Paths of analysis*

C62

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: 121.85

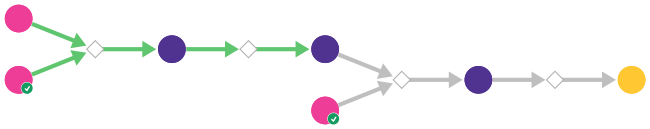
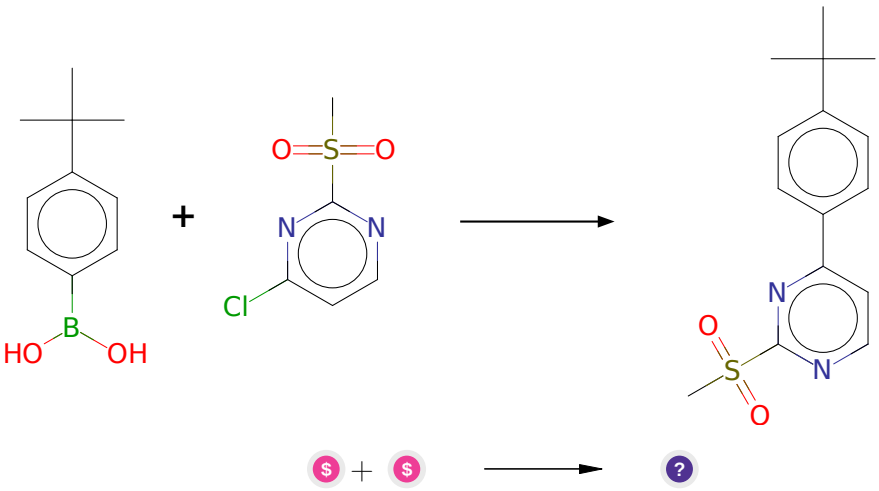


Figure 1: Outline of path 1

2.1.1 Suzuki coupling with aryl chlorides



Substrates:

1. 4-Chloro-2-(methylsulfonyl)pyrimidine - *Combi-Blocks*
2. 4-t-Butylphenylboronic acid - *available at Sigma-Aldrich*

Products:

1. CC(C)(C)c1ccc(-c2ccnc(S(C)(=O)=O)n2)cc1

Typical conditions: [Pd].catalyst.base.

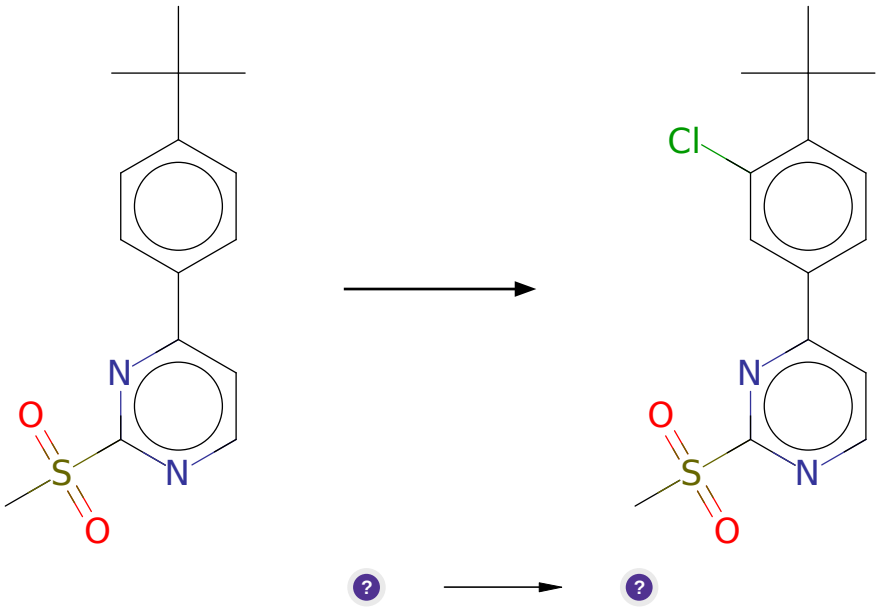
Protections: none

Yield: good

Reference: *10.1002/anie.201108608* and *10.1002/anie.200801465* and *10.1055/s-0033-1338293* and *10.1039/c1cc10708a* and *10.1055/s-0030-1260169* and *10.1016/j.tet.2005.05.071* and *10.1038/s41929-020-00564-z* (metal-free coupling)

Retrosynthesis ID: 26284

2.1.2 Chlorination of aromatic compounds



Substrates:

1. CC(C)(C)c1ccc(-c2ccnc(S(C)(=O)=O)n2)cc1

Products:

1. CC(C)(C)c1ccc(-c2ccnc(S(C)(=O)=O)n2)cc1Cl

Typical conditions: Cl2 or other chlorinating agent like NCS

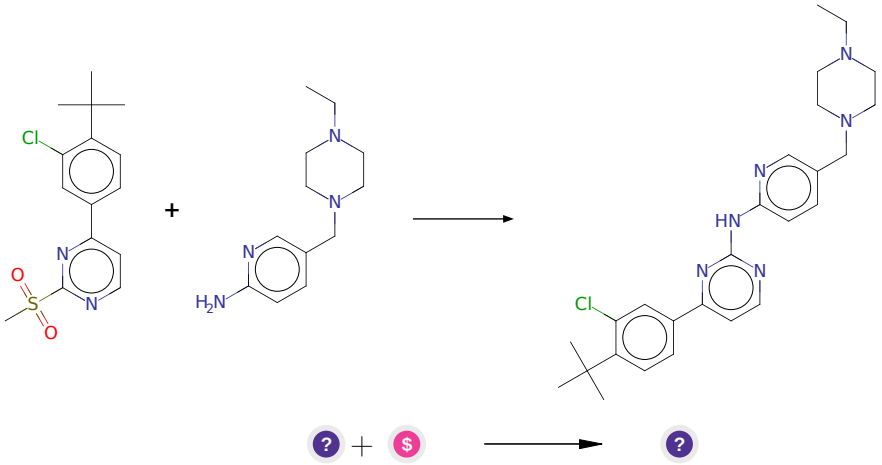
Protections: none

Yield: moderate

Reference: DOI: *10.1007/s11178-005-0256-1*

Retrosynthesis ID: 11125

2.1.3 Substiution of pyrimidinesulfones with amines



Substrates:

1. CC(C)(C)c1ccc(-c2ccnc(S(C)(=O)=O)n2)cc1Cl
2. 5-((4-Ethylpiperazin-1-yl)methyl)pyridin-2-amine - *available at Sigma-Aldrich*

Products:

1. CCN1CCN(Cc2ccc(Nc3nccc(-c4ccc(C(C)(C)C)c(Cl)c4)n3)nc2)CC1

Typical conditions: K2CO3.DMF

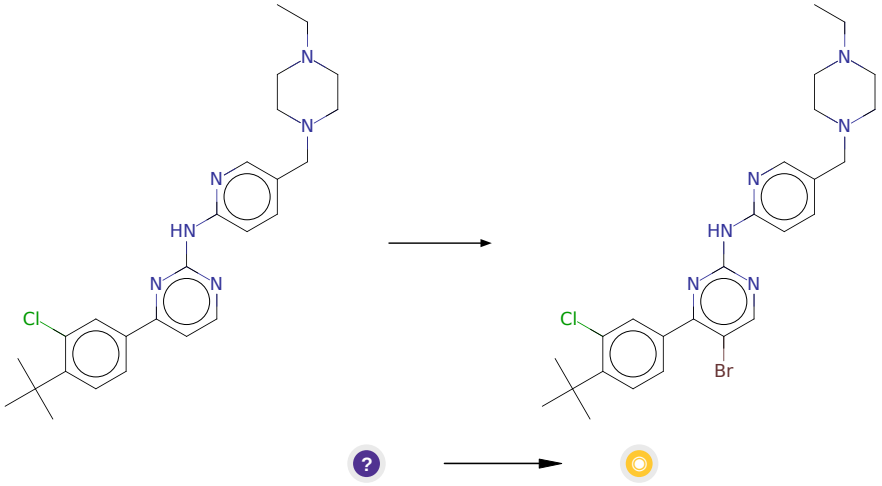
Protections: none

Yield: good

Reference: *10.1021/jm980222w* AND *10.1016/j.cclet.2014.10.007* AND *10.1002/jhet.5570280520* AND *10.1080/00397910701396930*

Retrosynthesis ID: 14936

2.1.4 Bromination of aromatic compounds



Substrates:

1. CCN1CCN(Cc2ccc(Nc3nccc(-c4ccc(C(C)(C)C)c(Cl)c4)n3)nc2)CC1

Products:

1. CCN1CCN(Cc2ccc(Nc3ncc(Br)c(-c4ccc(C(C)(C)C)c(Cl)c4)n3)nc2)CC1

Typical conditions: Br2.Fe

Protections: none

Yield: good

Reference: *10.1021/acs.accounts.6b00120*

Retrosynthesis ID: 7777000