Paths of analysis*

Analysis 6

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: 71.88

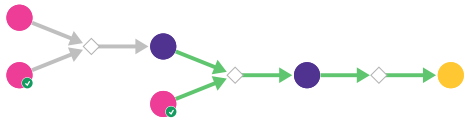
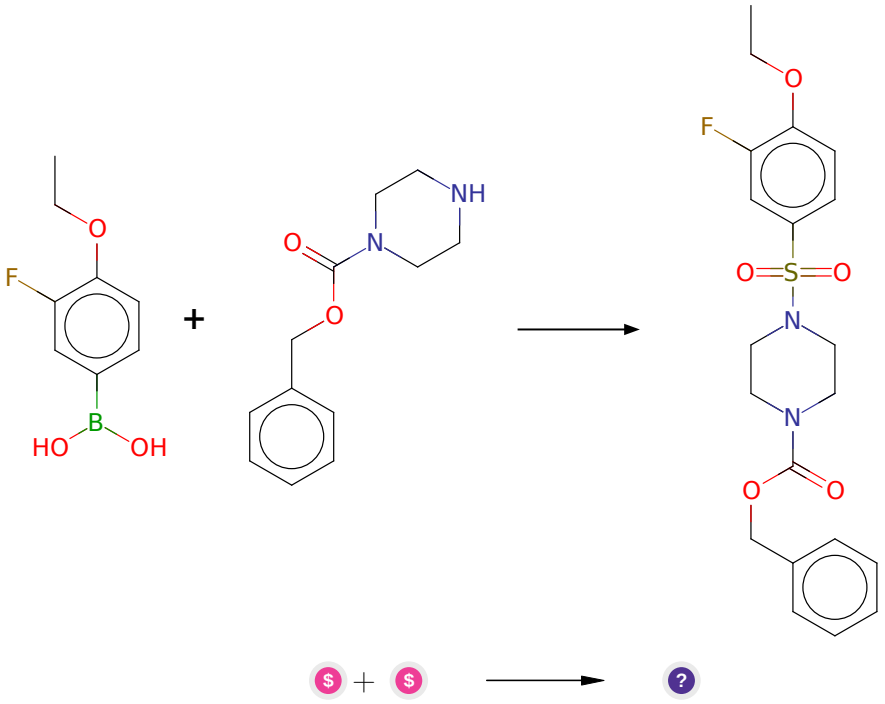


Figure 1: Outline of path 1

2.1.1 Synthesis of sulfonamides from boronic acids



Substrates:

1. 4-Ethoxy-3-fluorophenylboronic acid - *AOBChem*
2. 1-Z-Piperazine - *available at Sigma-Aldrich*

Products:

1. CCOc1ccc(S(=O)(=O)N2CCN(C(=O)OCc3ccccc3)CC2)cc1F

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

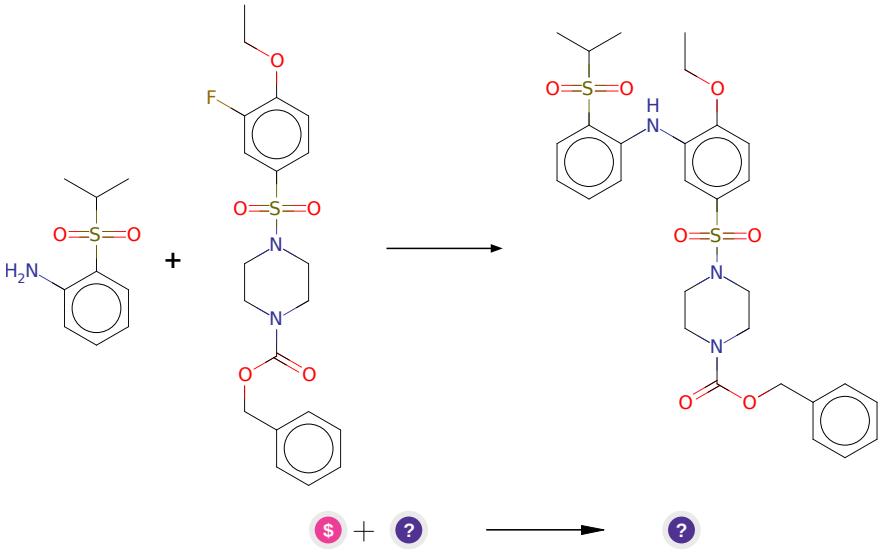
Protections: none

Yield: moderate

Reference: *10.1021/jacs.8b04532*

Retrosynthesis ID: 10029538

2.1.2 Nucleophilic aromatic substitution



Substrates:

1. 1-Amino-2-(isopropylsulphonyl)benzene - *available at Sigma-Aldrich*
2. CCOc1ccc(S(=O)(=O)N2CCN(C(=O)OCc3ccccc3)CC2)cc1F

Products:

1. CCOc1ccc(S(=O)(=O)N2CCN(C(=O)OCc3ccccc3)CC2)cc1Nc1ccccc1S(=O)(=O)C(C)C

Typical conditions: Solvent

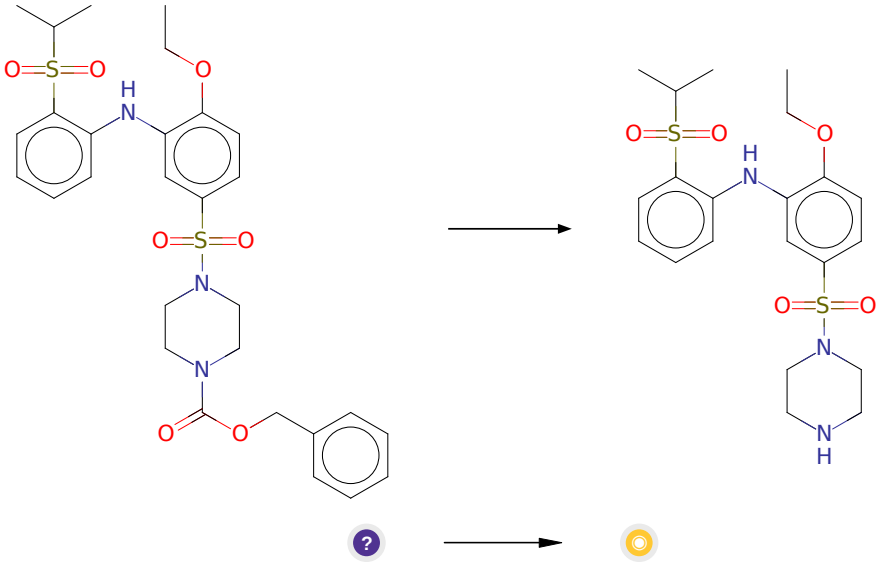
Protections: none

Yield: good

Reference: *10.1002/9781118093559.ch4*

Retrosynthesis ID: 49476

2.1.3 Cleavage of benzyloxycarbamates



Substrates:

1. CCOc1ccc(S(=O)(=O)N2CCN(C(=O)OCc3ccccc3)CC2)cc1Nc1ccccc1S(=O)(=O)C(C)C

Products:

1. CCOc1ccc(S(=O)(=O)N2CCNCC2)cc1Nc1ccccc1S(=O)(=O)C(C)C

Typical conditions: H2.Pd/C

Protections: none

Yield: moderate

Reference: *10.1021/jm070755h* and *10.1021/jm2016057* and *10.1055/s-0033-1340215* and *10.1016/S0040-4039(03)01181-X*

Retrosynthesis ID: 9990024