| SMILES | IC50 | Binary_Clas | pIC50 | | | | | |
|---|---|---|---|---|---|---|---|---|
| Oc1ccc(-c2 | 8 | 1 | 8.09691 | | | | | |
| C/C(=N\OC | 10 | 1 | 8 | | | | | |
| CC(C)c1ccc | 10 | 1 | 8 | | | | | |
| CC(=O)N(O | 13 | 1 | 7.886057 | | | | | |
| Oc1ccc(-c2 | 20 | 1 | 7.69897 | | | | | |
| Cc1cc(-c2c( | 22 | 1 | 7.657577 | | | | | |
| O=C(O)/C= | 22 | 1 | 7.657577 | | | | | |
| CC1Cc2c(O | 23 | 1 | 7.638272 | | | | | |
| C/C(=N\OC | 29 | 1 | 7.537602 | | | | | |
| CC/C(=N\O | 30 | 1 | 7.522879 | | | | | |
| CCOc1ccc(- | 30 | 1 | 7.522879 | | | | | |
| COC1(c2cc( | 40 | 1 | 7.39794 | | | | | |
| C/C(=C\CC/ | 40 | 1 | 7.39794 | | | | | |
| Cc1nsc(NC( | 44 | 1 | 7.356547 | | | | | |
| C/C(=C\CC/ | 50 | 1 | 7.30103 | | | | | |
| Oc1ccc(-c2 | 50 | 1 | 7.30103 | | | | | |
| O=[N+]([O- | 50 | 1 | 7.30103 | | | | | |
| CCCCC(O/N | 52 | 1 | 7.283997 | | | | | |
| O=C(Nc1nc | 53 | 1 | 7.275724 | | | | | |
| C/C(=C\CC/ | 57 | 1 | 7.244125 | | | | | |
| CC1Cc2c(O | 60 | 1 | 7.221849 | | | | | |
| CC(C)Cc1cc | 60 | 1 | 7.221849 | | | | | |
| O=C1N=C(c | 60 | 1 | 7.221849 | | | | | |
| CCCCCCCC( | 62 | 1 | 7.207608 | | | | | |
| COC(=O)c1 | 65 | 1 | 7.187087 | | | | | |
| COc1cc(/C= | 70 | 1 | 7.154902 | | | | | |
| C/C(=C\CC/ | 70 | 1 | 7.154902 | | | | | |
| COc1ccc2c( | 70 | 1 | 7.154902 | | | | | |
| CCOC(=O)C | 70 | 1 | 7.154902 | | | | | |
| O=C(Nc1cc | 71 | 1 | 7.148742 | | | | | |
| O=C(Nc1cc | 74 | 1 | 7.130768 | | | | | |
| COc1ccccc1 | 76 | 1 | 7.119186 | | | | | |
| O=C1N=C(c | 80 | 1 | 7.09691 | | | | | |
| O=C1N=C(c | 80 | 1 | 7.09691 | | | | | |
| CCCOc1ccc | 80 | 1 | 7.09691 | | | | | |
| Cc1c(C)c2c | 80 | 1 | 7.09691 | | | | | |
| COc1ccc(/C | 80 | 1 | 7.09691 | | | | | |
| COc1ccc(/C | 80 | 1 | 7.09691 | | | | | |
| NC(=O)N(O | 85 | 1 | 7.070581 | | | | | |
| CC(=O)N(O | 86 | 1 | 7.065502 | | | | | |
| COc1ccc(C2 | 90 | 1 | 7.045757 | | | | | |
| COc1ccc(C2 | 90 | 1 | 7.045757 | | | | | |
| C/C(=C\CC/ | 90 | 1 | 7.045757 | | | | | |
| O=C1N=C(c | 90 | 1 | 7.045757 | | | | | |
| C/C(=C\CC/ | 90 | 1 | 7.045757 | | | | | |
| O=C1N=C(c | 90 | 1 | 7.045757 | | | | | |
| COc1ccc(/C | 90 | 1 | 7.045757 | | | | | |
| CNC(=O)N( | 98 | 1 | 7.008774 | | | | | |
| CCc1cc(/C= | 100 | 1 | 7 | | | | | |
| COc1cc(/C= | 100 | 1 | 7 | | | | | |

| | | | |
|---|---|---|---|
| CC(=O)C1(c | 100 | 1 | 7 |
| NC(=O)N(O | 100 | 1 | 7 |
| COc1ccc(/C | 100 | 1 | 7 |
| CCC(OC)(c1 | 100 | 1 | 7 |
| C/C(=C\CC/ | 110 | 1 | 6.958607 |
| C/C(=C\CC/ | 110 | 1 | 6.958607 |
| COc1ccc(-n | 110 | 1 | 6.958607 |
| COc1cccc(C | 115 | 1 | 6.939302 |
| COc1ccccc1 | 119 | 1 | 6.924453 |
| C/C(=C\CC/ | 120 | 1 | 6.920819 |
| NC(=O)N(O | 120 | 1 | 6.920819 |
| CCOC(=O)c | 120 | 1 | 6.920819 |
| CCCCCCOc1 | 126 | 1 | 6.899629 |
