# Paths of analysis*

AS3

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

**Strategies:** none selected

**FGI Coeff:** 0

**Tunnels Coeff:** 0

**JSON Parameters:** {}

# 2 Paths

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

## 2.1 Path 1

**Score:** `323.01`

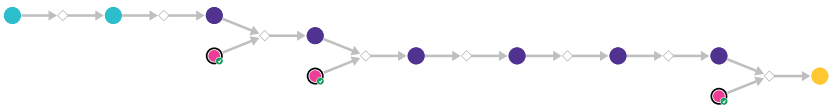
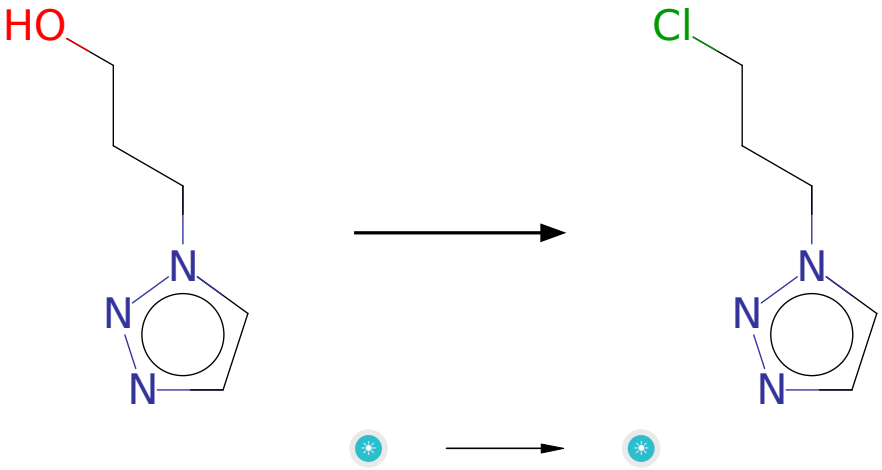


Figure 1: Outline of path 1

### 2.1.1 Synthesis of alkyl chlorides from alcohols




**Substrates:**

1. 3-[1,2,3]triazol-1-yl-propan-1-ol

**Products:**

1. C5H8ClN3

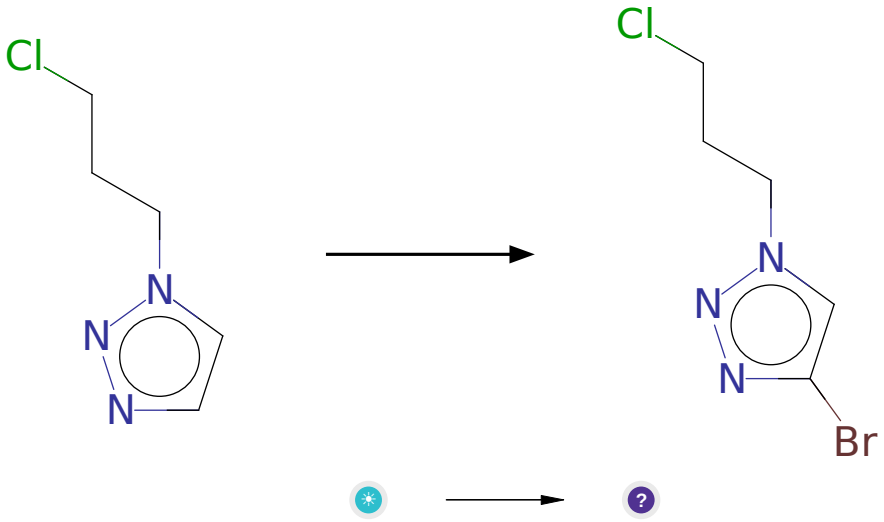
**Typical conditions:** cyanuric chloride.DMF.DCM.RT

