Paths of analysis*

C68

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: 88.21

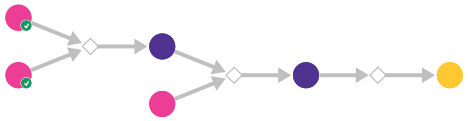
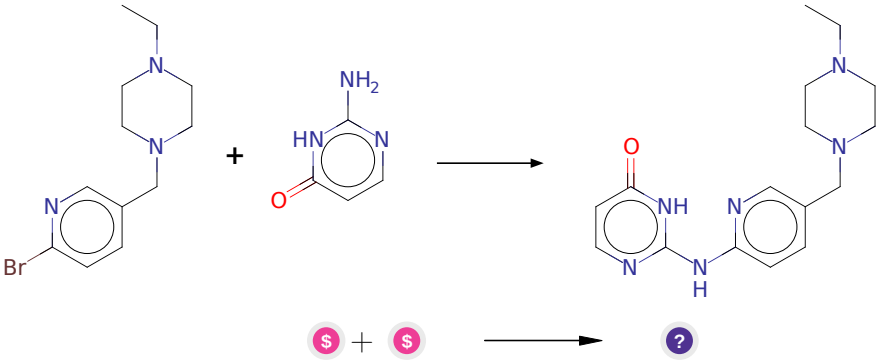


Figure 1: Outline of path 1

2.1.1 Buchwald-Hartwig amination



Substrates:

1. Isocytosine - *available at Sigma-Aldrich*
2. 1-((6-Bromopyridin-3-yl)methyl)-4-ethylpiperazine - *available at Sigma-Aldrich*

Products:

1. CCN1CCN(Cc2ccc(Nc3nccc(=O)[nH]3)nc2)CC1

Typical conditions: Pd(cat).toluene.100C.K2CO3

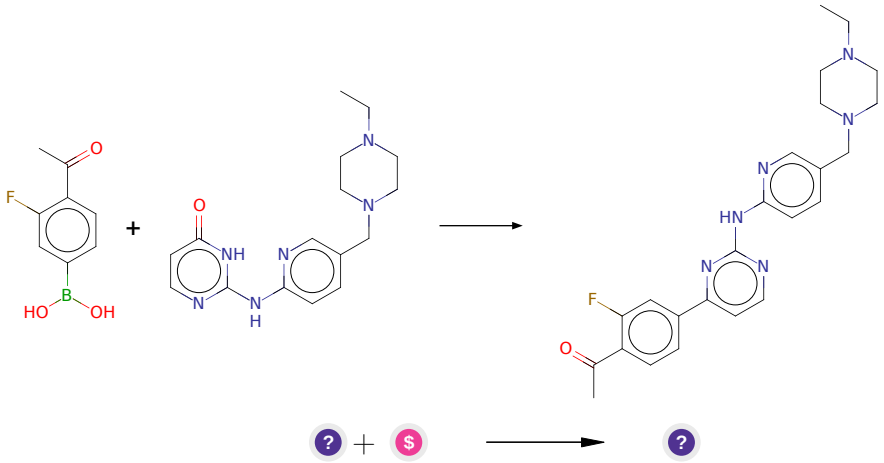
Protections: none

Yield: good

Reference: *10.1021/acs.oprd.9b00161* and *10.1002/anie.201904795* and *10.1021/acs.chemrev.6b00512*

Retrosynthesis ID: 31017518

2.1.2 Suzuki coupling



Substrates:

1. CCN1CCN(Cc2ccc(Nc3nccc(=O)[nH]3)nc2)CC1
2. 4-Acetyl-3-fluorophenylboronic acid - *AOBChem*

Products:

1. CCN1CCN(Cc2ccc(Nc3nccc(-c4ccc(C(C)=O)c(F)c4)n3)nc2)CC1

Typical conditions: 1.PyBroP.Et3N.dioxane.rt.2h.2.PhB(OH)2.[Pd]

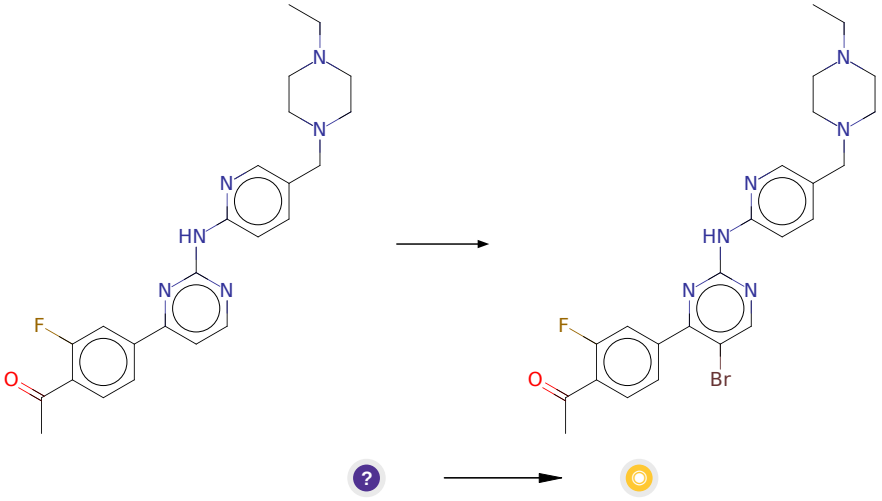
Protections: none

Yield: good

Reference: *10.1055/s-0031-1290826*

Retrosynthesis ID: 4774

2.1.3 Bromination of aromatic compounds



Substrates:

1. CCN1CCN(Cc2ccc(Nc3nccc(-c4ccc(C(C)=O)c(F)c4)n3)nc2)CC1

Products:

1. CCN1CCN(Cc2ccc(Nc3ncc(Br)c(-c4ccc(C(C)=O)c(F)c4)n3)nc2)CC1

Typical conditions: Br2.Fe

Protections: none

Yield: good

Reference: *10.1021/acs.accounts.6b00120*

Retrosynthesis ID: 7777000