

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.

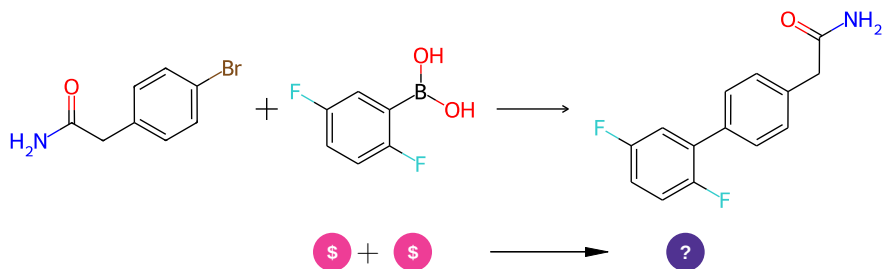
1. 4-Methyl-5-(methylsulfanyl)-1,3-thiazol-2-amine - *available at Sigma-Aldrich*

Protections: none

Reference: US20090143448A1

Retrosynthesis ID: 8454157

2.1.2 Suzuki coupling of arylboronic acids with aryl bromides



Substrates:

1. 2-(4-Bromophenyl)acetamide - *available at Sigma-Aldrich*
2. 2,5-Difluorophenylboronic acid - *Combi-Blocks*

Products:

1. NC(=O)Cc1ccc(-c2cc(F)ccc2F)cc1

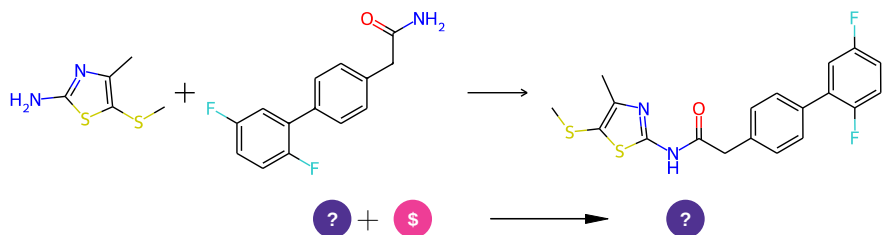
Typical conditions: Pd catalyst.base.solvent

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

2.1.3 Synthesis of N-arylamides from arenediazonium salts



Substrates:

1. NC(=O)Cc1ccc(-c2cc(F)ccc2F)cc1
2. 4-Methyl-5-(methylsulfanyl)-1,3-thiazol-2-amine - *available at Sigma-Aldrich*

Products:

1. CSc1sc(NC(=O)Cc2ccc(-c3cc(F)ccc3F)cc2)nc1C

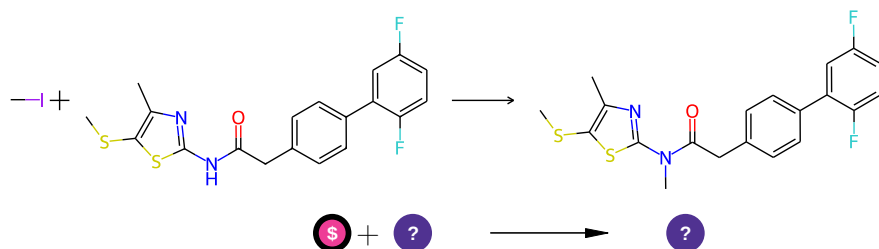
Typical conditions: 1) HCl.NaNO₂ 2) CuI.TBAI.N,N'-dimethylethane-1,2-diamine.K₂CO₃.DMSO.110C

Protections: none

Reference: DOI: [10.1055/s-0034-1378556](https://doi.org/10.1055/s-0034-1378556)

Retrosynthesis ID: 1922

2.1.4 N-alkylation of amides



Substrates:

1. Iodomethane - *available at Sigma-Aldrich*
2. CSc1sc(NC(=O)Cc2ccc(-c3cc(F)ccc3F)cc2)nc1C

Products:

1. CSc1sc(N(C)C(=O)Cc2ccc(-c3cc(F)ccc3F)cc2)nc1C

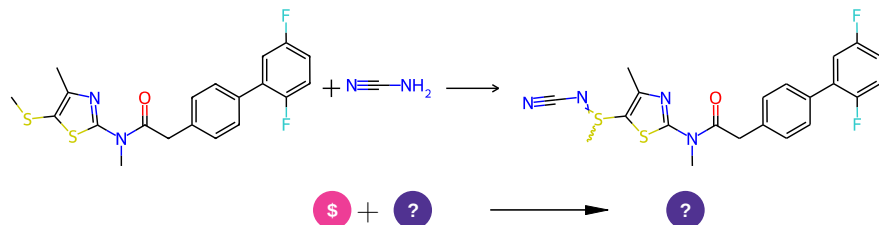
Typical conditions: NaH.DMF

Protections: none

Reference: DOI: [10.1016/j.bmc.2014.03.007](https://doi.org/10.1016/j.bmc.2014.03.007) and [10.1016/j.tetlet.2008.10.057](https://doi.org/10.1016/j.tetlet.2008.10.057)

