

# Paths of analysis\*

AS1

Synthia

October 10, 2022

## 1 Analysis parameters

**Analysis type:** Automatic Retrosynthesis

**Rules:** none selected

**Filters:** Exclude Diastereoselective 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:**  $\text{TUNNEL\_COEF} * \text{FGI\_COEF} * \text{STEP} * 20 + 1000 * (\text{CONFLICT} + \text{NON\_SELECTIVITY} + \text{FILTERS} + \text{PROTECT})$

**Chemical scoring formula:**  $\text{SMALLER}^3, \text{SMALLER}^{1.5}$

**Min. search width:** 400

**Max. reactions per product:** 60

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\*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

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

### 2.1 Path 1

**Score:** 396.84

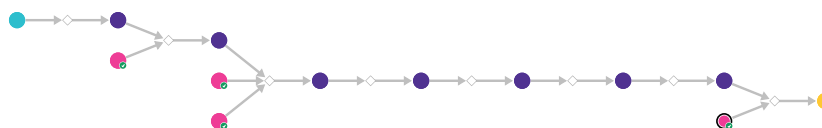
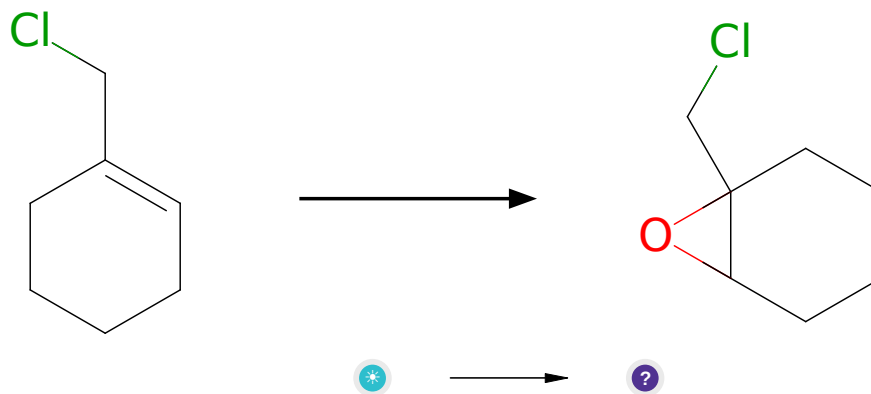


Figure 1: Outline of path 1

#### 2.1.1 Shi epoxidation



**Substrates:**

1. 1-chloromethyl-cyclohexene

**Products:**

1. ClCC12CCCCC1O2

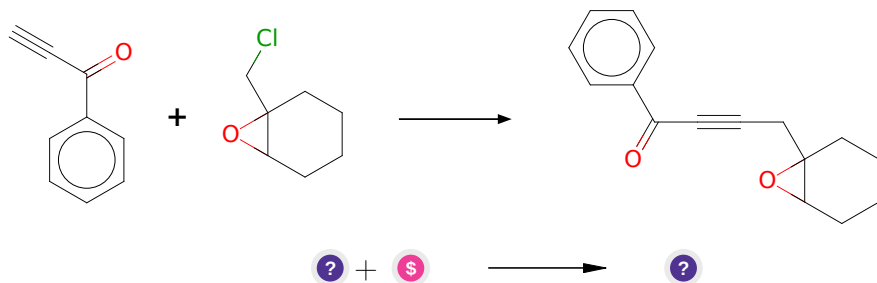
**Typical conditions:** sugar.based.catalyst.KHSO5.K2CO3.H2O.ACN.0C

**Protections:** none

**Reference:** [10.1055/s-0028-1083545](#) and [10.1021/ja972272g](#) and [10.1021/ja003049d](#) and [10.1021/jo972106r](#)

**Retrosynthesis ID:** 7430

### 2.1.2 Alkylation of terminal Alkynes



**Substrates:**

1. ClCC12CCCCC1O2
2. 1-Phenylpropynone - *available at Sigma-Aldrich*

**Products:**

1. O=C(C#CCCC12CCCCC1O2)c1ccccc1

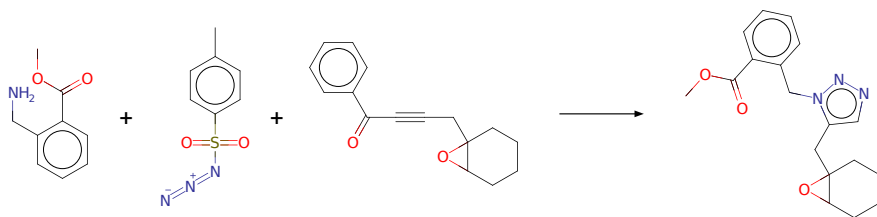
**Typical conditions:** K2CO3.CuI.TBAB.solvent

