

# Paths of analysis\*

OP\_Exp

Synthia

February 13, 2024

## 1 Analysis parameters

**Analysis type:** Automatic Retrosynthesis

**Rules:** Expert-Coded Rules

**Published Reactions:** none selected

**Filters:** Exclude Diastereoselective reactions, Tunnels, FGI, FGI with protections

**Max. paths returned:** 50

**Max. iterations:** 2000

**Commercial:**

1. Max. molecular weight - 1000 g/mol
2. Max. price - 1500 \$/g

**Published:**

1. Max. molecular weight - 1000 g/mol
2. Popularity - 5

**My Stockroom:**

1. Max. molecular weight - 1000 g/mol

**Shorter paths:** no

**Pathway linearity:** COMBO

**Protecting groups:** BALANCED

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\*The results stated herein were generated using the proprietary platform owned and maintained by Grzybowski Scientific Inventions, Inc., a subsidiary of Merck KGaA, Darmstadt Germany. The results are provided on an as is basis, and shall be used solely in connection with the rights afforded in the license agreement and for no other purpose.

**Reaction scoring formula:**  $\text{TUNNEL\_COEF} * \text{FGI\_COEF} * \text{STEP} * 20 + 100000 * (\text{FILTERS} + \text{CONFLICT} + \text{NON\_SELECTIVITY}) + 40 * \text{PROTECT}$

**Chemical scoring formula:**  $\text{SMALLER}^3, \text{SMALLER}^{1.5}$

**Min. search width:** 400

**Max. reactions per product:** 60

**Strategies:** none selected

**FGI Coeff:** 1

**Tunnels Coeff:** 1

**JSON Parameters:** {}

## 2 Paths

1 path found. *Paths are sorted by score. Reactions are sorted in appearance order for each path.*

### 2.1 Path 1

**Score:** 136.28

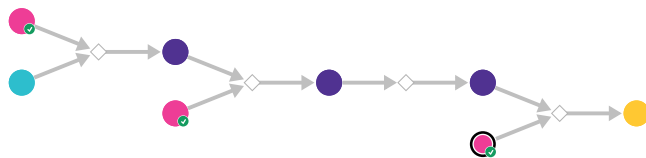
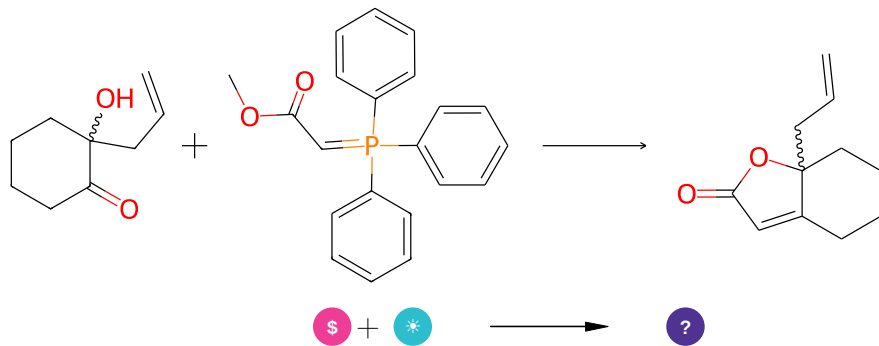


Figure 1: Outline of path 1

#### 2.1.1 Synthesis of lactones from hydroxyketones and Bestmann ylide



**Substrates:**

1. Methyl (triphenylphosphoranylidene)acetate - *available at Sigma-Aldrich*
2. 2-Allyl-2-hydroxycyclohexanone

**Products:**

1. C=CCC12CCCCC1=CC(=O)O2

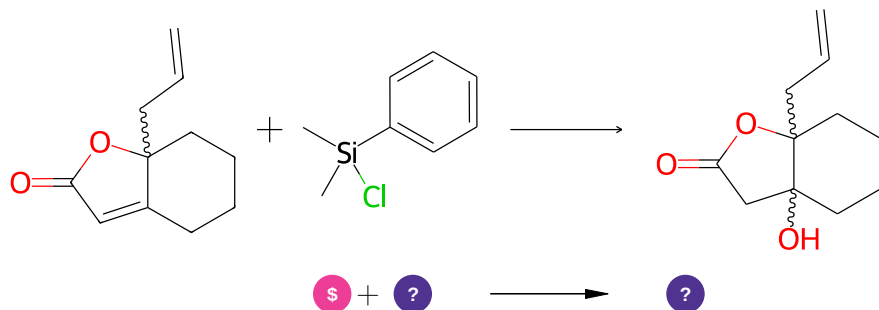
**Typical conditions:** toluene.heat

**Protections:** none

**Reference:** [10.1021/ol503150c](#) and [10.1002/anie.200704959](#) and [10.1016/S0040-4039\(02\)02535-2](#) and [10.1016/j.tetasy.2007.07.027](#) and [10.1016/S0040-4020\(97\)10428-8](#) and [10.1002/anie.201407788](#) and [10.1002/hlca.201300203](#) and reagent prep: [10.15227/orgsyn.082.0140](#)

