**SUPPLEMENTARY INFORMATION**



**Fig. S1**: Chart showing the top 5 ligands using AutoDock Vina (MCULE) and the correlating intersecting ligands using CCLCDDW



**Fig. S2:** Chart showing the top scored 5% ligands using CLCDDW and the correlating intersecting ligands using AutoDock Vina (MCULE).



**Fig. S3:** The binding modes of compound B in (a) Auto Dock VINA and (b) CLCDDW



Bond lengths are in Angstroms

**Fig. S4:** The molecular interactions of compound B in (a) Auto Dock VINA and (b) CLCDDW



**Fig. S5:** The binding modes of compound C in (a) Auto Dock VINA and (b) CLCDDW



Bond lengths are in Angstroms

**Fig. S6:** The molecular interactions of compound C in (a) Auto Dock VINA and (b) CLCDDW



**Fig. S7**: The binding modes of compound D in (a) Auto Dock VINA and (b) CLCDDW



Bond lengths are in Angstroms

**Fig. S8:** The molecular interactions of compound D in (a) Auto Dock VINA and (b) CLCDDW



**Fig. S9:** The binding modes of compound E in (a) Auto Dock VINA and (b) CLCDDW



Bond lengths are in Angstroms

**Fig. S10**: The molecular interactions of compound E in (a) Auto Dock VINA and (b) CLCDDW

**Table S1:** The docking results using AutoDock Vina via Mcule

|  |  |  |  |
| --- | --- | --- | --- |
| **S/N** | **SMILES** | **MCULE ID** | **SSCORE** |
| 1 | C(C1=CN=CN1C1=CC(C2C3SC4C=CC=CC=4C=3C=CC=2)=CC=C1)(=O)NCC1C(F)=CC=CC=1F | MCULE-8443281251-0-1 | -8.9 |
| 2 | C12SC(=CC=1C(=NN2C1C=CC=CC=1)C)C(=O)/C=C1\NCCC2=CC3=C(OCCCO3)C=C\12 | MCULE-9995974956-0-1 | -8.5 |
| 3 | C1=CC2=C(C=C1)N(C1C=CC=CC=1C=C2)C(=O)N[C@@H]1C[C@@H]2CC[C@@H](N2C)C1 | MCULE-1523073286-0-2 | -8.5 |
| 4 | C12C(=NC=NC=1N(N=N2)C)N1CCN(CC1)C(=O)COC1=CC=C2C(C=CC=C2)=C1 | MCULE-2821431762-0-1 | -8.4 |
| 5 | C12=NN=NN1[C@H](C=C(C1C=CC=CC=1)N2CC(=O)NCC1=CC=C(C=C1)F)C1=CC=C(C=C1)Cl | MCULE-1018045960-0-1 | -8.4 |
| 6 | N12N=C(SC1=NN=C2[C@H]1COC2C(=CC=CC=2)O1)C1=CC2=C(C=CC=C2)O1 | MCULE-8663107798-0-1 | -8.3 |
| 7 | FC1=CC(F)=C(C(NCC(NC2C3=C(C=CC=C3)OC3=C2C=CC=C3)=O)=O)C=C1 | MCULE-9565740349-0-1 | -8.2 |
