Paths of analysis*

AS7

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: `259.51`

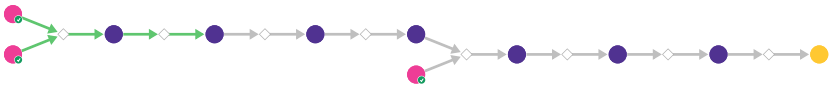
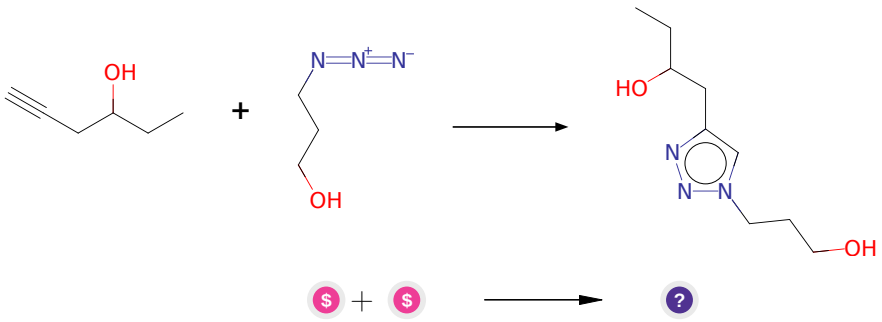


Figure 1: Outline of path 1

2.1.1 Huisgen Cycloaddition



Substrates:

1. 5-Hexyn-3-ol - *available at Sigma-Aldrich*
2. 3-Azido-1-propanol - *available at Sigma-Aldrich*

Products:

1. CCC(O)Cc1cn(CCCO)nn1

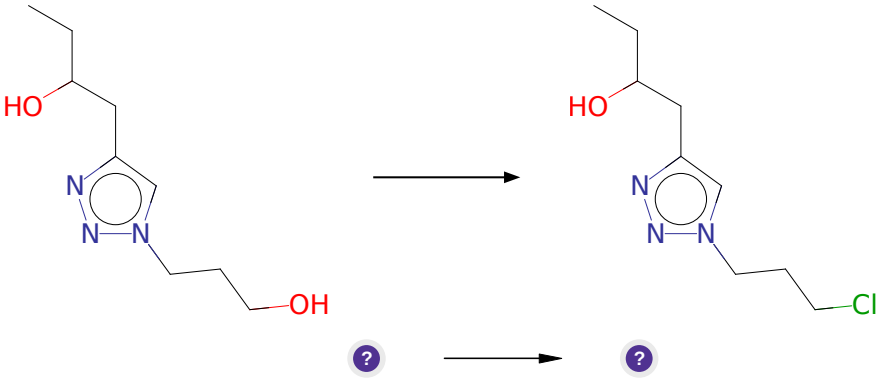
Typical conditions: Cu(I).H2O

Protections: none

Reference: *10.1039/PS9610000357* and *10.1016/S1359-6446(03)02933-7* and *10.1002/1521-3773(20010601)40:11<2004::AID-ANIE2004>3.0.CO;2-5*

Retrosynthesis ID: 10268

2.1.2 Appel Reaction



Substrates:

1. CCC(O)Cc1cn(CCCO)nn1

Products:

1. CCC(O)Cc1cn(CCCCl)nn1

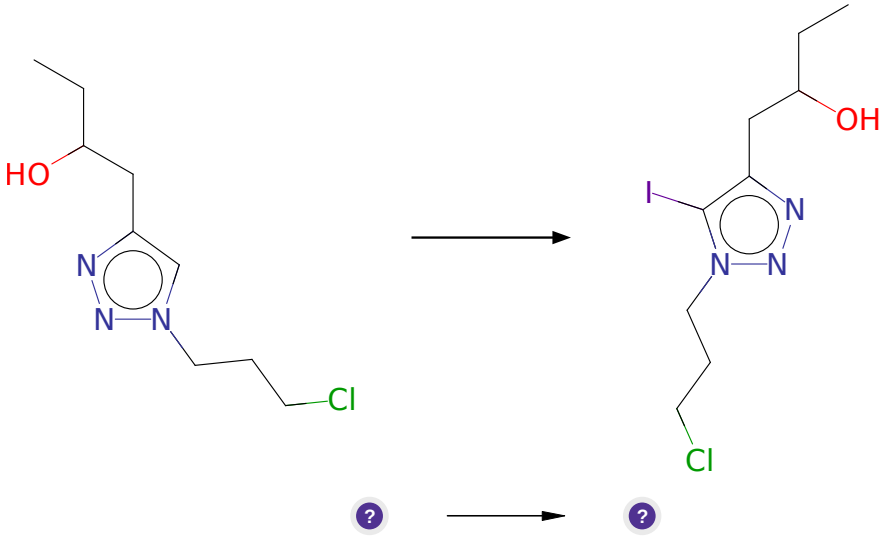
Typical conditions: PPh3.CCl4

Protections: none

Reference: *10.2174/1570179412666150305231358*

Retrosynthesis ID: 245593

2.1.3 Iodination of aromatic compounds



Substrates:

