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

*The results stated herein were generated using the proprietary platform owned and maintained by Grzybowski Scientific Inventions, Inc., a subsidiary of Merck KGaA, Darmstadt Germany. The results are provided on an as is basis, and shall be used solely in connection with the rights afforded in the license agreement and for no other purpose.

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: 77.91

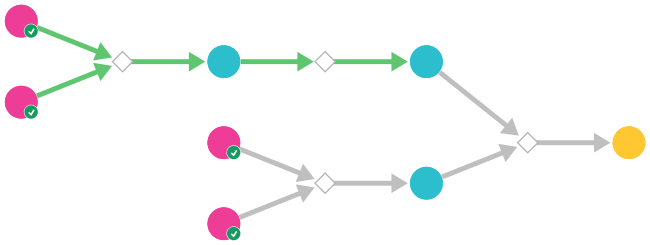
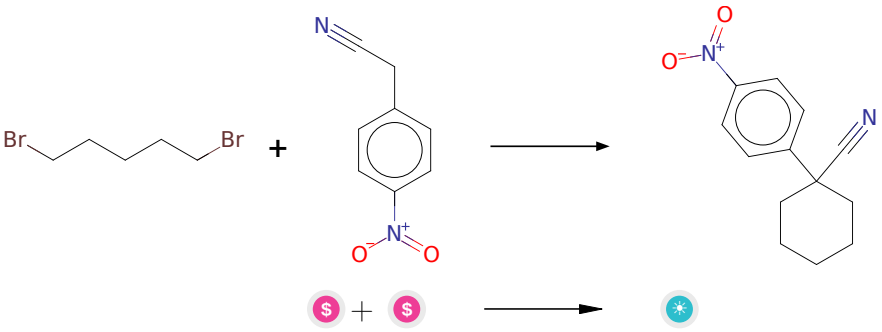


Figure 1: Outline of path 1

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

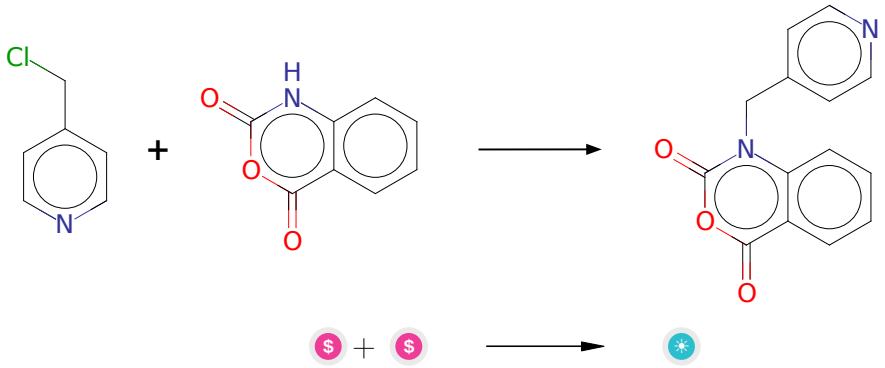
Protections: none

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 N-alkylation of Heterocycles



Substrates:

1. Isatoic anhydride - *available at Sigma-Aldrich*
2. 4-Picolyl chloride hydrochloride - *available at Sigma-Aldrich*

Products:

1. 1-pyridin-4-ylmethyl-1h-benzo[d][1,3]oxazine-2,4-dione

Typical conditions: NaH.DMF

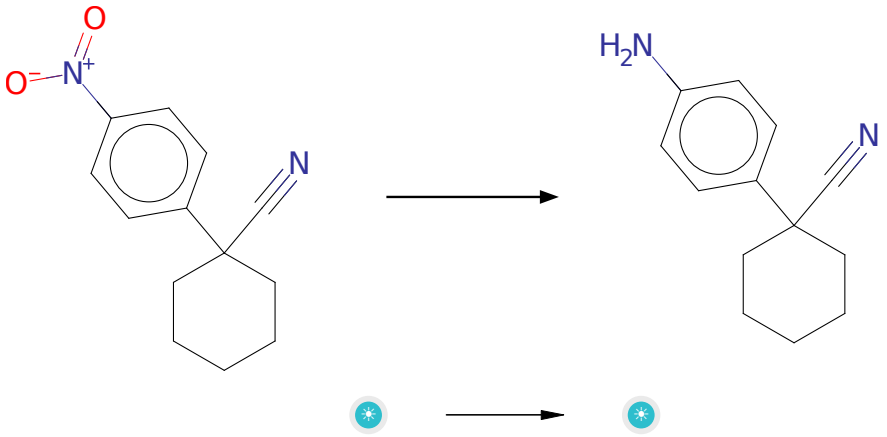
Protections: none

Yield: moderate

Reference: *10.1021/ol503625z* and *10.1081/SCC-120022467* (experimental) and *10.1021/ol2018328* (SI, p.5) and *10.1021/jo8026565* (SI, p.2)

Retrosynthesis ID: 28538

2.1.3 Reduction of nitro group



Substrates:

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

Products:

1. C13H16N2

Typical conditions: Zn. aq NH4. EtOH //Zn.Hcl

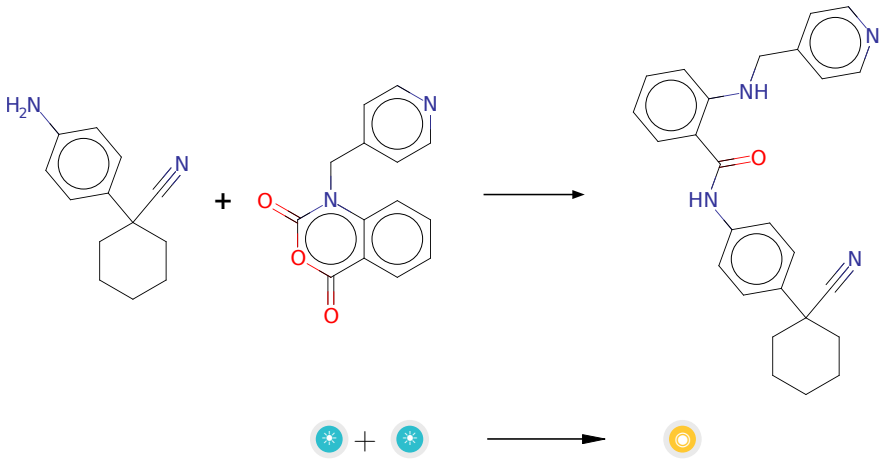
Protections: none

Yield: good

Reference: DOI: *10.1002/anie.201512005* and *10.1002/anie.201104681* and *10.3390/molecules17055497* and *10.3390/molecules19022655* and *10.1021/ol5033464* (SI,page 3) and *10.5012/bkcs.2013.34.4.1275*

Retrosynthesis ID: 6145

2.1.4 Acylation of amines by oxazolidine-2,4-dion



Substrates:

1. 1-pyridin-4-ylmethyl-1h-benzo[d][1,3]oxazine-2,4-dione
2. C13H16N2

Products:

1. N#CC1(c2ccc(NC(=O)c3ccccc3NCc3ccncc3)cc2)CCCCC1

Typical conditions: amine.K2CO3.DMF.heating

Protections: none

Yield: good

Reference: *10.1016/j.tetlet.2012.03.060* and *10.1055/s-2000-6252* and *10.1021/ja01560a041* and WO2015/189108 A1

Retrosynthesis ID: 23674