

Sample ID	IC50 (uM)	Curve Class	Efficacy (%)
NCGC00249758-02	19.18	-2.2	-90.55
NCGC00253871-01	15.24	-2.2	-88.89
NCGC00253874-01	17.10	-2.2	-87.52
NCGC00249752-01	21.52	-2.2	-86.36
NCGC00411091-01	44.08	-2.2	-83.34
NCGC00436585-01	21.52	-2.2	-82.60
NCGC00387565-01	21.52	-2.2	-80.87
NCGC00253872-01	21.52	-2.2	-77.14
NCGC00410042-01	35.01	-2.2	-76.88
NCGC00411065-01	27.81	-2.2	-75.31
NCGC00183457-01	7.64	-1.2	-73.41
NCGC00411059-01	11.07	-2.2	-72.43
NCGC00249756-01	10.79	-1.2	-72.04
NCGC00183901-01	13.58	-2.2	-71.74
NCGC00274169-01	6.07	-1.2	-71.48
NCGC00253873-01	3.83	-1.2	-71.12
NCGC00274168-01	6.81	-1.2	-69.99
NCGC00274172-01	9.61	-1.2	-69.96
NCGC00183552-01	13.58	-2.2	-68.70
NCGC00345601-01	10.79	-1.2	-68.04
NCGC00253910-01	21.52	-2.2	-67.93
NCGC00274163-01	17.10	-2.2	-64.03
NCGC00238532-01	55.48	-2.2	-63.66
NCGC00486043-01	42.94	-3	-62.95
NCGC00438901-01	21.52	-2.2	-59.82
NCGC00415526-01	62.26	-3	-59.71
NCGC00253870-02	15.24	-2.2	-58.99
NCGC00445126-01	5.41	-1.2	-58.07
NCGC00249685-01	24.15	-2.2	-56.01
NCGC00274159-01	13.58	-1.2	-55.36
NCGC00429546-01	30.40	-2.2	-53.10
NCGC00120665-01	19.18	-2.2	-53.09
NCGC00249286-01	21.52	-2.2	-52.85
NCGC00345209-01	27.10	-2.2	-51.26
NCGC00099510-01	9.61	-1.2	-50.92
NCGC00249385-01	6.81	-2.2	-50.85
NCGC00183578-01	30.40	-3	-49.29
NCGC00183897-01	30.40	-3	-49.16
NCGC00274158-01	24.15	-2.2	-48.73
NCGC00238495-01	17.54	-1.2	-48.53
NCGC00411254-01	22.09	-1.2	-47.22
NCGC00411080-01	35.01	-2.2	-46.64
NCGC00274171-38	27.10	-2.2	-46.00
NCGC00348340-01	30.40	-3	-43.93
NCGC00249381-01	17.10	-2.2	-43.90
NCGC00390961-01	19.18	-2.2	-42.67
NCGC00461841-01	15.24	-2.2	-42.23

NCGC00487199-01	3.83	-1.2	-41.92
NCGC00442771-01	21.52	-2.2	-41.50
NCGC00344500-01	19.18	-2.2	-39.39
NCGC00428589-01	21.52	-2.2	-38.43
NCGC00411178-01	39.28	-2.4	-37.49
NCGC00249295-01	21.52	-2.2	-36.96
NCGC00121701-01	24.15	-2.2	-36.96
NCGC00411172-01	44.08	-2.4	-35.51
NCGC00378200-01	27.10	-3	-35.50
NCGC00441250-01	24.15	-2.4	-35.41
NCGC00247746-01	5.41	-2.4	-35.38
NCGC00486912-01	10.79	-1.2	-35.23
NCGC00351354-01	27.10	-2.4	-35.03
NCGC00274170-01	24.15	-2.2	-34.65
NCGC00460844-01	27.10	-3	-33.11
NCGC00443003-01	21.52	-2.4	-32.63
NCGC00537668-01	24.15	-2.4	-32.48
NCGC00183576-01	17.10	-2.2	-31.71
NCGC00425516-01	19.18	-2.4	-31.67
NCGC00098573-01	21.52	-2.2	-30.89
NCGC00434725-01	19.18	-2.4	-30.18
NCGC00595033-01	42.94	3	36.34