**Protections:** none

**Reference:** DOI: *10.1021/ol017168p*

**Retrosynthesis ID:** 11617

### 2.1.2 Bromination of aromatic compounds




**Substrates:**

1. C5H8ClN3

**Products:**

1. ClCCCn1cc(Br)nn1

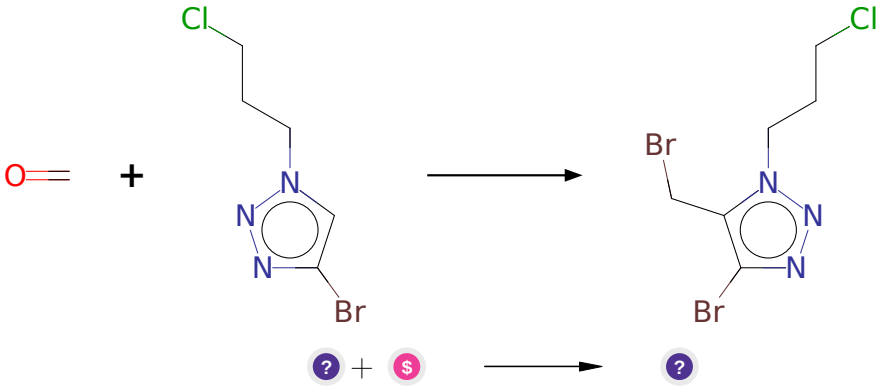
**Typical conditions:** Br2.Fe

**Protections:** none

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

**Retrosynthesis ID:** 7777000

### 2.1.3 Blanc bromomethylation




**Substrates:**

1. ClCCCn1cc(Br)nn1
2. Formalin - *available at Sigma-Aldrich*

**Products:**

1. ClCCCn1nnc(Br)c1CBr

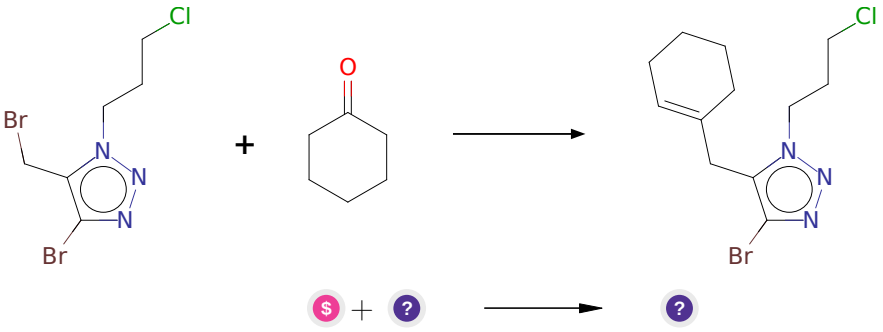
**Typical conditions:** HBr.heat

**Protections:** none

**Reference:** *10.1021/ja011493q* and *10.1021/ma012195g* and *10.1016/S0040-4039(02)01769-0* and *10.1021/ja002069c*

**Retrosynthesis ID:** 31010730

### 2.1.4 Shapiro reaction followed by alkyl bromide addition




**Substrates:**

1. Cyclohexanone - *available at Sigma-Aldrich*

2. ClCCCn1nnc(Br)c1CBr

**Products:**

1. ClCCCn1nnc(Br)c1CC1=CCCCC1

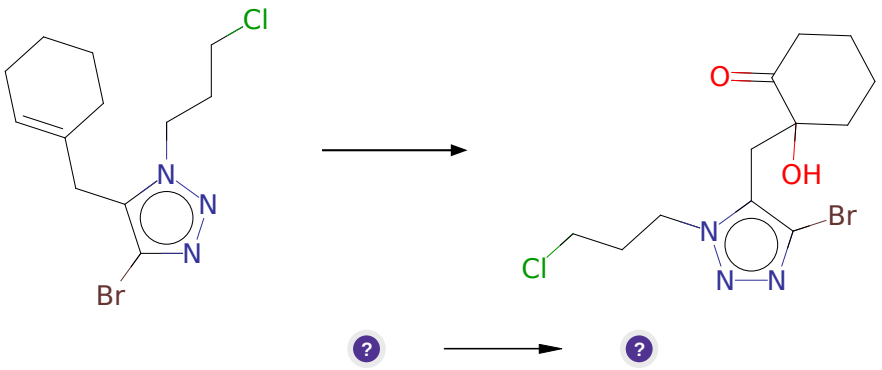
**Typical conditions:** 1.TsNH2NH2.2.Mes2Mg.LiCl.THF.heating then alkyl bromide.cooling

**Protections:** none

**Reference:** *10.1016/S0040-4039(00)75263-4* and *10.1021/ol300652k* and *10.1021/ja00299a037*

**Retrosynthesis ID:** 9990463

### 2.1.5 Oxohydroxylation of unsymmetric alkenes




**Substrates:**

1. ClCCCn1nnc(Br)c1CC1=CCCCC1

**Products:**

1. O=C1CCCCC1(O)Cc1c(Br)nnn1CCCCl

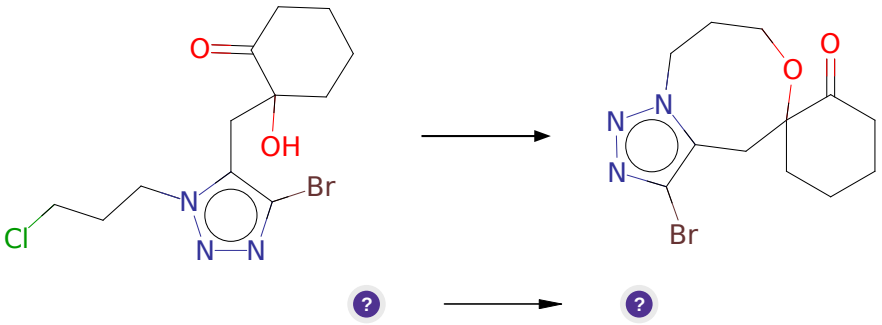
**Typical conditions:** KMnO4.Acetone/H2O.-10 deg C