| C/C(=C\CC/ | 129 | 1 | 6.88941 |
| CC(=O)c1cc | 130 | 1 | 6.886057 |
| COc1ccc(/C | 130 | 1 | 6.886057 |
| NC(=O)N(O | 130 | 1 | 6.886057 |
| O=C1N=C(c | 130 | 1 | 6.886057 |
| COc1ccc(/C | 140 | 1 | 6.853872 |
| COc1ccc(/C | 140 | 1 | 6.853872 |
| Cc1nc(NC(= | 140 | 1 | 6.853872 |
| O=C(NCc1c | 148 | 1 | 6.829738 |
| C/C(=C\CC/ | 150 | 1 | 6.823909 |
| C/C(=C\CC/ | 150 | 1 | 6.823909 |
| COc1ccc(/C | 150 | 1 | 6.823909 |
| CC(=O)Oc1 | 160 | 1 | 6.79588 |
| CC(C)(Cc1c | 160 | 1 | 6.79588 |
| CC(/C=C/c1 | 160 | 1 | 6.79588 |
| CC(=O)c1cc | 160 | 1 | 6.79588 |
| C/C(=C\CC/ | 170 | 1 | 6.769551 |
| C/C(=C\CC[ | 170 | 1 | 6.769551 |
| COc1ccc(/C | 170 | 1 | 6.769551 |
| NC(=O)N(O | 170 | 1 | 6.769551 |
| CCOC(=O)c | 170 | 1 | 6.769551 |
| C/C(=C\CC/ | 170 | 1 | 6.769551 |
| C/C(=C\CC[ | 170 | 1 | 6.769551 |
| COC(=O)C( | 170 | 1 | 6.769551 |
| C/C(=C\CC/ | 170 | 1 | 6.769551 |
| CC1(C)C2C( | 171 | 1 | 6.767004 |
| CC1(C)Cc2c | 180 | 1 | 6.744727 |
| COc1ccc(/C | 180 | 1 | 6.744727 |
| C#CCCCCC( | 180 | 1 | 6.744727 |
| C/C(=C/CC/ | 180 | 1 | 6.744727 |
| CCCCCCCC( | 190 | 1 | 6.721246 |
| CCOC(=O)C | 200 | 1 | 6.69897 |
| CC(C)c1cc(/ | 200 | 1 | 6.69897 |
| COc1ccc(/C | 200 | 1 | 6.69897 |
| COC1(c2cc( | 200 | 1 | 6.69897 |
| CC(=O)c1cc | 210 | 1 | 6.677781 |
| COc1ccc(C2 | 210 | 1 | 6.677781 |
| C/C(=C\CC/ | 210 | 1 | 6.677781 |

| | | | |
|---|---|---|---|
| COc1ccc(C2 | 210 | 1 | 6.677781 |
| CCCOc1ccc | 210 | 1 | 6.677781 |
| COc1cccc(C | 210 | 1 | 6.677781 |
| CCOC(=O)c | 220 | 1 | 6.657577 |
| CC1Oc2ccc | 220 | 1 | 6.657577 |
| Cc1nccn1-c | 230 | 1 | 6.638272 |
| CCOC(=O)c | 230 | 1 | 6.638272 |
| NC(=O)N(O | 230 | 1 | 6.638272 |
| CCCCCCCC( | 230 | 1 | 6.638272 |
| O=C1OCc2c | 240 | 1 | 6.619789 |
| Cc1nc(NC(= | 240 | 1 | 6.619789 |
| COc1ccccc1 | 250 | 1 | 6.60206 |
| CCOC(=O)c | 257 | 1 | 6.590067 |
| COc1cc(CC1 | 260 | 1 | 6.585027 |
| COc1ccc(/C | 260 | 1 | 6.585027 |
| COC1=CC(= | 280 | 1 | 6.552842 |
| CCOC(=O)c | 290 | 1 | 6.537602 |
| COC(=O)c1 | 300 | 1 | 6.522879 |
| C/C(=C\CC/ | 300 | 1 | 6.522879 |
| Fc1ccc(-c2[ | 300 | 1 | 6.522879 |
| CCOC(=O)c | 300 | 1 | 6.522879 |
| CCCC/C(=C | 300 | 1 | 6.522879 |
| O=C1C=C(C | 310 | 1 | 6.508638 |
| C/C(=C\CC/ | 310 | 1 | 6.508638 |
| CC1(C)Oc2c | 310 | 1 | 6.508638 |
| COc1ccc(/C | 320 | 1 | 6.49485 |
| O=C(/C=C/c | 330 | 1 | 6.481486 |
| CCCCCCCC( | 340 | 1 | 6.468521 |
| Cc1cc(OCC( | 351 | 1 | 6.454693 |
| C/C(=C\CC[ | 380 | 1 | 6.420216 |
| NC(=O)N(O | 380 | 1 | 6.420216 |
| CCCCCCCC( | 380 | 1 | 6.420216 |
| NC(=O)N(O | 390 | 1 | 6.408935 |
| CCCC/C(=C | 400 | 1 | 6.39794 |
| O=C(Nc1cc | 400 | 1 | 6.39794 |
| CCCCCCC(S | 400 | 1 | 6.39794 |
| O=C(O)c1cc | 400 | 1 | 6.39794 |
| C/C(=C\CC/ | 400 | 1 | 6.39794 |
