Paths of analysis*

C124

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: 160.73

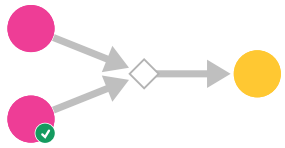
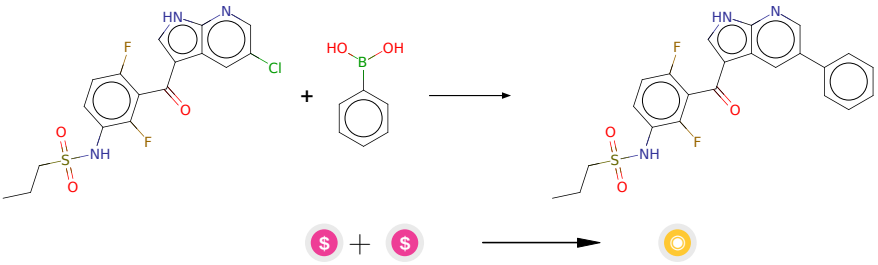


Figure 1: Outline of path 1

2.1.1 Suzuki coupling with aryl chlorides



Substrates:

1. N-[3-[(5-Chloro-1H-pyrrolo[2,3-b]pyridin-3-yl)carbonyl]-2,4-difluorophenyl]-1-propanesulfonamide - *AstaTech*
2. Phenylboric acid - *available at Sigma-Aldrich*

Products:

1. CCCS(=O)(=O)Nc1ccc(F)c(C(=O)c2c[nH]c3ncc(-c4ccccc4)cc23)c1F

Typical conditions: [Pd].catalyst.base.

Protections: none

Yield: good

Reference: *10.1002/anie.201108608* and *10.1002/anie.200801465* and *10.1055/s-0033-1338293* and *10.1039/c1cc10708a* and *10.1055/s-0030-1260169* and *10.1016/j.tet.2005.05.071* and *10.1038/s41929-020-00564-z* (metal-free coupling)

Retrosynthesis ID: 26284