Paths of analysis*

PG7

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

*The results stated herein were generated using the proprietary platform owned and maintained by Grzybowski Scientific Inventions, Inc., a subsidiary of Merck KGaA, Darmstadt Germany. The results are provided on an as is basis, and shall be used solely in connection with the rights afforded in the license agreement and for no other purpose.

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`

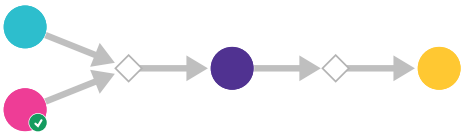
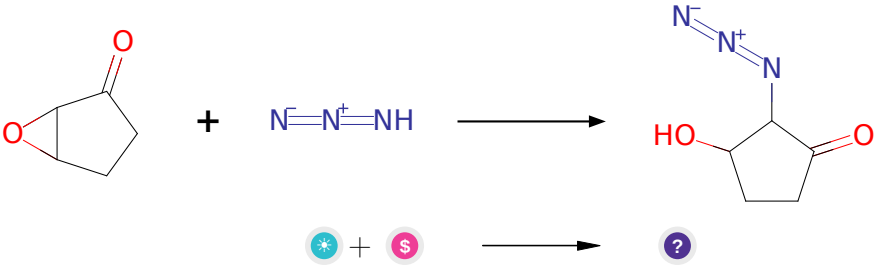


Figure 1: Outline of path 1

2.1.1 Ring-opening of epoxides or thiiranes with azides



Substrates:

1. hydrazoic acid
2. 6-OXABICYCLO[3.1.0]HEXAN-2-ONE - *available at Sigma-Aldrich*

Products:

1. [N-]=[N+]=NC1C(=O)CCC1O

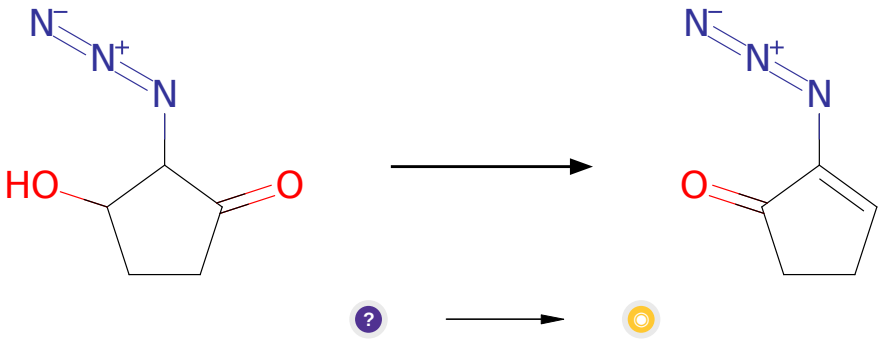
Typical conditions: NaN3.NH4Cl.MeOH.H2O.65 C

Protections: none

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

Retrosynthesis ID: 858

2.1.2 Dehydration of Beta Hydroxy Carbonyl Compounds



Substrates:

1. [N-]=[N+]=NC1C(=O)CCC1O

Products:

1. C5H5N3O

Typical conditions: TsOH

Protections: none

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

Retrosynthesis ID: 7731

2.2 Path 2

Score: 76.25

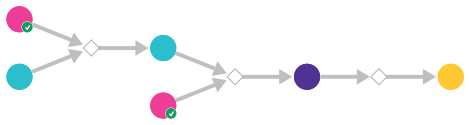
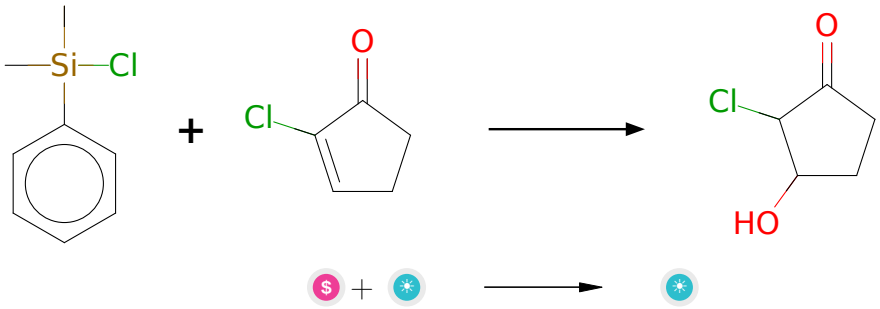