| Oc1cccc(-c1 | 400 | 1 | 6.39794 |
| CC(=O)c1c( | 420 | 1 | 6.376751 |
| NC(=O)N(O | 430 | 1 | 6.366532 |
| C/C(=C\CC[ | 440 | 1 | 6.356547 |
| C/C(=C\CC/ | 440 | 1 | 6.356547 |
| C#CCCCCC( | 470 | 1 | 6.327902 |
| C/C(=C\CC[ | 470 | 1 | 6.327902 |
| CCOC(=O)c | 470 | 1 | 6.327902 |
| CS(=O)(=O) | 500 | 1 | 6.30103 |
| O=C1Nc2cc | 500 | 1 | 6.30103 |
| O=C(O)C(Sc | 500 | 1 | 6.30103 |
| CCCCC(Sc1 | 500 | 1 | 6.30103 |
| CCCCCCC(S | 500 | 1 | 6.30103 |

| | | | |
|---|---|---|---|
| CC1=NN(c2 | 520 | 1 | 6.283997 |
| O=C(/C=C/( | 530 | 1 | 6.275724 |
| Cc1ccc(/C= | 540 | 1 | 6.267606 |
| COc1ccc(C( | 560 | 1 | 6.251812 |
| O=C(Nc1cc | 570 | 1 | 6.244125 |
| COc1ccc(C2 | 570 | 1 | 6.244125 |
| O=C1C=C(C | 580 | 1 | 6.236572 |
| CCCCC(Oc1 | 600 | 1 | 6.221849 |
| CC1C(=O)O | 600 | 1 | 6.221849 |
| CCCCCCC(S | 600 | 1 | 6.221849 |
| CCCCC(Sc1 | 600 | 1 | 6.221849 |
| CCCCCCC(S | 600 | 1 | 6.221849 |
| O=C(O)c1c( | 600 | 1 | 6.221849 |
| CC(=O)Oc1 | 600 | 1 | 6.221849 |
| Cc1ccc(S(=( | 600 | 1 | 6.221849 |
| COc1cc(/C= | 600 | 1 | 6.221849 |
| c1cn2c(NC3 | 610 | 1 | 6.21467 |
| CCCCCCCC( | 620 | 1 | 6.207608 |
| O=C(O/N=C | 620 | 1 | 6.207608 |
| CS(=O)(=O) | 620 | 1 | 6.207608 |
| COc1ccc(/C | 630 | 1 | 6.200659 |
| CC(=O)c1cc | 630 | 1 | 6.200659 |
| Cc1nc(NC(= | 640 | 1 | 6.19382 |
| CCOC(=O)c | 657 | 1 | 6.182435 |
| CC(C)CC(=C | 660 | 1 | 6.180456 |
| O=C(/C=C/( | 660 | 1 | 6.180456 |
| CC(C)(C)c1( | 690 | 1 | 6.161151 |
| CC(C)(C)c1( | 700 | 1 | 6.154902 |
| CCCC/C(=C | 700 | 1 | 6.154902 |
| COc1cc(/C= | 700 | 1 | 6.154902 |
| CCCCCCC(S | 700 | 1 | 6.154902 |
| CCOC(=O)c | 700 | 1 | 6.154902 |
| Oc1n[nH]c2 | 700 | 1 | 6.154902 |
| Cc1ccc(C2= | 730 | 1 | 6.136677 |
| COC1(c2cc( | 740 | 1 | 6.130768 |
| NC1=NN(c2 | 750 | 1 | 6.124939 |
| CCC(=O)Nc | 760 | 1 | 6.119186 |
| CCOC(=O)c | 780 | 1 | 6.107905 |
| O=C(/C=C/( | 790 | 1 | 6.102373 |
| O=C1N=C(c | 790 | 1 | 6.102373 |
| CCCC/C(=C | 800 | 1 | 6.09691 |
| CCOC(=O)c | 800 | 1 | 6.09691 |
| O=C(O)c1c( | 800 | 1 | 6.09691 |
| O=C1C=C(c | 800 | 1 | 6.09691 |
| COc1cc(C)c | 800 | 1 | 6.09691 |
| CCCOc1cc( | 800 | 1 | 6.09691 |
| CCCC/C(=C | 800 | 1 | 6.09691 |
| CCOC(=O)c | 800 | 1 | 6.09691 |
| CCCOc1cc( | 800 | 1 | 6.09691 |
| CCCCC(Sc1( | 800 | 1 | 6.09691 |
| CCCCCC[C@ | 800 | 1 | 6.09691 |

| | | | |
|---|---|---|---|
| O=C(O)/C= | 800 | 1 | 6.09691 |
| CCOC(=O)c | 800 | 1 | 6.09691 |
| C/C(=C\CC[ | 810 | 1 | 6.091515 |
| CC(=O)N(C) | 840 | 1 | 6.075721 |
| COc1ccc(Sc | 850 | 1 | 6.070581 |
| O=C(/C=C/( | 890 | 1 | 6.05061 |
| Oc1ccc(-c2 | 900 | 1 | 6.045757 |
| CCCCC1CC( | 900 | 1 | 6.045757 |
| COc1ccc(C2 | 900 | 1 | 6.045757 |
| COc1cc(C)c | 900 | 1 | 6.045757 |
| COc1cc(C(= | 900 | 1 | 6.045757 |
| CCOC(=O)c | 900 | 1 | 6.045757 |
