Paths of analysis*

AS2

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: 364.43

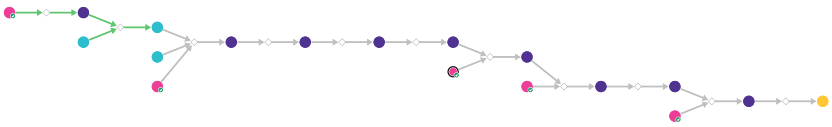
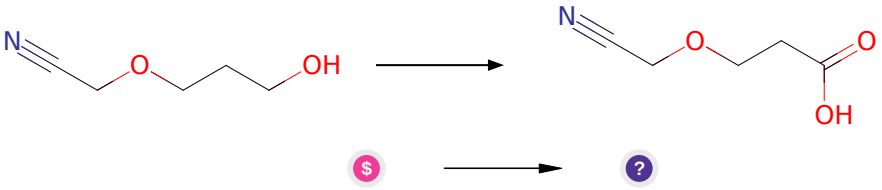


Figure 1: Outline of path 1

2.1.1 Jones Oxidation



Substrates:

1. 2-(3-Hydroxypropoxy)acetonitrile - *available at Sigma-Aldrich*

Products:

1. N#CCOCCC(=O)O

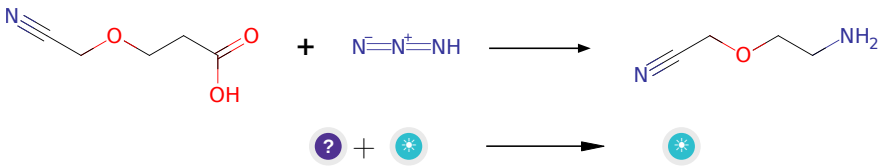
Typical conditions: cromate.sulfate.H2O.acetone

Protections: none

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

Retrosynthesis ID: 11160

2.1.2 Schmidt reaction



Substrates:

1. N#CCOCCC(=O)O
2. hydrazoic acid

Products:

1. C4H8N2O

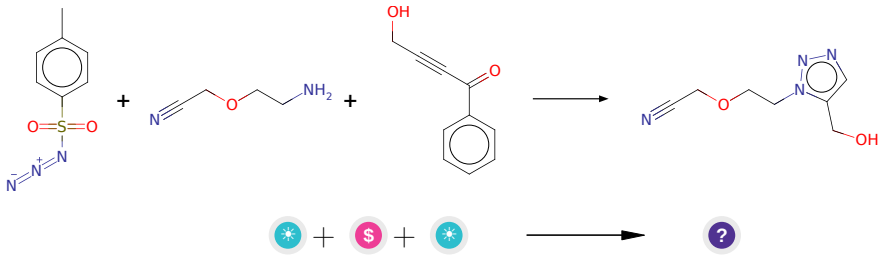
Typical conditions: azide.H+.40C

Protections: none

Reference: *10.1039/B505080D*

Retrosynthesis ID: 11702

2.1.3 Metal-free multicomponent synthesis of triazoles



Substrates:

1. 4-hydroxybut-2-ynophenone
2. Tosyl azide solution - *available at Sigma-Aldrich*
3. C4H8N2O

Products:

1. N#CCOCCn1nncc1CO

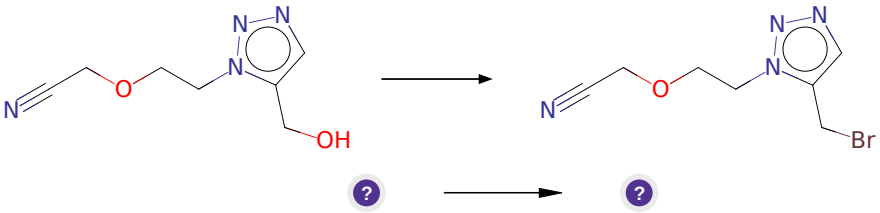
Typical conditions: 1. toluene.80C 2. LiOtBu.RT

Protections: none

Reference: DOI: *10.1002/anie.201307499*

Retrosynthesis ID: 6001

2.1.4 Appel Reaction



Substrates:

1. N#CCOCCn1nncc1CO

Products:

1. N#CCOCCn1nncc1CBr

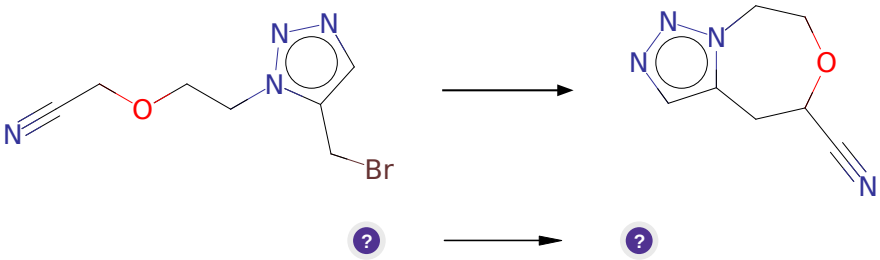
Typical conditions: PPh3.CBr4

Protections: none

Reference: *10.1021/ja800574m* and *10.1016/j.tet.2012.05.010* and *10.1016/j.tet.2004.09.021* (experimantal)

