Paths of analysis*

PG5A

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

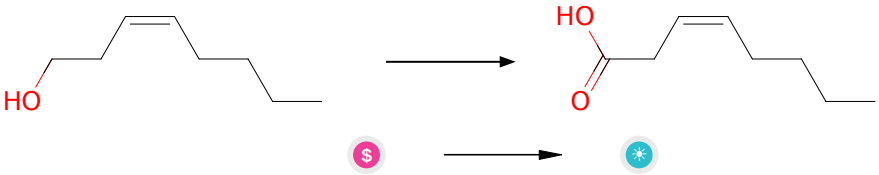
5 paths found. *Paths are sorted by score. Reactions are sorted in appearance order for each path.*

2.1 Path 1

Score: 45.00

Figure 1: Outline of path 1

2.1.1 Jones Oxidation



Substrates:

1. oct-3c-en-1-ol - *available at Sigma-Aldrich*

Products:

1. oct-3c-ensaeure

Typical conditions: cromate.sulfate.H2O.acetone

Protections: none

Reference: *10.1002/9780470638859.conrr349* and *10.1021/jm00270a004*

Retrosynthesis ID: 11160

2.1.2 Synthesis of alkyl chlorides from carboxylic acids

Substrates:

1. oct-3c-ensaeure

Products:

1. 1-chloro-hept-2c-ene

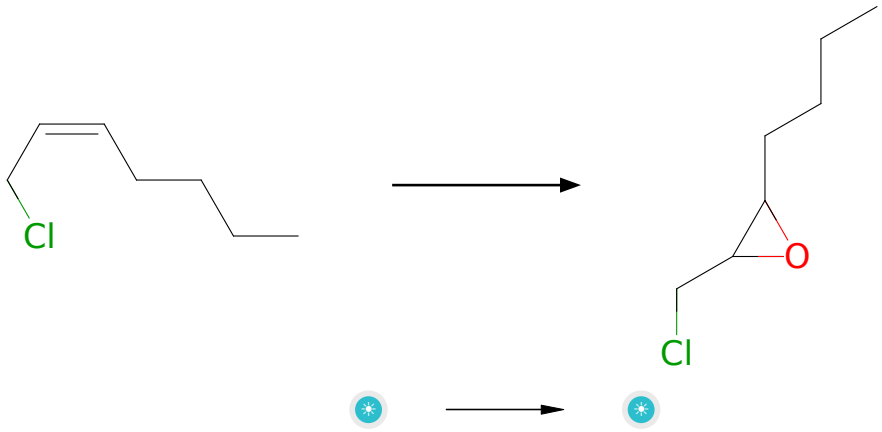
Typical conditions: Ag(Phen)2OTf.OtBu.Cl.acetonitrile.RT

Protections: none

Reference: DOI: *10.1021/ja210361z*

Retrosynthesis ID: 11619

2.1.3 Shi Epoxidation



Substrates:

1. 1-chloro-hept-2c-ene

Products:

1. C7H13ClO

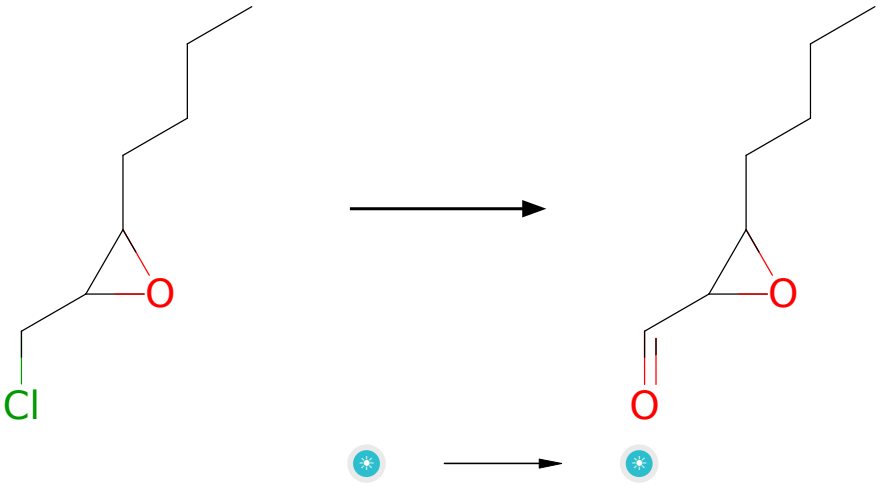
Typical conditions: chiral catalyst.oxone.NaHCO3.MeCN.Bu4NHSO4