| CCCCC(Cc1 | 900 | 1 | 6.045757 |
| CCCOc1cc( | 900 | 1 | 6.045757 |
| CCCC/C(=C | 900 | 1 | 6.045757 |
| CCCC/C(=C | 900 | 1 | 6.045757 |
| COc1ccc(C2 | 900 | 1 | 6.045757 |
| C/C(=C\CC[ | 920 | 1 | 6.036212 |
| C#CCCCCO( | 920 | 1 | 6.036212 |
| CC(C)C(=O) | 980 | 1 | 6.008774 |
| C/C(=C\CC/ | 998 | 1 | 6.000869 |
| CCc1cc(/C= | 1000 | 1 | 6 |
| O=C(NCC12 | 1000 | 1 | 6 |
| Cc1cc(CCc2 | 1000 | 1 | 6 |
| CC(C)c1cc(/ | 1000 | 1 | 6 |
| COC(=O)CC | 1000 | 1 | 6 |
| CCCC/C(=C | 1000 | 1 | 6 |
| Cc1ccc(/C= | 1000 | 1 | 6 |
| Cc1ccc(CN( | 1000 | 1 | 6 |
| COc1ccc(C2 | 1000 | 1 | 6 |
| C/C(=C\CC/ | 1000 | 1 | 6 |
| Cc1cc(O)cc | 1000 | 1 | 6 |
| NC(=O)C1(C | 1000 | 1 | 6 |
| Cc1cc(Cc2c | 1000 | 1 | 6 |
| Cc1cc(/C=C | 1000 | 1 | 6 |
| CCc1cc(/C= | 1000 | 1 | 6 |
| Cc1cc(/C=C | 1000 | 1 | 6 |
| Cc1cc(O)cc | 1000 | 1 | 6 |
| Cc1ccc(/C= | 1000 | 1 | 6 |
| O=C(Nc1cc | 1000 | 1 | 6 |
| Cc1cc(/C=C | 1000 | 1 | 6 |
| Cc1cc(/C=C | 1000 | 1 | 6 |
| Cc1cc(CCC( | 1000 | 1 | 6 |
| Cc1nccn1-c | 1000 | 1 | 6 |
| COC(=O)/C | 1000 | 1 | 6 |
| C/C(=C\CC/ | 1000 | 1 | 6 |
| Cc1cc(OCC | 1000 | 1 | 6 |
| COc1cc(/C= | 1000 | 1 | 6 |
| Cc1cc(/C=C | 1000 | 1 | 6 |
| COC(=O)C( | 1000 | 1 | 6 |
| CCCCCCCC( | 1000 | 1 | 6 |

| | | | |
|---|---|---|---|
| CCCCCc1cc | 1090 | 0 | 5.962574 |
| Oc1ccc(CC( | 1100 | 0 | 5.958607 |
| C=CCc1ccc( | 1100 | 0 | 5.958607 |
| CCCCC(Sc1 | 1100 | 0 | 5.958607 |
| O=C(O)c1c( | 1100 | 0 | 5.958607 |
| CCCCNC(=C | 1200 | 0 | 5.920819 |
| CC(C)(C)c1( | 1200 | 0 | 5.920819 |
| CCOC(=O)C | 1200 | 0 | 5.920819 |
| CCOC(=O)c | 1200 | 0 | 5.920819 |
| CCC(OC)(c1 | 1300 | 0 | 5.886057 |
| CCCCCC(=C | 1300 | 0 | 5.886057 |
| O=C(O)/C= | 1300 | 0 | 5.886057 |
| COc1cccc(C | 1300 | 0 | 5.886057 |
| CC(=O)Oc1 | 1300 | 0 | 5.886057 |
| Cc1ccc(Sc2 | 1400 | 0 | 5.853872 |
| CCCc1ccc(C | 1400 | 0 | 5.853872 |
| CCCCCCC(S | 1400 | 0 | 5.853872 |
| CCCCCCC1= | 1400 | 0 | 5.853872 |
| Cc1ccc2nc( | 1467 | 0 | 5.83357 |
| CC(C)(C)CN | 1480 | 0 | 5.829738 |
| CCCCCC[C@ | 1500 | 0 | 5.823909 |
| C=CCc1ccc( | 1500 | 0 | 5.823909 |
| CCCCCCN(c | 1500 | 0 | 5.823909 |
| CCCCCCC(S | 1500 | 0 | 5.823909 |
| Cc1ccc2nc( | 1540 | 0 | 5.812479 |
| CC(C)(C)c1( | 1600 | 0 | 5.79588 |
| CC1CN(c2c | 1600 | 0 | 5.79588 |
| CCCCCCCC( | 1600 | 0 | 5.79588 |
| CCCC/C(=C | 1600 | 0 | 5.79588 |
| CCCCCC(=C | 1600 | 0 | 5.79588 |
| CC(C)(C)c1( | 1700 | 0 | 5.769551 |
| CCCCCCC(S | 1700 | 0 | 5.769551 |
| Cc1ccccc1C | 1700 | 0 | 5.769551 |
| O=C1Nc2c( | 1700 | 0 | 5.769551 |
| CCOC(=O)c | 1700 | 0 | 5.769551 |
| O=C(O)c1c( | 1700 | 0 | 5.769551 |
| CC(=O)c1c( | 1700 | 0 | 5.769551 |
| CCCc1ccc(C | 1700 | 0 | 5.769551 |
| Cc1ccc(-c2( | 1720 | 0 | 5.764472 |
| CCOC(=O)C | 1800 | 0 | 5.744727 |
| CCOC(=O)c | 1800 | 0 | 5.744727 |