Figure 2: Outline of path 2

2.2.1 Addition of silanes to Michael acceptors followed by oxidation



Substrates:

1. DMPSCl - *available at Sigma-Aldrich*
2. 2-chloro-cyclopent-2-enone

Products:

1. C5H7ClO2

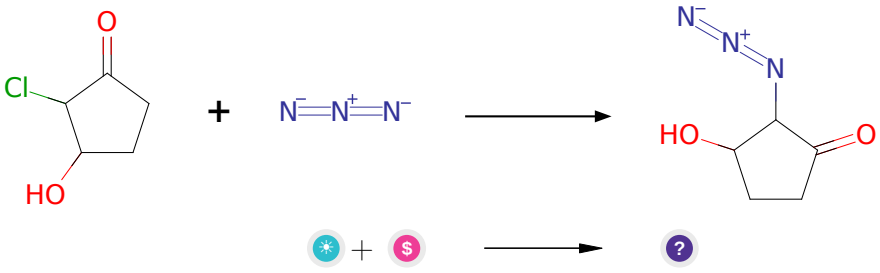
Typical conditions: 1.nBuLi.2.CuCN.3.electrophile.4.H2O2

Protections: none

Reference: *10.1021/ja058370g* AND (Oxidation) *10.1021/jo9905672* or *10.1021/ol300832f*

Retrosynthesis ID: 20295

2.2.2 Nucleophilic substitution with azides



Substrates:

1. C5H7ClO2
2. Potassium azide - *available at Sigma-Aldrich*

Products:

1. [N-]=[N+]=NC1C(=O)CCC1O

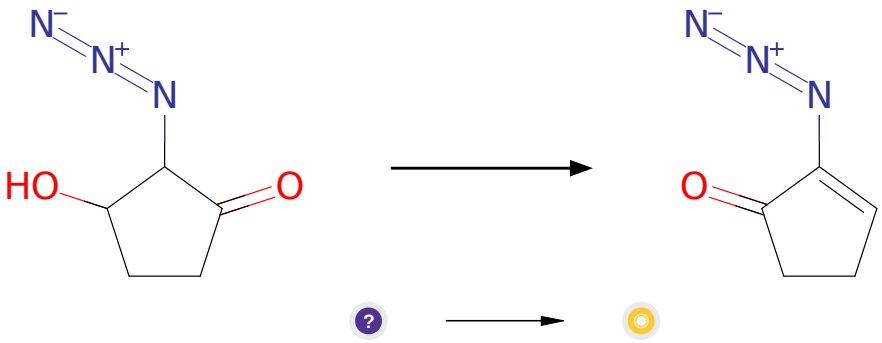
Typical conditions: DMF.heat

Protections: none

Reference: *10.1016/j.tet.2013.11.027* and *10.1021/jo015632y* and *10.3987/COM-06-S(K)18*

Retrosynthesis ID: 31011248

2.2.3 Dehydration of Beta Hydroxy Carbonyl Compounds



Substrates:

1. [N-]=[N+]=NC1C(=O)CCC1O

Products:

1. C5H5N3O

Typical conditions: TsOH

Protections: none

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

Retrosynthesis ID: 7731

2.3 Path 3

Score: 84.06

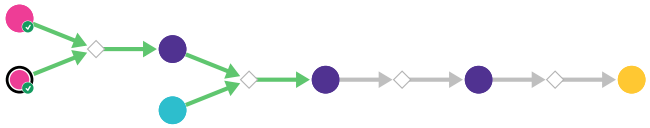
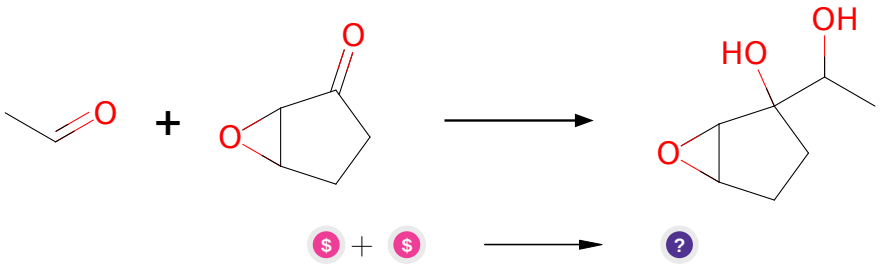