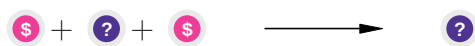
**Protections:** none

**Reference:** DOI: [10.1021/ja064223m](#) (SI, page S-3) AND [10.1016/j.tet.2008.01.139](#) AND [10.1021/ol049474j](#) AND Patent: US5231232 A1, page 4

**Retrosynthesis ID:** 10617

### 2.1.3 Metal-free multicomponent synthesis of triazoles





**Substrates:**

1. Tosyl azide solution - *available at Sigma-Aldrich*
2. O=C(C#CCCC1CCCCC1O2)c1ccccc1
3. methyl-2-aminomethylbenzoat - *available at Sigma-Aldrich*

**Products:**

1. COC(=O)c1ccccc1Cn1nccc1CC12CCCCC1O2

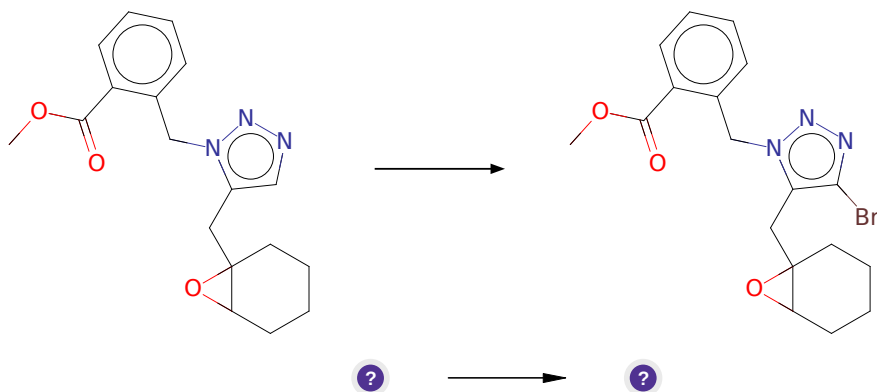
**Typical conditions:** 1. toluene.80C 2. LiOtBu.RT

**Protections:** none

**Reference:** DOI: [10.1002/anie.201307499](https://doi.org/10.1002/anie.201307499)

**Retrosynthesis ID:** 6001

**2.1.4 Bromination of aromatic compounds**



**Substrates:**

1. COC(=O)c1ccccc1Cn1nccc1CC12CCCCC1O2

**Products:**

1. COC(=O)c1ccccc1Cn1nnc(Br)c1CC12CCCCC1O2

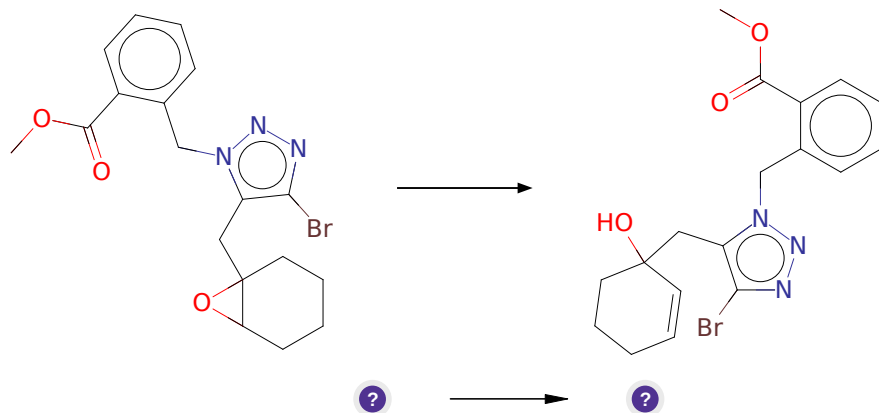
**Typical conditions:** Br<sub>2</sub>.Fe

