Paths of analysis*

C55

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: 373.35

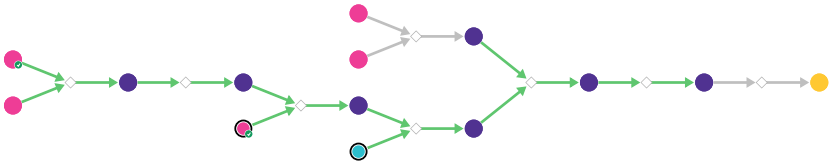
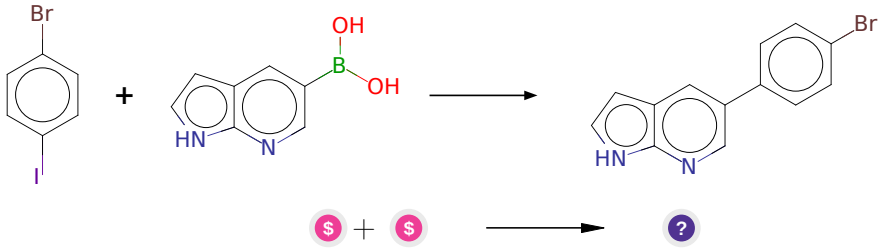


Figure 1: Outline of path 1

2.1.1 Suzuki coupling of arylboronic acids with aryl iodides



Substrates:

1. 1-Bromo-4-iodobenzene - *available at Sigma-Aldrich*
2. (1H-Pyrrolo[2,3-b]pyridin-5-yl)boronic acid - *Combi-Blocks*

Products:

1. Brc1ccc(-c2cnc3[nH]ccc3c2)cc1

Typical conditions: Pd catalyst.base.solvent

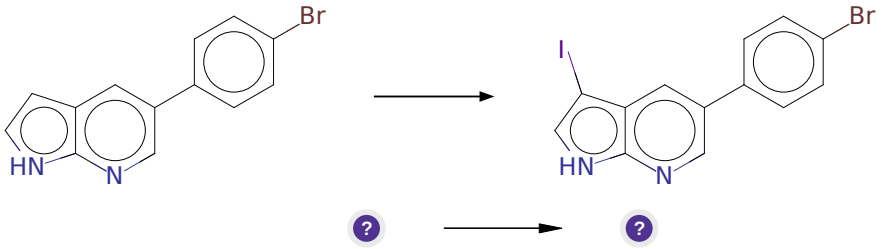
Protections: none

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: 25149

2.1.2 Iodination of aromatic compounds



Substrates:

1. Brc1ccc(-c2cnc3[nH]ccc3c2)cc1

Products:

1. Brc1ccc(-c2cnc3[nH]cc(I)c3c2)cc1

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

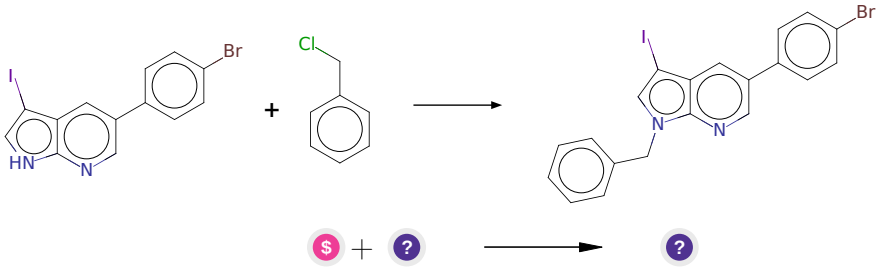
Protections: none

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

2.1.3 N-alkylation of Heterocycles



Substrates:

1. a-Chlorotoluene - *available at Sigma-Aldrich*

2. Brc1ccc(-c2cnc3[nH]cc(I)c3c2)cc1

Products:

1. Brc1ccc(-c2cnc3c(c2)c(I)cn3Cc2ccccc2)cc1

Typical conditions: NaH.DMF

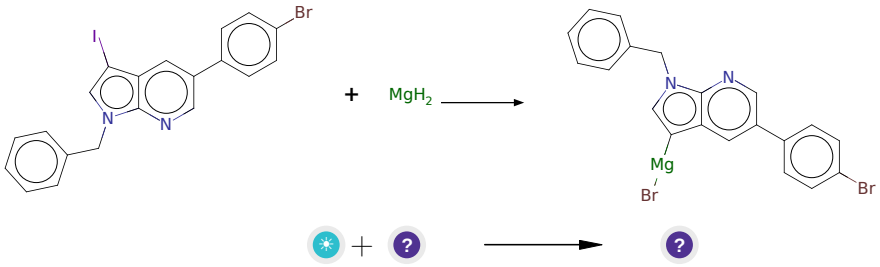
Protections: none

Yield: moderate

Reference: *10.1021/ol503625z* and *10.1081/SCC-120022467* (experimental) and *10.1021/ol2018328* (SI, p.5) and *10.1021/jo8026565* (SI, p.2)

Retrosynthesis ID: 28538

2.1.4 Synthesis of aryl Grignard reagents



Substrates:

1. magnesium
2. Brc1ccc(-c2cnc3c(c2)c(I)cn3Cc2ccccc2)cc1

Products:

1. Br[Mg]c1cn(Cc2ccccc2)c2ncc(-c3ccc(Br)cc3)cc12

Typical conditions: iPrMgCl.LiCl.THF or other conditions Mg.THF or tBuLi.MgBr2

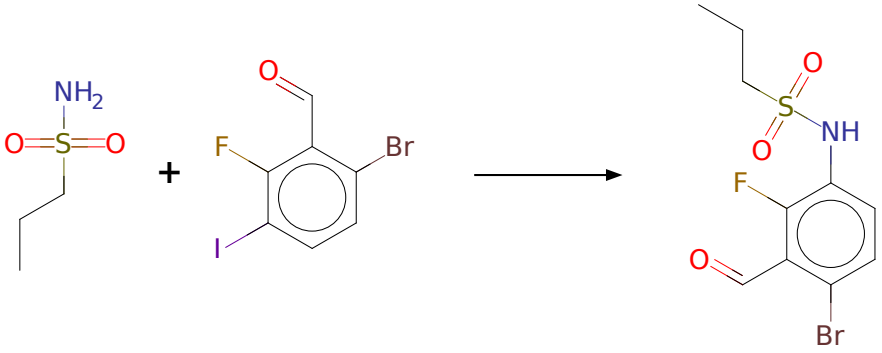
Protections: none

Yield: moderate

Reference: DOI: *10.1016/S0040-4039(99)01404-5* and *10.1021/jo0000574* and WO2014123793 p.137 and *10.1021/jm400491x* and *10.3762/bjoc.12.36*

Retrosynthesis ID: 10011460

2.1.5 Arylation of sulfonamides with aryl iodides



Substrates:

1. 6-Bromo-2-fluoro-3-iodobenzaldehyde - *AOBChem*
2. Propane-1-sulfonamide - *Combi-Blocks*

Products:

1. CCCS(=O)(=O)Nc1ccc(Br)c(C=O)c1F

Typical conditions: Cu.salt.diamine.base.DMF.heat

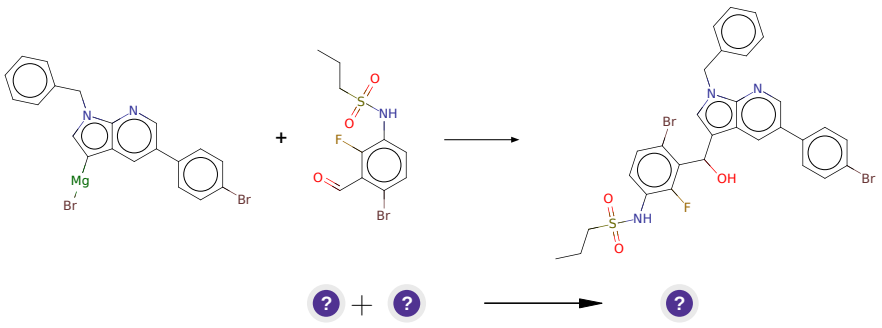
Protections: none

Yield: good

Reference: *10.1016/j.tetlet.2006.04.041* and *10.1016/j.tetlet.2011.10.113* and *10.1016/j.tetlet.2005.08.149* and *10.1021/ol035942y* and *10.1021/acs.jmedchem.6b00685*