Figure 3: Outline of path 3

2.3.1 Pinacol Coupling Reaction



Substrates:

1. 6-OXABICYCLO[3.1.0]HEXAN-2-ONE - *available at Sigma-Aldrich*
2. Ethanal - *available at Sigma-Aldrich*

Products:

1. CC(O)C1(O)CCC2OC21

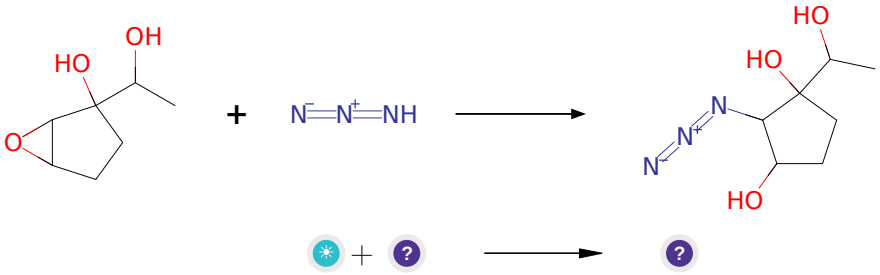
Typical conditions: Mg.NH4Cl.H2O or Mg.SmI2.TMSCl.THF.HMPA

Protections: none

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

Retrosynthesis ID: 10205

2.3.2 Ring-opening of epoxides or thiiranes with azides



Substrates:

1. hydrazoic acid
2. CC(O)C1(O)CCC2OC21

Products:

1. CC(O)C1(O)CCC(O)C1N=[N+]=[N-]

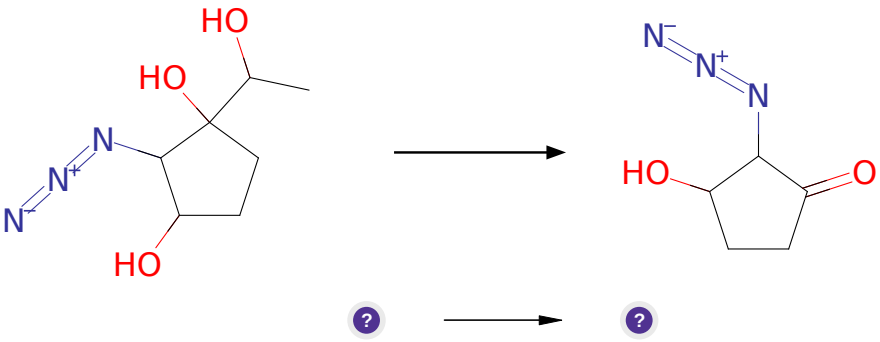
Typical conditions: NaN3.NH4Cl.MeOH.H2O.65 C

Protections: none

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

Retrosynthesis ID: 858

2.3.3 Cleavage of 1,2-diols with NaIO4



Substrates:

1. CC(O)C1(O)CCC(O)C1N=[N+]=[N-]

Products:

1. [N-]=[N+]=NC1C(=O)CCC1O

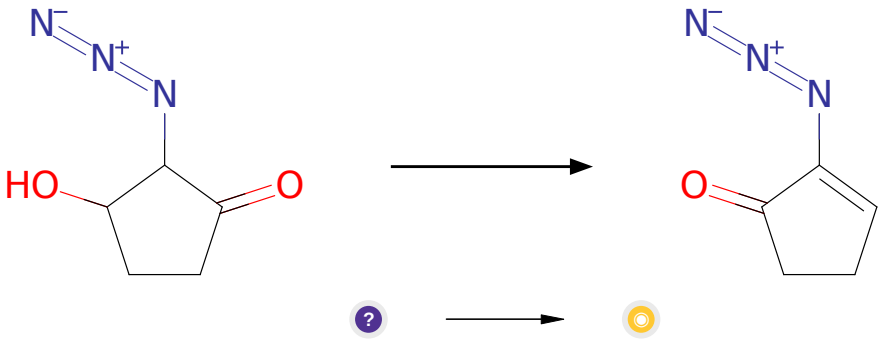
Typical conditions: NaIO4.solvent

Protections: none

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

Retrosynthesis ID: 31017508

2.3.4 Dehydration of Beta Hydroxy Carbonyl Compounds



Substrates:

1. [N-]=[N+]=NC1C(=O)CCC1O

Products:

1. C5H5N3O

Typical conditions: TsOH

Protections: none

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

Retrosynthesis ID: 7731

2.4 Path 4

Score: `84.06`

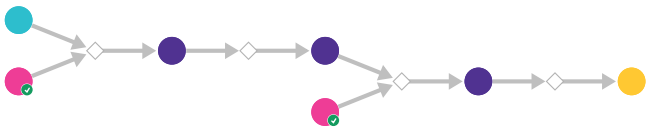
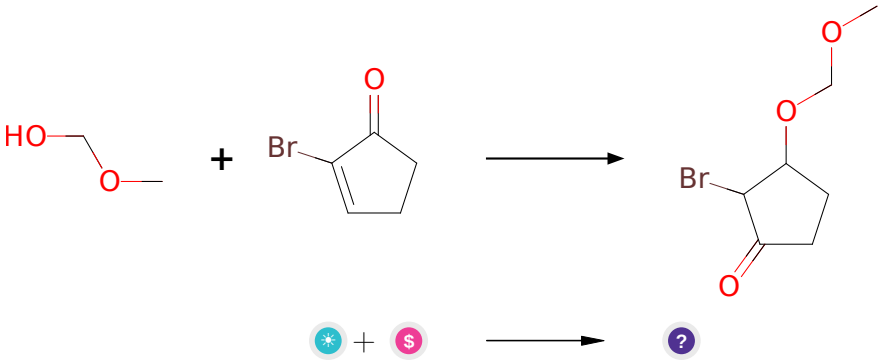


Figure 4: Outline of path 4

2.4.1 Addition of alcohols or phenols to Michael acceptors



Substrates:

1. methoxymethanol
2. 2-Bromocyclopent-2-enone - *available at Sigma-Aldrich*

Products:

1. COCOC1CCC(=O)C1Br

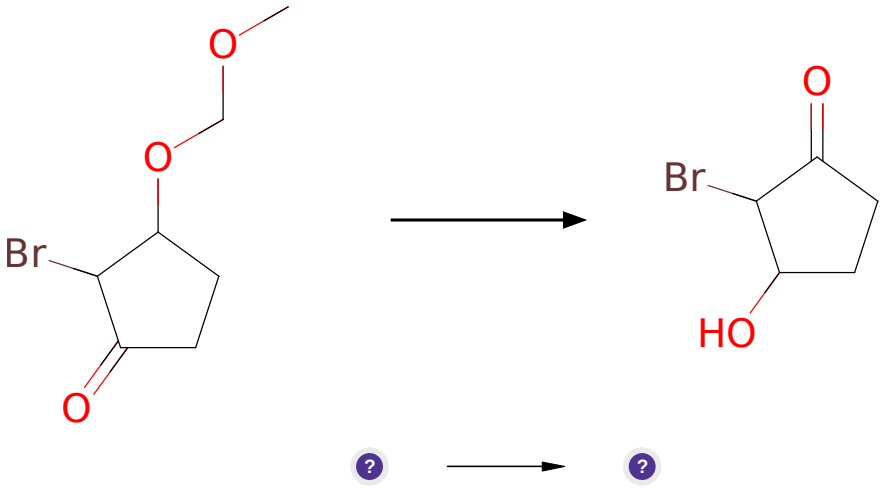
Typical conditions: cat.Na.DMF

Protections: none

Reference: 14.1016/S0957-4166(97)00479-5 AND *10.1016/S0040-4020(98)00817-5* AND *10.1021/np970346w*

Retrosynthesis ID: 12432

2.4.2 Hydrolysis of acetals



Substrates:

1. COCOC1CCC(=O)C1Br

Products:

1. O=C1CCC(O)C1Br

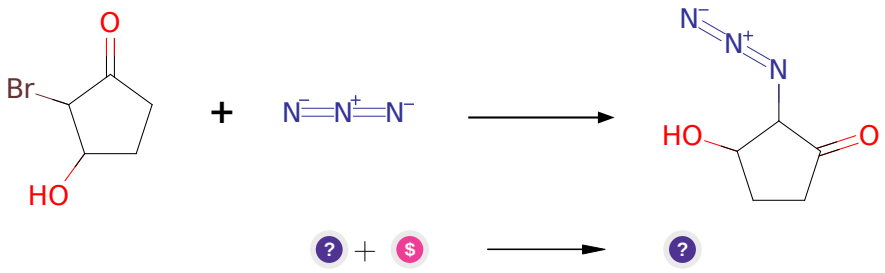
Typical conditions: HCl.THF ot TFA.DCM

Protections: none

Reference: *10.1002/ejoc.201301615* and *10.3762/bjoc.9.289* and *10.1080/00397919808004478* and *10.1016/S0040-4039(99)02200-5* and *10.1055/s-0030-1258583* and *10.1016/j.tet.2011.04.072*

