Paths of analysis*

PG2

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: `31.25`

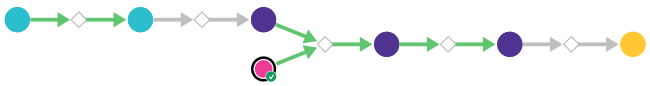
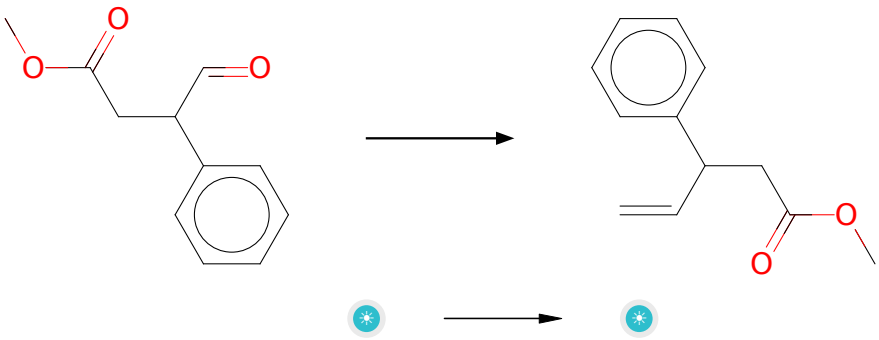


Figure 1: Outline of path 1

2.1.1 Tebbe Olefination



Substrates:

1. 4-oxo-3-phenylbutansaeure-methylester

Products:

1. methyl 3-phenyl-4-pentenoate

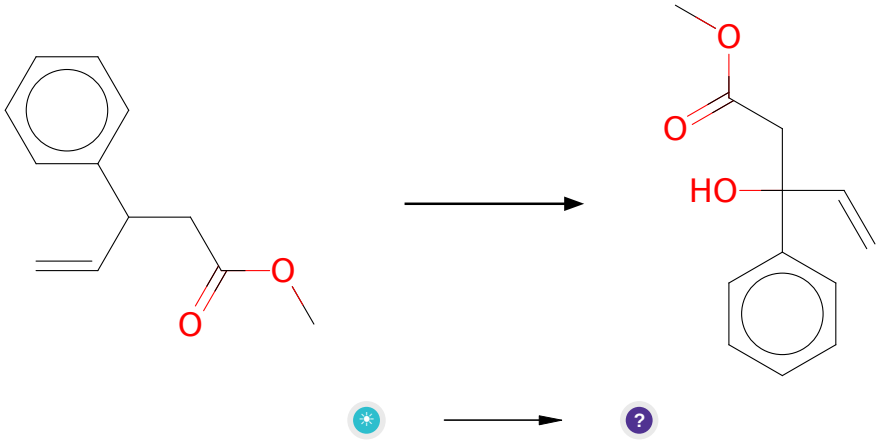
Typical conditions: Cp2TiCl2.AlMe3.toluene

Protections: none

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

Retrosynthesis ID: 11714

2.1.2 Allylic oxidation to alcohol



Substrates:

1. methyl 3-phenyl-4-pentenoate

Products:

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

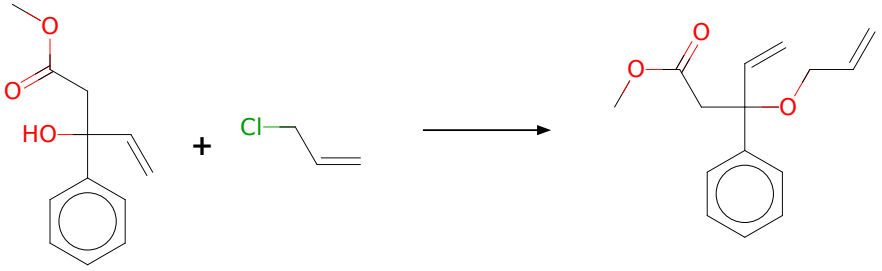
Typical conditions: ArCOOOH or t-BuOOOH

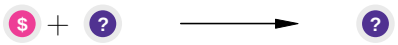
Protections: none

Reference: DOI: *10.1021/ja00458a072* AND *10.1016/j.tetlet.2013.03.046* AND *10.1039/b612423b*

Retrosynthesis ID: 7603

2.1.3 Alkylation of tertiary alcohols





Substrates:

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

Products:

