Paths of analysis*

Analysis 2

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: 59.03

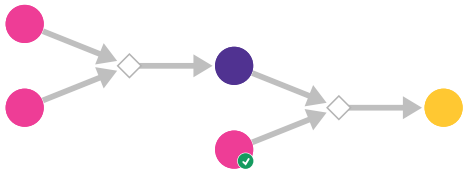
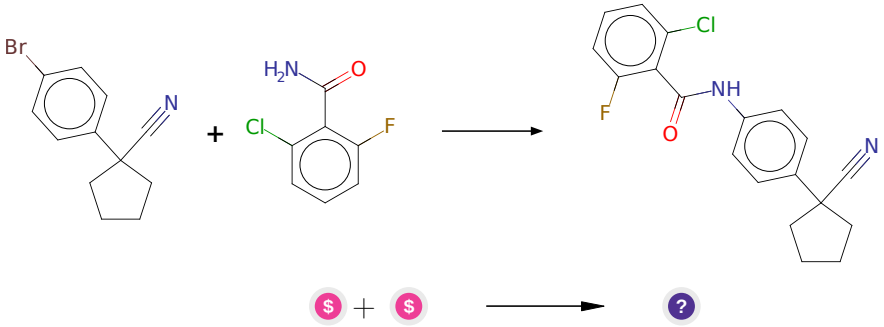


Figure 1: Outline of path 1

2.1.1 Arylation of amides with aryl bromides



Substrates:

1. 1-(4-bromophenyl)cyclopentanecarbonitrile - *Combi-Blocks*
2. 2-Chloro-6-fluorobenzamide 1g pack - *Combi-Blocks*

Products:

1. N#CC1(c2ccc(NC(=O)c3c(F)cccc3Cl)cc2)CCCC1

Typical conditions: Base.[Pd].catalyst.dioxane.heat or CuI.diamine.base.DMF.heat

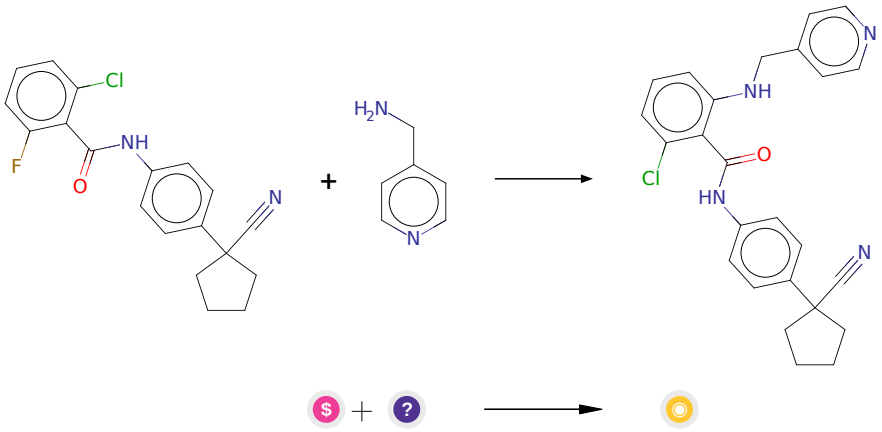
Protections: none

Yield: good

Reference: *10.1021/ja0717414* and *10.1080/00397911.2016.1195844* and *10.1055/s-0035-1560473* and *10.3390/molecules190913448*

Retrosynthesis ID: 10012553

2.1.2 Nucleophilic aromatic substitution



Substrates:

1. 4-Picolylamine - *available at Sigma-Aldrich*
2. N#CC1(c2ccc(NC(=O)c3c(F)cccc3Cl)cc2)CCCC1

Products:

1. N#CC1(c2ccc(NC(=O)c3c(Cl)cccc3NCc3ccncc3)cc2)CCCC1

Typical conditions: Solvent

Protections: none

Yield: good

Reference: *10.1002/9781118093559.ch4*

Retrosynthesis ID: 49476