Paths of analysis*

Analysis 4

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

2 paths found. *Paths are sorted by score. Reactions are sorted in appearance order for each path.*

2.1 Path 1

Score: `114.12`

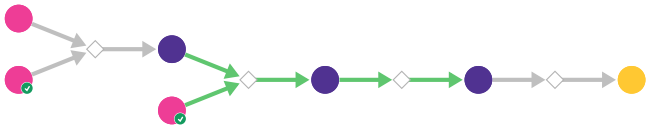
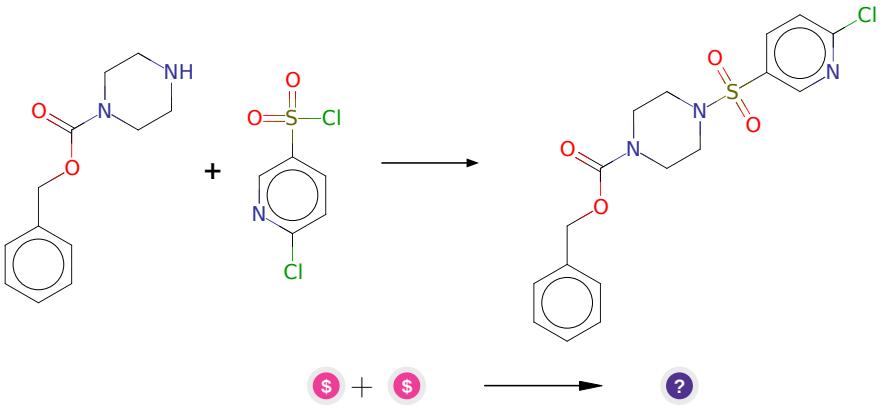


Figure 1: Outline of path 1

2.1.1 Synthesis of sulfonamides from sulfonyl chlorides



Substrates:

1. 2-Chloropyridine-5-sulfonyl chloride - *Combi-Blocks*
2. 1-Z-Piperazine - *available at Sigma-Aldrich*

Products:

1. O=C(OCc1ccccc1)N1CCN(S(=O)(=O)c2ccc(Cl)nc2)CC1

Typical conditions: Et3N

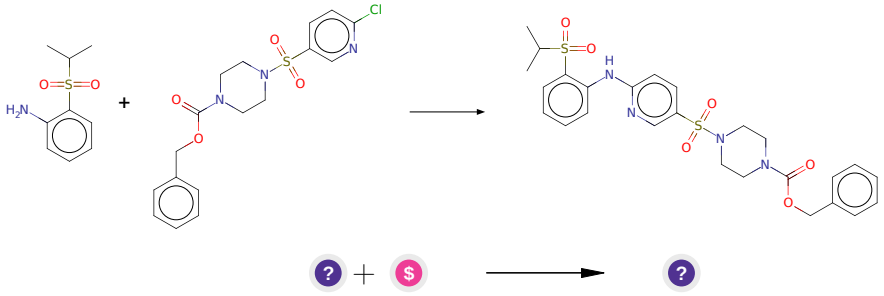
Protections: none

Yield: good

Reference: *10.1021/jm00395a010* and *10.1002/047084289X.rn00099* and *10.1016/j.jfluchem.2013.01.009*

Retrosynthesis ID: 247

2.1.2 Nucleophilic aromatic substitution



Substrates:

1. O=C(OCc1ccccc1)N1CCN(S(=O)(=O)c2ccc(Cl)nc2)CC1
2. 1-Amino-2-(isopropylsulphonyl)benzene - *available at Sigma-Aldrich*

Products:

1. CC(C)S(=O)(=O)c1ccccc1Nc1ccc(S(=O)(=O)N2CCN(C(=O)OCc3ccccc3)CC2)cn1

Typical conditions: solvent. Heating or pressure

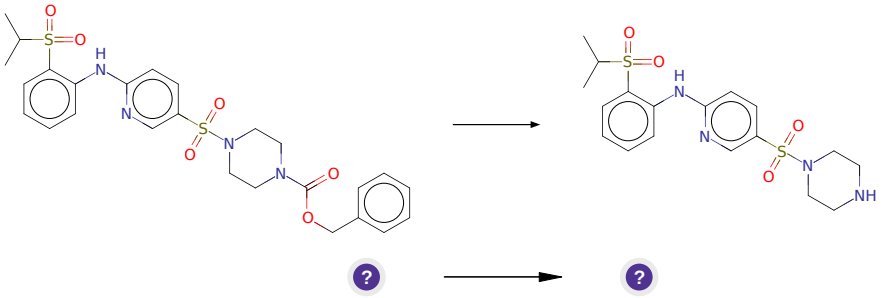
Protections: none

Yield: good

Reference: *10.1021/jm00040a009* or *10.1111/bph.12233* or *10.1246/cl.1987.1187*