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

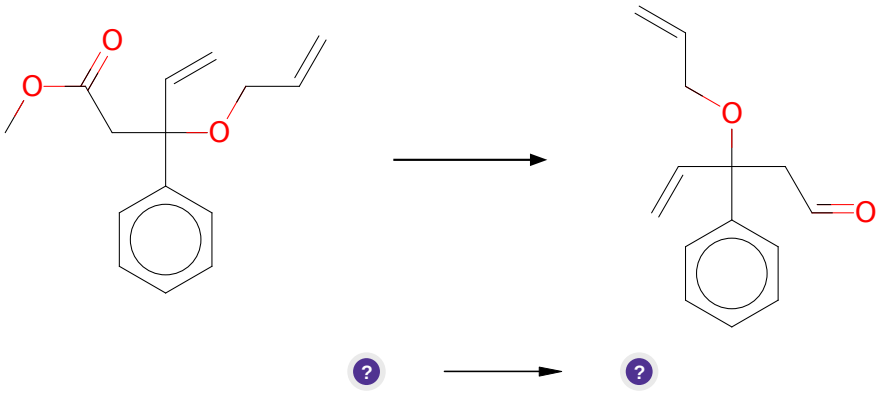
Typical conditions: K2CO3.acetone.heat

Protections: none

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

Retrosynthesis ID: 31010936

2.1.4 Aldehyde Formation



Substrates:

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

Products:

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

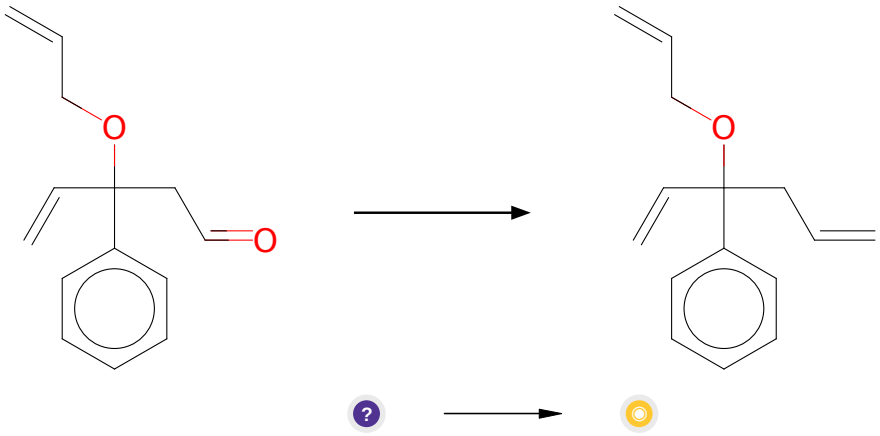
Typical conditions: DIBAL.solvent e.g. DCM

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

2.1.5 Tebbe Olefination



Substrates:

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

Products:

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

2.2 Path 2

Score: `45.00`

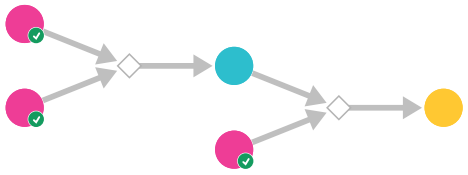
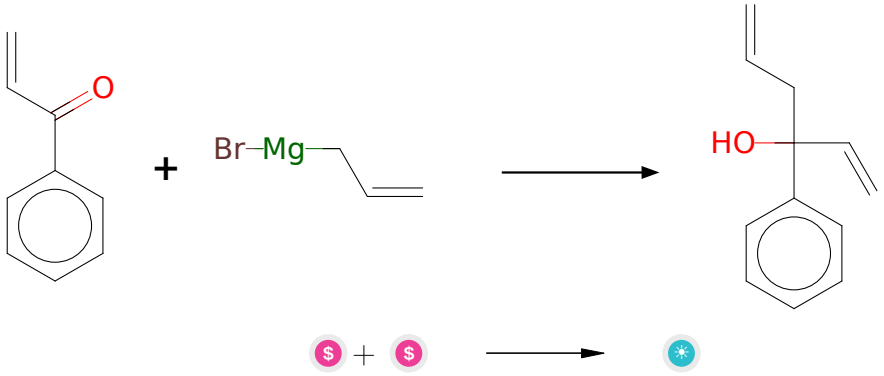


Figure 2: Outline of path 2

2.2.1 Grignard-Type Reaction



Substrates:

1. 1-Phenylprop-2-en-1-one - *available at Sigma-Aldrich*
2. Allylmagnesium bromide solution - *available at Sigma-Aldrich*

Products:

1. 3-phenyl-1,5-hexadien-3-ol

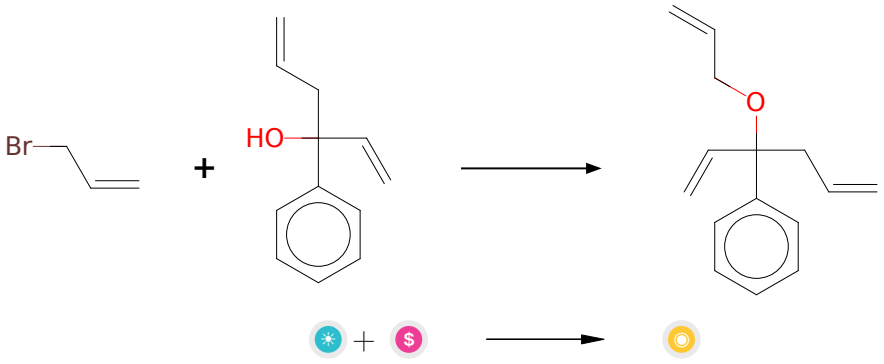
Typical conditions: Mg or Li.ether

Protections: none

Reference: *10.1021/jo010494y* or *10.1016/j.steroids.2015.09.009* or *10.1021/jo061349t* or *10.1021/ja056165v* (SI page 19)

Retrosynthesis ID: 25134

2.2.2 Alkylation of tertiary alcohols



Substrates:

1. 3-phenyl-1,5-hexadien-3-ol
2. Allyl bromide - *available at Sigma-Aldrich*

Products:

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

Typical conditions: K2CO3.acetone.heat

Protections: none

Reference: *10.1002/anie.201909177* and *10.1016/j.jfluchem.2019.109388* and *10.2174/1570178613106660077*

Retrosynthesis ID: 31010955

2.3 Path 3

Score: 45.00

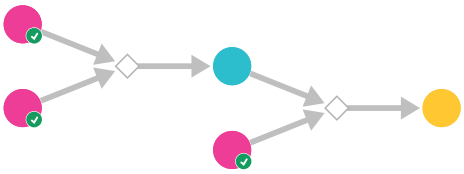
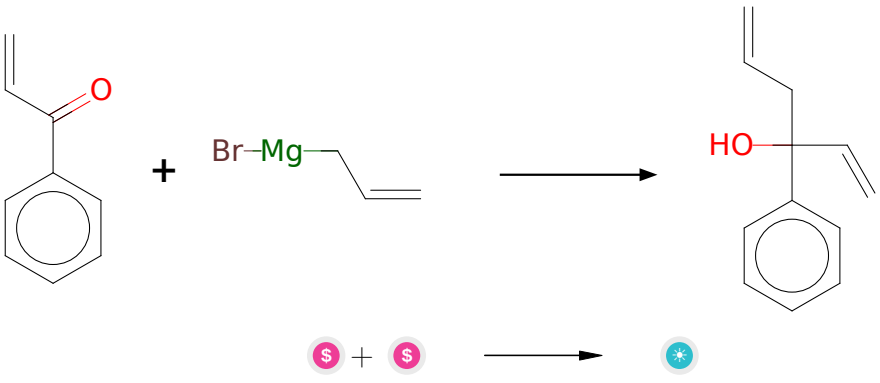


Figure 3: Outline of path 3

2.3.1 Grignard-Type Reaction



Substrates:

1. 1-Phenylprop-2-en-1-one - *available at Sigma-Aldrich*
2. Allylmagnesium bromide solution - *available at Sigma-Aldrich*

Products:

1. 3-phenyl-1,5-hexadien-3-ol

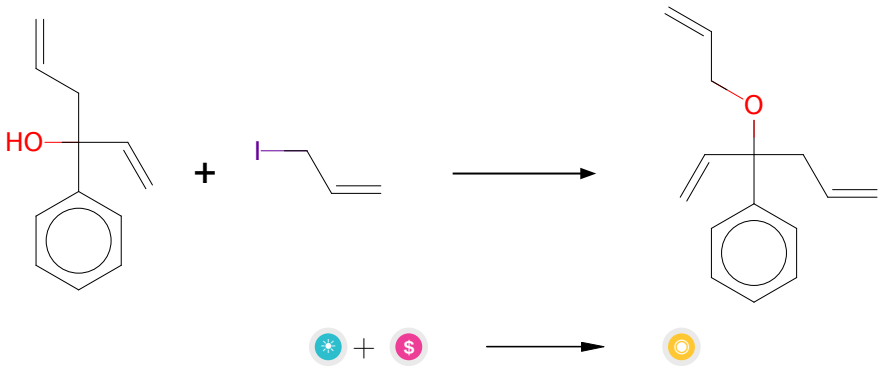
Typical conditions: Mg or Li.ether

Protections: none

Reference: *10.1021/jo010494y* or *10.1016/j.steroids.2015.09.009* or *10.1021/jo061349t* or *10.1021/ja056165v* (SI page 19)

