Paths of analysis*

PG1

Synthia

October 10, 2022

1 Analysis parameters

Analysis type: Automatic Retrosynthesis

Rules: 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

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

Chemical scoring formula: SMALLER^ 3,SMALLER^ 1.5

Min. search width: 400

Max. reactions per product: 60

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Strategies: none selected

FGI Coeff: 0

Tunnels Coeff: 0

JSON Parameters: {}

2 Paths

5 paths found. *Paths are sorted by score. Reactions are sorted in appearance order for each path.*

2.1 Path 1

Score: `20.00`

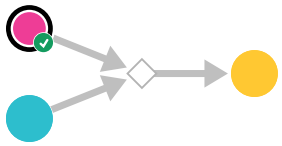
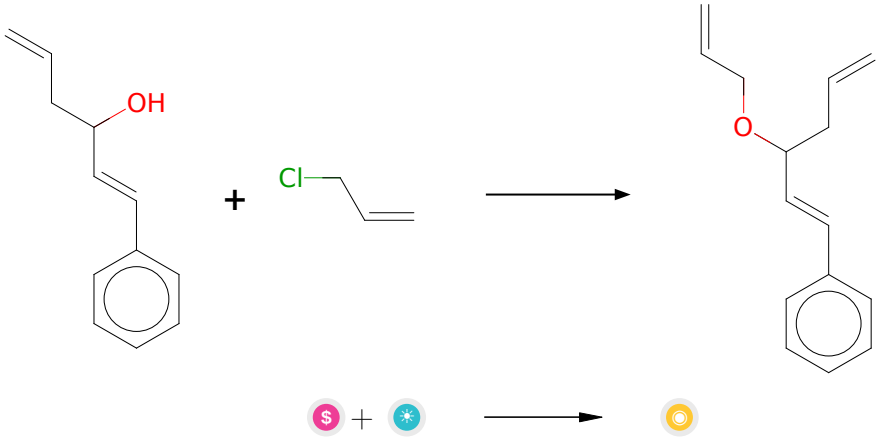


Figure 1: Outline of path 1

2.1.1 Alkylation of secondary unhindered alcohols



Substrates:

1. Chlorallylene - *available at Sigma-Aldrich*
2. (+-)-1t-phenyl-hexa-1,5-dien-3-ol

Products:

1. (3-allyloxyhexa-1,5-dienyl)-benzene

Typical conditions: K2CO3.acetone.heat

Protections: none

Reference: *10.1016/S0022-1139(00)85021-6* and

Retrosynthesis ID: 31011036

2.2 Path 2

Score: 31.25

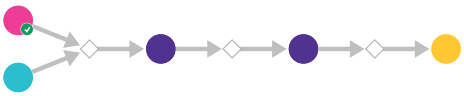
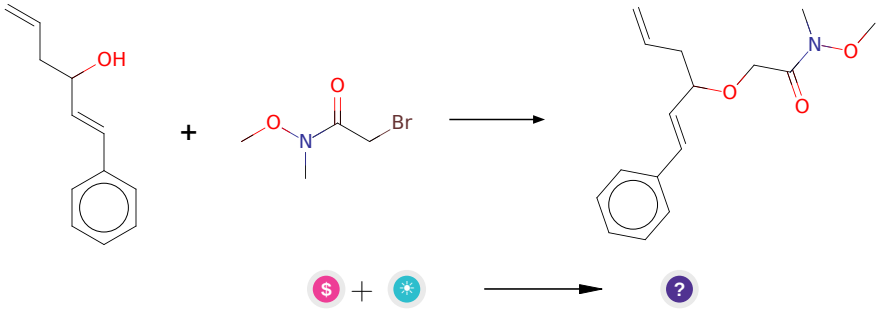


Figure 2: Outline of path 2

2.2.1 Reaction of alpha-bromo carbonyl compounds with alcohols or phenols



Substrates:

1. 2-Bromo-N-methoxy-N-methylacetamide - *available at Sigma-Aldrich*
2. (+-)-1t-phenyl-hexa-1,5-dien-3-ol

Products:

1. C=CCC(/C=C/c1ccccc1)OCC(=O)N(C)OC

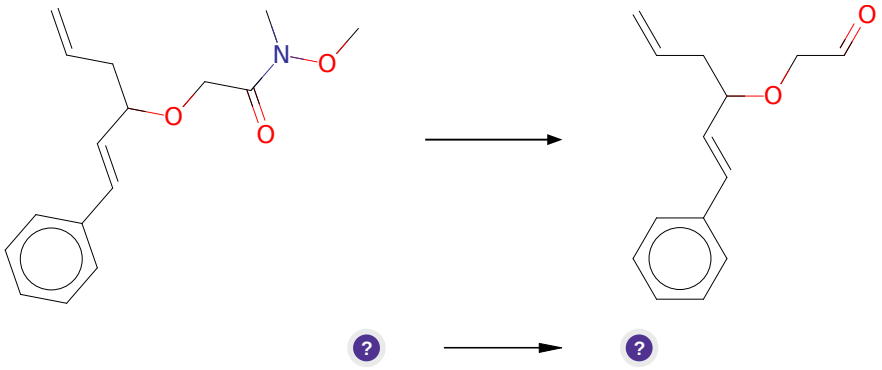
Typical conditions: NaOH.EtOH

Protections: none

Reference: *10.1021/jm070511x* AND *10.1021/op1002038* AND *10.1007/BF00758669* AND *10.1021/ja01117a054*

Retrosynthesis ID: 14804

2.2.2 Aldehyde Formation



Substrates:

1. C=CCC(/C=C/c1ccccc1)OCC(=O)N(C)OC

Products:

1. C=CCC(/C=C/c1ccccc1)OCC=O

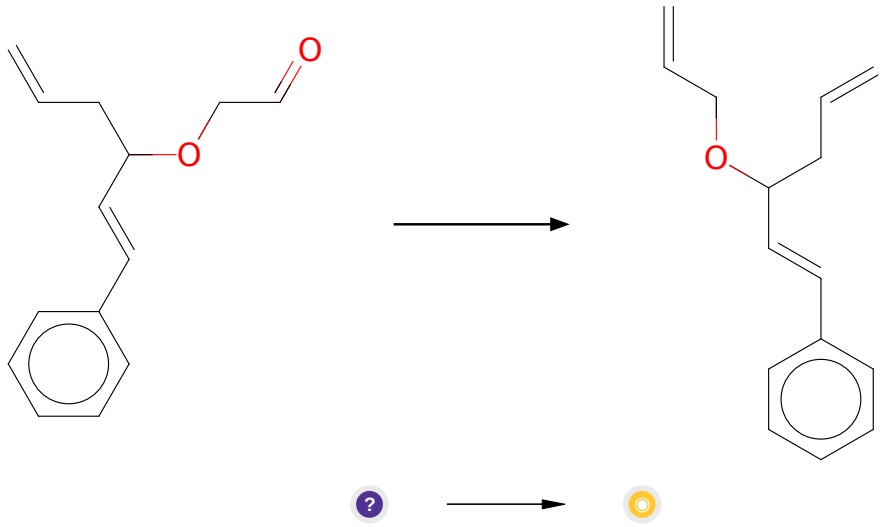
Typical conditions: DIBAL.toluene.CO

Protections: none

Reference: *10.1021/jo202652f*

Retrosynthesis ID: 11504

2.2.3 Tebbe Olefination



Substrates:

1. C=CCC(/C=C/c1ccccc1)OCC=O

Products:

1. (3-allyloxyhexa-1,5-dienyl)-benzene

Typical conditions: Cp2TiCl2.AlMe3.toluene

Protections: none

Reference: *10.1016/j.tet.2007.03.015* and *10.1002/9780470638859.conrr617*

Retrosynthesis ID: 11714

2.3 Path 3

Score: 31.25

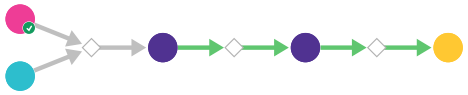
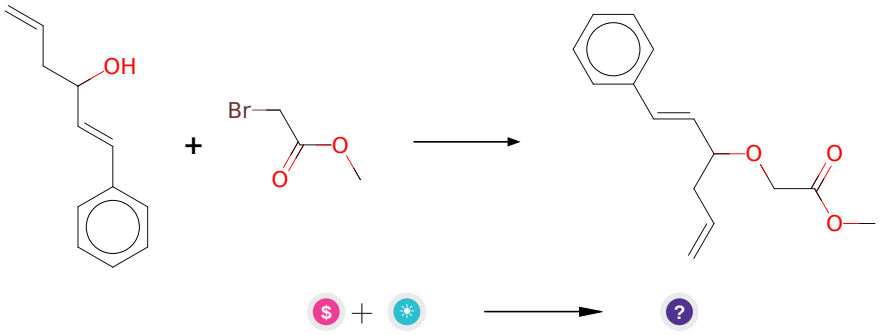


