



## Reaction Searching Questions

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### Practice questions #1-3

1. What is the structure of Aleve? What is its CAS Registry Number?
2. What has been reported in the patent literature since 2000 regarding the Wittig reaction? How many references cite multiple reactions?
3. Locate reactions in which sulfides are converted to sulfones.



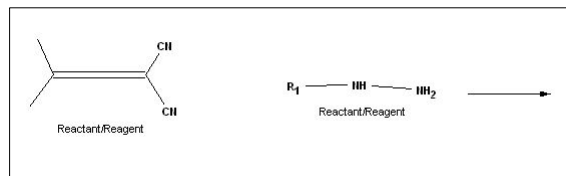
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## Practice question #4

- What type of products have been formed from the reaction of the following two starting materials?



R1 = May be a ring/chain except hydrogen



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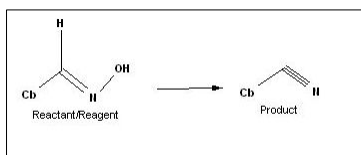
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## Practice question #5

- Locate reactions for carrying out the following transformation:



Restrict the results to single step reactions with yields greater than 60%

Utilize Zinc oxide (ZnO) and Acetyl Chloride (AcCl) as catalysts



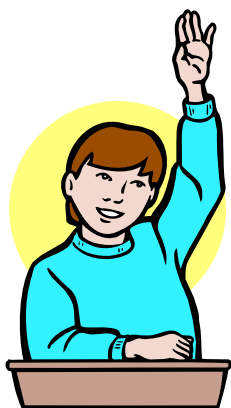
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## Practice question answers



**For the following questions:**  
Note searches were done on 1-4-08, due to the daily updating of SciFinder Scholar research results may vary when done in the future.



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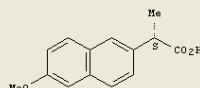
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## 1. What is the structure of Aleve? What is its CAS Registry Number?

Use Locate by Substance Identifier: Aleve

Registry Number: 26159-34-2

Absolute stereochemistry. Rotation (+).



Formula: C<sub>14</sub>H<sub>14</sub>O<sub>3</sub> · Na

CA Index Name: 2-Naphthaleneacetic acid, 6-methoxy- $\alpha$ -methyl-, sodium salt (1:1), ( $\alpha$ S)-

**Other Names:** 2-Naphthaleneacetic acid, 6-methoxy- $\alpha$ -methyl-, sodium salt, ( $\alpha$ S)- (9CI); 2-Naphthaleneacetic acid, 6-methoxy- $\alpha$ -methyl-, sodium salt, (S)-; 2-Naphthaleneacetic acid, 6-methoxy- $\alpha$ -methyl-, sodium salt, L-(-) (8CI); (2S)-2-(6-Methoxy-2-naphthyl)propanoic acid sodium salt, Aflaxen; Agilxen; Aleve; Anaprox; Anaprox DS; Anax; Apranax; Apraxin; Apronax; Axer; Daflofen; Duk-F; Flanax; Flanax Forte; Gynestrel; Lefaine; Licorax; Miranax; Naprelan; Naprogesic; Naprosyn sodium; Naproxen sodium; Narocin; Primaler; RS 3560; Sodium (+)-6-methoxy-2-naphthalenepropanoate; Sodium d-2-(6-methoxy-2-naphthyl)propionate; Sodium naprosyn; Sodium naproxen; Sutolin; Synflex; Uniflam; Xenobid



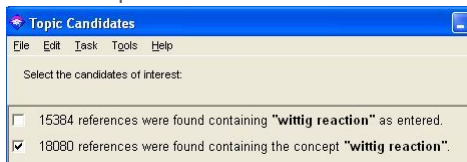
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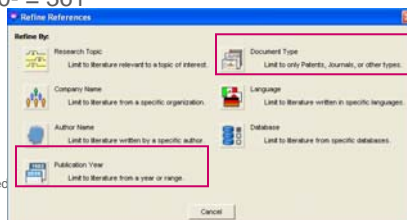
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## 2. What has been reported in the patent literature since 2000 regarding the Wittig reaction? How many related references cite multiple reactions?

