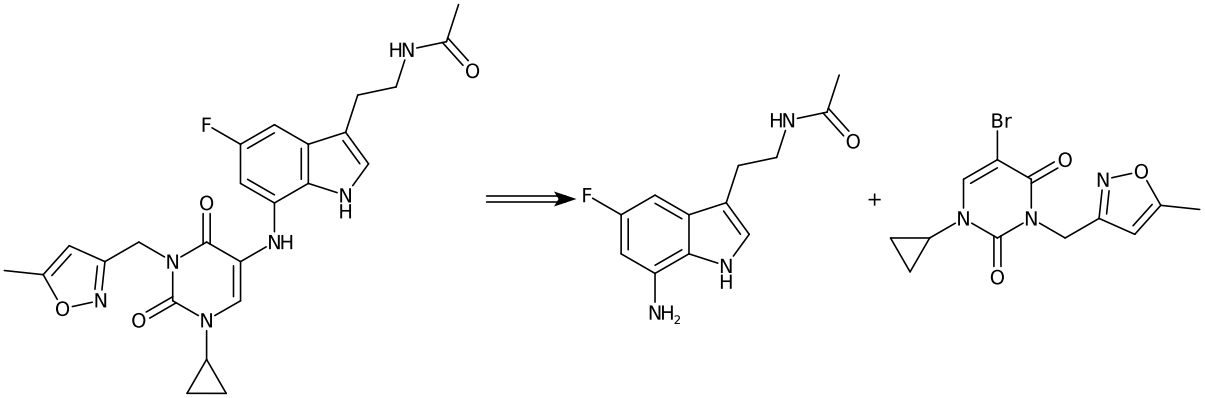
Sequence 0, Confidence: 0.714

Step 1

Type: Bromo N-arylation, Confidence: 0.898

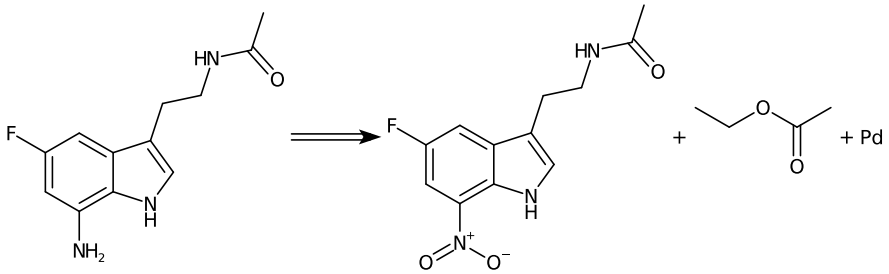
CC(=O)NCCc1c[nH]c2c(N)cc(F)cc12.Cc1cc(Cn2c(=O)c(Br)cn(C3CC3)c2=O)no1>>C1(C2C([H])=C(F)C([H])=C(N([H])C3=C([H])N(C([H])4C([H])([H])C4([H])[H])C(=O)N(C([H])([H])C4=NOC(C([H])([H])[H])=C4[H])C3=O)C=2N([H])C=1[H])C([H])([H])C([H])([H])N([H])C(=O)C([H])([H])[H]



Step 2

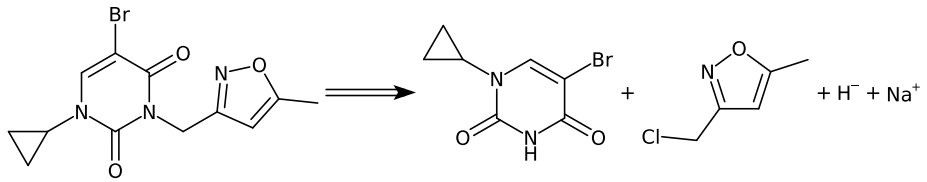
Type: Nitro to amino, Confidence: 0.978

CC(=O)NCCc1c[nH]c2c([N+](=O)[O-])cc(F)cc12.CCOC(C)=O.[Pd]>>CC(=O)NCCc1c[nH]c2c(N)cc(F)cc12



Type: Chloro N-alkylation, Confidence: 0.987

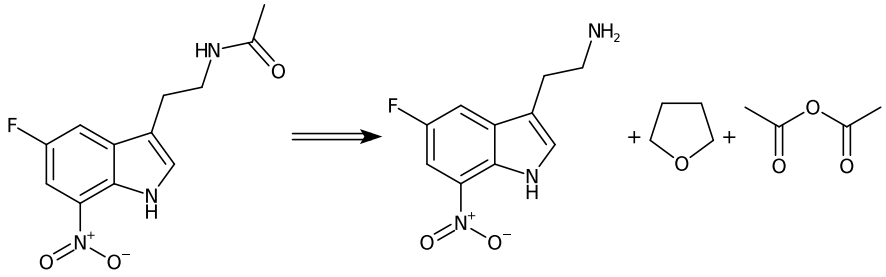
O=c1[nH]c(=O)n(C2CC2)cc1Br.Cc1cc(CCl)no1.[H-].[Na+]>>Cc1cc(Cn2c(=O)c(Br)cn(C3CC3)c2=O)no1



