Paths of analysis*

C136

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: 96.57

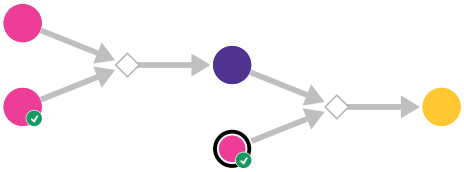
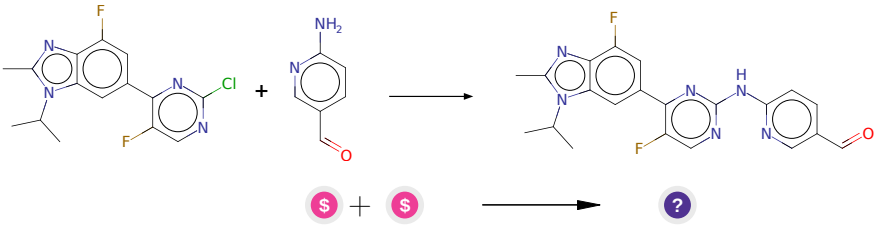


Figure 1: Outline of path 1

2.1.1 Amination of aryl chlorides



Substrates:

1. 6-Aminonicotinaldehyde - *Combi-Blocks*
2. 6-(2-Chloro-5-fluoropyrimidin-4-yl)-4-fluoro-1-isopropyl-2-methyl-1H-benzo[d]imidazole - *available at Sigma-Aldrich*

Products:

1. Cc1nc2c(F)cc(-c3nc(Nc4ccc(C=O)cn4)ncc3F)cc2n1C(C)C

Typical conditions: [Pd].Ligand.base

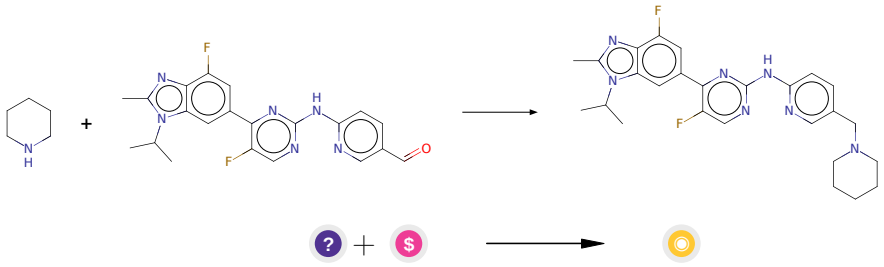
Protections: none

Yield: good

Reference: *10.1021/ja903049z* and *10.1021/jo060945k* and *10.1021/jo060190h* and *10.1021/ja8055358* and *10.1021/ja068926f* and *10.1002/anie.200601612* and *10.1021/acscatal.0c04280*

Retrosynthesis ID: 28545

2.1.2 Reductive Amination of Aldehydes with Secondary Amines



Substrates:

1. Cc1nc2c(F)cc(-c3nc(Nc4ccc(C=O)cn4)ncc3F)cc2n1C(C)C
2. Piperidine - *available at Sigma-Aldrich*

Products:

1. Cc1nc2c(F)cc(-c3nc(Nc4ccc(CN5CCCCC5)cn4)ncc3F)cc2n1C(C)C

Typical conditions: NaBH(OAc)3 or NaBH3CN

Protections: none

Yield: good

Reference: DOI: *10.1021/jo960057x* and *10.1021/jm7009292* and *10.1073/pnas.1405685111* and *10.1002/ejoc.201101063* and *10.1038/ja.2017.61* and *10.1021/jm4013906*

Retrosynthesis ID: 10019705