Paths of analysis*

PG2A

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

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: `173.93`

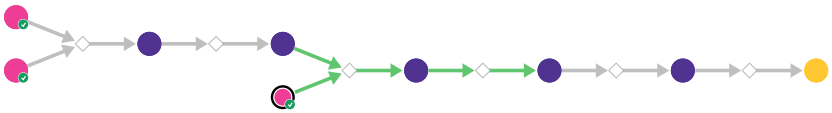
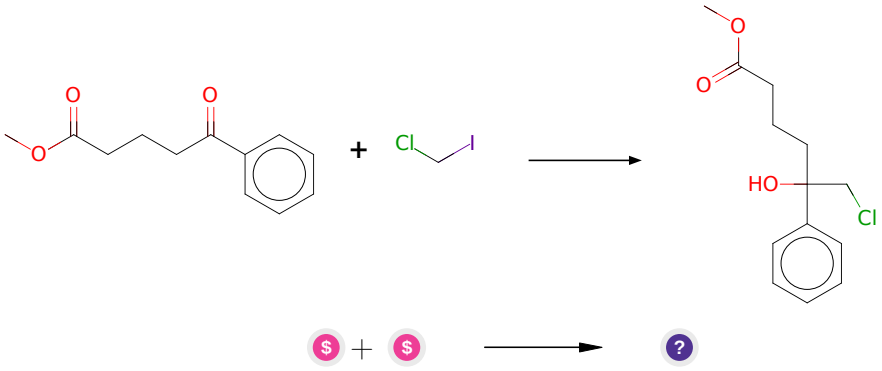


Figure 1: Outline of path 1

2.1.1 Addition of dihalomethane to ketone



Substrates:

1. Methyl 4-Benzoylbutyrate - *available at Sigma-Aldrich*
2. Chloroiodomethane - *available at Sigma-Aldrich*

Products:

1. COC(=O)CCCC(O)(CCl)c1ccccc1

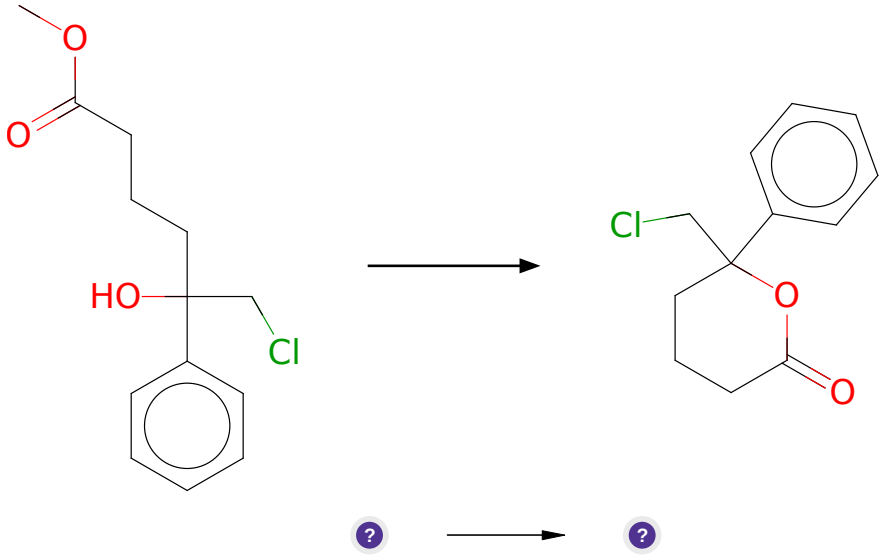
Typical conditions: SmI2.THF

Protections: none

Reference: *10.1016/S0040-4039(00)83908-8* and *10.1002/adsc.201301042* and *10.1039/P19910003127* and *10.1021/jo00068a021* and *10.1021/jm050194z* and *10.1021/ol300058t* and *10.1021/jo960335s*

Retrosynthesis ID: 25219

2.1.2 Acid catalyzed transesterification



Substrates:

1. COC(=O)CCCC(O)(CCl)c1ccccc1

Products:

1. O=C1CCCC(CCl)(c2ccccc2)O1

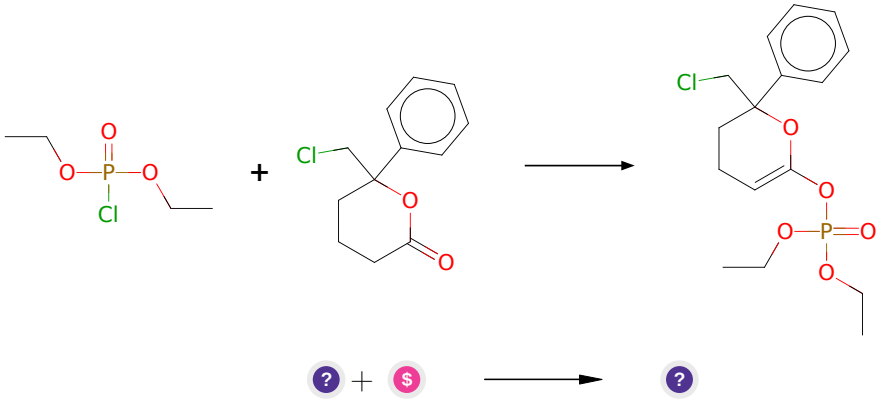
Typical conditions: H+

Protections: none

Reference: *10.1021/cr00020a004*

Retrosynthesis ID: 50438

2.1.3 Fosforylation of ketones



Substrates:

1. O=C1CCCC(CCl)(c2ccccc2)O1
2. Diethyl chlorophosphate - *available at Sigma-Aldrich*

Products:

1. CCOP(=O)(OCC)OC1=CCCC(CCl)(c2ccccc2)O1

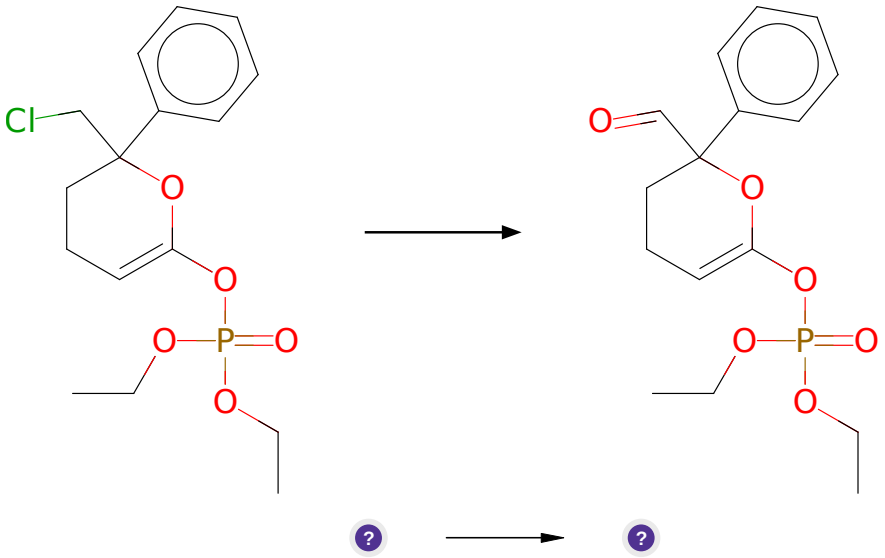
Typical conditions: KHMDS.HMPA.THF.cooling

Protections: none

Reference: *10.1021/ja970619+*

Retrosynthesis ID: 23009

2.1.4 Kornblum Oxidation



Substrates:

1. CCOP(=O)(OCC)OC1=CCCC(CCl)(c2ccccc2)O1

Products:

1. CCOP(=O)(OCC)OC1=CCCC(C=O)(c2ccccc2)O1

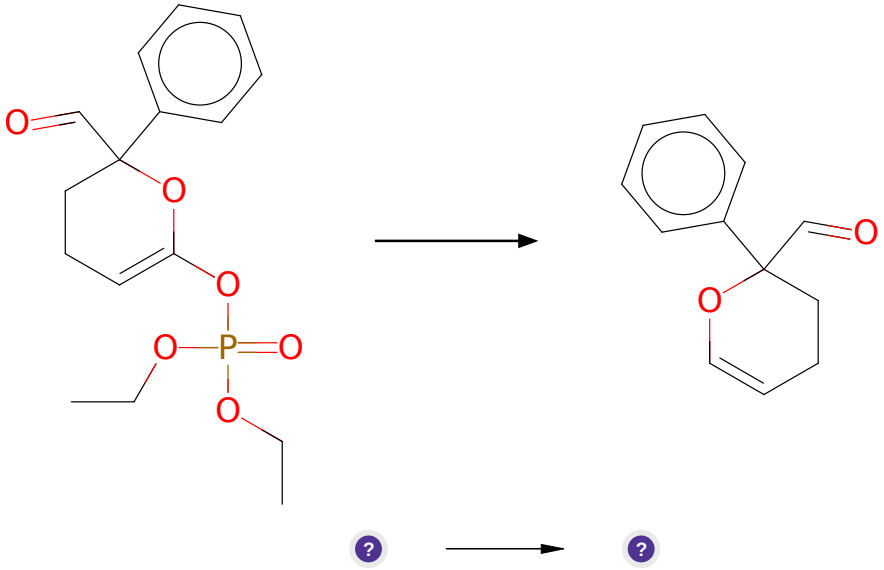
Typical conditions: DMSO.NEt3

Protections: none

Reference: *10.1080/00397918608056381* and *10.1002/9780470638859.conrr373*

Retrosynthesis ID: 11658

2.1.5 Reduction of enol phosphonates



Substrates:

1. CCOP(=O)(OCC)OC1=CCCC(C=O)(c2ccccc2)O1

Products:

1. O=CC1(c2ccccc2)CCC=CO1

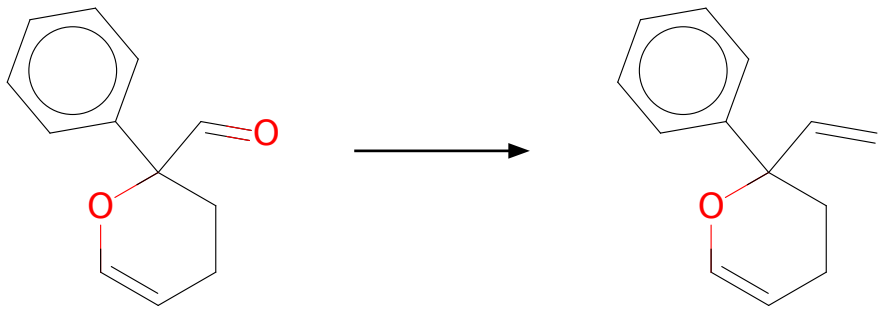
Typical conditions: Et3Al.Pd(PPh3)4

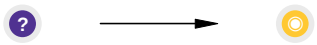
Protections: none

Reference: *10.1021/jo00387a038* AND *10.1021/jo00292a049* AND *10.1039/C1CS15100B*

Retrosynthesis ID: 23046

2.1.6 Tebbe Olefination





Substrates:

1. O=CC1(c2ccccc2)CCC=CO1

Products:

1. C=CC1(c2ccccc2)CCC=CO1

Typical conditions: Cp2TiCl2.AlMe3.toluene

Protections: none

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

Retrosynthesis ID: 11714