Retrosynthesis ID: 8841

2.1.5 Synthesis of N-cyano sulfilimines



Substrates:

1. Cyanamide - *available at Sigma-Aldrich*
2. CSc1sc(N(C)C(=O)Cc2ccc(-c3cc(F)ccc3F)cc2)nc1C

Products:

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

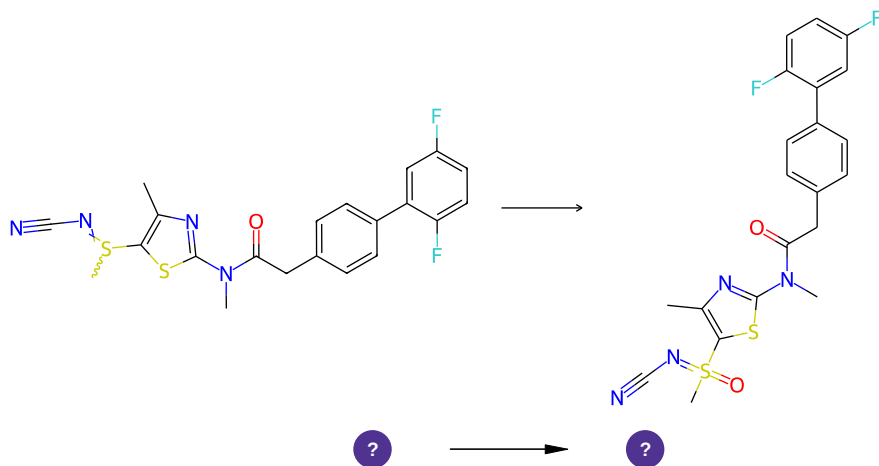
Typical conditions: PhI(OAc)2.CH3CN.0°C

Protections: none

Reference: US3505401A p.3-6 and *10.1021/ol7016577*

Retrosynthesis ID: 10033463

2.1.6 Synthesis of N-cyanosulfoximines by oxidation of N-cyano sulfilimines



Substrates:

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

Products:

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

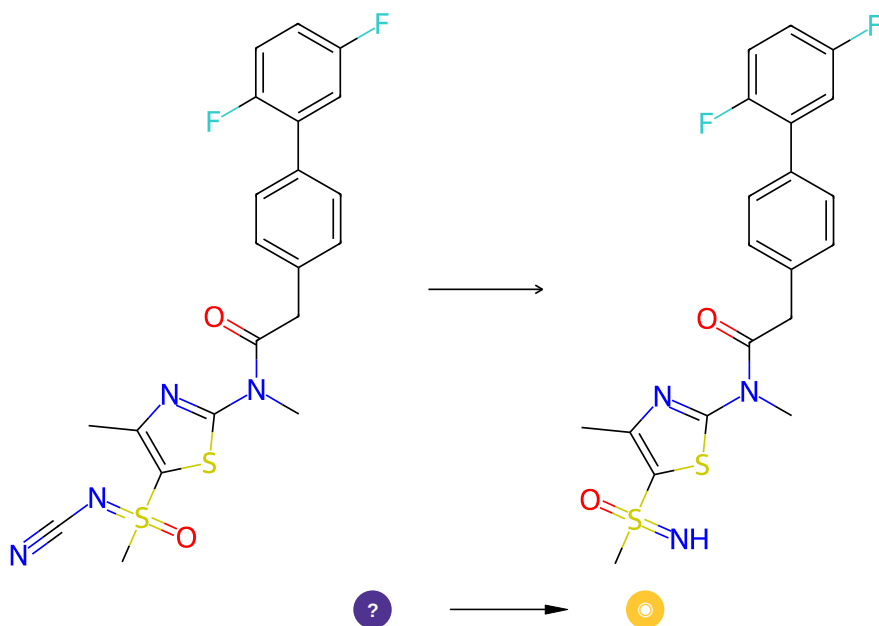
Typical conditions: mCPBA.MeOH.K₂CO₃

Protections: none

Reference: [10.1055/s-0030-1258192](#)

Retrosynthesis ID: 10037382

2.1.7 Synthesis of NH-sulfoximines by hydrolysis of N-cyano sulfoximines



Substrates:

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

Products:

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

Typical conditions: H₂SO₄.H₂O or HCl.dioxane.H₂O

Protections: none

Reference: [10.1055/s-0034-1378936](#) and US2009029863 p.11

Retrosynthesis ID: 10037380