Protections: none

Reference: *10.1021/ja972272g* and *10.1021/ja003049d*

Retrosynthesis ID: 9991499

2.1.4 Kornblum Oxidation



Substrates:

1. C7H13ClO

Products:

1. 2,3-epoxycyclohexanone

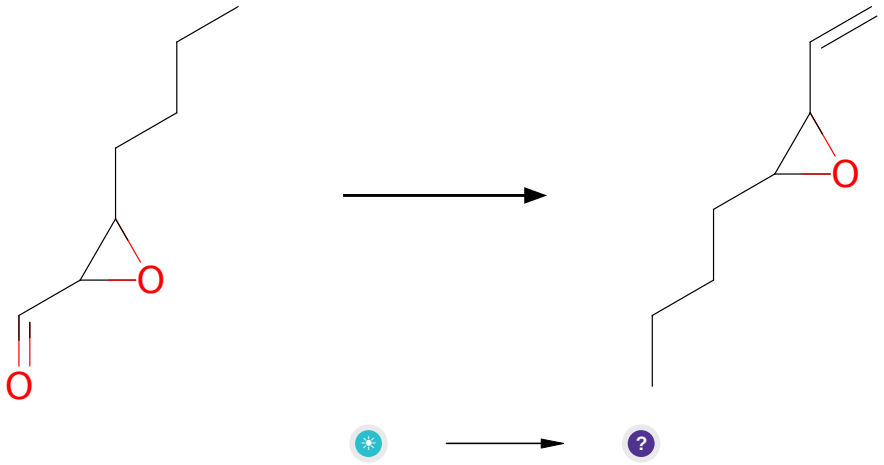
Typical conditions: DMSO.NEt3

Protections: none

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

Retrosynthesis ID: 11658

2.1.5 Tebbe Olefination



Substrates:

1. 2,3-epoxycyclohexanone

Products:

1. C=CC1OC1CCCC

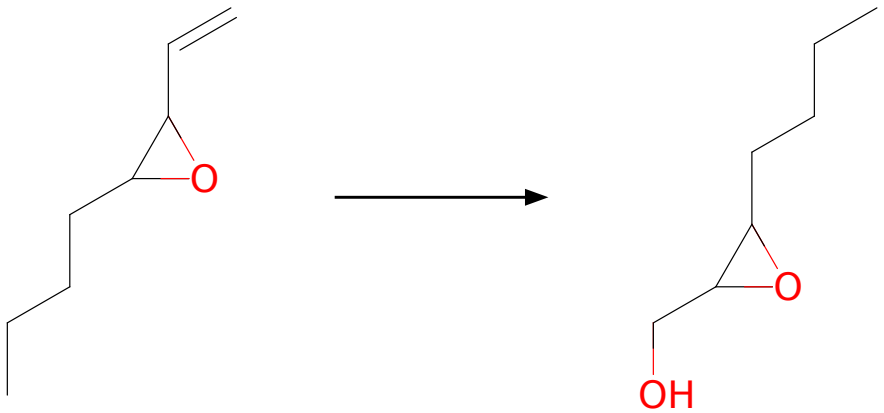
Typical conditions: Cp2TiCl2.AlMe3.toluene

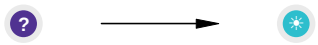
Protections: none

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

Retrosynthesis ID: 11714

2.1.6 Ozonolysis followed by reduction





Substrates:

1. C=CC1OC1CCCC

Products:

1. (3-butyl-oxiranyl)-methanol

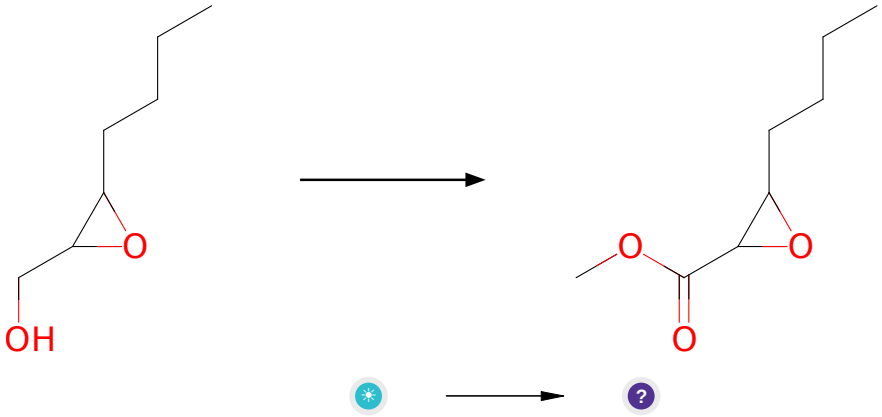
Typical conditions: O3.MeOH.CH2Cl2.NaBH4.low temperature

Protections: none

Reference: *10.1016/j.tet.2017.03.039*

Retrosynthesis ID: 5080

2.1.7 Tandem oxidation-esterification



Substrates:

1. (3-butyl-oxiranyl)-methanol

Products:

1. CCCCC1OC1C(=O)OC

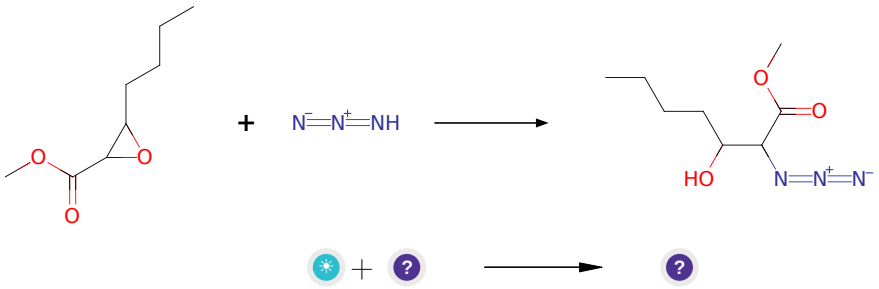
Typical conditions: Oxidant (eg. I2.K2CO3 or Ca(OCl)2).MeOH

Protections: none

Reference: *10.1016/S0040-4039(00)73550-7* and *10.1016/j.tet.2005.03.097* and *10.1021/ol062940f*

Retrosynthesis ID: 25234

2.1.8 Ring-opening of epoxides or thiiranes with azides



Substrates:

1. hydrazoic acid
2. CCCCC1OC1C(=O)OC

Products:

1. CCCCC(O)C(N=[N+]=[N-])C(=O)OC

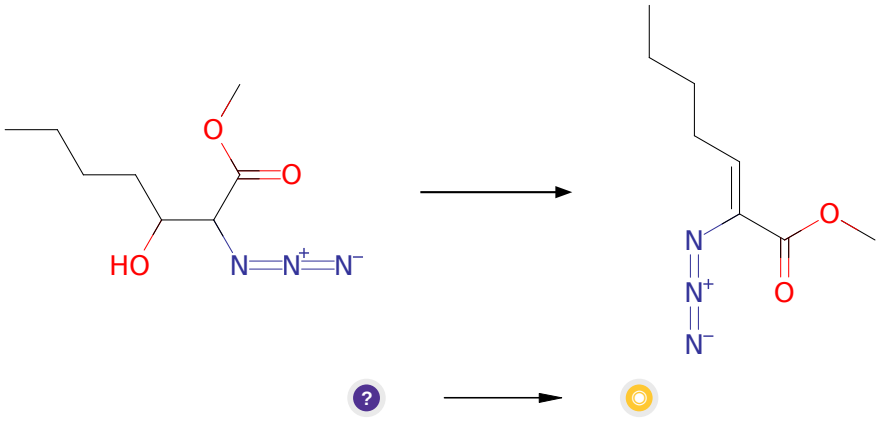
Typical conditions: NaN3.NH4Cl.MeOH.H2O.65 C

Protections: none

Reference: *10.1021/jm400529f* p. 4361, 4367 and *10.1021/ja003713q* p. 1590, 1594

Retrosynthesis ID: 858

2.1.9 Dehydration of Beta Hydroxy Carbonyl Compounds



Substrates:

1. CCCCC(O)C(N=[N+]=[N-])C(=O)OC

Products:

1. CCCC/C=C(\N=[N+]=[N-])C(=O)OC

Typical conditions: TsOH

Protections: none

Reference: DOI:*10.1002/anie.201204977* AND *10.1021/ol062777o*

Retrosynthesis ID: 7732

2.2 Path 2

Score: 76.25

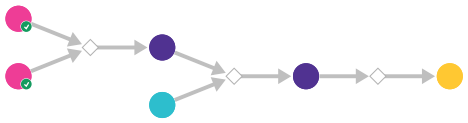
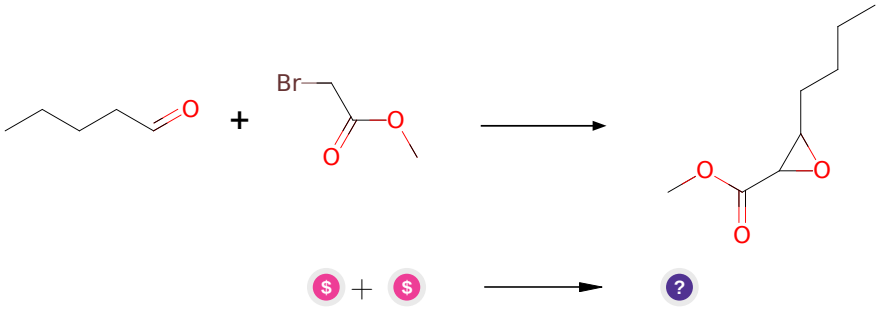


Figure 2: Outline of path 2

2.2.1 Darzens Condensation



Substrates:

1. Methyl bromoacetate - *available at Sigma-Aldrich*
2. Pentanal - *available at Sigma-Aldrich*

Products:

1. CCCCC1OC1C(=O)OC

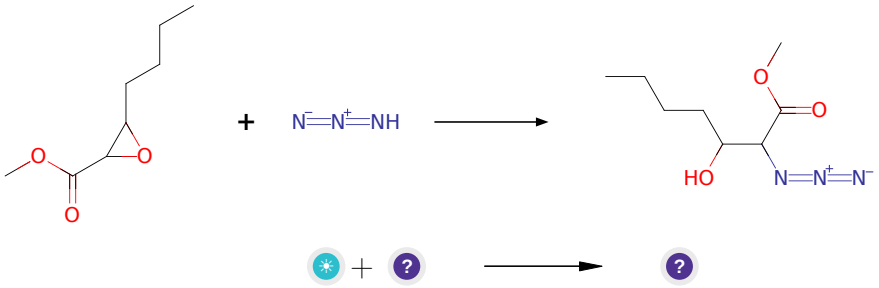
Typical conditions: KOtBu.HOtBu

Protections: none

Reference: *10.1002/0471264180.or005.10* and *10.1021/cr50002a002*

Retrosynthesis ID: 11625

2.2.2 Ring-opening of epoxides or thiiranes with azides



Substrates:

1. hydrazoic acid
2. CCCCC1OC1C(=O)OC

Products:

1. CCCCC(O)C(N=[N+]=[N-])C(=O)OC

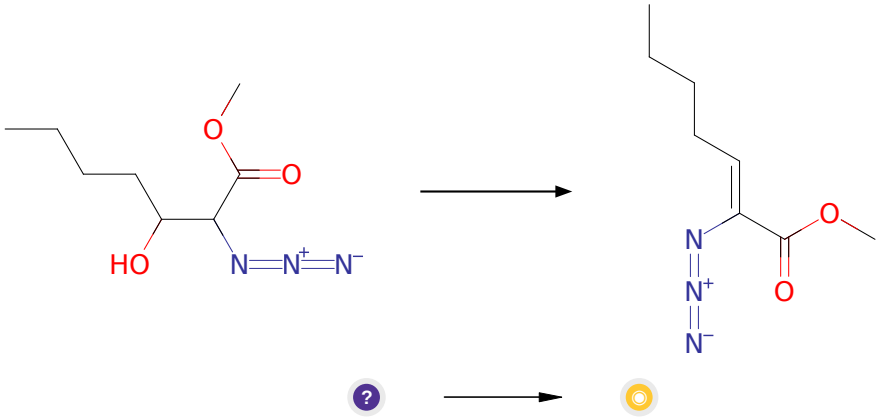
Typical conditions: NaN3.NH4Cl.MeOH.H2O.65 C

