Paths of analysis*

Analysis 7

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: 62.19

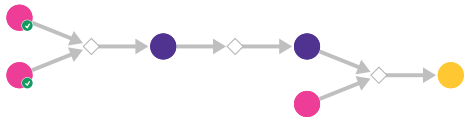
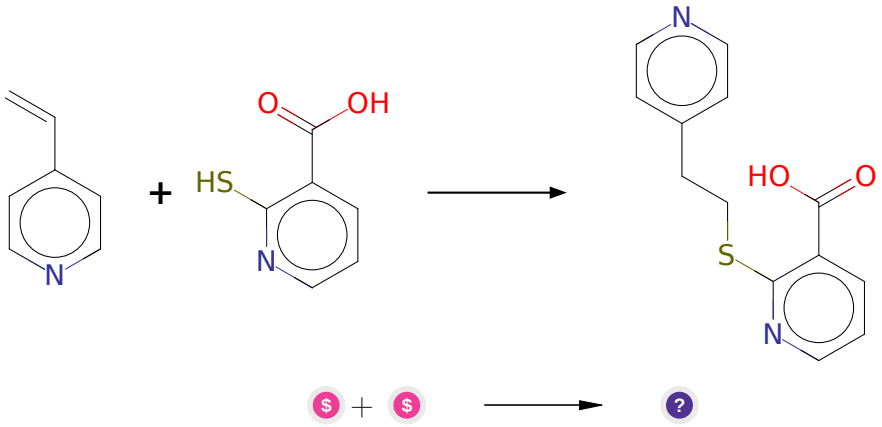


Figure 1: Outline of path 1

2.1.1 Hydrothiolation of alkenes



Substrates:

1. 2-Mercaptonicotinic acid - *available at Sigma-Aldrich*
2. 4-Vinylpyridine - *available at Sigma-Aldrich*

Products:

1. O=C(O)c1cccnc1SCCc1ccncc1

Typical conditions: acid.catalyst

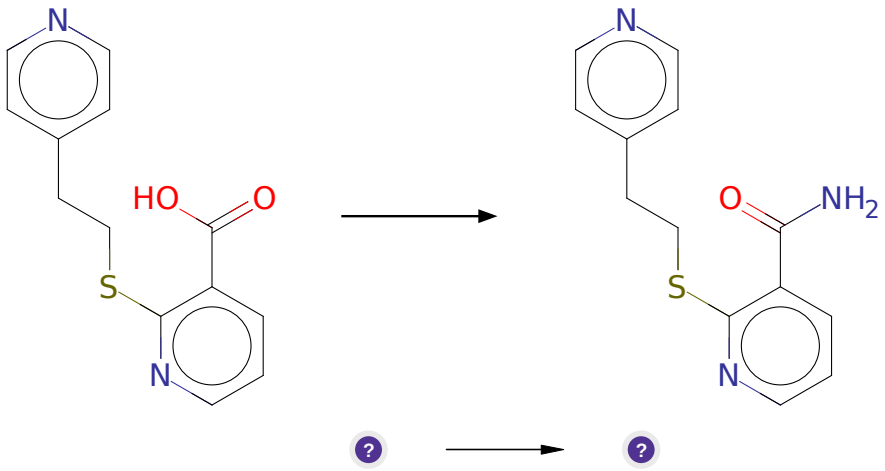
Protections: none

Yield: good

Reference: *10.1055/s-1999-2976* AND *10.1039/B9NJ00399A* AND *10.1016/j.catcom.2013.06.032*

Retrosynthesis ID: 15154

2.1.2 Synthesis of amides from carboxylic acids



Substrates:

1. O=C(O)c1cccnc1SCCc1ccncc1

Products:

1. NC(=O)c1cccnc1SCCc1ccncc1

Typical conditions: ammonia.coupling agent

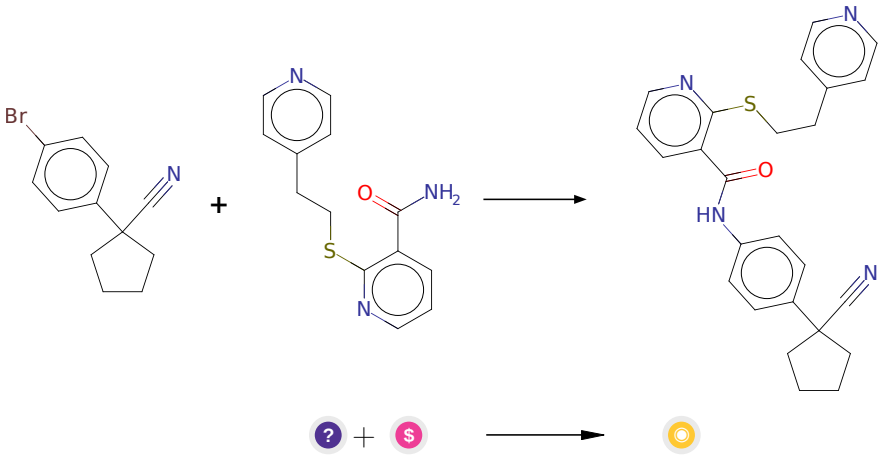
Protections: none

Yield: good

Reference: *10.1039/c1ob05430a* and *10.1016/j.tetlet.2005.08.021* and *10.3762/bjoc.12.55*

Retrosynthesis ID: 31360

2.1.3 Arylation of amides with aryl bromides



Substrates:

1. NC(=O)c1cccnc1SCCc1ccncc1
2. 1-(4-bromophenyl)cyclopentanecarbonitrile - *Combi-Blocks*

Products:

1. N#CC1(c2ccc(NC(=O)c3cccnc3SCCc3ccncc3)cc2)CCCC1

Typical conditions: Base.[Pd].catalyst.dioxane.heat or CuI.diamine.base.DMF.heat

Protections: none

Yield: good

Reference: *10.1021/ja0717414* and *10.1080/00397911.2016.1195844* and *10.1055/s-0035-1560473* and *10.3390/molecules190913448*

Retrosynthesis ID: 10012553