Paths of analysis*

AS6

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

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

2.1 Path 1

Score: 232.65

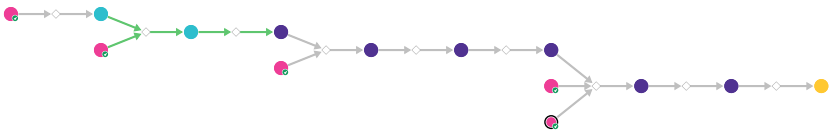
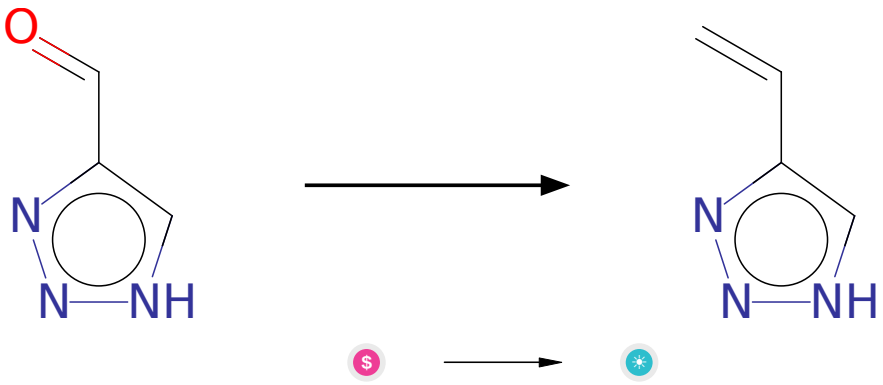


Figure 1: Outline of path 1

2.1.1 Tebbe Olefination



Substrates:

1. 1H-[1,2,3]Triazole-4-carbaldehyde - *available at Sigma-Aldrich*

Products:

1. 5-vinyl-1h-[1,2,3]triazole

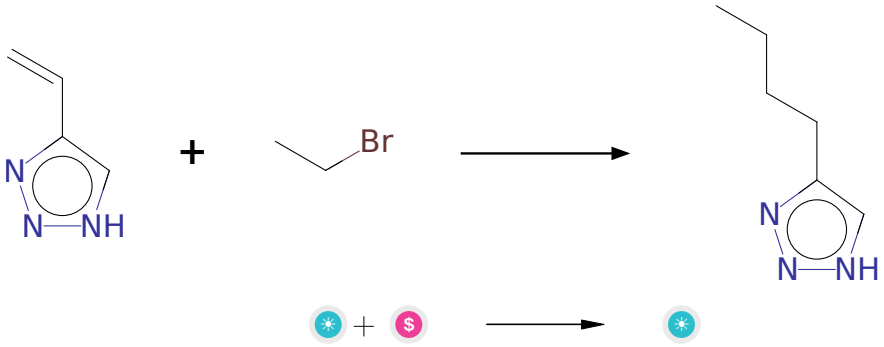
Typical conditions: Cp2TiCl2.AlMe3.toluene

Protections: none

Reference: *10.1016/j.tet.2007.03.015* and *10.1002/9780470638859.conrr617*

Retrosynthesis ID: 11714

2.1.2 Suzuki alkyl-alkyl coupling



Substrates:

1. 5-vinyl-1h-[1,2,3]triazole
2. Bromoethane - *available at Sigma-Aldrich*

Products:

1. 4-butyl-1h-[1,2,3]triazole

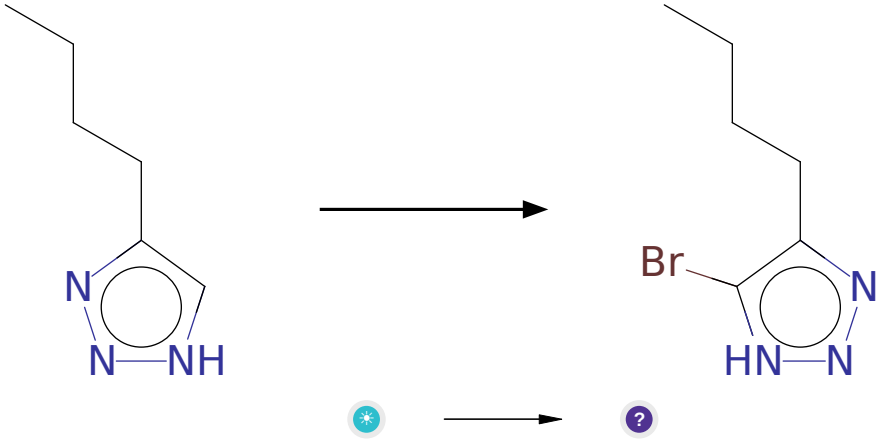
Typical conditions: 1.9BBN-H or pinB-Bpin.Cu 2.[Pd].ligand.base

