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: 90.31

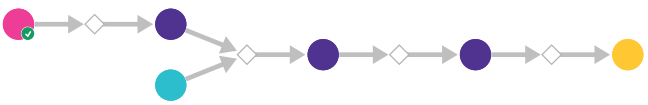
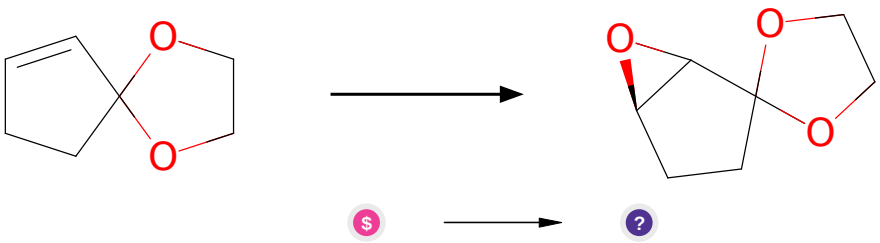


Figure 1: Outline of path 1

2.1.1 Shi epoxidation



Substrates:

1. 1,4-Dioxaspiro[4.4]non-6-ene - *available at Sigma-Aldrich*

Products:

1. C1COC2(CC[C@H]3OC32)O1

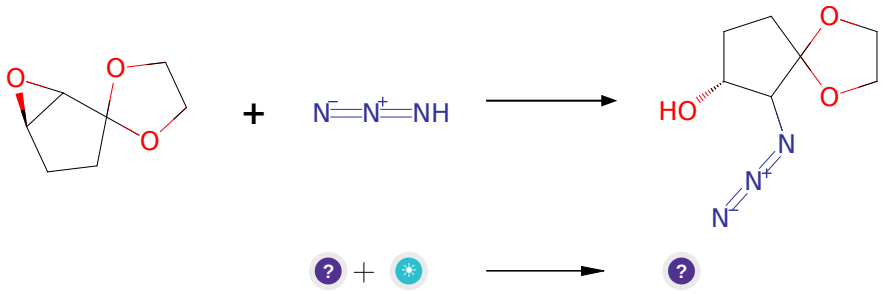
Typical conditions: sugar.based.catalyst.KHSO5.K2CO3.H2O.ACN.0C

Protections: none

Reference: *10.1055/s-0028-1083545* and *10.1021/ja972272g* and *10.1021/ja003049d* and *10.1021/jo972106r*

Retrosynthesis ID: 7429

2.1.2 Ring-opening of epoxides or thiiranes with azides



Substrates:

1. C1COC2(CC[C@H]3OC32)O1
2. hydrazoic acid

Products:

1. [N-]=[N+]=NC1[C@H](O)CCC12OCCO2

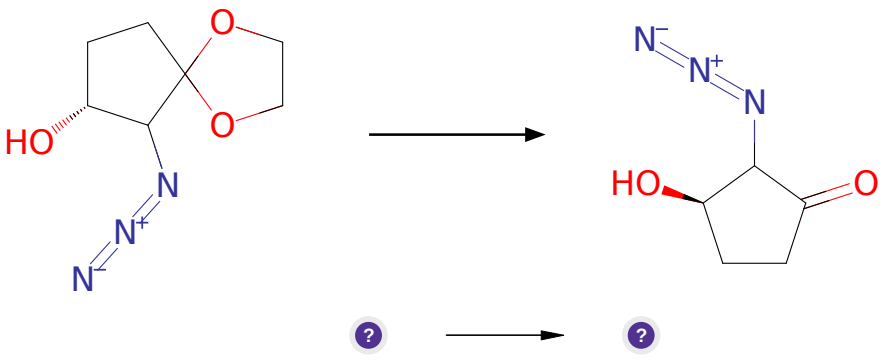
Typical conditions: NaN3.NH4Cl.MeOH.H2O.65 C

Protections: none

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

Retrosynthesis ID: 858

2.1.3 Hydrolysis of ketals



Substrates:

1. [N-]=[N+]=NC1[C@H](O)CCC12OCCO2

Products:

1. [N-]=[N+]=NC1C(=O)CC[C@H]1O

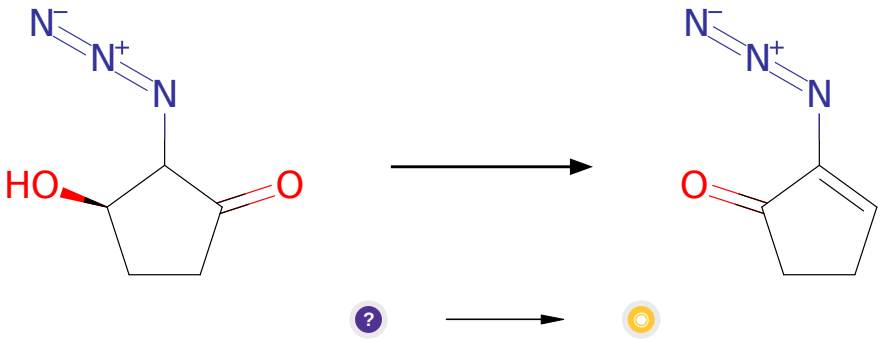
Typical conditions: H2O.HCl

Protections: none

Reference: *10.1021/jo0159035* and *10.1021/jo00194a003* and

Retrosynthesis ID: 31013139

2.1.4 Dehydration of beta-ketoalcohols



Substrates:

1. [N-]=[N+]=NC1C(=O)CC[C@H]1O

Products:

1. C5H5N3O

Typical conditions: 1.MsCl.NEt3

Protections: none

Reference: *10.1021/ol301090v* and *10.1021/ja00521a062* and *10.1002/ejoc.201201636* (SI)

Retrosynthesis ID: 20813

2.2 Path 2

Score: `90.31`

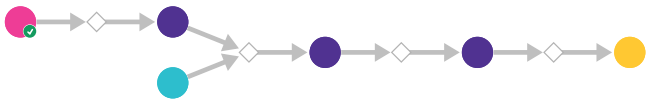
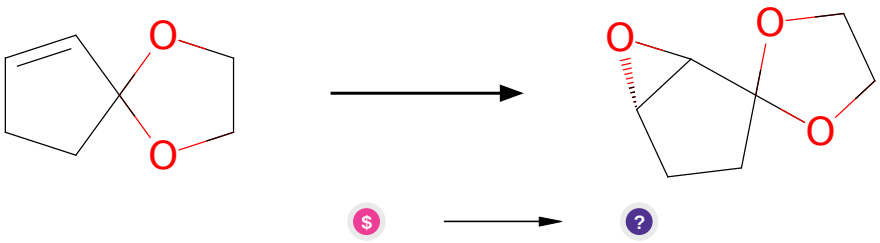


Figure 2: Outline of path 2

2.2.1 Shi epoxidation



Substrates:

1. 1,4-Dioxaspiro[4.4]non-6-ene - *available at Sigma-Aldrich*

Products:

1. C1COC2(CC[C@@H]3OC32)O1

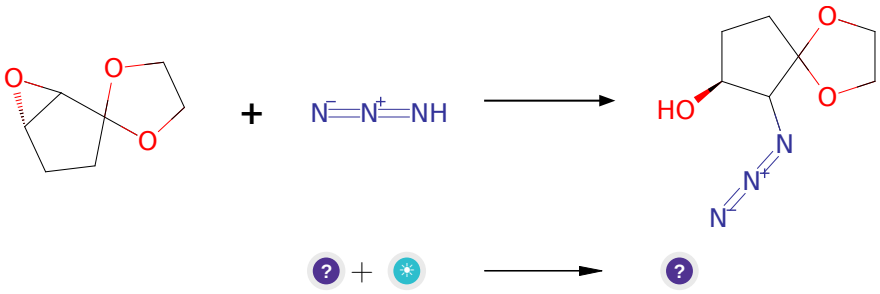
Typical conditions: sugar.based.catalyst.KHSO5.K2CO3.H2O.ACN.0C