| 8 | C12OC3=CC=C(C=C3CC=1C(N(C1=CC=CC=C1)N2CC(=O)NCC1C=CC=C(OC)C=1)=O)Br | MCULE-3439413100-0-1 | -8.2 |
| 9 | C1(=C(C(F)(F)F)OC(C)=C1)NC(=O)NC1C=CC(=NC=1)OC1=C2C=CC(Cl)=CC2=NC=N1 | MCULE-9087873656-0-1 | -8.2 |
| 10 | N12N[C@H](C3=CC=CC=C3)[C@@H](SC1=NN=C2C1=CC=CC=C1)C(=O)NCC1=CC=CO1 | MCULE-4860195799-0-2 | -8.2 |
| 11 | C1(C2=CC=C(C=C2)C(F)(F)F)C(=O)C2C(=CC=CC=2)C=1NC1C=CC(=C(F)C=1)C | MCULE-8279910233-0-1 | -8.1 |
| 12 | FC1=C(C2OC(C3=C(C(NC4=CC(Cl)=C(N5CC(=O)NCC5)C=C4)=O)C=CC=C3)=NC=2)C=CC=C1 | MCULE-8041377389-0-1 | -8.1 |
| 13 | CC1=CC=C(N2N=NC(C(NNC3=C4C(CCCC4)=CC=C3)=O)=C2)C=C1 | MCULE-7731866337-0-1 | -8.1 |
| 14 | C12NC(CCC(=O)N1N=C(CCC)C=2C1C=CC(=C(C=1)S(=O)(=O)NC1C=C(C)C=CC=1C)C)=O | MCULE-6762395817-0-1 | -8 |
| 15 | N1C2=CC=CC=C2CC[C@@H](SCCC(=O)NC2=CC=CC3=C2C=CC=N3)C=1O | MCULE-5929541522-0-41 | -8 |
| 16 | C1(=C/C(C2=CC=CC=C2)=O)/NC2=C(C=CC=N2)N=C/1CC(C1C=CC=CC=1)=O | MCULE-8372782252-0-1 | -8 |
| 17 | C12=C3C4=CC=CC=C4C(=O)C1=C(C=C(N1CCC(CC1)C)C2=NO3)NC1=CC=C(C=C1)N(C)C | MCULE-4741178768-0-1 | -8 |
| 18 | N12C(SCC(=O)N3CCN(CC3)C3=CC=C(F)C=C3)=NNC(=O)C1=CC(C1=CC=CS1)=N2 | MCULE-7246818590-0-1 | -8 |
| 19 | N1(C(NCC2=CC=C(C=C2)OC)=NC(C2C=CC=CC=2)=N1)S(=O)(=O)C1C=CC(=CC=1)C | MCULE-4190411975-0-2 | -7.9 |
| 20 | C12=C(C)C3OC(=C(C)C=3C=C1C(=C(CCC(=O)N1CCC3=C(N=CN3)C1)C(=O)O2)C)C | MCULE-7826929160-0-1 | -7.9 |
| 21 | C12C(C3=CC=C(C=C3)OC)=C(OC=1N=CN1N=C(COC3C=CC(=CC=3)C)N=C21)C1C=CC(=CC=1)OC | MCULE-4718215784-0-1 | -7.9 |
| 22 | [C@]12(CN(CC3C=CC=CC=3)C[C@](C3C=CC=CC=3C1=O)(N(=O)=O)[C@@H]2CC(C1C=CC=CC=1)=O)N(=O)=O | MCULE-2819757532-0-4 | -7.9 |
| 23 | C12[C@H](CC(=NC=1C(OC2=O)(C)C)O)C1C=CC(=C(OC)C=1)OCC1=CC=CC=C1 | MCULE-6256273847-0-2 | -7.9 |
| 24 | C1(N2CCOCC2)N=C(N/N=C/C2C=CC=C(C=2)N(=O)=O)N=C(NC2C=C(C)C=CC=2C)N=1 | MCULE-1343386283-0-3 | -7.9 |
| 25 | CC1=C(C)C2=C(C(=CC(O2)=O)CSC2N3C(C(=CC(C(F)(F)F)=C3)Cl)=NN=2)C=C1 | MCULE-8994798017-0-1 | -7.9 |
| 26 | N1(N=C(/C(=N\NC2=CC=CC(Br)=C2)/C1=O)C)C1SC=C(C2=CC=C(C=C2)Cl)N=1 | MCULE-6084272273-0-1 | -7.9 |
