



Information about the retrosynthesis

Created On: 2023-03-08T10:48:17.683000 UTC

Model: disconnection-aware-2022-06-24

Product: CC1N=C(N(C)C(=O)CC2C=CC(C3C(F)=CC=C(F)C=3)=CC=2)SC=1S(C)(=N)=O

Search strategy: hyper

MSSR: 15

MRP: 50

FAP: 0.65

SbP: 3

Availability pricing threshold: 20

Are materials exclusive: True

Enzymatic only: False

Available smiles:

Exclude smiles: CC1N=C(N(C)C(=O)CC2C=CC(C3C(F)=CC=C(F)C=3)=CC=2)SC=1S(C)(=N)=O

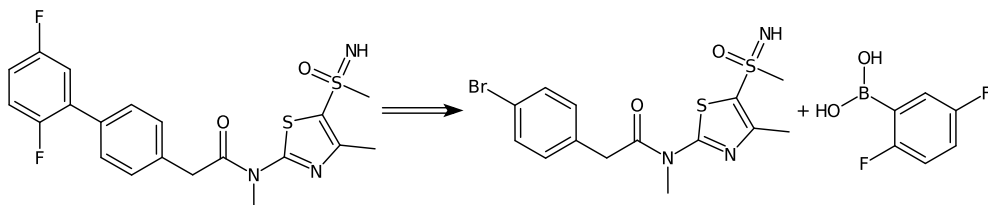
Exclude substructures:

Sequence 2, Confidence: 0.7014809338503818

Step 1

Type: Bromo Suzuki-type coupling, Confidence: 0.952

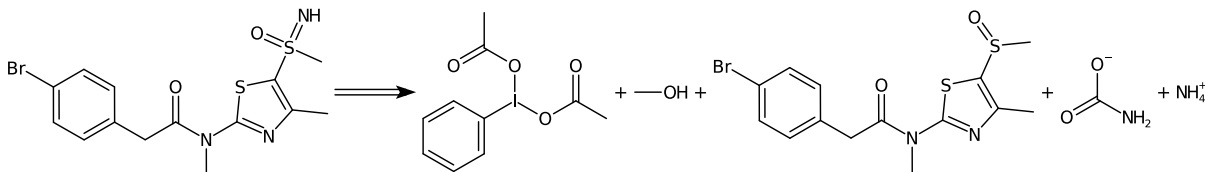
Cc1nc(N(C)C(=O)Cc2ccc(Br)cc2)sc1S(C)(=N)=O.OB(O)c1cc(F)ccc1F>>CC1N=C(N(C)C(=O)CC2C=CC(C3C(F)=CC=C(F)C=3)=CC=2)SC=1S(C)(=N)=O



Step 2

Type: Unrecognised, Confidence: 0.92

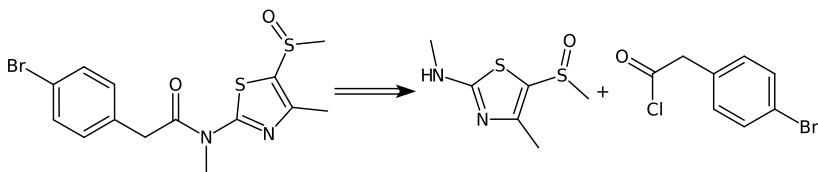
CC(=O)OI(OC(C)=O)c1ccccc1.CO.Cc1nc(N(C)C(=O)Cc2ccc(Br)cc2)sc1S(C)=O.NC(=O)[O-].[NH4+]>>Cc1nc(N(C)C(=O)Cc2ccc(Br)cc2)sc1S(C)(=N)=O



Step 3

Type: Amide Schotten-Baumann, Confidence: 0.969

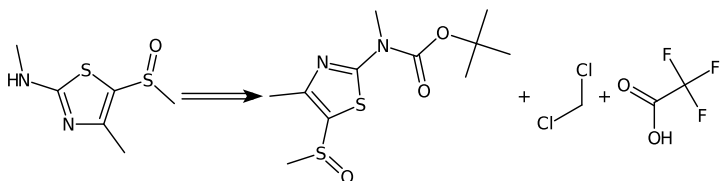
CNc1nc(C)c(S(C)=O)s1.O=C(Cl)Cc1ccc(Br)cc1>>Cc1nc(N(C)C(=O)Cc2ccc(Br)cc2)sc1S(C)=O



Step 4

Type: N-Boc deprotection, Confidence: 0.971

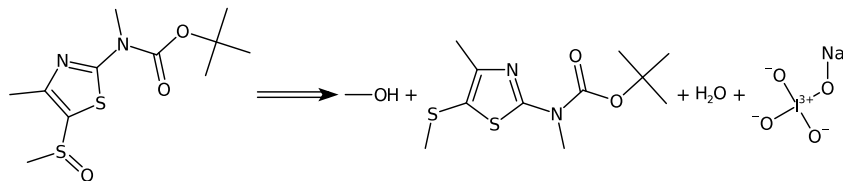
Cc1nc(N(C)C(=O)OC(C)(C)C)sc1S(C)=O.ClCCl.O=C(O)C(F)(F)F>>CNc1nc(C)c(S(C)=O)s1



Step 5

Type: Sulfanyl to sulfinyl, Confidence: 0.942

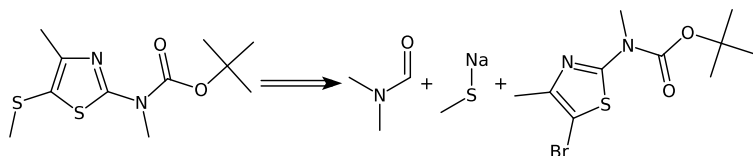
CO.CSc1sc(N(C)C(=O)OC(C)(C)C)nc1C.O.[O-][I+3]([O-])([O-])O[Na]>>Cc1nc(N(C)C(=O)OC(C)(C)C)sc1S(C)=O



Step 6

Type: Unrecognised, Confidence: 0.966

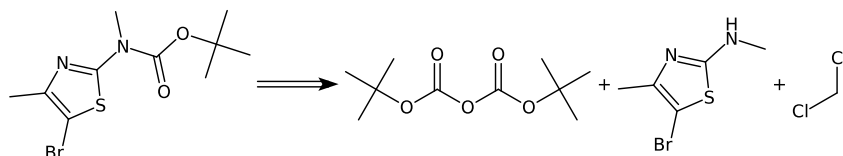
CN(C)C=O.CS[Na].Cc1nc(N(C)C(=O)OC(C)(C)C)sc1Br>>CSc1sc(N(C)C(=O)OC(C)(C)C)nc1C



Step 7

Type: N-Boc protection, Confidence: 0.972

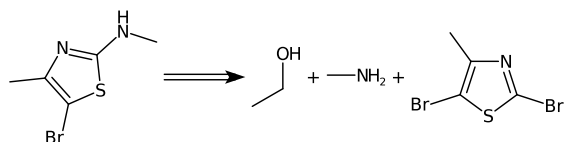
CC(C)(C)OC(=O)OC(=O)OC(C)(C)C.CNc1nc(C)c(Br)s1.ClCCl>>Cc1nc(N(C)C(=O)OC(C)(C)C)sc1Br



Step 8

Type: Bromo N-arylation, Confidence: 0.968

CCO.CN.Cc1nc(Br)sc1Br>>CNc1nc(C)c(Br)s1



Step 9

Type: Amino to bromo, Confidence: 0.993

Br[Cu]Br.CC#N.CC(C)(C)ON=O.Cc1nc(N)sc1Br>>Cc1nc(Br)sc1Br

