Paths of analysis*

L8_DIA

Synthia

October 11, 2022

1 Analysis parameters

Analysis type: Automatic Retrosynthesis

Rules: none selected

Filters: 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

Strategies: none selected

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FGI Coeff: 0

Tunnels Coeff: 0

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: `164.14`

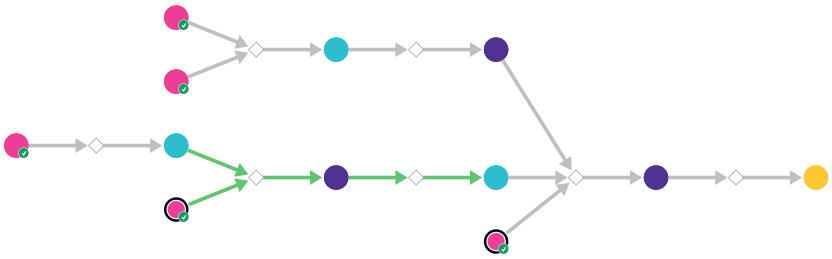
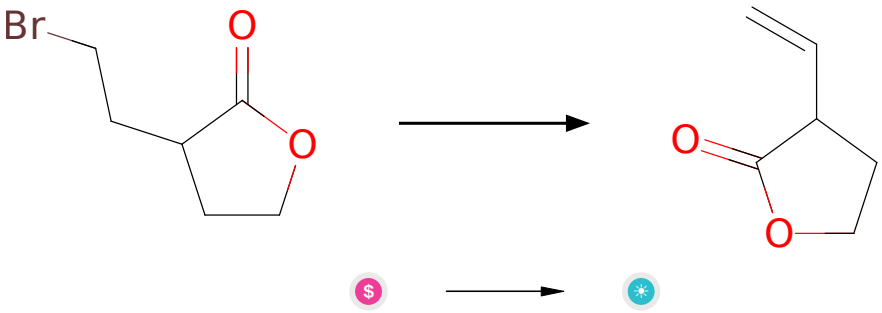


Figure 1: Outline of path 1

2.1.1 Elimination of primary bromides



Substrates:

1. 3-(2-bromoethyl)oxolan-2-one - *available at Sigma-Aldrich*

Products:

1. 3-vinyl-dihydro-furan-2-one

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

2.1.2 Enol esters and ethers synthesis

Substrates:

1. 3-vinyl-dihydro-furan-2-one
2. TMSCl - *available at Sigma-Aldrich*

Products:

1. C=CC1=C(O[Si](C)(C)C)OCC1

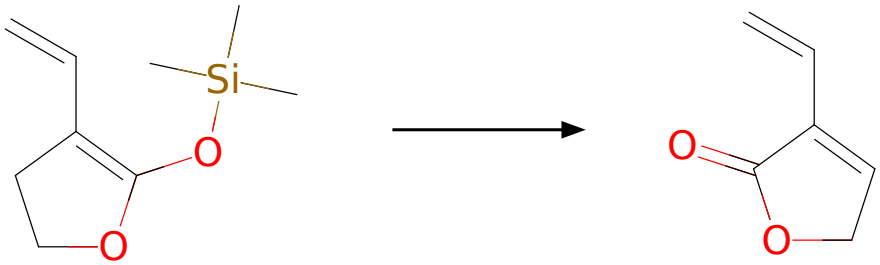
Typical conditions: 1. Et3N.Electrophile

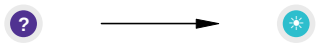
Protections: none

Reference: *10.1016/S0040-4020(03)00977-3* AND *10.1021/ja00056a002*

Retrosynthesis ID: 7799

2.1.3 Dehydrogenation of silyl enol ethers





Substrates:

1. C=CC1=C(O[Si](C)(C)C)OCC1

Products:

1. 3-vinyl-2(5h)-furanone

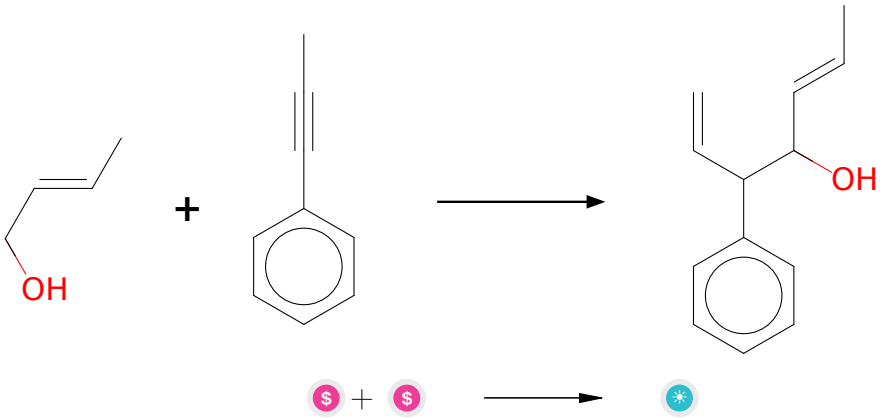
Typical conditions: Pd(OAc)2.Cu(OAc)2.O2.MeCN

Protections: none

Reference: *10.1271/bbb.60.405* and *10.1039/C3CC46778C* and US2015284405 p.40 and *10.1016/S0040-4039(01)81518-5* and US2010204477 p. 15-16 and *10.1016/0040-4039(95)00694-8* and *10.1021/jo00089a034* and *10.1016/S0040-4020(01)90587-3* and *10.1080/00397919008052802* and *10.1021/ja00218a060*

