Paths of analysis*

Analysis 1

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: 147.98

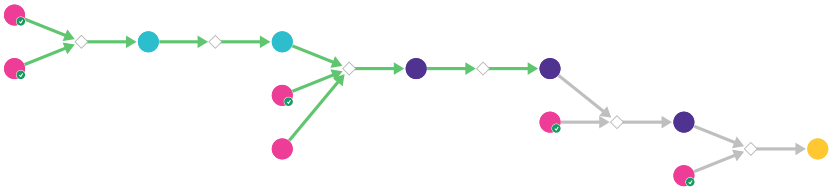
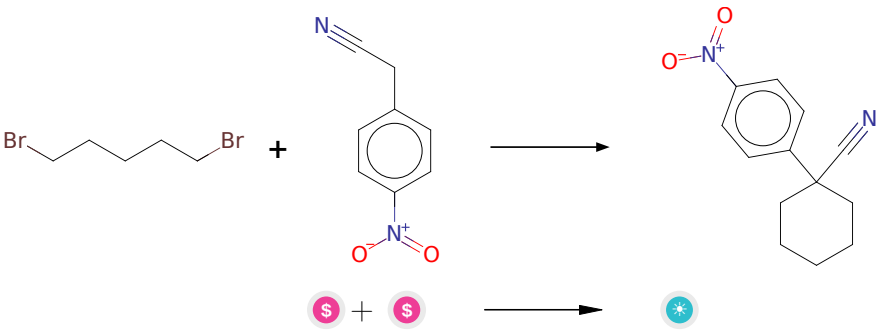


Figure 1: Outline of path 1

2.1.1 Dialkylation of nitrile



Substrates:

1. 4-Nitrobenzyl cyanide - *available at Sigma-Aldrich*
2. 1,5-Dibromopentane - *available at Sigma-Aldrich*

Products:

1. 1-(4-nitro-phenyl)-cyclohexan-carbonitril-(1)

Typical conditions: CsCO3.DMF

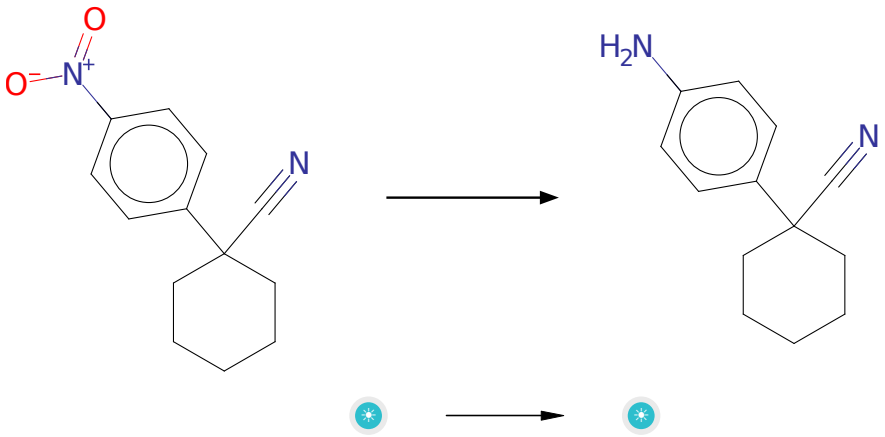
Protections: none

Yield: good

Reference: *10.1016/S0960-894X(98)00748-3* and *10.1016/j.tetasy.2012.02.021* and *10.1002/chem.201100305*

Retrosynthesis ID: 28568

2.1.2 Palladium-catalyzed reduction of nitro group



Substrates:

1. 1-(4-nitro-phenyl)-cyclohexan-carbonitril-(1)

Products:

1. C13H16N2

Typical conditions: H2.Pd/C

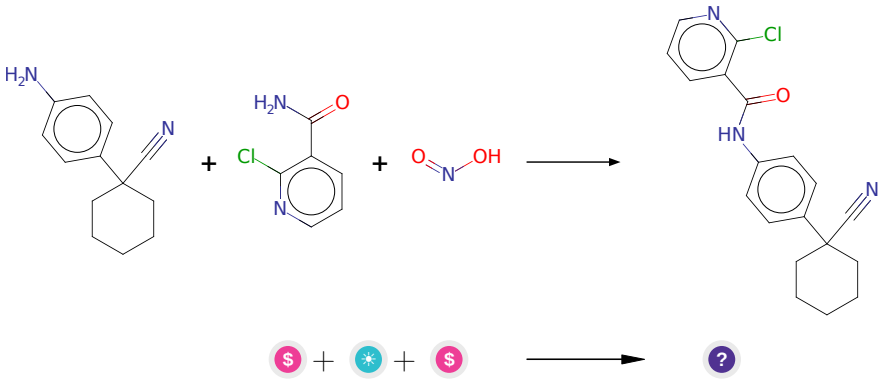
Protections: none

Yield: good

Reference: DOI: *10.1002/anie.200501738* and *10.1002/anie.200352175* and *10.1016/j.tetlet.2015.05.004* and *10.3390/molecules13061427* and *10.1016/S0968-0896(03)00459-0*

Retrosynthesis ID: 29908

2.1.3 Synthesis of N-arylamides from arenediazonium salts



Substrates:

1. Calcium nitrite solution - *available at Sigma-Aldrich*
2. C13H16N2
3. 2-Chloronicotinamide - *Combi-Blocks*

Products:

1. N#CC1(c2ccc(NC(=O)c3cccnc3Cl)cc2)CCCCC1

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

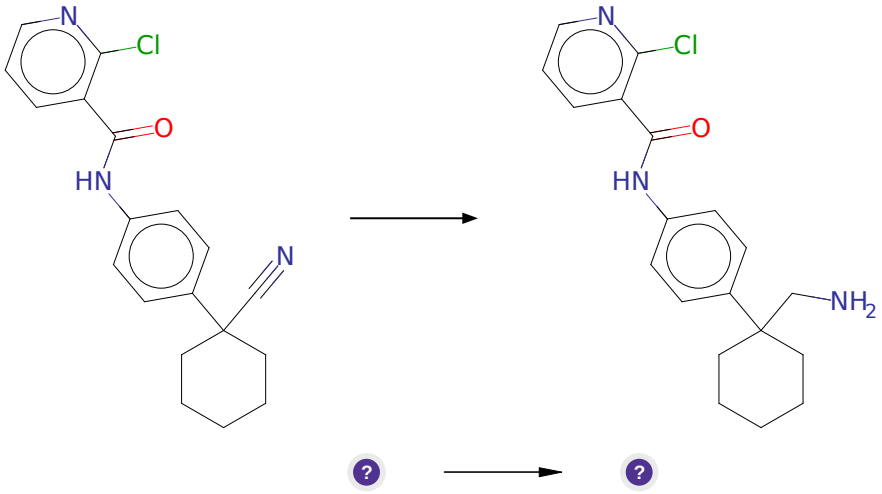
Protections: none

Yield: moderate

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

Retrosynthesis ID: 1922

2.1.4 Reduction of cyanides to amines



Substrates:

1. N#CC1(c2ccc(NC(=O)c3cccnc3Cl)cc2)CCCCC1

Products:

1. NCC1(c2ccc(NC(=O)c3cccnc3Cl)cc2)CCCCC1

Typical conditions: CoCl2.NaBH4

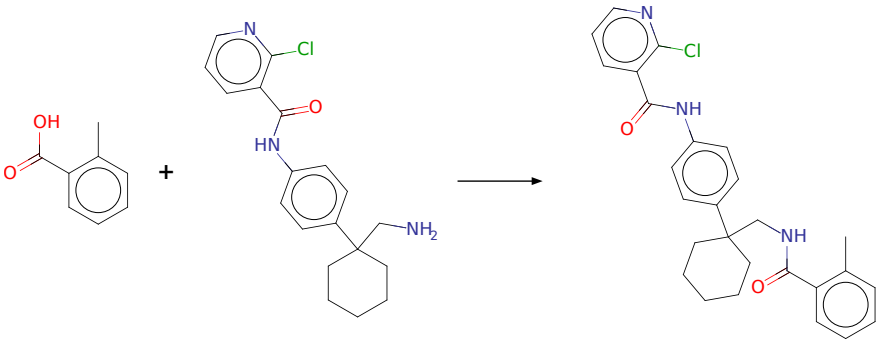
Protections: none

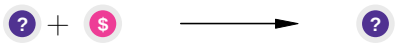
Yield: good

Reference: *10.1021/ol202535f*

Retrosynthesis ID: 9900034

2.1.5 Amide coupling





Substrates:

1. NCC1(c2ccc(NC(=O)c3cccnc3Cl)cc2)CCCCC1
2. o-Toluic acid - *available at Sigma-Aldrich*

Products:

1. Cc1ccccc1C(=O)NCC1(c2ccc(NC(=O)c3cccnc3Cl)cc2)CCCCC1

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

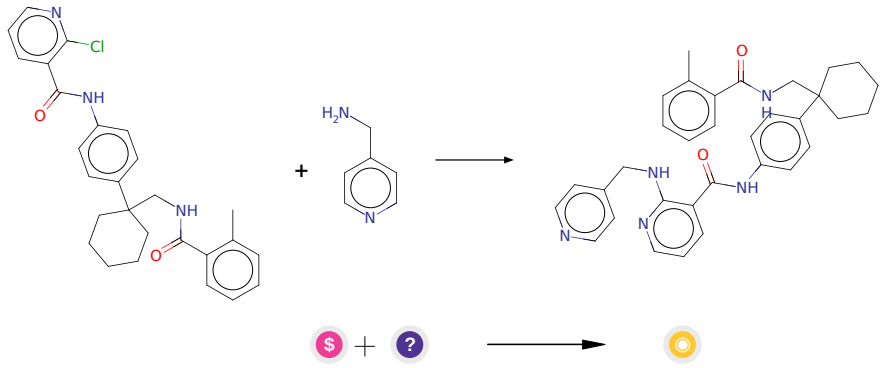
Protections: none

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: 10087

2.1.6 Nucleophilic aromatic substitution



Substrates:

1. 4-Picolylamine - *available at Sigma-Aldrich*
2. Cc1ccccc1C(=O)NCC1(c2ccc(NC(=O)c3cccnc3Cl)cc2)CCCCC1

Products:

1. Cc1ccccc1C(=O)NCC1(c2ccc(NC(=O)c3cccnc3NCc3ccncc3)cc2)CCCCC1

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