**Protections:** none

**Reference:** *10.1016/j.tetlet.2015.12.042* and *10.1021/jacs.5b05792*

**Retrosynthesis ID:** 10037547

### 2.1.6 Alkylation of tertiary alcohols




**Substrates:**

1. O=C1CCCCC1(O)Cc1c(Br)nnn1CCCCl

**Products:**

1. O=C1CCCCC12Cc1c(Br)nnn1CCCO2

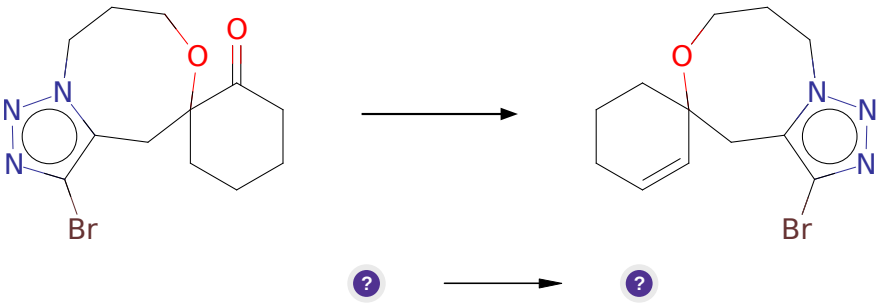
**Typical conditions:** K2CO3.acetone.heat

**Protections:** none

**Reference:** *10.1016/S0040-4020(01)90106-1* and *10.1021/acs.analchem.5b04461* and *10.3390/molecules24091643*

**Retrosynthesis ID:** 31010930

### 2.1.7 Shapiro reaction




**Substrates:**

1. O=C1CCCCC12Cc1c(Br)nnn1CCCO2

**Products:**

1. Brc1nnn2c1CC1(C=CCCC1)OCCC2

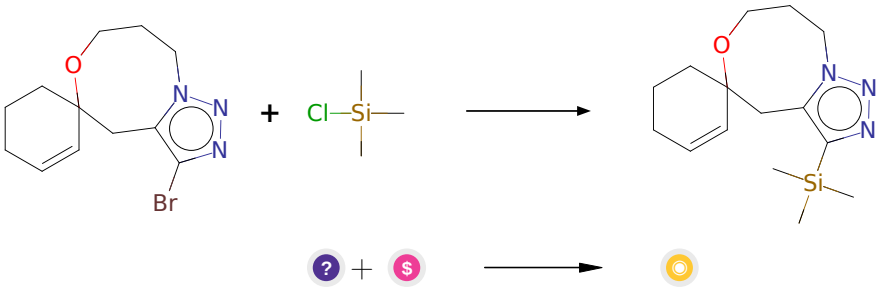
**Typical conditions:** 1.TsNH2NH2.2.N-BuLi

**Protections:** none

**Reference:** *10.1021/jm4008517* and *10.1016/j.bmc.2009.08.038* and *10.1021/jo00350a003*

**Retrosynthesis ID:** 9990398

### 2.1.8 Synthesis of arylsilanes




**Substrates:**

1. Brc1nnn2c1CC1(C=CCCC1)OCCC2
2. TMSCl - *available at Sigma-Aldrich*

**Products:**

1. C[Si](C)(C)c1nnn2c1CC1(C=CCCC1)OCCC2

**Typical conditions:** 1.nBuLi.2.ClSnR3

**Protections:** none

**Reference:** *10.1071/CH9851147*.

**Retrosynthesis ID:** 5370

## 2.2 Path 2

**Score:** `323.01`

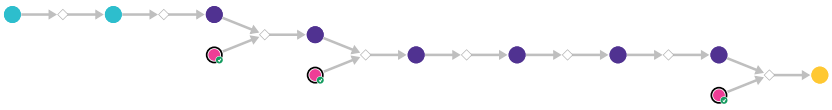
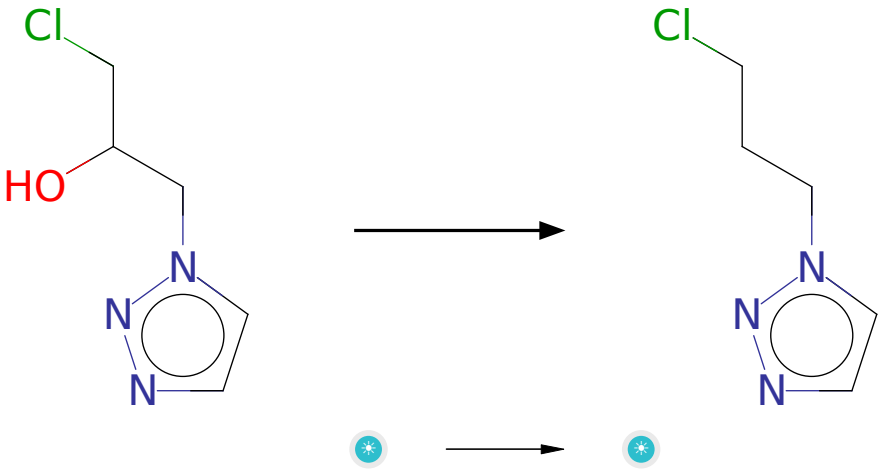