**Retrosynthesis ID:** 10030991

**2.1.2 Addition of silanes to Michael acceptors followed by oxidation**



**Substrates:**

1. DMPSCl - *available at Sigma-Aldrich*
2. C=CCC12CCCCC1=CC(=O)O2

**Products:**

1. C=CCC12CCCCC1(O)CC(=O)O2

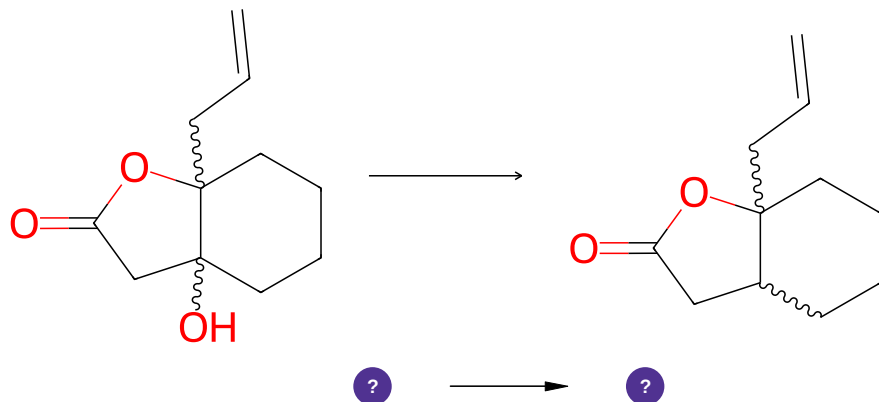
**Typical conditions:** 1.nBuLi.2.CuCN.3.electrophile.4.H<sub>2</sub>O<sub>2</sub>

**Protections:** none

**Reference:** [10.1021/ja058370g](#) AND (Oxidation) [10.1021/jo9905672](#) or [10.1021/ol300832f](#)

**Retrosynthesis ID:** 20296

### 2.1.3 Deoxygenation of alcohols with silanes



**Substrates:**

1. C=CCC12CCCCC1(O)CC(=O)O2

**Products:**

1. C=CCC12CCCCC1CC(=O)O2

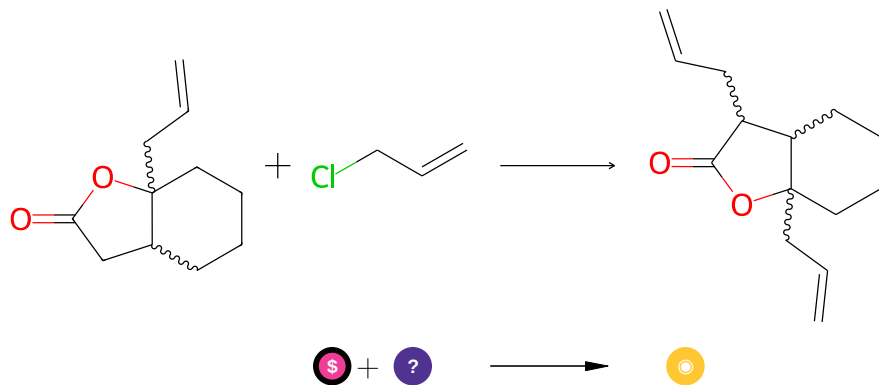
**Typical conditions:** Et<sub>3</sub>SiH.Lewis.or.Bronsted.Acid

**Protections:** none

**Reference:** [10.1021/jo0158534](#) AND [10.1021/ol3020144](#)

**Retrosynthesis ID:** 8163

### 2.1.4 Alkylation of Esters



**Substrates:**

1. Chloroallylene - *available at Sigma-Aldrich*

2. C=CCC12CCCCC1CC(=O)O2

**Products:**

1. C=CCC1C(=O)OC2(CC=C)CCCCC12

**Typical conditions:** base e.g. BuLi.THF

**Protections:** none

**Reference:** [10.1021/ja065404r](#) and [10.1016/S0040-4020\(01\)88337-X](#)  
and [10.1016/0040-4039\(95\)00562-Q](#) and [10.1021/acs.orglett.6b01901](#) and  
[10.1021/jo00073a034](#) and [10.1021/ol2023278](#)

**Retrosynthesis ID:** 31017152