Retrosynthesis ID: 9990037

2.1.5 Alkylation of Nitriles



Substrates:

1. N#CCOCCn1nncc1CBr

Products:

1. N#CC1Cc2cnnn2CCO1

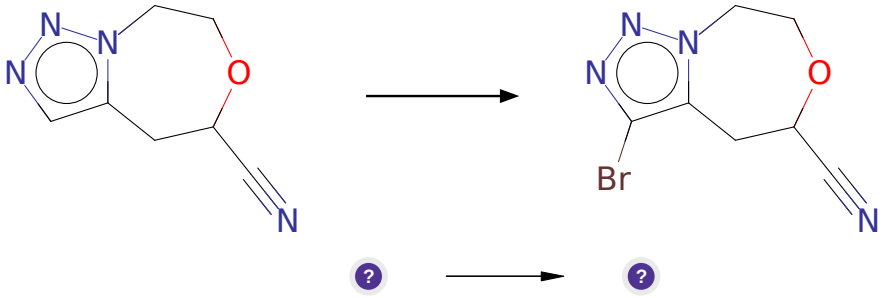
Typical conditions: base e.g. BuLi.THF

Protections: none

Reference: WO2016/71211A1 p. 47 and WO2017/25491A1 p. 36 and WO2014/150331A1 p. 57 and US2007/129379A1 p. 37 and *10.1021/ja058303m* and *10.1021/acs.orglett.9b03078* and *10.1016/S0040-4020(01)80336-7*

Retrosynthesis ID: 31017112

2.1.6 Bromination of aromatic compounds



Substrates:

1. N#CC1Cc2cnnn2CCO1

Products:

1. N#CC1Cc2c(Br)nnn2CCO1

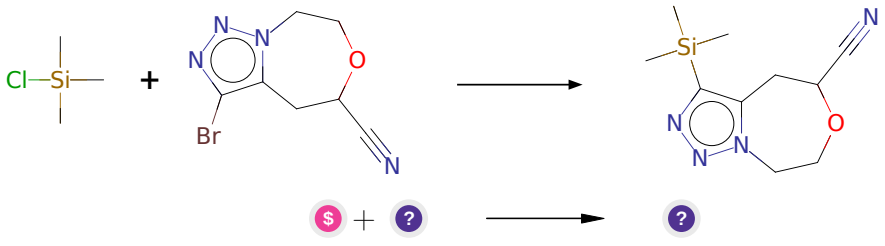
Typical conditions: Br2.Fe

Protections: none

Reference: *10.1021/acs.accounts.6b00120*

Retrosynthesis ID: 7777000

2.1.7 Synthesis of silanes,stannanes and germanes from Grignard reagents



Substrates:

1. TMSCl - *available at Sigma-Aldrich*
2. N#CC1Cc2c(Br)nnn2CCO1

Products:

1. C[Si](C)(C)c1nnn2c1CC(C#N)OCC2

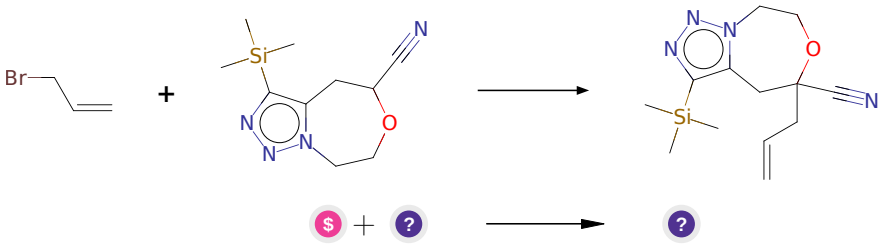
Typical conditions: 1.nBuLi.or.Mg.THF.-78C.2.Si-Cl.to.rt

Protections: none

Reference: *10.1021/jo802433t* AND *10.1021/ja01108a009*

Retrosynthesis ID: 5402

2.1.8 Alkylation of Nitriles



Substrates:

1. Allyl bromide - *available at Sigma-Aldrich*
2. C[Si](C)(C)c1nnn2c1CC(C#N)OCC2

Products:

1. C=CCC1(C#N)Cc2c([Si](C)(C)C)nnn2CCO1

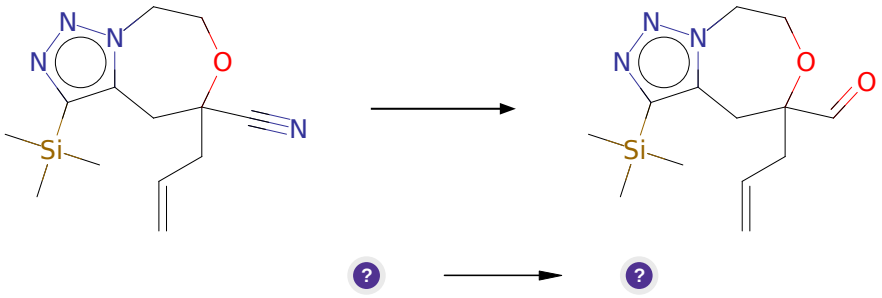
Typical conditions: base e.g. BuLi.THF

Protections: none

Reference: WO2016/71211A1 p. 47 and WO2017/25491A1 p. 36 and WO2014/150331A1 p. 57 and US2007/129379A1 p. 37 and *10.1021/ja058303m* and *10.1021/acs.orglett.9b03078* and *10.1016/S0040-4020(01)80336-7*

Retrosynthesis ID: 31017112

2.1.9 Reduction of nitriles to aldehydes



Substrates:

1. C=CCC1(C#N)Cc2c([Si](C)(C)C)nnn2CCO1

Products:

1. C=CCC1(C=O)Cc2c([Si](C)(C)C)nnn2CCO1

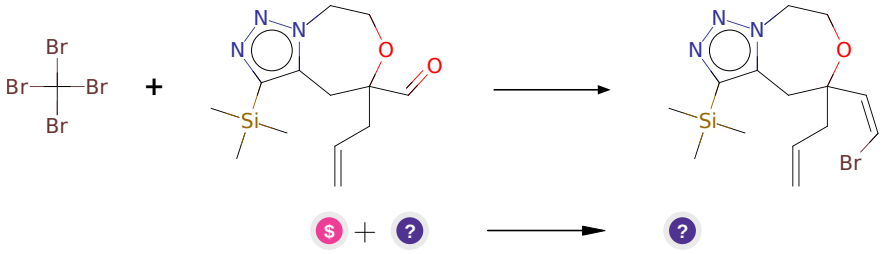
Typical conditions: DIBALH.DCM

Protections: none

Reference: *10.1016/j.bmc.2006.01.061* and *10.1016/j.tet.2012.07.022* and *10.1016/j.bmcl.2009.01.075* and *10.1016/j.bmcl.2007.09.081* and *10.1021/jo000502v*

Retrosynthesis ID: 31406

2.1.10 Synthesis of Z-bromoalkenes



Substrates:

1. Tetrabromomethane - *available at Sigma-Aldrich*
2. C=CCC1(C=O)Cc2c([Si](C)(C)C)nnn2CCO1

Products:

1. C=CCC1(/C=C\Br)Cc2c([Si](C)(C)C)nnn2CCO1

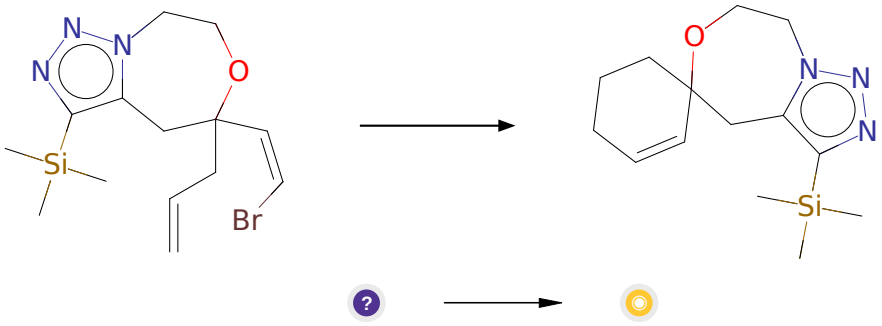
Typical conditions: 1.CBr4.Ph3P.TEA.THF.cooling to rt.2. nBu3SnH.Pd(PPh3)4.toluene.rt

Protections: none

Reference: *10.1002/chem.201101630* (SI p.13) and *10.1021/jo0498157* and *10.1016/j.tetlet.2004.01.151* and *10.1021/ol035127i*

Retrosynthesis ID: 10001762

2.1.11 Suzuki alkyl-vinyl coupling



Substrates:

1. C=CCC1(/C=C\Br)Cc2c([Si](C)(C)C)nnn2CCO1

Products:

1. C[Si](C)(C)c1nnn2c1CC1(C=CCCC1)OCC2

Typical conditions: 1. 9BBN-H. or. PinB-Bpin. Cu. 2. [Pd]. Ligand. Base

Protections: none

Reference: *10.1002/1521-3773(20011217)40:24<4544::AID-ANIE4544>3.0.CO;2-N* and *10.1021/ol300575d*

Retrosynthesis ID: 10034491