| O=C(O)C(Sc | 1800 | 0 | 5.744727 |
| C#CCCOC(= | 1800 | 0 | 5.744727 |
| c1cn2c(NC3 | 1800 | 0 | 5.744727 |
| O=C(O)/C= | 1800 | 0 | 5.744727 |
| CC(C)=CCC/ | 1800 | 0 | 5.744727 |
| COc1ccc(/C | 1860 | 0 | 5.730487 |
| O=C(O)c1c( | 1900 | 0 | 5.721246 |
| Cc1ccc(-c2( | 2000 | 0 | 5.69897 |
| CC1C(=O)O | 2000 | 0 | 5.69897 |
| O=C(O)/C= | 2000 | 0 | 5.69897 |

| | | | |
|---|---|---|---|
| CCCCC/C=C | 2000 | 0 | 5.69897 |
| CCCCCCC(S | 2000 | 0 | 5.69897 |
| CCCCC(Cc1 | 2000 | 0 | 5.69897 |
| C/C=C(/C=C | 2000 | 0 | 5.69897 |
| Oc1c(F)c(F) | 2000 | 0 | 5.69897 |
| COc1c(CC= | 2000 | 0 | 5.69897 |
| C=CCc1ccc( | 2100 | 0 | 5.677781 |
| O=C(O)c1cc | 2100 | 0 | 5.677781 |
| Oc1ccc(-c2 | 2100 | 0 | 5.677781 |
| O=C(/C=C/C | 2100 | 0 | 5.677781 |
| O=C(O)/C= | 2100 | 0 | 5.677781 |
| CCCOc1ccc | 2140 | 0 | 5.669586 |
| CCCCC1=C( | 2200 | 0 | 5.657577 |
| O=C(O)/C= | 2200 | 0 | 5.657577 |
| C=CCc1ccc( | 2200 | 0 | 5.657577 |
| CCOC(=O)c | 2300 | 0 | 5.638272 |
| O=C(c1cccc | 2300 | 0 | 5.638272 |
| CCOC(=O)c | 2300 | 0 | 5.638272 |
| O=C(/C=C/C | 2300 | 0 | 5.638272 |
| CCOC(=O)c | 2300 | 0 | 5.638272 |
| Oc1ccc(Cc2 | 2300 | 0 | 5.638272 |
| COc1c(CC= | 2300 | 0 | 5.638272 |
| CCCCNc1cc | 2400 | 0 | 5.619789 |
| CC(=O)c1c( | 2400 | 0 | 5.619789 |
| Cc1ccc(S(=C | 2400 | 0 | 5.619789 |
| CCCCC(Sc1 | 2400 | 0 | 5.619789 |
| CCOC(=O)C | 2400 | 0 | 5.619789 |
| COc1ccc(-c | 2400 | 0 | 5.619789 |
| CCOC(=O)c | 2400 | 0 | 5.619789 |
| CC(C)(C)c1c | 2500 | 0 | 5.60206 |
| O=C(O)/C= | 2500 | 0 | 5.60206 |
| O=C(O)/C= | 2500 | 0 | 5.60206 |
| C=C(C)[C@ | 2500 | 0 | 5.60206 |
| O=C(O)C(Sc | 2500 | 0 | 5.60206 |
| CC(C)CCNc | 2500 | 0 | 5.60206 |
| CC(C)=CCC/ | 2500 | 0 | 5.60206 |
| CC(c1cc2c( | 2500 | 0 | 5.60206 |
| CCOC(=O)C | 2600 | 0 | 5.585027 |
| O=C1Nc2cc | 2600 | 0 | 5.585027 |
| CC(C)(C)c1c | 2600 | 0 | 5.585027 |
| CC1(C)Cc2c | 2600 | 0 | 5.585027 |
| CC(=O)Oc1 | 2600 | 0 | 5.585027 |
| O=C(O)c1cc | 2600 | 0 | 5.585027 |
| CC(C)(C)c1c | 2700 | 0 | 5.568636 |
| COc1cc(/C= | 2700 | 0 | 5.568636 |
| CCCCCC(=C | 2700 | 0 | 5.568636 |
| Cc1cc(Oc2c | 2700 | 0 | 5.568636 |
| CC(=O)O[C | 2700 | 0 | 5.568636 |
| Cc1ccc(-c2c | 2700 | 0 | 5.568636 |
| CC(Nc1[nH | 2800 | 0 | 5.552842 |
| Cc1ccc(-c2c | 2800 | 0 | 5.552842 |

| | | | |
|---|---|---|---|
| CC(C)C(C1= | 2800 | 0 | 5.552842 |
| Cc1ccc(-n2 | 2800 | 0 | 5.552842 |
| CN(C)c1ccc | 2800 | 0 | 5.552842 |
| Oc1ccc(-c2 | 2800 | 0 | 5.552842 |
| CC(C)(C)c1 | 2800 | 0 | 5.552842 |
| CCCCCCc1c | 2800 | 0 | 5.552842 |
| O=C(O)/C= | 2800 | 0 | 5.552842 |
| CC(C)(C)c1 | 2900 | 0 | 5.537602 |
| CCOC(=O)c | 2900 | 0 | 5.537602 |
| Oc1nc(-c2c | 2900 | 0 | 5.537602 |
| Cc1ccc(-c2 | 2900 | 0 | 5.537602 |
| CC(C)(C)c1 | 2900 | 0 | 5.537602 |
