# 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:** 396.08

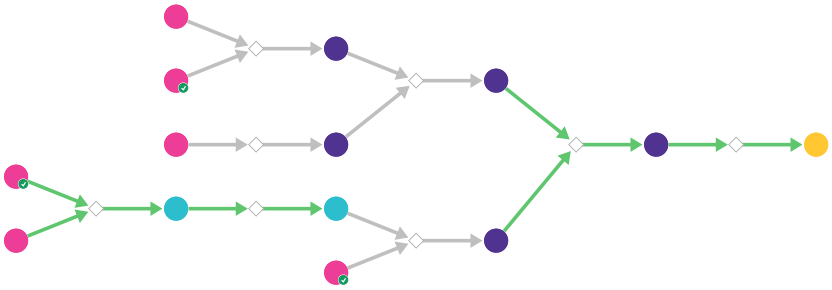
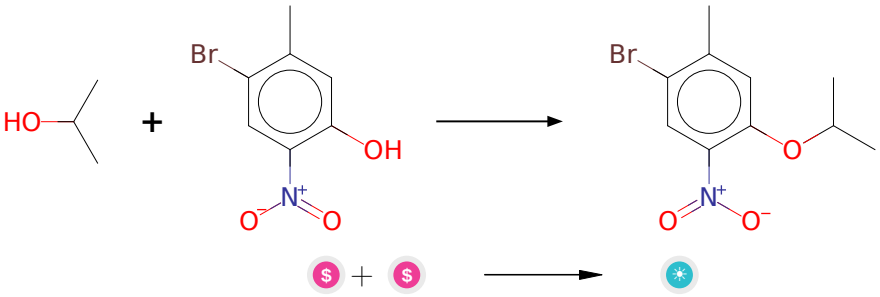


