Paths of analysis*

C41

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: 91.35

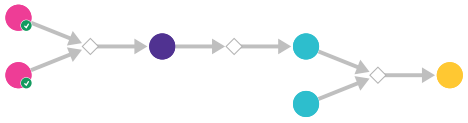
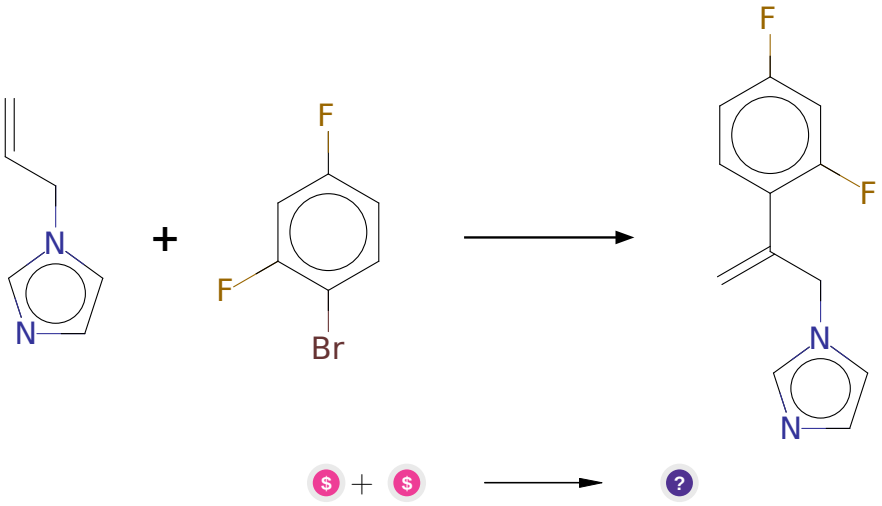


Figure 1: Outline of path 1

2.1.1 Heck Reaction



Substrates:

1. 1-(prop-2-en-1-yl)-1H-imidazole - *available at Sigma-Aldrich*
2. 1-Bromo-2,4-difluorobenzene - *available at Sigma-Aldrich*

Products:

1. C=C(Cn1ccnc1)c1ccc(F)cc1F

Typical conditions: Pd (cat). Ligand e.g. TXPTS. Base. Temp

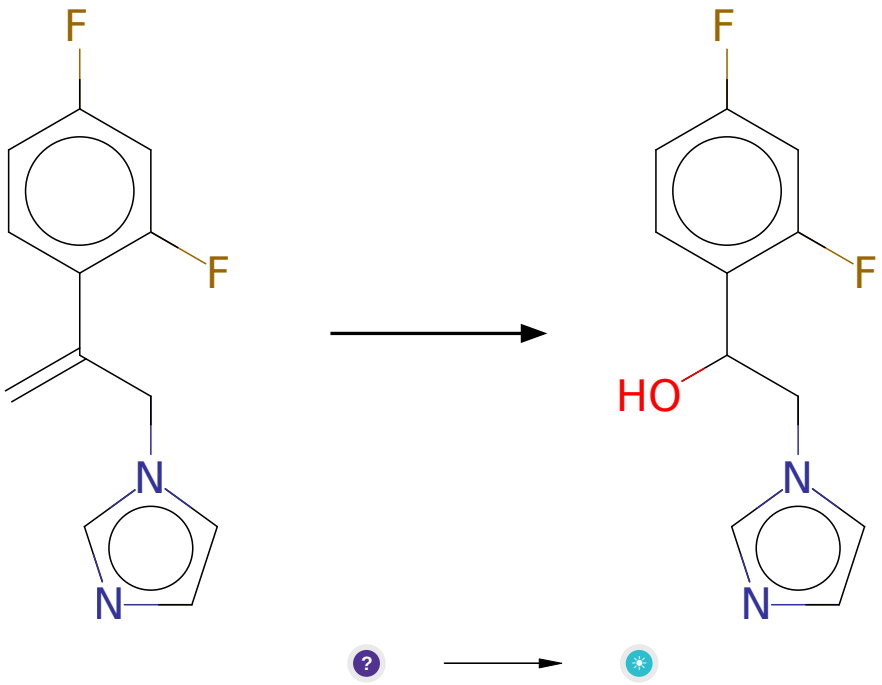
Protections: none

Yield: moderate

Reference: *10.1039/C3CC45911J* or *10.1021/ar00049a001* or *10.1002/anie.201201806* or *10.1002/9780470716076*

Retrosynthesis ID: 9266

2.1.2 Ozonolysis followed by reduction



Substrates:

1. C=C(Cn1ccnc1)c1ccc(F)cc1F

Products:

1. 1-(2,4-difluorophenyl)-2-(1h-imidazol-1-yl)ethan-1-ol

Typical conditions: O3.MeOH.CH2Cl2.NaBH4.low temperature

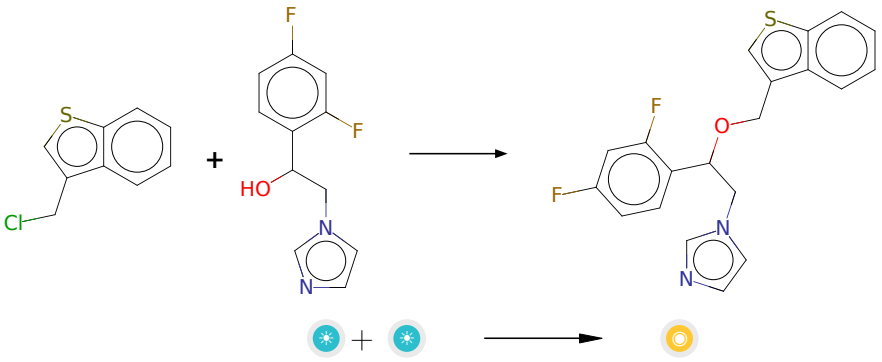
Protections: none

Yield: good

Reference: *10.1021/ja043506g*(SI,page S2) and *10.1016/j.jfluchem.2011.05.031* and *10.1021/ja304872j* and *10.1021/jo026004z*

Retrosynthesis ID: 28553

2.1.3 Alkylation of secondary alcohols



Substrates:

1. 3-chlormethyl-benzo[b]thiophen
2. 1-(2,4-difluorophenyl)-2-(1h-imidazol-1-yl)ethan-1-ol

Products:

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

Typical conditions: K2CO3.acetone.heat

Protections: none

Yield: moderate

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

Retrosynthesis ID: 31011106