| COc1cc(/C= | 3000 | 0 | 5.522879 |
| CCCOc1cc( | 3000 | 0 | 5.522879 |
| CCCCC/C=C | 3000 | 0 | 5.522879 |
| CCCCCCCC( | 3000 | 0 | 5.522879 |
| CC(C)(C)c1 | 3000 | 0 | 5.522879 |
| CC1C(=O)O | 3000 | 0 | 5.522879 |
| C[C@H]1[C | 3000 | 0 | 5.522879 |
| O=C(O)C(S | 3100 | 0 | 5.508638 |
| CCOC(=O)c | 3100 | 0 | 5.508638 |
| O=C(c1cccc | 3100 | 0 | 5.508638 |
| O=C1Nc2c( | 3100 | 0 | 5.508638 |
| O=C(O)c1c | 3200 | 0 | 5.49485 |
| O=C(O)c1c | 3200 | 0 | 5.49485 |
| COc1cc(CC | 3200 | 0 | 5.49485 |
| CCOC(=O)c | 3200 | 0 | 5.49485 |
| CCOC(=O)C | 3200 | 0 | 5.49485 |
| COc1ccc(-n | 3300 | 0 | 5.481486 |
| O=C1Nc2c( | 3300 | 0 | 5.481486 |
| O=C(O)c1c | 3300 | 0 | 5.481486 |
| COc1ccc(C( | 3300 | 0 | 5.481486 |
| COc1ccc(/C | 3340 | 0 | 5.476254 |
| CS(=O)(=O) | 3400 | 0 | 5.468521 |
| COC(=O)CN | 3500 | 0 | 5.455932 |
| Cc1ccc(S(= | 3500 | 0 | 5.455932 |
| Cc1ccc(-c2 | 3500 | 0 | 5.455932 |
| COc1ccc(C2 | 3550 | 0 | 5.449772 |
| CC(=O)c1c( | 3600 | 0 | 5.443697 |
| CCOCc1ccc | 3700 | 0 | 5.431798 |
| CCOC(=O)c | 3800 | 0 | 5.420216 |
| O=C(NC(=S | 3800 | 0 | 5.420216 |
| O=C(O)CSc | 3900 | 0 | 5.408935 |
| COc1cc(C)c | 4000 | 0 | 5.39794 |
| CCCCCCC1= | 4000 | 0 | 5.39794 |
| CCOC(=O)C | 4000 | 0 | 5.39794 |
| CCCCN(c1c | 4000 | 0 | 5.39794 |
| COc1ccccc1 | 4000 | 0 | 5.39794 |
| COC1=CC(= | 4100 | 0 | 5.387216 |
| Cc1ccsc1C( | 4100 | 0 | 5.387216 |
| O=C(O)/C= | 4200 | 0 | 5.376751 |

| | | | |
|---|---|---|---|
| CCOC(=O)c | 4200 | 0 | 5.376751 |
| O=C1NCc2( | 4200 | 0 | 5.376751 |
| C=CCc1ccc( | 4200 | 0 | 5.376751 |
| O=C(O)c1c( | 4400 | 0 | 5.356547 |
| O=C(O)C(Sc | 4400 | 0 | 5.356547 |
| CCCCCCCCI | 4500 | 0 | 5.346787 |
| COc1c(CC= | 4500 | 0 | 5.346787 |
| C=CCc1ccc( | 4500 | 0 | 5.346787 |
| O=C(O)/C= | 4500 | 0 | 5.346787 |
| O=C1C=C(c | 4600 | 0 | 5.337242 |
| COc1ccc(/C | 4660 | 0 | 5.331614 |
| CCCCC(Cc1 | 4700 | 0 | 5.327902 |
| Cc1ccc(NS( | 4700 | 0 | 5.327902 |
| CC(C)(C)c1( | 4800 | 0 | 5.318759 |
| CCCCC(Sc1( | 4800 | 0 | 5.318759 |
| Cc1ccc(S(=( | 4800 | 0 | 5.318759 |
| CCCCC(Sc1( | 4800 | 0 | 5.318759 |
| CCCCC(Sc1( | 4800 | 0 | 5.318759 |
| Cc1ccc(/C= | 4860 | 0 | 5.313364 |
| Oc1ccc(/C= | 4900 | 0 | 5.309804 |
| CCOC(=O)c | 5000 | 0 | 5.30103 |
| CCOC(=O)c | 5000 | 0 | 5.30103 |
| C=C(C)C1C( | 5000 | 0 | 5.30103 |
| Cc1cccc(Nc | 5000 | 0 | 5.30103 |
| O=C(O)c1c( | 5000 | 0 | 5.30103 |
| O=C(O)/C= | 5100 | 0 | 5.29243 |
| CCCCC(Sc1( | 5200 | 0 | 5.283997 |
| Nc1ccc(-c2 | 5300 | 0 | 5.275724 |
| COc1c(CC= | 5300 | 0 | 5.275724 |
| COc1c(CC= | 5300 | 0 | 5.275724 |
| COc1cc(CC( | 5400 | 0 | 5.267606 |
| COC(=O)[C( | 5460 | 0 | 5.262807 |
| CC(C)=CCC1 | 5900 | 0 | 5.229148 |
| CCOC(=O)c | 5900 | 0 | 5.229148 |
| CCOCCn1c( | 5920 | 0 | 5.227678 |