| 27 | C(/NC1C=CC(=CC=1)OC)(\NC1=NC(C)=CC(C)=N1)=N\C(=O)C1=CC=C(C=C1)N(=O)=O | MCULE-9606225094-0-1 | -7.8 |
| 28 | FC(C1=CC([C@@H]2OCCN(C(NN3C4=C(C=CC=C4)N=C3)=O)C2)=CC=C1)(F)F | MCULE-8714561085-0-1 | -7.8 |
| 29 | NC1N[C@@H](C2=CC=C(OCC3N=C4N(C=CC=C4)C=3)C=C2)N2C(=NC3=C2C=CC=C3)N=1 | MCULE-3254184720-0-1 | -7.8 |
| 30 | CN([C@@H](C1=CC=C(F)C=C1)C1=CC=CC=C1)CC1OC(C2C(C3=CC=CC=C3)=NOC=2C)=NN=1 | MCULE-8969405481-0-1 | -7.8 |
| 31 | O=C1[C@@H](SC2OC(C3C4=C(C=CC=C4)C(=O)N(CC4=CC=CC=C4)N=3)=NN=2)CCO1 | MCULE-2636033371-0-2 | -7.8 |
| 32 | C1(C(=O)N2CCCCC2)=NN(S/C/1=N\C(=O)C1=CC=C(C=C1Cl)Cl)C1=CC=C(C=C1)Cl | MCULE-4582733893-0-2 | -7.8 |
| 33 | C1C(F)=C(C=CC=1)C(=O)N1[C@H](C)CN(CC1)C1C2C=CC=CC=2OC2C(N=1)=CC=C(C=2)C | MCULE-3102850185-0-1 | -7.8 |
| 34 | C12=NC(=C(C(=O)NC3C=CC4=C(C=3)SC(=N4)C)N1CCS2(=O)=O)C1C=CC(=CC=1)Cl | MCULE-5830645399-0-1 | -7.8 |
| 35 | C1C=CC(=CC=1)C1=C(NC(C2C=CC(=C(Cl)C=2)Cl)=N1)C1=CC=CC=C1 | MCULE-1558157577-0-1 | -7.8 |
| 36 | C[C@H](C1OC(C2SC=CC=2)=NN=1)OC(C1OC(C2=CC(C(F)(F)F)=CC=C2)=CC=1)=O | MCULE-2635982406-0-1 | -7.7 |
| 37 | C12C(SC3C=CC(=CC=3)C)=NC=CN1C(N(CC(=O)NC1=C(OC)C=C(C(Cl)=C1)OC)N=2)=O | MCULE-9960939319-0-1 | -7.7 |
| 38 | C1(OCCSC=1)C(=O)NC1=CC=C(C=C1)C(=O)NC1C=CC(=C(C)C=1)C | MCULE-4580750146-0-2 | -7.7 |
| 39 | N1(C2=CC=CC=C2)[C@H](C2=CC=CC3=CC=CC=C23)N2N(CCC2)C1=S | MCULE-8912229689-0-1 | -7.7 |
| 40 | S1(=O)(=O)C(C2=CC=CC=C2)=C(C(N2CCC(CC2)NC(=O)CC2=CC=CC=C2C)=N1)C | MCULE-7231722824-0-1 | -7.7 |
| 41 | S(=O)(=O)(C1C=CC(=CC=1)C)N/N=C/C1C=C(Br)C=CC=1OC(C1=CC=CC=C1)=O | MCULE-4547957100-0-1 | -7.7 |
| 42 | N1(CC(=O)/N=C2\NN=C(CCC3C=CC=CC=3)S\2)C=NC2C(=CC=CC=2)C1=O | MCULE-3967939030-0-1 | -7.7 |
| 43 | C1(=CSC2[C@@H](C3C=CC(=CC=3)C(F)(F)F)CC(=O)NC1=2)S(=O)(=O)C1C=CC(Cl)=CC=1 | MCULE-1549237209-0-3 | -7.7 |
| 44 | C1C(C(=O)C2C(C)=CC=C3C=CC=CC=23)=C2C=CC=CC2=CC=1 | MCULE-7427577414-0-1 | -7.7 |
| 45 | S1(=O)(=O)C2C=CC=CC=2N=C(CC2(CCCC2)CC(NCCC2C=C(OC)C=CC=2OC)=O)N1 | MCULE-9973978696-0-3 | -7.6 |
