Paths of analysis*

L9_STEREO

Synthia

October 11, 2022

1 Analysis parameters

Analysis type: Automatic Retrosynthesis

Rules: none selected

Filters: 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

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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: `186.11`

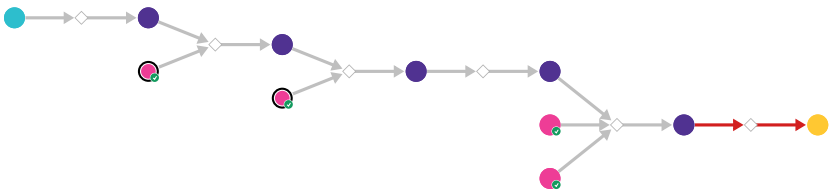
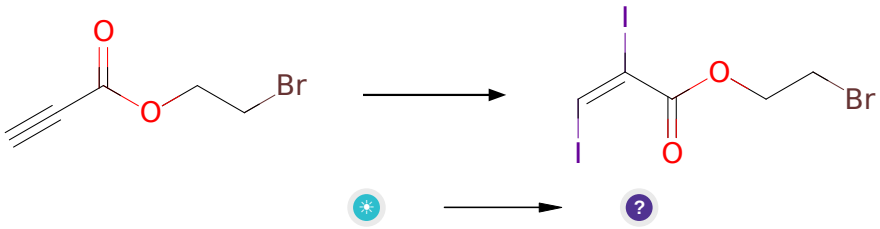


Figure 1: Outline of path 1

2.1.1 Iodination Of Alkynes



Substrates:

1. 2-bromoethyl 2-propynoate

Products:

1. O=C(OCCBr)/C(I)=C\I

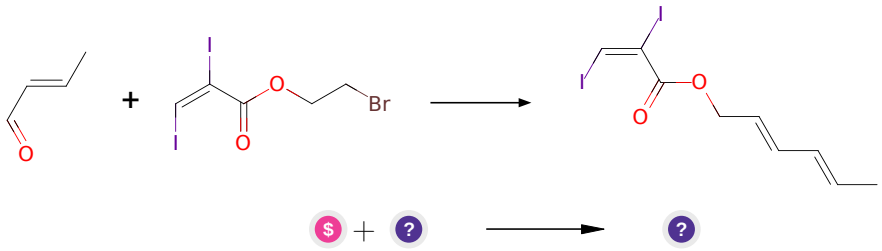
Typical conditions: I2.ACN

Protections: none

Reference: *10.1002/chem.201102570* AND *10.1055/s-2007-966043* AND *10.1021/ol800845r*

Retrosynthesis ID: 8998

2.1.2 Wittig-Schlosser olefination



Substrates:

1. 2-Butenal - *available at Sigma-Aldrich*
2. O=C(OCCBr)/C(I)=C\I

Products:

1. C/C=C/C=C/COC(=O)/C(I)=C\I

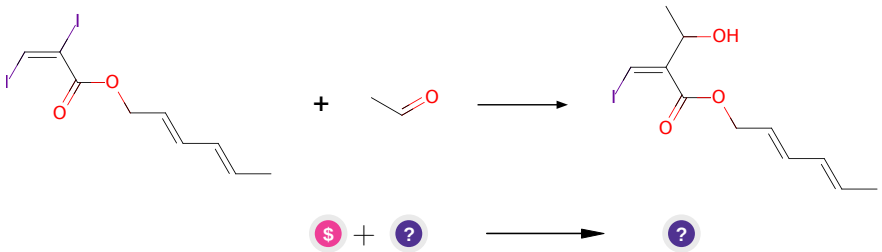
Typical conditions: 1.PPh3 or trialkylphosphite.2.base.aldehyde.3.base

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

2.1.3 Reformatsky Reaction



Substrates:

1. Ethanal - *available at Sigma-Aldrich*

2. C/C=C/C=C/COC(=O)/C(I)=C\I

Products:

1. C/C=C/C=C/COC(=O)/C(=C\I)C(C)O

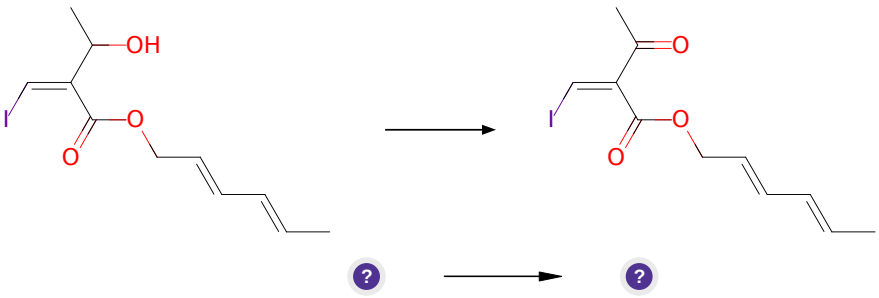
Typical conditions: Zn.THF

Protections: none

Reference: *10.1016/j.bmc.2016.07.052* p. 4521, 4520 and *10.1016/j.ejmech.2013.07.047* p. 214, 218

