Paths of analysis*

Analysis 10

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: 150.48

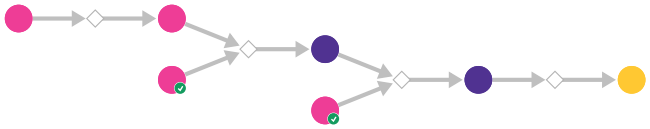
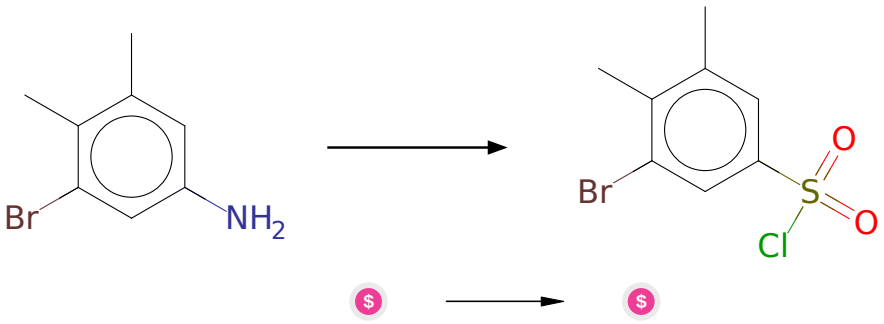


Figure 1: Outline of path 1

2.1.1 Sandmeyer Reaction



Substrates:

1. 3-BROMO-4,5-DIMETHYLANILINE - *Combi-Blocks*

Products:

1. 3-bromo-4,5-dimethylbenzene-1-sulfonyl chloride - *Enamine*

Typical conditions: NaNO2.HCl.CuCl.thionyl chloride

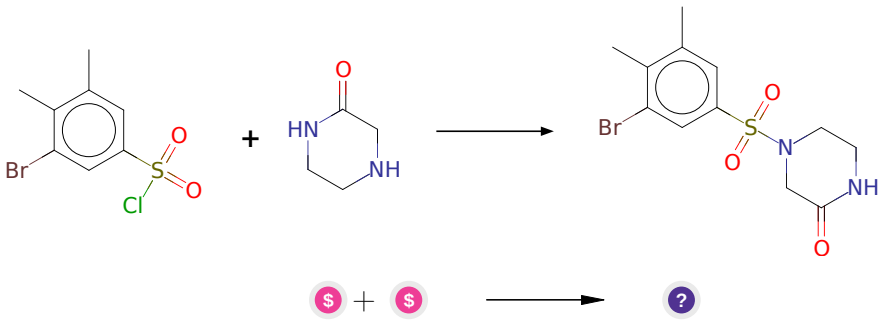
Protections: none

Yield: moderate

Reference: *10.1021/acs.jmedchem.5b01078* and *10.1016/j.bmcl.2013.04.049* and *10.1021/jm0503897*

Retrosynthesis ID: 29983

2.1.2 Synthesis of sulfonamides from sulfonyl chlorides



Substrates:

1. 2-Oxopiperazine - *available at Sigma-Aldrich*
2. 3-bromo-4,5-dimethylbenzene-1-sulfonyl chloride - *Enamine*

Products:

1. Cc1cc(S(=O)(=O)N2CCNC(=O)C2)cc(Br)c1C

Typical conditions: Et3N

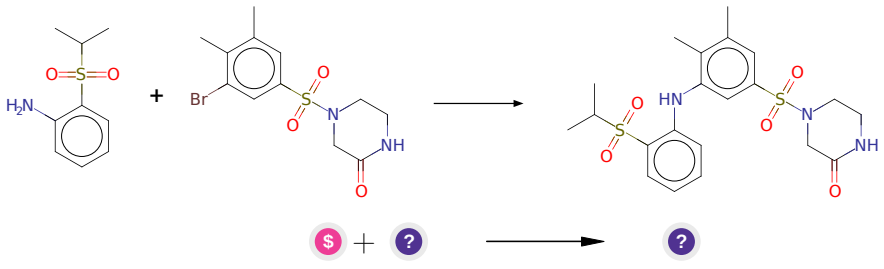
Protections: none

Yield: good

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

Retrosynthesis ID: 247

2.1.3 Amination of aryl bromides



Substrates:

1. 1-Amino-2-(isopropylsulphonyl)benzene - *available at Sigma-Aldrich*
2. Cc1cc(S(=O)(=O)N2CCNC(=O)C2)cc(Br)c1C

Products:

1. Cc1cc(S(=O)(=O)N2CCNC(=O)C2)cc(Nc2ccccc2S(=O)(=O)C(C)C)c1C

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

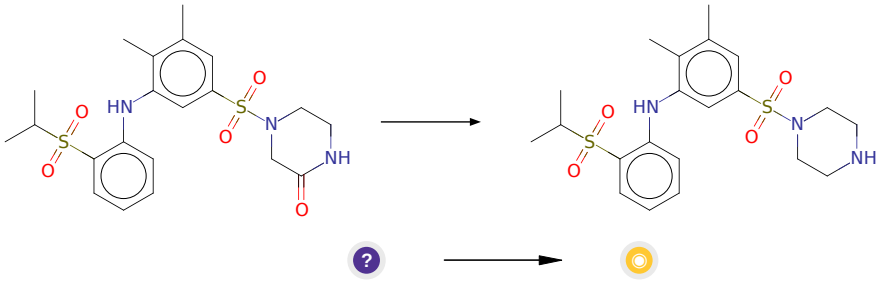
Protections: none

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 Reduction of amide to amine



Substrates:

1. Cc1cc(S(=O)(=O)N2CCNC(=O)C2)cc(Nc2ccccc2S(=O)(=O)C(C)C)c1C

Products:

1. Cc1cc(S(=O)(=O)N2CCNCC2)cc(Nc2ccccc2S(=O)(=O)C(C)C)c1C

Typical conditions: BH3.THF

Protections: none

Yield: good

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

Retrosynthesis ID: 9900018