

# RxnFinder

## ChemInform Reaction Library online search

The screenshot displays the ChemInform RxnFinder web interface. At the top left is the ChemInform RxnFinder logo, and at the top right, it indicates the user is logged in as "Wiley Information Services" and shows the Wiley logo. The interface is divided into several sections:

- Navigation Tabs:** Query, Results, Details, and Selected Hits.
- Left Sidebar:** Contains "Query Fields", "Saved Queries", and "Query History" sections, each with a plus or minus icon, and a "clear history" button.
- Query Editor:** Features a dropdown menu set to "AND", a large empty text input area, and three buttons: "open structure editor", "structure library", and "upload structure".
- Search Options:** A list of radio buttons for "exact", "similarity", "substructure", and "transformation". The "substructure" option is selected. A checkbox for "highlight match" is checked. There is also a small "X" button.
- Submit Button:** A "submit query" button is located at the bottom right of the search options area.

## Search: Structure Search with Accelrys JDraw

The screenshot displays the Accelrys JDraw Molecule Editor window. The main workspace shows a chemical structure with a carbonyl group and a chiral center. Two context menus are open:

- Atom Property** menu (open over the carbonyl oxygen):
  - Atom symbol...
  - Charge...
  - Isotope
  - Valence...
  - Radical
  - Number of nonhydrogen substituents...
  - Prevent hydrogen substituents
  - Unsaturated bond to atom
  - Ring bonds to atom
    - As drawn
    - 0 (no rings)
    - 2 (isolated ring)
    - 3 ring bonds
    - 4 ring bonds
    - Off
  - Allow these atoms
  - Prohibit these atoms
  - Remove Properties
  - No Structure
  - About...
- Bond Property** menu (open over the C-O single bond):
  - Bond order
  - Stereobond
  - Query bond type
    - Any
    - Aromatic
    - Single or Double
    - Single or Aromatic
    - Double or Aromatic
  - Chain or ring bond
  - Remove properties
  - No Structure
  - About...

At the bottom of the window, there are buttons for 'reset' and 'clear', and a status bar with 'cancel' and 'transfer for query' options.

define atom or bond properties per right-click

ChemInform RxnFinder

Query Results

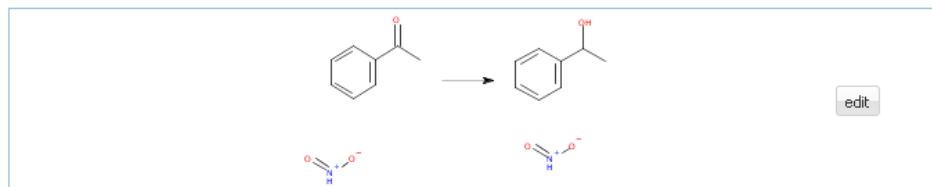
Query Fields

- Reaction
  - Structure
  - Enantiomeric Excess
  - Diastereomeric Excess
  - Yield
  - Temperature
  - Keyphrase
  - Green Chemistry
- Molecule
  - Structure
  - Name and Synonyms
  - Keyword
  - InChI
  - InChIKey
  - Formula
  - Molecular Weight
- Citation
  - Author
  - Journal
  - Title
  - Year

Saved Queries +  
 Query History +

## Search

by substructure



706 hits

refine query by various fields

AND

edit

AND Yield > 95%

85 hits

add molecules with defined roles

new save **save as**

AND

edit

exact  
 similarity  
 substructure  
 highlight match

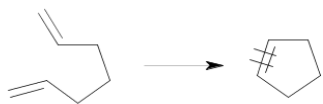
AND Name and Synonyms is NaBH4 Reagent

54 hits

Save queries, use saved queries, use queries from history

Query: ring closing metathesis

# Result List



is Grubbs II Catalyst

automatic cluster analysis over various fields

Cluster Analysis	
Author	+
Catalyst	+
Reagent	-
Reagent	n
none	123
H <sub>2</sub> C=CH <sub>2</sub>	2
molecular sieves	2
TosOH	1
1. none, 2. Et <sub>3</sub> N	1
1. none, 2. Ac-Cl	1