Step 3

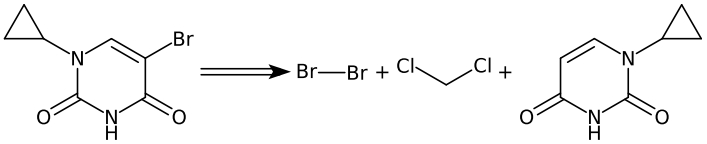
Type: N-acetylation, Confidence: 0.96

NCCc1c[nH]c2c([N+](=O)[O-])cc(F)cc12.C1CCOC1.CC(=O)OC(C)=O>>CC(=O)NCCc1c[nH]c2c([N+](=O)[O-])cc(F)cc12



Type: Bromination, Confidence: 0.986

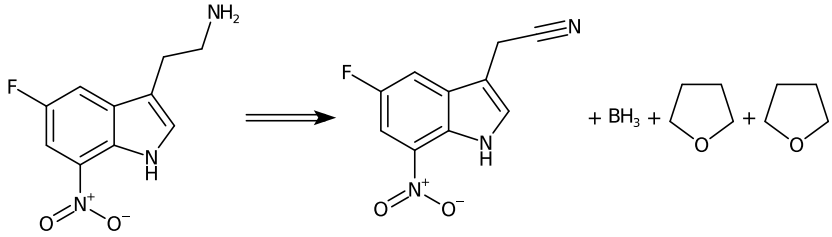
BrBr.ClCCl.O=c1ccn(C2CC2)c(=O)[nH]1>>O=c1[nH]c(=O)n(C2CC2)cc1Br



Step 4

Type: Nitrile reduction, Confidence: 0.957

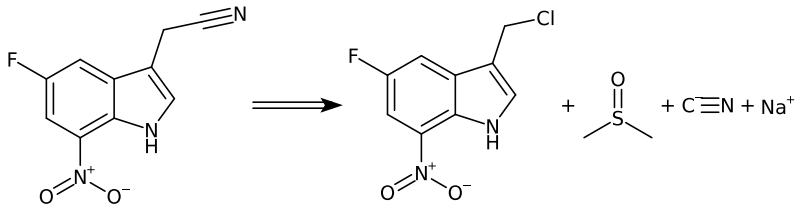
N#CCc1c[nH]c2c([N+](=O)[O-])cc(F)cc12.B.C1CCOC1.C1CCOC1>>NCCc1c[nH]c2c([N+](=O)[O-])cc(F)cc12



Step 5

Type: Chloro Kolbe nitrile synthesis, Confidence: 0.982

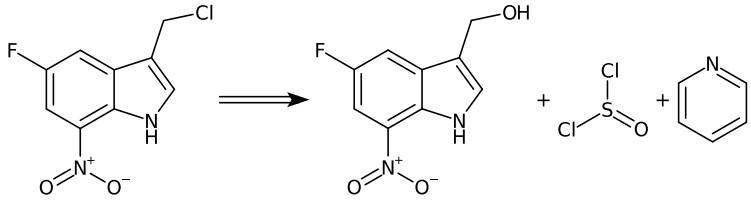
O=[N+]([O-])c1cc(F)cc2c(CCl)c[nH]c12.CS(C)=O.[C-]#N.[Na+]>>N#CCc1c[nH]c2c([N+](=O)[O-])cc(F)cc12



Step 6

Type: Hydroxy to chloro, Confidence: 0.978

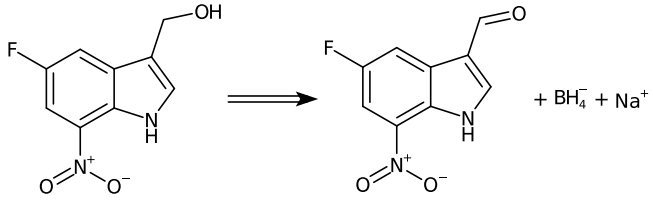
O=[N+]([O-])c1cc(F)cc2c(CO)c[nH]c12.O=S(Cl)Cl.c1ccncc1>>O=[N+]([O-])c1cc(F)cc2c(CCl)c[nH]c12



Step 7

Type: Aldehyde to alcohol reduction, Confidence: 0.965

O=Cc1c[nH]c2c([N+](=O)[O-])cc(F)cc12.[BH4-].[Na+]>>O=[N+]([O-])c1cc(F)cc2c(CO)c[nH]c12



Step 8

Type: Vilsmeier-Haack reaction, Confidence: 0.981

CN(C)C=O.O.O=P(Cl)(Cl)Cl.O=[N+]([O-])c1cc(F)cc2cc[nH]c12>>O=Cc1c[nH]c2c([N+](=O)[O-])cc(F)cc12