

Compound\_ID,SMILES,IC50 or other compound property (optional),Other compound property (optic

- 1 O=C(NCCC1=CC=C(OC)C=C1)NC2=C(C(O)=O)SC(C3=CC(Cl)=C(Cl)C=C3)=C2
- 2 O=C(N)NC1=C(C(O)=O)SC(C2=CC(Cl)=C(Cl)C=C2)=C1
- 3 O=C(NC(C)C)NC1=C(C(O)=O)SC(C2=CC(Cl)=C(Cl)C=C2)=C1
- 4 O=C(NCCCC)NC1=C(C(O)=O)SC(C2=CC(Cl)=C(Cl)C=C2)=C1
- 5 O=C(NCCCCC)NC1=C(C(O)=O)SC(C2=CC(Cl)=C(Cl)C=C2)=C1
- 6 O=C(NCCC(O)=O)NC1=C(C(O)=O)SC(C2=CC(Cl)=C(Cl)C=C2)=C1
- 7 O=C(NC1=CC=CC=C1)NC2=C(C(O)=O)SC(C3=CC(Cl)=C(Cl)C=C3)=C2
- 8 O=C(NCCC1=CC=CC=C1)NC2=C(C(O)=O)SC(C3=CC(Cl)=C(Cl)C=C3)=C2
- 9 O=C(NCCCC1=CC=CC=C1)NC2=C(C(O)=O)SC(C3=CC(Cl)=C(Cl)C=C3)=C2
- 10 O=C(NCCC1=NC=CC=C1)NC2=C(C(O)=O)SC(C3=CC(Cl)=C(Cl)C=C3)=C2
- 11 O=C(NCCC1=CN=CC=C1)NC2=C(C(O)=O)SC(C3=CC(Cl)=C(Cl)C=C3)=C2
- 12 O=C(NCCC1=CC=NC=C1)NC2=C(C(O)=O)SC(C3=CC(Cl)=C(Cl)C=C3)=C2
- 13 O=C(N(C)C1=CC=CC=C1)NC2=C(C(O)=O)SC(C3=CC(Cl)=C(Cl)C=C3)=C2
- 14 O=C(N(CC)C1=CC=CC=C1)NC2=C(C(O)=O)SC(C3=CC(Cl)=C(Cl)C=C3)=C2
- 15 O=C(N(CCCC)C1=CC=CC=C1)NC2=C(C(O)=O)SC(C3=CC(Cl)=C(Cl)C=C3)=C2
- 16 O=C(N(CCCC)CC1=CC=CC=C1)NC2=C(C(O)=O)SC(C3=CC(Cl)=C(Cl)C=C3)=C2
- 17 O=C(N(CCCC)CCC1=CC=CC=C1)NC2=C(C(O)=O)SC(C3=CC(Cl)=C(Cl)C=C3)=C2
- 18 O=C(N(C)CC1=CC=CC=C1)NC2=C(C(O)=O)SC(C3=CC(Cl)=C(Cl)C=C3)=C2
- 19 O=C(N(CC)CC1=CC=CC=C1)NC2=C(C(O)=O)SC(C3=CC(Cl)=C(Cl)C=C3)=C2
- 20 O=C(N(C1=CC=CC=C1)CC2=CC=CC=C2)NC3=C(C(O)=O)SC(C4=CC(Cl)=C(Cl)C=C4)=C3
- 21 O=C(N(CC1=CC=CC=C1)CC2=CC=CC=C2)NC3=C(C(O)=O)SC(C4=CC(Cl)=C(Cl)C=C4)=C3
- 22 O=C(NCCCCC)NC1=C(C(O)=O)SC(C2=CC=CC=C2)=C1
- 23 O=C(NCCCCC)NC1=C(C(O)=O)SC(C2=CC(Cl)=CC=C2)=C1
- 24 O=C(NCCCCC)NC1=C(C(O)=O)SC(C2=CC=C(Cl)C=C2)=C1
- 25 O=C(NCCCCC)NC1=C(C(O)=O)SC(C2=C(Cl)C=C(Cl)C=C2)=C1
- 26 O=C(NCCCCC)NC1=C(C(O)=O)SC(C2=C(Cl)C=CC(Cl)=C2)=C1
- 27 O=C(NCCCCC)NC1=C(C(O)=O)SC(C2=CC(C(F)(F)F)=C(Cl)C=C2)=C1
- 28 O=C(NCCCCC)NC1=C(C(O)=O)SC(C2=CC=C(OC)C=C2)=C1
- 29 O=C(NCCCCC)NC1=C(C(O)=O)SC(C2=CC([N+])([O-])=CC=C2)=C1
- 30 O=C(NCCCCC)NC1=C(C(O)=O)SC(C2=CC=C([N+])([O-])=C=C2)=C1
- 31 O=C(NCCCCC)NC1=C(C(O)=O)SC(C2=CC(C(F)(F)F)=CC=C2)=C1
- 32 O=C(NCCCCC)NC1=C(C(O)=O)SC(C2=CC=C(C(F)(F)F)C=C2)=C1
- 33 O=C(N(CC1=CC=CC=C1)CC)NC2=C(C(O)=O)SC(C3=CC(Cl)=CC(Cl)=C3)=C2
- 34 O=C(N(CC1=CC=CC=C1)CC)NC2=C(C(O)=O)SC(C3=CC=C(Br)C=C3)=C2
- 35 O=C(N(CC1=CC=CC=C1)CC)NC2=C(C(O)=O)SC(C3=CC=C(C)C=C3)=C2
- 36 O=C(N(CC1=CC=CC=C1)CC)NC2=C(C(O)=O)SC(C3=CC=C(OC(F)(F)F)C=C3)=C2
- 37 O=C(N(CC1=CC=CC=C1)CC)NC2=C(C(O)=O)SC(C3=CC=C(C#N)C=C3)=C2
- 38 O=C(N(CC1=CC=CC=C1)CC)NC2=C(C(O)=O)SC(C3=CC=C(OC4=CC=CC=C4)C=C3)=C2
- 39 O=C(NCCCCC)NC1=C(C(O)=O)C=C(C2=CC(Cl)=C(Cl)C=C2)S1
- 40 O=C(NCCCCC)NC1=C(C(O)=O)SC=C1C2=CC=C(Cl)C(Cl)=C2
- 41 ClC(Cl)=C1=CC=C1C2=CSC(NCCCCC)=O=C2C(O)=O
- 42 NC1=C(C(O)=O)SC=C1C2=CC=C(Cl)C(Cl)=C2
- 43 O=C(NCCCCC)NC1=C(C(O)=O)SC=C1
- 44 CCCCC(NC1=C(C(O)=O)SC=C1C2=CC=C(Cl)C(Cl)=C2)=O
- 45 CCCCCNC1=C(C(O)=O)SC=C1C2=CC=C(Cl)C(Cl)=C2
- 46 ClC1=CC=C(C2=C(NC(NCCCCC)=O)C(C(O)=O)=CC=C2)C=C1Cl
- 47 O=C(N(CCCC)C1=CC=CC=C1)NC2=C(C(O)=O)SC=C2C3=C(Cl)C=CC(Cl)=C3
- 48 O=C(N(CCCC)C1=CC=CC=C1)NC2=C(C(O)=O)SC=C2C3=CC=C(OC4=CC=CC=C4)C=C3

onal),Other compound property (optional)