Figure 1: Outline of path 1

### 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

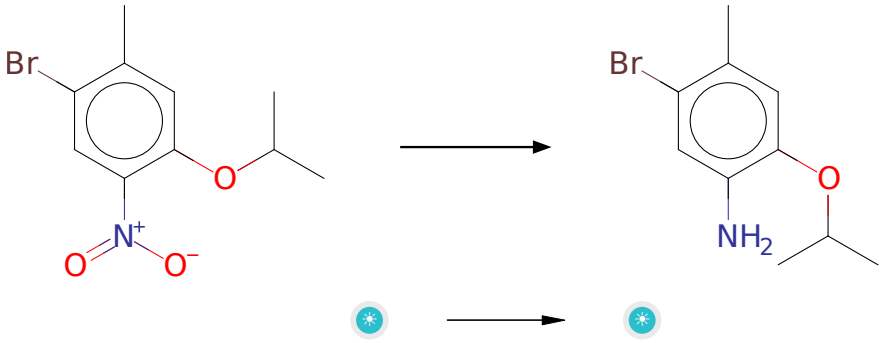
**Protections:** none

**Yield:** moderate

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

**Retrosynthesis ID:** 7562

### 2.1.2 Reduction of nitro group




**Substrates:**

1. C10H12BrNO3

**Products:**

1. C10H14BrNO

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

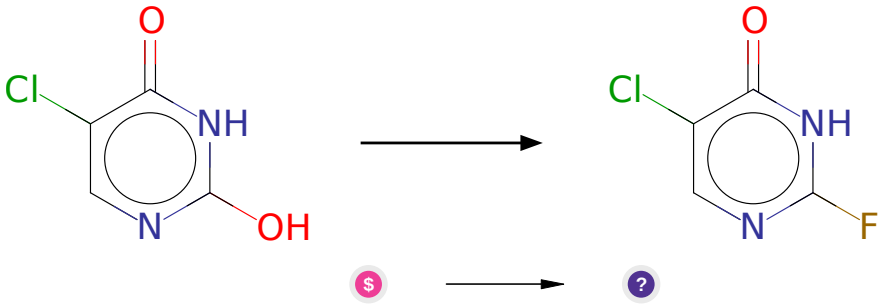
**Protections:** none

**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

### 2.1.3 Synthesis of haloarenes via triflates




**Substrates:**

1. 5-chloro-uracil - *Combi-Blocks*

**Products:**

1. O=c1[nH]c(F)ncc1Cl

**Typical conditions:** 1.Tf2O 2. [Pd].MX

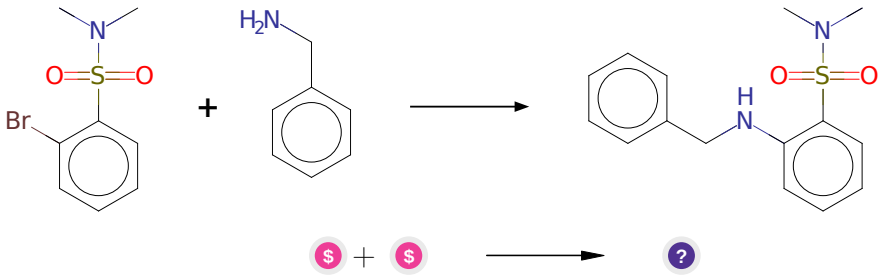
**Protections:** none

**Yield:** moderate

**Reference:** *10.1016/j.tetasy.2012.04.008* and WO2007/136577 (p46) and *10.1021/ol202098h* and *10.1021/ol402859k* and *10.1021/jacs.5b09308*

**Retrosynthesis ID:** 23940

### 2.1.4 Amination of aryl bromides




**Substrates:**

1. 2-Bromo-N,N-dimethylbenzenesulphonamide 1g pack - *Combi-Blocks*
2. Benzylamine - *available at Sigma-Aldrich*

**Products:**

1. CN(C)S(=O)(=O)c1ccccc1NCc1ccccc1

**Typical conditions:** Pd.ligand.base or CuI.ligand.base

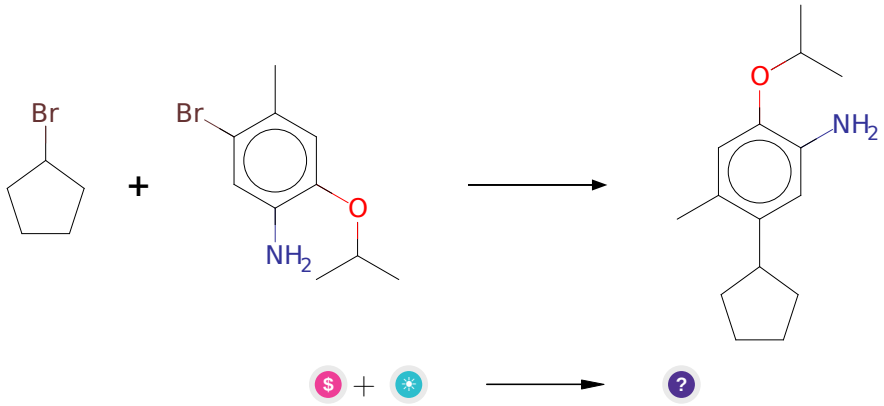
**Protections:** none

**Yield:** good

**Reference:** *10.1021/ja903049z* and *10.1021/jo060945k* and *10.1021/jo060190h* and *10.1039/B923255A* and *10.1021/jm8003625* and *10.1021/jo9006738*

