

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

*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: $\text{TUNNEL_COEF} * \text{FGI_COEF} * \text{STEP} * 20 + 1000 * (\text{FILTERS} + \text{CONFLICT} + \text{NON_SELECTIVITY}) + 40 * \text{PROTECT}$

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: 164.90

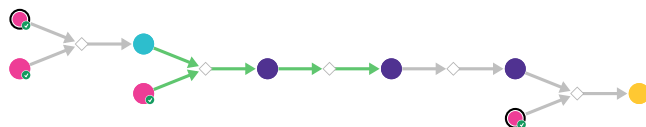
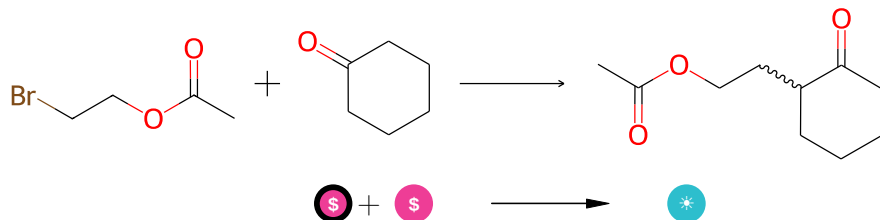


Figure 1: Outline of path 1

2.1.1 Alkylation of ketones



Substrates:

1. Hexanon - *available at Sigma-Aldrich*
2. 2-Bromoethyl acetate - *available at Sigma-Aldrich*

Products:

1. 2-(2-Acetoxy-ethyl)-cyclohexanone

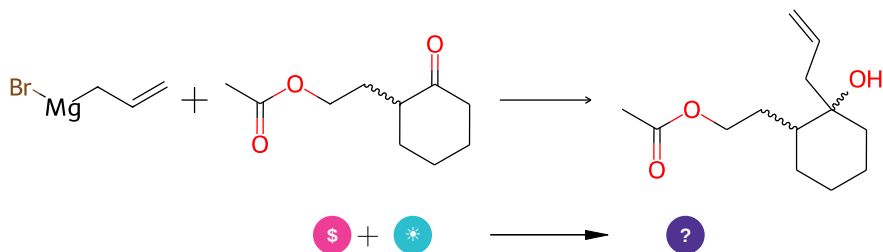
Typical conditions: LDA or other base.THF.-78C

Protections: none

Reference: DOI: [10.1021/ja0123554](https://doi.org/10.1021/ja0123554)

Retrosynthesis ID: 1868

2.1.2 Addition of Grignard reagents



Substrates:

1. Allylmagnesium bromide - *available at Sigma-Aldrich*
2. 2-(2-Acetoxy-ethyl)-cyclohexanone

Products:

1. C=CCC1(O)CCCCC1CCOC(C)=O

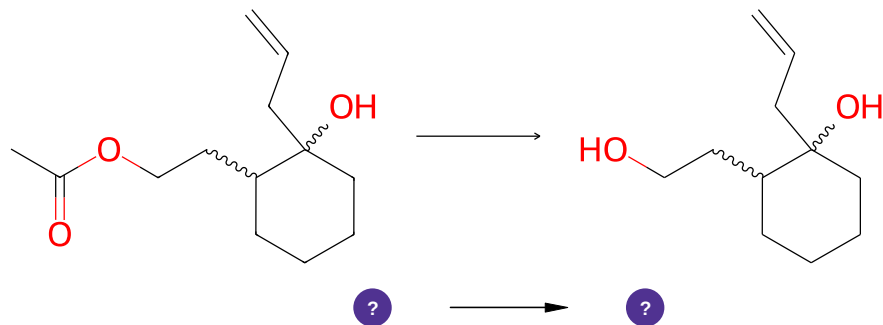
Typical conditions: THF.cooling

Protections: none

Reference: [10.1021/jo010494y](https://doi.org/10.1021/jo010494y) or [10.1016/j.steroids.2015.09.009](https://doi.org/10.1016/j.steroids.2015.09.009) or [10.1021/jo061349t](https://doi.org/10.1021/jo061349t) or [10.1021/ja056165v](https://doi.org/10.1021/ja056165v) (SI page 19)

Retrosynthesis ID: 25134

2.1.3 Deacylation of primary alcohols



Substrates:

1. C=CCC1(O)CCCCC1CCOC(C)=O

Products:

1. C=CCC1(O)CCCCC1CCO

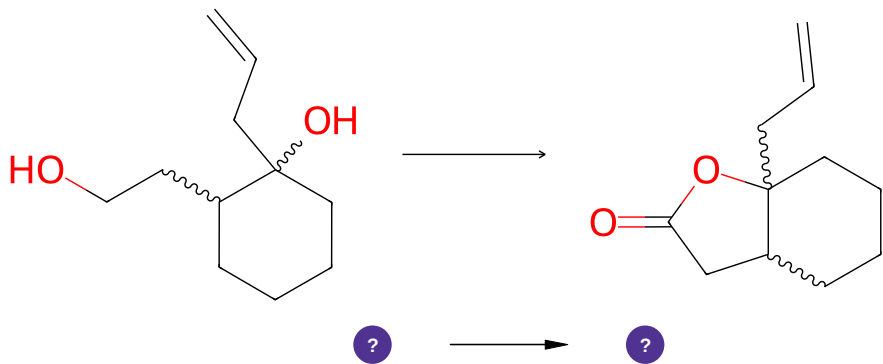
Typical conditions: Acid.heat or MeONa.MeOH.rt

Protections: none

Reference: [10.1016/j.carres.2015.04.008](#) and [10.3390/molecules201219789](#)

Retrosynthesis ID: 31019469

2.1.4 Oxidative lactonization of 1,4-diols



Substrates:

1. C=CCC1(O)CCCCC1CCO

Products:

1. C=CCC12CCCCC1CC(=O)O2

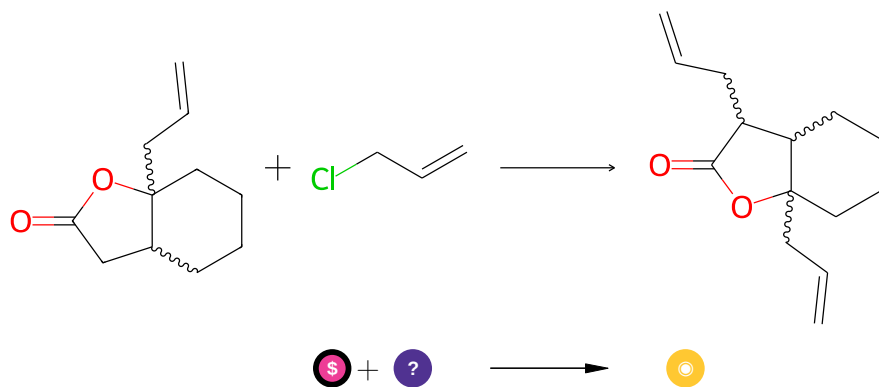
Typical conditions: Cp(st)RuCl(cod).tBuOK.acetone.30C

Protections: none

Reference: DOI: [10.1021/ol0706408](https://doi.org/10.1021/ol0706408)

Retrosynthesis ID: 1501

2.1.5 Alkylation of Esters



Substrates:

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

Retrosynthesis ID: 31017152