Figure 2: Outline of path 2

### 2.2.1 Deoxygenation of alcohols with silanes




**Substrates:**

1. 1-chloro-3(1,2,3)triazol-1-ylpropan-2-ol

**Products:**

1. C5H8ClN3

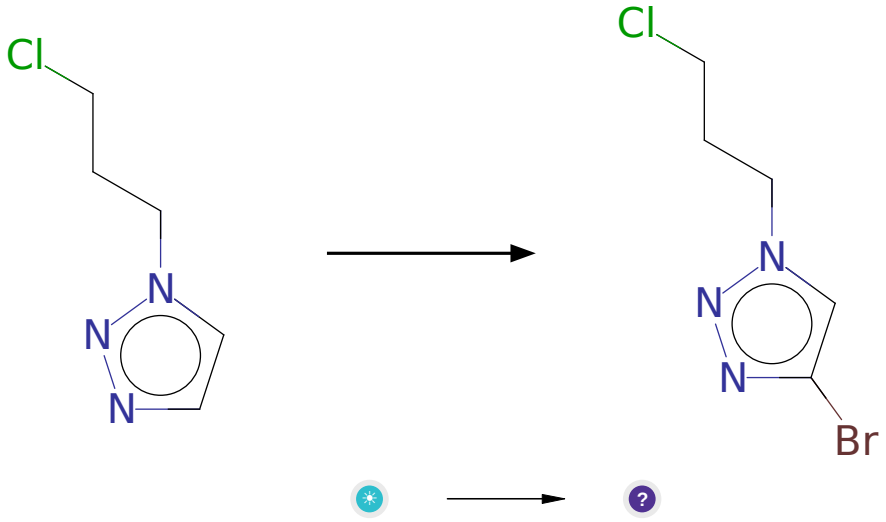
**Typical conditions:** Et3SiH.Lewis.or.Bronsted.Acid

