

Compound, SMILES

1, [H]C(C1=CC=CC=C1Br)=O
 2, OC1(CCC(CC1)=O)C2=CC=CC=C2CC(OC)OC
 3, O=C(CC1)CCC21C3=CC=CC=C3C=CO2
 4a, [H][C@@](CC1)(NCC2CCCCC2)CC[C@]31OC=CC4=CC=CC=C43
 4b, [H][C@](CC1)(NCC2CCCCC2)CC[C@]31OC=CC4=CC=CC=C43
 5a, [H][C@@](CC1)(N(C)CC2CCCCC2)CC[C@]31OC=CC4=CC=CC=C43
 5b, [H][C@](CC1)(N(C)CC2CCCCC2)CC[C@]31OC=CC4=CC=CC=C43
 6, CCOC1OC2(CCC(CC2)=O)C3=CC=CC=C3C1
 7a, [H][C@@](CC1)(NCC2CCCCC2)CC[C@]31OC(OCC)CC4=CC=CC=C43
 7b, [H][C@](CC1)(NCC2CCCCC2)CC[C@]31OC(OCC)CC4=CC=CC=C43
 8a, [H][C@@](CC1)(N(C)CC2CCCCC2)CC[C@]31OC(OCC)CC4=CC=CC=C43
 8b, [H][C@](CC1)(N(C)CC2CCCCC2)CC[C@]31OC(OCC)CC4=CC=CC=C43
 9, O=C(CC1)CCC21C3=CC=CC=C3CC(OC)O2
 10a, [H][C@@](CC1)(NCC2CCCCC2)CC[C@]31OC(OC)CC4=CC=CC=C43
 10b, [H][C@](CC1)(NCC2CCCCC2)CC[C@]31OC(OC)CC4=CC=CC=C43
 11a, [H][C@@](CC1)(N(C)CC2CCCCC2)CC[C@]31OC(OC)CC4=CC=CC=C43
 11b, [H][C@](CC1)(N(C)CC2CCCCC2)CC[C@]31OC(OC)CC4=CC=CC=C43
 12, BrC1=CC=CC=C1C(OC)OC
 13, O=C(CC1)CCC21C3=CC=CC=C3C(OC)O2
 14a, [H][C@@](CC1)(NCC2CCCCC2)CC[C@@]31C(C=CC=C4)=C4C(OC)O3
 14b, [H][C@](CC1)(NCC2CCCCC2)CC[C@@]31C(C=CC=C4)=C4C(OC)O3
 15a, [H][C@@](CC1)(N(C)CC2CCCCC2)CC[C@@]31C(C=CC=C4)=C4C(OC)O3
 15b, [H][C@](CC1)(N(C)CC2CCCCC2)CC[C@@]31C(C=CC=C4)=C4C(OC)O3
 16, OCCC1=CC=CC=C1Br
 17, C12=CC=CC=C1CCOC23CCC4(OCCO4)CC3
 18, O=C(CC1)CCC21C3=CC=CC=C3CCO2
 19a, [H][C@@](CC1)(NCC2CCCCC2)CC[C@]31OCCC4=CC=CC=C43
 19b, [H][C@](CC1)(NCC2CCCCC2)CC[C@]31OCCC4=CC=CC=C43
 20a, [H][C@@](CC1)(N(C)CC2CCCCC2)CC[C@]31OCCC4=CC=CC=C43
 20b, [H][C@](CC1)(N(C)CC2CCCCC2)CC[C@]31OCCC4=CC=CC=C43
 21a, [H][C@@](CC1)(NCC2=CC=CC=C2)CC[C@]31OC(OC)CC4=CC=CC=C43
 21b, [H][C@](CC1)(NCC2=CC=CC=C2)CC[C@]31OC(OC)CC4=CC=CC=C43
 22a, [H][C@@](CC1)(N(C)CC2=CC=CC=C2)CC[C@]31OC(OC)CC4=CC=CC=C43
 22b, [H][C@](CC1)(N(C)CC2=CC=CC=C2)CC[C@]31OC(OC)CC4=CC=CC=C43
 23a, [H][C@@](CC1)(NCC2=CC=CC=C2)CC[C@@]31C(C=CC=C4)=C4C(OC)O3
 23b, [H][C@](CC1)(NCC2=CC=CC=C2)CC[C@@]31C(C=CC=C4)=C4C(OC)O3
 24a, [H][C@@](CC1)(NCC2=CC=CC=C2)CC[C@]31OCCC4=CC=CC=C43
 24b, [H][C@](CC1)(NCC2=CC=CC=C2)CC[C@]31OCCC4=CC=CC=C43