Paths of analysis*

L11

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: `388.52`

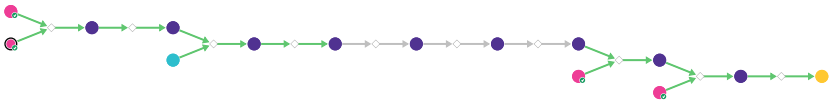
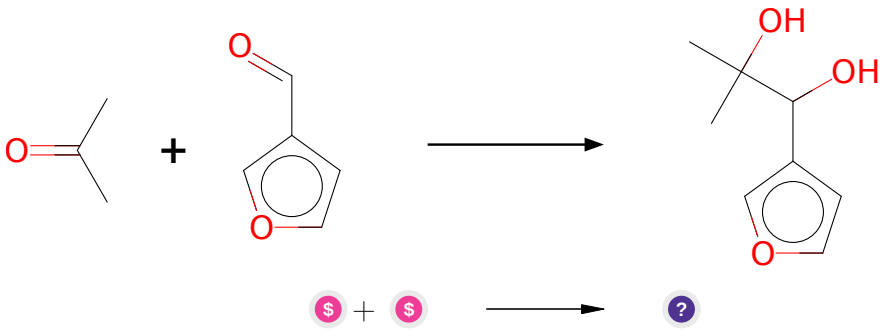


Figure 1: Outline of path 1

2.1.1 Pinacol Coupling Reaction



Substrates:

1. 3-Furaldehyde - *available at Sigma-Aldrich*
2. Acetone - *available at Sigma-Aldrich*

Products:

1. CC(C)(O)C(O)c1ccoc1

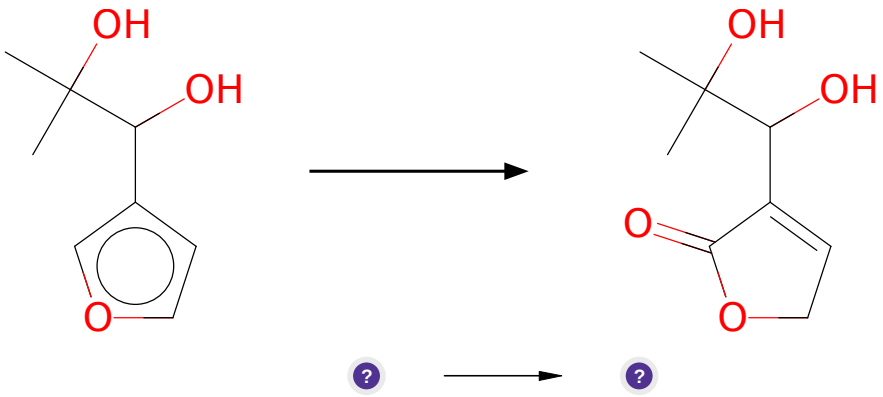
Typical conditions: Mg.NH4Cl.H2O or Mg.SmI2.TMSCl.THF.HMPA

Protections: none

Reference: *10.1021/jo982497p* p. 3234, 3236 and *10.1021/ol0506258* p. 2366, SI p. S12

Retrosynthesis ID: 10205

2.1.2 NBS-promoted oxidation of furans to lactones



Substrates:

1. CC(C)(O)C(O)c1ccoc1

Products:

1. CC(C)(O)C(O)C1=CCOC1=O

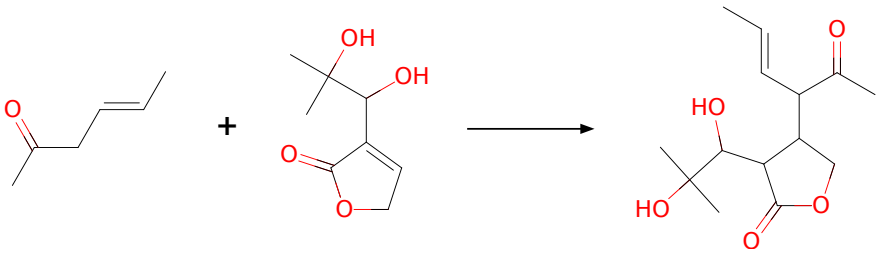
Typical conditions: NBS.MW.MeOH

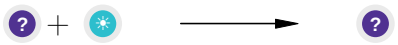
Protections: none

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

Retrosynthesis ID: 49766

2.1.3 Michael addition





Substrates:

1. CC(C)(O)C(O)C1=CCOC1=O
2. hex-4t-en-2-one

Products:

1. C/C=C/C(C(C)=O)C1COC(=O)C1C(O)C(C)(C)O

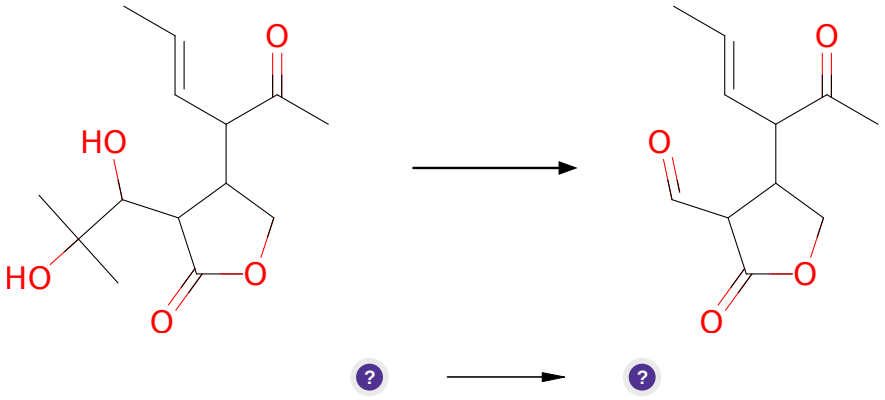
Typical conditions: EtONa or other base

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

2.1.4 Cleavage of 1,2-diols with NaIO4



Substrates:

1. C/C=C/C(C(C)=O)C1COC(=O)C1C(O)C(C)(C)O

Products:

1. C/C=C/C(C(C)=O)C1COC(=O)C1C=O

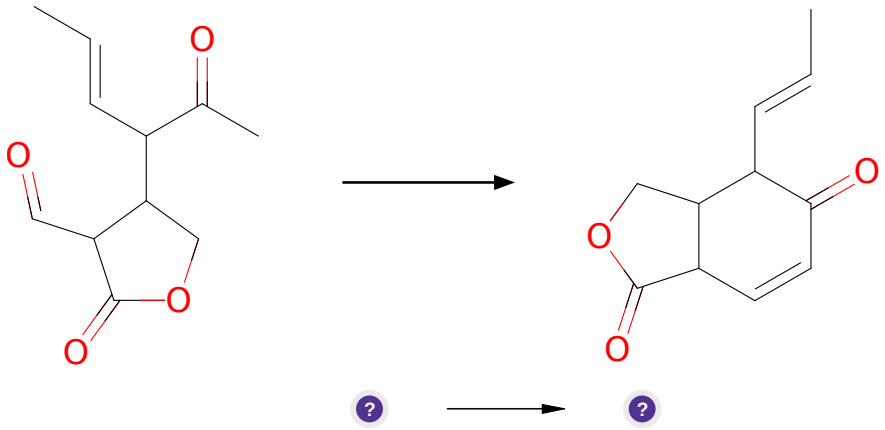
Typical conditions: NaIO4.solvent

Protections: none

Reference: *10.1039/C5OB00238A* and *10.1002/chem.201301371* and *10.1021/ol052106a*

Retrosynthesis ID: 31017509

2.1.5 Aldol Condensation



Substrates:

1. C/C=C/C(C(C)=O)C1COC(=O)C1C=O

Products:

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

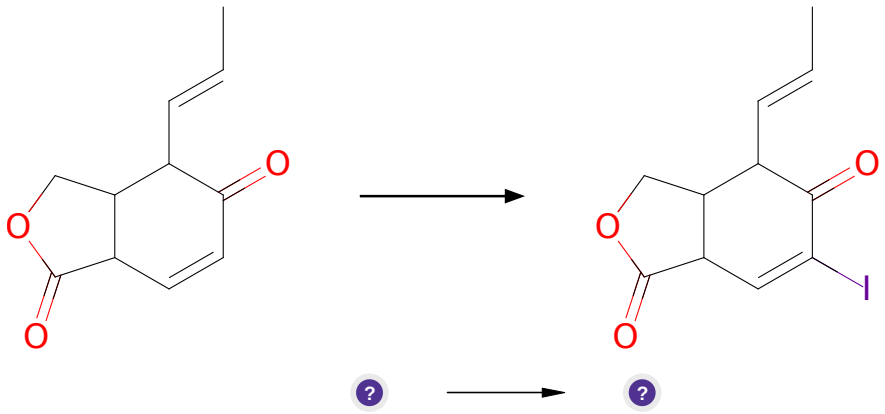
Typical conditions: NaOEt.base

Protections: none

Reference: *10.1080/00397911.2016.1206938*

Retrosynthesis ID: 10896

2.1.6 Alpha-iodination of alpha-beta-unsaturated carbonyl compounds



Substrates:

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

Products:

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

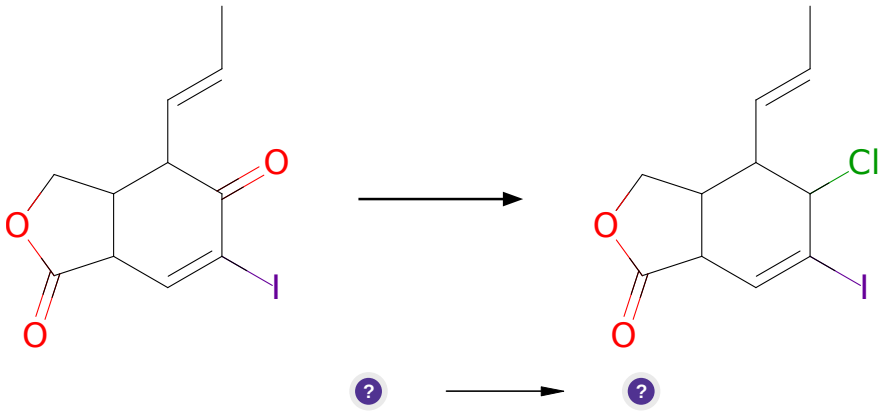
Typical conditions: DMAP.K2CO3.H2O.THF

Protections: none

Reference: DOI: *10.1055/s-2005-868495*

Retrosynthesis ID: 786

2.1.7 Synthesis of alkyl chlorides from ketones



Substrates:

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

Products:

1. C/C=C/C1C(Cl)C(I)=CC2C(=O)OCC21

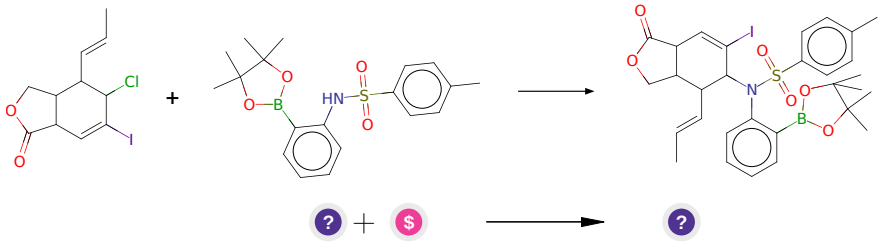
Typical conditions: InO3.chloroform.SiMe2Cl

Protections: none

Reference: DOI: *10.1021/ja0283246*

Retrosynthesis ID: 11620

2.1.8 Alkylation of sulfonamides with alkyl chlorides



Substrates:

1. C/C=C/C1C(Cl)C(I)=CC2C(=O)OCC21
2. 2-(p-Toluenesulfonylamino)phenylboronic acid pinacol ester - *available at Sigma-Aldrich*

