Paths of analysis*
Analysis 5

Synthia

March 3, 2022

1 Analysis parameters

Analysis type: Automatic Retrosynthesis

Rules: none selected

Filters: FGI, FGI with protections

Max. paths returned: 5

Max. iterations: 300

Commercial:

1. Max. molecular weight - 1000 g/mol

2. Max. price - 1000 $/g

Published:

1. Max. molecular weight - 1000 g/mol

2. Popularity - 10

My Stockroom:

1. Max. molecular weight - 1000 g/mol

Reaction scoring formula: TUNNEL_COEF*FGI_COEF*STEP*20+1000 000*(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

JSON Parameters: {}

2 Paths

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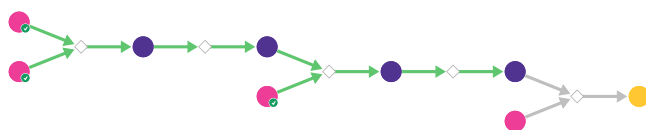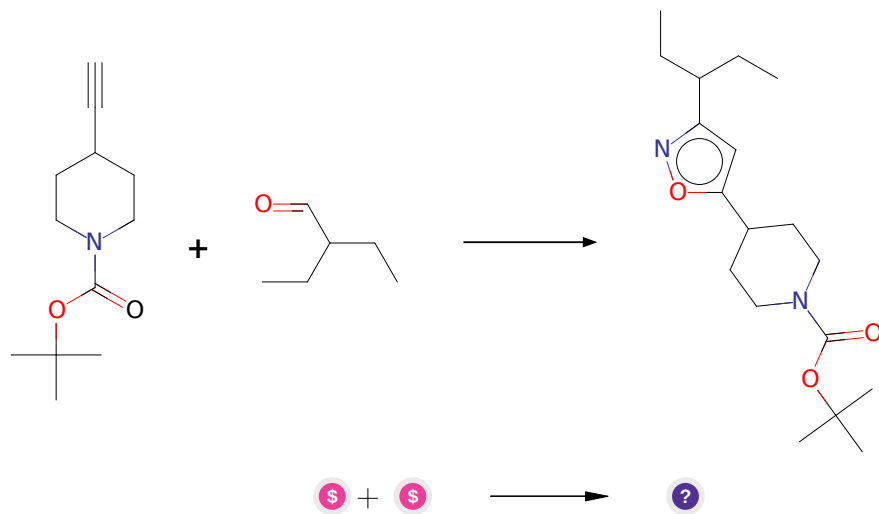
2.1 Path 1

Score: 122.50

Figure 1: Outline of path 1

2.1.1 Synthesis of isoxazoles from aldehydes and hydrazines

Substrates:

1. 2-Ethylbutanal -   *available at Sigma-Aldrich*

2. 4-Ethynylpiperidine-1-carboxylic acid tert-butyl ester -   *available at Sigma-Aldrich*

Products:

1. CCC(CC)c1cc(C2CCN(C(=O)OC(C)(C)C)CC2)on1
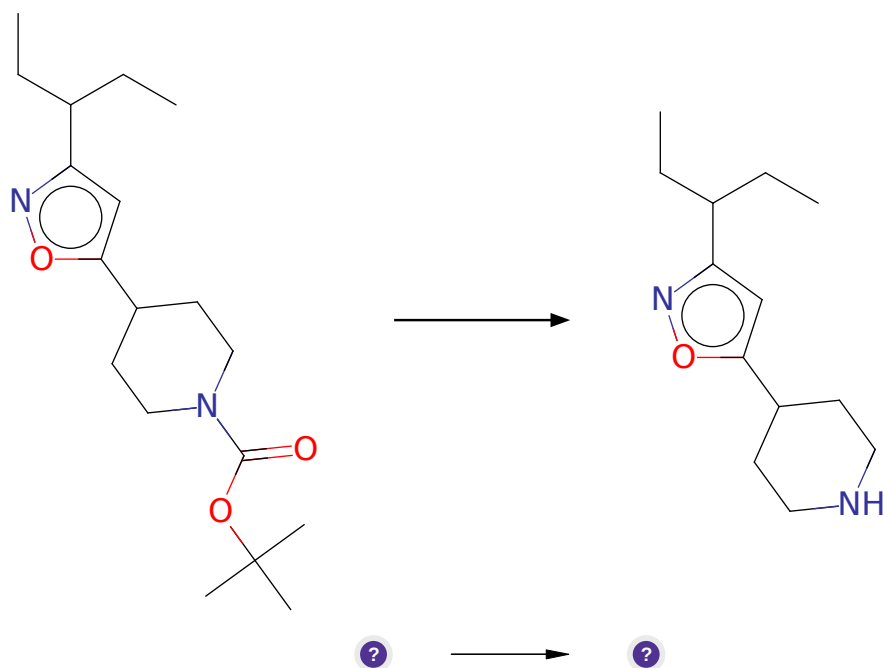
Typical conditions: 1. nBuLi 2. I2.K2CO3