**Protections:** none

**Reference:** *10.1021/jo0158534* AND *10.1021/ol3020144*

**Retrosynthesis ID:** 8162

### 2.2.2 Bromination of aromatic compounds




**Substrates:**

1. C5H8ClN3

**Products:**

1. ClCCCn1cc(Br)nn1

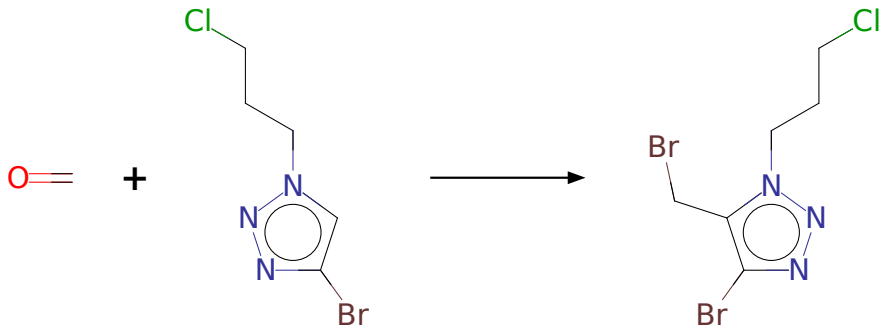
**Typical conditions:** Br2.Fe

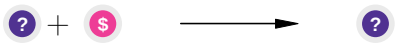
**Protections:** none

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

**Retrosynthesis ID:** 7777000

### 2.2.3 Blanc bromomethylation





**Substrates:**

1. ClCCCn1cc(Br)nn1
2. Formalin - *available at Sigma-Aldrich*

**Products:**

1. ClCCCn1nnc(Br)c1CBr

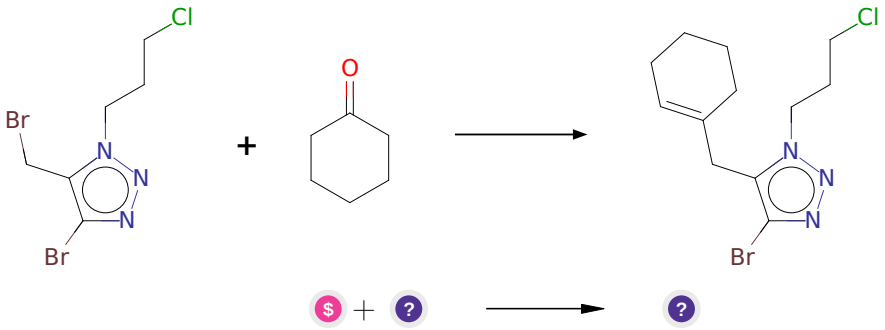
**Typical conditions:** HBr.heat

**Protections:** none

**Reference:** *10.1021/ja011493q* and *10.1021/ma012195g* and *10.1016/S0040-4039(02)01769-0* and *10.1021/ja002069c*

**Retrosynthesis ID:** 31010730

### 2.2.4 Shapiro reaction followed by alkyl bromide addition




**Substrates:**

1. Cyclohexanone - *available at Sigma-Aldrich*
2. ClCCCn1nnc(Br)c1CBr

**Products:**

1. ClCCCn1nnc(Br)c1CC1=CCCCC1

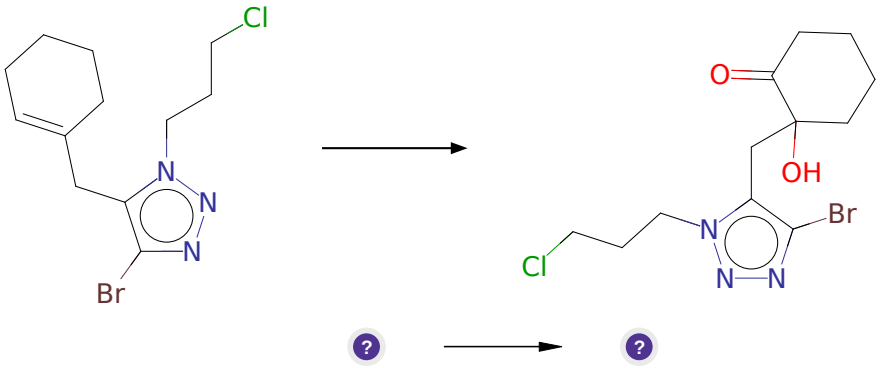
**Typical conditions:** 1.TsNH2NH2.2.Mes2Mg.LiCl.THF.heating then alkyl bromide.cooling

**Protections:** none

**Reference:** *10.1016/S0040-4039(00)75263-4* and *10.1021/ol300652k* and *10.1021/ja00299a037*

**Retrosynthesis ID:** 9990463

### 2.2.5 Oxohydroxylation of unsymmetric alkenes




**Substrates:**

1. ClCCCn1nnc(Br)c1CC1=CCCCC1

**Products:**

1. O=C1CCCCC1(O)Cc1c(Br)nnn1CCCCl

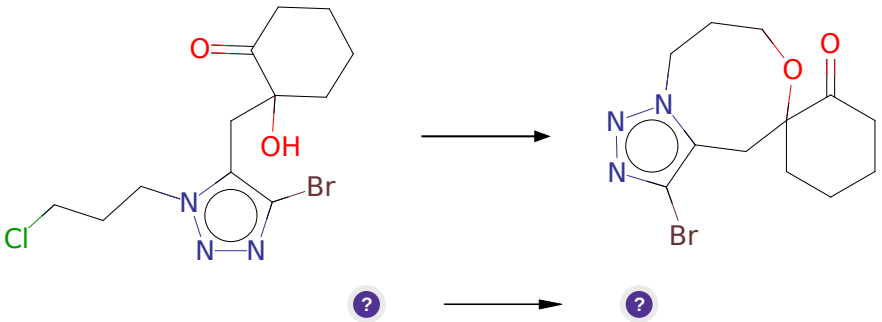
**Typical conditions:** KMnO4.Acetone/H2O.-10 deg C

**Protections:** none

**Reference:** *10.1016/j.tetlet.2015.12.042* and *10.1021/jacs.5b05792*

**Retrosynthesis ID:** 10037547

### 2.2.6 Alkylation of tertiary alcohols




**Substrates:**

1. O=C1CCCCC1(O)Cc1c(Br)nnn1CCCCl

**Products:**

1. O=C1CCCCC12Cc1c(Br)nnn1CCCO2

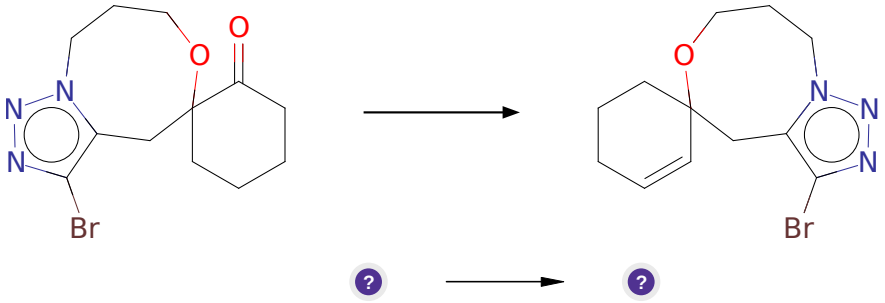
**Typical conditions:** K2CO3.acetone.heat

**Protections:** none

**Reference:** *10.1016/S0040-4020(01)90106-1* and *10.1021/acs.analchem.5b04461* and *10.3390/molecules24091643*

**Retrosynthesis ID:** 31010930

### 2.2.7 Shapiro reaction




**Substrates:**

1. O=C1CCCCC12Cc1c(Br)nnn1CCCO2

**Products:**

1. Brc1nnn2c1CC1(C=CCCC1)OCCC2

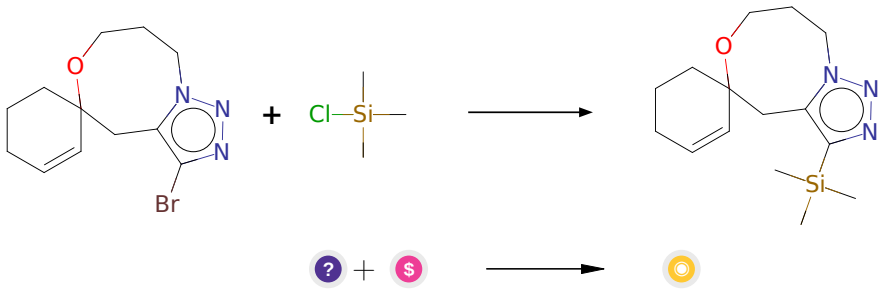
**Typical conditions:** 1.TsNH2NH2.2.N-BuLi

