



Information about the retrosynthesis

Created On: 2023-03-08T10:28:07.696000 UTC

Model: disconnection-aware-2022-06-24

Product: CC1=C(S(=O)(=N)C)SC(N(C(CC2C=CC(C3=CC(F)=CC=C3F)=CC=2)=O)C)=N1

Search strategy: hyper

MSSR: 10

MRP: 50

FAP: 0.65

SbP: 3

Availability pricing threshold: 0

Are materials exclusive: True

Enzymatic only: False

Available smiles:

Exclude smiles: CC1=C(S(=O)(=N)C)SC(N(C(CC2C=CC(C3=CC(F)=CC=C3F)=CC=2)=O)C)=N1

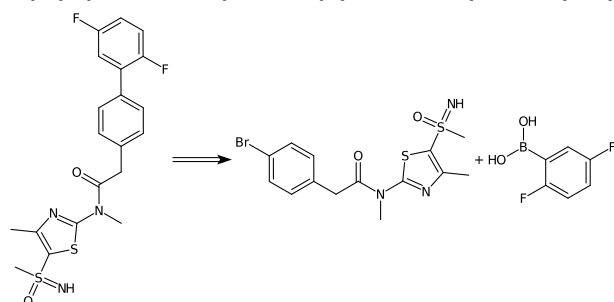
Exclude substructures:

Sequence 2, Confidence: 0.7447737231863633

Step 1

Type: Bromo Suzuki-type coupling, Confidence: 0.952

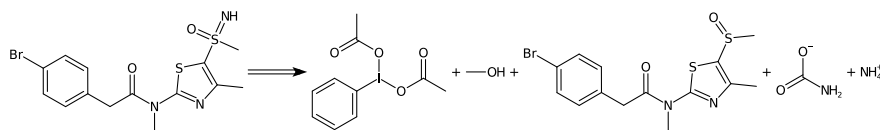
Cc1nc(N(C)C(=O)Cc2ccc(Br)cc2)sc1S(C)(=N)=O.OB(O)c1cc(F)ccc1F>>CC1=C(S(=O)(=N)C)S
C(N(C)C(Cc2cc(C3=CC(F)=CC=C3F)=CC=2)=O)C)=N1



Step 2

Type: Unrecognised, Confidence: 0.92

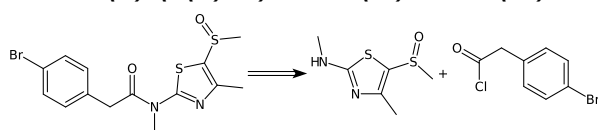
CC(=O)OI(OC(C)=O)c1ccccc1.CO.Cc1nc(N(C)C(=O)Cc2ccc(Br)cc2)sc1S(C)=O.NC(=O)[O-].[NH4+]>>Cc1nc(N(C)C(=O)Cc2ccc(Br)cc2)sc1S(C)(=N)=O



Step 3

Type: Amide Schotten-Baumann, Confidence: 0.969

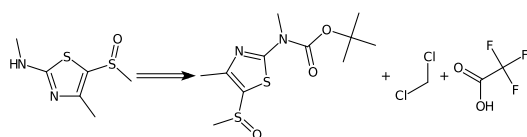
CNc1nc(C)c(S(C)=O)s1.O=C(Cl)Cc1ccc(Br)cc1>>Cc1nc(N(C)C(=O)Cc2ccc(Br)cc2)sc1S(C)=O



Step 4

Type: N-Boc deprotection, Confidence: 0.971

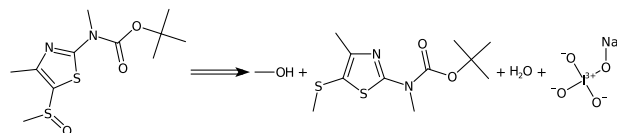
Cc1nc(N(C)C(=O)OC(C)(C)C)sc1S(C)=O.ClCCl.O=C(O)C(F)(F)F>>CNc1nc(C)c(S(C)=O)s1



Step 5

Type: Sulfanyl to sulfinyl, Confidence: 0.942

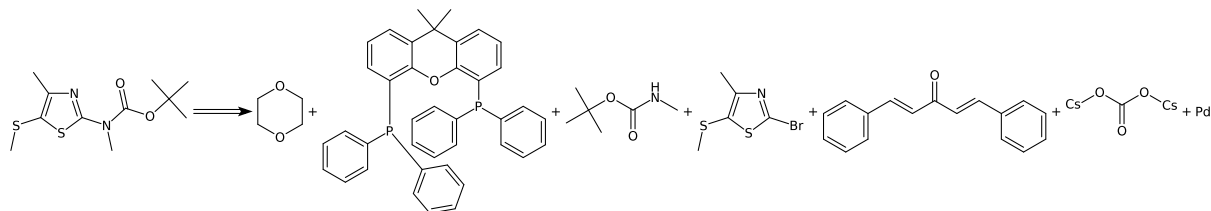
CO.CSc1sc(N(C)C(=O)OC(C)(C)C)nc1C.O.[O-][I+3]([O-])([O-])O[Na]>>Cc1nc(N(C)C(=O)OC(C)(C)C)sc1S(C)=O



Step 6

Type: Bromo Buchwald-Hartwig amination, Confidence: 0.962

C1COCCO1.CC1(C)c2cccc(P(c3ccccc3)c3ccccc3)c2Oc2c(P(c3ccccc3)c3ccccc3)cccc21.CNC(=O)OC(C)(C)C.CSc1sc(Br)nc1C.O=C(/C=C/c1ccccc1)/C=C/c1ccccc1.O=C(O[Cs])O[Cs].[Pd]>>CSc1sc(N(C)C(=O)OC(C)(C)C)nc1C



Step 7

Type: Amino to bromo, Confidence: 0.996

Br[Cu]Br.CC#N.CC(C)(C)ON=O.CCOC(C)=O.CSc1sc(N)nc1C>>CSc1sc(Br)nc1C

