Paths of analysis*

AS5

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

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

2.1 Path 1

Score: `209.18`

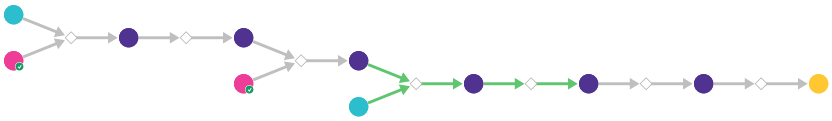
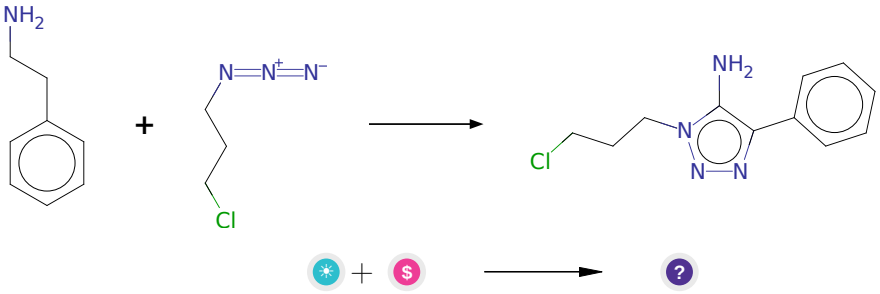


Figure 1: Outline of path 1

2.1.1 Synthesis of 1,2,3-triazoles from azides and nitrile derivatives



Substrates:

1. 1-azido-3-chlor-propan
2. Phenethylamine - *available at Sigma-Aldrich*

Products:

1. Nc1c(-c2ccccc2)nnn1CCCCl

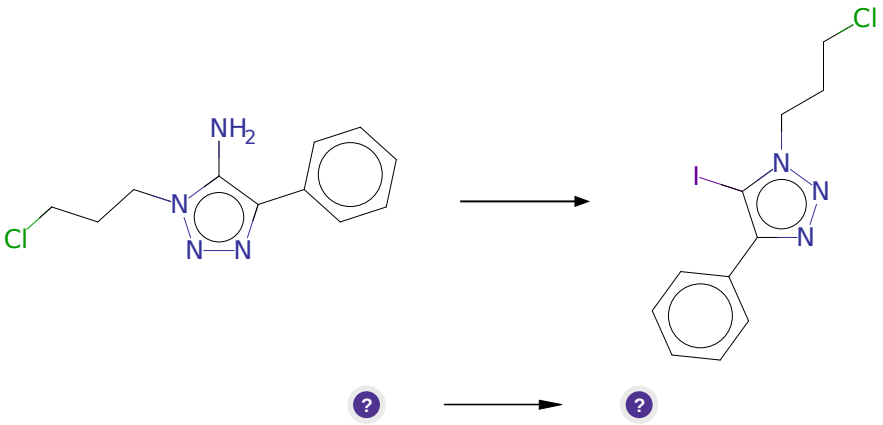
Typical conditions: anhydrous potassium carbonate.DMSO

Protections: none

Reference: DOI: *10.1002/jhet.5570280216*

Retrosynthesis ID: 295117

2.1.2 Synthesis of iodoarenes



Substrates:

1. Nc1c(-c2ccccc2)nnn1CCCCl

Products:

1. ClCCCn1nnc(-c2ccccc2)c1I

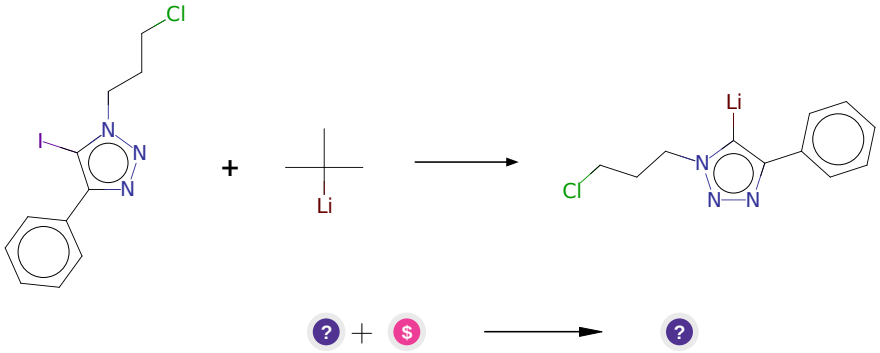
Typical conditions: MeCN.p-TSOH.NaNO2.KI.0 to 25C

Protections: none

Reference: *10.1002/anie.201407653* (SI, page S2) and *10.1002/anie.201409691* and *10.1021/ja312148q* and *10.1021/op300198a* and *10.1002/ejoc.201001436* and *10.1055/s-0028-1087981* and *10.1016/j.bmcl.2011.08.006* and *10.1021/ja0446404* and *10.3762/bjoc.12.36* and *10.1021/acs.orglett.5b01248* and *10.1055/s-2006-958936*

Retrosynthesis ID: 29903

2.1.3 I/Li exchange



Substrates:

1. ClCCCn1nnc(-c2ccccc2)c1I
2. t-BuLi - *available at Sigma-Aldrich*

Products:

1. [Li]c1c(-c2ccccc2)nnn1CCCCl

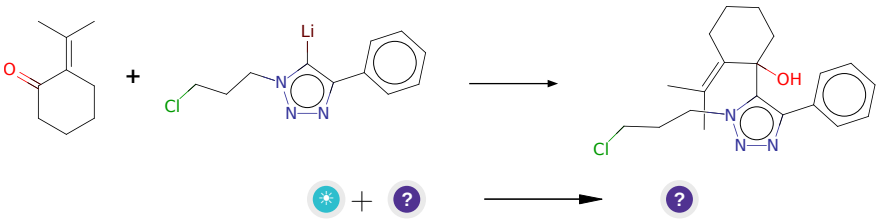
Typical conditions: nBuLi.or.tBuLi.THF.-78C

Protections: none

Reference: *10.1016/j.tet.2004.09.111* and *10.1039/c3ob41082j* And *10.1016/j.bmc.2012.03.056* And *10.1002/chem.201300292*

Retrosynthesis ID: 30673

2.1.4 Addition of electrophiles to lithiated arenes/heteroarenes



Substrates:

1. 2-isopropylidene-cyclohexanone
2. [Li]c1c(-c2ccccc2)nnn1CCCCl

Products:

1. CC(C)=C1CCCCC1(O)c1c(-c2ccccc2)nnn1CCCCl

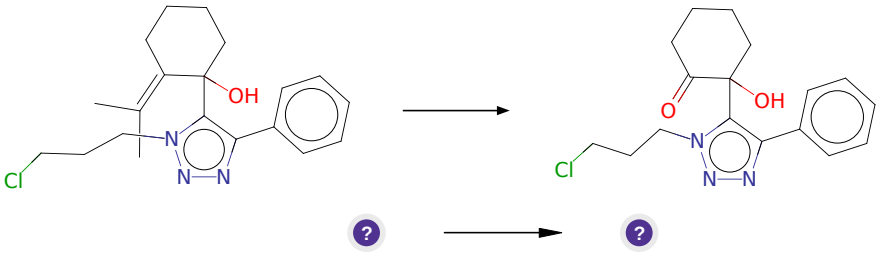
Typical conditions: THF.-78 deg C

Protections: none

Reference: *10.1021/ml300335r* and *10.1021/acs.jmedchem.6b00866*

Retrosynthesis ID: 31008139

2.1.5 Ozonolysis



Substrates:

1. CC(C)=C1CCCCC1(O)c1c(-c2ccccc2)nnn1CCCCl

Products:

1. O=C1CCCCC1(O)c1c(-c2ccccc2)nnn1CCCCl

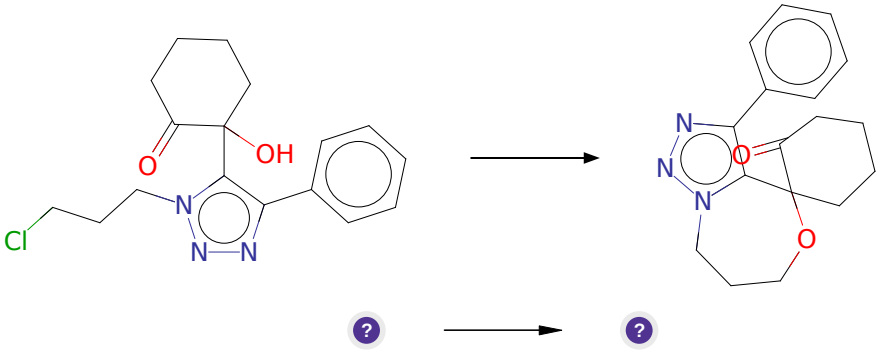
Typical conditions: O3.MeOH.CH2Cl2.PPh3 or Me2S.low temperature

Protections: none

Reference: *10.1016/j.tet.2017.03.039*

Retrosynthesis ID: 5079

2.1.6 Alkylation of tertiary alcohols



Substrates:

1. O=C1CCCCC1(O)c1c(-c2ccccc2)nnn1CCCCl

Products:

1. O=C1CCCCC12OCCCn1nnc(-c3ccccc3)c12

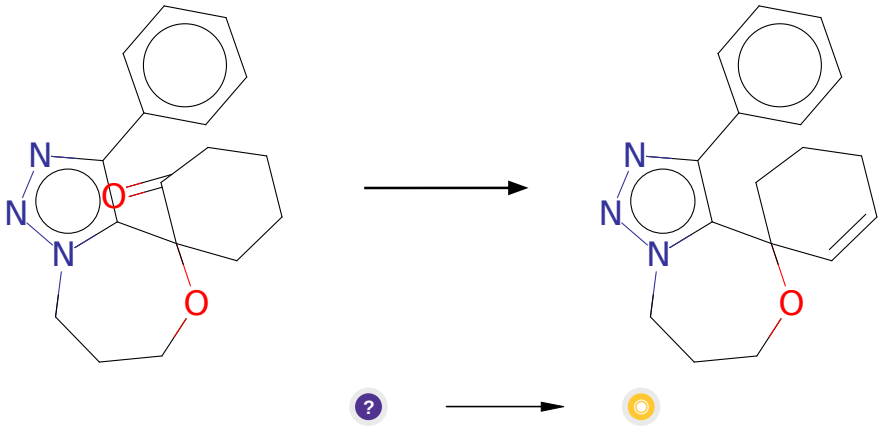
Typical conditions: K2CO3.acetone.heat

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=C1CCCCC12OCCCn1nnc(-c3ccccc3)c12

Products:

1. C1=CC2(CCC1)OCCCn1nnc(-c3ccccc3)c12

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