Products:

1. C/C=C/C1C2COC(=O)C2C=C(I)C1N(c1ccccc1B1OC(C)(C)C(C)(C)O1)S(=O)(=O)c1ccc(C)cc1

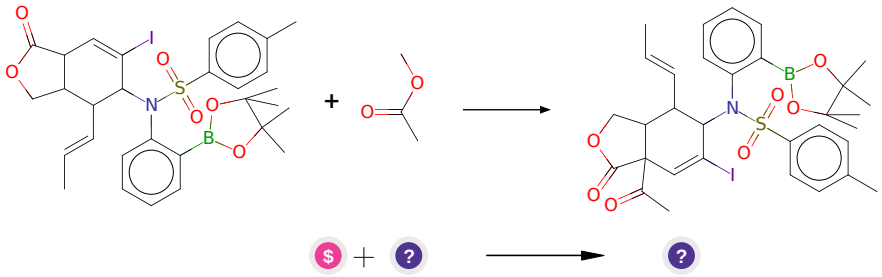
Typical conditions: LDA

Protections: none

Reference: *10.1002/1099-0690(200101)2001:2<323::AID-EJOC323>3.0.CO;2-A*

Retrosynthesis ID: 7727

2.1.9 Claisen Condensation



Substrates:

1. Methyl acetate - *available at Sigma-Aldrich*
2. C/C=C/C1C2COC(=O)C2C=C(I)C1N(c1ccccc1B1OC(C)(C)C(C)(C)O1)S(=O)(=O)c1ccc(C)cc1

Products:

1. C/C=C/C1C(N(c2ccccc2B2OC(C)(C)C(C)(C)O2)S(=O)(=O)c2ccc(C)cc2)C(I)=CC2(C(C)=O)C(=O)C

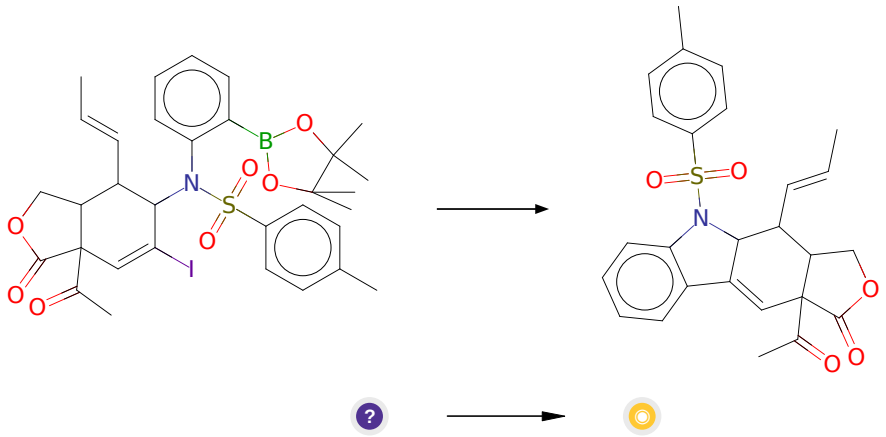
Typical conditions: Base.Solvent

Protections: none

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

Retrosynthesis ID: 5015

2.1.10 Suzuki coupling of arylboronic pinacol esters with vinyl iodides



Substrates:

1. C/C=C/C1C(N(c2ccccc2B2OC(C)(C)C(C)(C)O2)S(=O)(=O)c2ccc(C)cc2)C(I)=CC2(C(C)=O)C(=O)C

Products:

1. C/C=C/C1C2C(=CC3(C(C)=O)C(=O)OCC13)c1ccccc1N2S(=O)(=O)c1ccc(C)cc1

Typical conditions: Pd catalyst.base.solvent

Protections: none

Reference: *10.1021/cr00039a007* and *10.1007/3418_2012_32* and *10.1021/cr0505268* and *10.1016/j.jfluchem.2016.01.018* and *10.1039/C3CS60197H*

Retrosynthesis ID: 10176