Paths of analysis*

PG3

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

*The results stated herein were generated using the proprietary platform owned and maintained by Grzybowski Scientific Inventions, Inc., a subsidiary of Merck KGaA, Darmstadt Germany. The results are provided on an as is basis, and shall be used solely in connection with the rights afforded in the license agreement and for no other purpose.

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: `45.00`

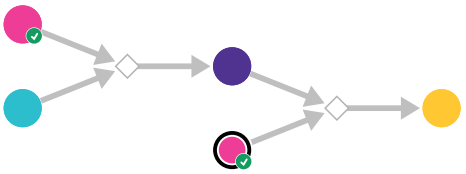
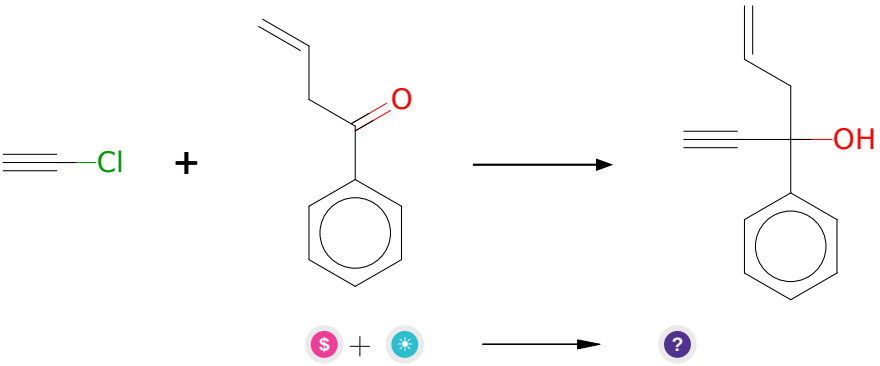


Figure 1: Outline of path 1

2.1.1 Grignard Reaction



Substrates:

1. 1-phenylbut-3-en-1-one - *available at Sigma-Aldrich*
2. chloroethyne

Products:

1. C#CC(O)(CC=C)c1ccccc1

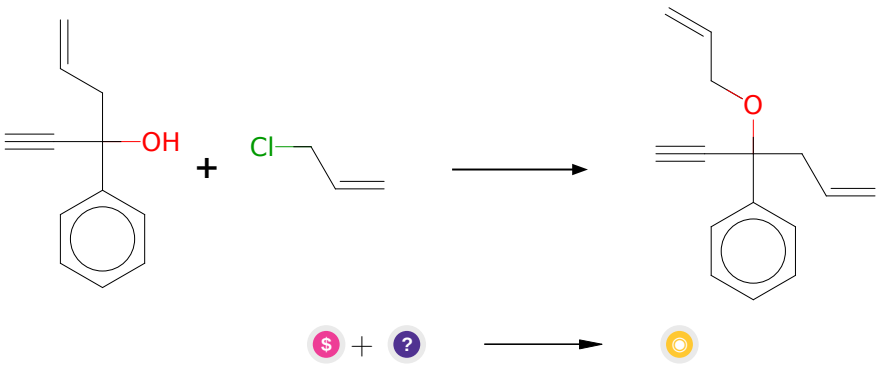
Typical conditions: Mg.ether

Protections: none

Reference: *10.1039/C0CC02612C* or *10.1002/cber.19681011029*

Retrosynthesis ID: 10219

2.1.2 Alkylation of tertiary alcohols



Substrates:

1. Chlorallylene - *available at Sigma-Aldrich*
2. C#CC(O)(CC=C)c1ccccc1

Products:

1. C#CC(CC=C)(OCC=C)c1ccccc1

Typical conditions: K2CO3.acetone.heat

Protections: none

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

Retrosynthesis ID: 31010936

2.2 Path 2

Score: `48.83`

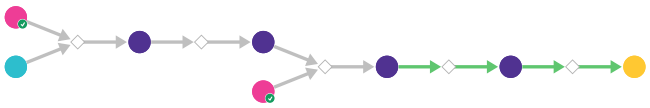
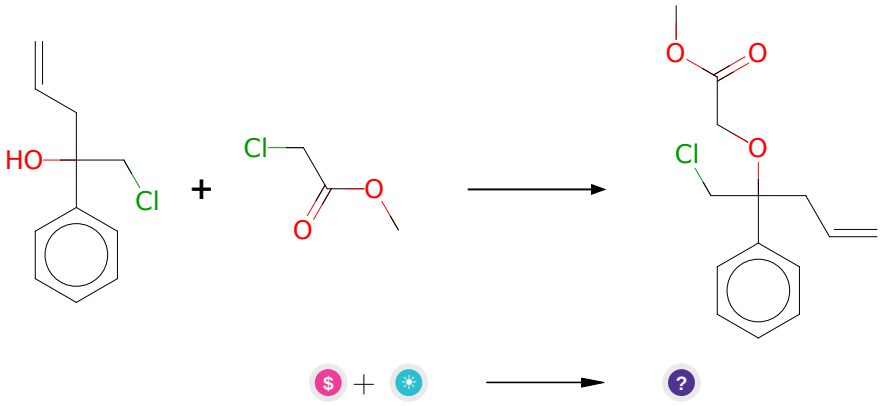


Figure 2: Outline of path 2

2.2.1 Alkylation of tertiary alcohols



Substrates:

1. Methyl chloroacetate - *available at Sigma-Aldrich*
2. 1-chloro-2-phenyl-pent-4-en-2-ol

Products:

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

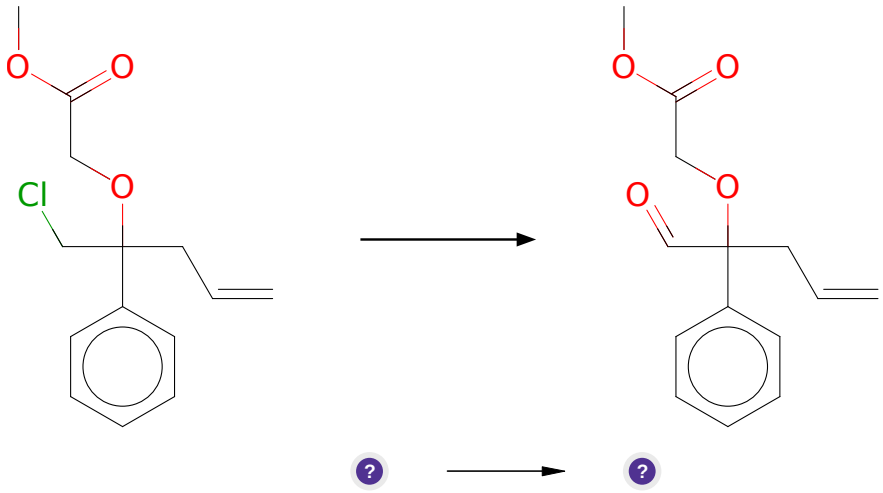
Typical conditions: K2CO3.acetone.heat

Protections: none

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

Retrosynthesis ID: 31010936

2.2.2 Kornblum Oxidation



Substrates:

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

Products:

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

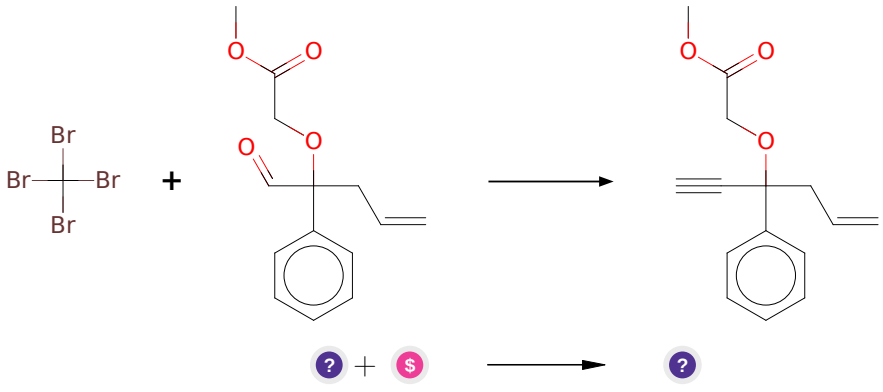
Typical conditions: DMSO.NEt3

Protections: none

Reference: *10.1080/00397918608056381* and *10.1002/9780470638859.conrr373*

Retrosynthesis ID: 11658

2.2.3 Corey-Fuchs reaction



Substrates:

1. C=CCC(C=O)(OCC(=O)OC)c1ccccc1
2. Tetrabromomethane - *available at Sigma-Aldrich*

Products:

1. C#CC(CC=C)(OCC(=O)OC)c1ccccc1

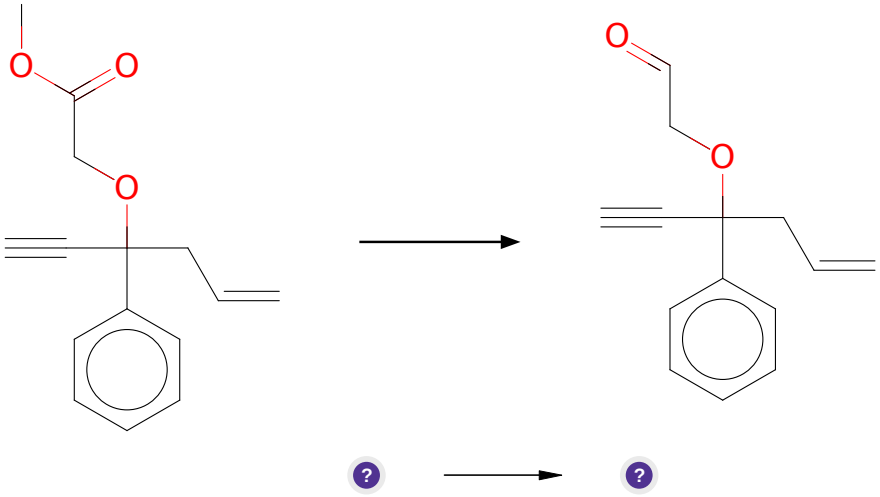
Typical conditions: PPh3.BuLi.CBr4

Protections: none

Reference: *10.1002/ejoc.200601137* and *10.1016/S0040-4039(01)94157-7*

Retrosynthesis ID: 10912

2.2.4 Aldehyde Formation



Substrates:

1. C#CC(CC=C)(OCC(=O)OC)c1ccccc1

Products:

1. C#CC(CC=C)(OCC=O)c1ccccc1

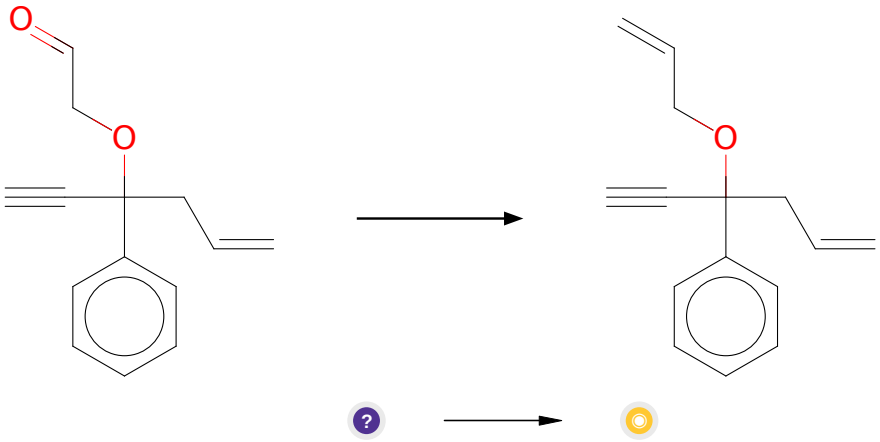
Typical conditions: DIBAL.solvent e.g. DCM

