Paths of analysis*

L1

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

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

2.1 Path 1

Score: 234.45

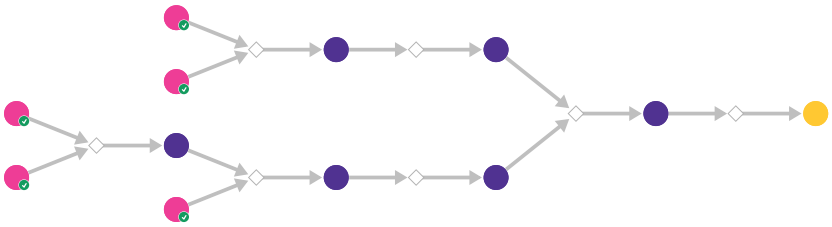
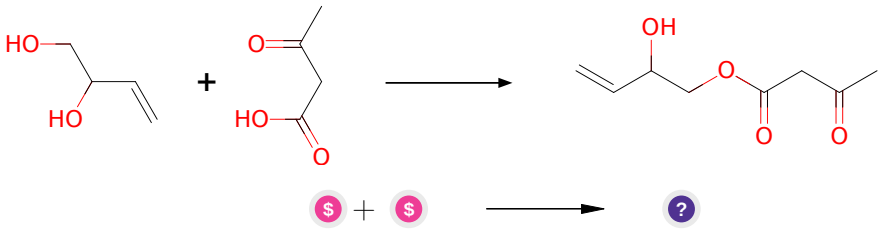


Figure 1: Outline of path 1

2.1.1 Acylation of primary alcohols



Substrates:

1. 3-Butene-1,2-diol - *available at Sigma-Aldrich*
2. Lithium acetoacetate - *available at Sigma-Aldrich*

Products:

1. C=CC(O)COC(=O)CC(C)=O

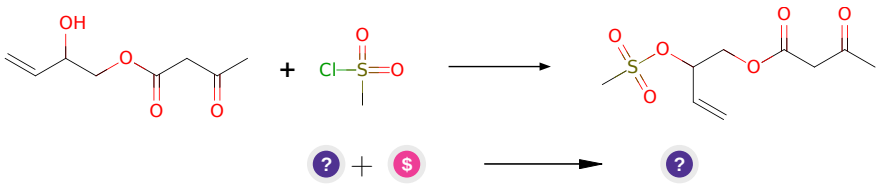
Typical conditions: DCC.DMAP.DCM

Protections: none

Reference: *10.1016/j.molstruc.2016.10.087* and *10.1016/j.bmc.2014.12.043* and *10.1016/j.steroids.2013.03.004* and *10.3390/molecules21091123*

Retrosynthesis ID: 9998689

2.1.2 Sulfonation of secondary alcohols



Substrates:

1. C=CC(O)COC(=O)CC(C)=O
2. Mesyl chloride - *available at Sigma-Aldrich*

Products:

1. C=CC(COC(=O)CC(C)=O)OS(C)(=O)=O

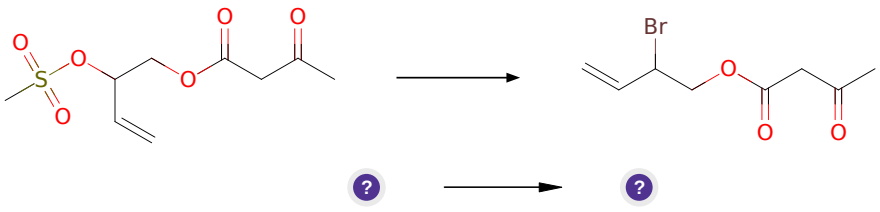
Typical conditions: Et3N.DMAP.DCM

Protections: none

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

Retrosynthesis ID: 24386

2.1.3 Substitution of secondary mesyl group with bromide



Substrates:

1. C=CC(COC(=O)CC(C)=O)OS(C)(=O)=O

Products:

1. C=CC(Br)COC(=O)CC(C)=O

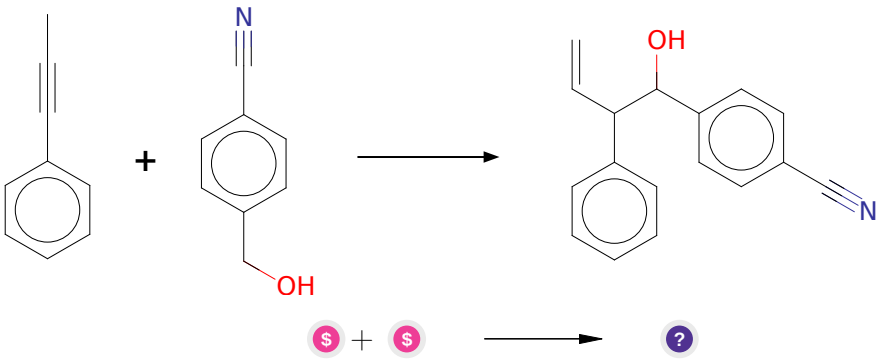
Typical conditions: LiBr.DMF

Protections: none

Reference: *10.1021/jo00068a037* and *10.1016/S0040-4020(03)00140-6*

Retrosynthesis ID: 29713

2.1.4 Coupling of alkynes and alcohols



Substrates:

1. 4-Cyanobenzyl alcohol - *available at Sigma-Aldrich*
2. 1-Phenyl-1-propyne - *available at Sigma-Aldrich*

Products:

1. C=CC(c1ccccc1)C(O)c1ccc(C#N)cc1

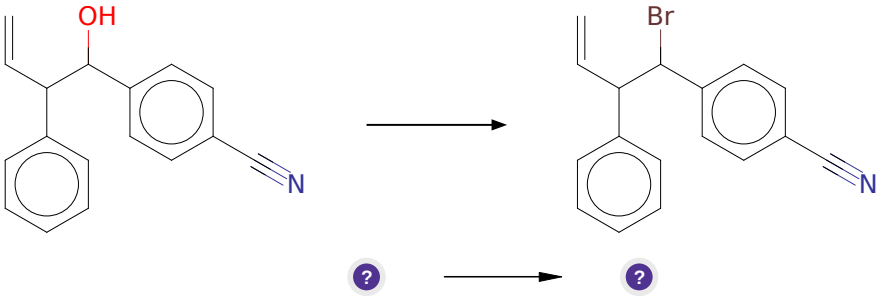
Typical conditions: H2Ru(CO)(PPh3)3.2,4,6-(iPr)3PhSO3H.SL-J009-1.TBAI.IPA.THF.95C

Protections: none

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

Retrosynthesis ID: 9894

2.1.5 Appel Reaction



Substrates:

1. C=CC(c1ccccc1)C(O)c1ccc(C#N)cc1

Products:

1. C=CC(c1ccccc1)C(Br)c1ccc(C#N)cc1

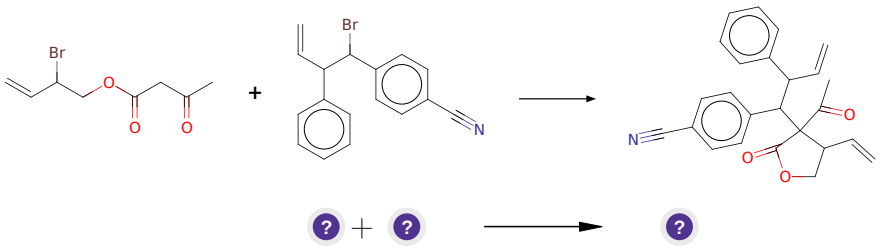
Typical conditions: PPh3.CBr4

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 Acetoacetic Ester Synthesis



Substrates:

1. C=CC(Br)COC(=O)CC(C)=O
2. C=CC(c1ccccc1)C(Br)c1ccc(C#N)cc1

Products:

1. C=CC(c1ccccc1)C(c1ccc(C#N)cc1)C1(C(C)=O)C(=O)OCC1C=C

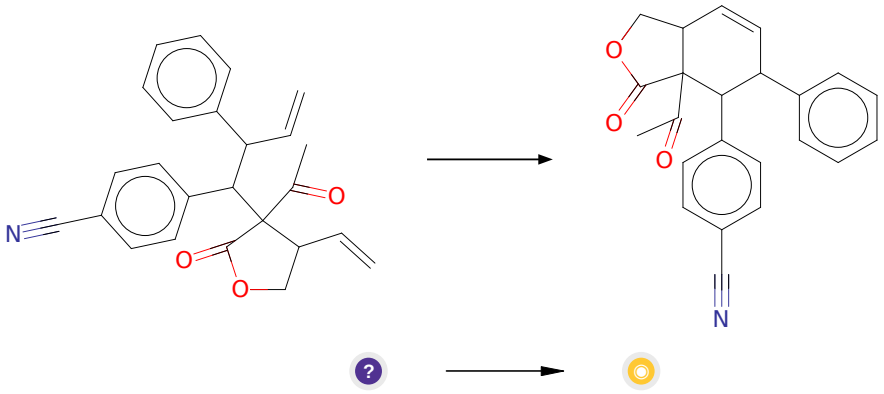
Typical conditions: Exess Typical bases LDA, NaHMDS, LiHMDS.THF

Protections: none

Reference: *10.1002/9780470638859.conrr003*

Retrosynthesis ID: 5037

2.1.7 Ring-Closing Metathesis



Substrates:

1. C=CC(c1ccccc1)C(c1ccc(C#N)cc1)C1(C(C)=O)C(=O)OCC1C=C

Products:

1. CC(=O)C12C(=O)OCC1C=CC(c1ccccc1)C2c1ccc(C#N)cc1

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