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

*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`

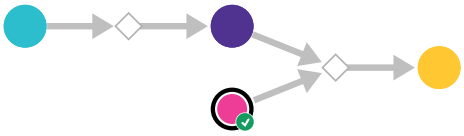
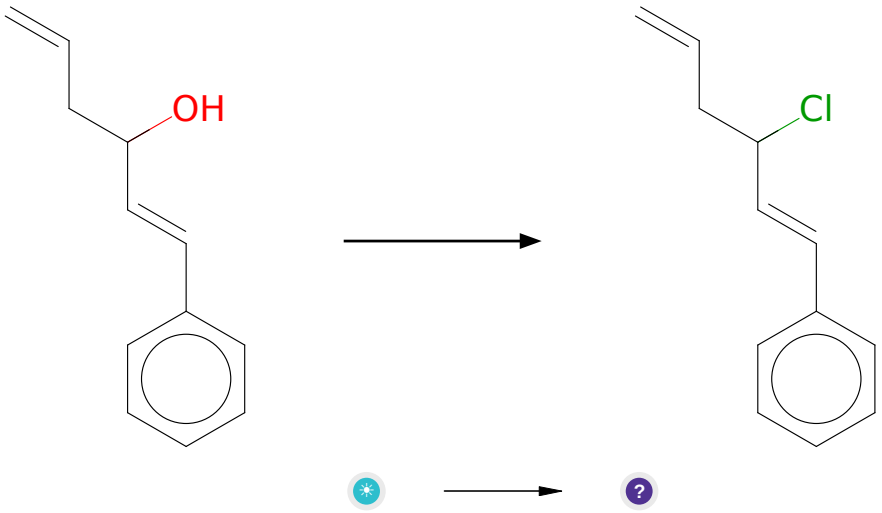


Figure 1: Outline of path 1

2.1.1 Appel Reaction



Substrates:

1. (+-)-1t-phenyl-hexa-1,5-dien-3-ol

Products:

1. C=CCC(Cl)/C=C/c1ccccc1

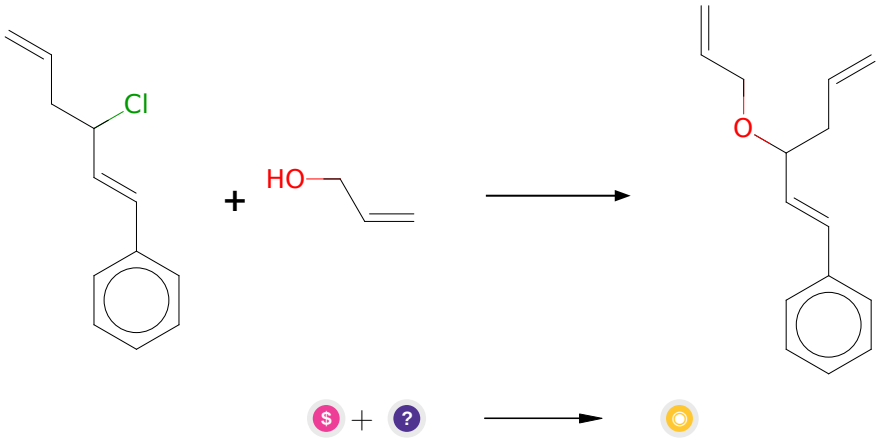
Typical conditions: PPh3.CHCl3

Protections: none

Reference: *10.1021/ja0470158* and *10.1016/j.tet.2015.03.108* and *10.1021/ol9016595* and *10.1081/CAR-120021700*

Retrosynthesis ID: 9990041

2.1.2 Alkylation of primary alcohols



Substrates:

1. 2-Propen-1-ol - *available at Sigma-Aldrich*
2. C=CCC(Cl)/C=C/c1ccccc1

Products:

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

Typical conditions: K2CO3.acetone.heat

Protections: none

Reference: *10.1021/jo00161a028* and *10.1021/acs.orglett.8b03053*

Retrosynthesis ID: 31010998

2.2 Path 2

Score: 45.00

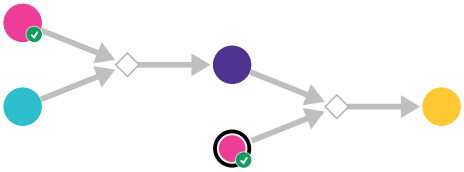
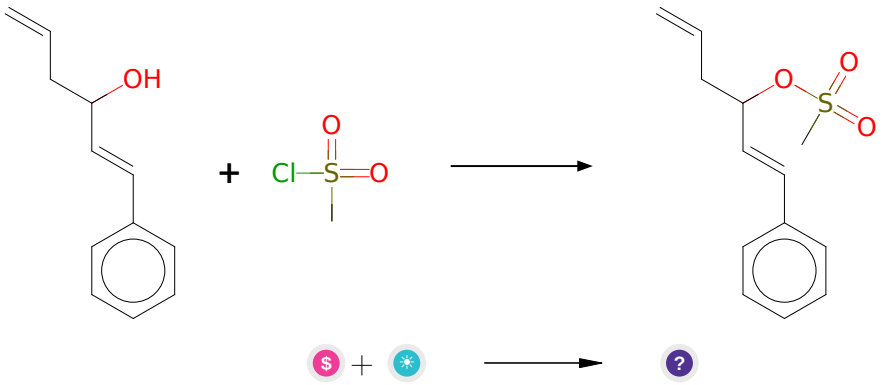


Figure 2: Outline of path 2

2.2.1 Sulfonation of secondary alcohols



Substrates:

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

Products:

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

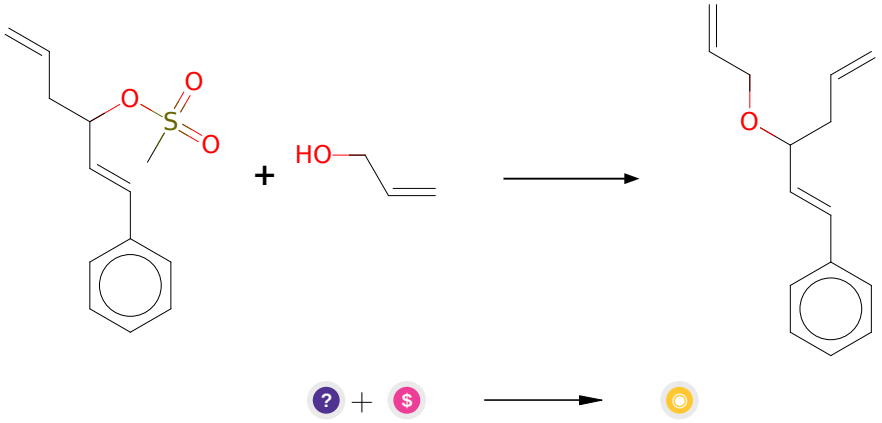
Typical conditions: Et3N.DMAP.DCM

Protections: none

Reference: *10.1021/jo048289g* and *10.1021/ja9617808* and *10.1016/j.steroids.2005.10.004*

Retrosynthesis ID: 24386

2.2.2 Alkylation of primary alcohols



Substrates:

1. C=CCC(/C=C/c1ccccc1)OS(C)(=O)=O
2. 2-Propen-1-ol - *available at Sigma-Aldrich*

Products:

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

Typical conditions: K2CO3.acetone.heat

Protections: none

Reference: *10.1021/jacs.7b02326* and *10.1021/ja01160a042* and *10.1016/S0040-4020(01)88330-7*