**Protections:** none

**Reference:** *10.1021/jm4008517* and *10.1016/j.bmc.2009.08.038* and *10.1021/jo00350a003*

**Retrosynthesis ID:** 9990398

### 2.2.8 Synthesis of arylsilanes



**Substrates:**

1. Brc1nnn2c1CC1(C=CCCC1)OCCC2
2. TMSCl - *available at Sigma-Aldrich*

**Products:**

1. C[Si](C)(C)c1nnn2c1CC1(C=CCCC1)OCCC2

**Typical conditions:** 1.nBuLi.2.ClSnR3

**Protections:** none

**Reference:** *10.1071/CH9851147*.

**Retrosynthesis ID:** 5370

## 2.3 Path 3

**Score:** 326.52

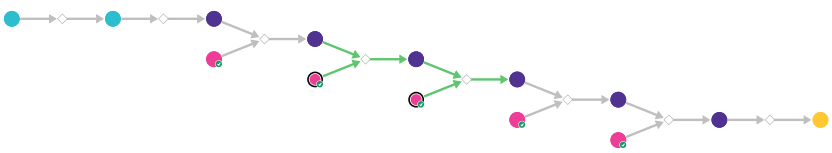
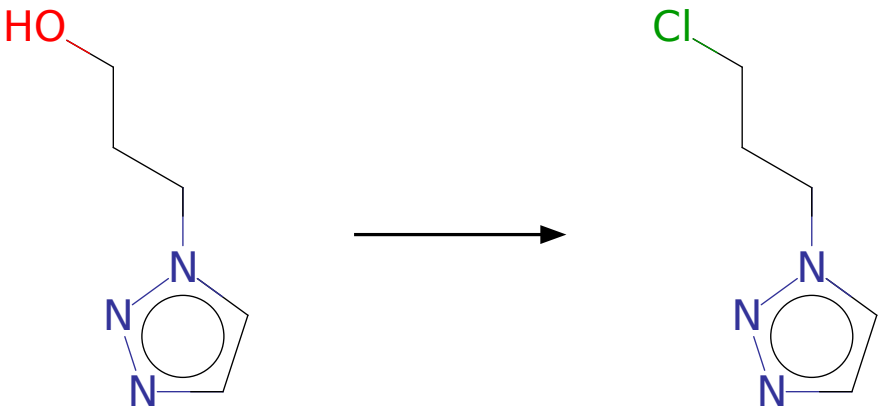
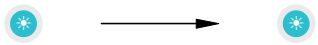


Figure 3: Outline of path 3

### 2.3.1 Synthesis of alkyl chlorides from alcohols





**Substrates:**

1. 3-[1,2,3]triazol-1-yl-propan-1-ol

**Products:**

1. C5H8ClN3

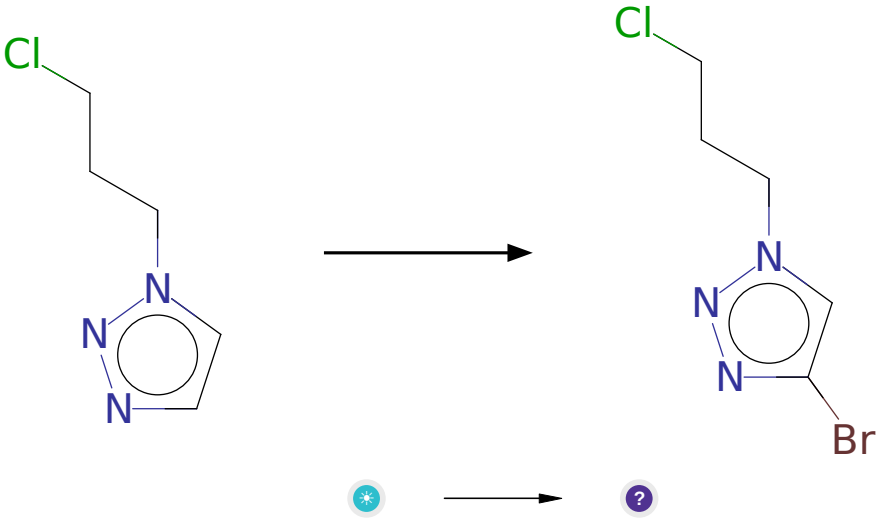
**Typical conditions:** cyanuric chloride.DMF.DCM.RT