Figure 3: Outline of path 3

2.3.1 Reaction of alpha-bromo carbonyl compounds with alcohols or phenols



Substrates:

1. Methyl bromoacetate - *available at Sigma-Aldrich*
2. (+-)-1t-phenyl-hexa-1,5-dien-3-ol

Products:

1. C=CCC(/C=C/c1ccccc1)OCC(=O)OC

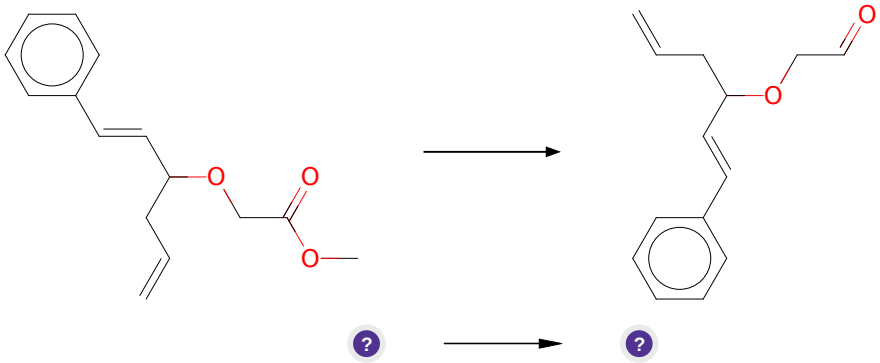
Typical conditions: NaOH.EtOH

Protections: none

Reference: *10.1021/jm070511x* AND *10.1021/op1002038* AND *10.1007/BF00758669* AND *10.1021/ja01117a054*

Retrosynthesis ID: 14804

2.3.2 Aldehyde Formation



Substrates:

1. C=CCC(/C=C/c1ccccc1)OCC(=O)OC

Products:

1. C=CCC(/C=C/c1ccccc1)OCC=O

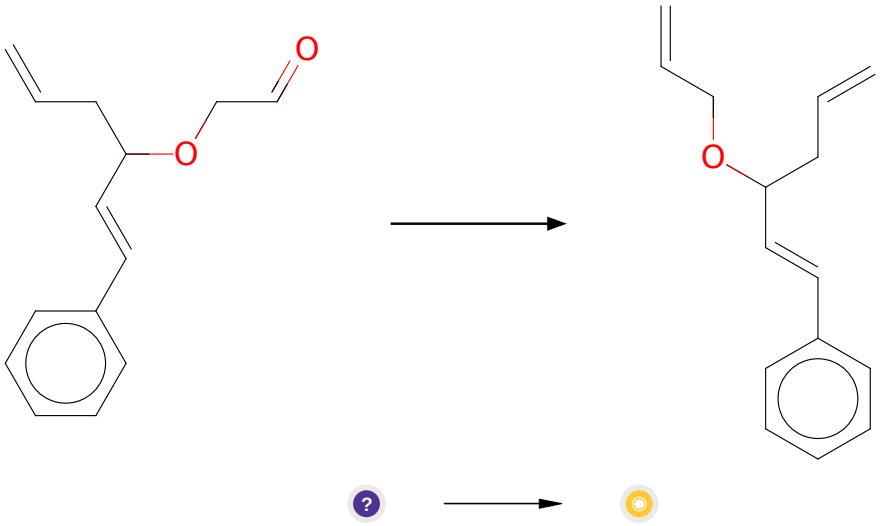
Typical conditions: DIBAL.solvent e.g. DCM

Protections: none

Reference: *10.1039/C39940000483* and *10.1039/C3CC47867J* and *10.1021/jo00222a054* and *10.1021/ja9934908* and *10.1021/jo902426z*

Retrosynthesis ID: 28551

2.3.3 Tebbe Olefination



Substrates:

1. C=CCC(/C=C/c1ccccc1)OCC=O

Products:

1. (3-allyloxyhexa-1,5-dienyl)-benzene

Typical conditions: Cp2TiCl2.AlMe3.toluene

Protections: none

Reference: *10.1016/j.tet.2007.03.015* and *10.1002/9780470638859.conrr617*

Retrosynthesis ID: 11714

2.4 Path 4

Score: 31.25

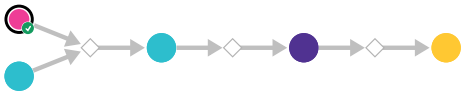
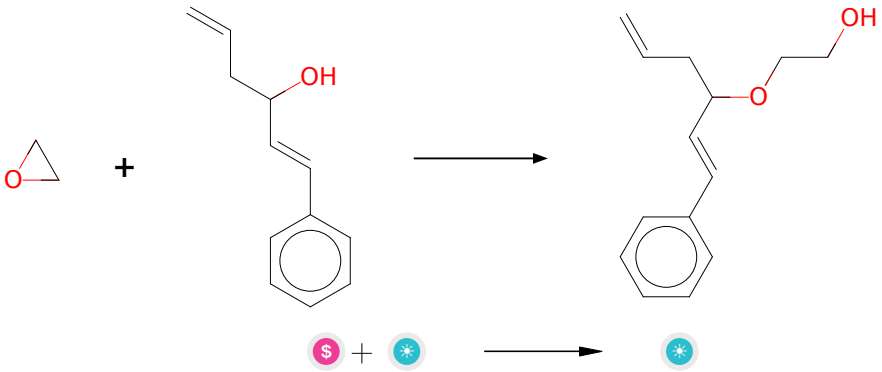


Figure 4: Outline of path 4

2.4.1 Ring-opening of epoxides or thiiranes with alkoxides



Substrates:

1. Oxirane - *available at Sigma-Aldrich*
2. (+-)-1t-phenyl-hexa-1,5-dien-3-ol

Products:

1. trans-3-(2-hydroxyethoxy)-1-phenyl-1,5-hexadiene

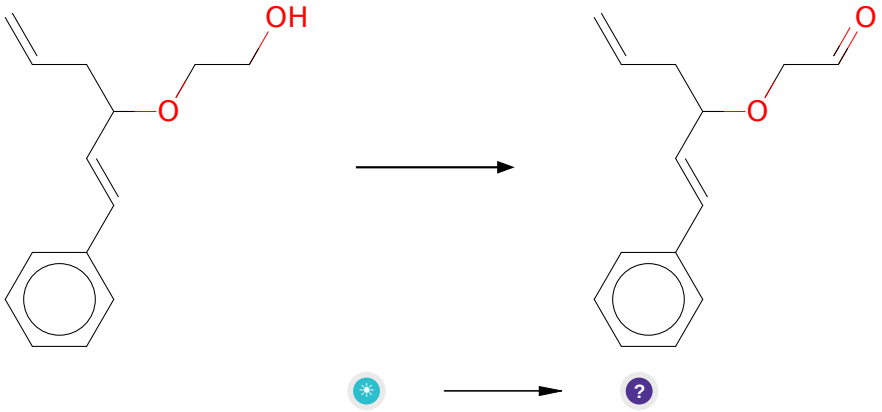
Typical conditions: NaH.THF or K2CO3.DMF.110 C

Protections: none

Reference: *10.1021/acs.orglett.7b00756* SI p. S4, S5 and *10.1021/jm401625b* p. 873, 878

Retrosynthesis ID: 833

2.4.2 Oxidation of primary alcohols with DMP



Substrates:

1. trans-3-(2-hydroxyethoxy)-1-phenyl-1,5-hexadiene

Products:

1. C=CCC(/C=C/c1ccccc1)OCC=O

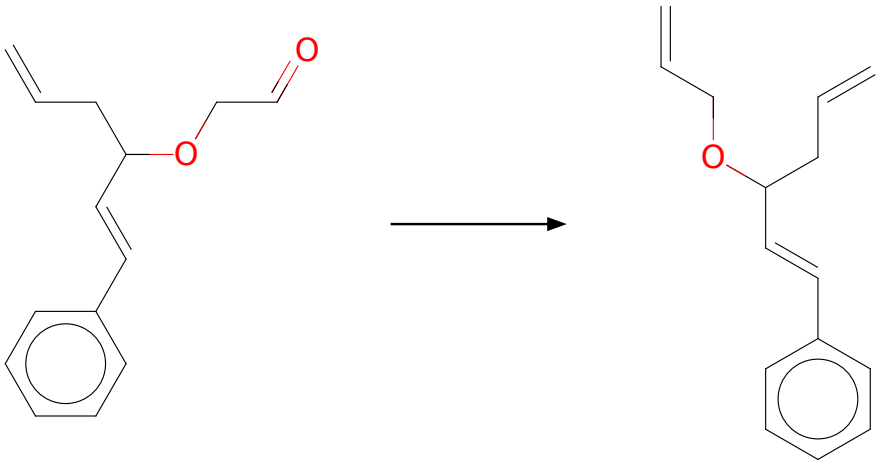
Typical conditions: DMP.DCM.0-25 C

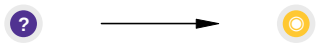
Protections: none

Reference: *10.1016/j.bmc.2020.115469* p. 3, 9 and *10.1021/acs.jmedchem.8b01878* SI p. S43

Retrosynthesis ID: 50426

2.4.3 Tebbe Olefination





Substrates:

1. C=CCC(/C=C/c1ccccc1)OCC=O

Products:

1. (3-allyloxyhexa-1,5-dienyl)-benzene

Typical conditions: Cp2TiCl2.AlMe3.toluene

Protections: none

Reference: *10.1016/j.tet.2007.03.015* and *10.1002/9780470638859.conrr617*

Retrosynthesis ID: 11714

2.5 Path 5

Score: 39.06

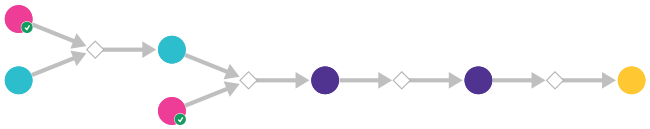
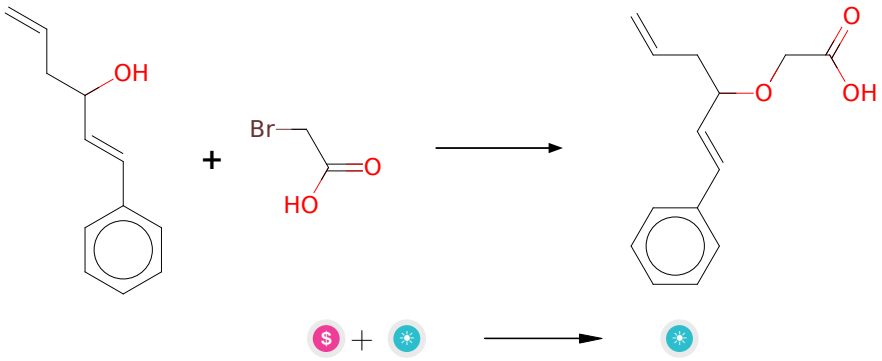


Figure 5: Outline of path 5

2.5.1 Reaction of alpha-bromo carbonyl compounds with alcohols or phenols



Substrates:

1. Bromoacetic acid - *available at Sigma-Aldrich*
2. (+-)-1t-phenyl-hexa-1,5-dien-3-ol

Products:

1. trans-3-(carboxymethoxy)-1-phenyl-1,5-hexadiene

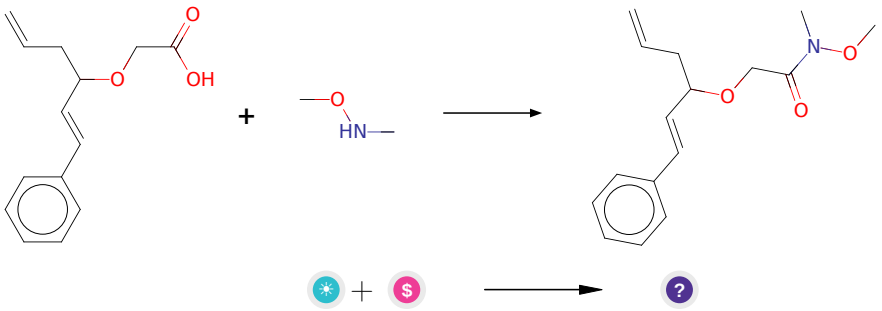
Typical conditions: NaOH.EtOH

Protections: none

Reference: *10.1021/jm070511x* AND *10.1021/op1002038* AND *10.1007/BF00758669* AND *10.1021/ja01117a054*