Protections: none

Reference: *10.1021/ja074008l* and *10.1021/ja011306o* and *10.1002/1521-3773(20011217)40:24<4544::AID-ANIE4544>3.0.CO;2-N* and *10.1021/ol300575d*

Retrosynthesis ID: 8325

2.1.3 Bromination of aromatic compounds



Substrates:

1. 4-butyl-1h-[1,2,3]triazole

Products:

1. CCCCc1nn[nH]c1Br

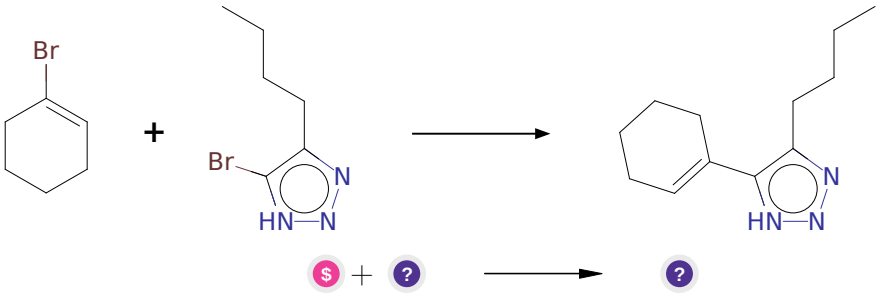
Typical conditions: Br2.Fe

Protections: none

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

Retrosynthesis ID: 7777000

2.1.4 Kumada-Corriu reaction



Substrates:

1. 1-Bromocyclohex-1-ene - *available at Sigma-Aldrich*
2. CCCCc1nn[nH]c1Br

Products:

1. CCCCc1nn[nH]c1C1=CCCCC1

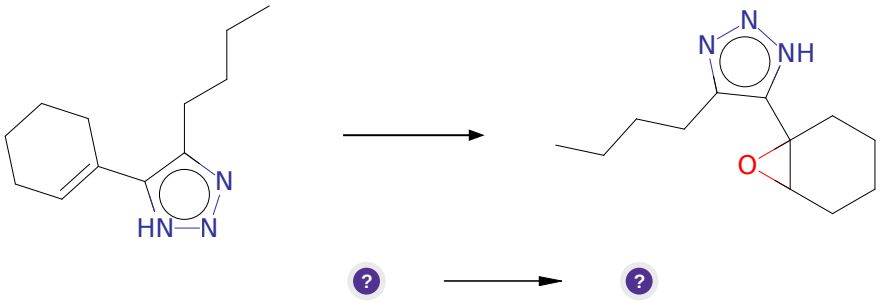
Typical conditions: 1. (nBu)3MgLi.THF.0C 2. NiCl2-dppp.THF.0C

Protections: none

Reference: DOI: *10.1021/ol070841b*

Retrosynthesis ID: 1971

2.1.5 Shi epoxidation



Substrates:

1. CCCCc1nn[nH]c1C1=CCCCC1

Products:

1. CCCCc1nn[nH]c1C12CCCCC1O2

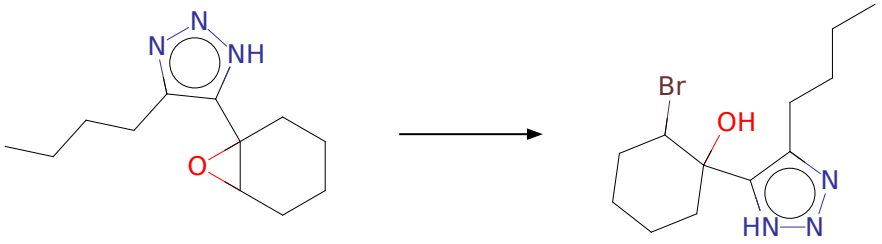
Typical conditions: sugar.based.catalyst.KHSO5.K2CO3.H2O.ACN.0C