Retrosynthesis ID: 5003

2.1.3 Cleavage of benzyloxycarbamates



Substrates:

1. CC(C)S(=O)(=O)c1ccccc1Nc1ccc(S(=O)(=O)N2CCN(C(=O)OCc3ccccc3)CC2)cn1

Products:

1. CC(C)S(=O)(=O)c1ccccc1Nc1ccc(S(=O)(=O)N2CCNCC2)cn1

Typical conditions: H2.Pd/C

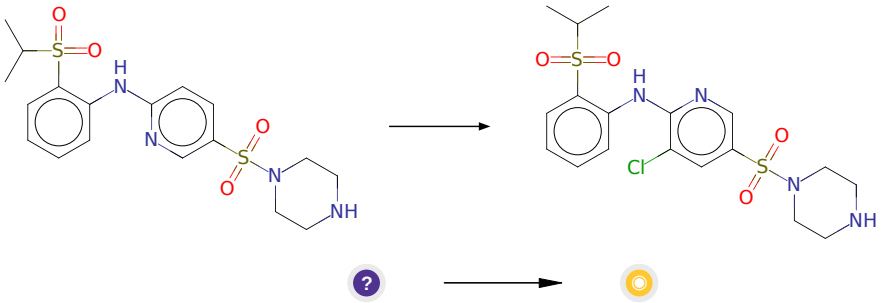
Protections: none

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

2.1.4 Chlorination of aromatic compounds



Substrates:

1. CC(C)S(=O)(=O)c1ccccc1Nc1ccc(S(=O)(=O)N2CCNCC2)cn1

Products:

1. CC(C)S(=O)(=O)c1ccccc1Nc1ncc(S(=O)(=O)N2CCNCC2)cc1Cl

Typical conditions: Cl2 or other chlorinating agent like NCS

Protections: none

Yield: moderate

Reference: DOI: *10.1007/s11178-005-0256-1*

Retrosynthesis ID: 11125

2.2 Path 2

Score: `127.01`

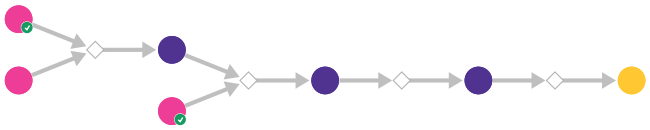
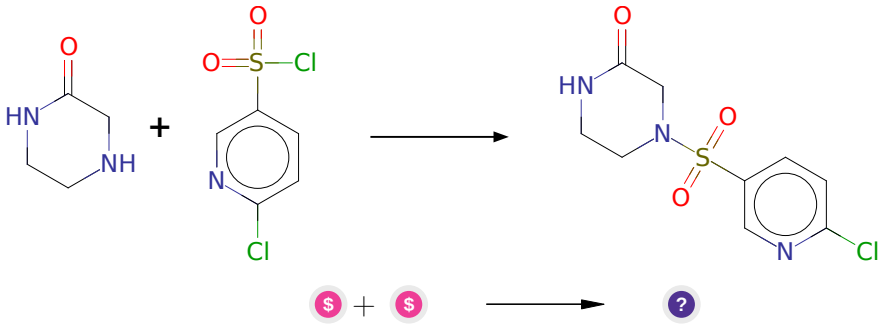


Figure 2: Outline of path 2

2.2.1 Synthesis of sulfonamides from sulfonyl chlorides



Substrates:

1. 2-Oxopiperazine - *available at Sigma-Aldrich*
2. 2-Chloropyridine-5-sulfonyl chloride - *Combi-Blocks*

Products:

1. O=C1CN(S(=O)(=O)c2ccc(Cl)nc2)CCN1

Typical conditions: Et3N

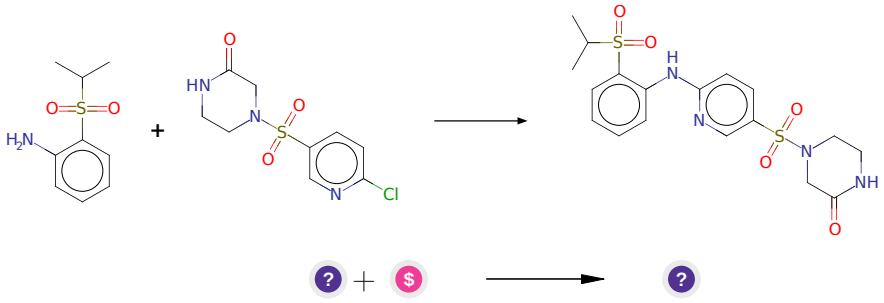
Protections: none

Yield: good

Reference: *10.1021/jm00395a010* and *10.1002/047084289X.rn00099* and *10.1016/j.jfluchem.2013.01.009*

