# Paths of analysis*

C42

Synthia

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## 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:** 128.97

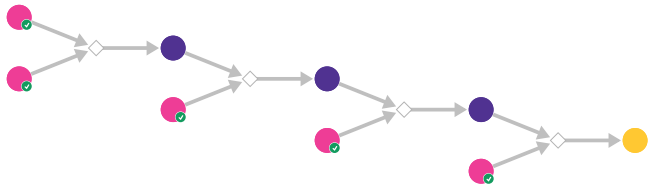
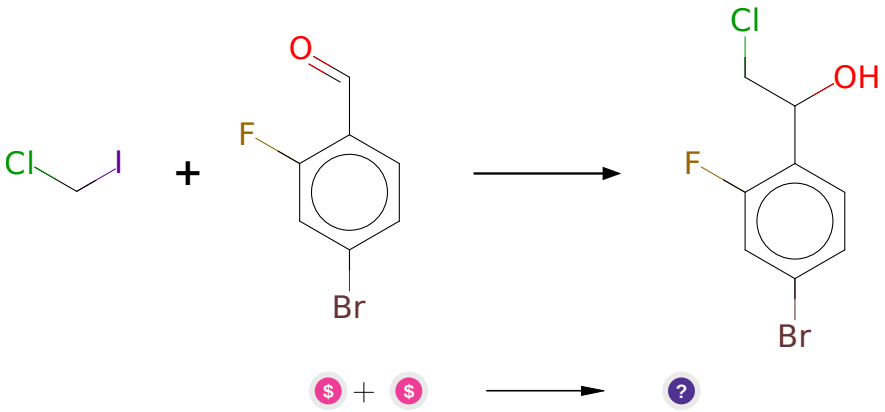


Figure 1: Outline of path 1

### 2.1.1 Addition of dihalomethane to aldehyde




**Substrates:**

1. Chloroiodomethane - *available at Sigma-Aldrich*
2. 4-Bromo-2-fluorobenzaldehyde - *available at Sigma-Aldrich*

**Products:**

1. OC(CCl)c1ccc(Br)cc1F

**Typical conditions:** SmI2.THF

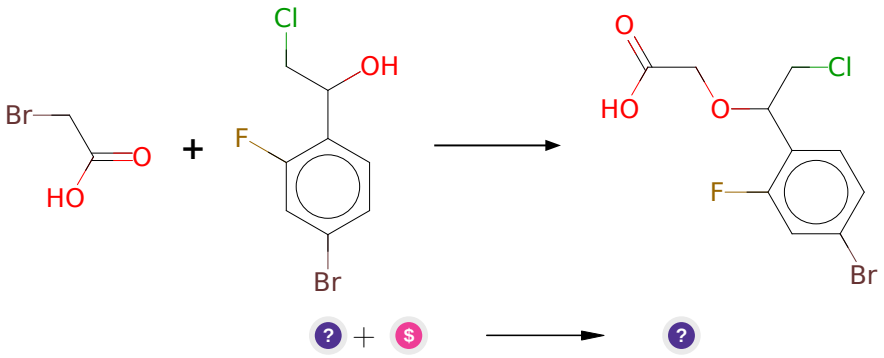
**Protections:** none

**Yield:** good

**Reference:** *10.1016/j.tet.2012.02.033* and *10.1016/j.tetlet.2005.02.093* and *10.1021/jo970318i*

**Retrosynthesis ID:** 25218

### 2.1.2 Reaction of alpha-bromo carbonyl compounds with alcohols or phenols




**Substrates:**

1. OC(CCl)c1ccc(Br)cc1F
2. Bromoacetic acid - *available at Sigma-Aldrich*

**Products:**

1. O=C(O)COC(CCl)c1ccc(Br)cc1F

**Typical conditions:** NaOH.EtOH

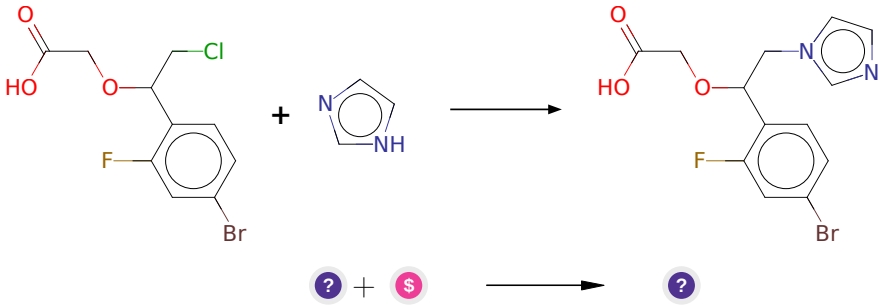
**Protections:** none

**Yield:** good

**Reference:** *10.1021/jm070511x* AND *10.1021/op1002038* AND *10.1007/BF00758669* AND *10.1021/ja01117a054*

**Retrosynthesis ID:** 14804

### 2.1.3 N-alkylation of Heterocycles




**Substrates:**

1. O=C(O)COC(CCl)c1ccc(Br)cc1F
2. Imidazole - *available at Sigma-Aldrich*

**Products:**

1. O=C(O)COC(Cn1ccnc1)c1ccc(Br)cc1F

**Typical conditions:** NaH.DMF

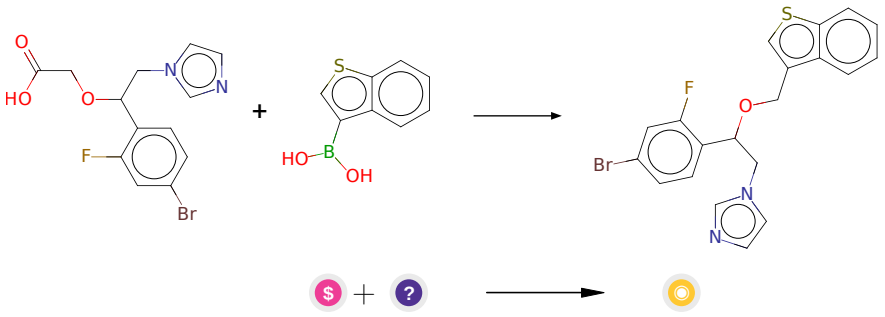
**Protections:** none

**Yield:** good

**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

### 2.1.4 Decarboxylative arylation of redox-active esters




**Substrates:**

1. Thianaphthene-3-boronic acid - *available at Sigma-Aldrich*

2. O=C(O)COC(Cn1ccnc1)c1ccc(Br)cc1F

**Products:**

1. Fc1cc(Br)ccc1C(Cn1ccnc1)OCc1csc2ccccc12

**Typical conditions:** 1. TCNHPI.DCC 2.NiCl2.TEA.dioxane.DMF

**Protections:** none

**Yield:** moderate

**Reference:** *10.1002/anie.201605463*

**Retrosynthesis ID:** 10008335