Protections: none

Reference: *10.1055/s-0028-1083545* and *10.1021/ja972272g* and *10.1021/ja003049d* and *10.1021/jo972106r*

Retrosynthesis ID: 7433

2.2.2 Ring-opening of epoxides or thiiranes with azides



Substrates:

1. C1COC2(CC[C@@H]3OC32)O1

2. hydrazoic acid

Products:

1. [N-]=[N+]=NC1[C@@H](O)CCC12OCCO2

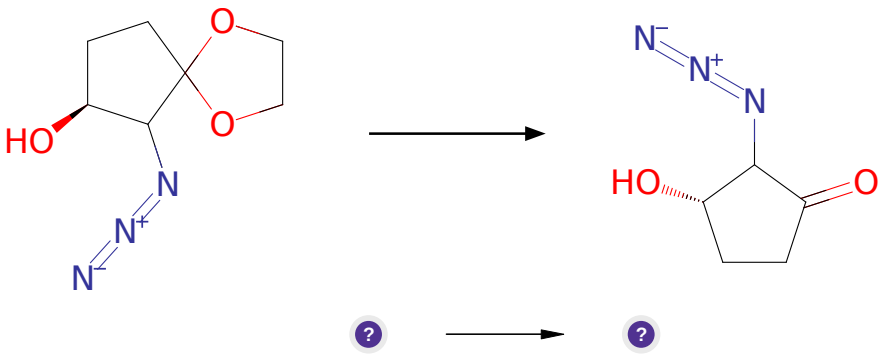
Typical conditions: NaN3.NH4Cl.MeOH.H2O.65 C

Protections: none

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

Retrosynthesis ID: 859

2.2.3 Hydrolysis of ketals



Substrates:

1. [N-]=[N+]=NC1[C@@H](O)CCC12OCCO2

Products:

1. [N-]=[N+]=NC1C(=O)CC[C@@H]1O

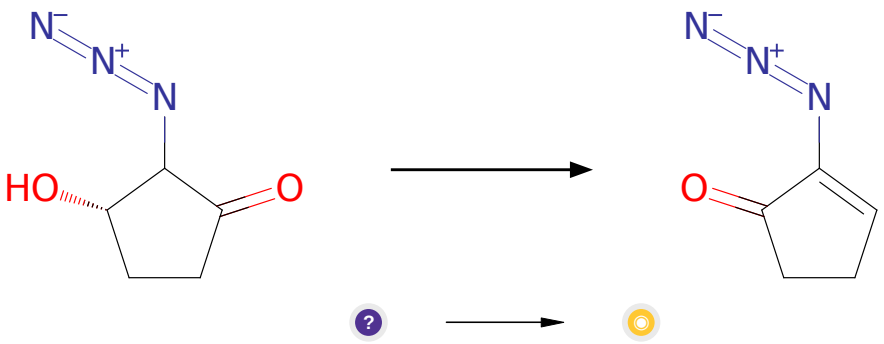
Typical conditions: H2O.HCl

Protections: none

Reference: *10.1021/jo0159035* and *10.1021/jo00194a003* and

Retrosynthesis ID: 31013139

2.2.4 Dehydration of beta-ketoalcohols



Substrates:

1. [N-]=[N+]=NC1C(=O)CC[C@@H]1O

Products:

1. C5H5N3O

Typical conditions: 1.MsCl.NEt3

Protections: none

Reference: *10.1021/ol301090v* and *10.1021/ja00521a062* and *10.1002/ejoc.201201636* (SI)