1. CCC(O)Cc1cn(CCCCl)nn1

Products:

1. CCC(O)Cc1nnn(CCCCl)c1I

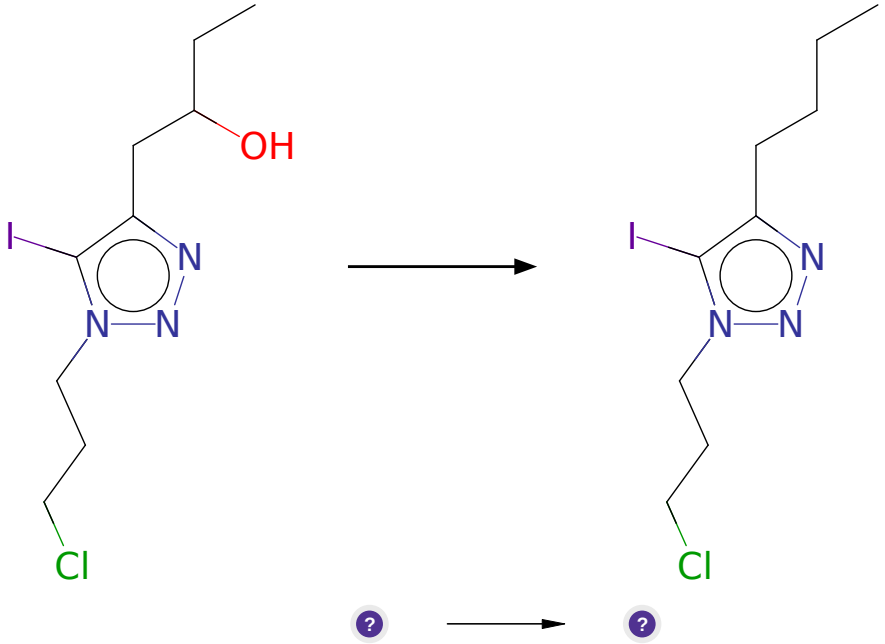
Typical conditions: I2 or other iodinating agent e.g. NIS

Protections: none

Reference: DOI: *10.1039/C5SC00964B* and *10.1016/j.tetlet.2005.05.117* and *10.1007/s11178-005-0256-1*

Retrosynthesis ID: 10697

2.1.4 Deoxygenation of alcohols with silanes



Substrates:

1. CCC(O)Cc1nnn(CCCCl)c1I

Products:

1. CCCCc1nnn(CCCCl)c1I

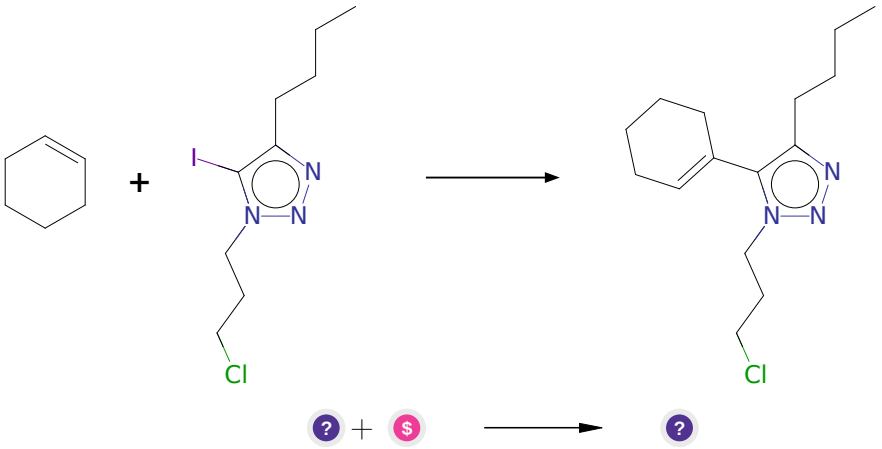
Typical conditions: Et3SiH.Lewis.or.Bronsted.Acid

