

Paths of analysis*

(re)Analysis 1381 - No Filter - Rerun

Synthia

November 28, 2023

1 Analysis parameters

Analysis type: Automatic Retrosynthesis

Saved Configuration: General

Rules: Expert-Coded Rules

Published Reactions: SPRESI by DeepMatter, USPTO, Enzyme-Catalyzed Reactions

Filters: none selected

Max. paths returned: 50

Max. iterations: 2000

Commercial:

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

Published:

1. Max. molecular weight - 1000 g/mol
2. Popularity - 15

My Stockroom:

1. Max. molecular weight - 1000 g/mol

Shorter paths: no

Pathway linearity: COMBO

Protecting groups: BALANCED

*The results stated herein were generated using the proprietary platform owned and maintained by Grzybowski Scientific Inventions, Inc., a subsidiary of Merck KGaA, Darmstadt Germany. The results are provided on an as is basis, and shall be used solely in connection with the rights afforded in the license agreement and for no other purpose.

1. 4-Methyl-5-(methylsulfanyl)-1,3-thiazol-2-amine - *available at Sigma-Aldrich*

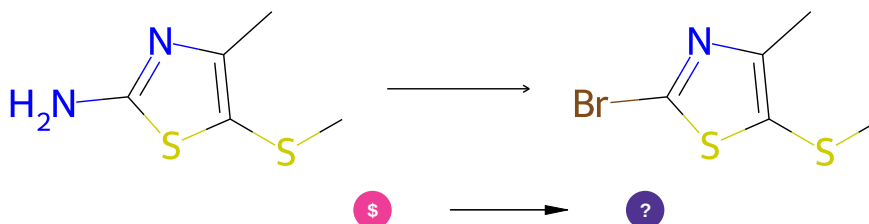
Typical conditions: Pd(OAc)₂.tBuONa.DME.110C

Protections: none

Reference: [10.1021/ja0580340](#)

Retrosynthesis ID: 1299

2.1.2 Sandmeyer Reaction



Substrates:

1. 4-Methyl-5-(methylsulfanyl)-1,3-thiazol-2-amine - *available at Sigma-Aldrich*

Products:

1. CSc1sc(Br)nc1C

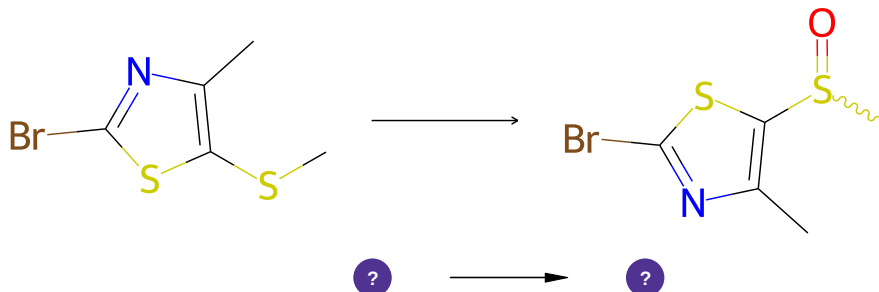
Typical conditions: IsoAmONO or t-BuONO.CuBr₂.MeCN or HBr.CuBr₂.NaNO₂

Protections: none

Reference: [10.1002/chem.201600278](#) and [10.1016/j.bmcl.2011.12.131](#) and [10.1016/j.ejmech.2013.01.046](#) and [10.1021/jm0002782](#) and [10.1002/ejoc.201300443](#) and [10.1021/jo052589w](#) (SI, page S3) and [10.1021/jm800527x](#) and [10.1016/j.bmcl.2015.04.098](#) and [10.1021/ja034563x](#)

Retrosynthesis ID: 29904

2.1.3 Oxidation of sulfides to sulfoxides



Substrates:

1. CSc1sc(Br)nc1C

Products:

1. Cc1nc(Br)sc1S(C)=O

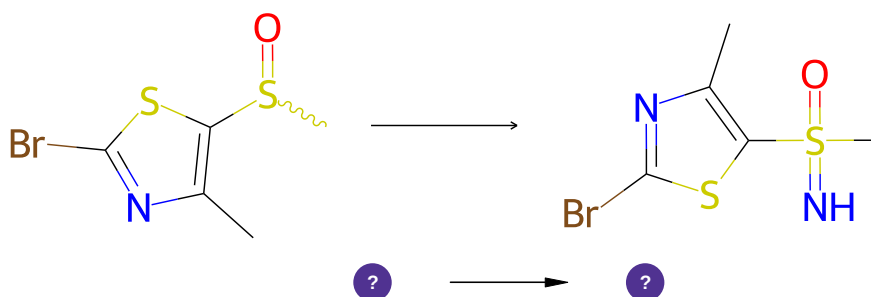
Typical conditions: TaC.H2O2.MeOH.45C

Protections: none

Reference: DOI: [10.1055/s-0029-1219947](https://doi.org/10.1055/s-0029-1219947) or DOI: [10.1055/s-2008-1067019](https://doi.org/10.1055/s-2008-1067019)