- Explore Research Topic – wittig reaction
- Select Research Topic candidates for references containing concept = 18080



- Refine by Document Type: Patent = 2876
- Refine by Publication Year: 2000- = 361



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## What has been reported in the patent literature since 2000 regarding the Wittig reaction? How many related references cite multiple reactions?

- Click Get Related Information – select Reactions = 11634 reactions
- Click View – select One Reaction per reference = 171 references

SciFinder Scholar

File Edit View Task Tools Help

View

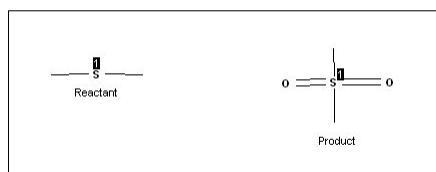
- Compact
- Standard
- Summary
- Full
- All Reactions
- One Reaction per Reference
- ✓ Show Reaction Substructure Highlighting
- Accession Number Order
- Title Order
- Year, Title Order
- Score Order
- ✓ Reverse Order

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### 3. Locate reactions in which sulfides are converted to sulfones

- Unable to use Functional Groups – too broad but search will run to completion
- Use Atom Mapping tool after drawing structures and assigning roles – see below
- Select variable only at specified positions, but no other filters
- Results = 62 reactions



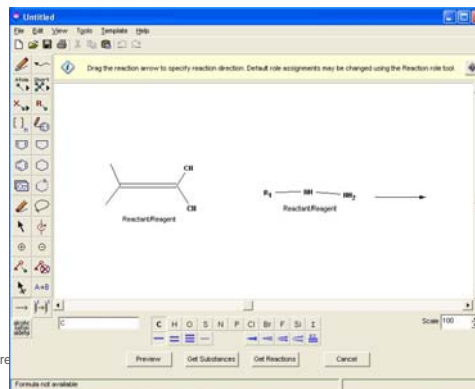
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### 4. What type of products have been formed from the reaction of the following two starting materials?

- Draw structures & click Get Reactions
- Select substructures and no other filters
- Results = 175 reactions

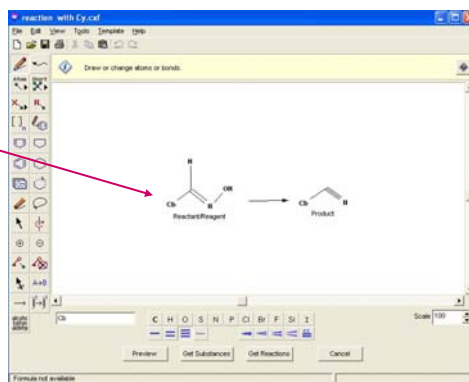


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## 5. Locate reactions for carrying out the following transformation and restrict the results to single step reactions with yields greater than 60% that use ZnO and AcCl as catalysts

- Draw the structure
- Use variables



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## Apply reaction search filters

- Apply filter: 1 reaction step
- Substructures feature
- Click OK
- Results = 851 reactions

Get Reactions

Get reactions where the structure(s) are:

variable only at the specified positions

substructures of more complex structures

Filters

Reaction steps: Only return reactions having this number or range of steps: 1

Reaction classification: Only return reactions of the following type(s):

Biotransformation  Non-catalyzed

Catalyzed  Photochemical

Chemoselective  Radiochemical

Combinatorial  Regioselective

Electrochemical  Stereoselective

Gas-phase

Patents: Only return reactions from these sources:

Patents

Sources other than patents

Publication year: Only return reactions published in this year or range of years:

OK Cancel



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# Refine Reaction by Product Yield

**Analyze or Refine**

Select One:

- Analyze  
Display histograms by Journal, Number of steps, Publication Year, etc.
- Refine**  
Narrow your answer set by Structure, Yield, Number of steps, Classifications, etc.

