Paths of analysis*

Analysis 10

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: 79.69

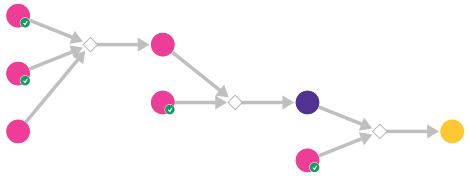
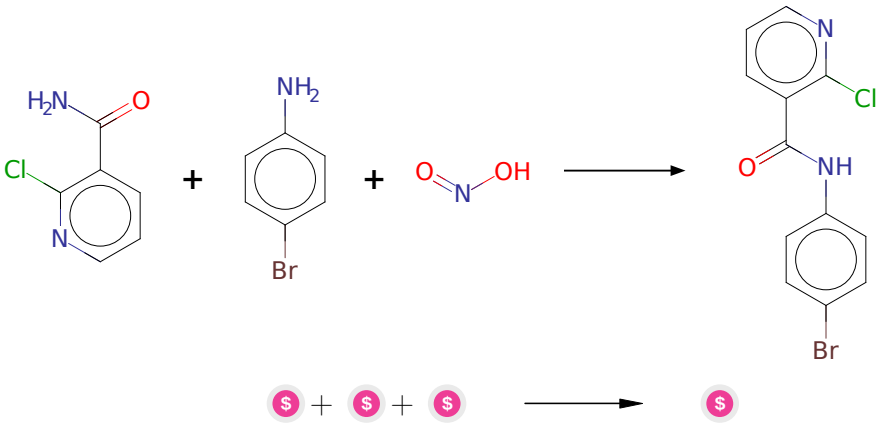


Figure 1: Outline of path 1

2.1.1 Synthesis of N-arylamides from arenediazonium salts



Substrates:

1. 4-Bromoaniline - *available at Sigma-Aldrich*
2. Calcium nitrite solution - *available at Sigma-Aldrich*
3. 2-Chloronicotinamide - *Combi-Blocks*

Products:

1. n-(4-bromo-phenyl)-2-chloro-nicotinamide - *Enamine*

Typical conditions: 1) HCl.NaNO2 2) CuI.TBAI.N,N'-dimethylethane-1,2-diamine.K2CO3.DMSO.110C

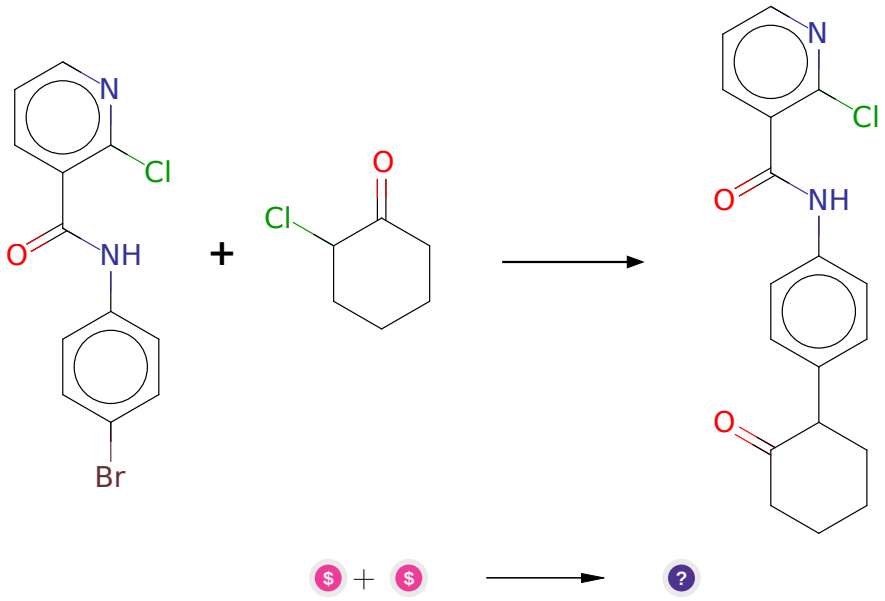
Protections: none

Yield: moderate

Reference: DOI: *10.1055/s-0034-1378556*

Retrosynthesis ID: 1922

2.1.2 Photoredox Cross-Electrophile Coupling of alpha-Chloro Carbonyls with Aryl Halides



Substrates:

1. n-(4-bromo-phenyl)-2-chloro-nicotinamide - *Enamine*
2. 2-Chlorocyclohexanone - *available at Sigma-Aldrich*

Products:

1. O=C(Nc1ccc(C2CCCCC2=O)cc1)c1cccnc1Cl

Typical conditions: [Ir]-photocat.[Ni]-cat.silane reagent.base.blue light

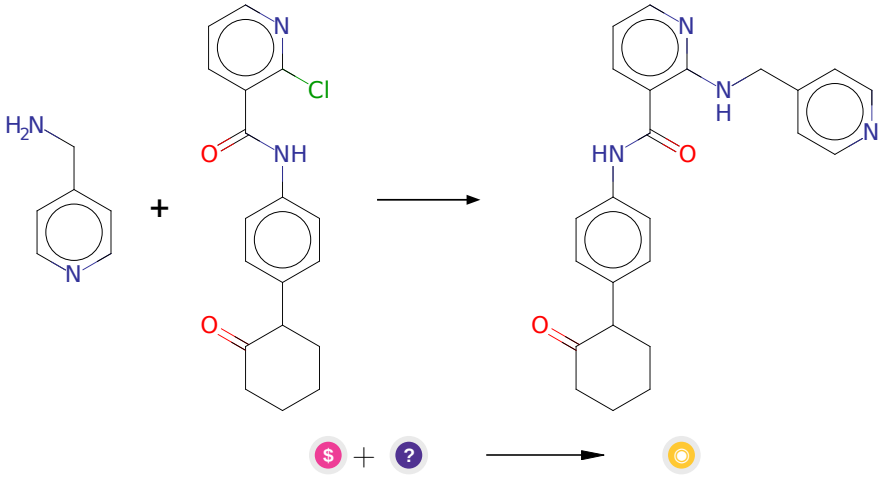
Protections: none

Yield: good

Reference: *10.1002/anie.201909072*

Retrosynthesis ID: 31016951

2.1.3 Nucleophilic aromatic substitution



Substrates:

1. 4-Picolylamine - *available at Sigma-Aldrich*
2. O=C(Nc1ccc(C2CCCCC2=O)cc1)c1cccnc1Cl

Products:

1. O=C(Nc1ccc(C2CCCCC2=O)cc1)c1cccnc1NCc1ccncc1

Typical conditions: solvent. Heating or pressure

Protections: none

Yield: good

Reference: *10.1021/jm00040a009* or *10.1111/bph.12233* or *10.1246/cl.1987.1187*

Retrosynthesis ID: 5003