Retrosynthesis ID: 247

2.2.2 Nucleophilic aromatic substitution



Substrates:

1. O=C1CN(S(=O)(=O)c2ccc(Cl)nc2)CCN1
2. 1-Amino-2-(isopropylsulphonyl)benzene - *available at Sigma-Aldrich*

Products:

1. CC(C)S(=O)(=O)c1ccccc1Nc1ccc(S(=O)(=O)N2CCNC(=O)C2)cn1

Typical conditions: solvent. Heating or pressure

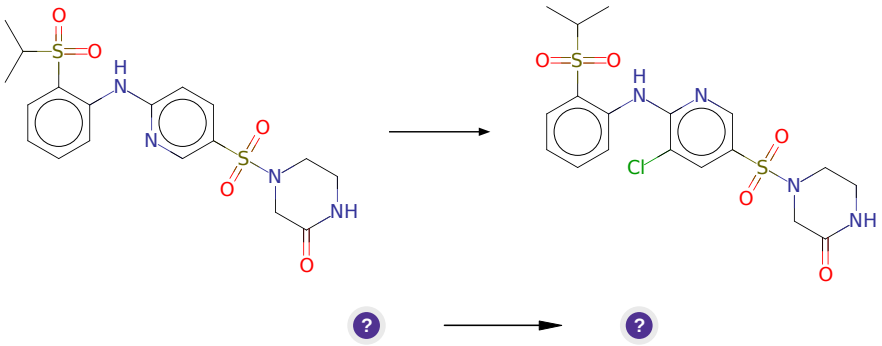
Protections: none

Yield: good

Reference: *10.1021/jm00040a009* or *10.1111/bph.12233* or *10.1246/cl.1987.1187*

Retrosynthesis ID: 5003

2.2.3 Chlorination of aromatic compounds



Substrates:

1. CC(C)S(=O)(=O)c1ccccc1Nc1ccc(S(=O)(=O)N2CCNC(=O)C2)cn1

Products:

1. CC(C)S(=O)(=O)c1ccccc1Nc1ncc(S(=O)(=O)N2CCNC(=O)C2)cc1Cl

Typical conditions: Cl2 or other chlorinating agent like NCS

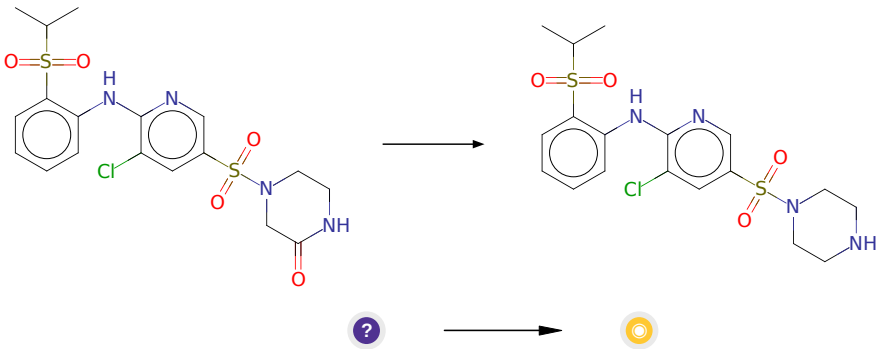
Protections: none

Yield: moderate

Reference: DOI: *10.1007/s11178-005-0256-1*

Retrosynthesis ID: 11125

2.2.4 Reduction of amide to amine



Substrates:

1. CC(C)S(=O)(=O)c1ccccc1Nc1ncc(S(=O)(=O)N2CCNC(=O)C2)cc1Cl

Products:

1. CC(C)S(=O)(=O)c1ccccc1Nc1ncc(S(=O)(=O)N2CCNCC2)cc1Cl

Typical conditions: BH3.THF

Protections: none

Yield: good

Reference: *10.1016/S0957-4166(02)00111-8*

Retrosynthesis ID: 9900018