**Refine Reactions**

Refine by:

- Reaction Structure  
Limit results by structural information.
- Product Yield**  
Limit results by product yield.
- Number of Steps  
Limit results by number of steps.
- Reaction Classification  
Limit results by reaction classification.

Cancel

**Refine by Product Yield**

Please enter the minimum and maximum product yield values.

60 Minimum product yield.

100 Maximum product yield.

Include reactions that do not have yield data.

OK Back



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# Transformation with 60% yield results in 646 reactions

Still need to limit reactions by type of catalyst used.

Reaction 1: C1=CC=C(C=C1)C=C >> C1=CC=C(C=C1)C(=O)O  
C:344708-88-7, 2,0-Styrene, 1.0 h, 145°C  
NOTE: catalyst prepared and used, Reagents: 1, Catalysts: 1, Solvents: 1, Steps: 1, Stages: 1  
Angewandte Chemie International Edition, 46(21), 3922-3926, 2007  
CASREACT

Reaction 2: C1=CC=C(C=C1)C(=O)O >> C1=CC=C(C=C1)C(=O)O  
Reagents: 1, Reagents: 2, Solvents: 2, Steps: 1, Stages: 1  
Journal of Medicinal Chemistry, 50(11), 2672-2679, 2007  
CASREACT

Reaction 3: C1=CC=C(C=C1)C(=O)O >> C1=CC=C(C=C1)C(=O)O  
Reagents: 1, Solvents: 1, Steps: 1, Stages: 1  
Journal of Medicinal Chemistry, 50(10), 2468-2495, 2007  
CASREACT

Get References Analyze/Refine

Reaction 29-32 of 646



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## Limit reactions to those that use ZnO and AcCl as catalysts

- Select Analyze/Refine
- Analyze by Catalyst
- Check both ZnO and AcCl

**Analyze Reactions**

Analyze By:

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

Analyze only selected reactions

Analyze all reactions

Sort results alphabetically

Sort results by frequency

OK Cancel

**Catalyst Analysis**

Select the candidates of interest:

<input type="checkbox"/>	MgSO4	7
<input type="checkbox"/>	Montmorillonite	8
<input type="checkbox"/>	Na2SO4	7
<input type="checkbox"/>	p-MeC6H4SO3H	1
<input type="checkbox"/>	P2O5	4
<input type="checkbox"/>	Reactions not containing information for this analysis	459
<input type="checkbox"/>	SiO2	12
<input type="checkbox"/>	Zn	6
<input type="checkbox"/>	ZnCl2	1
<input checked="" type="checkbox"/>	ZnO	15

Get Reactions Back

Histogram Entries 30-39 of 39

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## 15 Reactions use ZnO and AcCl as catalysts

**Reaction 1:** 4-nitrobenzaldehyde  $\xrightarrow{\text{C:ZnO, C:AcCl, 20 h, 80}^\circ\text{C}}$  4-cyanoacetophenone (87%)

NOTE: no solvent, Reactants: 1, Catalysts: 2, Steps: 1, Stages: 1

Synthesis\_ (5)\_787-790\_2005 CASREACT

**Reaction 2:** 4-aminobenzaldehyde  $\xrightarrow{\text{C:ZnO, C:AcCl, 20 h, 80}^\circ\text{C}}$  4-aminobenzonitrile (90%)

NOTE: no solvent, Reactants: 1, Catalysts: 2, Steps: 1, Stages: 1

Synthesis\_ (5)\_787-790\_2005 CASREACT

**Reaction 3:** 2,4-dichlorobenzaldehyde  $\xrightarrow{\text{C:ZnO, C:AcCl, 10 h, 80}^\circ\text{C}}$  2,4-dichlorobenzonitrile (94%)

NOTE: no solvent, Reactants: 1, Catalysts: 2, Steps: 1, Stages: 1

Get References Analyze/Refine

Reactions 1-4 of 15

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