Retrosynthesis ID: 25134

2.3.2 Alkylation of tertiary alcohols



Substrates:

1. 3-phenyl-1,5-hexadien-3-ol
2. Allyl iodide - *available at Sigma-Aldrich*

Products:

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

Typical conditions: K2CO3.acetone.heat

Protections: none

Reference: *10.1039/P29910000147* and *10.1038/ncomms7703*

Retrosynthesis ID: 31010959

2.4 Path 4

Score: 45.00

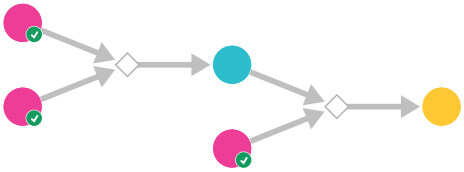
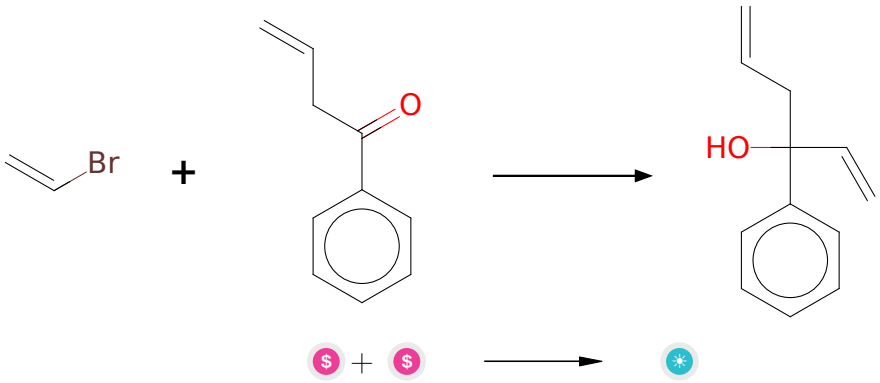


Figure 4: Outline of path 4

2.4.1 Grignard addition to ketone



Substrates:

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

Products:

1. 3-phenyl-1,5-hexadien-3-ol

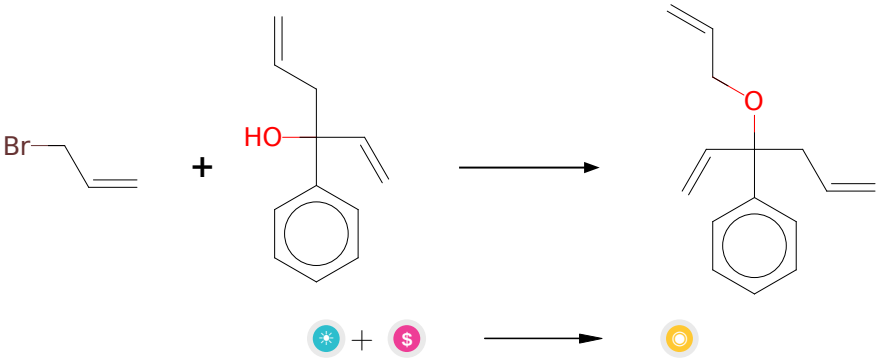
Typical conditions: Mg.THF.or.iPrMgClxLiCl

Protections: none

Reference: *10.3762/bjoc.9.175* and *10.1016/j.tetlet.2012.08.088* and *10.1002/anie.200504247* (supporting info)

Retrosynthesis ID: 18170

2.4.2 Alkylation of tertiary alcohols



Substrates:

1. 3-phenyl-1,5-hexadien-3-ol
2. Allyl bromide - *available at Sigma-Aldrich*

Products:

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

Typical conditions: K2CO3.acetone.heat

Protections: none

Reference: *10.1002/anie.201909177* and *10.1016/j.jfluchem.2019.109388* and *10.2174/1570178613106660077*

