refine

Analyze by: Index Term

Click bar to view only those references within the current answer set

<b>Suzuki coupling reaction</b>	351
Human	216
Suzuki coupling reaction catalysts	175
Antitumor agents	148
Neoplasm	129
Inflammation	123
Anti-inflammatory agents	108
Disease, animal	99

## Find out what Suzuki reactions are reported in these patents

SciFinder®

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Create Keep Me Posted Research Topic "suzuki" > references (12340) > keep analysis "Document Type" (851) > keep analysis "Index Term" (351)

References **Get Substances** **Get Reactions** Get Cited Get Citing Get Full Text Combine Answer Sets

351 References 0 Selected Keep Selected Remove Selected Remove Duplicates Add Tags Save Print Export

Select All Deselect All Sort by: Accession Number

1. Preparation of  
By Nishino, Shigeyoshi  
From Ger. Offen. (2010)  
Title compds. I  
(II) mediated Su  
Substances

2. Diaryl and hetero  
for Suzuki coupl  
By Richter, Andreas M.,  
From Ger. Offen. (2010)  
Diarylbutadiynes,  
[5, Ar1, Ar2 = (borono, (cyclic)  
substituted 1,3  
benzodiazaborola  
reagents for Suz  
Substances

SciFinder®

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Create Keep Me Posted Research Topic "SUZUKI" > references (12340) > get reactions (2225)

Reactions **Get References** Find Additional Reactions NEW Combine Answer Sets

2225 Reactions 0 Selected Keep Selected Remove Selected Save Print Export

262 reactions with the Document Types Patent are displayed Keep Analysis Clear Analysis

Select All Deselect All Sort by: Entry Order Answers per Page [15] 1 2 3 4 5 6 ... 18 Display: [Icons]

671. Reaction Detail Link Similar Reactions

**But some reactions from these patents are not Suzuki**

1.1 R: SO<sub>3</sub>, R: H<sub>2</sub>SO<sub>4</sub>, S: CH<sub>2</sub>Cl<sub>2</sub>, rt → 0°C; 0°C; 0°C → rt; 24 h, rt; rt → 0°C

1.2 R: NaOH, S: H<sub>2</sub>O, cooled, pH 7

HO<sub>3</sub>S Pr-i

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# Actual Suzuki reactions can be isolated with the Refine tool

**Analysis**      **Refine**

**Refine by:** ⓘ

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

**Reaction Structure:**

B  
any role

Click image to change structure  
view details

Search type: **Substructure**

**Refine**

**Reaction editor** [X]

Draw or change atoms or bonds.      Shortcut Keys

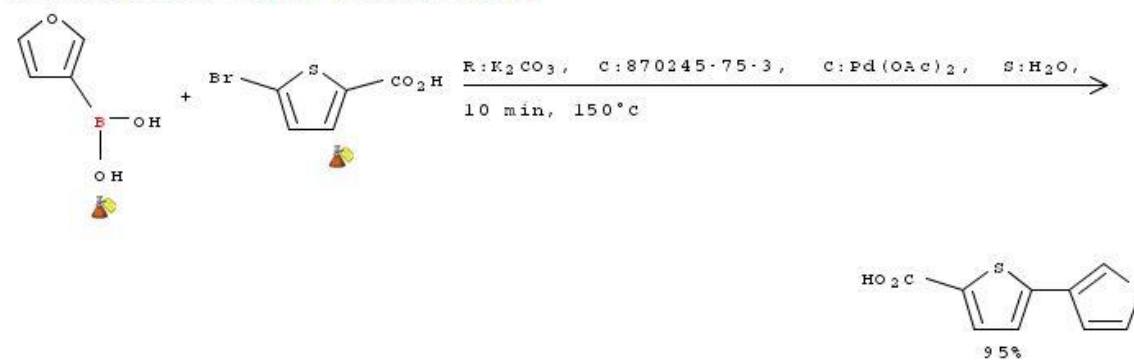
**Reactions**      [Get References](#)      [Combine Answer Sets](#)

1541 Reactions      0 Selected      [Keep Selected](#)      [Remove Selected](#)      [Save](#)

132 reactions with the Document Types **Patent** are displayed      [Keep Analysis](#)      [Clear Analysis](#)

[Select All](#)      [Deselect All](#)      Sort by: Entry Order      Answers per Page [15]      1 2 3 4

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



**NOTE:** microwave irradiation, Suzuki-Miyaura coupling,  
**Reactants:** 2, **Reagents:** 1, **Catalysts:** 2, **Solvents:** 1,  
**Steps:** 1, **Stages:** 1

Transition-metal-catalyzed carbon-nitrogen and carbon-carbon bond-forming reactions  
 By Buchwald, Stephen L. and Anderson, Kevin W.  
 From PCT Int. Appl., 2006074315, 13 Jul 2006

## Keyword searching can be an effective starting point for reactions with “difficult” chemistry

- Found over 12000 references mentioning Suzuki in the scientific literature
  - > 800 references from patents
- Found > 2000 reactions covered in these patents
- Isolated > 100 actual Suzuki reactions for review

## SciFinder is a valuable resource for locating reaction information

- **Timely** – reactions are added each week
- **Flexible** – reaction information is seamlessly integrated with reference and substance information
- **Comprehensive** – reaction coverage has expanded by addition of older reactions at the same time editorial scientists keep up with current literature

# SciFinder is the premier enterprise-wide research discovery tool used by scientists around the world



## Questions