| 46 | O=S(C1=C2C(C=NC=C2)=CC=C1)(N1C2=C(C=CC=C2)CN2C(=CN=N2)C1)=O | MCULE-2602756469-0-1 | -7.6 |
| 47 | C12=NN=NN1CCCC[C@@H]2C(=O)N(C)CC1=NC2=CC=CC=C2C(=O)N1 | MCULE-6169724363-0-1 | -7.6 |
| 48 | C[C@@H](C(NNC([C@@H](SC1=CC=CC=C1)C)=O)=O)OC1=CC2=C(C=CC=C2)C=C1 | MCULE-6217345482-0-1 | -7.6 |
| 49 | C1(=CC2=CC(=CC=C2OC1=O)C(=O)NC1C=C(C)C=C(C)C=1)S(=O)(=O)C1=CC=C(C=C1)F | MCULE-2173184013-0-1 | -7.6 |
| 50 | N1=C(C2=CC=CC=C2)OC(=O)[C@H]1C1C=CC2=C(C=CC=C2)N=1 | MCULE-1309971741-0-1 | -7.6 |
| 51 | CC1=C(OC(C2=CC3=C(N4C(=NS3(=O)=O)CCCCC4)C=C2)=O)C=CC(Cl)=C1 | MCULE-7037072833-0-1 | -7.6 |
| 52 | [N+]1(CCCCC1)(CC#CC(O)(C1C=CC=CC=1)C1C=CC=CC=1)CC1C=CC=CC=1Cl | MCULE-9346699773-0-1 | -7.6 |
| 53 | COC1=CC(C(NNC(C2=C3C(CCC3)=CC=C2)=O)=O)=C(Br)C=C1 | MCULE-5689264030-0-1 | -7.6 |
| 54 | N1C(CC2=CC=C(C=C2)OC)=NNC=1NC(=O)[C@@H](C)C1C=CC(=CC=1)C[C@@H]1CCCC1=O | MCULE-9207274769-0-1 | -7.6 |
| 55 | COC1=CC=C(C2N=C3N(C(/C(/S3)=C3/SC(C)=C(C)S/3)=O)[C@@H](C3=CC=CC=C3)C=2)C=C1 | MCULE-7834508649-0-1 | -7.6 |
| 56 | N1NC(C2C=CC(=CC=2)OC)=NC2C=CC(Cl)=CC=2C=1C1C=CC(OCC)=CC=1 | MCULE-1429070077-0-1 | -7.5 |
| 57 | S1(=O)(=O)C2=CC=CC=C2N(C=C1C(=O)C1C=CC(=CC=1)OCC)C1=CC=C(C=C1)OC1=CC=CC=C1 | MCULE-7950872117-0-1 | -7.5 |
| 58 | CC1=C(C2=CC=CC=C2)C(=O)C2=C(C=C(C=C2)OC2=C(N(=O)=O)N3C(C=CC=C3)=N2)O1 | MCULE-5693530085-0-1 | -7.5 |
| 59 | C12N=C(C3CCN(CC3)S(=O)(=O)C3=CC=C(C=C3)OC(F)(F)F)N=C(O)C=1N=NN2CC1=CC=CC=C1F | MCULE-2264653472-0-1 | -7.5 |
| 60 | COC1=C(NC(C#CC2=CC=CC=C2)=O)C=C(S(C(F)(F)F)(=O)=O)C=C1 | MCULE-7976254688-0-1 | -7.5 |
| 61 | S1C(COC2C=CC3=C(C=2)C(C)=CC(=O)O3)=NN=C1NC1C=CC(=CC=1)Br | MCULE-7247419279-0-1 | -7.5 |
| 62 | CC1=CC(OCC2OC(C3(C4=CC=CC=C4)CCOCC3)=NN=2)=CC=C1 | MCULE-6277098690-0-1 | -7.5 |
| 63 | CC(N1[C@H](CC2ON=C(C3=CC=CC=C3)N=2)C2=C(C=CC=C2)C=C1)=O | MCULE-1341291914-0-1 | -7.5 |
| 64 | C1(NC(=O)C2=CC=CO2)=C2C[S@](CC2=NN1C1C=CC=C(C)C=1C)=O | MCULE-3362868466-0-1 | -7.5 |
| 65 | C[C@H]1C2=C(C=CC(OCC3N=C4N(C=CC(=C4)C)C(=O)C=3)=C2C(=O)C1)Cl | MCULE-7539618691-0-2 | -7.5 |
