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 Diastereoselecitve 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

Reaction scoring formula: TUNNEL_COEF*FGI_COEF*STEP*20+1000000*(FILTERS+CONFLICT+NON_SELECTIVITY)+40*PROTECT

Chemical scoring formula: SMALLER^ 3,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`

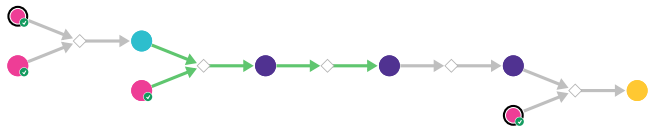
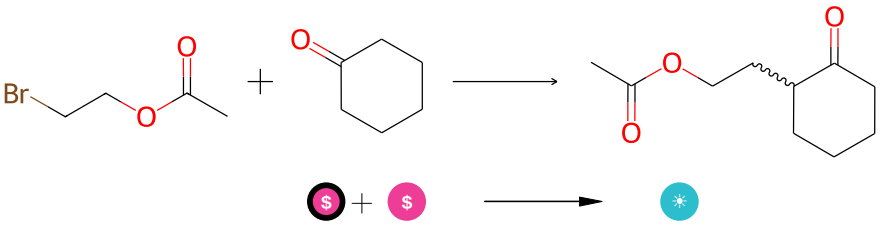


Figure 1: Outline of path 1

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

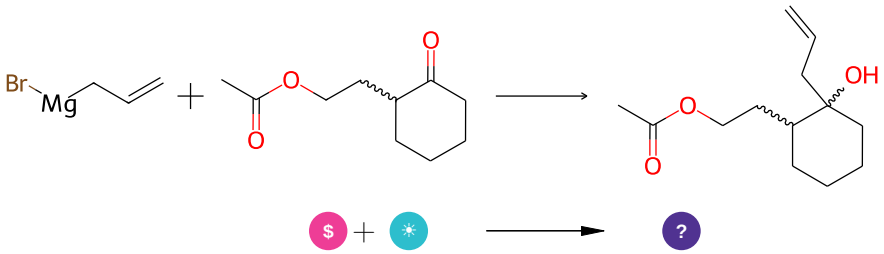
Typical conditions: LDA or other base.THF.-78C

Protections: none

Reference: DOI: *10.1021/ja0123554*

Retrosynthesis ID: 1868

2.1.2 Addition of Grignard reagents



Substrates:

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

Products:

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

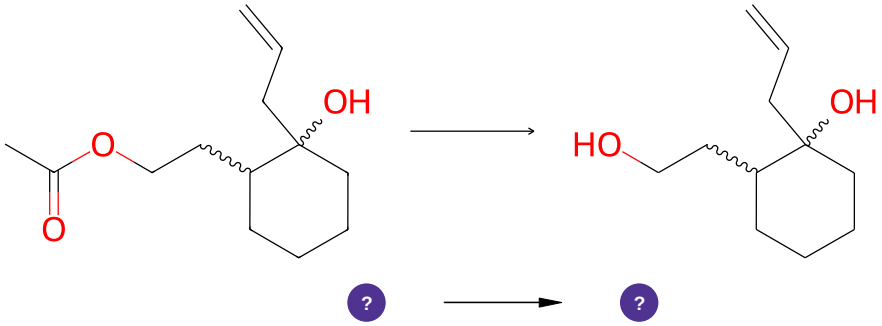
Typical conditions: THF.cooling

Protections: none

Reference: *10.1021/jo010494y* or *10.1016/j.steroids.2015.09.009* or *10.1021/jo061349t* or *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

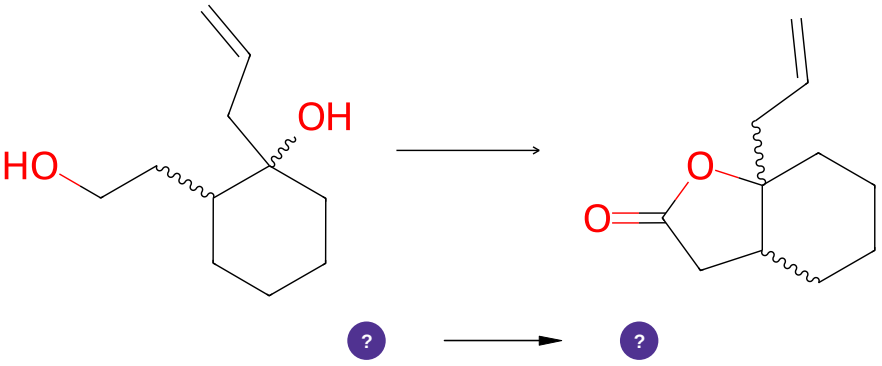
Typical conditions: Acid.heat or MeONa.MeOH.rt

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

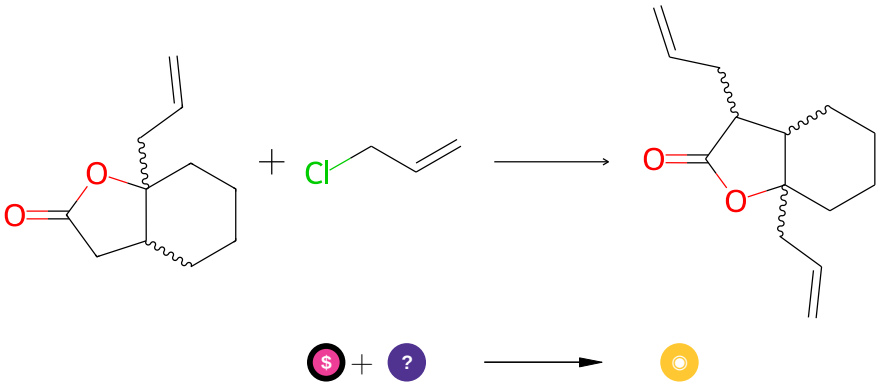
Typical conditions: Cp(st)RuCl(cod).tBuOK.acetone.30C

Protections: none

Reference: DOI: *10.1021/ol0706408*

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* 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