Retrosynthesis ID: 11539

2.1.4 Swern Oxidation



Substrates:

1. C/C=C/C=C/COC(=O)/C(=C\I)C(C)O

Products:

1. C/C=C/C=C/COC(=O)/C(=C\I)C(C)=O

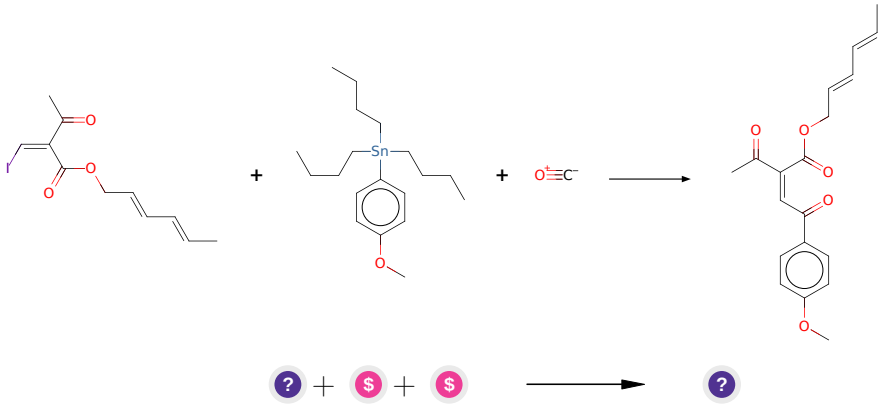
Typical conditions: oxalyl chloride.DMSO.DCM.NMe3.-40C

Protections: none

Reference: *10.1055/s-1990-27036*

Retrosynthesis ID: 11163

2.1.5 Stille Carbonylative Cross-Coupling



Substrates:

1. C/C=C/C=C/COC(=O)/C(=C\I)C(C)=O
2. Tributyl(4-methoxyphenyl)stannane - *available at Sigma-Aldrich*
3. CORM-2 - *available at Sigma-Aldrich*

Products:

1. C/C=C/C=C/COC(=O)/C(=C\C(=O)c1ccc(OC)cc1)C(C)=O

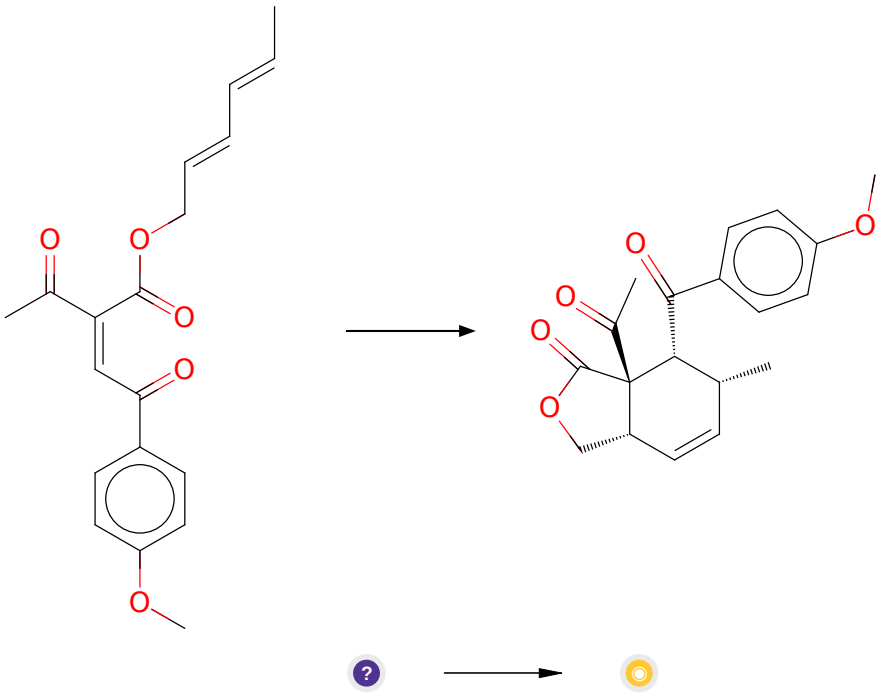
Typical conditions: Pd(0) complex

Protections: none

Reference: DOI: *10.1002/anie.198605081*

Retrosynthesis ID: 245571

2.1.6 Diels-Alder



Substrates:

1. C/C=C/C=C/COC(=O)/C(=C\C(=O)c1ccc(OC)cc1)C(C)=O

Products:

1. COc1ccc(C(=O)[C@@H]2[C@H](C)C=C[C@@H]3COC(=O)[C@@]32C(C)=O)cc1

Typical conditions: Lewis acid or chiral Lewis acid. Solvent.

Protections: none

Reference: DOI: *10.1002/1521-3773(20020517)41:10<1668::AID-ANIE1668>3.0.CO;2-Z* AND *10.1021/ja062508t*

Retrosynthesis ID: 18116