Retrosynthesis ID: 20812

2.3 Path 3

Score: `100.08`

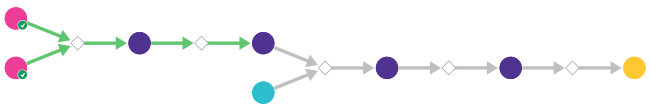
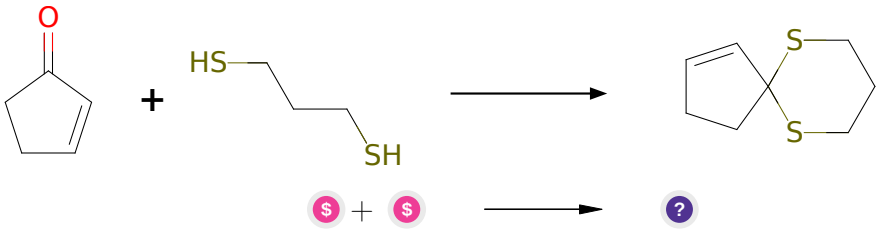


Figure 3: Outline of path 3

2.3.1 Synthesis of ketals and acetals



Substrates:

1. 2-Cyclopenten-1-one - *available at Sigma-Aldrich*
2. 1,3-Propanedithiol - *available at Sigma-Aldrich*

Products:

1. C1=CC2(CC1)SCCCS2

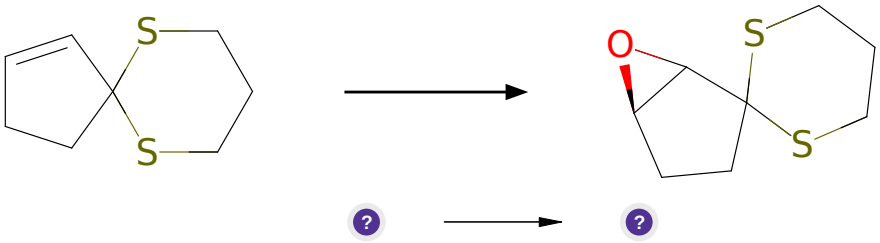
Typical conditions: pTsOH.toluene.heat

Protections: none

Reference: *10.1039/P19880000817* AND *10.1016/j.tetlet.2012.07.052* AND *10.1039/C0CC00110D* AND *10.1002/1521-3765(20010504)7:9<2007::AID-CHEM2007>3.0.CO;2-7*

Retrosynthesis ID: 14599

2.3.2 Shi epoxidation



Substrates:

1. C1=CC2(CC1)SCCCS2

Products:

1. C1CSC2(CC[C@H]3OC32)SC1

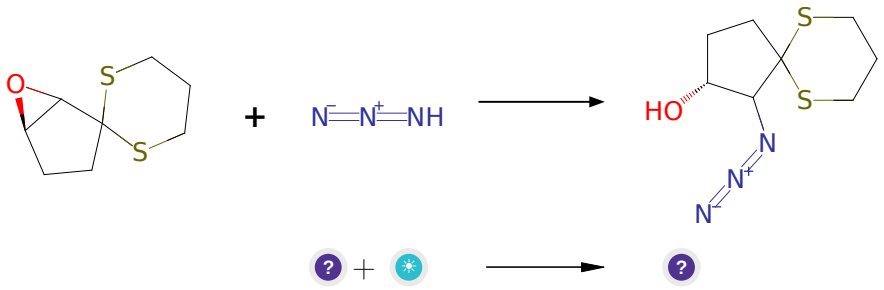
Typical conditions: sugar.based.catalyst.KHSO5.K2CO3.H2O.ACN.0C

Protections: none

Reference: *10.1055/s-0028-1083545* and *10.1021/ja972272g* and *10.1021/ja003049d* and *10.1021/jo972106r*

Retrosynthesis ID: 7429

2.3.3 Ring-opening of epoxides or thiiranes with azides



Substrates:

1. C1CSC2(CC[C@H]3OC32)SC1
2. hydrazoic acid

Products:

1. [N-]=[N+]=NC1[C@H](O)CCC12SCCCS2

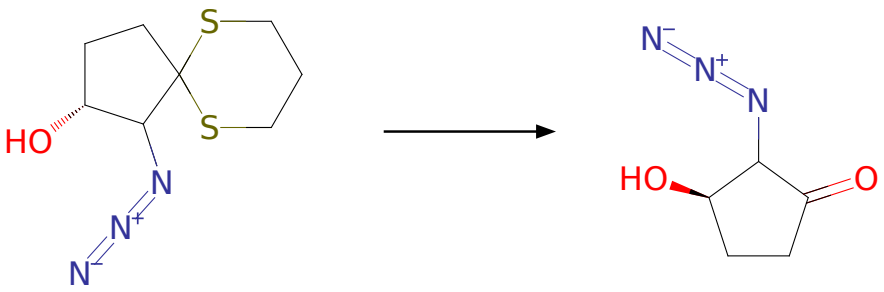
Typical conditions: NaN3.NH4Cl.MeOH.H2O.65 C

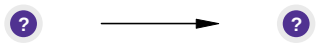
Protections: none

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

Retrosynthesis ID: 858

2.3.4 Synthesis of ketones from dithianes





Substrates:

1. [N-]=[N+]=NC1[C@H](O)CCC12SCCCS2

Products:

1. [N-]=[N+]=NC1C(=O)CC[C@H]1O

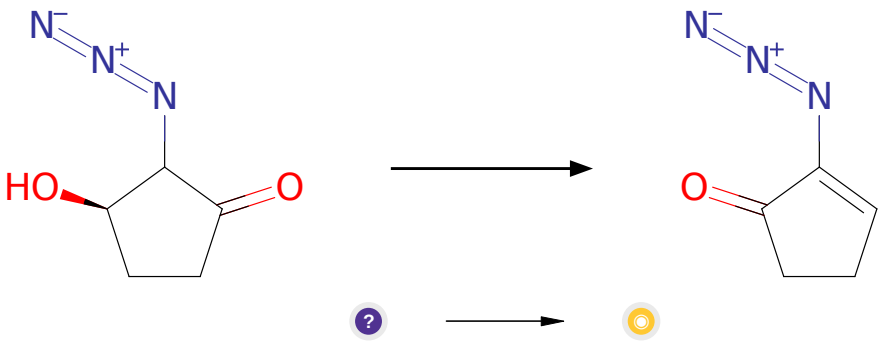
Typical conditions: MeI.CaCO3

Protections: none

Reference: *10.1016/j.tet.2013.09.075* and *10.1021/jo00007a015* and *10.1021/jo0610412* and *10.1021/ol901024t* and *10.1021/ol500553x* and *10.1021/jo0626459*

Retrosynthesis ID: 31724

2.3.5 Dehydration of beta-ketoalcohols



Substrates:

1. [N-]=[N+]=NC1C(=O)CC[C@H]1O

Products:

1. C5H5N3O

Typical conditions: 1.MsCl.NEt3

Protections: none

Reference: *10.1021/ol301090v* and *10.1021/ja00521a062* and *10.1002/ejoc.201201636* (SI)

Retrosynthesis ID: 20813

2.4 Path 4

Score: 100.08

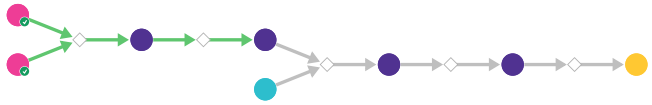
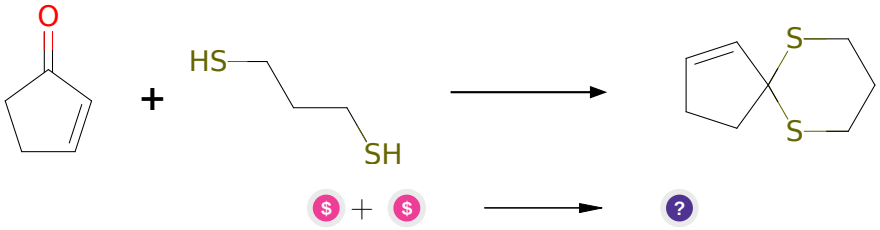