| OC1(c2cccc | 6000 | 0 | 5.221849 |
| O=Cc1ccc(- | 6000 | 0 | 5.221849 |
| COc1ccc(C( | 6000 | 0 | 5.221849 |
| COc1c(CC= | 6000 | 0 | 5.221849 |
| O=C(O)/C= | 6000 | 0 | 5.221849 |
| CCCCC(Cc1 | 6000 | 0 | 5.221849 |
| CC1(C)Cc2( | 6100 | 0 | 5.21467 |
| CN(C)c1ccc | 6100 | 0 | 5.21467 |
| Oc1ccc(-c2 | 6300 | 0 | 5.200659 |
| O=C(O)c1c( | 6700 | 0 | 5.173925 |
| O=C(O)c1c( | 6800 | 0 | 5.167491 |
| O=C(Cc1cc( | 6800 | 0 | 5.167491 |
| COc1ccc2c( | 7000 | 0 | 5.154902 |
| C=CCN(CC= | 7100 | 0 | 5.148742 |
| CC(=O)Oc1 | 7600 | 0 | 5.119186 |
| O=C(O)CSc | 7600 | 0 | 5.119186 |

| | | | |
|---|---|---|---|
| CC(C)(C)c1c | 8000 | 0 | 5.09691 |
| CC1C(=O)O | 8000 | 0 | 5.09691 |
| COc1ccc(-n | 8000 | 0 | 5.09691 |
| Cc1ccc(-c2c | 8000 | 0 | 5.09691 |
| CCCC(Sc1n | 8000 | 0 | 5.09691 |
| COc1cc(C)c | 8000 | 0 | 5.09691 |
| CC(=O)c1c( | 8100 | 0 | 5.091515 |
| CC(C)C(=O) | 8100 | 0 | 5.091515 |
| O=Nc1c(-c2 | 8200 | 0 | 5.086186 |
| C#CCCNC(= | 8230 | 0 | 5.0846 |
| COC(=O)CC | 8330 | 0 | 5.079355 |
| O=C(O)c1c | 8400 | 0 | 5.075721 |
| O=C(O)/C= | 8500 | 0 | 5.070581 |
| CC(C)C(C1= | 8600 | 0 | 5.065502 |
| FC(F)(F)c1c | 8800 | 0 | 5.055517 |
| CCCCCc1cc | 8900 | 0 | 5.05061 |
| O=C1C=C(C | 9000 | 0 | 5.045757 |
| O=C(O)/C= | 9200 | 0 | 5.036212 |
| OC[C@@H | 9200 | 0 | 5.036212 |
| CC1(C)CC(= | 9200 | 0 | 5.036212 |
| O=C(OCc1c | 9300 | 0 | 5.031517 |
| CC(C)=CCC | 9300 | 0 | 5.031517 |
| COc1cc(O)c | 9300 | 0 | 5.031517 |
| Oc1ccc(Cc2 | 9400 | 0 | 5.026872 |
| CCCCC(Sc1 | 9500 | 0 | 5.022276 |
| COC1=CC(= | 10000 | 0 | 5 |
| O=C(O)c1c | 10000 | 0 | 5 |
| O=C(O)c1c | 10000 | 0 | 5 |
| O=[N+]([O- | 10000 | 0 | 5 |
| O=C(/C=C/ | 10000 | 0 | 5 |
| CS(=O)(=O) | 10000 | 0 | 5 |
| O=C(O)c1c | 10000 | 0 | 5 |
| O=C1C=C(C | 10000 | 0 | 5 |
| CC(C)=CCc1 | 10000 | 0 | 5 |
| COc1cc2c(c | 10000 | 0 | 5 |
| CCOC(=O)c | 10000 | 0 | 5 |
| CCCCC(Sc1 | 10000 | 0 | 5 |
| CCCCC(Sc1 | 10000 | 0 | 5 |
| CS(=O)(=O) | 10000 | 0 | 5 |
| CCOC(=O)c | 10000 | 0 | 5 |
| O=C1C=C(C | 10000 | 0 | 5 |
| Cc1cccc(OC | 10000 | 0 | 5 |
| Cc1cccc(OC | 10000 | 0 | 5 |
| Cc1ccc(-c2c | 10000 | 0 | 5 |
| CC(C)=CCC | 10000 | 0 | 5 |
| COC1=CC(= | 10000 | 0 | 5 |
| CC(C)C(C1= | 10000 | 0 | 5 |
| COCCOc1c | 10000 | 0 | 5 |
| CCCCC(Sc1 | 10000 | 0 | 5 |
| CCCCC1=C( | 10000 | 0 | 5 |
| C#CCCOC(= | 10000 | 0 | 5 |

| | | | |
|---|---|---|---|
| Oc1ccc(-c2 | 10000 | 0 | 5 |
| Nc1ccc(-c2 | 10000 | 0 | 5 |
| O=C(O)c1c | 10000 | 0 | 5 |
| CCCCC1=C( | 10000 | 0 | 5 |
| CCCCC(Sc1 | 10000 | 0 | 5 |
| CCCCCCC1= | 10000 | 0 | 5 |
| CC(=O)c1c( | 10000 | 0 | 5 |
| CCCCC(Sc1 | 10000 | 0 | 5 |
| COc1cc(-c2 | 10000 | 0 | 5 |
| CC(C)C(=O) | 10000 | 0 | 5 |
| COc1cccc( | 10000 | 0 | 5 |
| COc1cccc( | 10000 | 0 | 5 |
| O=C(O)c1c | 10000 | 0 | 5 |
