Paths of analysis*

C59

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

*The results stated herein were generated using the proprietary platform owned and maintained by Grzybowski Scientific Inventions, Inc., a subsidiary of Merck KGaA, Darmstadt Germany. The results are provided on an as is basis, and shall be used solely in connection with the rights afforded in the license agreement and for no other purpose.

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: 245.70

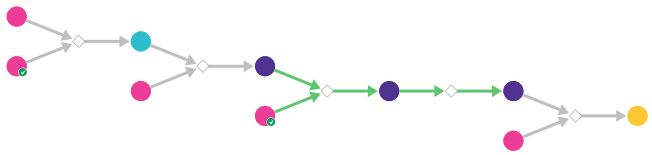
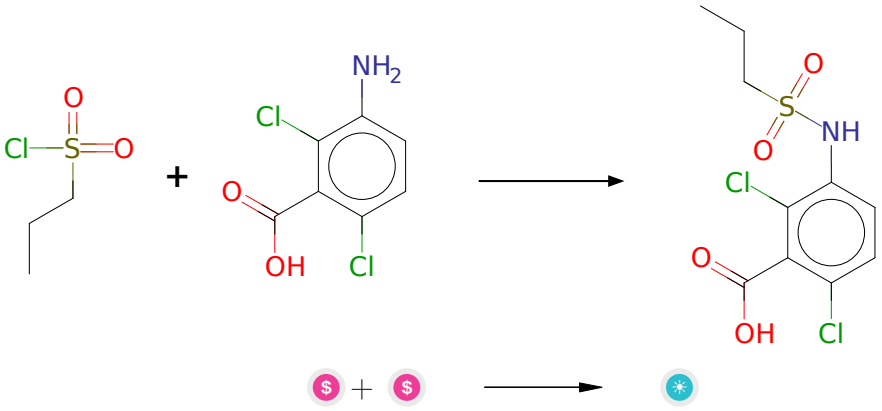


Figure 1: Outline of path 1

2.1.1 N-Sulfonylation



Substrates:

1. 3-Amino-2,6-dichlorobenzoic acid - *Combi-Blocks*
2. 1-Propanesulfonyl chloride - *available at Sigma-Aldrich*

Products:

1. C10H11Cl2NO4S

Typical conditions: THF.rt

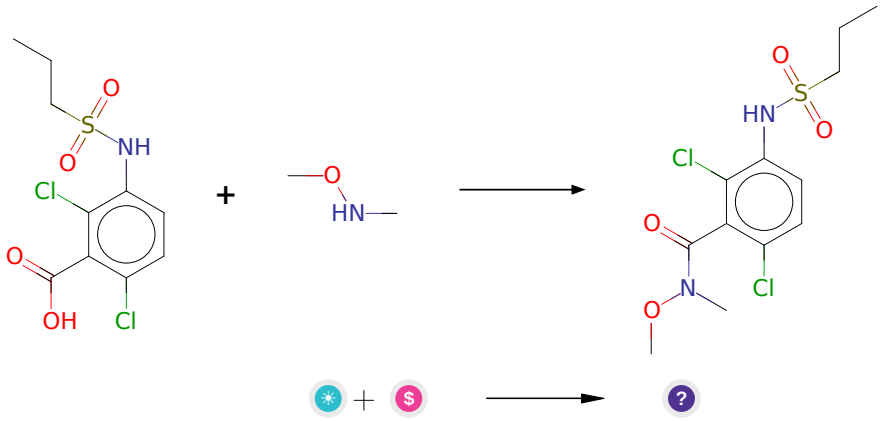
Protections: none

Yield: good

Reference: *10.1055/s-0029-1217565* and *10.1002/(SICI)1099-0690(199806)1998:6<945::AID-EJOC945>3.0.CO;2-3* and *10.1055/s-2001-14567* and *10.1016/j.bmc.2014.07.022*

Retrosynthesis ID: 14717

2.1.2 Synthesis of O-substituted N-substituted hydroxamic acids



Substrates:

1. C10H11Cl2NO4S
2. n-methoxymethylamine - *ChemImpexInternational*

Products:

1. CCCS(=O)(=O)Nc1ccc(Cl)c(C(=O)N(C)OC)c1Cl

Typical conditions: DCC.DMAP or CDI.TEA.DCM

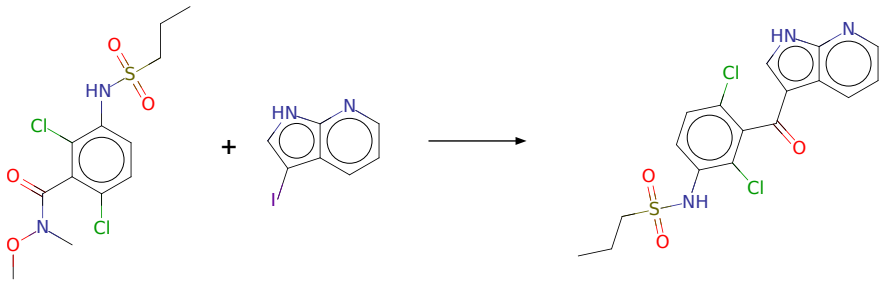
Protections: none

Yield: good

Reference: Patent: WO2007/67333A2, 2007 & *10.1016/j.bmcl.2008.09.100*

Retrosynthesis ID: 1152

2.1.3 Synthesis of ketones from Weinreb amides



Substrates:

1. 3-Iodo-7-azaindole - *available at Sigma-Aldrich*
2. CCCS(=O)(=O)Nc1ccc(Cl)c(C(=O)N(C)OC)c1Cl

Products:

1. CCCS(=O)(=O)Nc1ccc(Cl)c(C(=O)c2c[nH]c3ncccc23)c1Cl

Typical conditions: 1.RmgBr.THF 2.TFA.DCM

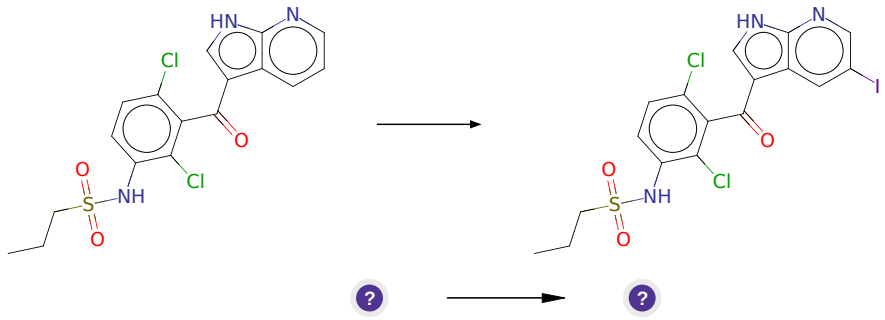
Protections: none

Yield: good

Reference: *10.1021/jm051185t* and *10.1021/ol101021v* (supporting info)

Retrosynthesis ID: 5060

2.1.4 Iodination of aromatic compounds



Substrates:

1. CCCS(=O)(=O)Nc1ccc(Cl)c(C(=O)c2c[nH]c3ncccc23)c1Cl

Products:

1. CCCS(=O)(=O)Nc1ccc(Cl)c(C(=O)c2c[nH]c3ncc(I)cc23)c1Cl

Typical conditions: I2 or other iodinating agent e.g. NIS

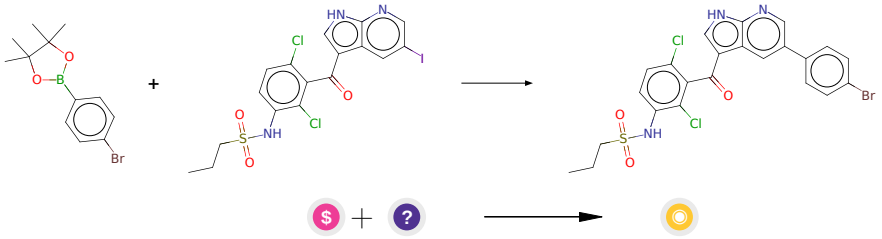
Protections: none

Yield: good

Reference: DOI: *10.1039/C5SC00964B* and *10.1016/j.tetlet.2005.05.117* and *10.1007/s11178-005-0256-1*

Retrosynthesis ID: 10697

2.1.5 Suzuki coupling of arylboronic acids pinacol esters with aryl iodides



Substrates:

1. 2-(4-Bromophenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane - *AOBChem*
2. CCCS(=O)(=O)Nc1ccc(Cl)c(C(=O)c2c[nH]c3ncc(I)cc23)c1Cl

Products:

1. CCCS(=O)(=O)Nc1ccc(Cl)c(C(=O)c2c[nH]c3ncc(-c4ccc(Br)cc4)cc23)c1Cl

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*

Retrosynthesis ID: 25152