| 66 | C1(C#N)(C#N)[C@H](C2=CC=C(C=C2F)F)[C@H](N2C3=C(C=CC=C3)C=C[C@@]21[H])C(C1=CC=CC=C1)=O | MCULE-8658699071-0-1 | -7.5 |
| 67 | [C@@]1(CC2C=CC=CC=2)(NC(C2=CC=CC=C2)=O)C(=O)NC(C2C=CC=CC=2)=N1 | MCULE-4182318424-0-38 | -7.5 |
| 68 | C12C(SCC3=CC=CC(Br)=C3)=NC=CN1N=C(C1C=C(C)C=CC=1C)C=2 | MCULE-2894347504-0-1 | -7.5 |
| 69 | C(=O)(C(C1=CC=CC=C1)C1C=CC=CC=1)N/N=C(/C=C/C1C=CC=CC=1)\C=C\C1=CC=CC=C1 | MCULE-1522865047-0-1 | -7.5 |
| 70 | C12NN=C(O)C=1[C@H](C1C(C[C@@H](C3=CC=CS3)CC=1N2)=O)C1C(=CC=CC=1Cl)Cl | MCULE-8226146640-0-1 | -7.5 |
| 71 | FC1=CC=C(/C=C/S(N2C3=C(C=C(C=C3)F)NC(=O)CC2)(=O)=O)C=C1 | MCULE-9007015866-0-1 | -7.5 |
| 72 | C1(C=CN(CC2C=CC(=CC=2Cl)Cl)N=1)C(=O)N/N=C/C1=CC=CC=C1Cl | MCULE-3389288402-0-1 | -7.5 |
| 73 | CC1=NN(C2N(N)C(SCC3=C4C(C=CC=C4)=CC=C3)=NN=2)C(C)=C1 | MCULE-9998470483-0-1 | -7.5 |
| 74 | C12C=CC=CC=1C=CC(/N=N/C1C=CC3C=CC=CC=3C=1)=C2 | MCULE-9976836886-0-1 | -7.5 |
| 75 | C1(C2C=CC=CC=2C2=CC=CC=C12)C(=O)N1CCN2[C@H](C(=O)NCC2)C1 | MCULE-1626453876-0-1 | -7.4 |
| 76 | S1(=O)(=O)C2=CC=C(C=C2N(N=C1C(=O)N1CCCCCC1)CC1C(C)=NOC=1C)C | MCULE-1127544270-0-2 | -7.4 |
| 77 | C1(SC2C(=O)NC3=C(C=C(C=C3)N(=O)=O)C=2C2C=CC=CC=2)=NN=NN1C | MCULE-5624146770-0-1 | -7.4 |
| 78 | N1([C@H]2CC(=O)[C@@H]3OC[C@H]2O3)N=NN(C2C=CC(=C(C)C=2)C)C1=S | MCULE-2930104442-0-2 | -7.4 |
| 79 | C(C1=C(COC2=CC=CC=C2)C=CC=C1)NC1=NN2C(=NN=N2)C=C1 | MCULE-3128059000-0-1 | -7.4 |
| 80 | O=N(C1OC(/C=N/NP(C2=CC=CC=C2)(C2=CC=CC=C2)=S)=CC=1)=O | MCULE-8566994915-0-1 | -7.4 |
| 81 | C1(SC(=O)C2=CC=CC=C2C)=C(NC2=CC=CC=C2)SC(C2=CC=C(C=C2)Cl)=N1 | MCULE-1603455942-0-1 | -7.4 |
| 82 | C1C2=C3C(=CC=C(C3=CC=1)NC1C(C(=O)O)=CC=CC=1)CC2 | MCULE-3663386420-0-1 | -7.4 |
| 83 | C1(N(=O)=O)C=CC(SC2C(=O)CC(C)(C)CC=2OC([C@]23C[C@H]4C[C@H](C[C@H](C4)C2)C3)=O)=CC=1 | MCULE-3135305105-0-1 | -7.4 |
| 84 | N12C3C=CC=CC=3N=C1N[C@H]([C@H](C)CC1C=CC3=C(OCO3)C=1)C(C#N)=C2N | MCULE-1969516429-0-1 | -7.4 |
| 85 | N1=C(SCC(=O)NC2C=CC=C(C)C=2)C(=NC21CCN(CC2)CC)C1C=CC(=CC=1)F | MCULE-9410581573-0-1 | -7.4 |
