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: `150.04`

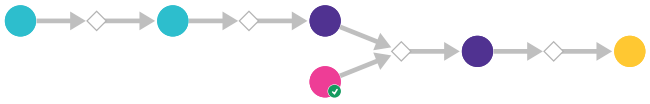
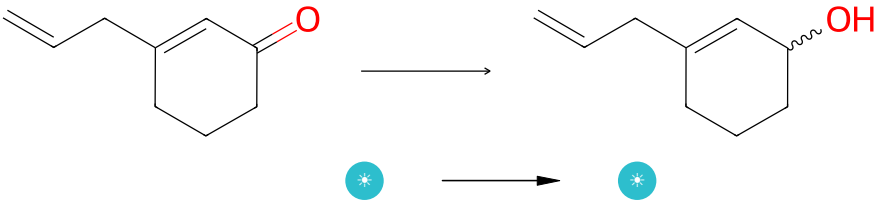


Figure 1: Outline of path 1

2.1.1 Luche Reduction



Substrates:

1. 3-Allyl-2-cyclohexen-1-one

Products:

1. 3-Allyl-cyclohex-2-enol

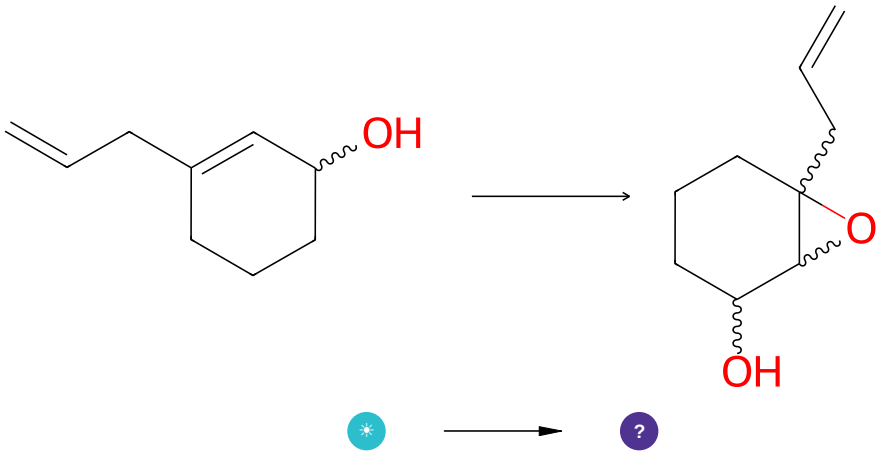
Typical conditions: CeCl3.NaBH4.MeOH

Protections: none

Reference: *10.1002/9780470638859.conrr400*

Retrosynthesis ID: 10180

2.1.2 Asymmetric epoxidation



Substrates:

1. 3-Allyl-cyclohex-2-enol

Products:

1. C=CCC12CCCC(O)C1O2

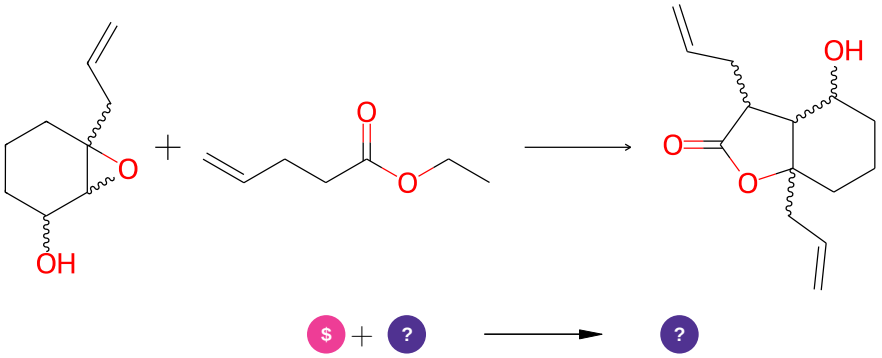
Typical conditions: MCPBA.DCM

Protections: none

Reference: *10.1021/ja00341a055* and *10.1002/chem.200901735* and *10.1021/ol102586w* and *10.1016/j.tetasy.2012.03.001*

Retrosynthesis ID: 29184

2.1.3 Synthesis of lactones from epoxides



Substrates:

1. Ethyl 4-pentenoate - *available at Sigma-Aldrich*
2. C=CCC12CCCC(O)C1O2

Products:

1. C=CCC1C(=O)OC2(CC=C)CCCC(O)C12

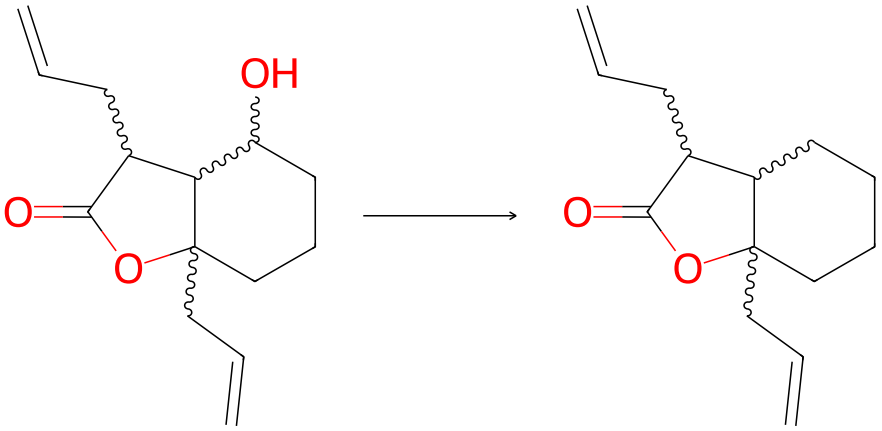
Typical conditions: EtONa.EtOH.rt

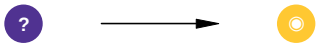
Protections: none

Reference: *10.1021/ja9049959* and *10.1016/j.tetlet.2014.12.024* and *10.1021/jo00077a012* and *10.1016/0040-4039(96)00494-7* and *10.1002/chem.201403294*

Retrosynthesis ID: 21259

2.1.4 Deoxygenation of alcohols with silanes





Substrates:

1. C=CCC1C(=O)OC2(CC=C)CCCC(O)C12

Products:

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

Typical conditions: Et3SiH.Lewis.or.Bronsted.Acid

Protections: none

Reference: *10.1021/jo0158534* AND *10.1021/ol3020144*

Retrosynthesis ID: 8162