Paths of analysis*

Synthia

October 10, 2022

1 Analysis parameters

Analysis type: Automatic Retrosynthesis

Rules: none selected

Filters: Exclude Diastereoselecitve reactions, Tunnels, FGI, FGI with protec-

tions

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+1000 000*(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.

 ${f Strategies:}\ {f none}\ {f selected}$

FGI Coeff: 0

Tunnels Coeff: 0

JSON Parameters: {}

2 Paths

 $1~\mathrm{path}$ found. Paths are sorted by score. Reactions are sorted in appearance order for each path.

2.1 Path 1

Score: 154.38

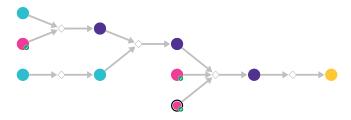
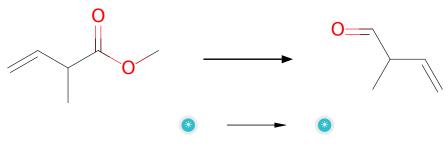


Figure 1: Outline of path 1

2.1.1 Aldehyde Formation



Substrates:

 $1. \ \ 2\text{-methylbut-}3\text{-ensaeuremethylester}$

Products:

 $1. \ \, \hbox{$2$-methyl-but-$3$-enal}$

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

2.1.2 Conjugate addition of organocuprate

Substrates:

 $1. \ \, \hbox{a-diethoxyphosphinyl-da,b-butenolide}$

 $2. \ \ Vinylmagnesium \ bromide \ solution \ - \quad \ \ \it{available at Sigma-Aldrich}$

Products:

1. C=CC1COC(=O)C1P(=O)(OCC)OCC

Typical conditions: 1.CuCN.LiCl.2.Eletrophile.3.NH4Cl

Protections: none

Reference: 10.1021/ol036071v AND 10.1016/j.tet.2011.12.046 AND 10.1002/anie.201007644 AND 10.1002/anie.201007644 AND 10.1055/s-1997-1371

Retrosynthesis ID: 10003577

2.1.3 Wittig-Horner Reaction

Substrates:

- 1. C=CC1COC(=O)C1P(=O)(OCC)OCC
- 2. 2-methyl-but-3-enal

Products:

1. C=CC(C)C=C1C(=O)OCC1C=C

Typical conditions: NaH.THF.0 C or NaH.DMF.0-50 C

Protections: none

Reference: 10.1021/acs.jmedchem.5b01239 p. 63, 71 and 10.1021/jm950725r p.

3150, 3153

Retrosynthesis ID: 11549

2.1.4 Alkenylation-Acylation of enones and enoate esters

Substrates:

1. C=CC(C)C=C1C(=O)OCC1C=C

2. b-Bromostyrene - available at Sigma-Aldrich

3. Acetyl chloride - available at Sigma-Aldrich

Products:

 $1. \ C=CC(C)C(/C=C/c1ccccc1)C1(C(C)=O)C(=O)OCC1C=C$

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

Protections: none

Reference: 10.1016/S0040-4039(01)80891-1 AND 10.1016/S0040-4020(01)82115-3 AND 10.1021/ja0320018 AND 10.1246/cl.1989.1063 AND 10.1248/cpb.33.1815

Retrosynthesis ID: 20532

2.1.5 Ring-Closing Metathesis

Substrates:

 $1. \ C{=}CC(C)C(/C{=}C/c1ccccc1)C1(C(C){=}O)C({=}O)OCC1C{=}C$

Products:

 $1. \ \mathrm{CC(=O)C12C(=O)OCC1C=CC(C)C2/C=C/c1ccccc1}$

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