Paths of analysis*

Analysis 1

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: `145.31`

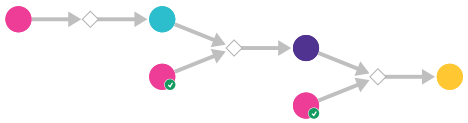
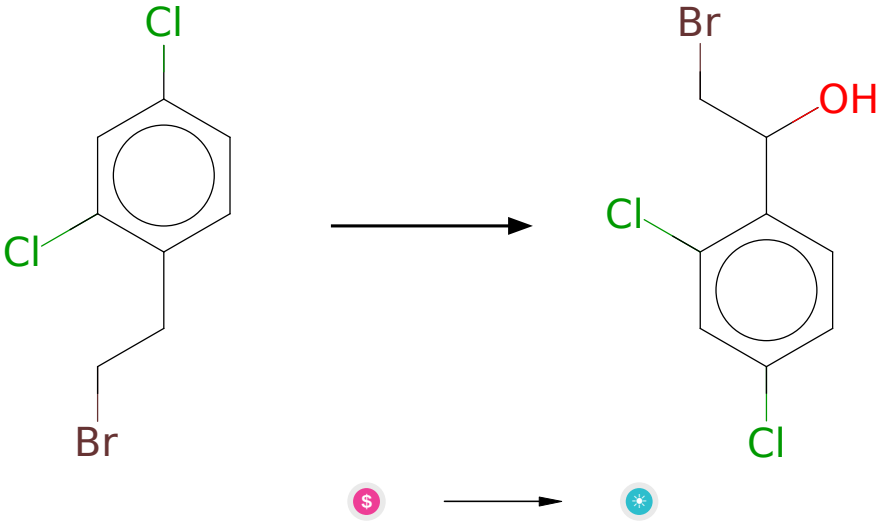


Figure 1: Outline of path 1

2.1.1 Hydroxylation of benzylic position



Substrates:

1. 2,4-Dichlorophenethyl bromide - *Combi-Blocks*

Products:

1. 2-bromo-1-(2,4-dichloro-phenyl)-ethanol

Typical conditions: 1.Ce(OTf)4.MeCN.2.NaBH4

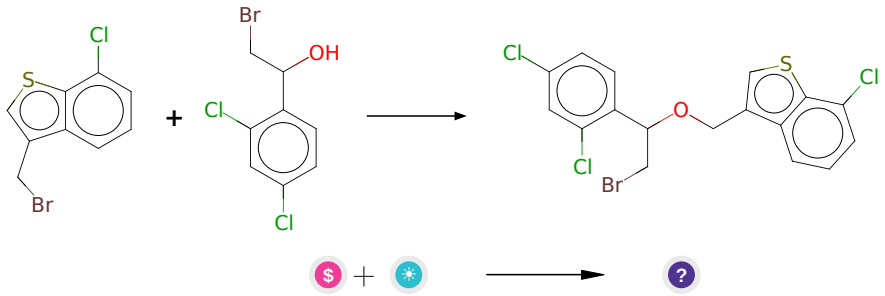
Protections: none

Yield: moderate

Reference: *10.1039/B008843I* and WO2012137047 p.12

Retrosynthesis ID: 27140

2.1.2 Alkylation of secondary alcohols



Substrates:

1. 3-(Bromomethyl)-7-chloro-1-benzothiophene - *available at Sigma-Aldrich*
2. 2-bromo-1-(2,4-dichloro-phenyl)-ethanol

Products:

1. Clc1ccc(C(CBr)OCc2csc3c(Cl)cccc23)c(Cl)c1

Typical conditions: K2CO3.acetone.heat

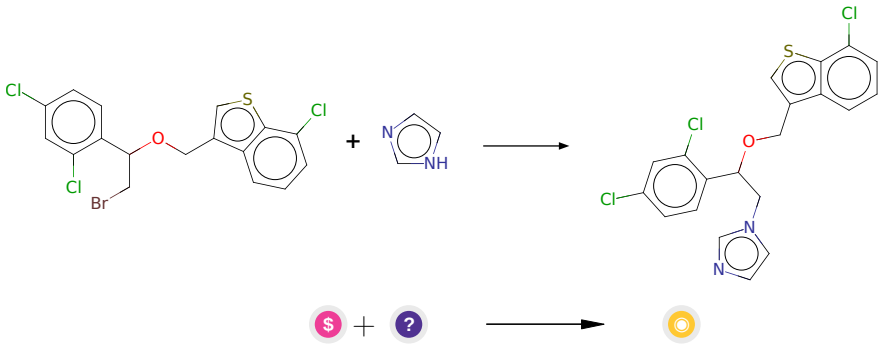
Protections: none

Yield: moderate

Reference: *10.1002/anie.201909177* and *10.1016/j.jfluchem.2019.109388* and *10.2174/1570178613106660077*

Retrosynthesis ID: 31011124

2.1.3 N-alkylation of heterocycles



Substrates:

1. Imidazole - *available at Sigma-Aldrich*
2. Clc1ccc(C(CBr)OCc2csc3c(Cl)cccc23)c(Cl)c1

Products:

1. 1-2-[(7-chloro-1-benzothiophen-3-yl)methoxy]-2-(2,4-dichlorophenyl)ethyl-1H-imidazole - *Combi-Blocks*

Typical conditions: NaH. DMF

Protections: none

Yield: good

Reference: *10.1016/j.ejmech.2010.11.014* or *10.1039/C6OB01149G* (SI) or *10.1246/cl.2005.442* or *10.1021/ol403570z* (SI) or *10.1016/S0040-4020(01)00360-X*

Retrosynthesis ID: 10000414