Paths of analysis*

C40

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: 450.50

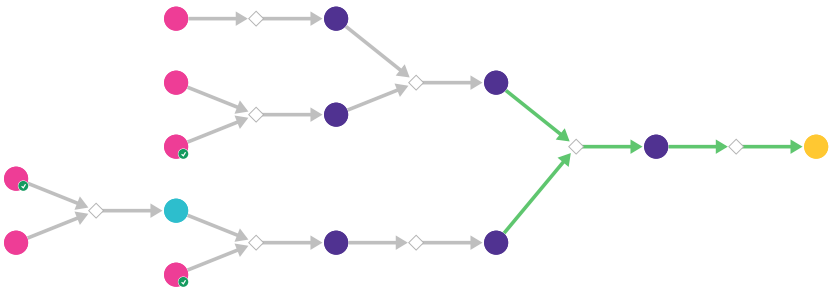
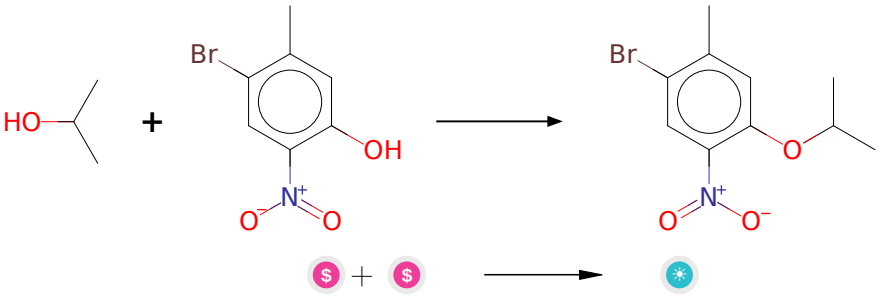


Figure 1: Outline of path 1

2.1.1 Mitsunobu reaction



Substrates:

1. 2-Propanol - *available at Sigma-Aldrich*
2. 4-Bromo-5-methyl-2-nitrophenol - *Combi-Blocks*

Products:

1. C10H12BrNO3

Typical conditions: DEAD.or.DCAD.or.DIAD.PPh3

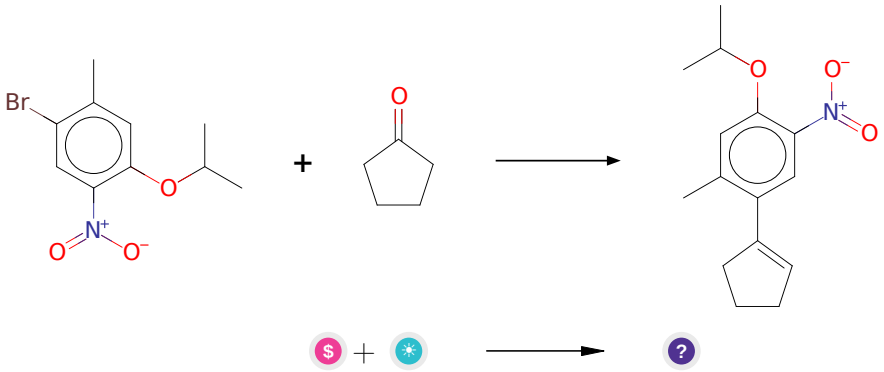
Protections: none

Yield: moderate

Reference: DOI: *10.1021/jo0345751* AND *10.1021/ol0618757*

Retrosynthesis ID: 7562

2.1.2 Arylation of hydrazones with bromoarene



Substrates:

1. Cyclopentanone - *available at Sigma-Aldrich*
2. C10H12BrNO3

Products:

1. Cc1cc(OC(C)C)c([N+](=O)[O-])cc1C1=CCCC1

Typical conditions: 1.TsNH2NH2.2.PdCl2(MeCN)2/Xphos.tBuOLi.ArX.dioxane.heating

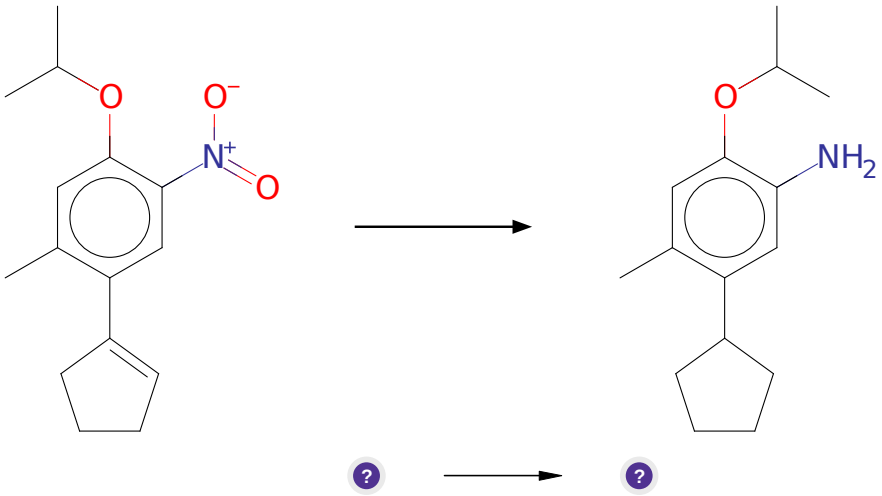
Protections: none

Yield: good

Reference: *10.1021/jo301987c* and *10.1021/acs.oprd.5b00211* and *10.1002/anie.201003450*