Retrosynthesis ID: 10012567

2.1.6 Grignard-Type Reaction



Substrates:

1. Br[Mg]c1cn(Cc2ccccc2)c2ncc(-c3ccc(Br)cc3)cc12
2. CCCS(=O)(=O)Nc1ccc(Br)c(C=O)c1F

Products:

1. CCCS(=O)(=O)Nc1ccc(Br)c(C(O)c2cn(Cc3ccccc3)c3ncc(-c4ccc(Br)cc4)cc23)c1F

Typical conditions: Mg or Li.ether

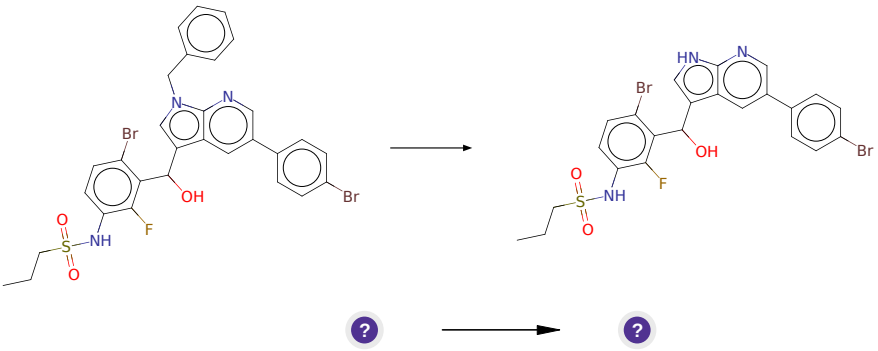
Protections: none

Yield: good

Reference: *10.1055/s-0030-1260809* or *10.1021/jm061429p* or *10.1021/jo0621423* or *10.1021/ja00373a036* or *10.1016/S0040-4020(01)00457-4*

Retrosynthesis ID: 25123

2.1.7 N-debenzylation of indoles



Substrates:

1. CCCS(=O)(=O)Nc1ccc(Br)c(C(O)c2cn(Cc3ccccc3)c3ncc(-c4ccc(Br)cc4)cc23)c1F

Products:

1. CCCS(=O)(=O)Nc1ccc(Br)c(C(O)c2c[nH]c3ncc(-c4ccc(Br)cc4)cc23)c1F

Typical conditions: Na.NH3

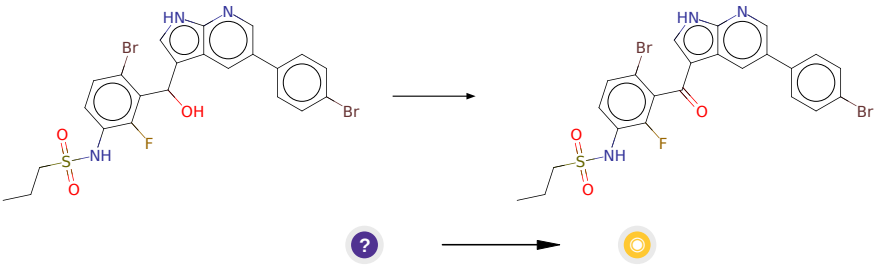
Protections: none

Yield: good

Reference: DOI: *10.1021/jo0110597*

Retrosynthesis ID: 356

2.1.8 Parikh-Doering Oxidation



Substrates:

1. CCCS(=O)(=O)Nc1ccc(Br)c(C(O)c2c[nH]c3ncc(-c4ccc(Br)cc4)cc23)c1F

Products:

1. CCCS(=O)(=O)Nc1ccc(Br)c(C(=O)c2c[nH]c3ncc(-c4ccc(Br)cc4)cc23)c1F

Typical conditions: DMSO. sulfur trioxide pyridine complex. NEt3

Protections: none

Yield: good

Reference: *10.1021/ja00997a067*

Retrosynthesis ID: 10257