Retrosynthesis ID: 31011004

2.3 Path 3

Score: 45.00

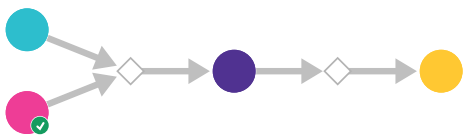
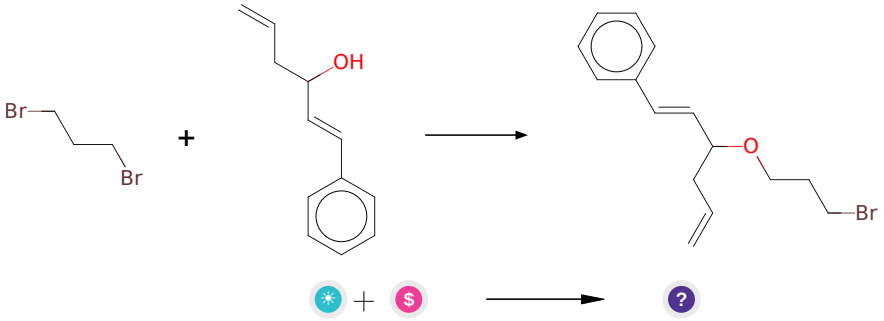


Figure 3: Outline of path 3

2.3.1 Alkylation of secondary unhindered alcohols



Substrates:

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

Products:

1. C=CCC(/C=C/c1ccccc1)OCCCBr

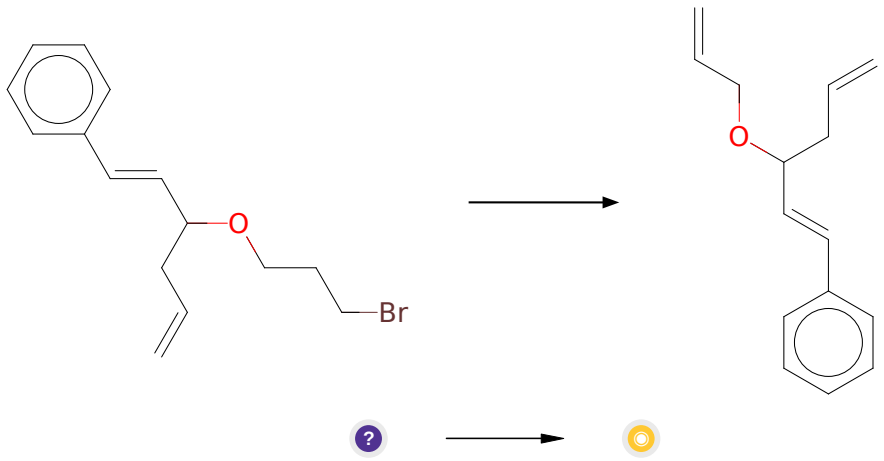
Typical conditions: K2CO3.acetone.heat

Protections: none

Reference: *10.1021/ja01212a043* and *10.1039/C0DT01321H* and *10.1002/macp.201600138*

Retrosynthesis ID: 31011052

2.3.2 Elimination of primary bromides



Substrates:

1. C=CCC(/C=C/c1ccccc1)OCCCBr

Products:

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

Typical conditions: NaOH.PTC.rt

Protections: none

Reference: *10.1021/jo00133a056* and *10.1016/j.tet.2004.06.086* and *10.1039/C6CC01880G* (suppl. Info) and *10.1080/00397919908085979* and *10.1021/jo00133a056* and *10.1002/pola.27990*