Solvent	+
Temperature (min.)	+
Temperature (max.)	+
Year	+
Yield	+

**Resultset** 130 Hits

Yield	Condition	Reference
100	Ph-CH=RuCl <sub>2</sub> (PCy <sub>3</sub> )(1,3-dimesitylimidazol-2-ylidene) (cat.) 1-butyl-3-methylimidazolium tetrafluoroborate	MAYO, K. G.; NAEPHVOOT, S. H.; KIDDLE, J. J.; Org Lett [ORLEF7] 2002, 4 (9), 1567-1570. <a href="#">[ open scheme ]</a> <a href="#">[ open article ]</a> <a href="#">[ save pdf ]</a> <a href="#">[ show details ]</a>
99	Ph-CH=RuCl <sub>2</sub> (H <sub>2</sub> IMes)(PCy <sub>3</sub> ) (cat.) CH <sub>2</sub> Cl <sub>2</sub>	LEE, K. Y.; MA, J. E.; LEE, J. Y.; KIM, J. N.; Bull Korean Chem Soc [BKCSDE] 2004, 25 (8), 1280-1282. <a href="#">[ open scheme ]</a> <a href="#">[ open article ]</a> <a href="#">[ save pdf ]</a> <a href="#">[ show details ]</a>

add to clipboard

link to the original paper

**Abstract 200503083**

**Synthesis of Substituted Cyclopentenes from the Baylis-Hillman Adducts via Ring-Closing Metathesis Reaction.**

Baylis-Hillman adducts [(I) or (VI)] are converted to the corresponding addition-elimination products [(III) or (VIII)], resp. which subsequently undergo an ROM reaction to form cyclopentenes [(IV) or (IX)], resp. using a second generation Grubbs' catalyst.

A): 1.2 equiv. DABCO, MeCN, 25°C; B): Ph-CH=RuCl<sub>2</sub>(H<sub>2</sub>IMes)(PCy<sub>3</sub>) (cat.), CH<sub>2</sub>Cl<sub>2</sub>, reflux

Ph-CH=RuCl<sub>2</sub>(H<sub>2</sub>IMes)(PCy<sub>3</sub>)

IV  $\xrightarrow[\text{MeOH, 25}^\circ\text{C}]{\text{H}_2, \text{Pd-C (cat.)}}$  V ~100%

VI  $\xrightarrow[\text{K}_2\text{CO}_3, 30-40^\circ\text{C}]{\text{1. A) Eoc-CH=CH}_2, \text{Eoc-CH=CH}_2}$  VIII

Eoc: -CO-O-Et

a R<sup>1</sup>: -Ph; R<sup>2</sup>: -CO-O-Et; X: -Br 80%  
b R<sup>1</sup>: -Ph; R<sup>2</sup>: -CN; X: -Br 69%  
c R<sup>1</sup>: -Ph; R<sup>2</sup>: -CO-Me; X: -Br 60%  
d R<sup>1</sup>: -H; R<sup>2</sup>: -CO-O-Et; X: -O-Ac 58%

show this rxn enlarged  
create a new query from this rxn

# Result List

choose fields to be displayed and sort results

Resultset

reset filter    add filter to query

130 Hits

Yield	Condition	Reference
100	Ph-CH=RuCl <sub>2</sub> (PCy <sub>3</sub> )(1,3-dimesitylimidazolin-2-ylidene) (cat.) 1-butyl-3-methylimidazolium tetrafluoroborate	MAYO, K. G.; NAERHOOF, E. H.; KIDDLE, J. J.; Org Lett [ORLEF7] 2002, 4 (9), 1567-1570. <a href="#">[ open scheme ]</a> <a href="#">[ open article ]</a> <a href="#">[ save pdf ]</a> <a href="#">[ show details ]</a>
99	Ph-CH=RuCl <sub>2</sub> (H <sub>2</sub> IMes)(PCy <sub>3</sub> ) (cat.) CH <sub>2</sub> Cl <sub>2</sub>	LEE, K. Y.; NA, J. E.; LEE, J. Y.; KIM, J. N.; Bull Korean Chem Soc [BKCSDE] 2004, 25 (8), 12 <a href="#">[ open scheme ]</a> <a href="#">[ open article ]</a> <a href="#">[ save pdf ]</a> <a href="#">[ show details ]</a>
99	Ph-CH=RuCl <sub>2</sub> (H <sub>2</sub> IMes)(PCy <sub>3</sub> ) (cat.) CH <sub>2</sub> Cl <sub>2</sub>	MIZUTANI, H.; WATANABE, M.; HONDA, T.; Synlett [SYNLES] 2005, (5), 793-796. <a href="#">[ open scheme ]</a> <a href="#">[ open article ]</a> <a href="#">[ save pdf ]</a> <a href="#">[ show details ]</a>

