Paths of analysis*

C29

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: 128.02

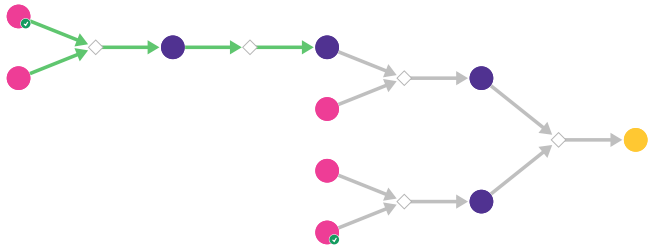
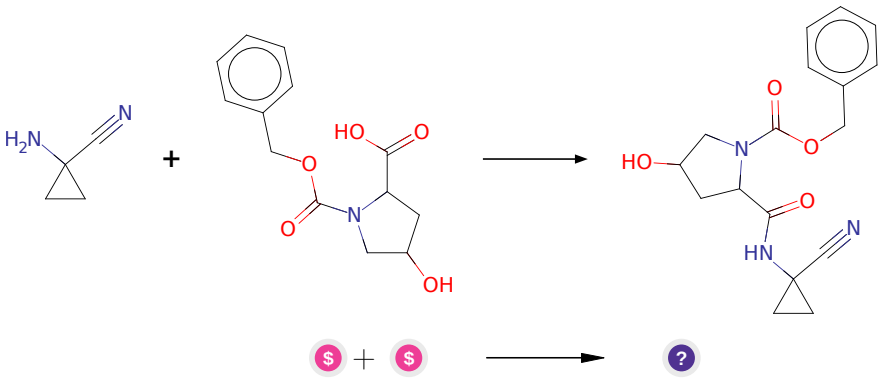


Figure 1: Outline of path 1

2.1.1 Amide coupling



Substrates:

1. Z-Hyp-OH - *available at Sigma-Aldrich*
2. 1-Amino-cyclopropanecarbonitrile - *Combi-Blocks*

Products:

1. N#CC1(NC(=O)C2CC(O)CN2C(=O)OCc2ccccc2)CC1

Typical conditions: DCC.DCM or EDC.DCM or SOCl2.DCM

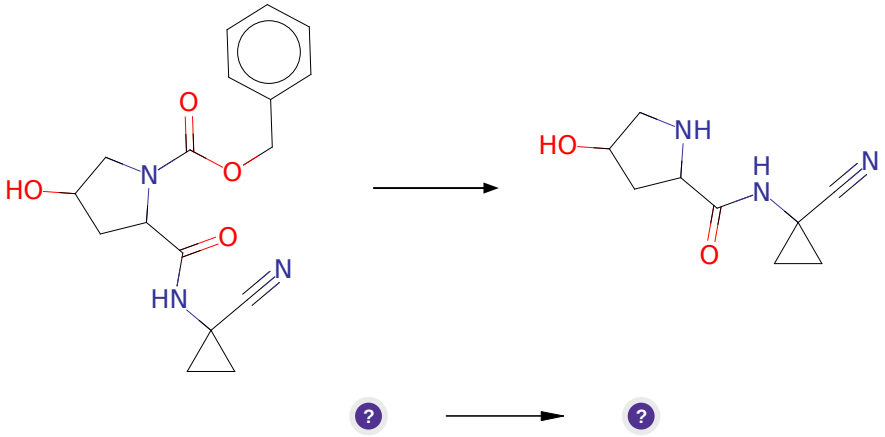
Protections: none

Yield: good

Reference: *10.1021/cr100048w* and *10.1039/B701677H* and *10.1039/C5RA24527C* and *10.3727/000000006783981206* and *10.1021/np060007f* and *10.1021/jo00012a058* and *10.1016/j.bmcl.2007.08.037* and *10.1039/C0OB00355G* and *10.1021/jm500031w* (p.3056) and *10.1016/j.tet.2011.03.046*

Retrosynthesis ID: 10087

2.1.2 Cleavage of benzyloxycarbamates



Substrates:

1. N#CC1(NC(=O)C2CC(O)CN2C(=O)OCc2ccccc2)CC1

Products:

1. N#CC1(NC(=O)C2CC(O)CN2)CC1

Typical conditions: H2.Pd/C

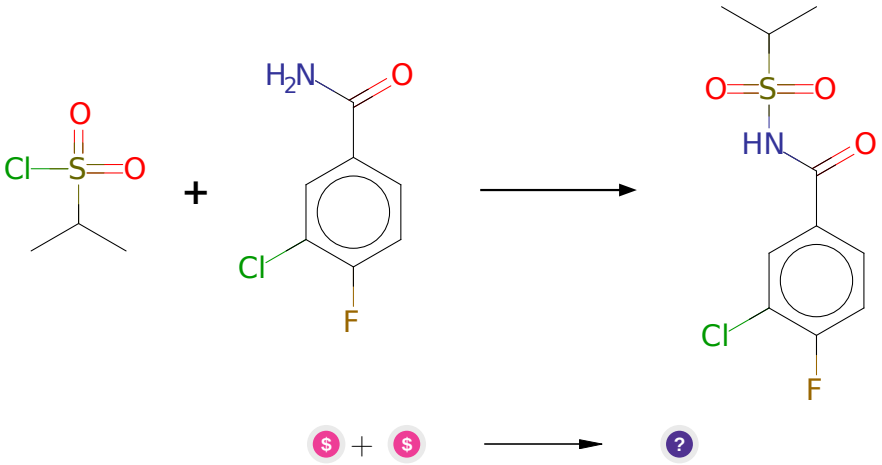
Protections: none

Yield: good

Reference: *10.1021/jm070755h* and *10.1021/jm2016057* and *10.1055/s-0033-1340215* and *10.1016/S0040-4039(03)01181-X*