| 86 | N12N=C(SC1=NC1=CC(=CC=C1C2=O)C(OC)=O)NC1C=CC(=C(C)C=1)C | MCULE-6470395655-0-1 | -7.4 |
| 87 | N1(CC(=O)NC2C=CC(=CC=2)CC)C2C=CC=CC=2N=C(C2C=CC(=CC=2)F)CC1=O | MCULE-2254917819-0-1 | -7.4 |
| 88 | C1(=C/C2C3C=CC=CC=3N(C)C=2)/C(=O)C2C(=C(C)C(=CC=2)OCC2=CC=C(C=C2Cl)F)O/1 | MCULE-5728035127-0-1 | -7.4 |
| 89 | C12C(=O)N(CC3C=CC(=CC=3)Br)C(N(C)C=1N=C1OC(C3C=CC(=CC=3)F)=CN21)=O | MCULE-2639921006-0-1 | -7.4 |
| 90 | CC(OCCCC1=CC(NC(C2=C(Cl)C=C(F)C(F)=C2)=O)=CC=C1)=O | MCULE-5886489196-0-1 | -7.4 |
| 91 | CCN1C(=O)CN(C(C2=CC3=C(C(O[C@@H](C4=CC=CC=C4)C3)=O)C=C2)=O)CCC1 | MCULE-6887869192-0-1 | -7.4 |
| 92 | O=C1C2=C(C=CC=C2)CS(=O)(=O)N1CCOC1=CC(C#N)=CC=C1 | MCULE-8128999844-0-1 | -7.4 |
| 93 | FC(C1=CC=C(C2OC=C(CO/N=C3\CCOCCC\3)N=2)C=C1)(F)F | MCULE-3843892892-0-1 | -7.4 |
| 94 | C12=C(C3C=CC=CC=3)C=C(C=C1SC(=O)O2)OC(COC1C=CC(=C(C)C=1)C)=O | MCULE-1054176167-0-1 | -7.3 |
| 95 | CCCCOC1=CC=C(NP(OC2=CC=C(C)C=C2)(OC2=CC=C(C)C=C2)=O)C=C1 | MCULE-2987506470-0-1 | -7.3 |
| 96 | C12C(SCC3=C(C)OC(C4=CC=CC=C4F)=N3)=NN=C(CC)N1C1=C(SC=C1)C=2 | MCULE-6122270640-0-2 | -7.3 |
| 97 | N1(C2=CC=CS2)C(=O)NN=C1CC1CCN(CC1)C(=O)CC1C2C=CC=CC=2ON=1 | MCULE-2004433404-0-1 | -7.3 |
| 98 | CC1=CC(N2N(CC3=C4C(COCO4)=CC(N(=O)=O)=C3)C(=O)N=C2)=C(C)C=C1 | MCULE-5420487886-0-1 | -7.3 |
| 99 | BrC1=CC2=C(C(=CC(O2)=O)CN2C(=O)NN=C2C2=CC=CC=C2)C=C1 | MCULE-4678986600-0-1 | -7.3 |
| 100 | S(=O)(=O)(C1=CC=C(C=C1)NC(=O)C1=CC=C(C=C1)C1C=CC=CC=1)NC1N=CC=NC=1OC | MCULE-3144366771-0-1 | -7.3 |
| 101 | N(C1=CC=C(F)C=C1)C(=S)N/N=C/C1C(=O)C2C=C(Cl)C=CC=2OC=1 | MCULE-7962068695-0-1 | -7.3 |
| 102 | C12N=C(C)C=C(SCC(=O)NC3CCN(CC3)C(OCC)=O)N1N=C(C)C=2C1=CC=CC=C1OC | MCULE-8440683563-0-1 | -7.3 |
| 103 | C1(C(OC)=O)=NOC(C)=C1C1C=CC=C(C=1)C(NCCCN1C=CN=N1)=O | MCULE-5273153078-0-1 | -7.3 |
| 104 | COC1=CC(NC2SC(=S)N(CN3C[C@@H](C4N5C(CCCCC5)=NN=4)CCC3)N=2)=CC=C1 | MCULE-1486436428-0-1 | -7.3 |
| 105 | C1(C2C=CC=CN=2)ON=C(C[C@@H]2CC[C@@H]([C@H](O2)CNS(=O)(=O)C2C=CC(C)=CC=2)O)C=1 | MCULE-5883354014-0-1 | -7.3 |