Figure 4: Outline of path 4

2.4.1 Synthesis of ketals and acetals



Substrates:

1. 2-Cyclopenten-1-one - *available at Sigma-Aldrich*
2. 1,3-Propanedithiol - *available at Sigma-Aldrich*

Products:

1. C1=CC2(CC1)SCCCS2

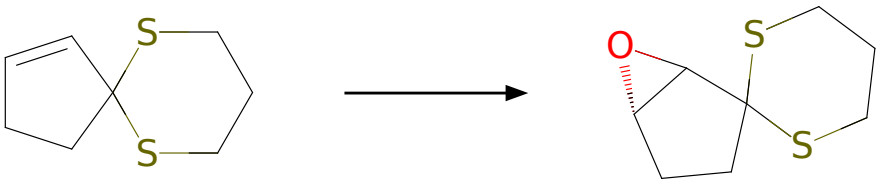
Typical conditions: pTsOH.toluene.heat

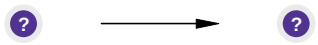
Protections: none

Reference: *10.1039/P19880000817* AND *10.1016/j.tetlet.2012.07.052* AND *10.1039/C0CC00110D* AND *10.1002/1521-3765(20010504)7:9<2007::AID-CHEM2007>3.0.CO;2-7*

Retrosynthesis ID: 14599

2.4.2 Shi epoxidation





Substrates:

1. C1=CC2(CC1)SCCCS2

Products:

1. C1CSC2(CC[C@@H]3OC32)SC1

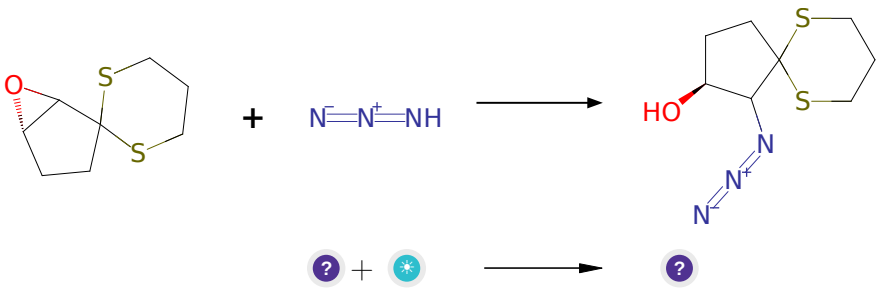
Typical conditions: sugar.based.catalyst.KHSO5.K2CO3.H2O.ACN.0C

Protections: none

Reference: *10.1055/s-0028-1083545* and *10.1021/ja972272g* and *10.1021/ja003049d* and *10.1021/jo972106r*

Retrosynthesis ID: 7433

2.4.3 Ring-opening of epoxides or thiiranes with azides



Substrates:

1. C1CSC2(CC[C@@H]3OC32)SC1
2. hydrazoic acid

Products:

1. [N-]=[N+]=NC1[C@@H](O)CCC12SCCCS2

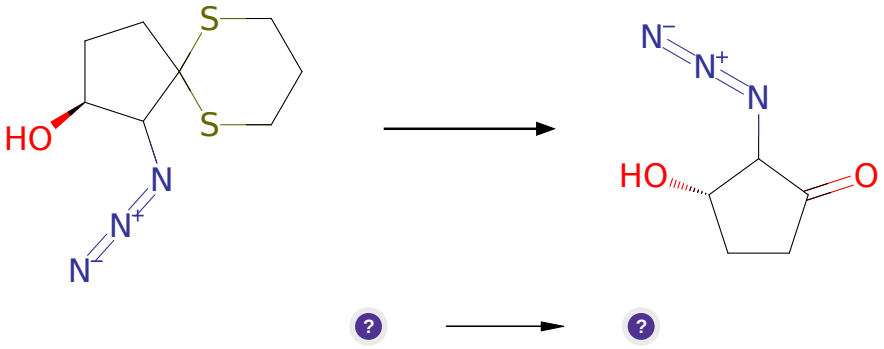
Typical conditions: NaN3.NH4Cl.MeOH.H2O.65 C

