Paths of analysis*

C47

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

*The results stated herein were generated using the proprietary platform owned and maintained by Grzybowski Scientific Inventions, Inc., a subsidiary of Merck KGaA, Darmstadt Germany. The results are provided on an as is basis, and shall be used solely in connection with the rights afforded in the license agreement and for no other purpose.

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: 257.19

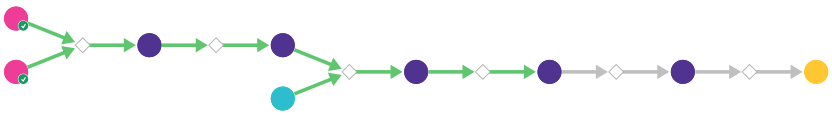
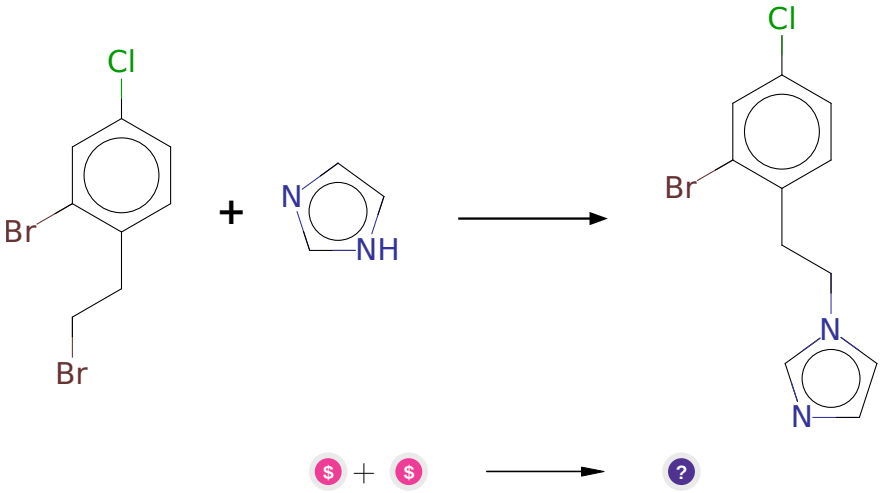


Figure 1: Outline of path 1

2.1.1 N-alkylation of heterocycles



Substrates:

1. 2-Bromo-1-(2-bromoethyl)-4-chlorobenzene - *available at Sigma-Aldrich*
2. Imidazole - *available at Sigma-Aldrich*

Products:

1. Clc1ccc(CCn2ccnc2)c(Br)c1

Typical conditions: NaH. DMF

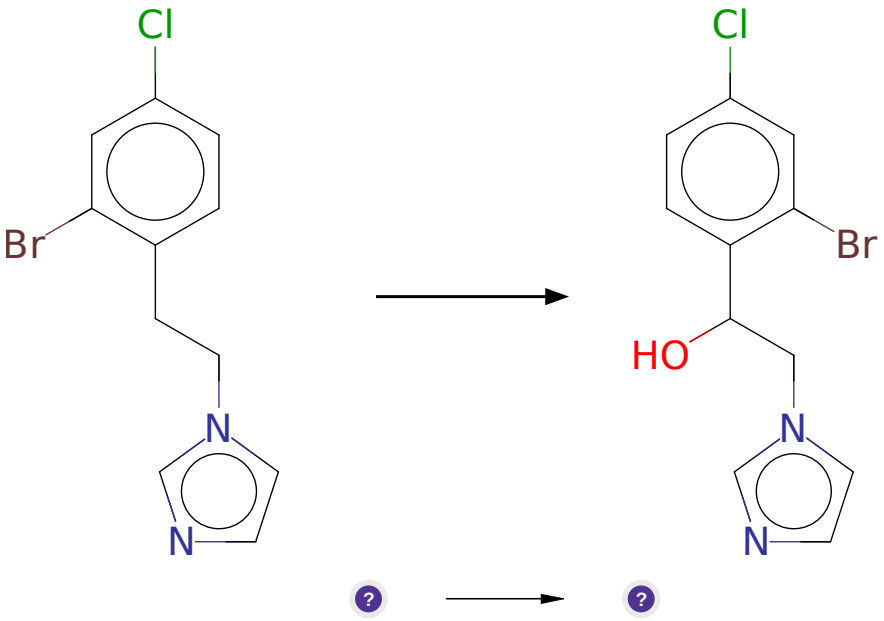
Protections: none

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

2.1.2 Hydroxylation of benzylic position



Substrates:

1. Clc1ccc(CCn2ccnc2)c(Br)c1

Products:

1. OC(Cn1ccnc1)c1ccc(Cl)cc1Br

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

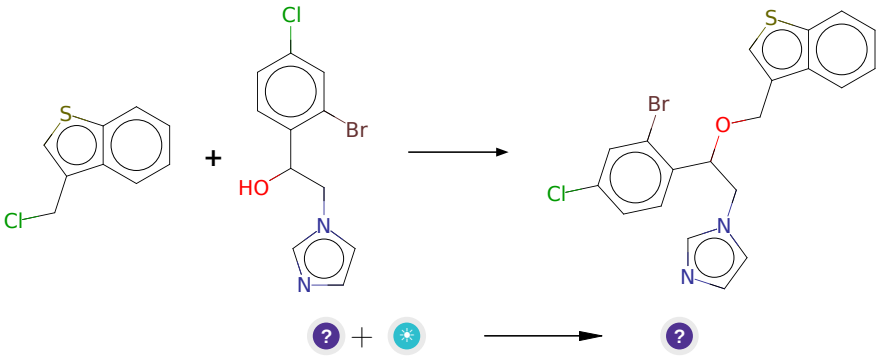
Protections: none

Yield: moderate

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

Retrosynthesis ID: 27140

2.1.3 Alkylation of secondary alcohols



Substrates:

1. OC(Cn1ccnc1)c1ccc(Cl)cc1Br
2. 3-chlormethyl-benzo[b]thiophen

Products:

1. Clc1ccc(C(Cn2ccnc2)OCc2csc3ccccc23)c(Br)c1

Typical conditions: K2CO3.acetone.heat

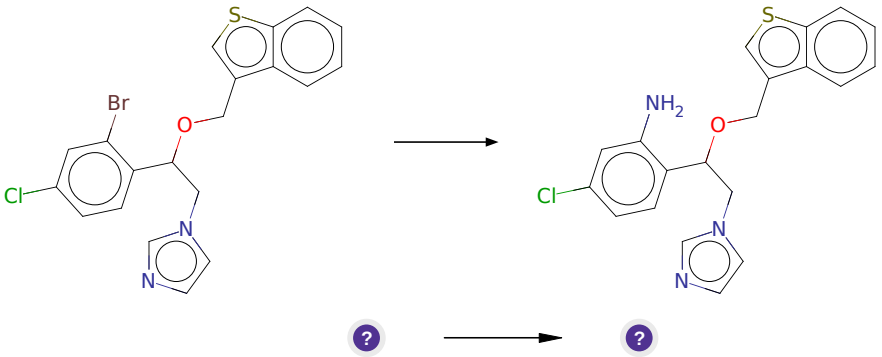
Protections: none

Yield: moderate

Reference: *10.1016/S0022-1139(00)85021-6* and

Retrosynthesis ID: 31011106

2.1.4 Coupling of Ammonia with Aryl Halides



Substrates:

1. Clc1ccc(C(Cn2ccnc2)OCc2csc3ccccc23)c(Br)c1

Products:

1. Nc1cc(Cl)ccc1C(Cn1ccnc1)OCc1csc2ccccc12

Typical conditions: Pd[(P(p-tol)3]2.NaOtBu.dioxane.heat

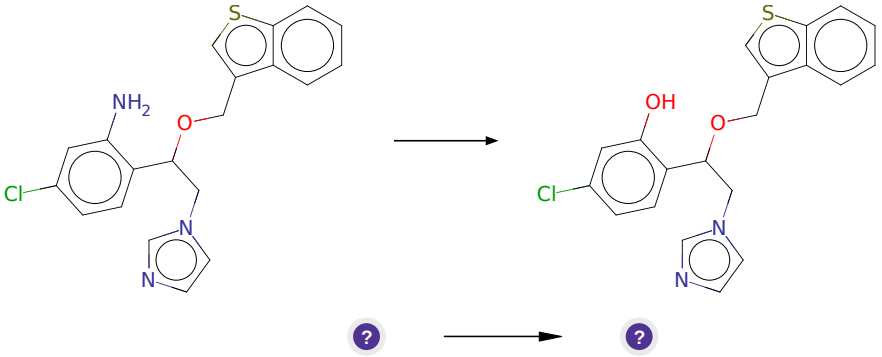
Protections: none

Yield: good

Reference: *10.1021/ja903049z* and *10.1021/ol027119s* and *10.1021/jo9006738*

Retrosynthesis ID: 31016463

2.1.5 Synthesis of phenols from amines - Sandmeyer reaction



Substrates:

1. Nc1cc(Cl)ccc1C(Cn1ccnc1)OCc1csc2ccccc12

Products:

1. Oc1cc(Cl)ccc1C(Cn1ccnc1)OCc1csc2ccccc12

Typical conditions: 1) NaNO2.HCl.aq 2) base.heat

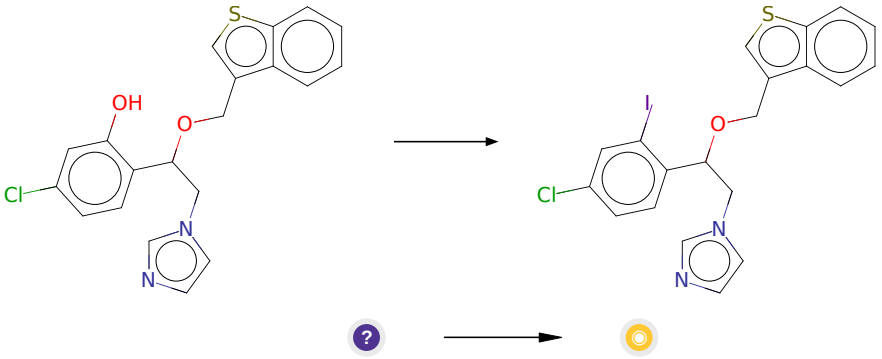
Protections: none

Yield: moderate

Reference: *10.1016/j.ejmech.2010.09.022* and *10.1021/jm00131a010*

Retrosynthesis ID: 7274

2.1.6 Synthesis of haloarenes via triflates



Substrates:

1. Oc1cc(Cl)ccc1C(Cn1ccnc1)OCc1csc2ccccc12

Products:

1. Clc1ccc(C(Cn2ccnc2)OCc2csc3ccccc23)c(I)c1

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