**Retrosynthesis ID:** 28544

### 2.1.5 Photoredox Cross-Electrophile Coupling of Unactivated Alkyl Bromides




**Substrates:**

1. Bromocyclopentane - *available at Sigma-Aldrich*
2. C10H14BrNO

**Products:**

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

**Typical conditions:** [Ir]-photocat.[Ni]-cat.TTMSS.base.blue light

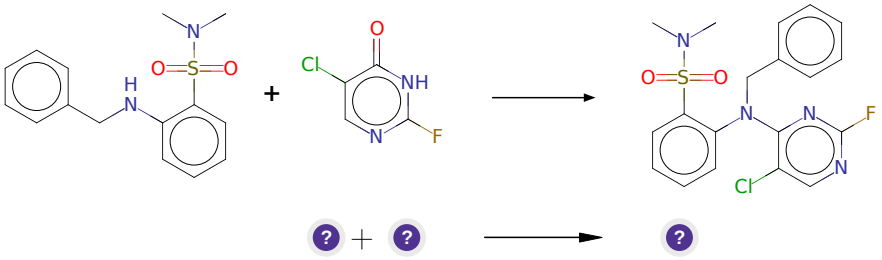
**Protections:** none

**Yield:** good

**Reference:** *10.1021/jacs.6b04818* and *10.1016/j.bbrc.2020.04.028* and *10.1021/acsmedchemlett.8b00183*

**Retrosynthesis ID:** 31016940

### 2.1.6 Amination of pyridones



**Substrates:**

1. CN(C)S(=O)(=O)c1ccccc1NCc1ccccc1
2. O=c1[nH]c(F)ncc1Cl

**Products:**

1. CN(C)S(=O)(=O)c1ccccc1N(Cc1ccccc1)c1nc(F)ncc1Cl

**Typical conditions:** 1.PCl5.2.amine

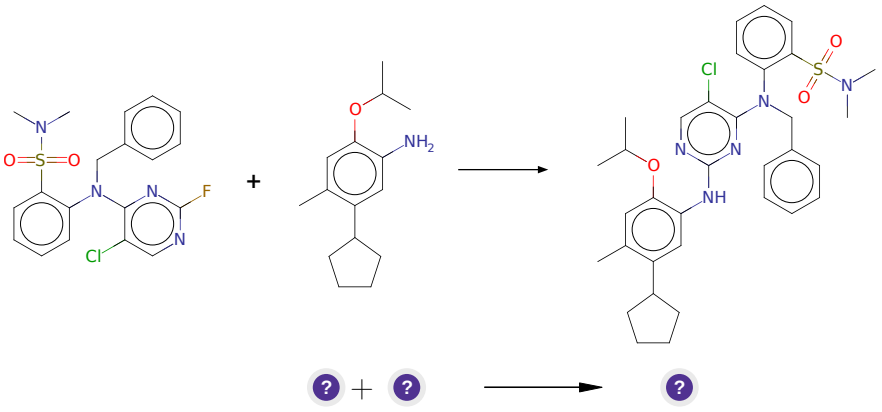
**Protections:** none

**Yield:** moderate

**Reference:** *10.1021/jm300780p* AND *10.3390/molecules170910902* AND *10.1021/jm00392a017*

**Retrosynthesis ID:** 14895

### 2.1.7 Nucleophilic aromatic substitution



**Substrates:**

1. Cc1cc(OC(C)C)c(N)cc1C1CCCC1
2. CN(C)S(=O)(=O)c1ccccc1N(Cc1ccccc1)c1nc(F)ncc1Cl

**Products:**

1. Cc1cc(OC(C)C)c(Nc2ncc(Cl)c(N(Cc3ccccc3)c3ccccc3S(=O)(=O)N(C)C)n2)cc1C1CCCC1

**Typical conditions:** Solvent

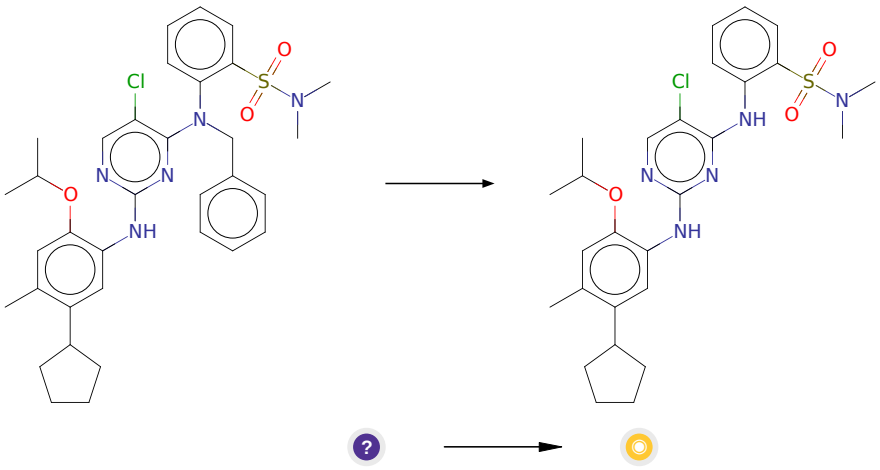
**Protections:** none

**Yield:** good

**Reference:** *10.1002/9781118093559.ch4*

**Retrosynthesis ID:** 49476

### 2.1.8 Debenzylation



**Substrates:**

1. Cc1cc(OC(C)C)c(Nc2ncc(Cl)c(N(Cc3ccccc3)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:** H2. Pd/C or Pd(OH)2

**Protections:** none

**Yield:** good

**Reference:** DOI: *10.1002/1521-3773(20020603)41:11<1895::AID-ANIE1895>3.0.CO;2-3* and *10.1021/jo400589j* and *10.1021/jm8012932* (SI,page S6) and *10.1080/00397911.2016.1261164*

**Retrosynthesis ID:** 9995661