Paths of analysis*

Y3A

Synthia

October 10, 2022

1 Analysis parameters

Analysis type: Automatic Retrosynthesis

Rules: none selected

Filters: Exclude Diastereoselecitve reactions, Tunnels, FGI, FGI with protections

Max. paths returned: 50

Max. iterations: 2000

Commercial:

1. Max. molecular weight - 1000 g/mol
2. Max. price - 1500 $/g

Published:

1. Max. molecular weight - 1000 g/mol
2. Popularity - 5

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

FGI Coeff: 0

Tunnels 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: `1000161.11`

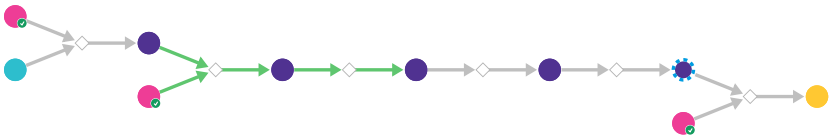
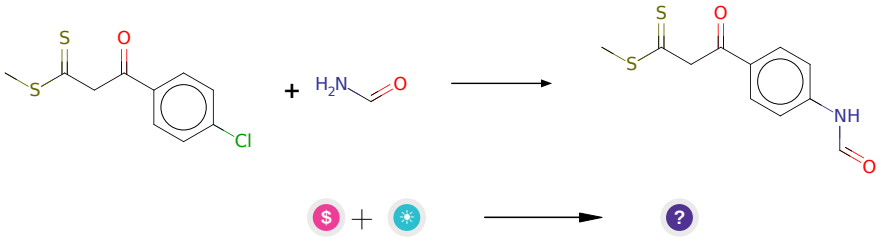


Figure 1: Outline of path 1

2.1.1 Arylation of amides with aryl chlorides



Substrates:

1. Amide C1 - *available at Sigma-Aldrich*
2. p-chlor-benzoyl-dithioessigsaeure-methylester

Products:

1. CSC(=S)CC(=O)c1ccc(NC=O)cc1

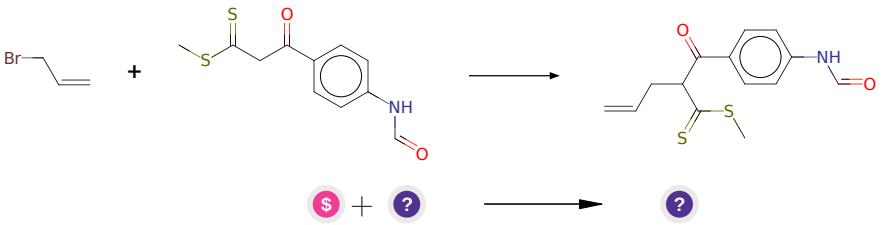
Typical conditions: Base.[Pd].catalyst.dioxane.heat or CuI.diamine.base.DMF.heat

Protections: none

Reference: *10.1021/ja0717414* and *10.1016/j.tet.2009.04.096* and *10.1002/chem.201302453* and *10.1080/00397911.2016.1195844*

Retrosynthesis ID: 10012552

2.1.2 Alkylation of ketones



Substrates:

1. Allyl bromide - *available at Sigma-Aldrich*
2. CSC(=S)CC(=O)c1ccc(NC=O)cc1

Products:

1. C=CCC(C(=O)c1ccc(NC=O)cc1)C(=S)SC

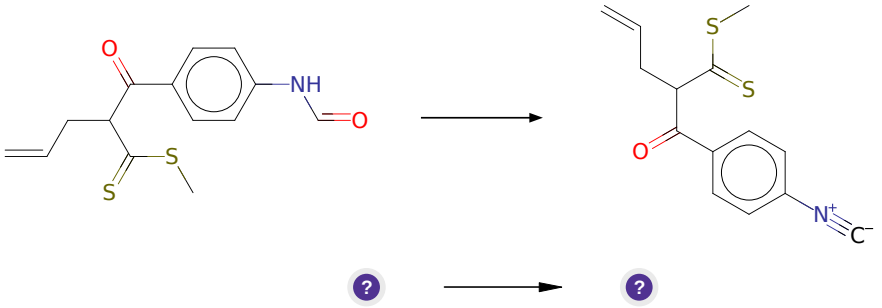
Typical conditions: LDA or other base.THF.-78C

Protections: none

Reference: DOI: *10.1021/jo1019738* OR DOI: *10.1021/jm00114a016*

Retrosynthesis ID: 1866

2.1.3 Synthesis of isocyanides from formamides



Substrates:

1. C=CCC(C(=O)c1ccc(NC=O)cc1)C(=S)SC

Products:

1. [C-]#[N+]c1ccc(C(=O)C(CC=C)C(=S)SC)cc1

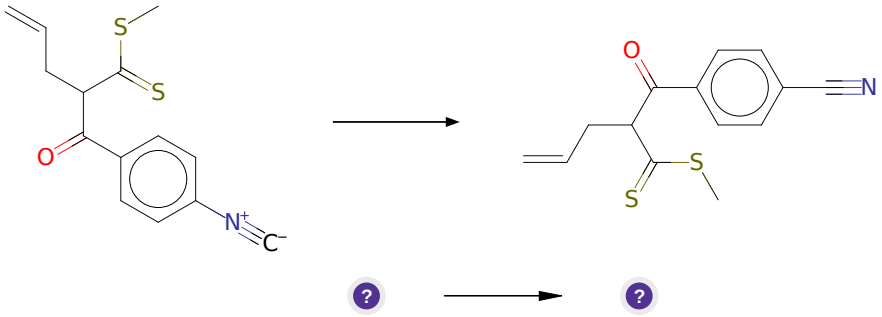
Typical conditions: TCT.DCM.TEA.MW.50-100C

Protections: none

Reference: DOI: *10.1021/jo047924f*

Retrosynthesis ID: 245867

2.1.4 Isonitrile-Nitrile Rearrangement



Substrates:

1. [C-]#[N+]c1ccc(C(=O)C(CC=C)C(=S)SC)cc1

Products:

1. C=CCC(C(=O)c1ccc(C#N)cc1)C(=S)SC

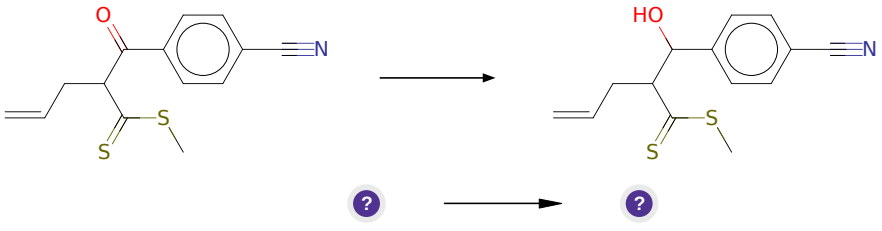
Typical conditions: (1-phenylethenyl)benzene.50C

Protections: none

Reference: DOI:*10.1021/jo00380a028*

Retrosynthesis ID: 10398

2.1.5 Reduction of ketones with NaBH4



Substrates:

1. C=CCC(C(=O)c1ccc(C#N)cc1)C(=S)SC

Products:

1. C=CCC(C(=S)SC)C(O)c1ccc(C#N)cc1

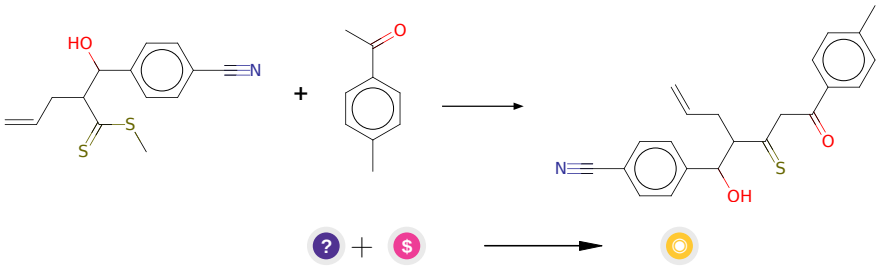
Typical conditions: NaBH4.EtOH.0-20 C

Protections: none

Reference: *10.1016/j.ejmech.2020.112360* p. 3, 8 and *10.1016/j.ejmech.2010.10.012* p. 434, 436

Retrosynthesis ID: 50432

2.1.6 Condensation of ketones with dithioesters



Substrates:

1. C=CCC(C(=S)SC)C(O)c1ccc(C#N)cc1
2. Methyl p-tolyl ketone - *available at Sigma-Aldrich*

Products:

1. C=CCC(C(=S)CC(=O)c1ccc(C)cc1)C(O)c1ccc(C#N)cc1

Typical conditions: NaH.DMF

Protections:

Functional group SMARTS	Classification	Protecting groups
[#6][CH]([#6])[OH]	alcohols	Methoxymethyl Ether (MOM) 2-Methoxyethoxymethyl Ether (MEM) Tetrahydropyranyl Ether (THP) Benzyl Ether (PMB) t-Butyldimethylsilyl Ether (TBDMS) Methyl Ether

Reference: *10.1021/jo400599e* and *10.1002/ejoc.201301667*

Retrosynthesis ID: 9996413