Protections: none

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

Retrosynthesis ID: 859

2.4.4 Synthesis of ketones from dithianes



Substrates:

1. [N-]=[N+]=NC1[C@@H](O)CCC12SCCCS2

Products:

1. [N-]=[N+]=NC1C(=O)CC[C@@H]1O

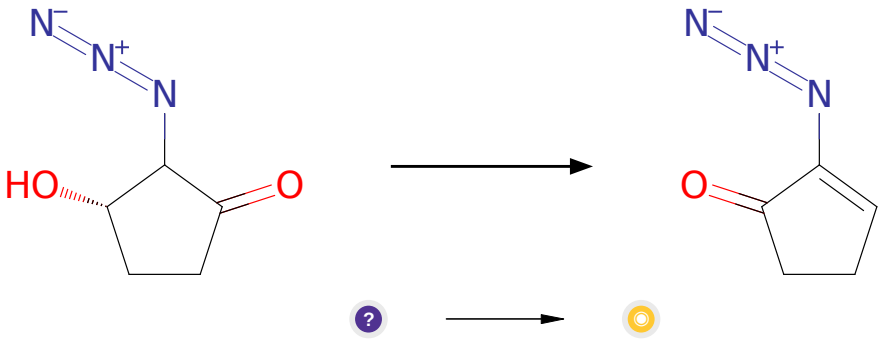
Typical conditions: MeI.CaCO3

Protections: none

Reference: *10.1016/j.tet.2013.09.075* and *10.1021/jo00007a015* and *10.1021/jo0610412* and *10.1021/ol901024t* and *10.1021/ol500553x* and *10.1021/jo0626459*

Retrosynthesis ID: 31724

2.4.5 Dehydration of beta-ketoalcohols



Substrates:

1. [N-]=[N+]=NC1C(=O)CC[C@@H]1O

Products:

1. C5H5N3O

Typical conditions: 1.MsCl.NEt3

Protections: none

Reference: *10.1021/ol301090v* and *10.1021/ja00521a062* and *10.1002/ejoc.201201636* (SI)

Retrosynthesis ID: 20812

2.5 Path 5

Score: `115.31`

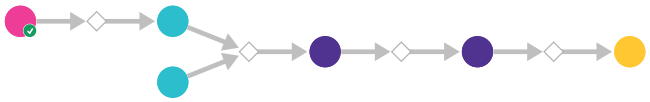
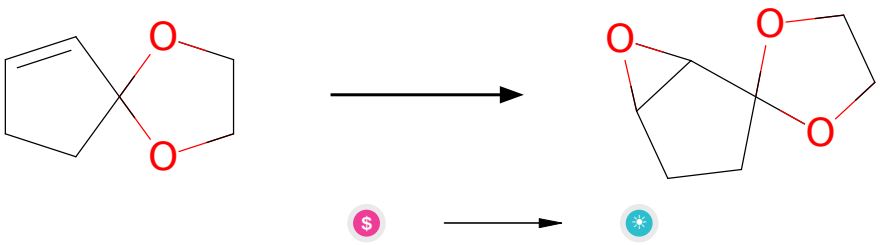


Figure 5: Outline of path 5

2.5.1 Shi epoxidation



Substrates:

1. 1,4-Dioxaspiro[4.4]non-6-ene - *available at Sigma-Aldrich*

Products:

1. 6,7-epoxy-1,4-dioxa-spiro[4.4]nonane

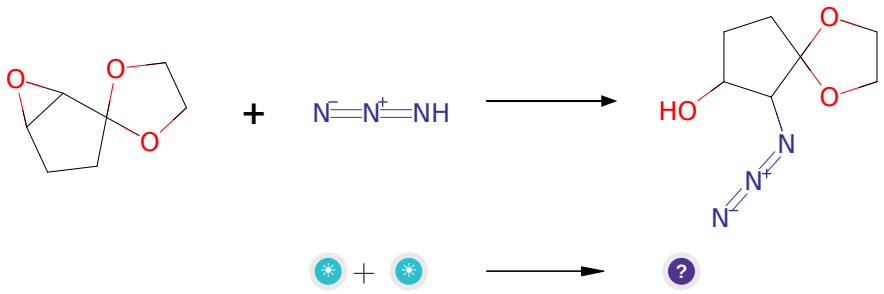
Typical conditions: sugar.based.catalyst.KHSO5.K2CO3.H2O.ACN.0C

Protections: none

Reference: *10.1055/s-0028-1083545* and *10.1021/ja972272g* and *10.1021/ja003049d* and *10.1021/jo972106r*

Retrosynthesis ID: 7429

2.5.2 Ring-opening of epoxides or thiiranes with azides



Substrates:

1. 6,7-epoxy-1,4-dioxa-spiro[4.4]nonane
2. hydrazoic acid

Products:

1. [N-]=[N+]=NC1C(O)CCC12OCCO2

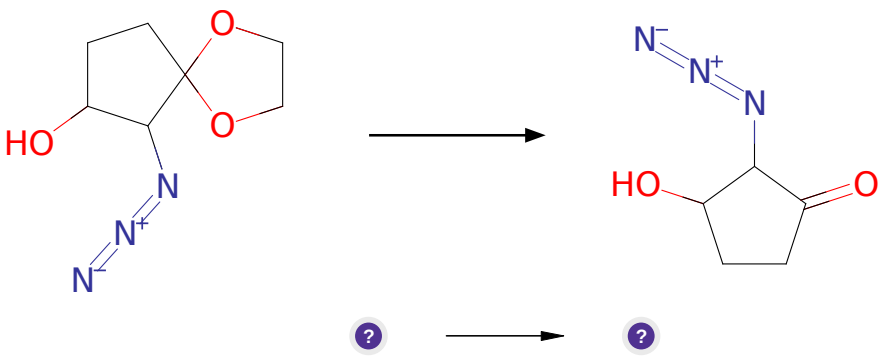
Typical conditions: NaN3.NH4Cl.MeOH.H2O.65 C

Protections: none

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

Retrosynthesis ID: 858

2.5.3 Hydrolysis of ketals



Substrates:

1. [N-]=[N+]=NC1C(O)CCC12OCCO2

Products:

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

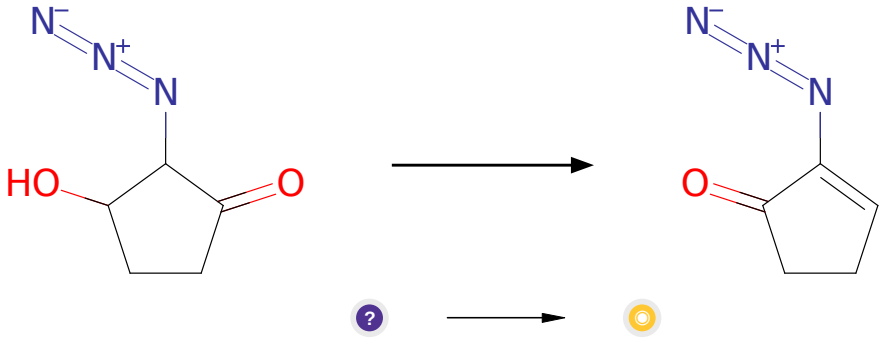
Typical conditions: H2O.HCl

Protections: none

Reference: *10.1021/jo0159035* and *10.1021/jo00194a003* and

Retrosynthesis ID: 31013139

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