Protections: none

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

Retrosynthesis ID: 8162

2.1.5 Heck Reaction



Substrates:

1. CCCCc1nnn(CCCCl)c1I
2. Cyclohexene - *available at Sigma-Aldrich*

Products:

1. CCCCc1nnn(CCCCl)c1C1=CCCCC1

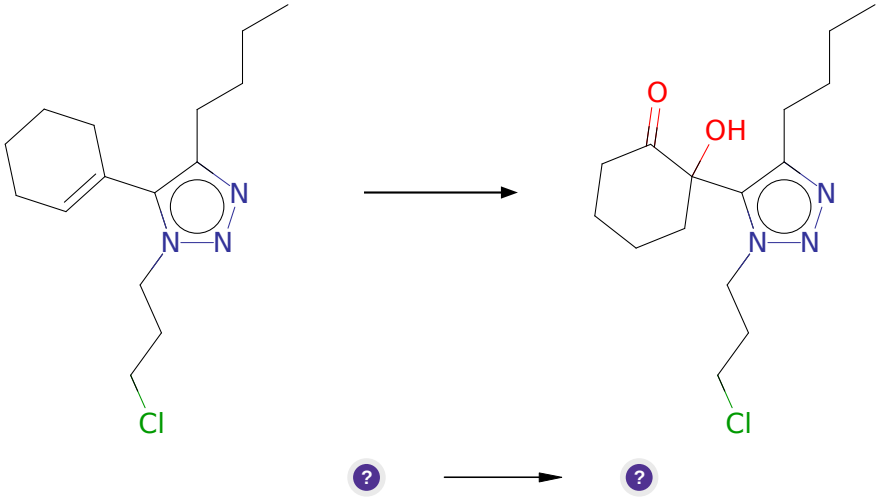
Typical conditions: Pd (cat). Ligand e.g. TXPTS. Base. Temp

Protections: none

Reference: *10.1016/j.tetlet.2013.01.077* or *10.1002/9780470716076* or *10.1021/op050106k* or *10.1021/ol0360288* or *10.1021/ol702755g* or *10.1055/s-0033-1340319* or *10.1016/j.tet.2004.10.049*

Retrosynthesis ID: 9186

2.1.6 Oxohydroxylation of unsymmetric alkenes



Substrates:

1. CCCCc1nnn(CCCCl)c1C1=CCCCC1

Products:

1. CCCCc1nnn(CCCCl)c1C1(O)CCCCC1=O

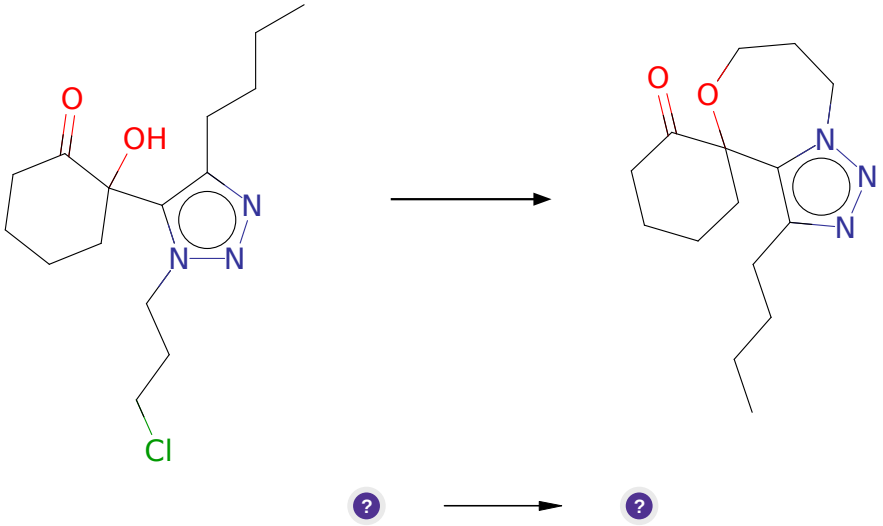
Typical conditions: KMnO4.Acetone/H2O.-10 deg C

Protections: none

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

Retrosynthesis ID: 10037547

2.1.7 Alkylation of tertiary alcohols



Substrates:

1. CCCCc1nnn(CCCCl)c1C1(O)CCCCC1=O

Products:

1. CCCCc1nnn2c1C1(CCCCC1=O)OCCC2

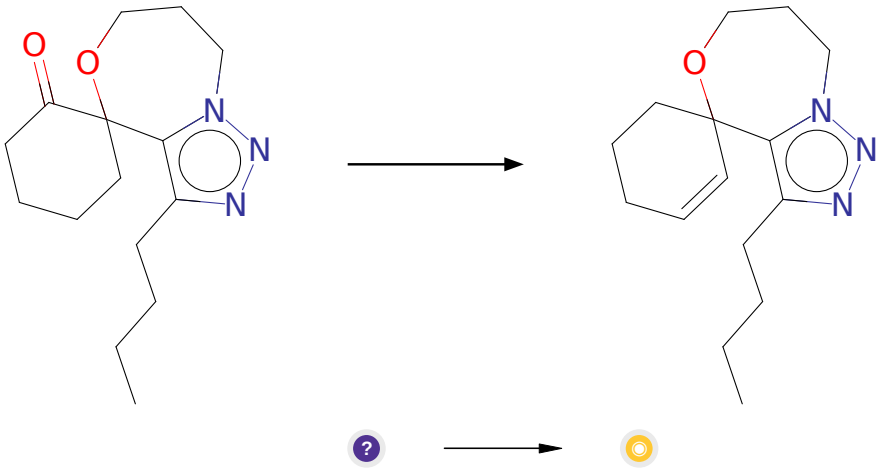
Typical conditions: K2CO3.acetone.heat

Protections: none

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

Retrosynthesis ID: 31010930

2.1.8 Shapiro reaction



Substrates:

1. CCCCc1nnn2c1C1(CCCCC1=O)OCCC2

Products:

1. CCCCc1nnn2c1C1(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 Path 2

Score: `262.41`

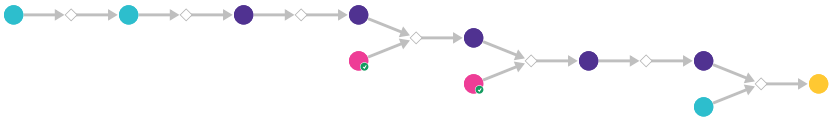
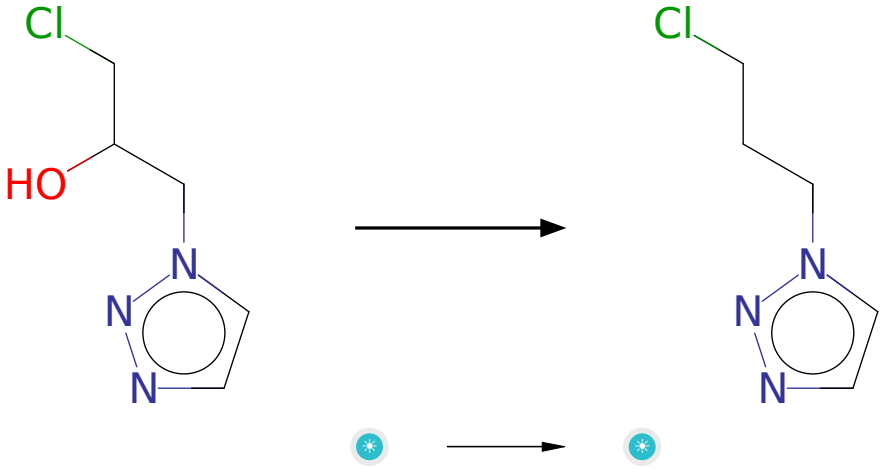


Figure 2: Outline of path 2

2.2.1 Deoxygenation of alcohols with silanes



Substrates:

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

Products:

1. C5H8ClN3

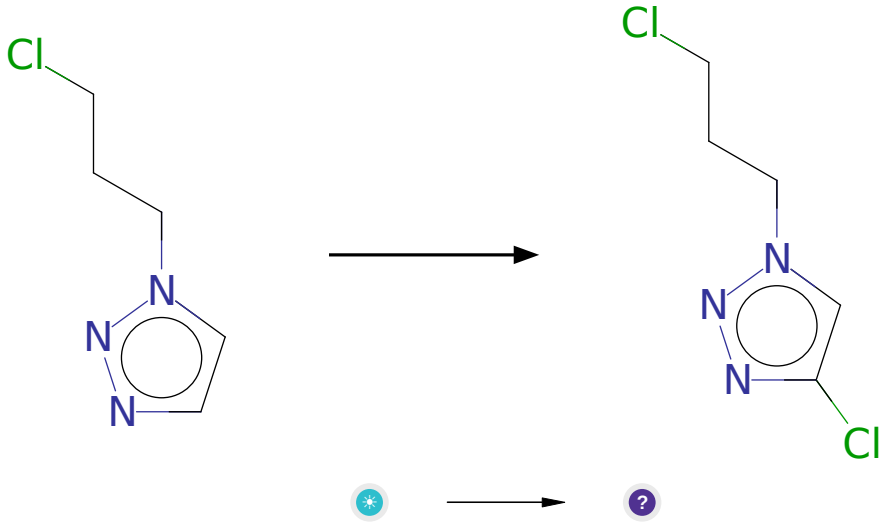
Typical conditions: Et3SiH.Lewis.or.Bronsted.Acid

