



## 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

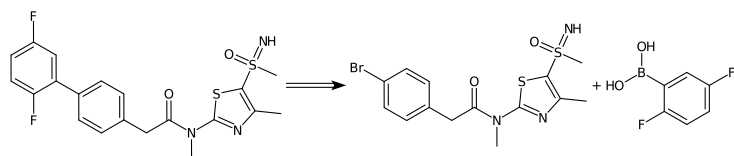
Exclude substructures:

## Sequence 0, Confidence: 0.7262175309184802

### Step 1

Type: Bromo Suzuki-type coupling, Confidence: 0.952

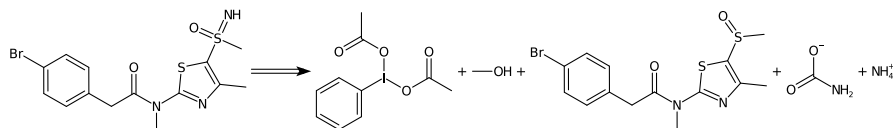
Cc1nc(N(C)C(=O)Cc2ccc(Br)cc2)sc1S(C)(=N)=O.OB(O)c1cc(F)ccc1F>>CC1N=C(N(C)C(=O)CC2C=CC(C3C(F)=CC=C(F)C=3)=CC=2)SC(=N)=O



### Step 2

Type: Unrecognised, Confidence: 0.92

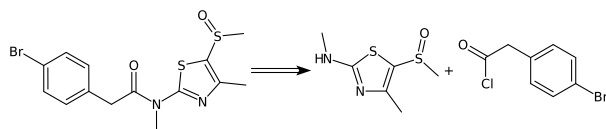
CC(=O)OI(OC(C)=O)c1ccccc1.CO.Cc1nc(N(C)C(=O)Cc2ccc(Br)cc2)sc1S(C)=O.NC(=O)[O-].[NH4+]>>Cc1nc(N(C)C(=O)Cc2ccc(Br)cc2)sc1S(C)(=N)=O



### Step 3

Type: Amide Schotten-Baumann, Confidence: 0.969

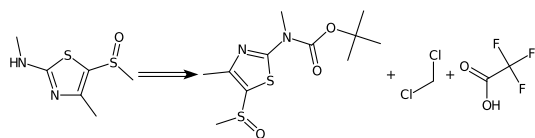
CNc1nc(C)c(S(C)=O)s1.O=C(Cl)Cc1ccc(Br)cc1>>Cc1nc(N(C)C(=O)Cc2ccc(Br)cc2)sc1S(C)=O



### 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

CC1=C(C)N(C(=O)OC(C)(C)C)C2=CC(=C(C)S2)S(=O)(=O)C1>>CC1=C(C)N(C(=O)OC(C)(C)C)C2=CC(=C(C)S2)S(=O)(=O)C1.[OH-].[Na+].[O-]P([O-])([O-])[O-].O

**Type: Unrecognised, Confidence: 0.97**

CC(C)(C)OC(=O)N1C(C)N=C(S1)SC2=CC=CC=C2.CC(C)(C)OC(=O)N1C(C)N=C(S1)SC2=CC=CC=C2>>C1CCOC1.CS.SC.CC(C)(C)OC(=O)N1C(C)N=C(S1)SC2=CC=CC=C2.CCCC[Li]

**Type: Bromo Buchwald-Hartwig amination, Confidence: 0.964**

Chemical reaction scheme showing the synthesis of a phosphonium salt. The reaction involves 4-methyl-5-(tert-butoxycarbonylamino)thiazole, 1,3,4,5-tetra-tert-butylphosphonium hexafluorophosphate, 4-bromothiazole, 4,4'-diphenyl-1,3-diene, and cesium fluoride in the presence of a palladium catalyst. The product is a phosphonium salt where the thiazole ring is coupled to the biphenyl system.