Retrosynthesis ID: 31010955

2.5 Path 5

Score: `45.00`

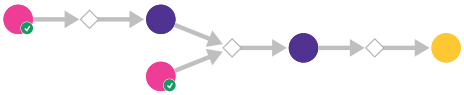
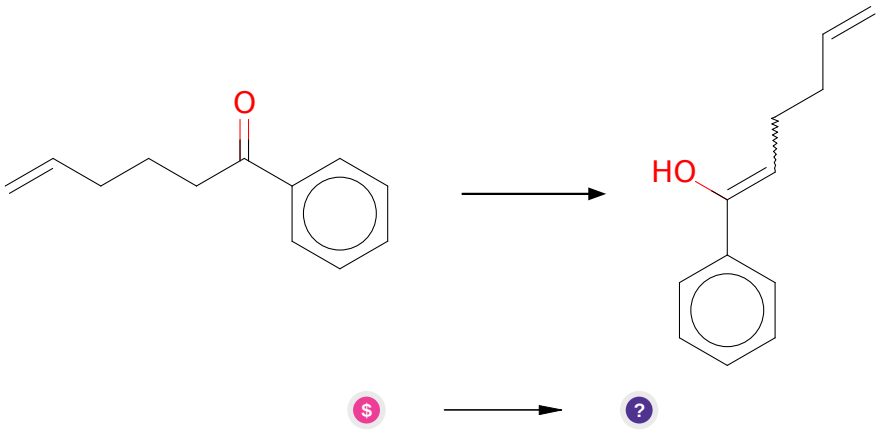


Figure 5: Outline of path 5

2.5.1 Keto-enol Tautomerism



Substrates:

1. 1-phenylhex-5-en-1-one - *available at Sigma-Aldrich*

Products:

1. C=CCCC=C(O)c1ccccc1

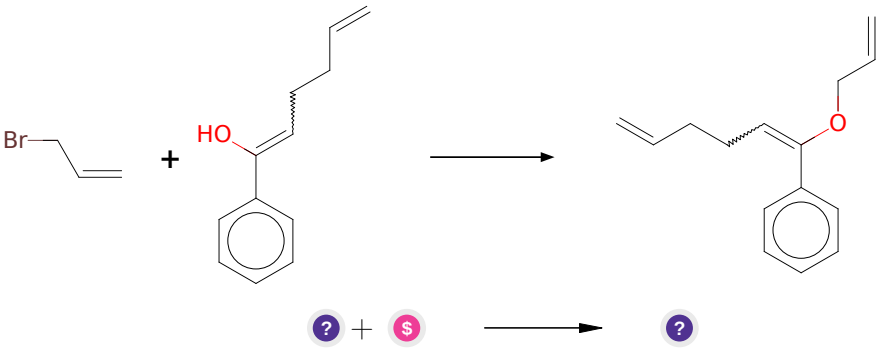
Typical conditions: solvent

Protections: none

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

Retrosynthesis ID: 7780

2.5.2 Enolate O-Alkylation



Substrates:

1. C=CCCC=C(O)c1ccccc1

2. Allyl bromide - *available at Sigma-Aldrich*

Products:

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

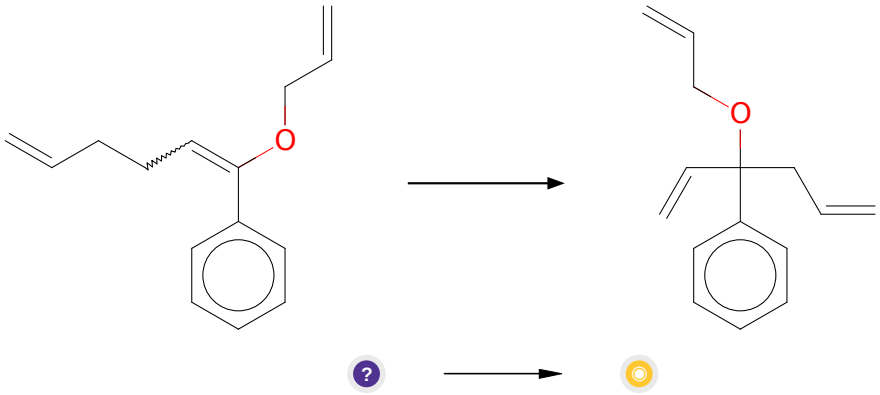
Typical conditions: Cs2CO3.DMF

Protections: none

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

Retrosynthesis ID: 14841

2.5.3 Cope rearrangement



Substrates:

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

Products:

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

Typical conditions: KH.THF.or.heat

Protections: none

Reference: *10.1021/jo2013753* AND *10.1021/ja00849a054* AND *10.1039/C0CC05215A* AND *10.1016/B978-0-08-095167-6.00213-5*

Retrosynthesis ID: 19824