Paths of analysis*

Analysis 7

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: 82.08

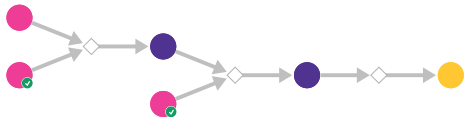
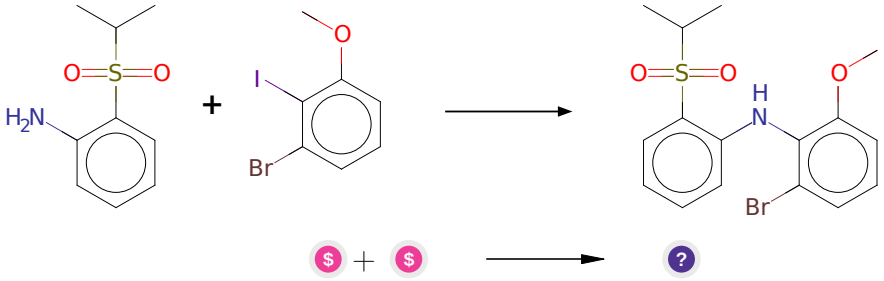


Figure 1: Outline of path 1

2.1.1 Amination of aryl iodides



Substrates:

1. 1-Bromo-2-iodo-3-methoxybenzene - *AOBChem*
2. 1-Amino-2-(isopropylsulphonyl)benzene - *available at Sigma-Aldrich*

Products:

1. COc1cccc(Br)c1Nc1ccccc1S(=O)(=O)C(C)C

Typical conditions: [Pd] or CuI.base.solvent

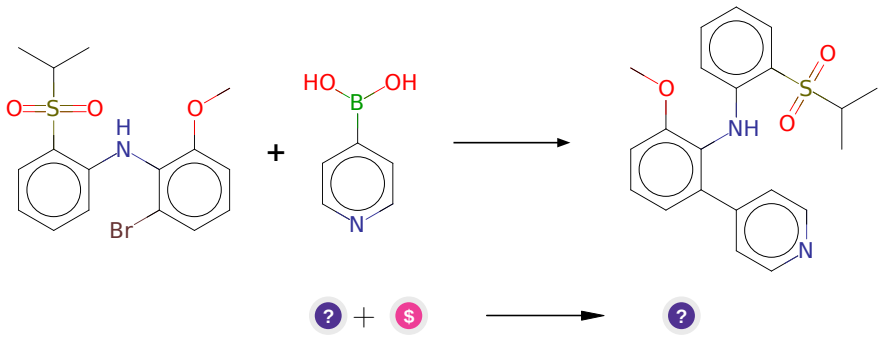
Protections: none

Yield: good

Reference: *10.1016/j.tet.2013.02.040* and *10.1021/ic200966f* (SI) and *10.1021/jo034994y*

Retrosynthesis ID: 1230

2.1.2 Suzuki coupling of arylboronic acids with aryl bromides



Substrates:

1. COc1cccc(Br)c1Nc1ccccc1S(=O)(=O)C(C)C
2. 4-Pyridylboronic acid - *available at Sigma-Aldrich*

Products:

1. COc1cccc(-c2ccncc2)c1Nc1ccccc1S(=O)(=O)C(C)C

Typical conditions: Pd catalyst.base.solvent

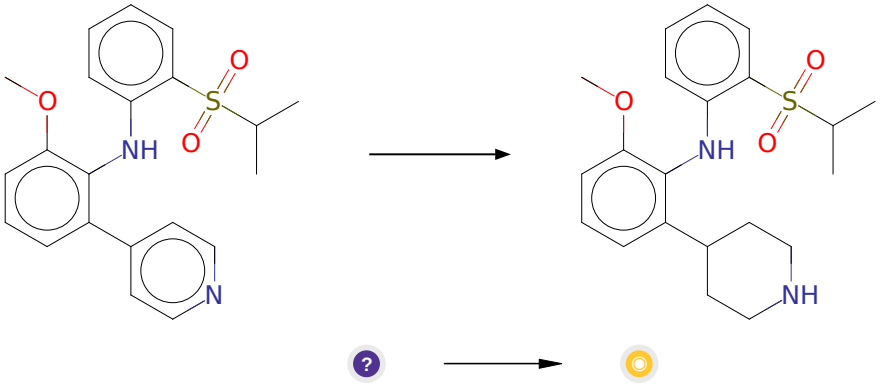
Protections: none

Yield: good

Reference: *10.1021/cr00039a007* and *10.1007/3418_2012_32* and *10.1021/cr0505268* and *10.1016/j.jfluchem.2016.01.018* and *10.1039/C3CS60197H* and *10.1016/j.ejmech.2018.08.092* and *10.1038/s41929-020-00564-z* (metal-free coupling)

Retrosynthesis ID: 25150

2.1.3 Reduction of pyridines with PtO2



Substrates:

1. COc1cccc(-c2ccncc2)c1Nc1ccccc1S(=O)(=O)C(C)C

Products:

1. COc1cccc(C2CCNCC2)c1Nc1ccccc1S(=O)(=O)C(C)C

Typical conditions: PtO2. H2. Acetic acid. Pressure

Protections: none

Yield: good

Reference: *10.1016/S0960-894X(01)00443-7* or *10.1002/jhet.5570390424* or *10.1055/s-2008-1072717* or *10.1002/ejoc.200801047* or *10.1016/0040-4020(95)00618-I* or *10.1021/acs.jmedchem.6b01694* or *10.3987/COM-92-6075*

Retrosynthesis ID: 10019874