Retrosynthesis ID: 9990491

2.1.3 Tandem alkene/nitro reduction



Substrates:

1. Cc1cc(OC(C)C)c([N+](=O)[O-])cc1C1=CCCC1

Products:

1. Cc1cc(OC(C)C)c(N)cc1C1CCCC1

Typical conditions: H2.Pd/C

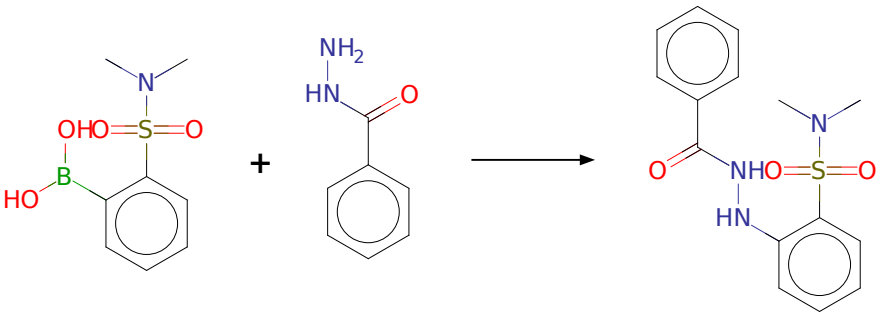
Protections: none

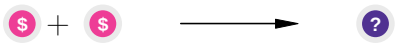
Yield: good

Reference: *10.1016/j.bmc.2009.05.066* and *10.1016/j.cclet.2015.05.003* and *10.1016/j.bmc.2012.12.025*

Retrosynthesis ID: 31351

2.1.4 Chan-Lam Coupling





Substrates:

1. 2-(N,N-DIMETHYLSULPHAMOYL)BENZENEBORONIC ACID - *Combi-Blocks*
2. Benzhydrazide - *available at Sigma-Aldrich*

Products:

1. CN(C)S(=O)(=O)c1ccccc1NNC(=O)c1ccccc1

Typical conditions: Cu(Oac)2.dioxane

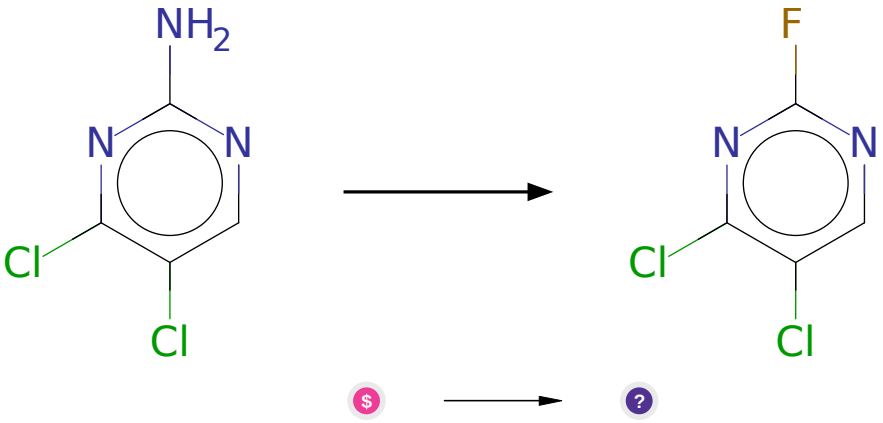
Protections: none

Yield: good

Reference: *10.1039/C4OB02343A*

Retrosynthesis ID: 31015967

2.1.5 Balz-Schiemann Reaction



Substrates:

1. 4,5-Dichloropyrimidin-2-amine - *Combi-Blocks*

Products:

1. Fc1ncc(Cl)c(Cl)n1

Typical conditions: NaNO2.HF-pyridine.-25 to 0C

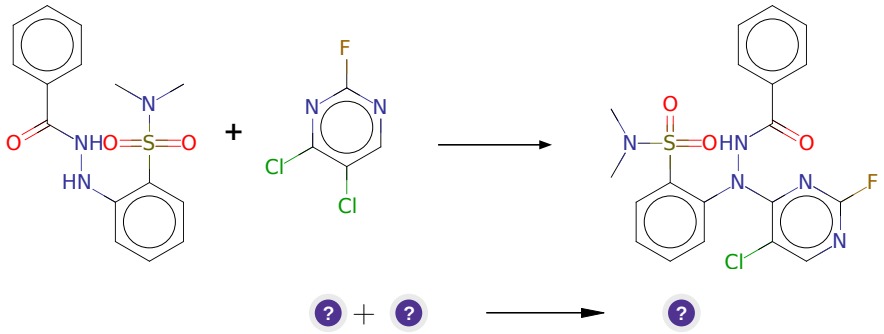
Protections: none

Yield: moderate

Reference: *10.1021/jm100432w* and *10.1021/jm5008177* and *10.1021/ol401540k* and *10.1021/jm401551n* (main text and SI, page S8) and *10.1515/chempap-2016-0033* and *10.1021/jm0311442* and *10.1016/j.jfluchem.2007.03.012* and *10.1021/jo00185a023*

