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: 136.25

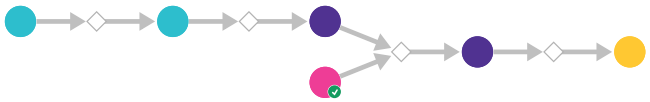
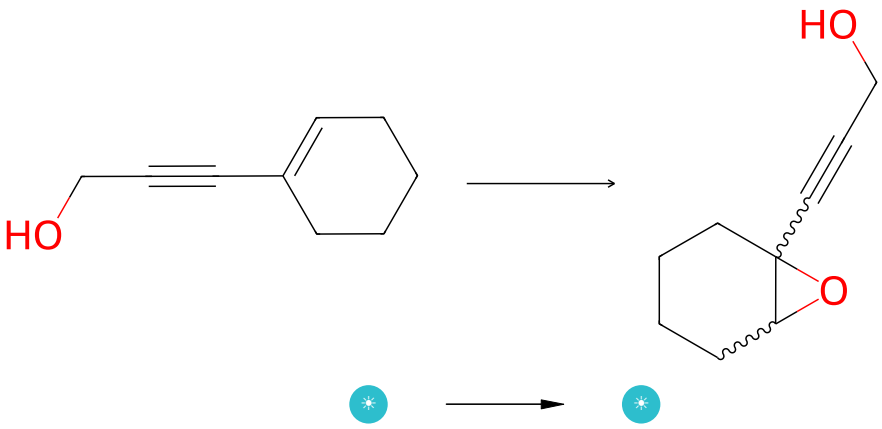


Figure 1: Outline of path 1

2.1.1 Epoxidation of trisubstituted alkene



Substrates:

1. 3-(Cyclohex-1-enyl)prop-2-yn-1-ol

Products:

1. 3-(7-Oxa-bicyclo[4.1.0]hept-1-yl)-prop-2-yn-1-ol

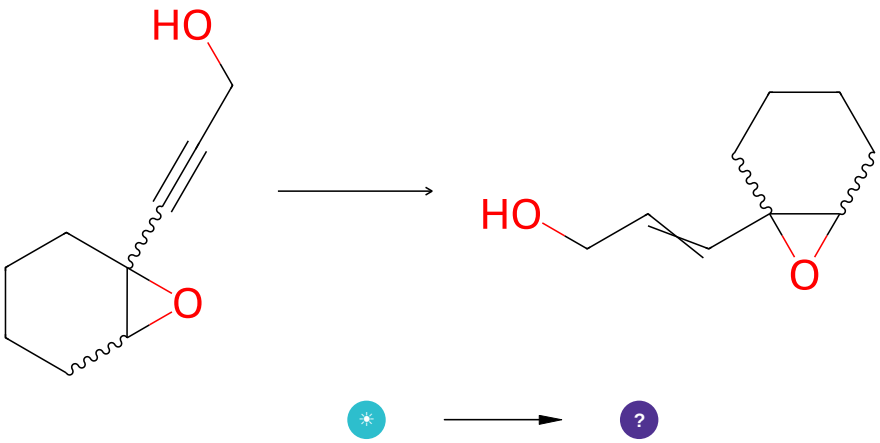
Typical conditions: MCPBA.DCM

Protections: none

Reference: *10.1016/0040-4039(95)01307-4* and *10.1016/j.tet.2011.09.067* and *10.1016/j.tetasy.2011.09.008* and *10.1016/j.jorganchem.2011.02.024* and *10.1021/acs.jmedchem.5b01292* and *10.1016/j.bmcl.2011.03.092* and *10.1016/j.tet.2010.11.076* and *10.1016/S0040-4039(00)79649-3*

Retrosynthesis ID: 9990243

2.1.2 Reduction of alkynes to Z-alkenes



Substrates:

1. 3-(7-Oxa-bicyclo[4.1.0]hept-1-yl)-prop-2-yn-1-ol

Products:

1. OCC=CC12CCCCC1O2

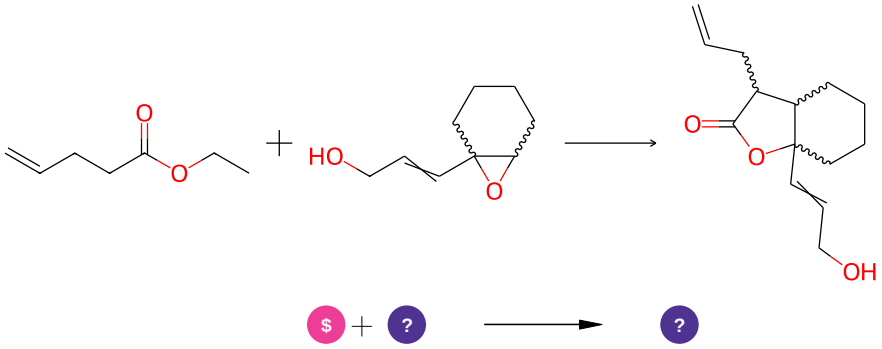
Typical conditions: H2.Lindlar's catalyst

Protections: none

Reference: *10.1021/ja035538u* and *10.1021/ja00006a029* and *10.1021/jo026511g* and *10.1021/jm9604437* and *10.1021/jo991395b* and *10.1002/chem.201403255*

Retrosynthesis ID: 10011832

2.1.3 Synthesis of lactones from epoxides



Substrates:

1. Ethyl 4-pentenoate - *available at Sigma-Aldrich*
2. OCC=CC12CCCCC1O2

Products:

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

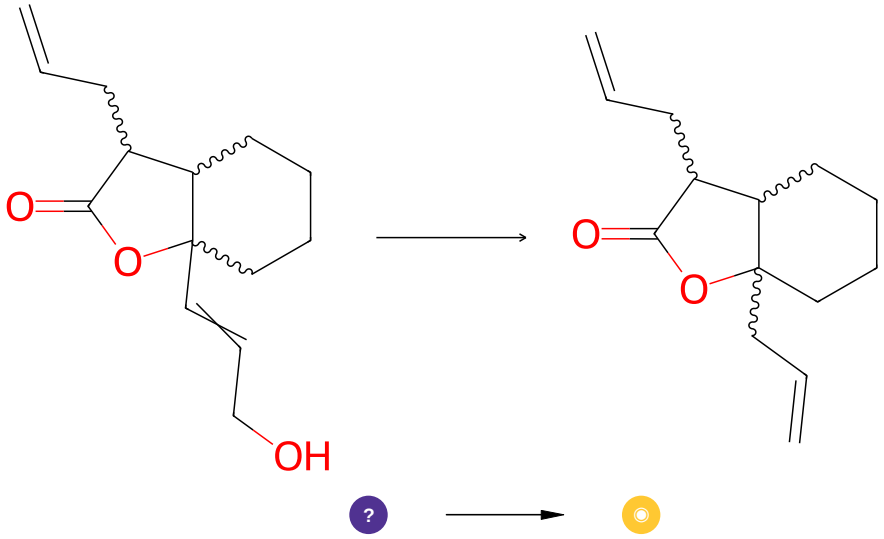
Typical conditions: EtONa.EtOH.rt

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 Allyl Alcohol Transposition



Substrates:

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

Products:

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

Typical conditions: PPh3. DEAD. NBSH or IPNBSH. Solvent e.g. THF

Protections: none

Reference: DOI: *10.1038/ja.2017.127* and *10.1021/jo062325p* and *10.1016/0040-4039(96)00965-3* and *10.1021/acs.orglett.8b03889* (cmpd 8)

Retrosynthesis ID: 31006955