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

2.2.5 Tebbe Olefination



Substrates:

1. C#CC(CC=C)(OCC=O)c1ccccc1

Products:

1. C#CC(CC=C)(OCC=C)c1ccccc1

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: 48.83

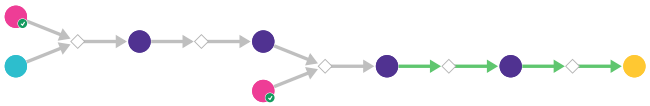
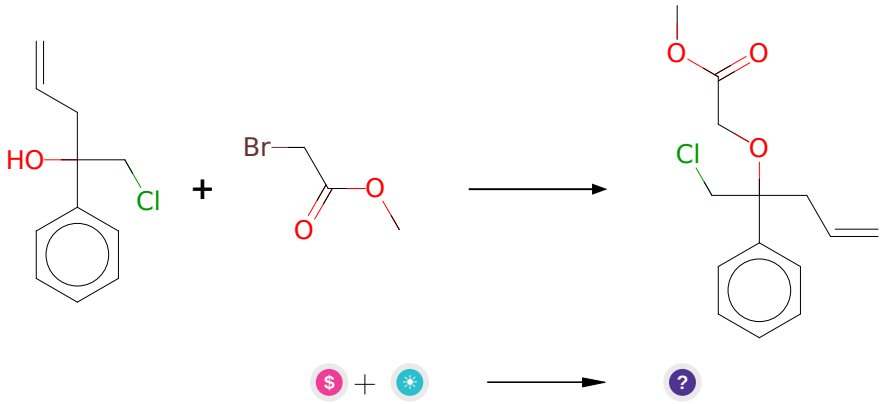


Figure 3: Outline of path 3

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



Substrates:

1. Methyl bromoacetate - *available at Sigma-Aldrich*
2. 1-chloro-2-phenyl-pent-4-en-2-ol

Products:

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

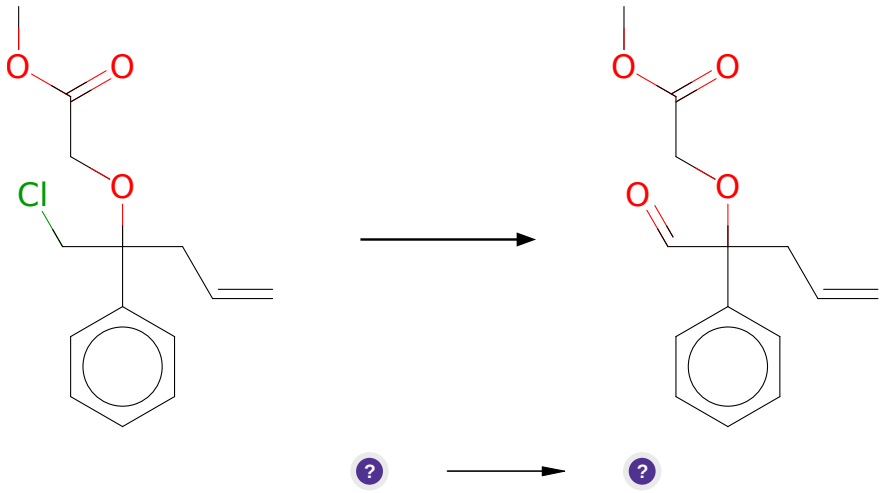
Typical conditions: NaOH.EtOH

Protections: none

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

Retrosynthesis ID: 14804

2.3.2 Kornblum Oxidation



Substrates:

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

Products:

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

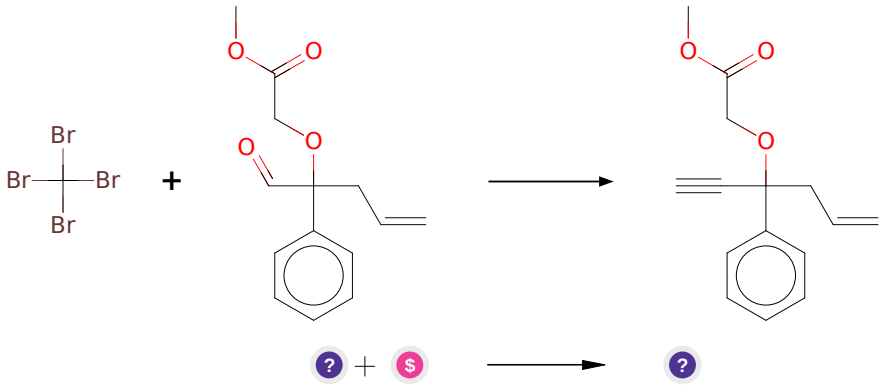
Typical conditions: DMSO.NEt3

Protections: none

Reference: *10.1080/00397918608056381* and *10.1002/9780470638859.conrr373*

Retrosynthesis ID: 11658

2.3.3 Corey-Fuchs reaction



Substrates:

1. C=CCC(C=O)(OCC(=O)OC)c1ccccc1
2. Tetrabromomethane - *available at Sigma-Aldrich*

Products:

1. C#CC(CC=C)(OCC(=O)OC)c1ccccc1

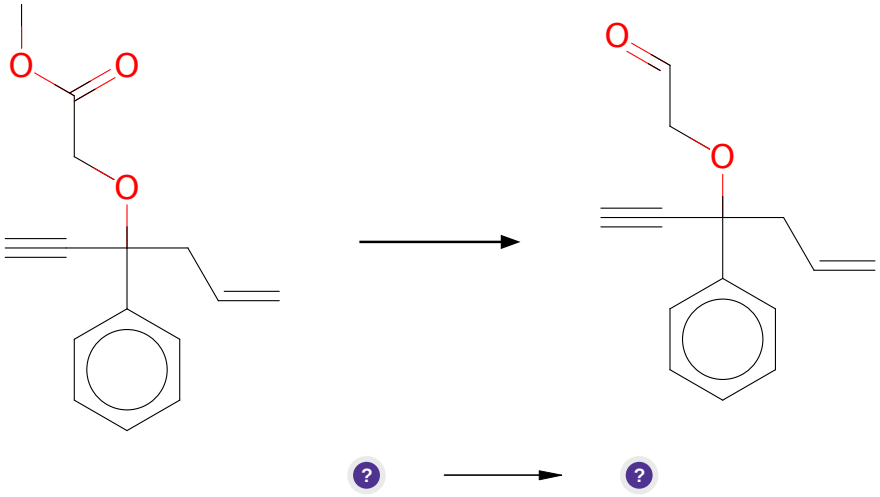
Typical conditions: PPh3.BuLi.CBr4

Protections: none

Reference: *10.1002/ejoc.200601137* and *10.1016/S0040-4039(01)94157-7*

Retrosynthesis ID: 10912

2.3.4 Aldehyde Formation



Substrates:

1. C#CC(CC=C)(OCC(=O)OC)c1ccccc1

Products:

1. C#CC(CC=C)(OCC=O)c1ccccc1

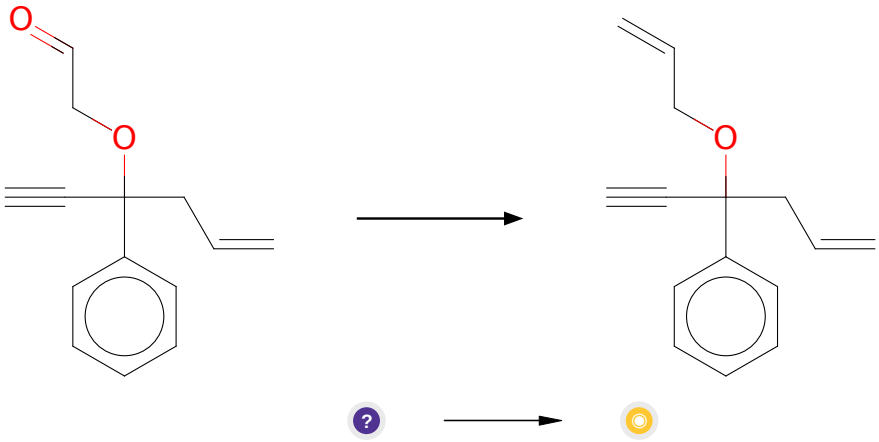
Typical conditions: DIBAL.solvent e.g. DCM