Yield    Condition    Reference

Sort Ascending  
Sort Descending

Columns

- Yield
- Condition
- Reference
- Variation ID
- Reaction ID
- Catalyst
- Reagent
- DOI
- Abstract No.
- max. Temp. [°C]
- min. Temp. [°C]
- Year
- Solvent
- Actions

Page 1 of 7

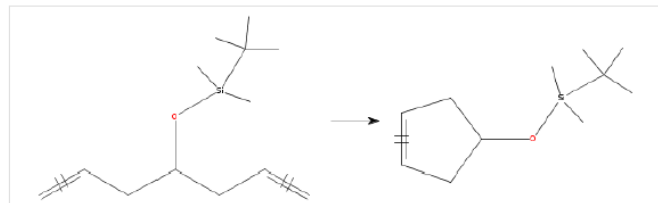
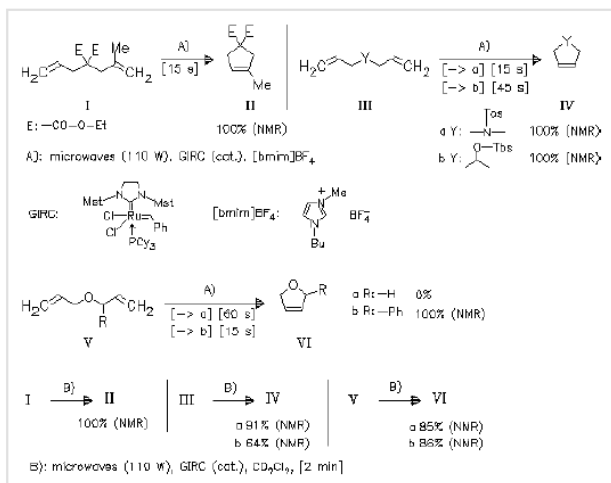
Displaying Variations 1 - 20 of 130

# Result

[save as pdf] (single hit)

## Microwave-Accelerated Ruthenium-Catalyzed Olefin Metathesis.

MAYO, K. G.; NAERHOOF, E. H.; KIDDLE, J. J.; Org Lett 4 (2002) 9, 1567-1570; doi:[10.1021/ol025789s](https://doi.org/10.1021/ol025789s)



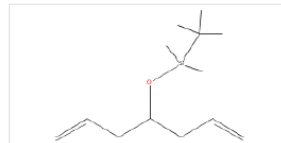
operation	steps	max. overall yield	keyphrases	conversion <sub>min</sub>	conversion <sub>max</sub>	comments
---	1	100	alkylation, C-alkylation	---	---	---

### Reaction Condition

step	temp <sub>min</sub>	temp <sub>max</sub>	time <sub>min</sub>	time <sub>max</sub>	pressure <sub>min</sub>	pressure <sub>max</sub>	pH <sub>min</sub>	pH <sub>max</sub>	other
---	---	---	---	---	---	---	---	---	---

1 --- -- .013 .013 --- -- -- -- microwaves (110 W)

### Reactants



C<sub>13</sub>H<sub>26</sub>OSi (mw: 226.43044)  
 CAS: 139656-31-8  
 InChI: InChI=1S/C13H26OSi/c1-8-10-12(11-9-2)14-15(6,7)13(3,4)5/h8-9,12H,1-2,10-11H2,3-7H3  
 InChIKey: MHOVRSQQGEURJ-UHFFFAOYSA-N