Retrosynthesis ID: 23927

2.4 Path 4

Score: 45.00

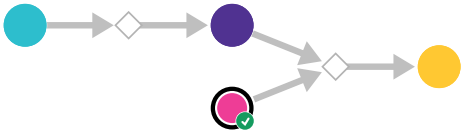
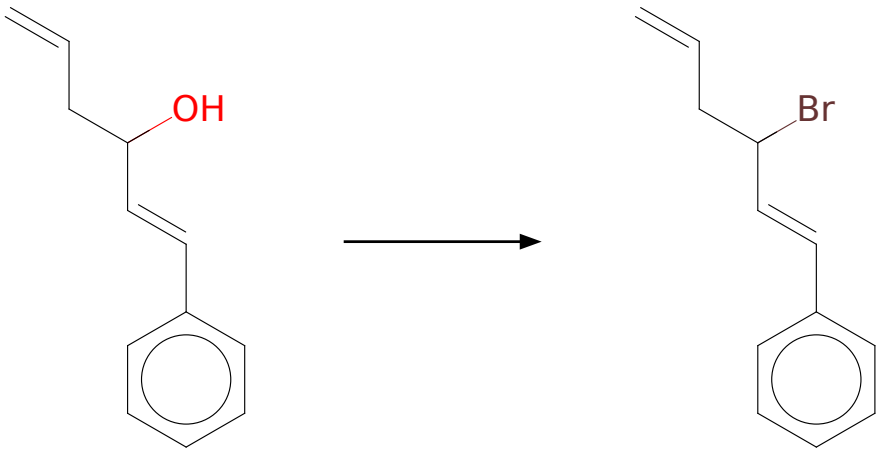
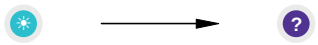


Figure 4: Outline of path 4

2.4.1 Appel Reaction





Substrates:

1. (+-)-1t-phenyl-hexa-1,5-dien-3-ol

Products:

1. C=CCC(Br)/C=C/c1ccccc1

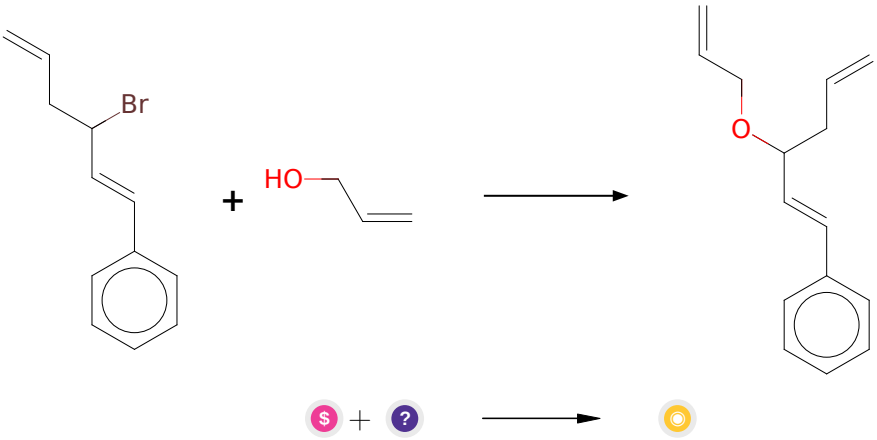
Typical conditions: PPh3.CBr4

Protections: none

Reference: *10.1016/j.jfluchem.2015.03.009* and *10.1016/j.tet.2005.12.006* and *10.1021/jm00161a029* and *10.1055/s-1995-5215*

Retrosynthesis ID: 9990042

2.4.2 Alkylation of primary alcohols



Substrates:

1. 2-Propen-1-ol - *available at Sigma-Aldrich*
2. C=CCC(Br)/C=C/c1ccccc1

Products:

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

Typical conditions: K2CO3.acetone.heat

Protections: none

Reference: *10.1016/S0040-4020(01)89360-1* and *10.1039/C4GC00005F*

Retrosynthesis ID: 31011000

2.5 Path 5

Score: 45.00

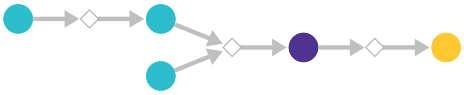
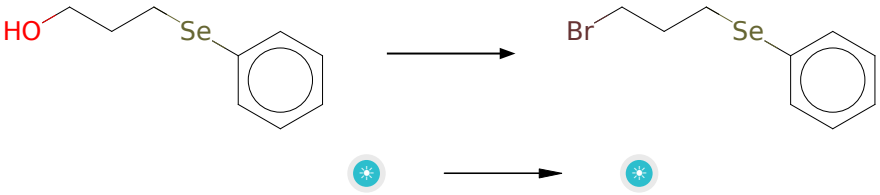