Structure

CCC1=CC(=CC(=C1)NC(=O)CN)C2=NN3C(=O)C=C(N=C3S2)N4CCNCC4  
CC(=C)C1=CC(=CC(=C1)NC(=O)CN)C2=NN3C(=O)C=C(N=C3S2)N4CCNCC4  
CC(O)C1=CC(=CC(=C1)NC(=O)CN)C2=NN3C(=O)C=C(N=C3S2)N4CCNCC4  
NCC(=O)NC1=CC(=CC(=C1)\C2=N\N/3C(=O)\C=C(/N=C3S2)N4CCNCC4)C(F)(F)F  
C1CN(CC2=CSC=C2)CC3=C(N1)C=C(NC4=CC=CC=C4)N=C3  
CC1=C(CNC(=O)C2=C(O)C3=NC=CC=C3C=C2)C4=C(CNCC4)C=N1  
O[C@@H]1[C@@H](O)[C@H](OCCCC[N]2C=C(C(=O)C3=C4C=CC=CC4=CC=C3)C5=C2C=CC=C5)O[C@@H]([C@H]1O)C(O)=C  
CC(C)C1=CC(=CC(=C1)NC(=O)CN)C2=NN3C(=O)C=C(N=C3S2)N4CCNCC4  
OC1=CC=C(CN2[C@H]3CCN(CC[C@H]3OCC2=O)CC4=CC=C5[NH]C=CC5=C4)C=C1  
CN(C)C1=CC=C(CN2CCN3=C(C2)C=NC(=C3)NC4=CC=CC=C4)C=C1  
NC1=CC=C(C=C1)C2=CC=CC(=C2)C3=N/N/4C(=O)\C=C(/N=C4S3)N5CCNCC5  
C1CN(CC2CC2)CC3=C(N1)C=C(NC4=CC=CC=C4)N=C3  
NCC(=O)NC1=CC(=CC(=C1)C2=NN/3C(=O)\C=C(/N=C3S2)N4CCNCC4)Br  
O=C1\C=C(/N=C\2S\C(=N/N12)C3=CC(=CC=C3)NCC4=CC=NC=C4)N5CCNCC5  
C[C@H](O)C1=CC(=CC(=C1)NC(=O)CN)\C2=N\N/3C(=O)\C=C(/N=C3S2)N4CCNCC4  
CC(=O)C1=CC(=CC(=C1)NC(=O)CN)C2=NN3C(=O)C=C(N=C3S2)N4CCNCC4  
C[C@H](O)C1=CC(=CC(=C1)NC(=O)CN)\C2=N\N/3C(=O)\C=C(/N=C3S2)N4CCNCC4  
NNC(=O)NC1=CC=CC(=C1)\C2=N\N/3C(=O)\C=C(/N=C3S2)N4CCNCC4  
NC(=O)C1CCN(CC1)C2=NC(=CS2)C3=CC=CC=C3  
O=C1\C=C(/N=C\2S\C(=N\N12)/C3=CC(=NC=C3)NC4CCCNC4)N5CCNCC5  
NC1=CC(=CC(=C1)\C2=N\N/3C(=O)\C=C(/N=C3S2)N4CCNCC4)C(F)(F)F  
NCC(=O)NC1=CC(=CC(=C1)B(O)O)\C2=N\N/3C(=O)\C=C(/N=C3S2)N4CCNCC4  
ClC1=C(OC2=CC=CC=C12)C(=O)NC3=CC=C4OC(=NC4=C3)C5=CC=CN=C5  
C(C(C([2H]))([2H]))([2H])NC(=N)NC(=N)NC1=CC=C(Cl)C=C1)([2H])([2H])[2H]  
C1CNCC2=CC(=N[N]2C1)C3=NC=C[N]3CCC[N]4N=CC5=C4C=CC=C5  
CC1(N(CC(O)=O)C(=O)OC12CCN(CC2)C(=O)CC3=CC=CC=N3)C4=CC=CC=C4  
NCC(=O)NC1=CC=CC(=C1)C2=NN3C(=O)C=C(N=C3S2)C4CCNCC4  
C1CN(CCC1C2CCN(C2)CC3=CC=C[NH]3)CC4=CC=CN=C4  
CN1CCN(CC1)C2=CC3=C([NH]C(=N3)C/4=C(\N)C5=C(F)C=CC=C5NC4=O)C=C2  
NCC(=O)NC1=CC(=CC(=C1)O)\C2=N\N/3C(=O)\C=C(/N=C3S2)N4CCNCC4  
O=C(CCC[C@@H]1[C@H]2CCN3CCC[C@@H](CN1C(=O)C4=CN=CC=C4)[C@@H]23)N5CCCCC5  
FC1=CC(=CC=C1)C(=O)NCC(N2CCC3=C2C=CC=C3)C4=CN=CC=C4  
BrC1=CC=C2[NH]C(=NC2=C1)NC3=CC=C(C=C3)C(=O)NCC4=CN=CC=C4  
[O-][S+](=O)(N1CCOCC1)C2=CC=C(NC(=O)C3=CC=C(CN4CCC5=CC=CC=C5C4)C=C3)C=C2  
ClC1=C(Cl)C(=CC=C1)C2=CC=C(O2)C(=O)NC3=CC=CC(=C3)C4=NC5=C(O4)C=CC=N5  
OC1=CC(=CC2=CC=CN=C12)C3=CC(=CC=C3)C(=O)NCCCCN4CCOCC4  
NC(=O)C1CCN(CC1)C2=NC(=CS2)C3=C4C=CC=CC4=CC=C3  
O=C1\C=C(/N=C\2S\C(=N/N12)C3=CC(=CC=C3)C4=CN=CN=C4)N5CCNCC5  
NCC(=O)NC1=CC(=CC(=C1)CO)\C2=N\N/3C(=O)\C=C(/N=C3S2)N4CCNCC4  
ClC1=CC=CC(=C1)C2=NC3=CC(=CC=C3O2)NC(=O)C4=CC=CN=C4  
CCCN1CCNC2=C(C1)C=NC(=C2)NC3=CC=CC=C3  
COC1=CC=C(CN2CCN3=C(C2)C=NC(=C3)NC4=CC=CC=C4)C=N1  
NCC(=O)NC1=CC(=CN=C1)C2=N/N/3C(S2)=N/C(=C\C3=O)N4CCNCC4  
[O-][S+](=O)(N1CCOCC1)C2=CC=C(NC(=O)C3=CC=C(CCN4CCC5=C(C4)C=CC=C5)C=C3)C=C2  
CC1=CC=CC(=C1)CN2CCN(CC2)C3=CN=C4C(=CC=C(C(O)=O)C4=C3)O  
OC(=O)C[C@@H]1CCN(C[C@@H]1CCN2CCN(CC2)C3=CC=CC=C3)C(=O)C4CCCCC4  
COCC1CN(CC2=C[NH]C3=CC=CC=C23)CC14CCNCC4

