Paths of analysis*

Analysis 2

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: 89.93

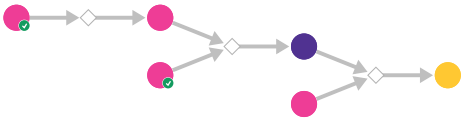
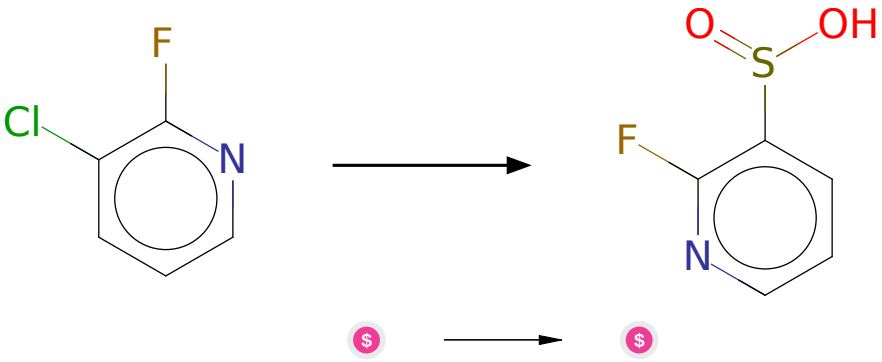


Figure 1: Outline of path 1

2.1.1 Synthesis of sulfinyl acids from alkyl or aryl halides



Substrates:

1. 3-Chloro-2-fluoropyridine - *available at Sigma-Aldrich*

Products:

1. C5H4FNO2S - *Enamine*

Typical conditions: 1. Mg.THF 2. SOCl2.THF

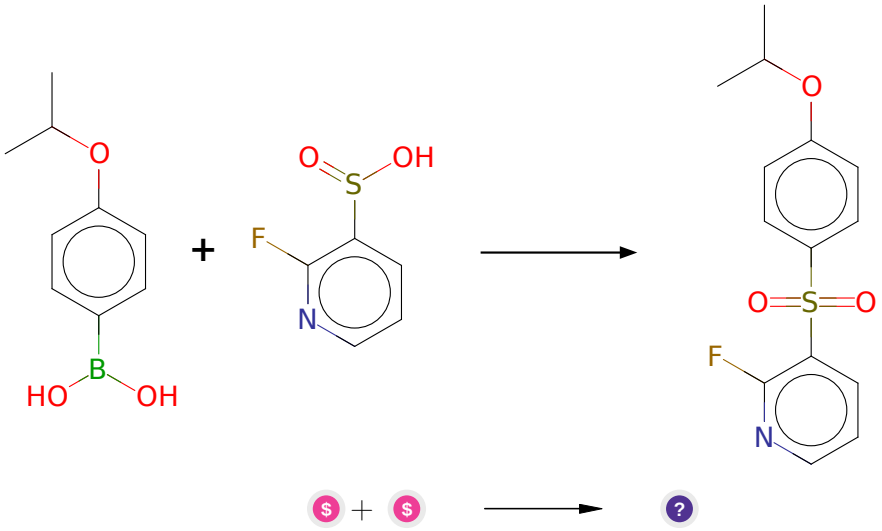
Protections: none

Yield: moderate

Reference: DOI: *10.1021/jo971455i* (experimental section)

Retrosynthesis ID: 1995

2.1.2 Synthesis of sulfones from boronic acids



Substrates:

1. 4-Isopropoxyphenylboronic acid - *available at Sigma-Aldrich*
2. C5H4FNO2S - *Enamine*

Products:

1. CC(C)Oc1ccc(S(=O)(=O)c2cccnc2F)cc1

Typical conditions: Cu(OAc)2.K2CO3.MS 4A.DMSO.rt

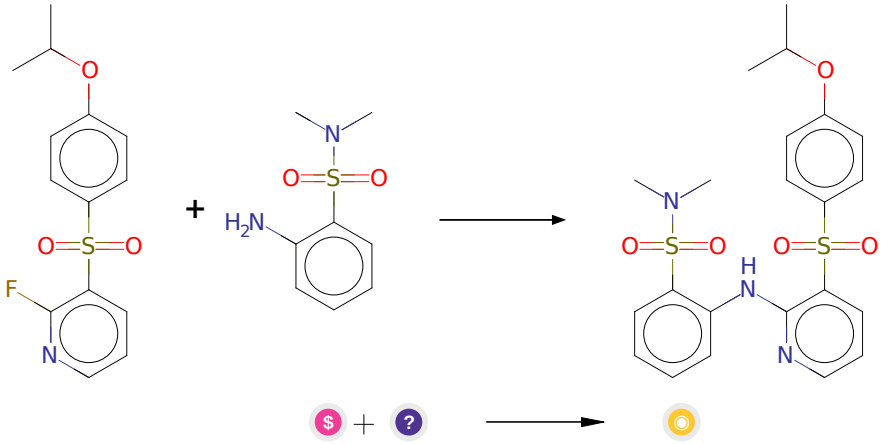
Protections: none

Yield: moderate

Reference: DOI: *10.1016/j.tetlet.2004.02.127*

Retrosynthesis ID: 1985

2.1.3 Nucleophilic aromatic substitution



Substrates:

1. 2-Amino-N,N-dimethylbenzenesulfonamide - *Combi-Blocks*
2. CC(C)Oc1ccc(S(=O)(=O)c2cccnc2F)cc1

Products:

1. CC(C)Oc1ccc(S(=O)(=O)c2cccnc2Nc2ccccc2S(=O)(=O)N(C)C)cc1

Typical conditions: Solvent

Protections: none

Yield: good

Reference: *10.1002/9781118093559.ch4*

Retrosynthesis ID: 49476