### Products

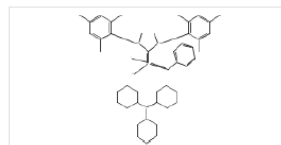


C<sub>11</sub>H<sub>22</sub>OSi (mw: 198.37728)  
 InChI: InChI=1S/C11H22OSi/c1-11(2,3)13(4,5)12-10-8-6-7-9-10/h6-7,10H,8-9H2,1-5H3  
 InChIKey: GVFFPKSGXMBWKM-UHFFFAOYSA-N

CS <sub>min</sub>	CS <sub>max</sub>	DE <sub>min</sub>	DE <sub>max</sub>	DS <sub>min</sub>	DS <sub>max</sub>	EE <sub>min</sub>	EE <sub>max</sub>	yield <sub>min</sub>	yield <sub>max</sub>	grade
100	100	---	---	---	---	---	---	100	100	(NMR)

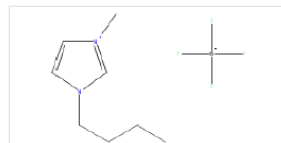
### Auxiliary Molecules

#### Catalyst



Grubbs II  
 C<sub>28</sub>H<sub>32</sub>Cl<sub>2</sub>N<sub>2</sub>Ru.C<sub>18</sub>H<sub>33</sub>P (mw: 848.9714599999999)  
 InChI: InChI=1S/C21H26N2.C18H33P.C7H6.2ClH.Ru/c1-14-9-16(3)20(17(4)10-14)22-7-8-23(13-22)21-18(5)11-15(2)12-19(21)6:1-4-10-16(11-5-1)19(17-12-6-2-7-13-17)18-14-8-3-9-15-18:1-7-5-3-2-4-6-7;;/h9-12H,7-8H2,1-6H3;16-18H,1-15H2;1-6H;2\*1H;/q;+2/p-2  
 InChIKey: FCDPQMAOJARMTG-UHFFFAOYSA-L

#### Solvent



[bim]BF<sub>4</sub>  
 C<sub>8</sub>H<sub>15</sub>N<sub>2</sub>.BF<sub>4</sub> (mw: 226.0227)  
 InChI: InChI=1S/C8H15N2.BF4/c1-3-4-5-10-7-6-9(2)8-10;2-1(3,4)5/h6-8H,3-5H2,1-2H3;/q+1;-1  
 InChIKey: LSBXQLQATZTAPE-UHFFFAOYSA-N

RXC102056905 / 200238060

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# Result

[show details] (single hit)

ChemInform RxnFinder you are logged in as "Wiley Information Services" WILEY

Query Results Details Selected Hits

Source Information: RANJITH, C.; SRINIVASAN, G. V.; VIDAYAN, K. K.; Bull Chem Soc Jpn 83 (2010) 3, 288-290; doi: 10.1246/bcsj.20090275 [ open scheme ]

Source Synthesis Steps: Step 1 of 1

Reaction RXCI10054478

max. overall yield: 89%

Reactants

- PhCHO**  
C<sub>7</sub>H<sub>6</sub>O (mw: 106.12194)  
Keywords: aldehyde, phenyl  
InChI: InChI=15/C7H6O/c8-6-7-4-2-1-3-5-7/h1-  
InChIKey: HUMNYLRZRPJDN-UHFFFAOYSA-N
- Ph-CO-CH<sub>2</sub>-CO-Me**  
C<sub>10</sub>H<sub>10</sub>O<sub>2</sub> (mw: 162.1852)  
Keywords: ketone, phenyl  
InChI: InChI=15/C10H10O2/c1-8(11)7-10(12)9-5-3-2-4-6-9/h2-6H,7H2,1H3  
InChIKey: CVBUKMMMLRLOKQR-UHFFFAOYSA-N
- H<sub>2</sub>N-CO-NH<sub>2</sub>**  
CH<sub>4</sub>N<sub>2</sub>O (mw: 60.05526)  
Keywords: amide, urea  
InChI: InChI=15/CH4N2O/c2-1(3)4/h(H,2,3,4)  
InChIKey: XSQUKJJFZCRTR-UHFFFAOYSA-N