Retrosynthesis ID: 29906

2.1.6 Nucleophilic aromatic substitution



Substrates:

1. Fc1ncc(Cl)c(Cl)n1
2. CN(C)S(=O)(=O)c1ccccc1NNC(=O)c1ccccc1

Products:

1. CN(C)S(=O)(=O)c1ccccc1N(NC(=O)c1ccccc1)c1nc(F)ncc1Cl

Typical conditions: EtOH.Heat or DMF.K2CO3

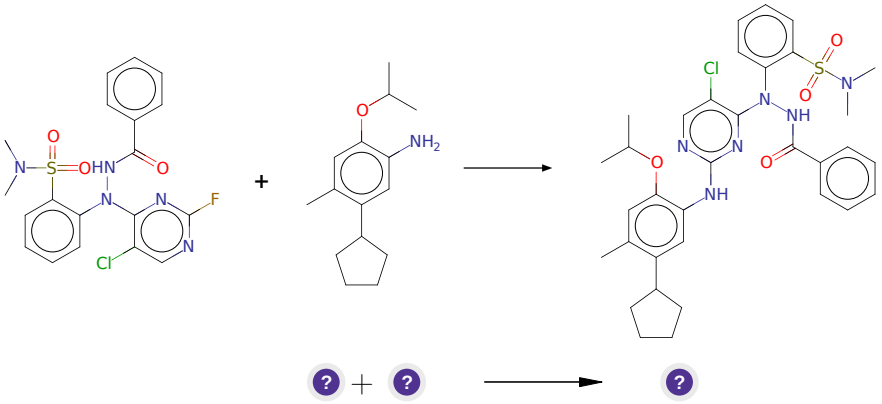
Protections: none

Yield: good

Reference: *10.1016/0040-4020(95)00966-3* and *10.1002/jhet.5570220420* and *10.1021/jo402481t*

Retrosynthesis ID: 29647

2.1.7 Nucleophilic aromatic substitution



Substrates:

1. CN(C)S(=O)(=O)c1ccccc1N(NC(=O)c1ccccc1)c1nc(F)ncc1Cl
2. Cc1cc(OC(C)C)c(N)cc1C1CCCC1

Products:

1. Cc1cc(OC(C)C)c(Nc2ncc(Cl)c(N(NC(=O)c3ccccc3)c3ccccc3S(=O)(=O)N(C)C)n2)cc1C1CCCC1

Typical conditions: Solvent

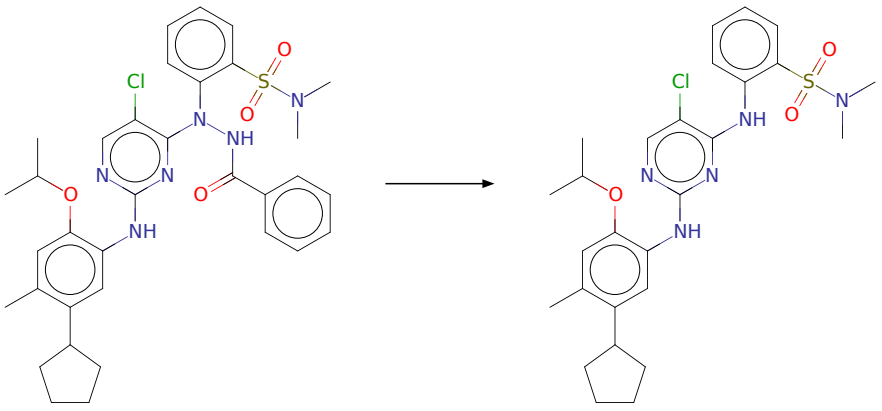
Protections: none

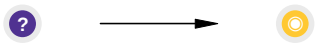
Yield: good

Reference: *10.1002/9781118093559.ch4*

Retrosynthesis ID: 49476

2.1.8 Reduction of phenylhydrazines





Substrates:

1. Cc1cc(OC(C)C)c(Nc2ncc(Cl)c(N(NC(=O)c3ccccc3)c3ccccc3S(=O)(=O)N(C)C)n2)cc1C1CCCC1

Products:

1. Cc1cc(OC(C)C)c(Nc2ncc(Cl)c(Nc3ccccc3S(=O)(=O)N(C)C)n2)cc1C1CCCC1

Typical conditions: RaNi.H2.MeOH

Protections: none

Yield: moderate

Reference: DOI: *10.1021/ol501424f*

Retrosynthesis ID: 1808