Protections: none

Yield: moderate

Reference: DOI:

Retrosynthesis ID: 49545

2.1.2 Boc removal

Substrates:

1. CCC(CC)c1cc(C2CCN(C(=O)OC(C)(C)C)CC2)on1

Products:

1. CCC(CC)c1cc(C2CCNCC2)on1
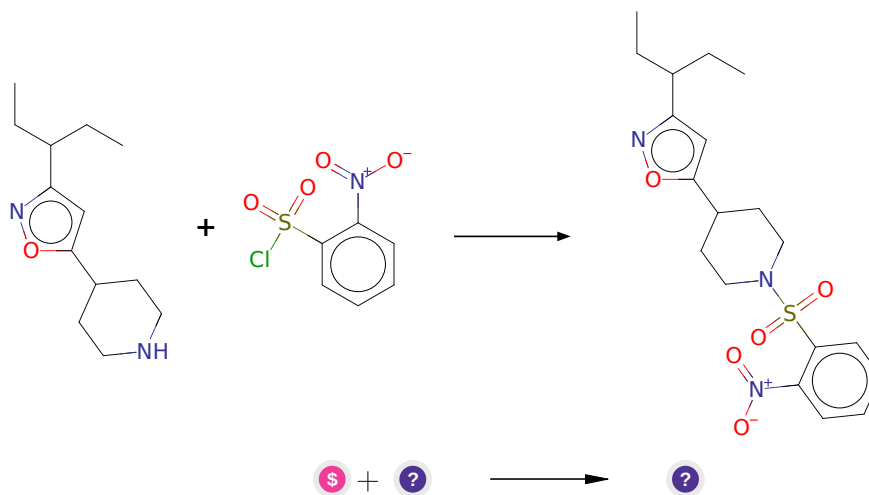
Typical conditions: TFA.DCM or HCl.EtOH

Protections: none

Yield: good

Retrosynthesis ID: 10025810

2.1.3 Synthesis of sulfonamides from sulfonyl chlorides

Substrates:

1. 2-Nitrobenzenesulfonyl chloride - *available at Sigma-Aldrich*

2. CCC(CC)c1cc(C2CCNCC2)on1

Products:

1. CCC(CC)c1cc(C2CCN(S(=O)(=O)c3ccccc3[N+](=O)[O-])CC2)on1
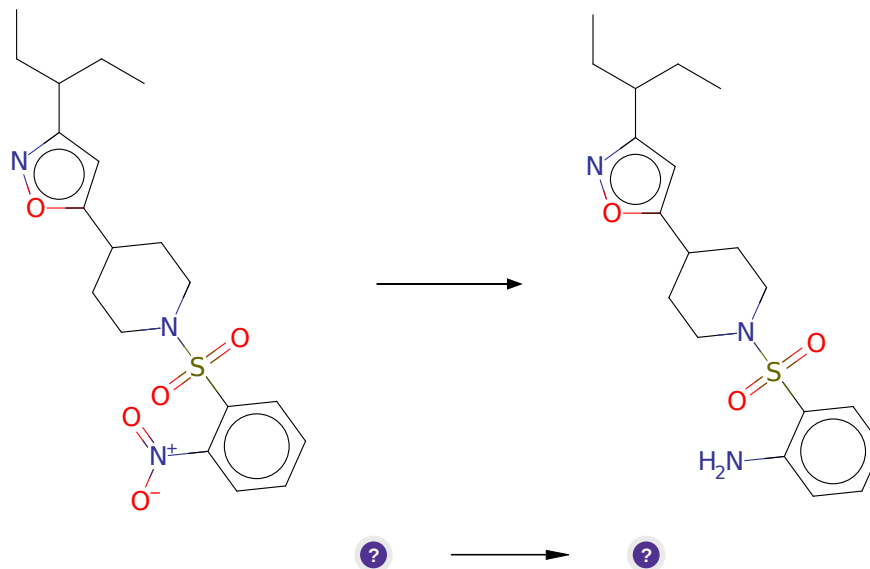
Typical conditions: Et3N

