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: `180.44`

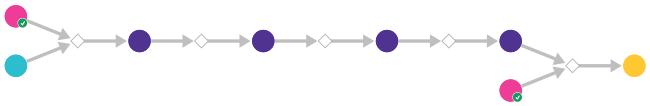
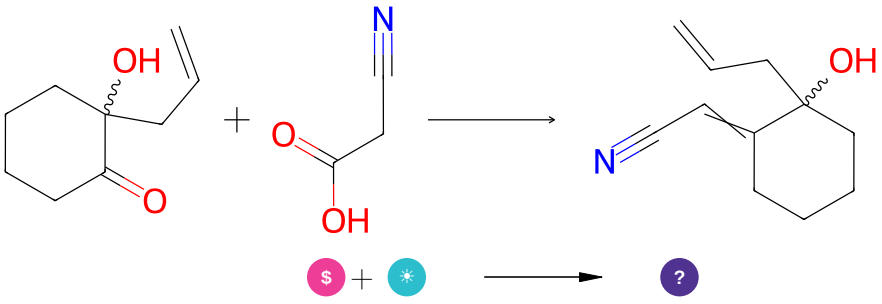


Figure 1: Outline of path 1

2.1.1 Knoevenagel condenstation



Substrates:

1. Cyanoacetic acid - *available at Sigma-Aldrich*

2. 2-Allyl-2-hydroxycyclohexanone

Products:

1. C=CCC1(O)CCCCC1=CC#N

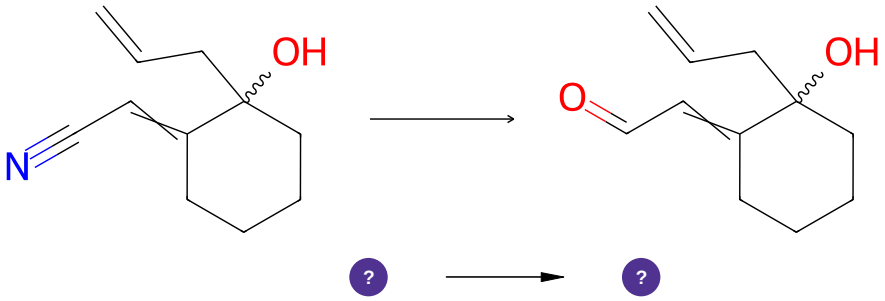
Typical conditions: NH4OAc.AcOH.heat

Protections: none

Reference: WO2005/44008 p.96 and *10.1002/hlca.201200162* and *10.1002/chem.200903053* and WO2005/44008 p.90 and US4012377 p.

Retrosynthesis ID: 32838

2.1.2 Reduction of nitriles to aldehydes



Substrates:

1. C=CCC1(O)CCCCC1=CC#N

Products:

1. C=CCC1(O)CCCCC1=CC=O

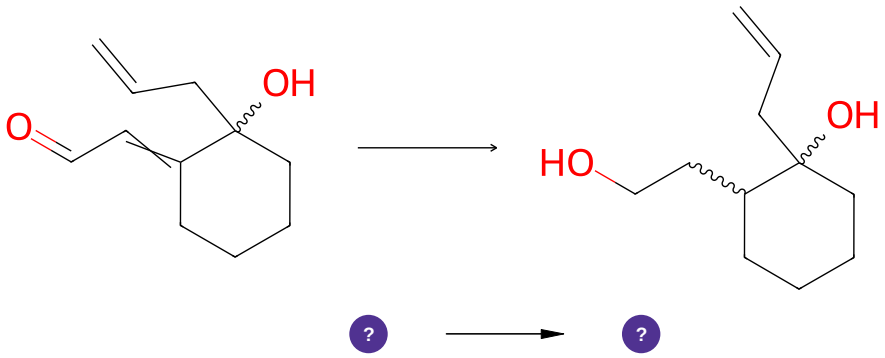
Typical conditions: DIBALH.DCM

Protections: none

Reference: *10.1016/j.bmc.2006.01.061* and *10.1016/j.tet.2012.07.022* and *10.1016/j.bmcl.2009.01.075* and *10.1016/j.bmcl.2007.09.081* and *10.1021/jo000502v*

