Paths of analysis*

Analysis 5

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: 78.53

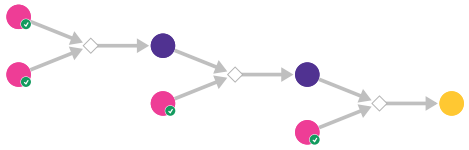
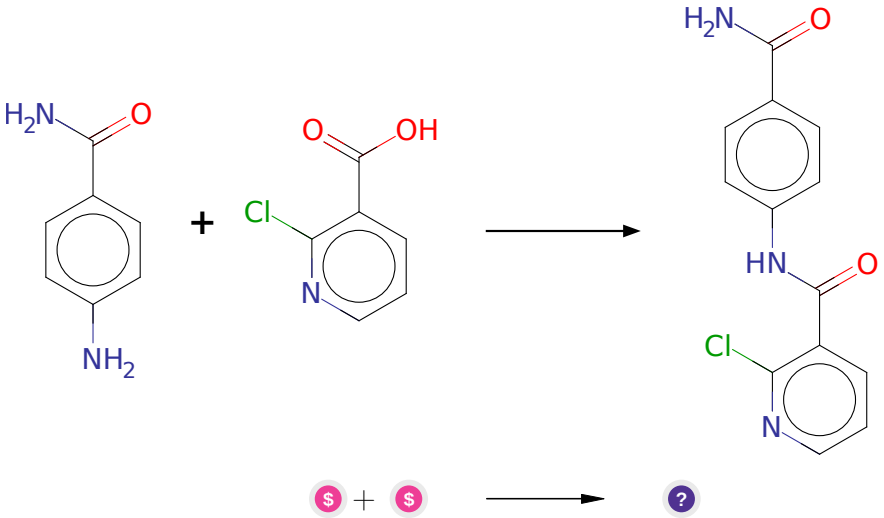


Figure 1: Outline of path 1

2.1.1 Amide coupling



Substrates:

1. 4-Aminobenzamide - *available at Sigma-Aldrich*
2. 2-Chloronicotinic acid - *available at Sigma-Aldrich*

Products:

1. NC(=O)c1ccc(NC(=O)c2cccnc2Cl)cc1

Typical conditions: DCC.DCM or EDC.DCM or SOCl2.DCM

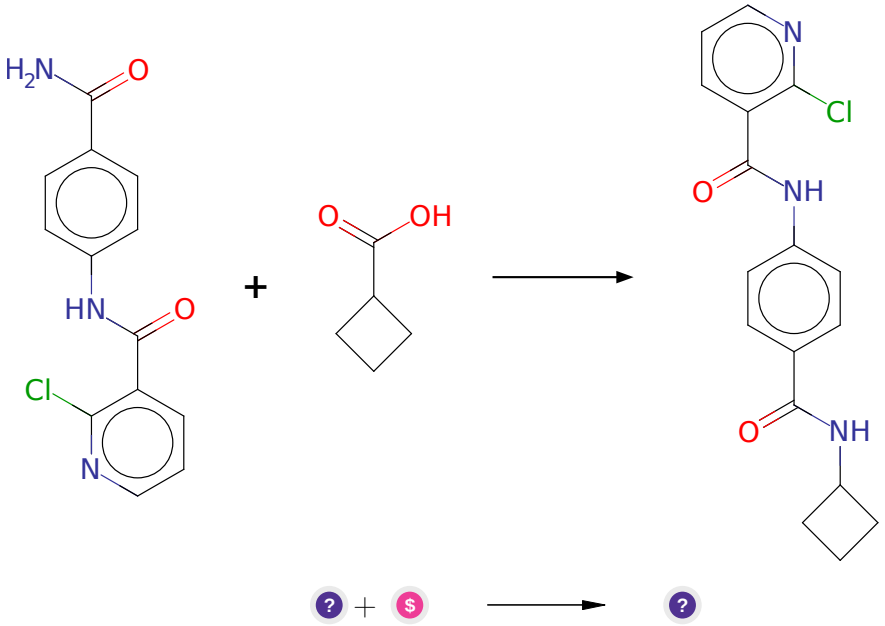
Protections: none

Yield: good

Reference: *10.1021/cr100048w* and *10.1039/B701677H* and *10.1039/C5RA24527C* and *10.3727/000000006783981206* and *10.1021/np060007f* and *10.1021/jo00012a058* and *10.1016/j.bmcl.2007.08.037* and *10.1039/C0OB00355G* and *10.1021/jm500031w* (p.3056) and *10.1016/j.tet.2011.03.046*

Retrosynthesis ID: 28548

2.1.2 Decarboxylative sp3 C-N coupling using photoredox catalysis of Aromatic Carboxylic acids



Substrates:

1. NC(=O)c1ccc(NC(=O)c2cccnc2Cl)cc1
2. Cyclobutanecarboxylic acid - *available at Sigma-Aldrich*

Products:

1. O=C(NC1CCC1)c1ccc(NC(=O)c2cccnc2Cl)cc1

Typical conditions: 1.MesI(OAc)2 2.[Ir]-photocatalyst.[Cu]-photocatalyst.Bphen.BTMG.Dioxane.Blue Led.rt

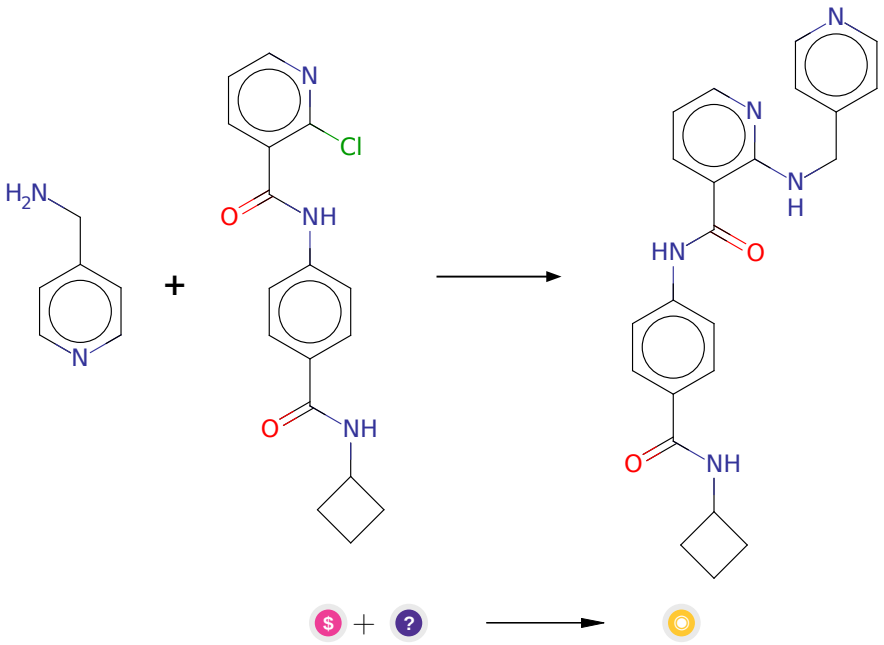
Protections: none

Yield: good

Reference: *10.1038/s41586-018-0234-8*

Retrosynthesis ID: 10029980

2.1.3 Nucleophilic aromatic substitution



Substrates:

1. 4-Picolylamine - *available at Sigma-Aldrich*
2. O=C(NC1CCC1)c1ccc(NC(=O)c2cccnc2Cl)cc1

Products:

1. O=C(NC1CCC1)c1ccc(NC(=O)c2cccnc2NCc2ccncc2)cc1

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