CC1=CC(=C(CNC(=N)NC(=O)C2=C(N)N=C(NCC3=CC=C(Cl)C=C3)C(=N2)Cl)C=C1)C  
CN1C(=O)CC(C(O)=O)C12CCN(CC2)C/C=C/C3=CC=CC=C3  
NC1=CC(=CC=N1)\C2=N\N/3C(=O)\C=C(/N=C3S2)N4CCNCC4  
O=C(CCC[C@H]1NC[C@@H]2C[C@H]1CN(C2)CC3=CC=CC=C3)N4CCN(CC4)C5=NC=CC=N5  
COC1=CC=C(NC2=CC3=C(CN(CCN3)CCC4=CC=CC=C4)C=N2)C=C1OC  
BrC1=CC=C2[NH]C(=NC2=C1)NC3=CC=C(C=C3)C(=O)NCN4CCOCC4  
CC1=CC=C(C=C1)C2=C[N]3C(=N2)SC4=CC(=CC=C34)C(=O)NCCCN5CCCCC5  
COC1=CC(=CC=C1)CN2CCNC3=C(C2)C=NC(=C3)NC4=CC=CC=C4  
N[C@H](C(=O)N1CCC2(CC1)N(CNC2=O)C(=O)CC3=C[NH]C4=C3C=CC=C4)C5=CC=CC=C5  
CC1=N[N](CCC[N]2C=CN=C2C3=N[N]4CCCNCC4=C3)C(=N1)C  
CN(C)CCCN1CCN(CC1)C(=O)C2=CC=CC(=C2)C3=CC4=CC=CN=C4C(=C3)O  
OC1=CC=CC(=C1)NC2=CC=NC3=C2SC(=C3)C4=CC=CC(=C4)CN5CCOCC5  
[O-][S+](=O)(N1CCOCC1)C2=CC=C(NC(=O)C3=CC=C(CN4CCC(CC4)C5=CC=CC=C5)C=C3)C=C2  
NCC(=O)NC1=CC(=CC(=C1)C(O)=O)\C2=N\N/3C(=O)\C=C(/N=C3S2)N4CCNCC4  
COC1=CC=C2[NH]C3=C(CCN34CCN(CC4)CC5=CC=C(C)O5)C2=C1  
CCN1CCCC1C[N]2C=CN=C2C3=N[N]4CCCNCC4=C3  
CC(=O)NCC(=O)NC1=CN=CC(=C1)/C2=N/N/3C(=O)\C=C(/N=C3S2)N4CCNCC4  
CC1=CC=CC(=C1)C2=CSC(=N2)N3CCC(CC3)C(N)=O  
CC1=C(CN2CCCC(CNC(=O)C3=CC=CC4=C3C=CC=C4)C2)[NH]C5=CC=CC=C15  
CC[N]1C2=C(C=CC=C2)C3=C1C=CC(=C3)CN4CCN(CC4)CC5=CC=C(OC)C(=C5)OC  
CC1=C(CNC(=O)C2=CC=CC=C2N3CCOCC3)C4=C(CNCC4)C=N1  
CC1=CC=C(C2=NC3=CC(NC(=O)C4=CC=CO4)=CC=C3O2)C(C)=C1

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