Retrosynthesis ID: 9990024

2.1.3 Sulfonylation of amides



Substrates:

1. 3-Chloro-4-fluorobenzamide 1g pack - *Combi-Blocks*
2. 2-Propanesulfonyl chloride - *available at Sigma-Aldrich*

Products:

1. CC(C)S(=O)(=O)NC(=O)c1ccc(F)c(Cl)c1

Typical conditions: Py.RSO2Cl

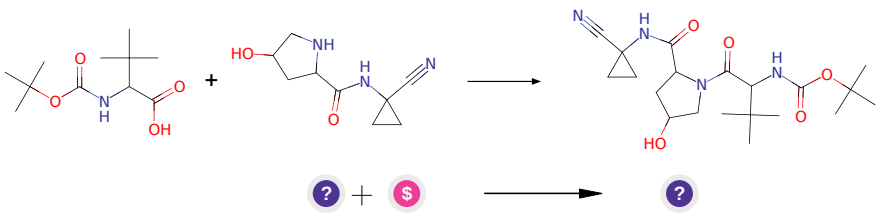
Protections: none

Yield: good

Reference: *10.1021/ja9945313* AND *10.1016/j.ejmech.2013.04.028* AND *10.1039/c5ra14001c* AND *10.1016/j.bmcl.2013.12.043* AND *10.1016/j.tetasy.2012.08.013*

Retrosynthesis ID: 14787

2.1.4 Amide coupling



Substrates:

1. N#CC1(NC(=O)C2CC(O)CN2)CC1
2. 2-[(tert-butoxy)carbonyl]amino-3,3-dimethylbutanoic acid - *Enamine*

Products:

1. CC(C)(C)OC(=O)NC(C(=O)N1CC(O)CC1C(=O)NC1(C#N)CC1)C(C)(C)C

Typical conditions: DCC.DCM or EDC.DCM or SOCl2.DCM

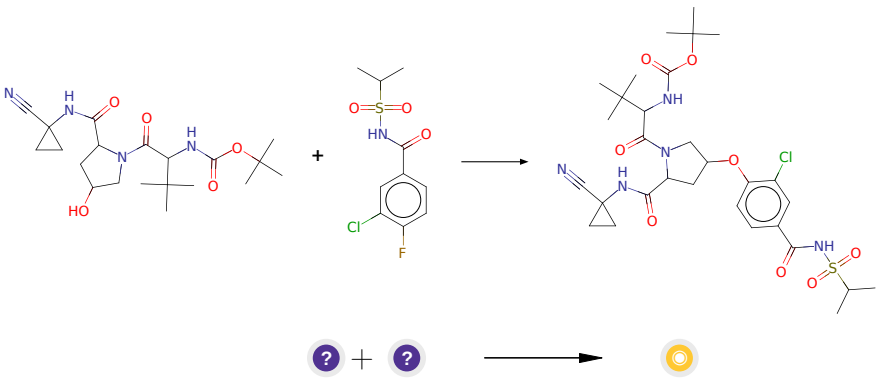
Protections: none

Yield: good

Reference: *10.1021/ol400686f* and *10.1021/jo00200a057* and *10.1021/cr100048w* and *10.1039/B701677H* and *10.1039/C5RA24527C* and *10.3727/000000006783981206* and *10.1021/np060007f* and *10.1021/jo00012a058* and *10.1016/j.bmcl.2007.08.037* and *10.1039/C0OB00355G* and *10.1021/jm500031w* (p.3056) and *10.1016/j.tet.2011.03.046*

Retrosynthesis ID: 9147

2.1.5 Nucleophilic aromatic substitution



Substrates:

1. CC(C)(C)OC(=O)NC(C(=O)N1CC(O)CC1C(=O)NC1(C#N)CC1)C(C)(C)C
2. CC(C)S(=O)(=O)NC(=O)c1ccc(F)c(Cl)c1

Products:

1. CC(C)S(=O)(=O)NC(=O)c1ccc(OC2CC(C(=O)NC3(C#N)CC3)N(C(=O)C(NC(=O)OC(C)(C)C)C(C

Typical conditions: NaH.THF.0-80 C or K2CO3.DMF.110 C

Protections: none

Yield: good

Reference: *10.1016/j.tetlet.2015.10.008* p. 6479, 6483 and *10.1016/j.ejmech.2016.06.056* p. 82, 85

Retrosynthesis ID: 49475