Paths of analysis*

Analysis 8

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+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

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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: 103.81

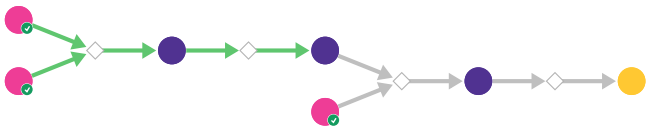
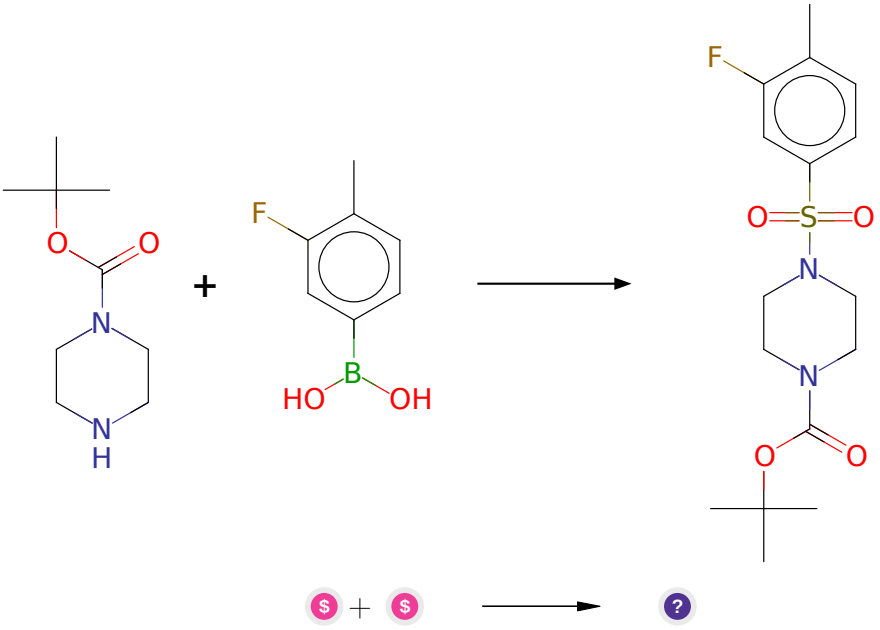


Figure 1: Outline of path 1

2.1.1 Synthesis of sulfonamides from boronic acids



Substrates:

1. 1-Boc-piperazine - *available at Sigma-Aldrich*

2. 3-Fluoro-4-methylphenylboronic acid - *available at Sigma-Aldrich*

Products:

1. Cc1ccc(S(=O)(=O)N2CCN(C(=O)OC(C)(C)C)CC2)cc1F

Typical conditions: Cu(OTf)2.ligand.Cs2CO3.DMSO.heat

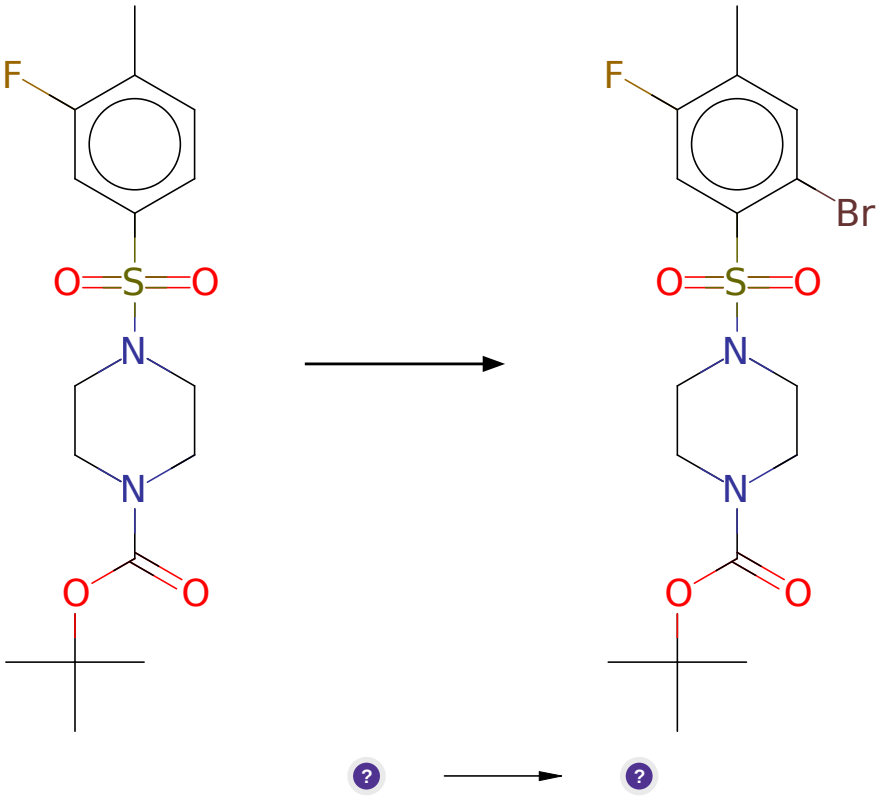
Protections: none

Yield: moderate

Reference: *10.1021/jacs.8b04532*

Retrosynthesis ID: 10029538

2.1.2 Bromination of aromatic compounds



Substrates:

1. Cc1ccc(S(=O)(=O)N2CCN(C(=O)OC(C)(C)C)CC2)cc1F

Products:

1. Cc1cc(Br)c(S(=O)(=O)N2CCN(C(=O)OC(C)(C)C)CC2)cc1F

Typical conditions: Br2.Fe

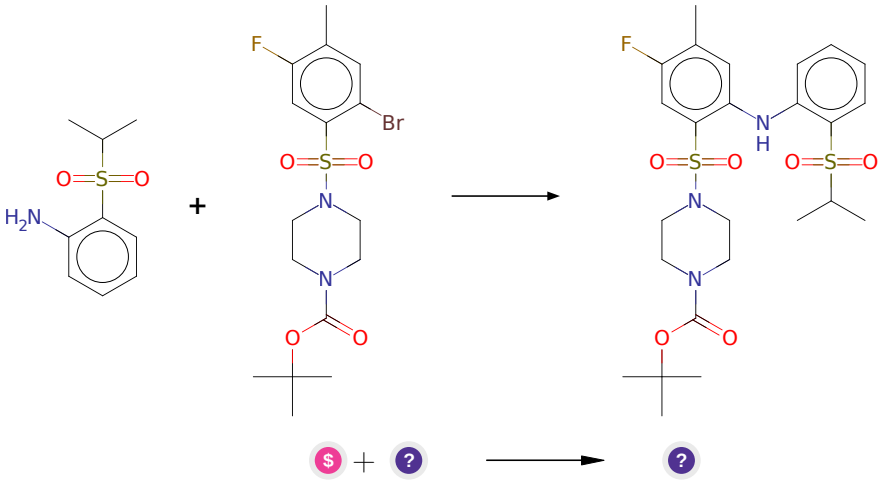
Protections: none

Yield: good

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

Retrosynthesis ID: 7777000

2.1.3 Amination of aryl bromides



Substrates:

1. 1-Amino-2-(isopropylsulphonyl)benzene - *available at Sigma-Aldrich*
2. Cc1cc(Br)c(S(=O)(=O)N2CCN(C(=O)OC(C)(C)C)CC2)cc1F

Products:

1. Cc1cc(Nc2ccccc2S(=O)(=O)C(C)C)c(S(=O)(=O)N2CCN(C(=O)OC(C)(C)C)CC2)cc1F

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

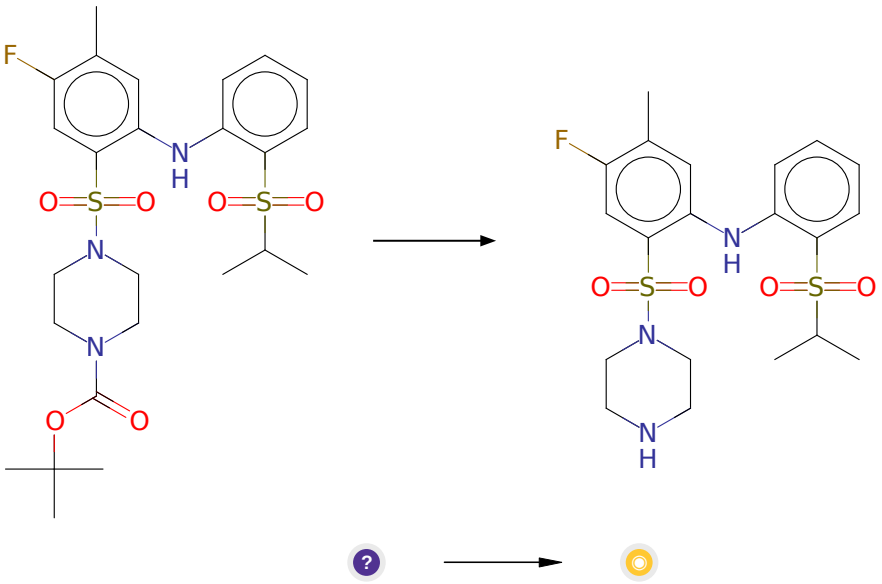
Protections: none

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

2.1.4 Boc removal



Substrates:

1. Cc1cc(Nc2ccccc2S(=O)(=O)C(C)C)c(S(=O)(=O)N2CCN(C(=O)OC(C)(C)C)CC2)cc1F

Products:

1. Cc1cc(Nc2ccccc2S(=O)(=O)C(C)C)c(S(=O)(=O)N2CCNCC2)cc1F

Typical conditions: TFA.DCM or HCl.EtOH

Protections: none

Yield: good

Reference: *10.1021/jm0707941* and *10.1021/jm020598g* and *10.1021/acs.oprd.5b00144* and *10.1016/j.bmc.2003.08.022*

Retrosynthesis ID: 10025810