Protections: none

Yield: good

Retrosynthesis ID: 247

2.1.4 Reduction of nitro group

Substrates:

1. CCC(CC)c1cc(C2CCN(S(=O)(=O)c3ccccc3[N+](=O)[O-])CC2)on1

Products:

1. CCC(CC)c1cc(C2CCN(S(=O)(=O)c3ccccc3N)CC2)on1
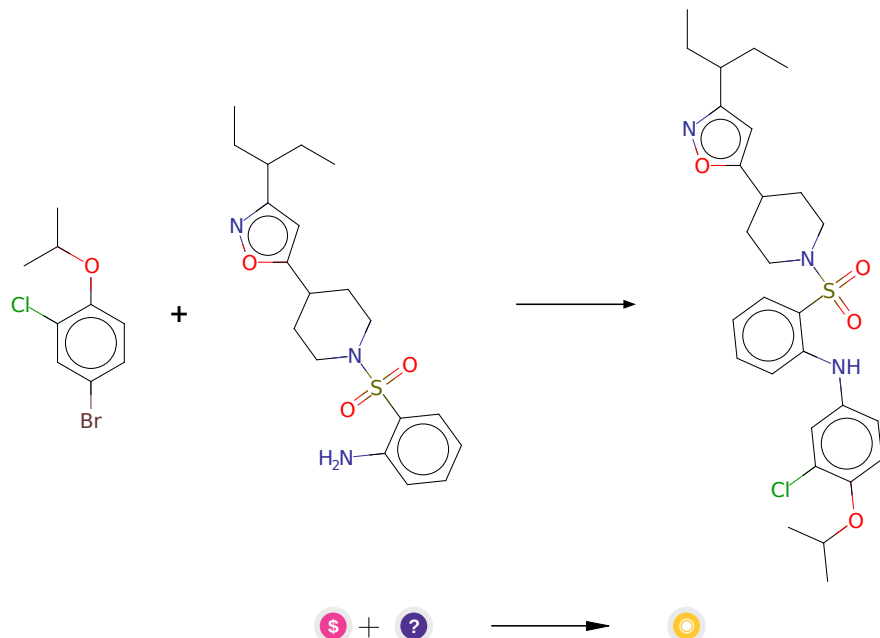
Typical conditions: Zn. aq NH4. EtOH //Zn.Hcl

Protections: none

Yield: good

Reference: DOI: *10.1002/anie.201512005* and *10.1002/anie.201104681* and *10.3390/molecules17055497* and *10.3390/molecules19022655* and *10.1021/ol5033464* (SI,page 3) and *10.5012/bkcs.2013.34.4.1275*

Retrosynthesis ID: 6145

2.1.5 Amination of aryl bromides

Substrates:

1. 4-Bromo-2-chloro-1-isopropoxybenzene - *AOBChem*

2. CCC(CC)c1cc(C2CCN(S(=O)(=O)c3ccccc3N)CC2)on1

Products:

1. CCC(CC)c1cc(C2CCN(S(=O)(=O)c3ccccc3Nc3ccc(OC(C)C)c(Cl)c3)CC2)on1

Typical conditions: Pd.ligand.base or CuI.ligand.base

Protections: none

Yield: good

Reference: *10.1021/ja903049z* and *10.1021/jo060945k* and *10.1021/jo060190h* and *10.1039/B923255A* and *10.1021/jm8003625* and *10.1021/jo9006738*

Retrosynthesis ID: 28544