Paths of analysis*

C46

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: `126.49`

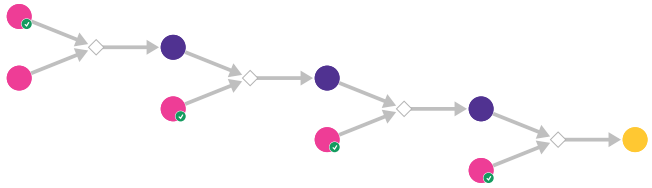
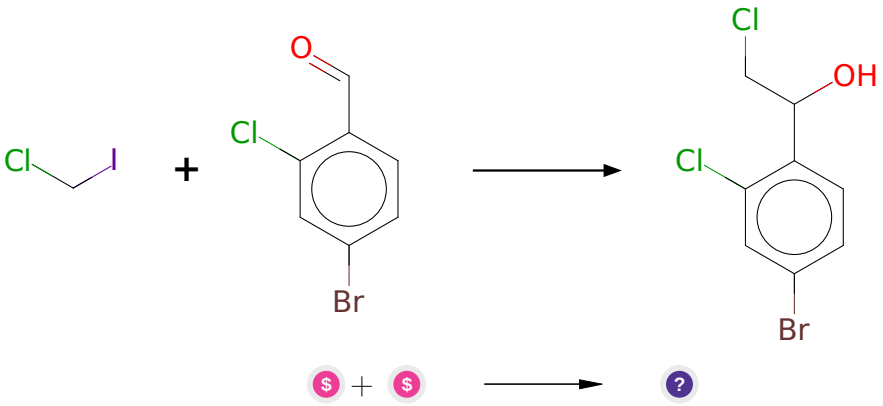


Figure 1: Outline of path 1

2.1.1 Addition of dihalomethane to aldehyde



Substrates:

1. Chloroiodomethane - *available at Sigma-Aldrich*
2. 2-Chloro-4-bromobenzaldehyde - *AstaTech*

Products:

1. OC(CCl)c1ccc(Br)cc1Cl

Typical conditions: SmI2.THF

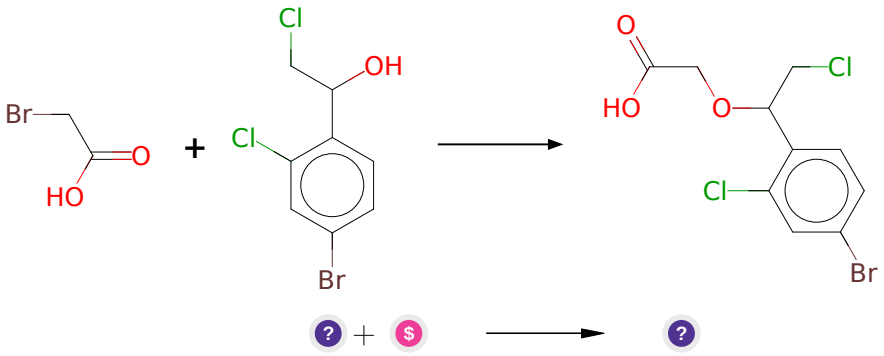
Protections: none

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)cc1Cl
2. Bromoacetic acid - *available at Sigma-Aldrich*

Products:

1. O=C(O)COC(CCl)c1ccc(Br)cc1Cl

Typical conditions: NaOH.EtOH

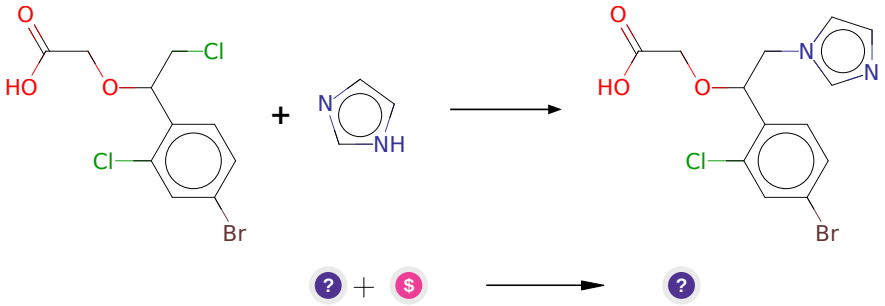
Protections: none

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)cc1Cl
2. Imidazole - *available at Sigma-Aldrich*

Products:

1. O=C(O)COC(Cn1ccnc1)c1ccc(Br)cc1Cl

Typical conditions: NaH.DMF

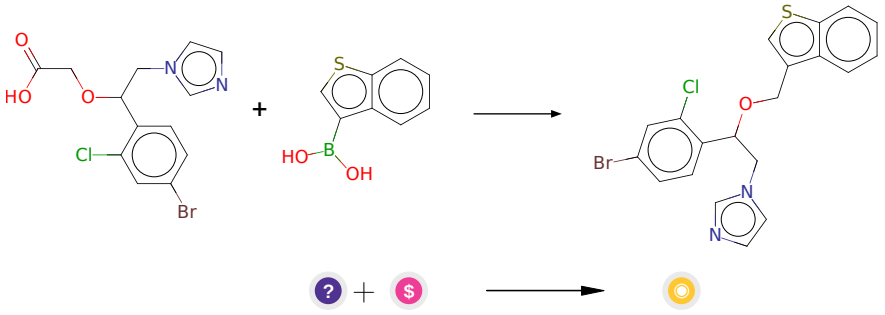
Protections: none

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. O=C(O)COC(Cn1ccnc1)c1ccc(Br)cc1Cl

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

Products:

1. Clc1cc(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