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

2.3.5 Tebbe Olefination



Substrates:

1. C#CC(CC=C)(OCC=O)c1ccccc1

Products:

1. C#CC(CC=C)(OCC=C)c1ccccc1

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: `51.25`

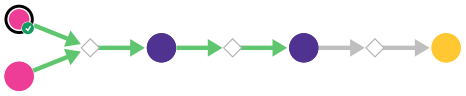
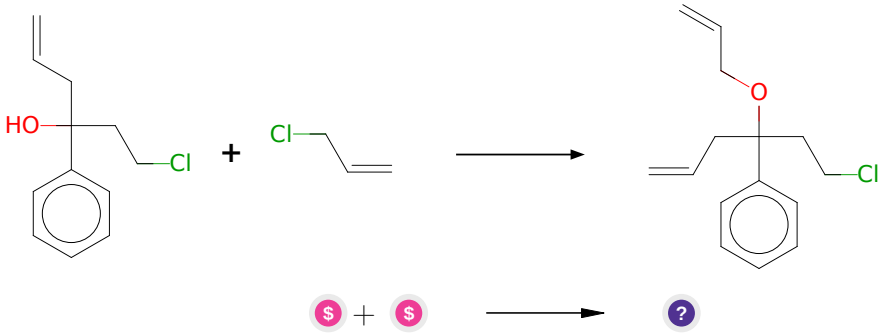


Figure 4: Outline of path 4

2.4.1 Alkylation of tertiary alcohols



Substrates:

1. Chlorallylene - *available at Sigma-Aldrich*
2. 1-chloro-3-phenyl-5-hexen-3-ol - *A1BioChemLabs*

Products:

1. C=CCOC(CC=C)(CCCl)c1ccccc1

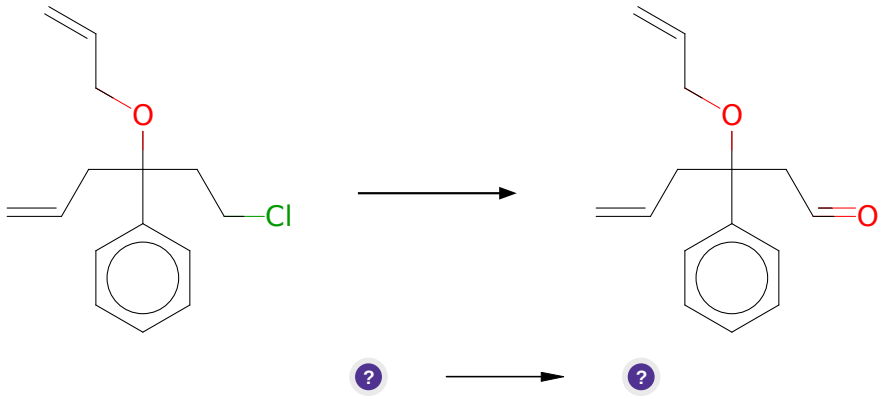
Typical conditions: K2CO3.acetone.heat

Protections: none

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

Retrosynthesis ID: 31010936

2.4.2 Kornblum Oxidation



Substrates:

1. C=CCOC(CC=C)(CCCl)c1ccccc1

Products:

1. C=CCOC(CC=C)(CC=O)c1ccccc1

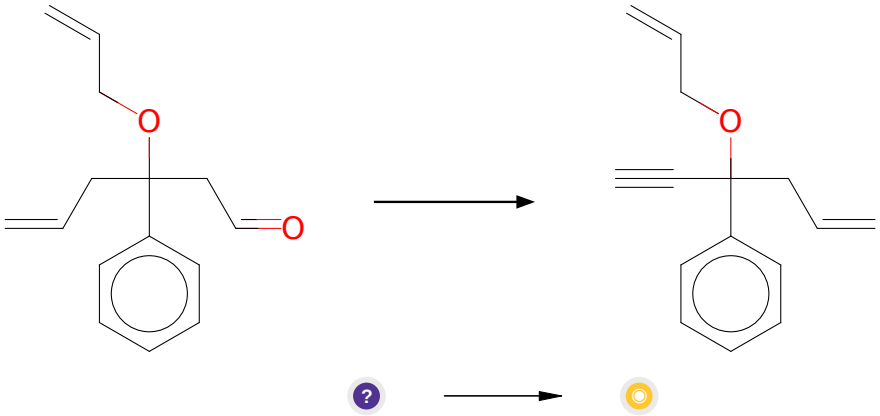
Typical conditions: DMSO.NEt3

Protections: none

Reference: *10.1080/00397918608056381* and *10.1002/9780470638859.conrr373*

Retrosynthesis ID: 11658

2.4.3 Synthesis of alkynes from aldehydes



Substrates:

1. C=CCOC(CC=C)(CC=O)c1ccccc1

Products:

1. C#CC(CC=C)(OCC=C)c1ccccc1

Typical conditions: P1-base.DMF

Protections: none

Reference: *10.1055/s-0028-1087919*

Retrosynthesis ID: 15028

2.5 Path 5

Score: 56.25

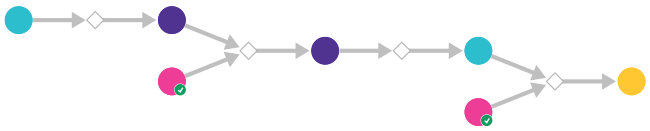
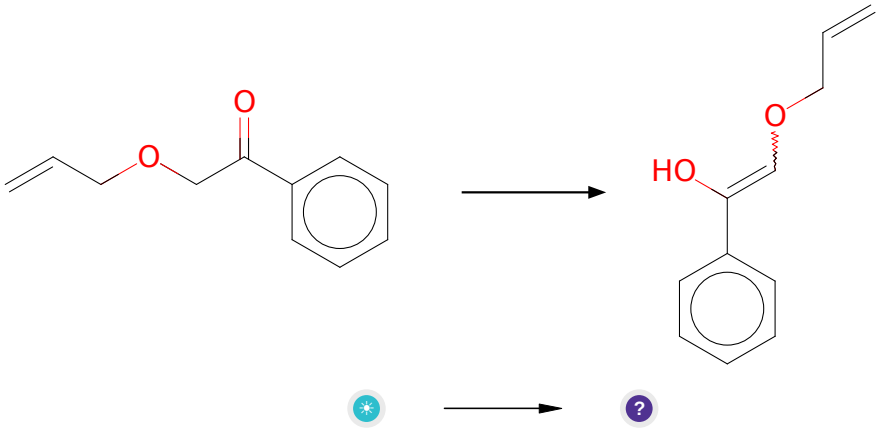


Figure 5: Outline of path 5

2.5.1 Keto-enol Tautomerism



Substrates:

1. allyl-phenacyl-ether

Products:

1. C=CCOC=C(O)c1ccccc1

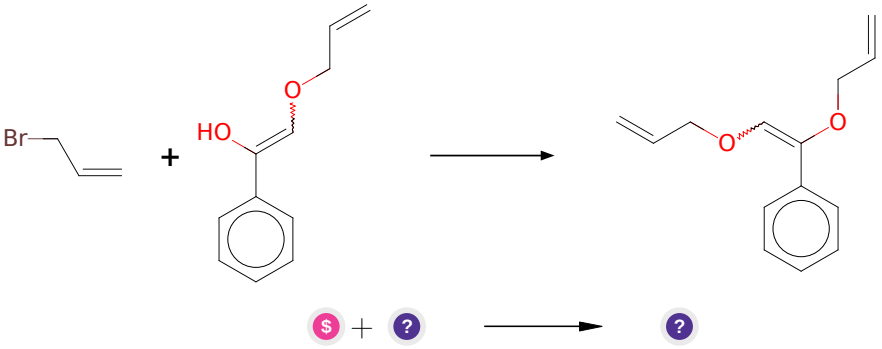
Typical conditions: solvent

Protections: none

Reference: *10.1021/ja01065a003* AND *10.1021/jo8012385*

Retrosynthesis ID: 7780

2.5.2 Enolate O-Alkylation



Substrates:

1. Allyl bromide - *available at Sigma-Aldrich*
2. C=CCOC=C(O)c1ccccc1

Products:

1. C=CCOC=C(OCC=C)c1ccccc1

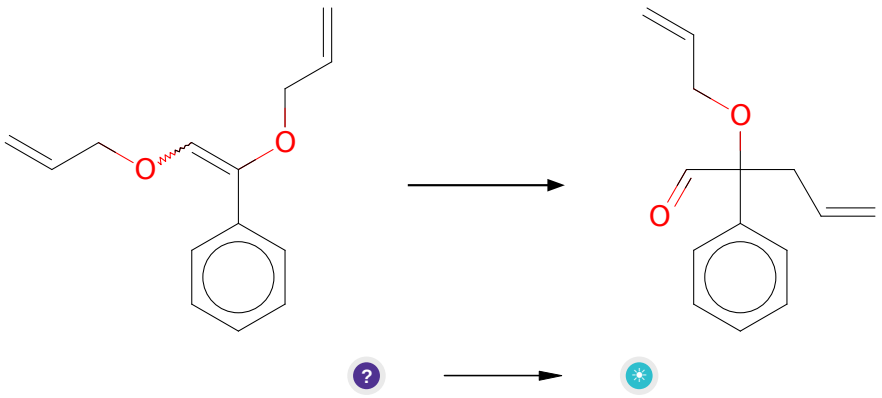
Typical conditions: Cs2CO3.DMF

Protections: none

Reference: *10.1016/j.bmcl.2012.05.070* and *10.1039/b612336h*

Retrosynthesis ID: 14841

2.5.3 Claisen Rearrangement



Substrates:

1. C=CCOC=C(OCC=C)c1ccccc1

Products:

1. rac-2-allyloxy-2-phenylpent-4-enal

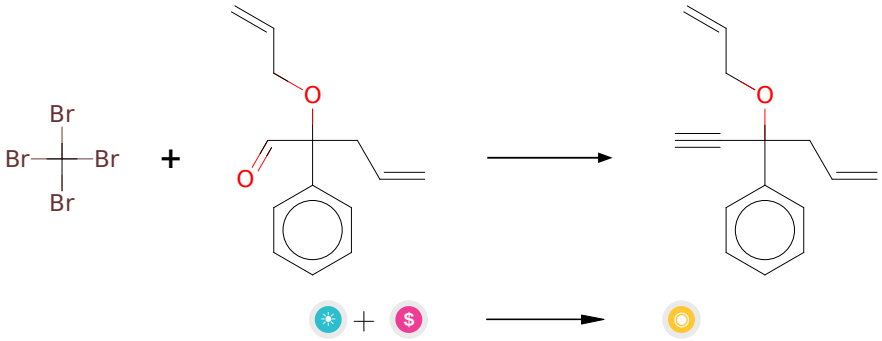
Typical conditions: heat

Protections: none

Reference: DOI: *10.1021/ja00206a017* and *10.1016/S0022-1139(98)00313-3*

Retrosynthesis ID: 1226

2.5.4 Corey-Fuchs reaction



Substrates:

1. rac-2-allyloxy-2-phenylpent-4-enal
2. Tetrabromomethane - *available at Sigma-Aldrich*

Products:

1. C#CC(CC=C)(OCC=C)c1ccccc1

Typical conditions: PPh3.BuLi.CBr4

Protections: none

Reference: *10.1002/ejoc.200601137* and *10.1016/S0040-4039(01)94157-7*

Retrosynthesis ID: 10912