Retrosynthesis ID: 9999877

2.1.4 Coupling of alkynes and alcohols



Substrates:

1. 2-Buten-1-ol - *available at Sigma-Aldrich*
2. 1-Phenyl-1-propyne - *available at Sigma-Aldrich*

Products:

1. C13H16O

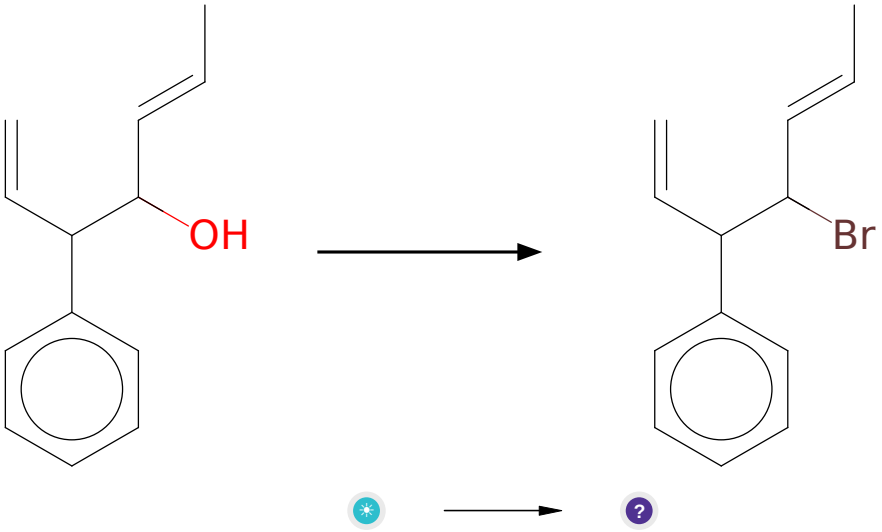
Typical conditions: H2Ru(CO)(PPh3)3.2,4,6-(iPr)3PhSO3H.SL-J009-1.TBAI.IPA.THF.95C

Protections: none

Reference: DOI: *10.1021/jacs.5b00747*

Retrosynthesis ID: 9895

2.1.5 Appel Reaction



Substrates:

1. C13H16O

Products:

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

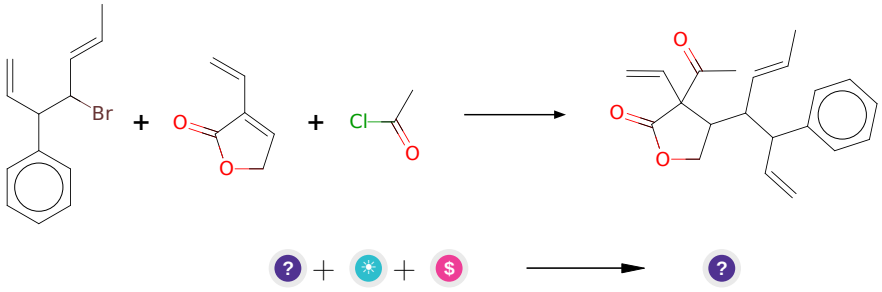
Typical conditions: PPh3.CBr4

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

2.1.6 Conjugated addition of organocuprate-acylation of enones and enoate esters



Substrates:

1. C=CC(c1ccccc1)C(Br)/C=C/C
2. 3-vinyl-2(5h)-furanone
3. Acetyl chloride - *available at Sigma-Aldrich*

Products:

1. C=CC(c1ccccc1)C(/C=C/C)C1COC(=O)C1(C=C)C(C)=O

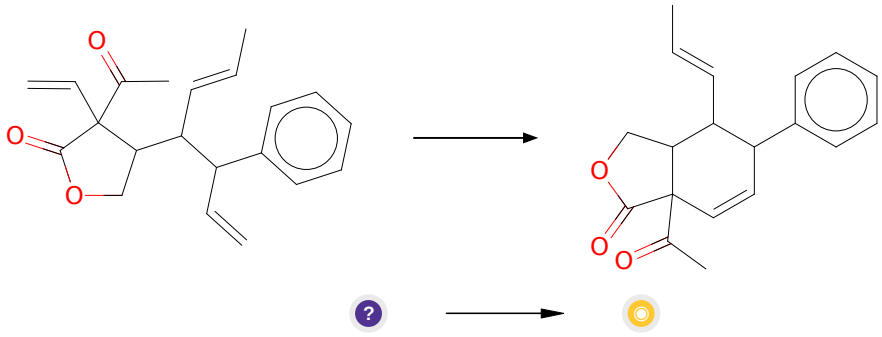
Typical conditions: 1.RCuLi.2.AcCl.HMPA

Protections: none

Reference: *10.3987/COM-99-S143* AND *10.1021/ja00148a023* AND *10.1016/S0040-4039(01)80891-1*

Retrosynthesis ID: 20523

2.1.7 Ring-Closing Metathesis



Substrates:

1. C=CC(c1ccccc1)C(/C=C/C)C1COC(=O)C1(C=C)C(C)=O

Products:

1. C/C=C/C1C(c2ccccc2)C=CC2(C(C)=O)C(=O)OCC12

Typical conditions: catalyst e.g. Hoveyda-Grubbs . solvent e.g. CH2Cl2

Protections: none

Reference: DOI: *10.1002/anie.200800693* and *10.1021/acs.orglett.8b04003* and *10.1021/jo0264729* and *10.1021/ja072334v* and *10.1002/ejoc.201001102*

Retrosynthesis ID: 31014187