Protections: none

Reference: *10.1021/jm400529f* p. 4361, 4367 and *10.1021/ja003713q* p. 1590, 1594

Retrosynthesis ID: 858

2.2.3 Dehydration of Beta Hydroxy Carbonyl Compounds



Substrates:

1. CCCCC(O)C(N=[N+]=[N-])C(=O)OC

Products:

1. CCCC/C=C(\N=[N+]=[N-])C(=O)OC

Typical conditions: TsOH

Protections: none

Reference: DOI:*10.1002/anie.201204977* AND *10.1021/ol062777o*

Retrosynthesis ID: 7732

2.3 Path 3

Score: 76.25

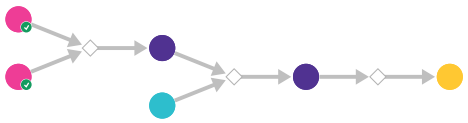
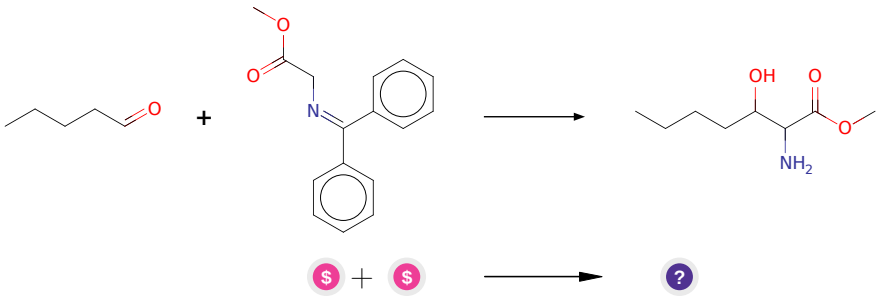


Figure 3: Outline of path 3

2.3.1 Enantioselective addition of enolates to aldehydes followed by deprotection



Substrates:

1. Methyl 2-((diphenylmethylene)amino)acetate - *available at Sigma-Aldrich*
2. Pentanal - *available at Sigma-Aldrich*

Products:

1. CCCCC(O)C(N)C(=O)OC

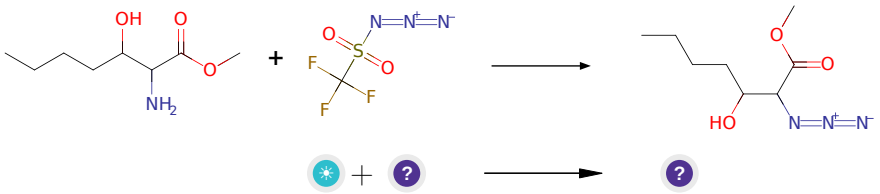
Typical conditions: ProPhenol.Et2Zn.MS4A.toluene.rt then NaBH3CN.AcOH.MeOH deprotection: Pd/C.H2

Protections: none

Reference: *10.1021/ja4129394*

Retrosynthesis ID: 9998198

2.3.2 Synthesis of alkyl azides from alkyl amines and TfN3



Substrates:

1. trifluoromethanesulfonyl azide
2. CCCCC(O)C(N)C(=O)OC

Products:

1. CCCCC(O)C(N=[N+]=[N-])C(=O)OC

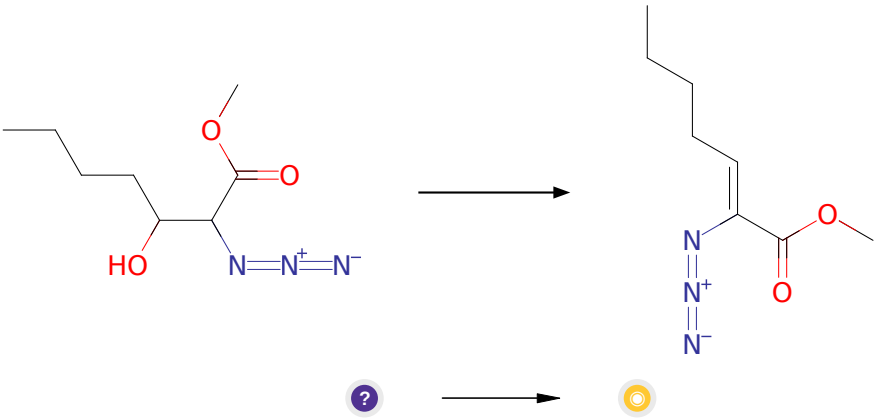
Typical conditions: H2O.K2CO3.CH2Cl2.CuSO4.MeOH