Figure 5: Outline of path 5

2.5.1 Appel Reaction



Substrates:

1. 3-phenylselenuro-1-propanol

Products:

1. 1-bromo-3-phenylselenopropane

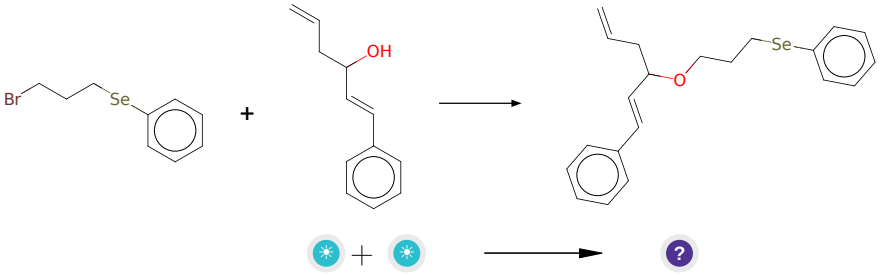
Typical conditions: PPh3.CBr4

Protections: none

Reference: *10.1021/ja800574m* and *10.1016/j.tet.2012.05.010* and *10.1016/j.tet.2004.09.021* (experimantal)

Retrosynthesis ID: 9990037

2.5.2 Alkylation of secondary unhindered alcohols



Substrates:

1. 1-bromo-3-phenylselenopropane
2. (+-)-1t-phenyl-hexa-1,5-dien-3-ol

Products:

1. C=CCC(/C=C/c1ccccc1)OCCC[Se]c1ccccc1

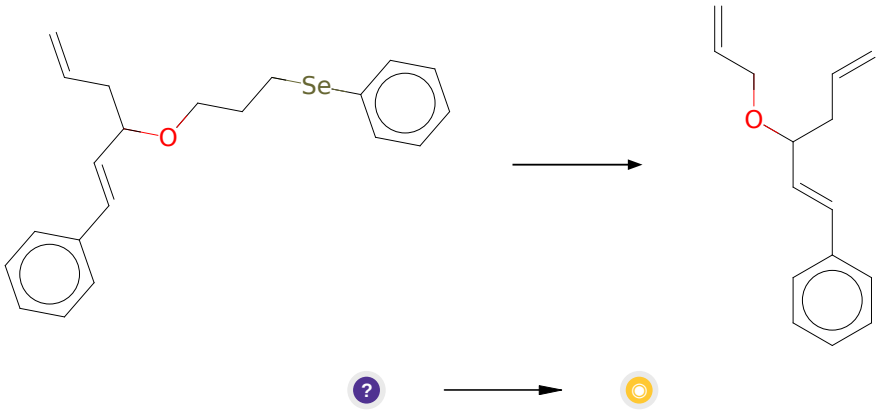
Typical conditions: K2CO3.acetone.heat

Protections: none

Reference: *10.1038/s41467-018-06099-z* and *10.1039/A808980I*

Retrosynthesis ID: 31011050

2.5.3 Selenoxide Elimination



Substrates:

1. C=CCC(/C=C/c1ccccc1)OCCC[Se]c1ccccc1

Products:

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

Typical conditions: 1) O3 or H2O2 or NaIO4. low temperature. 2) pyridine or Et3N

Protections: none

Reference: DOI: *10.1021/ja00852a019* or DOI: *10.1021/ja00258a056* or DOI: *10.1039/B716256A* or DOI: *10.1055/s-1998-1970* or DOI: *10.1016/S0040-4039(00)76646-9*

Retrosynthesis ID: 8381