Product

CS: 100 %, Yield: 89 %  
C<sub>18</sub>H<sub>16</sub>N<sub>2</sub>O<sub>2</sub> (mw: 292.33184)  
Keywords: alkene, amide, enamide, enone, heterocycle, lactam, phenyl, urea  
InChI: InChI=15/C18H16N2O2/c1-12-15(17)14-10-6-3-7-11-14)16(20-18(22)19-12)13-8-4-2-5-9-13/h2-11,16H,1H3,(H2,19,20,22)

Clipboard: Reference: BORDOLOI, A.; HALLIGUDI, S. B.;... DEFOIN, A.; Synthesis [SYNTBF] 2... ZHAO, D.; JOHANSSON, M.; BAEC...

Override current Query?  
? Would you like to search for RxnPaths for this compound? This will overwrite your current query!  
OK Cancel

Look up syntheses of reactants when available

note: your current query is in the history

## Selected Hits

ChemInform RxnFinder you are logged in as "Wiley Information Services" WILEY

Query Results Details Selected Hits

untitled list\*

Clipboard

transfer all / selected reactions to current list

remove selected

5 ring closing 0

Bignelli 0

new save remove print

	Yield	Condition	Reference
<input type="checkbox"/> 98		1. Bi(NO <sub>3</sub> ) <sub>3</sub> ·5H <sub>2</sub> O Bu <sub>4</sub> NF	KHODAEI, M. M.; KHOSROPOUR, A. R.; JOWKAR, M.; Synthesis [SYNTBF] 2005, (8), 1301-1304. [ open scheme ] [ open article ] [ save pdf ] [ show details ]
<input type="checkbox"/> 98		HClO <sub>4</sub> ·SiO <sub>2</sub> (cat.) neat	MAHESWARA, M.; OH, S. H.; KIM, K.; DO, J. Y.; Bull Korean Chem Soc [BKCSDE] 2008, 29 (9), 1752-1754. [ open scheme ] [ open article ] [ save pdf ] [ show details ]
<input type="checkbox"/> 98		[bmim]Cl·2AlCl <sub>3</sub>	BAHEKAR, S. S.; KOTHARKAR, S. A.; SHINDE, D. B.; Mendeleev Commun [MENCEX] 2004, (5), 210-212. [ open scheme ] [ open article ] [ save pdf ] [ show details ]
<input type="checkbox"/> 98		Sm(NO <sub>3</sub> ) <sub>3</sub> ·6H <sub>2</sub> O (cat.) neat	XU, H.; WANG, Y.-G.; J Chem Res, Synop [JRPSDC] 2003, (6), 377-379. [ open scheme ] [ open article ] [ save pdf ] [ show details ]
<input type="checkbox"/> 98		CAN (cat.) polyethylene glycol 400	KIDWAI, M.; BHATNAGAR, D.; KUMAR, R.; LUTHRA, P. M.; Chem Pharm Bull [CPBTAL] 2010, 58 (10), 1320-1323. [ open scheme ] [ save pdf ] [ show details ]

Up to now, it is only possible to save hitlists. Further export and print functionalities are planned



ChemInform RxnFinder you are logged in as "Wiley Information Services" WILEY

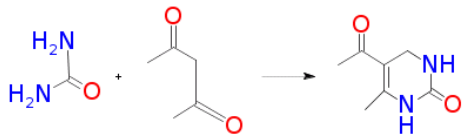
Query Results Details Selected Hits

Query Fields + Query: [Default] tools

Saved Queries - new save save as save as default

remove selected

- amine ox
- Biginelli
- kinetic resolution
- metathesis
- sel. nitro red.
- sel.keto/nitro reduction.

AND  edit

exact  
 similarity  
 substructure  
 highlight match  
 transformation

import query  
export query  
**send feedback**

AND Yield >= 95% submit query

Send Feedback for query

Recipient: rxnfinder-feedback@rxnfinder.com

Message:

Send feedback report with current query attached

Please use ,send feedback' button for any questions