Protections: none

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

Retrosynthesis ID: 8162

2.2.2 Chlorination of aromatic compounds



Substrates:

1. C5H8ClN3

Products:

1. ClCCCn1cc(Cl)nn1

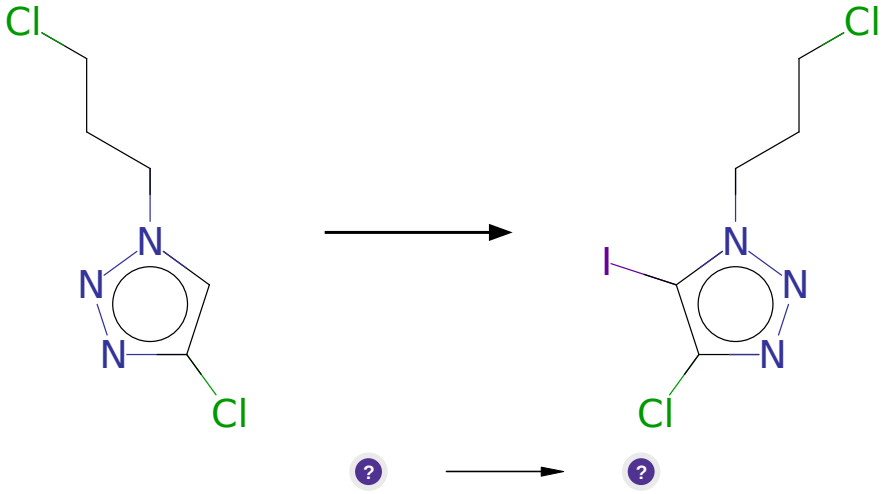
Typical conditions: Cl2 or other chlorinating agent like NCS

Protections: none

Reference: DOI: *10.1007/s11178-005-0256-1*

Retrosynthesis ID: 11125

2.2.3 Iodination of aromatic compounds



Substrates:

1. ClCCCn1cc(Cl)nn1

Products:

1. ClCCCn1nnc(Cl)c1I

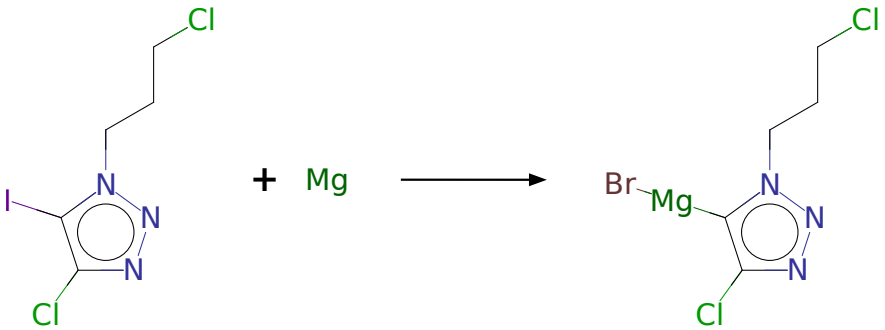
Typical conditions: I2 or other iodinating agent e.g. NIS

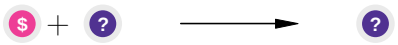
Protections: none

Reference: DOI: *10.1039/C5SC00964B* and *10.1016/j.tetlet.2005.05.117* and *10.1007/s11178-005-0256-1*

Retrosynthesis ID: 10697

2.2.4 Synthesis of aryl Grignard reagents





Substrates:

1. Magnesium - *available at Sigma-Aldrich*
2. ClCCCn1nnc(Cl)c1I

Products:

1. ClCCCn1nnc(Cl)c1[Mg]Br

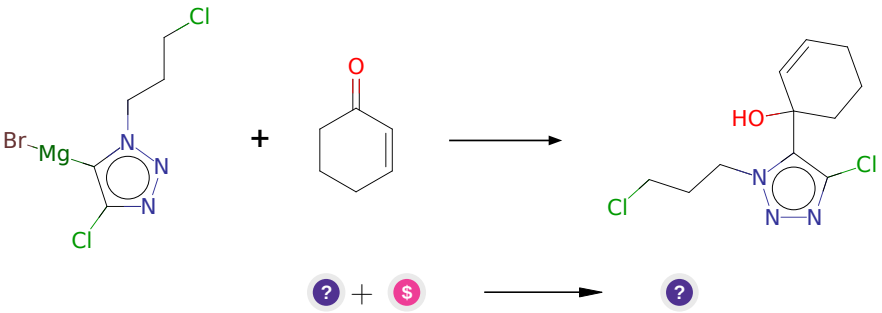
Typical conditions: iPrMgCl.LiCl.THF or other conditions Mg.THF or tBuLi.MgBr2

Protections: none

Reference: DOI: *10.1016/S0040-4039(99)01404-5* and *10.1021/jo0000574* and WO2014123793 p.137 and *10.1021/jm400491x* and *10.3762/bjoc.12.36*

Retrosynthesis ID: 10011460

2.2.5 Grignard-Type Reaction



Substrates:

1. ClCCCn1nnc(Cl)c1[Mg]Br
2. 2-Cyclohexen-1-one - *available at Sigma-Aldrich*

Products:

1. OC1(c2c(Cl)nnn2CCCCl)C=CCCC1

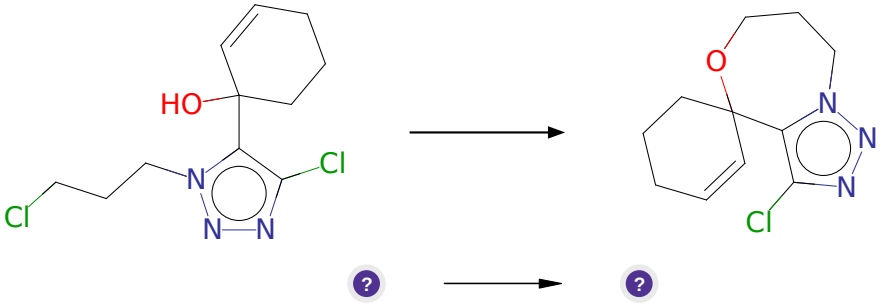
Typical conditions: Mg or Li.ether

Protections: none

Reference: *10.1021/jm061429p* or *10.1016/j.bmc.2012.11.015* or *10.1016/j.tetasy.2012.05.024*

Retrosynthesis ID: 25133

2.2.6 Alkylation of tertiary alcohols



Substrates:

1. OC1(c2c(Cl)nnn2CCCCl)C=CCCC1

Products:

1. Clc1nnn2c1C1(C=CCCC1)OCCC2

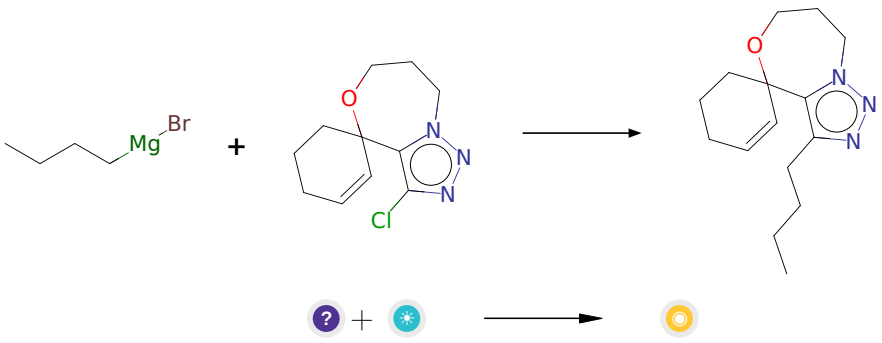
Typical conditions: K2CO3.acetone.heat

Protections: none

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

Retrosynthesis ID: 31010930

2.2.7 Kumada-Corriu reaction



Substrates:

1. Clc1nnn2c1C1(C=CCCC1)OCCC2
2. butylmagnesium bromide

Products:

1. CCCCc1nnn2c1C1(C=CCCC1)OCCC2

Typical conditions: NMP.Pd(OAc)2.PCy3

Protections: none

Reference: DOI: *10.1002/1521-3773(20021104)41:21<4056::AID-ANIE4056>3.0.CO;2-8*

Retrosynthesis ID: 1963