Paths of analysis*

L8

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: 220.45

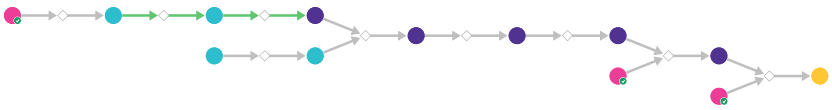
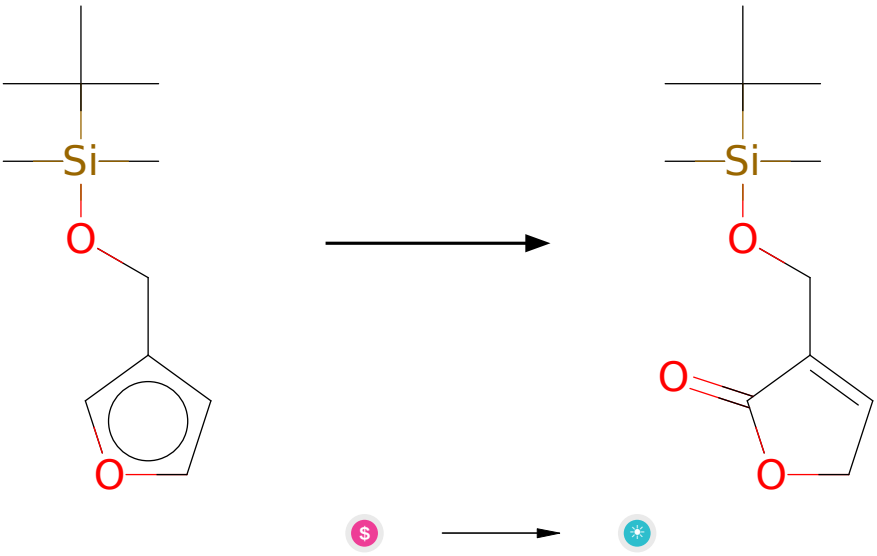


Figure 1: Outline of path 1

2.1.1 NBS-promoted oxidation of furans to lactones



Substrates:

1. tert-Butyl(furan-3-ylmethoxy)dimethylsilane - *available at Sigma-Aldrich*

Products:

1. 3-(tert-butyl-dimethyl-silanyloxymethyl)-5h-furan-2-one

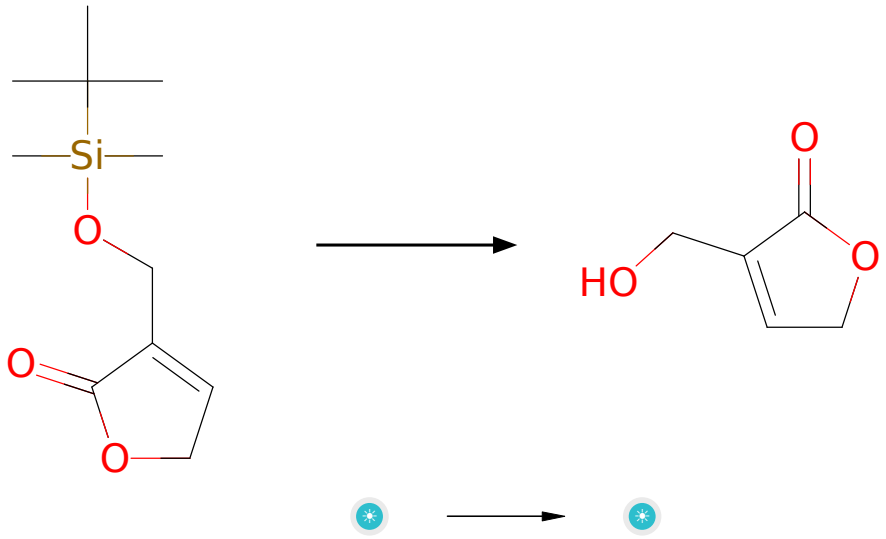
Typical conditions: NBS.MW.MeOH

Protections: none

Reference: DOI: *10.1016/S0040-4039(01)01261-8*

Retrosynthesis ID: 49766

2.1.2 Deprotection of TBS ethers



Substrates:

1. 3-(tert-butyl-dimethyl-silanyloxymethyl)-5h-furan-2-one

Products:

1. 3-(1-hydroxymethyl)-5h-furan-2-one

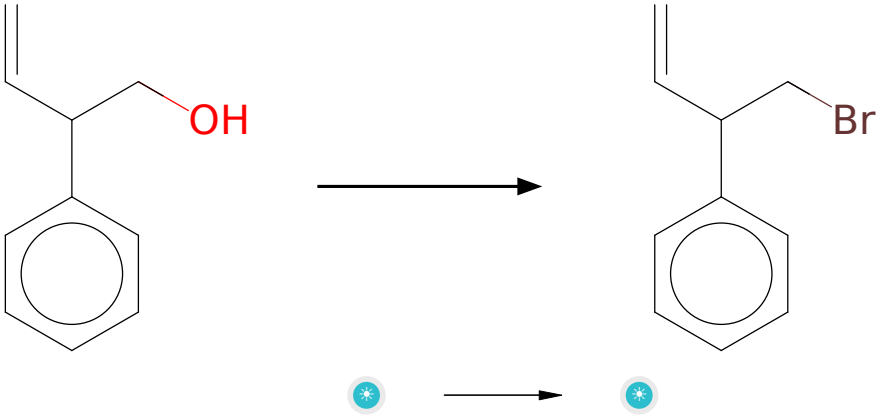
Typical conditions: TBAF.THF

Protections: none

Reference: *10.1016/j.tet.2013.01.017* and *10.1016/j.tet.2004.04.042*

Retrosynthesis ID: 31010160

2.1.3 Appel Reaction



Substrates:

1. 2-phenylbut-3-en-1-ol

Products:

1. 2-phenyl-1-bromo-3-buten

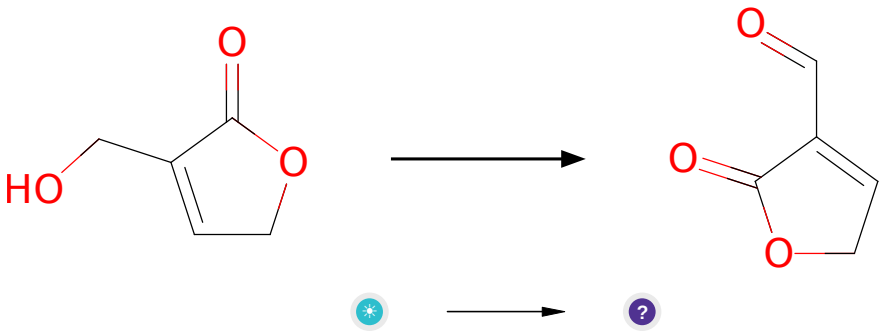
Typical conditions: PPh3.CBr4

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

2.1.4 Oxidation of primary alcohols with DMP



Substrates:

1. 3-(1-hydroxymethyl)-5h-furan-2-one

Products:

1. O=CC1=CCOC1=O

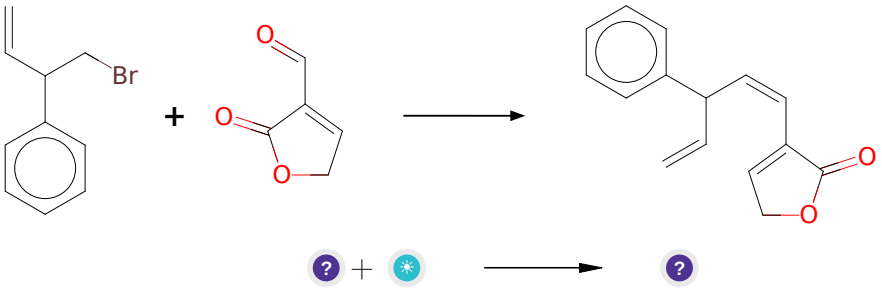
Typical conditions: DMP.DCM.0-25 C

Protections: none

Reference: *10.1016/j.bmc.2020.115469* p. 3, 9 and *10.1021/acs.jmedchem.8b01878* SI p. S43

Retrosynthesis ID: 50426

2.1.5 Wittig olefination



Substrates:

1. O=CC1=CCOC1=O
2. 2-phenyl-1-bromo-3-buten

Products:

1. C=CC(/C=C\C1=CCOC1=O)c1ccccc1

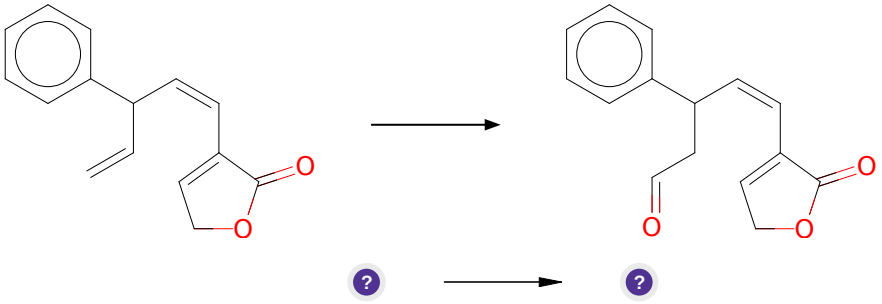
Typical conditions: 1.PPh3 or trialkylphosphite.2.basealdehyde

Protections: none

Reference: *10.1021/ja0015287* and *10.1021/ja404673s* and *10.1021/ol901979x*

Retrosynthesis ID: 9544

2.1.6 Tsuji-Wacker Oxidation of alkenes



Substrates:

1. C=CC(/C=C\C1=CCOC1=O)c1ccccc1

Products:

1. O=CCC(/C=C\C1=CCOC1=O)c1ccccc1

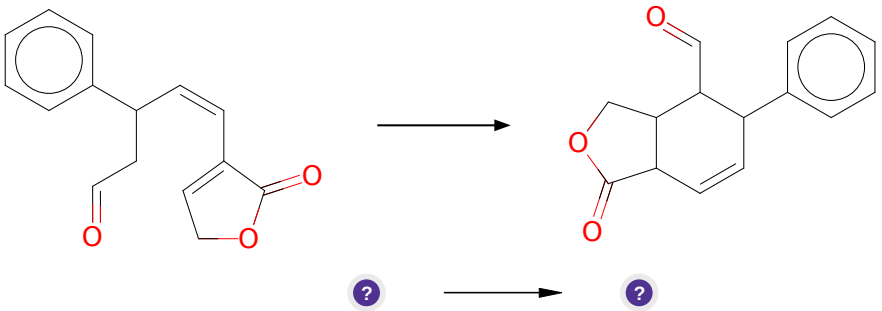
Typical conditions: PdCl2(PhCn)2.CuCl2.AgNO2.O2.tBuOH.MeNO2.rt

Protections: none

Reference: *10.1021/jacs.6b08788* and *10.1021/ja411749k*and *10.1002/anie.201306756* and *10.1016/S0040-4039(03)01709-X* and *10.1021/acs.orglett.6b01165*

Retrosynthesis ID: 28273

2.1.7 Michael addition



Substrates:

1. O=CCC(/C=C\C1=CCOC1=O)c1ccccc1

Products:

1. O=CC1C(c2ccccc2)C=CC2C(=O)OCC21

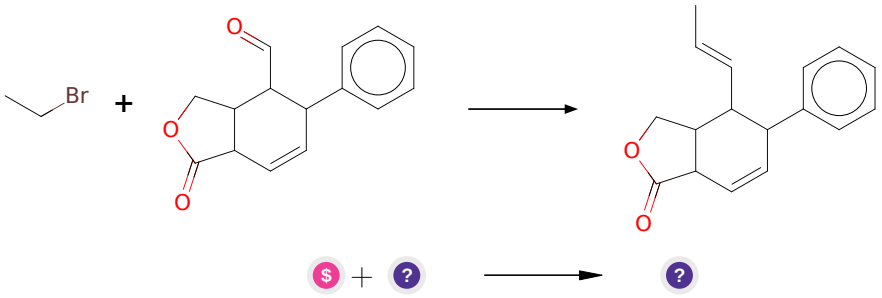
Typical conditions: EtONa or other base

Protections: none

Reference: *10.1016/j.tetlet.2011.02.073* AND *10.1016/j.molstruc.2010.12.005* AND *10.1016/S0040-4039(97)00695-3* AND *10.1021/ol016401g* AND *10.1002/ejoc.200500330*

Retrosynthesis ID: 15774

2.1.8 Wittig-Schlosser olefination



Substrates:

1. Bromoethane - *available at Sigma-Aldrich*
2. O=CC1C(c2ccccc2)C=CC2C(=O)OCC21

Products:

1. C/C=C/C1C(c2ccccc2)C=CC2C(=O)OCC21

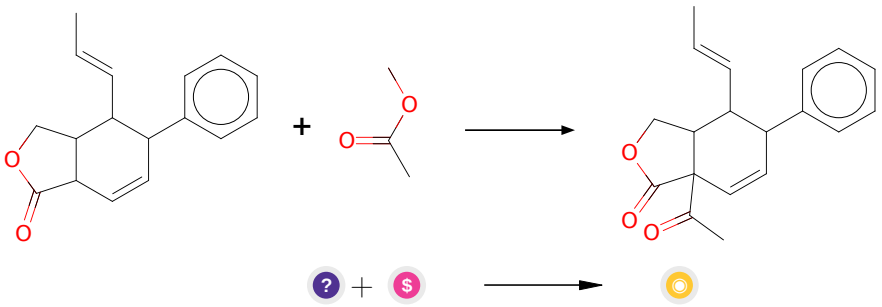
Typical conditions: 1.PPh3 or trialkylphosphite.2.base.aldehyde.3.base

Protections: none

Reference: *10.1021/ol049701h* and *10.1021/ja00535a063* and Kurti and Czako; Strategic Applications of Named Reactions in Organic Synthesis. 1st edn., 488-489.

Retrosynthesis ID: 9546

2.1.9 Claisen Condensation



Substrates:

1. C/C=C/C1C(c2ccccc2)C=CC2C(=O)OCC21
2. Methyl acetate - *available at Sigma-Aldrich*

Products:

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

Typical conditions: Base.Solvent

Protections: none

Reference: *10.1021/cr020703u* and *10.1021/cr60088a002*

Retrosynthesis ID: 5015