Paths of analysis*

Analysis 1

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: 125.03

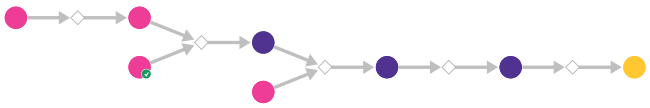
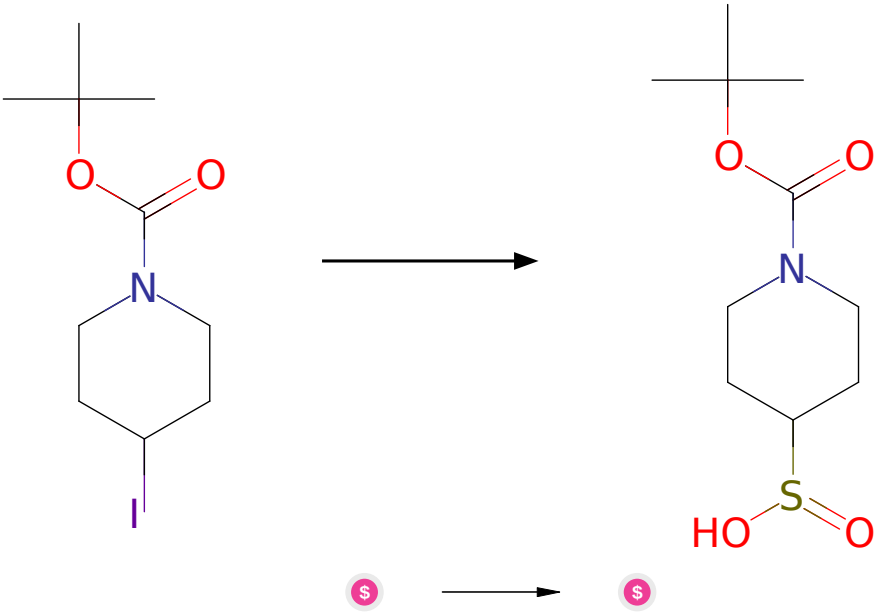


Figure 1: Outline of path 1

2.1.1 Synthesis of sulfinic acids from alkyl or aryl halides



Substrates:

1. 4-iodo-1-(tert-butoxycarbonyl)piperidine - *ManchesterOrganics*

Products:

1. C10H19NO4S - *Enamine*

Typical conditions: 1. BuLi 2. SO2 3. HCl

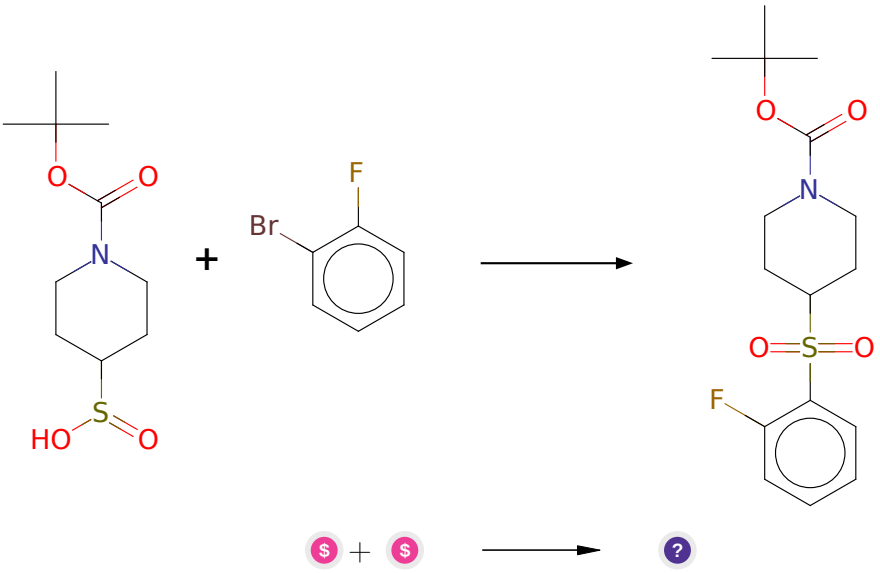
Protections: none

Yield: moderate

Reference: DOI: *10.1021/ol402235v*

Retrosynthesis ID: 1981

2.1.2 Synthesis of sulfones from sulfinic acids



Substrates:

1. C10H19NO4S - *Enamine*
2. 1-Bromo-2-fluorobenzene - *available at Sigma-Aldrich*

Products:

1. CC(C)(C)OC(=O)N1CCC(S(=O)(=O)c2ccccc2F)CC1

Typical conditions: CuI.DMSO.110C

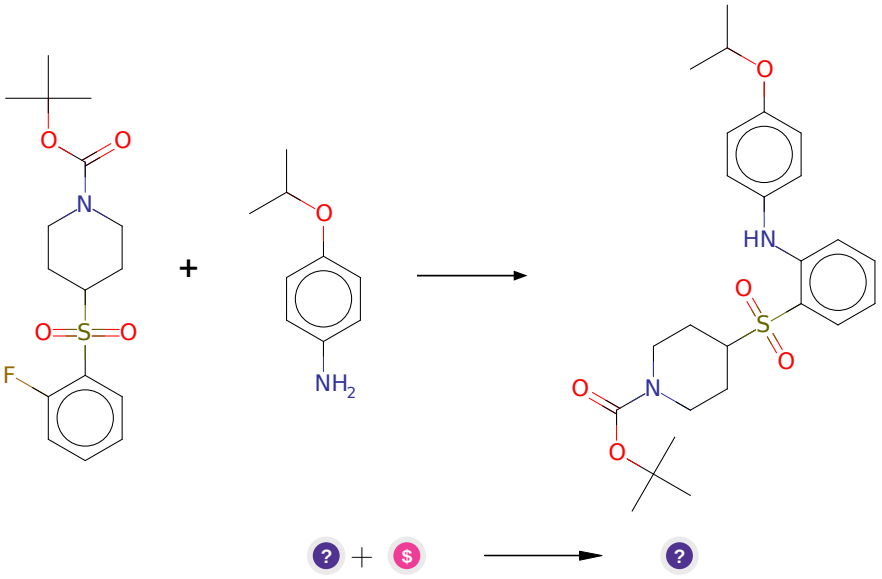
Protections: none

Yield: good

Reference: DOI: *10.1016/S0040-4039(02)02073-7*

Retrosynthesis ID: 1989

2.1.3 Nucleophilic aromatic substitution



Substrates:

1. CC(C)(C)OC(=O)N1CCC(S(=O)(=O)c2ccccc2F)CC1
2. 4-Isopropoxyaniline - *Combi-Blocks*

Products:

1. CC(C)Oc1ccc(Nc2ccccc2S(=O)(=O)C2CCN(C(=O)OC(C)(C)C)CC2)cc1

Typical conditions: Solvent

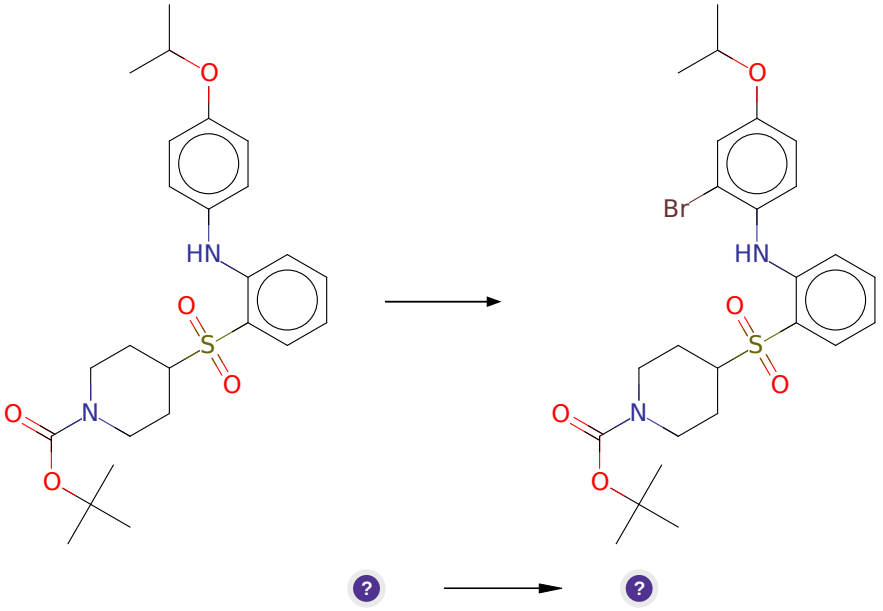
Protections: none

Yield: good

Reference: *10.1002/9781118093559.ch4*

Retrosynthesis ID: 49476

2.1.4 Bromination of aromatic compounds



Substrates:

1. CC(C)Oc1ccc(Nc2ccccc2S(=O)(=O)C2CCN(C(=O)OC(C)(C)C)CC2)cc1

Products:

1. CC(C)Oc1ccc(Nc2ccccc2S(=O)(=O)C2CCN(C(=O)OC(C)(C)C)CC2)c(Br)c1

Typical conditions: Br2.Fe

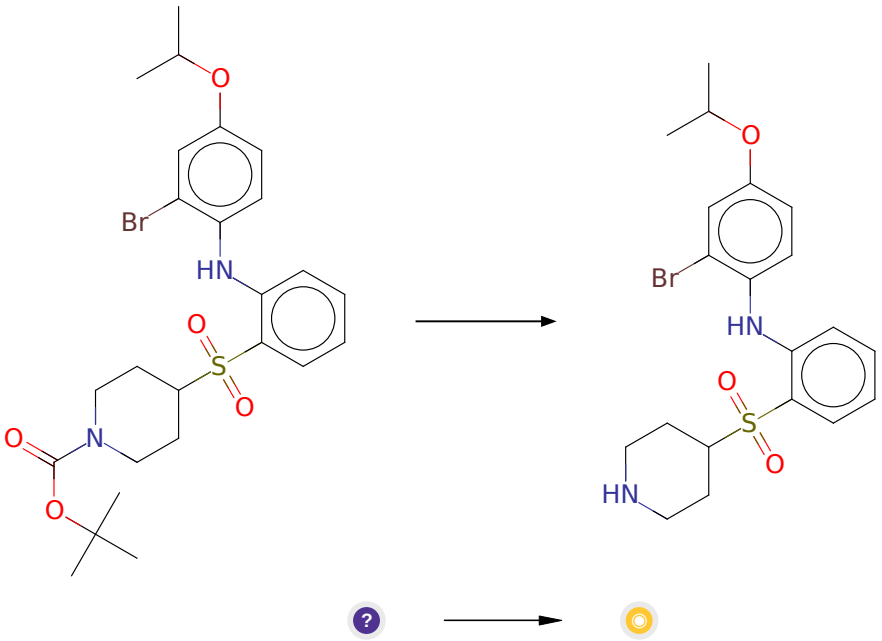
Protections: none

Yield: good

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

Retrosynthesis ID: 7777000

2.1.5 Boc removal



Substrates:

1. CC(C)Oc1ccc(Nc2ccccc2S(=O)(=O)C2CCN(C(=O)OC(C)(C)C)CC2)c(Br)c1

Products:

1. CC(C)Oc1ccc(Nc2ccccc2S(=O)(=O)C2CCNCC2)c(Br)c1

Typical conditions: TFA.DCM or HCl.EtOH

Protections: none

Yield: good

Reference: *10.1021/jm070794t* and *10.1021/jm020598g* and *10.1021/acs.oprd.5b00144* and *10.1016/j.bmc.2003.08.022*

Retrosynthesis ID: 10025810