Retrosynthesis ID: 31013131

2.4.3 Nucleophilic substitution with azides



Substrates:

1. O=C1CCC(O)C1Br
2. Potassium azide - *available at Sigma-Aldrich*

Products:

1. [N-]=[N+]=NC1C(=O)CCC1O

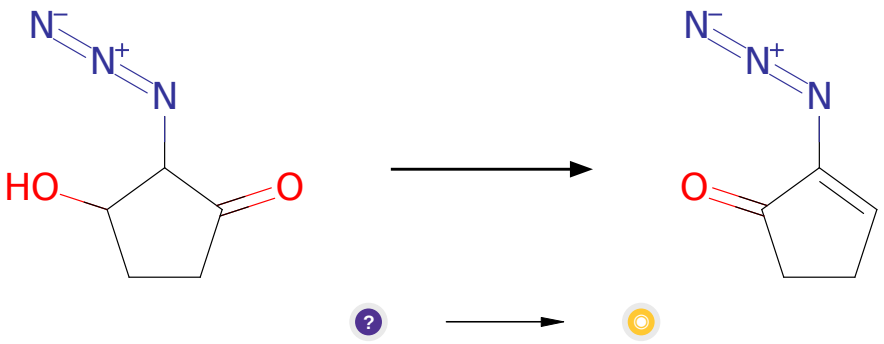
Typical conditions: DMF.heat

Protections: none

Reference: *10.1021/ol049369+* and *10.1016/S0040-4039(00)61343-6* and *10.1016/j.bmcl.2005.03.055*

Retrosynthesis ID: 31011250

2.4.4 Dehydration of Beta Hydroxy Carbonyl Compounds



Substrates:

1. [N-]=[N+]=NC1C(=O)CCC1O

Products:

1. C5H5N3O

Typical conditions: TsOH

Protections: none

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

Retrosynthesis ID: 7731

2.5 Path 5

Score: 84.06

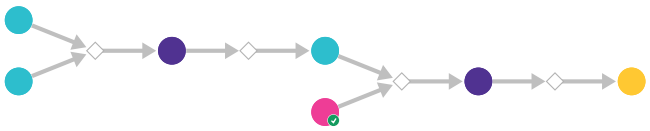
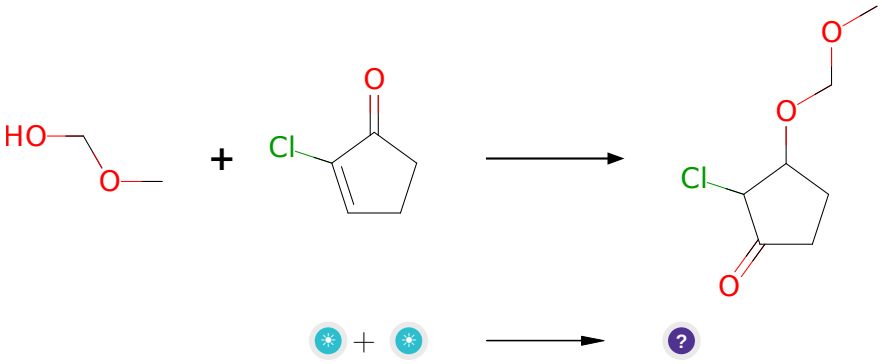


Figure 5: Outline of path 5

2.5.1 Addition of alcohols or phenols to Michael acceptors



Substrates:

1. methoxymethanol
2. 2-chloro-cyclopent-2-enone

Products:

1. COCOC1CCC(=O)C1Cl

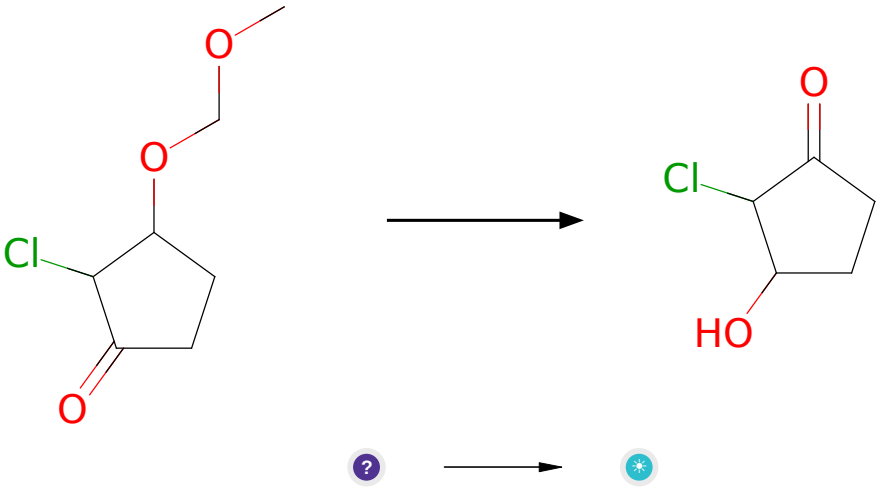
Typical conditions: cat.Na.DMF

Protections: none

Reference: 14.1016/S0957-4166(97)00479-5 AND *10.1016/S0040-4020(98)00817-5* AND *10.1021/np970346w*

Retrosynthesis ID: 12432

2.5.2 Hydrolysis of acetals



Substrates:

1. COCOC1CCC(=O)C1Cl

Products:

1. C5H7ClO2

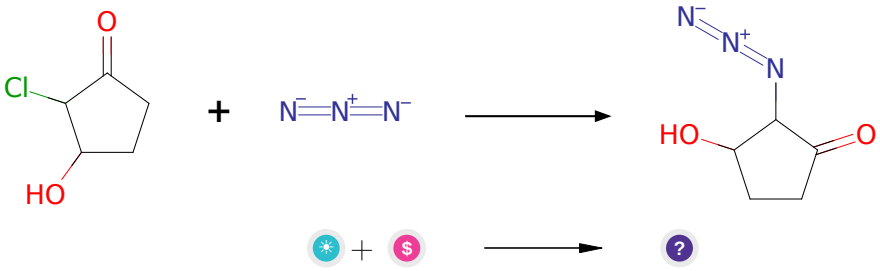
Typical conditions: HCl.THF ot TFA.DCM

Protections: none

Reference: *10.1002/ejoc.201301615* and *10.3762/bjoc.9.289* and *10.1080/00397919808004478* and *10.1016/S0040-4039(99)02200-5* and *10.1055/s-0030-1258583* and *10.1016/j.tet.2011.04.072*

Retrosynthesis ID: 31013131

2.5.3 Nucleophilic substitution with azides



Substrates:

1. C5H7ClO2
2. Potassium azide - *available at Sigma-Aldrich*

Products:

1. [N-]=[N+]=NC1C(=O)CCC1O

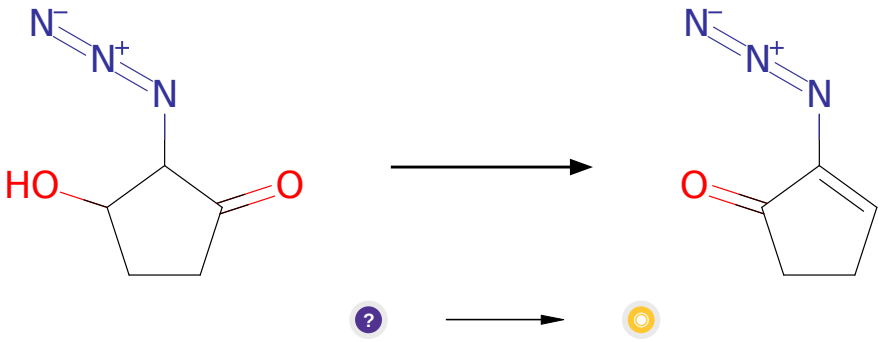
Typical conditions: DMF.heat

Protections: none

Reference: *10.1016/j.tet.2013.11.027* and *10.1021/jo015632y* and *10.3987/COM-06-S(K)18*

Retrosynthesis ID: 31011248

2.5.4 Dehydration of Beta Hydroxy Carbonyl Compounds



Substrates:

1. [N-]=[N+]=NC1C(=O)CCC1O

Products:

1. C5H5N3O

Typical conditions: TsOH

Protections: none

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

Retrosynthesis ID: 7731