Retrosynthesis ID: 10584

2.1.4 Synthesis of NH-sulfoximines



Substrates:

1. Cc1nc(Br)sc1S(C)=O

Products:

1. Cc1nc(Br)sc1S(C)(=N)=O

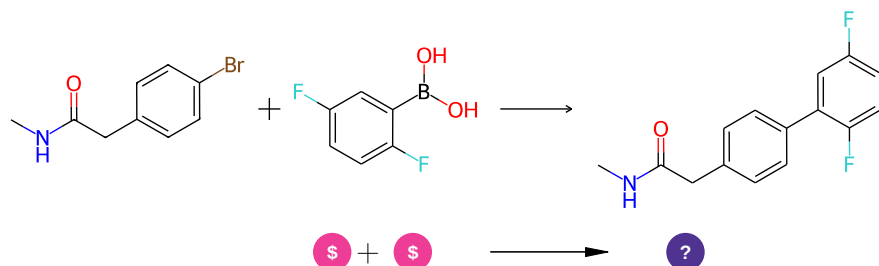
Typical conditions: NaN3.Eaton's reagent.50C or FeSO4.1,10-phen.NbzONH2*TfOH.MeCN or H2NCO2NH4.PhI(OAc)2.MeOH

Protections: none

Reference: [10.1016/j.tetlet.2016.12.031](#) and [10.1002/anie.201710498](#) and [10.1002/anie.201602320](#) and [10.1055/s-0036-1590874](#) and [10.1039/C7CC03386A](#)

Retrosynthesis ID: 31016630

2.1.5 Suzuki coupling of arylboronic acids with aryl bromides



Substrates:

- 2,5-Difluorophenylboronic acid - *Combi-Blocks*
- 2-(4-Bromophenyl)-N-methylacetamide - *available at Sigma-Aldrich*

Products:

- CNC(=O)Cc1ccc(-c2cc(F)ccc2F)cc1

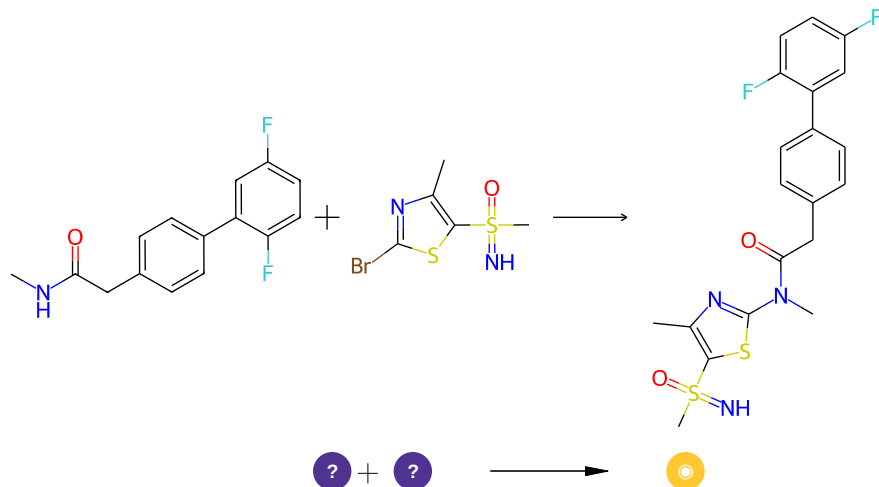
Typical conditions: Pd catalyst.base.solvent

Protections: none

Reference: [10.1021/cr00039a007](#) and [10.1007/3418_2012_32](#) and [10.1021/cr0505268](#) and [10.1016/j.jfluchem.2016.01.018](#) and [10.1039/C3CS60197H](#) and [10.1016/j.ejmech.2018.08.092](#) and [10.1038/s41929-020-00564-z](#) (metal-free coupling)

Retrosynthesis ID: 25150

2.1.6 N-arylation of amides



Substrates:

1. CNC(=O)Cc1ccc(-c2cc(F)ccc2F)cc1
2. Cc1nc(Br)sc1S(C)(=N)=O

Products:

1. Cc1nc(N(C)C(=O)Cc2ccc(-c3cc(F)ccc3F)cc2)sc1S(C)(=N)=O

Typical conditions: Cs₂CO₃.CuX₂/CuX.toluene.130C

Protections: none

Reference: [10.1021/ja012610k](#) and [10.1002/adsc.200700133](#) and [10.1021/jo701573w](#)

Retrosynthesis ID: 10207