**Protections:** none

**Reference:** [10.1021/acs.accounts.6b00120](https://doi.org/10.1021/acs.accounts.6b00120)

**Retrosynthesis ID:** 7777000

### 2.1.5 Synthesis of allyl alcohols from epoxides



**Substrates:**

1. COC(=O)c1ccccc1Cn1nnc(Br)c1CC12CCCCC1O2

**Products:**

1. COC(=O)c1ccccc1Cn1nnc(Br)c1CC1(O)C=CCCC1

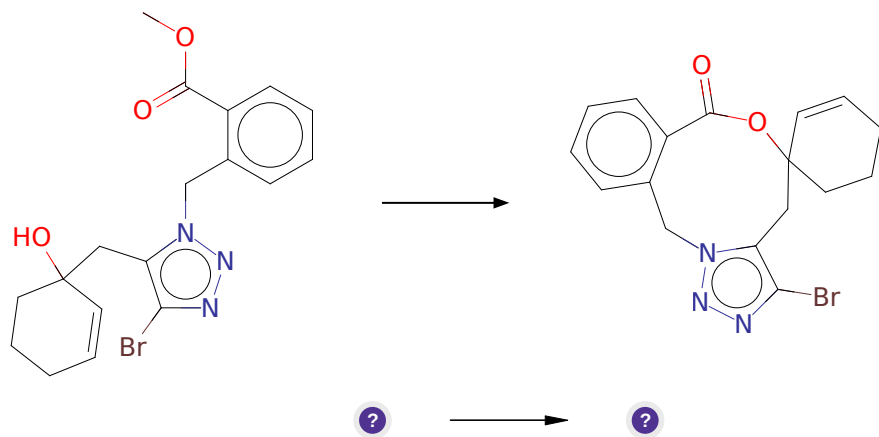
**Typical conditions:** PhSeNa, then H<sub>2</sub>O<sub>2</sub>

**Protections:** none

**Reference:** [10.1016/j.tetlet.2005.02.058](https://doi.org/10.1016/j.tetlet.2005.02.058) and [10.1016/0040-4020\(82\)85157-0](https://doi.org/10.1016/0040-4020(82)85157-0) and [10.1016/j.bmc.2008.05.034](https://doi.org/10.1016/j.bmc.2008.05.034) and [10.1021/ja070022m](https://doi.org/10.1021/ja070022m)

**Retrosynthesis ID:** 27837

### 2.1.6 Acid catalyzed transesterification



**Substrates:**

1. COC(=O)c1ccccc1Cn1nnc(Br)c1CC1(O)C=CCCC1

**Products:**

1. O=C1OC2(C=CCCC2)Cc2c(Br)nnn2Cc2ccccc21

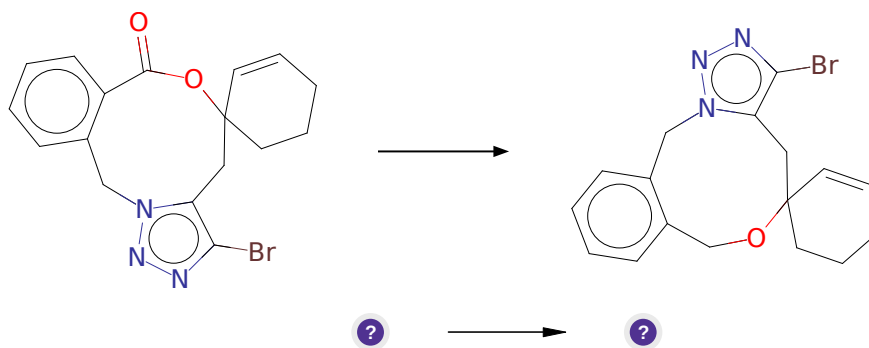
**Typical conditions:** H<sup>+</sup>

**Protections:** none

**Reference:** [10.1021/cr00020a004](#)

**Retrosynthesis ID:** 50438

**2.1.7 Reduction of lactones to ethers**



**Substrates:**

1. O=C1OC2(C=CCCC2)Cc2c(Br)nnn2Cc2ccccc21

**Products:**

1. BrC1nnn2c1CC1(C=CCCC1)OCc1ccccc1C2

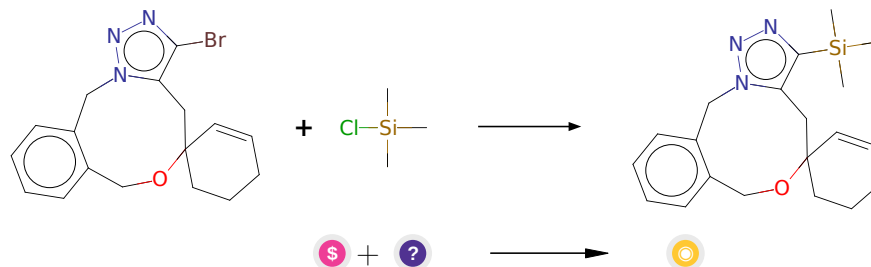
**Typical conditions:** LAH.THF.reflux

**Protections:** none

**Reference:** [10.1002/anie.200352705](#) and [10.1016/j.tet.2016.07.036](#) and [10.5012/bkcs.2013.34.8.2495](#) and [10.1080/10286020.2016.1232251](#)

**Retrosynthesis ID:** 9999753

### 2.1.8 Synthesis of arylsilanes



#### Substrates:

1. TMS-Cl - *available at Sigma-Aldrich*
2. BrC1=NN=C(C=C1)OCc2ccccc2C3

#### Products:

1. C[Si](C)(C)C1=NN=C(C=C1)OCc2ccccc2C3

**Typical conditions:** 1. nBuLi. 2. ClSnR<sub>3</sub>

**Protections:** none

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

**Retrosynthesis ID:** 5370