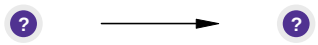
Protections: none

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

Retrosynthesis ID: 7430

2.1.6 Opening of epoxides with bromide via SN2 reaction





Substrates:

1. CCCCc1nn[nH]c1C12CCCCC1O2

Products:

1. CCCCc1nn[nH]c1C1(O)CCCCC1Br

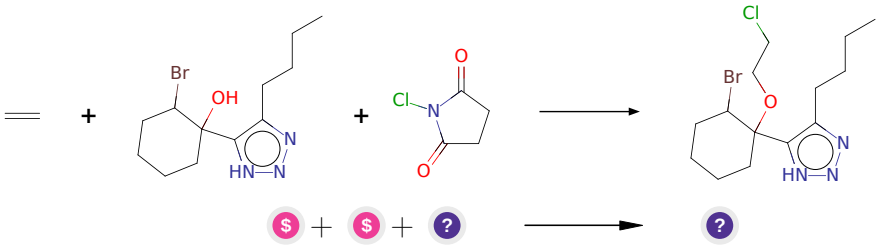
Typical conditions: NaBr.MeCN.TsOH.rt

Protections: none

Reference: *10.1021/ja00413a059* and *10.1016/j.tet.2013.06.046* and *10.1002/anie.200603806* and *10.1055/s-1996-4214* and *10.1016/S0040-4039(98)00390-6* and *10.1021/jo0156215* and *10.1021/ja0296531* and *10.1016/S0040-4039(00)89110-8* and *10.1021/jo00265a028*

Retrosynthesis ID: 23746

2.1.7 Synthesis of bromo and chloroalkoxyalkanes



Substrates:

1. Succinchlorimide - *available at Sigma-Aldrich*
2. Ethene - *available at Sigma-Aldrich*
3. CCCCc1nn[nH]c1C1(O)CCCCC1Br

Products:

1. CCCCc1nn[nH]c1C1(OCCCl)CCCCC1Br

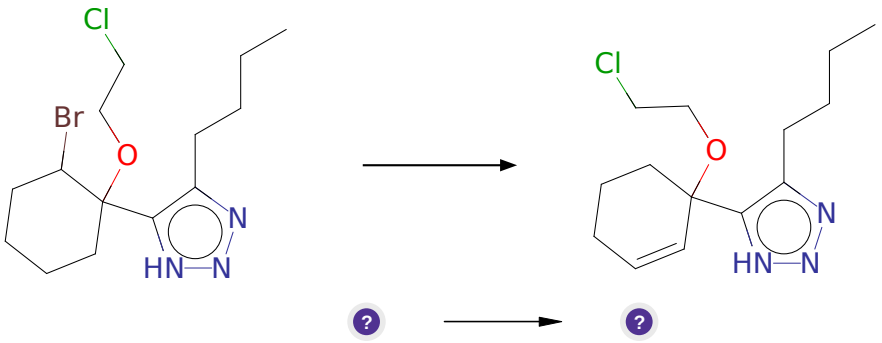
Typical conditions: NBS(NCS).alcohol

Protections: none

Reference: *10.1002/chem.200390180* and *10.1055/s-0037-1611277* and *10.1016/0040-4020(95)00352-9* and *10.1002/ange.19850970430*

Retrosynthesis ID: 245562

2.1.8 Elimination of bromide



Substrates:

1. CCCCc1nn[nH]c1C1(OCCCl)CCCCC1Br

Products:

1. CCCCc1nn[nH]c1C1(OCCCl)C=CCCC1

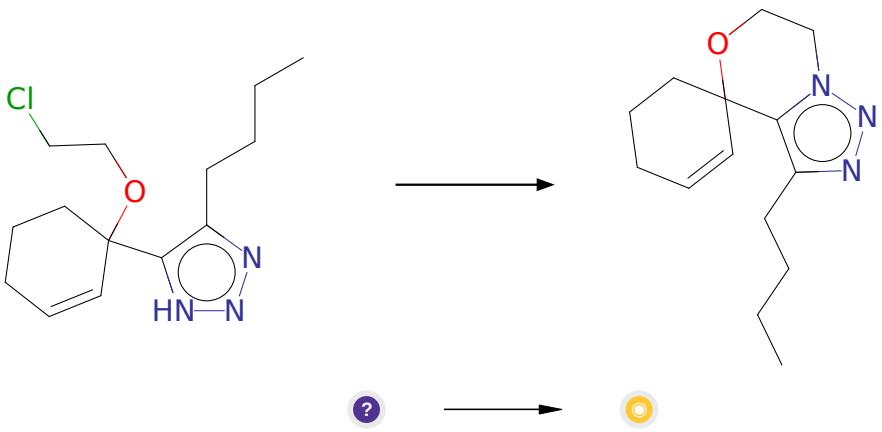
Typical conditions: K2CO3.DMF

Protections: none

Reference: *10.1016/j.jfluchem.2011.08.011* and *10.1039/P19920002971* and *10.1002/cber.19841170909* and *10.1021/ja01570a042*

Retrosynthesis ID: 23585

2.1.9 N-alkylation of Heterocycles



Substrates:

1. CCCCc1nn[nH]c1C1(OCCCl)C=CCCC1

Products:

1. CCCCc1nnn2c1C1(C=CCCC1)OCC2

Typical conditions: NaH.DMF

Protections: none

Reference: *10.1021/ol503625z* and *10.1081/SCC-120022467* (experimental) and *10.1021/ol2018328* (SI, p.5) and *10.1021/jo8026565* (SI, p.2)

Retrosynthesis ID: 28538

2.2 Path 2

Score: 252.64

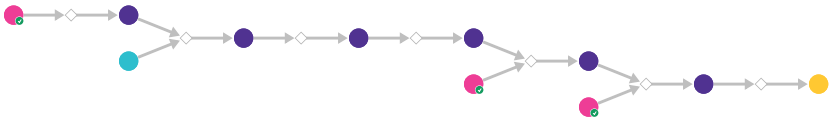
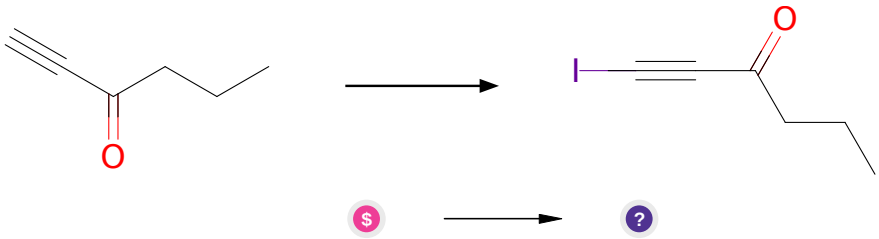


Figure 2: Outline of path 2

2.2.1 Iodination of acetylene



Substrates:

1. hex-1-yn-3-one - *available at Sigma-Aldrich*

Products:

1. CCCC(=O)C#CI

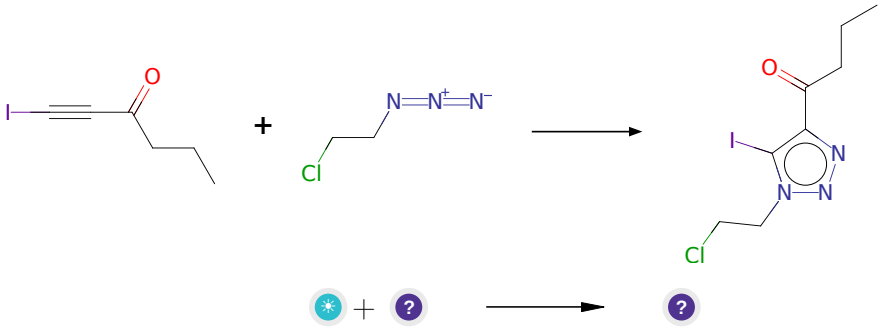
Typical conditions: AgNO3.NIS.THF.rt

Protections: none

Reference: *10.1021/ja960040w*

Retrosynthesis ID: 9900044

2.2.2 Synthesis of triazoles from azides and haloalkynes



Substrates:

1. 1-azido-2-chlor-aethan
2. CCCC(=O)C#CI

Products:

1. CCCC(=O)c1nnn(CCCl)c1I

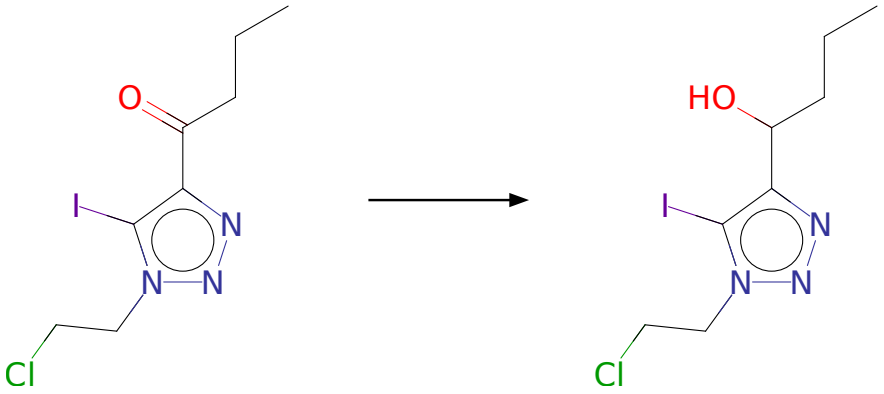
Typical conditions: CpRuCl(cod).ACN

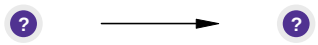
Protections: none

Reference: *10.1002/chem.201402559*

Retrosynthesis ID: 31456

2.2.3 Reduction of ketones with NaBH4





Substrates:

1. CCCC(=O)c1nnn(CCCl)c1I

Products:

1. CCCC(O)c1nnn(CCCl)c1I

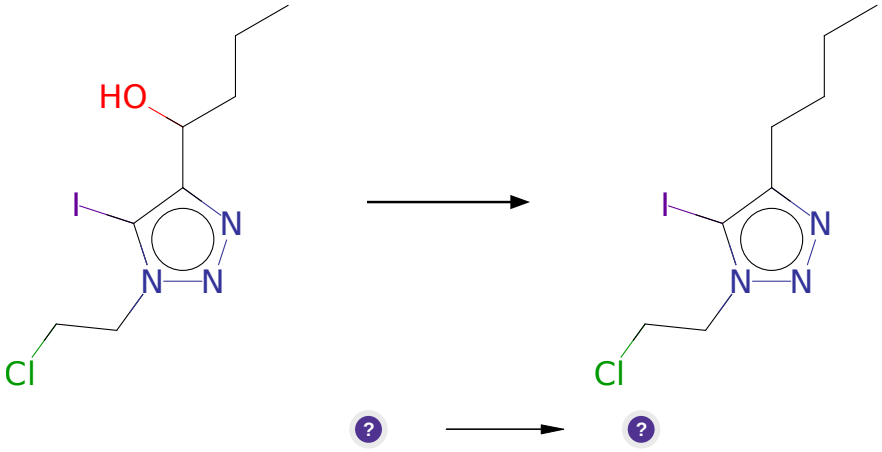
Typical conditions: NaBH4.EtOH.0-20 C

Protections: none

Reference: *10.1016/j.ejmech.2020.112360* p. 3, 8 and *10.1016/j.ejmech.2010.10.012* p. 434, 436

Retrosynthesis ID: 50432

2.2.4 Deoxygenation of alcohols with silanes



Substrates:

1. CCCC(O)c1nnn(CCCl)c1I

Products:

1. CCCCc1nnn(CCCl)c1I

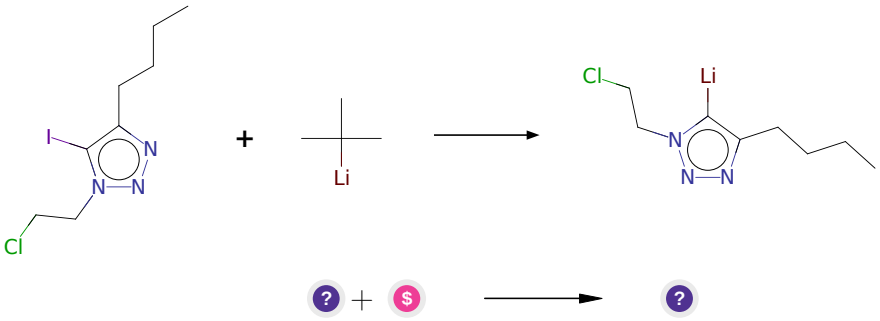
Typical conditions: Et3SiH.Lewis.or.Bronsted.Acid

Protections: none

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

Retrosynthesis ID: 8162

2.2.5 I/Li exchange



Substrates:

1. CCCCc1nnn(CCCl)c1I
2. t-BuLi - *available at Sigma-Aldrich*

Products:

1. [Li]c1c(CCCC)nnn1CCCl

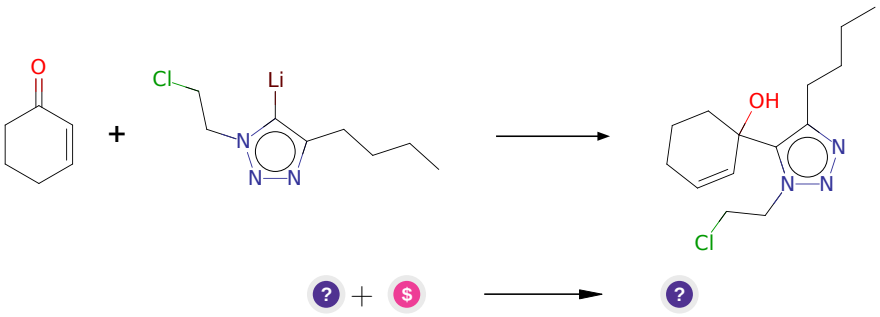
Typical conditions: nBuLi.or.tBuLi.THF.-78C

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

2.2.6 Addition of electrophiles to lithiated arenes/heteroarenes



Substrates:

1. [Li]c1c(CCCC)nnn1CCCl
2. 2-Cyclohexen-1-one - *available at Sigma-Aldrich*

Products:

1. CCCCc1nnn(CCCl)c1C1(O)C=CCCC1

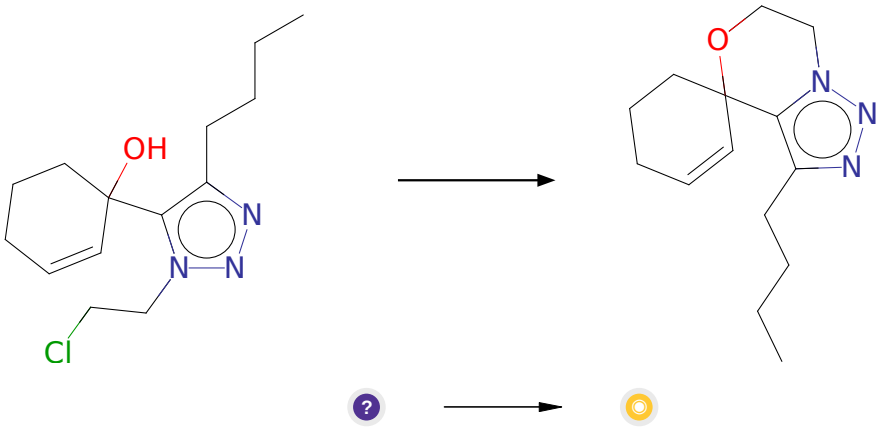
Typical conditions: THF.-78 deg C

Protections: none

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

Retrosynthesis ID: 31008139

2.2.7 Alkylation of tertiary alcohols



Substrates:

1. CCCCc1nnn(CCCl)c1C1(O)C=CCCC1

Products:

1. CCCCc1nnn2c1C1(C=CCCC1)OCC2

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