Retrosynthesis ID: 14804

2.5.2 Synthesis of O-substituted N-substituted hydroxamic acids



Substrates:

1. trans-3-(carboxymethoxy)-1-phenyl-1,5-hexadiene
2. n-methoxymethylamine - *available at Sigma-Aldrich*

Products:

1. C=CCC(/C=C/c1ccccc1)OCC(=O)N(C)OC

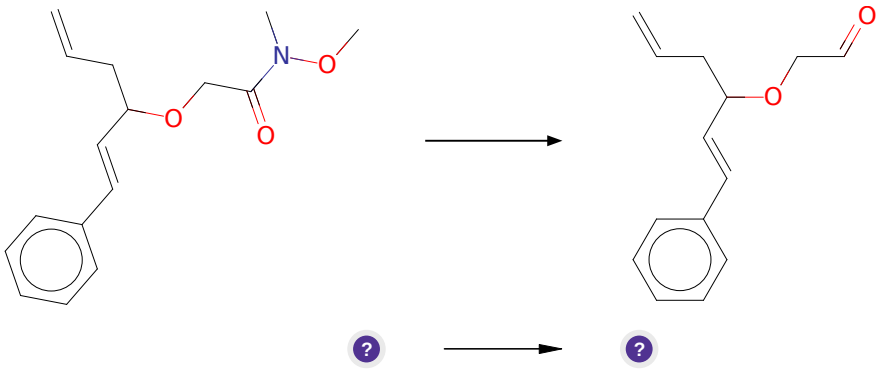
Typical conditions: DCC.DMAP or CDI.TEA.DCM

Protections: none

Reference: Patent: WO2007/67333A2, 2007 & *10.1016/j.bmcl.2008.09.100*

Retrosynthesis ID: 1152

2.5.3 Aldehyde Formation



Substrates:

1. C=CCC(/C=C/c1ccccc1)OCC(=O)N(C)OC

Products:

1. C=CCC(/C=C/c1ccccc1)OCC=O

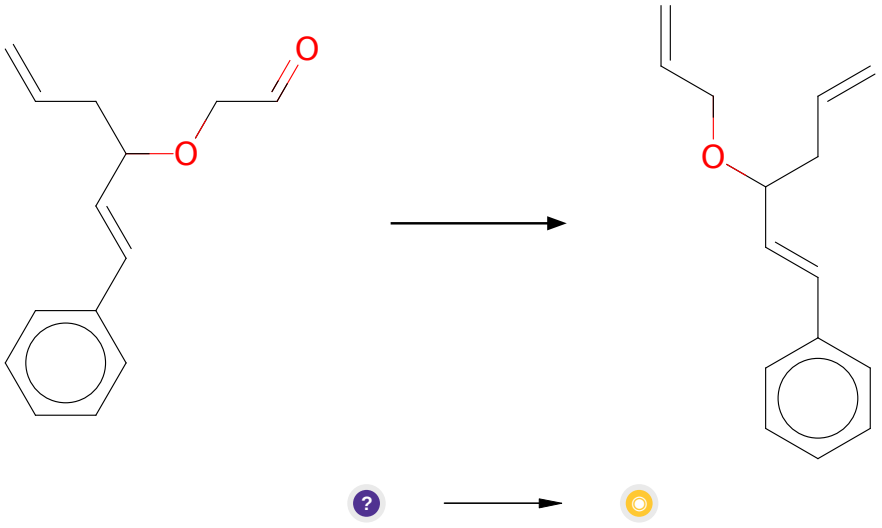
Typical conditions: DIBAL.toluene.CO

Protections: none

Reference: *10.1021/jo202652f*

Retrosynthesis ID: 11504

2.5.4 Tebbe Olefination



Substrates:

1. C=CCC(/C=C/c1ccccc1)OCC=O

Products:

1. (3-allyloxyhexa-1,5-dienyl)-benzene

Typical conditions: Cp2TiCl2.AlMe3.toluene

Protections: none

Reference: *10.1016/j.tet.2007.03.015* and *10.1002/9780470638859.conrr617*

Retrosynthesis ID: 11714