Paths of analysis*

C48

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: `114.48`

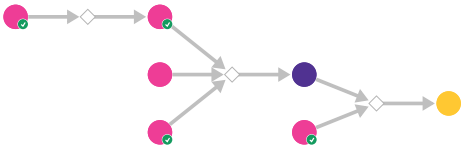
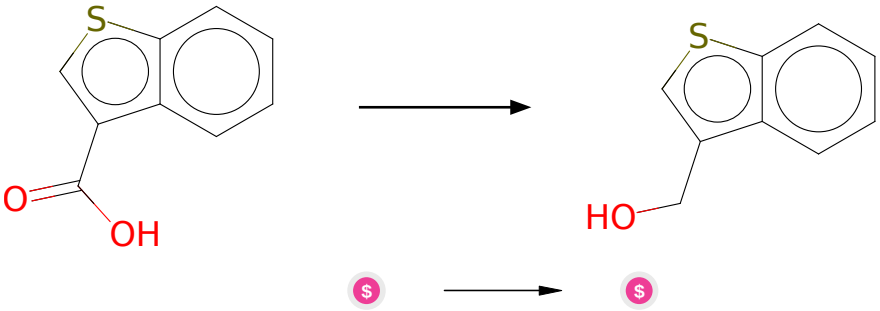


Figure 1: Outline of path 1

2.1.1 Reduction of carboxylic acids to alcohols



Substrates:

1. 1-Benzothiophene-3-carboxylic acid - *available at Sigma-Aldrich*

Products:

1. 1-benzothien-3-ylmethanol - *available at Sigma-Aldrich*

Typical conditions: BH3.THF

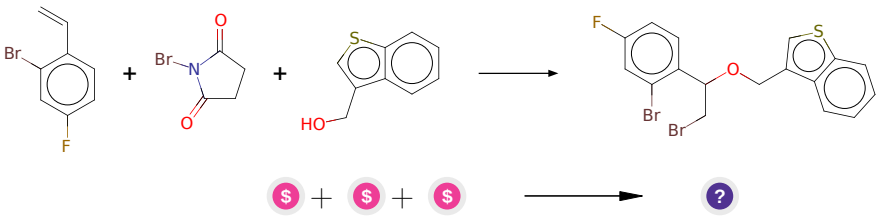
Protections: none

Yield: good

Reference: DOI: *10.1021/jo00956a011* and *10.1016/S0040-4039(98)01781-X* and *10.1021/ja508846g* and *10.1016/j.bmc.2011.07.054*

Retrosynthesis ID: 9141

2.1.2 Synthesis of bromo and chloroalkoxyalkanes



Substrates:

1. 2-Bromo-4-fluorostyrene 1g pack - *Enamine*
2. N-Bromosuccinimide - *available at Sigma-Aldrich*
3. 1-benzothien-3-ylmethanol - *available at Sigma-Aldrich*

Products:

1. Fc1ccc(C(CBr)OCc2csc3ccccc23)c(Br)c1

Typical conditions: NBS(NCS).alcohol

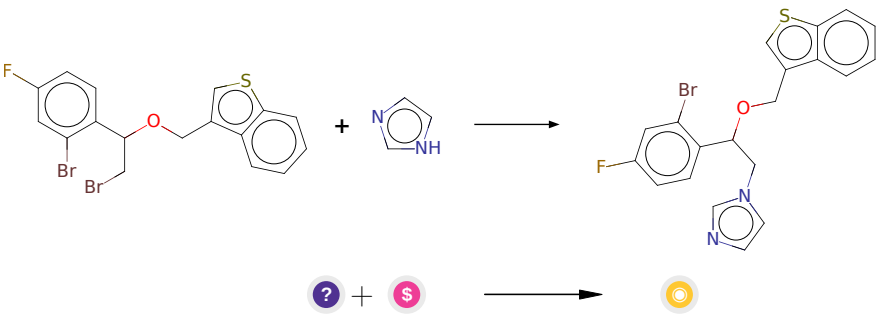
Protections: none

Yield: moderate

Reference: *10.1002/chem.200390180* and *10.1055/s-0037-1611277*

Retrosynthesis ID: 245562

2.1.3 N-alkylation of heterocycles



Substrates:

1. Fc1ccc(C(CBr)OCc2csc3ccccc23)c(Br)c1
2. Imidazole - *available at Sigma-Aldrich*

Products:

1. Fc1ccc(C(Cn2ccnc2)OCc2csc3ccccc23)c(Br)c1

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