**Protections:** none

**Reference:** DOI: *10.1021/ol017168p*

**Retrosynthesis ID:** 11617

### 2.3.2 Bromination of aromatic compounds




**Substrates:**

1. C5H8ClN3

**Products:**

1. ClCCCn1cc(Br)nn1

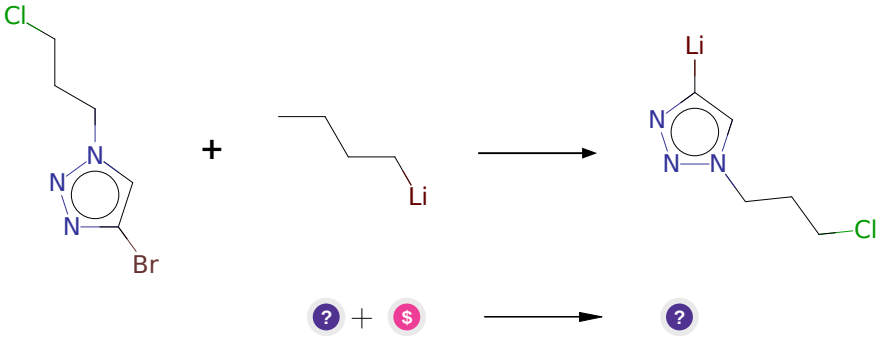
**Typical conditions:** Br2.Fe

**Protections:** none

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

**Retrosynthesis ID:** 7777000

### 2.3.3 Br/Li exchange




**Substrates:**

1. ClCCCn1cc(Br)nn1
2. n-BuLi - *available at Sigma-Aldrich*

**Products:**

1. [Li]c1cn(CCCCl)nn1

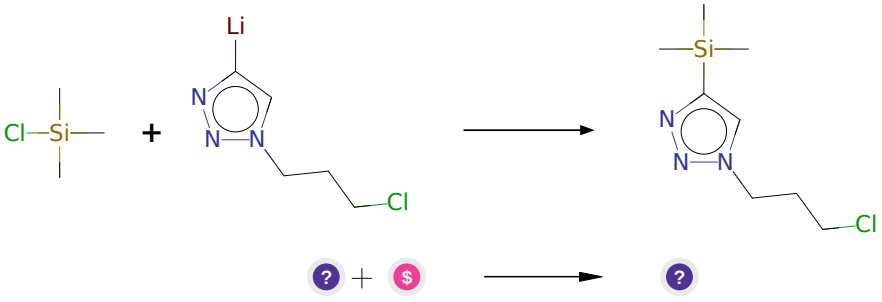
**Typical conditions:** nBuLi.or.tBuLi.THF.-78C

**Protections:** none

**Reference:** *10.1002/ejoc.201101490* and *10.1016/j.tet.2012.03.058* and *10.1016/j.tetlet.2015.01.032* and *10.1021/ja0541175* and *10.1016/j.tetlet.2016.06.123*

**Retrosynthesis ID:** 30672

### 2.3.4 Addition of electrophiles to lithiated arenes/heteroarenes




**Substrates:**

1. [Li]c1cn(CCCCl)nn1

2. TMSCl - *available at Sigma-Aldrich*

**Products:**

1. C[Si](C)(C)c1cn(CCCCl)nn1

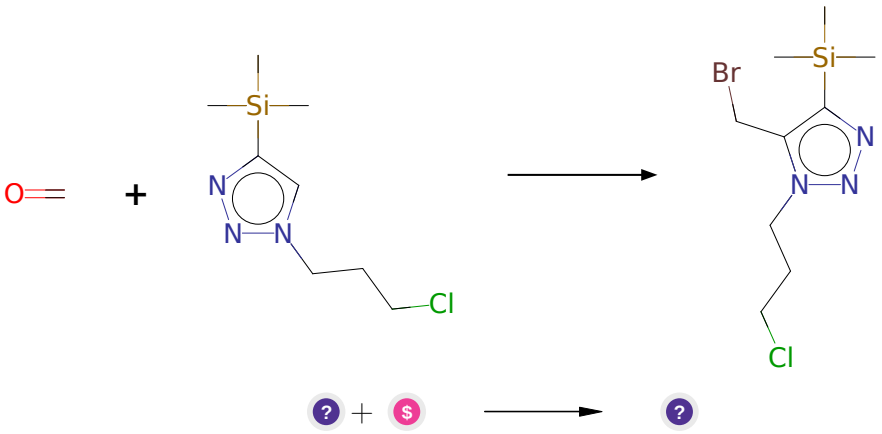
**Typical conditions:** THF

**Protections:** none

**Reference:** *10.1002/ejoc.200600589* and *10.1055/s-0036-1588863* and *10.1002/1099-0690(200107)2001:14<2771::AID-EJOC2771>3.0.CO;2-Y* and *10.1021/ol202873d* (SI)