| CCCCCc1cc | 10000 | 0 | 5 |
| COc1ccc(-c | 10000 | 0 | 5 |
| CCCCC(Cc1 | 10000 | 0 | 5 |
| CC(=O)Oc1 | 10000 | 0 | 5 |
| Cc1nnsc1C | 10000 | 0 | 5 |
| CC(=O)Oc1 | 10000 | 0 | 5 |
| CCOC(=O)c | 10000 | 0 | 5 |
| O=C1COCC | 10000 | 0 | 5 |
| COc1cc(F)c | 10000 | 0 | 5 |
| COc1ccc(-n | 10000 | 0 | 5 |
| CCOC(=O)C | 10000 | 0 | 5 |
| Cc1occc(=S | 11000 | 0 | 4.958607 |
| OCCc1ccc( | 13000 | 0 | 4.886057 |
| COc1cc(/C= | 13900 | 0 | 4.856985 |
| CC(C)=CCC | 14000 | 0 | 4.853872 |
| Cc1cccc(C2 | 14200 | 0 | 4.847712 |
| C=CCc1ccc | 15000 | 0 | 4.823909 |
| O=C([O-])/ | 17000 | 0 | 4.769551 |
| CC(C)Cc1cc | 17000 | 0 | 4.769551 |
| C/C=C/c1cc | 18400 | 0 | 4.735182 |
| COC1(c2cc | 19000 | 0 | 4.721246 |
| CCCCC/C=C | 20000 | 0 | 4.69897 |
| CCCCC/C=C | 20000 | 0 | 4.69897 |
| CN(C)c1ccc | 20000 | 0 | 4.69897 |
| COc1cc(-c2 | 20900 | 0 | 4.679854 |
| NS(=O)(=O) | 21310 | 0 | 4.671417 |
| COc1cc(-c2 | 22800 | 0 | 4.642065 |
| COc1ccc(N | 23500 | 0 | 4.628932 |
| Nc1ccccc1- | 24300 | 0 | 4.614394 |
| CC1(C)[C@ | 24800 | 0 | 4.605548 |
| CC1(C)[C@ | 25700 | 0 | 4.590067 |
| COc1ccc(-c | 27200 | 0 | 4.565431 |
| CCCCC/C=C | 28000 | 0 | 4.552842 |
| Cc1ccc(/C= | 30000 | 0 | 4.522879 |
| O=C1/C(=C | 30000 | 0 | 4.522879 |
| Oc1ccc(-c2 | 30000 | 0 | 4.522879 |
| c1ccc(CCCr | 30000 | 0 | 4.522879 |
| COc1ccc(/C | 30000 | 0 | 4.522879 |

| | | | |
|---|---|---|---|
| O=C1N=C(N | 30000 | 0 | 4.522879 |
| Cc1ccccc1C | 30000 | 0 | 4.522879 |
| c1ccc(CCCr | 30000 | 0 | 4.522879 |
| c1ccc(CCCr | 30000 | 0 | 4.522879 |
| Cc1ccccc1C | 30000 | 0 | 4.522879 |
| CC1(C)CC[C | 30400 | 0 | 4.517126 |
| CC1(C)CC[C | 30600 | 0 | 4.514279 |
| CCCCCCC(S | 31000 | 0 | 4.508638 |
| CC1(C)[C@ | 31800 | 0 | 4.497573 |
| O=c1/c(=C/ | 33800 | 0 | 4.471083 |
| CCCCCCC(S | 34000 | 0 | 4.468521 |
| CC1(C)CC[C | 40000 | 0 | 4.39794 |
| CC1(C)CC[C | 40000 | 0 | 4.39794 |
| CC1(C)CC[C | 40000 | 0 | 4.39794 |
| C[C@H]1[C | 40000 | 0 | 4.39794 |
| C[C@H]1[C | 40000 | 0 | 4.39794 |
| C[C@H]1[C | 40000 | 0 | 4.39794 |
| CC1(C)CC[C | 40000 | 0 | 4.39794 |
| CC1(C)CC[C | 40000 | 0 | 4.39794 |
| CC(=O)O[C | 40000 | 0 | 4.39794 |
| CC1(C)CC[C | 40000 | 0 | 4.39794 |
| CC(=O)O[C | 40000 | 0 | 4.39794 |
| C[C@H]1[C | 40000 | 0 | 4.39794 |
| C[C@H]1[C | 40000 | 0 | 4.39794 |
| CC1(C)CC[C | 40000 | 0 | 4.39794 |
| COc1cc(O)c | 41400 | 0 | 4.383 |
| CC1(C)CC[C | 42000 | 0 | 4.376751 |
| CC1(C)CC[C | 42000 | 0 | 4.376751 |
| CC1(C)[C@ | 42000 | 0 | 4.376751 |
| C[C@H]1[C | 42000 | 0 | 4.376751 |
| O=C(O)c1c | 50000 | 0 | 4.30103 |
| CCCNC(=O) | 50000 | 0 | 4.30103 |
| O=C(/C=C/ | 54000 | 0 | 4.267606 |
| CCCCC/C=C | 65000 | 0 | 4.187087 |
| COc1cc(Cl)c | 68000 | 0 | 4.167491 |
| O=C(O)c1c | 75000 | 0 | 4.124939 |
| COc1ccc2c | 81400 | 0 | 4.089376 |