Protections: none

Reference: DOI: *10.1016/0040-4039(96)01307-X*

Retrosynthesis ID: 9920002

2.3.3 Dehydration of Beta Hydroxy Carbonyl Compounds



Substrates:

1. CCCCC(O)C(N=[N+]=[N-])C(=O)OC

Products:

1. CCCC/C=C(\N=[N+]=[N-])C(=O)OC

Typical conditions: TsOH

Protections: none

Reference: DOI:*10.1002/anie.201204977* AND *10.1021/ol062777o*

Retrosynthesis ID: 7732

2.4 Path 4

Score: 84.06

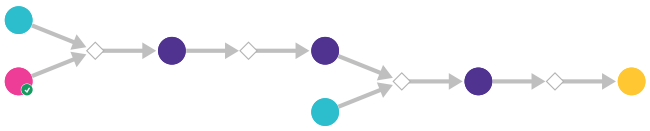
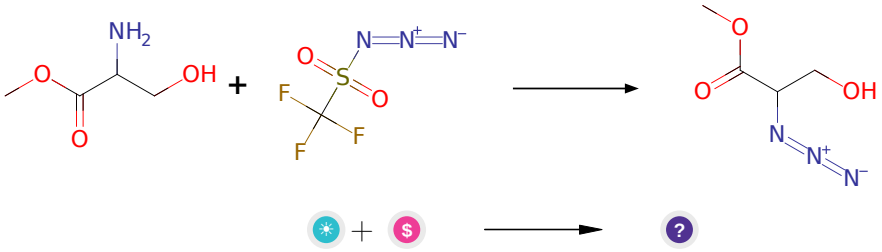


Figure 4: Outline of path 4

2.4.1 Synthesis of alkyl azides from alkyl amines and TfN3



Substrates:

1. trifluoromethanesulfonyl azide
2. DL-Serine methyl ester hydrochloride - *available at Sigma-Aldrich*

Products:

1. COC(=O)C(CO)N=[N+]=[N-]

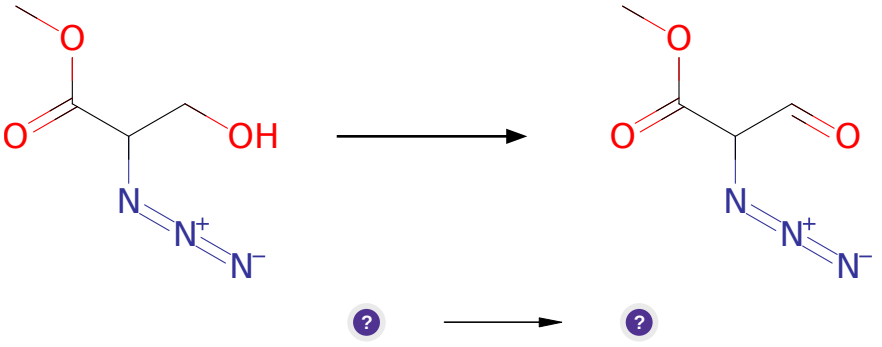
Typical conditions: H2O.K2CO3.CH2Cl2.CuSO4.MeOH

Protections: none

Reference: DOI: *10.1016/0040-4039(96)01307-X*

Retrosynthesis ID: 9920002

2.4.2 Oxidation of primary alcohols with DMP



Substrates:

1. COC(=O)C(CO)N=[N+]=[N-]

Products:

1. COC(=O)C(C=O)N=[N+]=[N-]

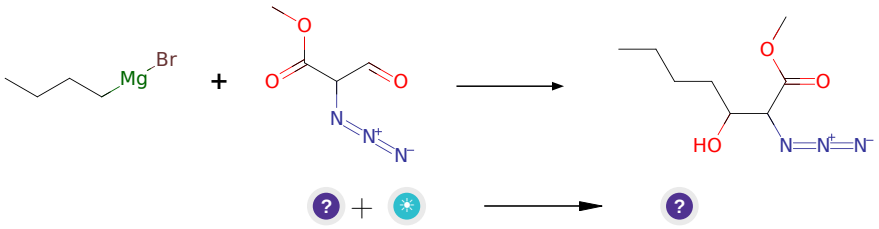
Typical conditions: DMP.DCM.0-25 C

Protections: none

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

Retrosynthesis ID: 50426

2.4.3 Grignard-Type Reaction



Substrates:

1. COC(=O)C(C=O)N=[N+]=[N-]
2. butylmagnesium bromide

Products:

1. CCCCC(O)C(N=[N+]=[N-])C(=O)OC

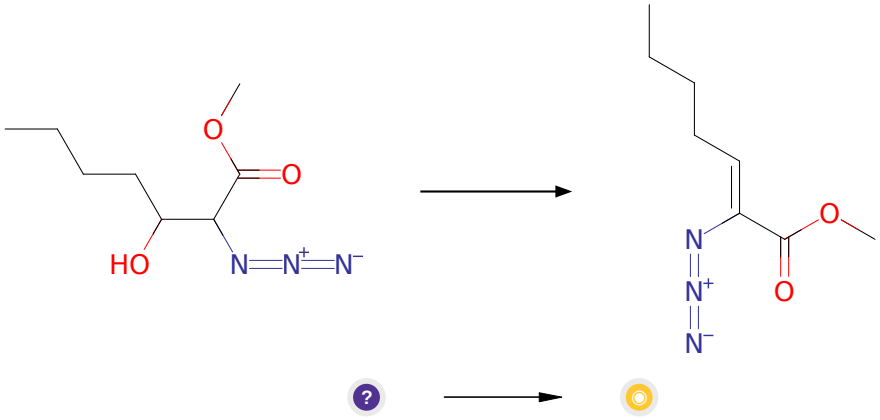
Typical conditions: Mg or Li.ether

Protections: none

Reference: *10.1016/S0040-4020(99)00197-0* or *10.1055/s-0030-1260809* or *10.1021/ol703056u*

Retrosynthesis ID: 25124

2.4.4 Dehydration of Beta Hydroxy Carbonyl Compounds



Substrates:

1. CCCCC(O)C(N=[N+]=[N-])C(=O)OC

Products:

1. CCCC/C=C(\N=[N+]=[N-])C(=O)OC

Typical conditions: TsOH

Protections: none

Reference: DOI:*10.1002/anie.201204977* AND *10.1021/ol062777o*

Retrosynthesis ID: 7732

2.5 Path 5

Score: 84.06

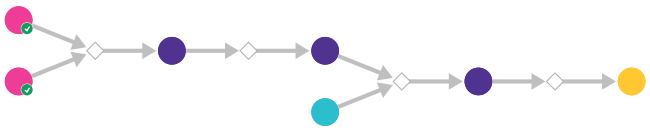
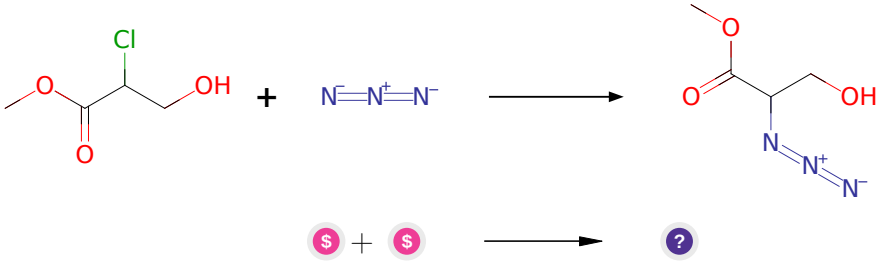


Figure 5: Outline of path 5

2.5.1 Nucleophilic substitution with azides



Substrates:

1. Potassium azide - *available at Sigma-Aldrich*
2. Methyl 2-chloro-3-hydroxypropionate - *available at Sigma-Aldrich*

Products:

1. COC(=O)C(CO)N=[N+]=[N-]

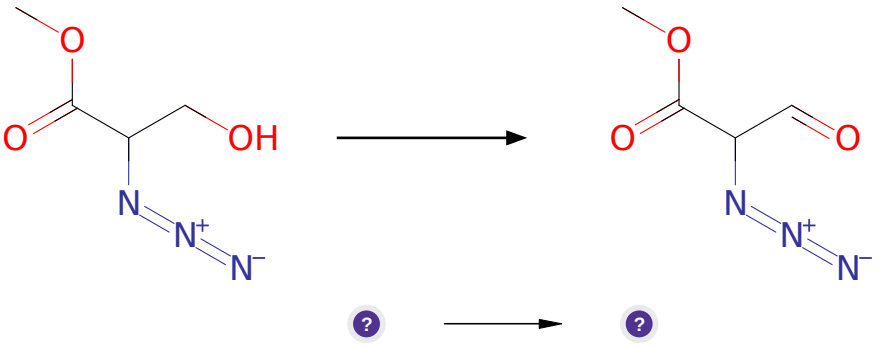
Typical conditions: DMF.heat

Protections: none

Reference: *10.1021/jo990445+* and *10.1002/adsc.200404102*

Retrosynthesis ID: 31011206

2.5.2 Oxidation of primary alcohols with DMP



Substrates:

1. COC(=O)C(CO)N=[N+]=[N-]

Products:

1. COC(=O)C(C=O)N=[N+]=[N-]

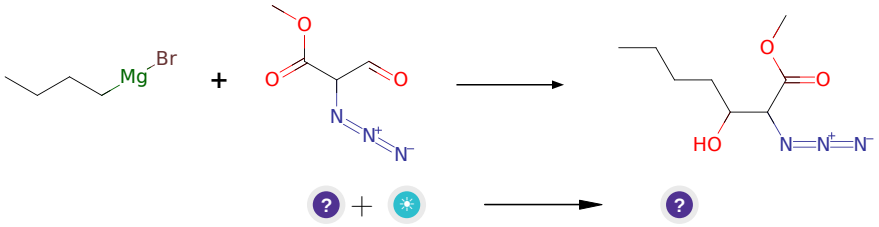
Typical conditions: DMP.DCM.0-25 C

Protections: none

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

Retrosynthesis ID: 50426

2.5.3 Grignard-Type Reaction



Substrates:

1. COC(=O)C(C=O)N=[N+]=[N-]
2. butylmagnesium bromide

Products:

1. CCCCC(O)C(N=[N+]=[N-])C(=O)OC

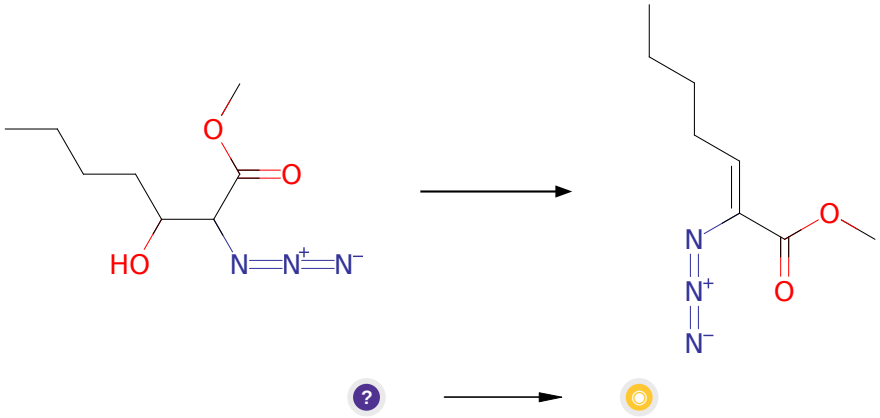
Typical conditions: Mg or Li.ether

Protections: none

Reference: *10.1016/S0040-4020(99)00197-0* or *10.1055/s-0030-1260809* or *10.1021/ol703056u*

Retrosynthesis ID: 25124

2.5.4 Dehydration of Beta Hydroxy Carbonyl Compounds



Substrates:

1. CCCCC(O)C(N=[N+]=[N-])C(=O)OC

Products:

1. CCCC/C=C(\N=[N+]=[N-])C(=O)OC

Typical conditions: TsOH

Protections: none

Reference: DOI:*10.1002/anie.201204977* AND *10.1021/ol062777o*

Retrosynthesis ID: 7732