**Retrosynthesis ID:** 10019541

### 2.3.5 Blanc bromomethylation




**Substrates:**

1. C[Si](C)(C)c1cn(CCCCl)nn1
2. Formalin - *available at Sigma-Aldrich*

**Products:**

1. C[Si](C)(C)c1nnn(CCCCl)c1CBr

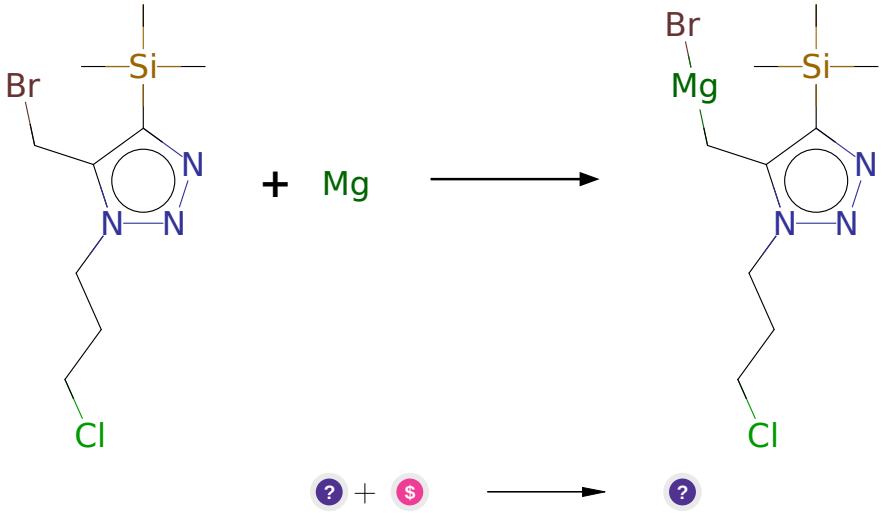
**Typical conditions:** HBr.heat

**Protections:** none

**Reference:** *10.1021/ja011493q* and *10.1021/ma012195g* and *10.1016/S0040-4039(02)01769-0* and *10.1021/ja002069c*

**Retrosynthesis ID:** 31010730

### 2.3.6 Synthesis of alkyl Grignard reagents




**Substrates:**

1. C[Si](C)(C)c1nnn(CCCCl)c1CBr
2. Magnesium - *available at Sigma-Aldrich*

**Products:**

1. C[Si](C)(C)c1nnn(CCCCl)c1C[Mg]Br

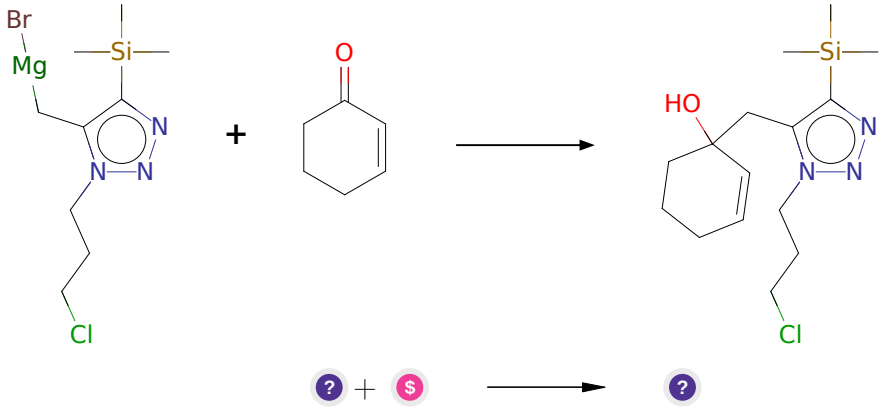
**Typical conditions:** Mg.THF or iPrMgBr

**Protections:** none

**Reference:** DOI: *10.1021/jo00002a039* and *10.1021/jo047877r* and *10.1021/ol006618v*

**Retrosynthesis ID:** 10011828

### 2.3.7 Grignard-Type Reaction




**Substrates:**

1. C[Si](C)(C)c1nnn(CCCCl)c1C[Mg]Br
2. 2-Cyclohexen-1-one - *available at Sigma-Aldrich*

**Products:**

1. C[Si](C)(C)c1nnn(CCCCl)c1CC1(O)C=CCCC1

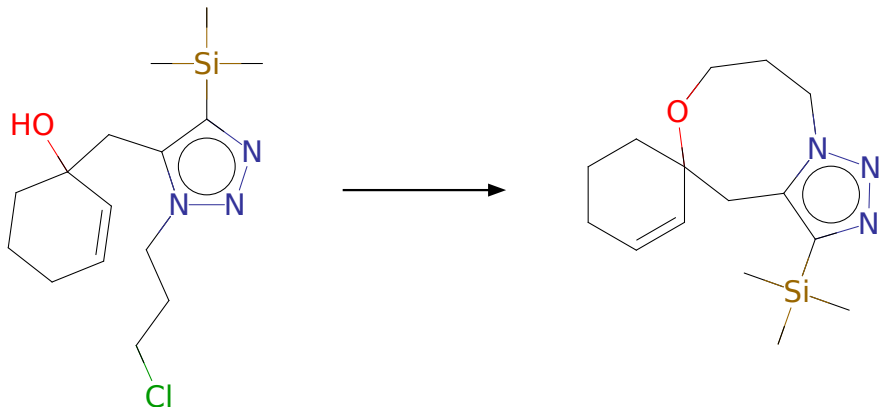
**Typical conditions:** Mg or Li.ether

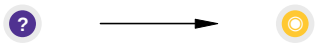
**Protections:** none

**Reference:** *10.1021/jo010494y* or *10.1016/j.steroids.2015.09.009* or *10.1021/jo061349t* or *10.1021/ja056165v* (SI page 19)

**Retrosynthesis ID:** 25134

### 2.3.8 Alkylation of tertiary alcohols





**Substrates:**

1. C[Si](C)(C)c1nnn(CCCCl)c1CC1(O)C=CCCC1

**Products:**

1. C[Si](C)(C)c1nnn2c1CC1(C=CCCC1)OCCC2

**Typical conditions:** K2CO3.acetone.heat

**Protections:** none

**Reference:** *10.1016/S0040-4020(01)90106-1* and *10.1021/acs.analchem.5b04461* and *10.3390/molecules24091643*

**Retrosynthesis ID:** 31010930