Paths of analysis*

Analysis 3

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

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: `121.03`

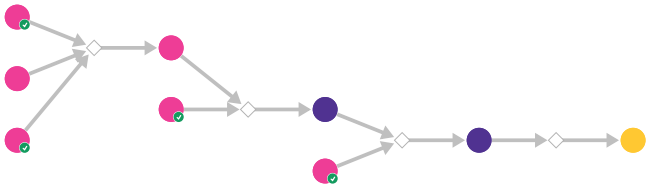
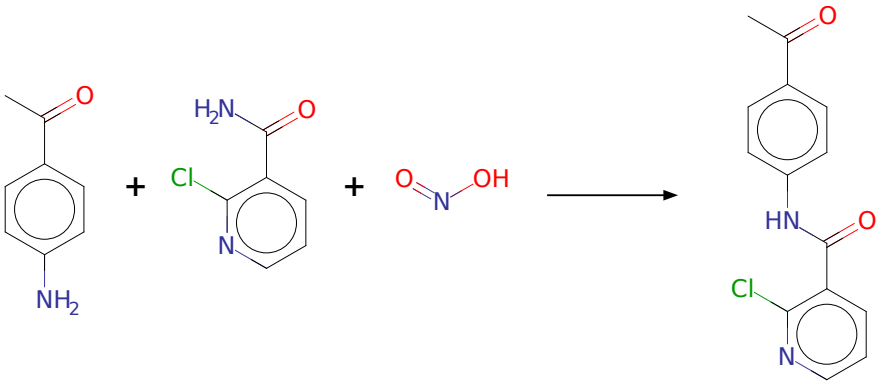


Figure 1: Outline of path 1

2.1.1 Synthesis of N-arylamides from arenediazonium salts



Substrates:

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

Products:

1. n-(4-acetylphenyl)-2-chloronicotinamide - *Vitas-MLaboratory*

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

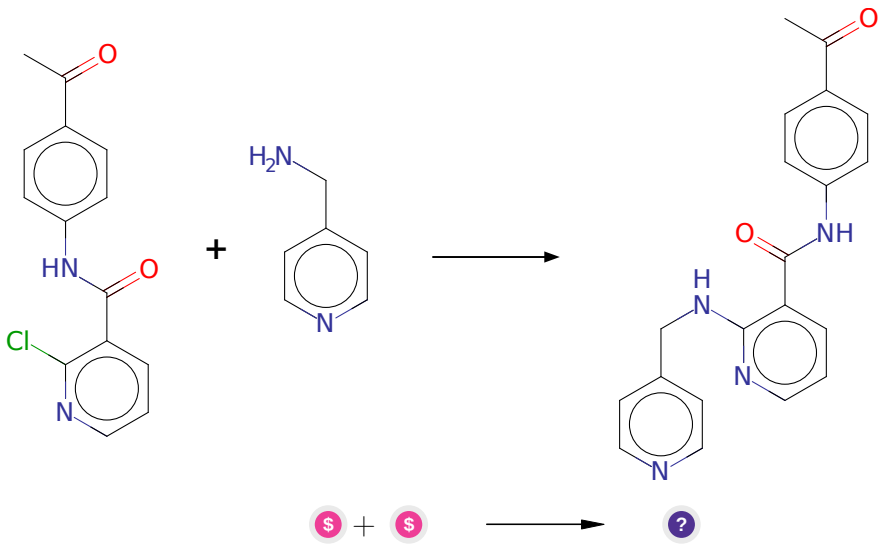
Protections: none

Yield: moderate

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

Retrosynthesis ID: 1922

2.1.2 Nucleophilic aromatic substitution



Substrates:

1. 4-Picolylamine - *available at Sigma-Aldrich*
2. n-(4-acetylphenyl)-2-chloronicotinamide - *Vitas-MLaboratory*

Products:

1. CC(=O)c1ccc(NC(=O)c2cccnc2NCc2ccncc2)cc1

Typical conditions: solvent. Heating or pressure

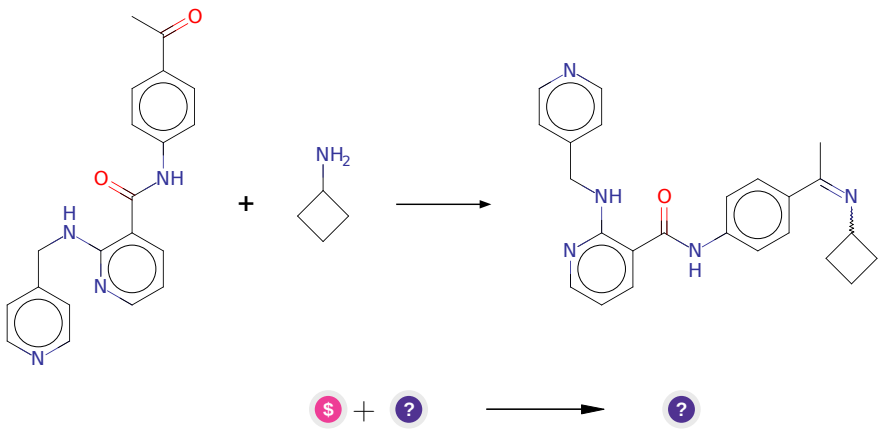
Protections: none

Yield: good

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

Retrosynthesis ID: 5003

2.1.3 Synthesis of imines



Substrates:

1. Cyclobutylamine - *available at Sigma-Aldrich*
2. CC(=O)c1ccc(NC(=O)c2cccnc2NCc2ccncc2)cc1

Products:

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

Typical conditions: pyridine.Na2SO4.DCM

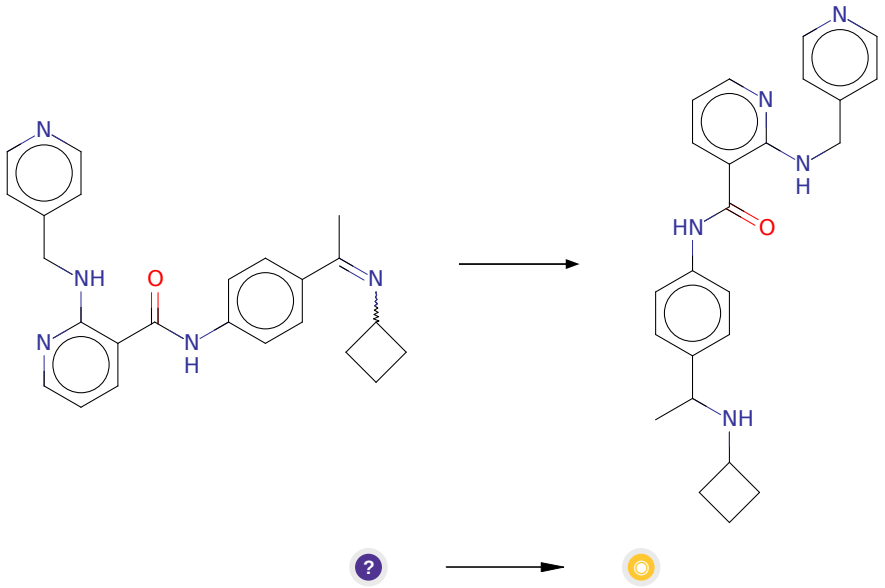
Protections: none

Yield: moderate

Reference: *10.1016/j.tet.2011.04.083* AND *10.1016/j.tet.2015.05.090* AND *10.1021/cc100084b* AND *10.3390/molecules20047245* AND *10.1016/j.tet.2011.12.005*

Retrosynthesis ID: 14699

2.1.4 Reduction of imines to amines



Substrates:

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

Products:

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

Typical conditions: NaBH3CN.AcOH

Protections: none

Yield: good

Reference: *10.1080/00397918908050701* AND *10.1016/S0040-4039(01)00219-2* AND *10.1016/S0040-4039(02)01905-6* AND *10.1002/ejoc.200901312* AND *10.1021/ja903319r* AND *10.1021/jo061140f*

Retrosynthesis ID: 14656