Retrosynthesis ID: 31406

2.1.3 Reduction of enones to saturated alcohols



Substrates:

1. C=CCC1(O)CCCCC1=CC=O

Products:

1. C=CCC1(O)CCCCC1CCO

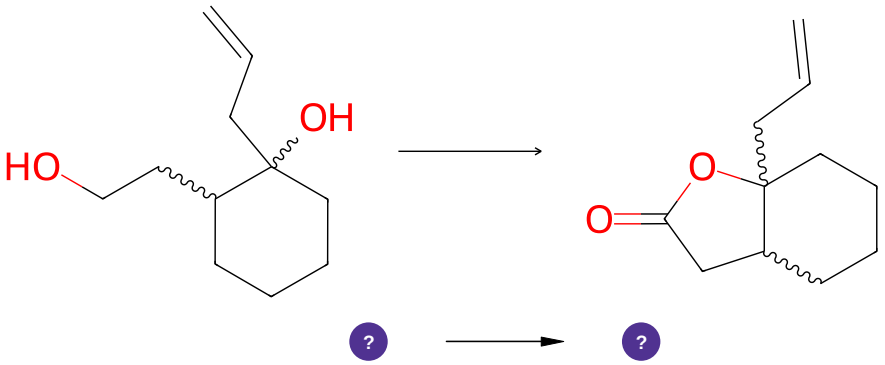
Typical conditions: NaBH4.transition.metal.salt.(eg.Pd(OAc)2.or.CeCl3)

Protections: none

Reference: *10.1080/00397910902788117* AND *10.1021/jo00235a009* AND *10.1016/0040-4020(95)00125-R* AND *10.1021/ja01327a041* AND *10.1021/jo00302a056* AND *10.1002/adsc.200900628*

Retrosynthesis ID: 15309

2.1.4 Oxidative lactonization of 1,4-diols



Substrates:

1. C=CCC1(O)CCCCC1CCO

Products:

1. C=CCC12CCCCC1CC(=O)O2

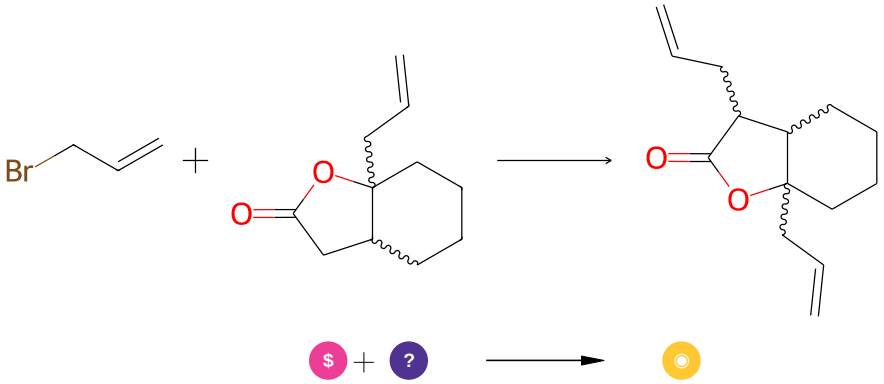
Typical conditions: Cp(st)RuCl(cod).tBuOK.acetone.30C

Protections: none

Reference: DOI: *10.1021/ol0706408*

Retrosynthesis ID: 1501

2.1.5 Alkylation of Esters



Substrates:

1. Allyl bromide - *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 *10.1021/ja058303m* and *10.1021/acs.orglett.9b03078* and *10.1016/S0040-4020(01)80336-7*

Retrosynthesis ID: 31017104