| 106 | C/C(/C1SC2=C(C=CC=C2)N=1)=N/NC([C@H]1OC2=C(C=CC=C2)OC1)=O | MCULE-7308674377-0-4 | -7.3 |
| 107 | FC(C1=NC(C2=CN=CC=C2)=NC(NNC(NC2=NC=CC=C2)=O)=C1)(F)F | MCULE-9092693054-0-1 | -7.3 |
| 108 | CC1=CC=C(NC2=NC(CSC3=CC(Cl)=C(F)C=C3)=NC(N)=N2)C=C1 | MCULE-3289368793-0-1 | -7.3 |
| 109 | N(=O)(=O)C1=CC=CC(=C1)[C@H](SC1=CC=C(SCC)S1)CC(C1=CC=CC=C1)=O | MCULE-1509614166-0-3 | -7.3 |
| 110 | COC1=CC2=C(C=C(C=C2)CN(C(CSC2N[C@H]3[C@H](CCCC3)N=2)=O)C)C=C1 | MCULE-7560305677-0-1 | -7.3 |
| 111 | C1(C(=O)C2C=CC(=CC=2)OC)=C(C)C2C(=CC(=CC=2)NC(CCC2ON=C(OC)C=2)=O)O1 | MCULE-4590635244-0-1 | -7.3 |
| 112 | O=C(NC1=CC2=C(NC(CC2)=O)C=C1)NNC1=CC=C(C#N)C=C1 | MCULE-8491581618-0-1 | -7.3 |
| 113 | C1(N2C=CN=C2)=NC(N2CCN(CC2)C(=O)/C=C/C2C=CC=CC=2)=NC(N2CCOCC2)=N1 | MCULE-4765178291-0-1 | -7.3 |
| 114 | CC(C1SC(C(/N=C2/N(CC3=CC=C(C)C=C3)C=CC=C/2)=O)=CN=1)C | MCULE-7578904639-0-1 | -7.3 |
| 115 | C(/C1C=CC=CC=1)(=N/NC(N)=O)\C(=S)NC1C=CC=CC=1 | MCULE-9917554113-0-1 | -7.3 |
| 116 | C1(=N/N=C/C2C(=CC=CC=2Cl)Cl)\SC2=C(C=CC=C2)N\1CC1C=CC=CC=1 | MCULE-5199506278-0-1 | -7.3 |
| 117 | C1(/C=C(\C#N)/C(=O)N2CCCCC2)C(=O)N2C=CC=C(C)C2=NC=1OC1=CC=C(C=C1Cl)Cl | MCULE-9684614732-0-1 | -7.3 |
| 118 | N1(C2=CC=C(C(C)=C2)Br)C(=O)/C(=C\NC2C=CC3=C(C=2)N=C(N3)O)/C(NC1=O)=O | MCULE-4685390061-0-1 | -7.2 |
| 119 | CC1C(CC(NCCN2C(=O)C3=C(C=CC=C3)CC2)=O)=C(Cl)ON=1 | MCULE-2293480961-0-1 | -7.2 |
| 120 | CC1=C(C(N)=O)C=CC=C1NC(C1C[C@H](C2=CC=CC=C2)ON=1)=O | MCULE-4057545493-0-3 | -7.2 |
| 121 | C1(SC=C(C2=CC=CC(C)=C2)C=1N1C=CC=C1)C1ON=C(C2=CC=C(C(OC)=C2)OC)N=1 | MCULE-4686635848-0-1 | -7.2 |
| 122 | N1(C2C=CC=CC=2C(/C(/C#N)=C\C2=CC=CC=C2Cl)=C1)C1=C(Cl)C=C(C=N1)C(F)(F)F | MCULE-5242809155-0-1 | -7.2 |
| 123 | N12C(CN(C3C=CC(=CC=3)F)C1=O)=NC(=O)N2CC(=O)NCC1=CC=CC=N1 | MCULE-2634744591-0-1 | -7.2 |
| 124 | CC1SC(S(NCCNC(C2=NOC(C3=CN=CC=C3)=C2)=O)(=O)=O)=CC=1 | MCULE-6979373962-0-1 | -7.2 |
| 125 | CC1=CC(C)=C(NC(CNC(COC(C2SC3=C(SC4=C3C=CC=C4)C=2)=O)=O)=O)C(C)=C1 | MCULE-2114638567-0-2 | -7.2 |
| 126 | C1(/C(/N)=N/OC(=O)C2=CC=CC(Cl)=C2)N=C(OC=1C(F)(F)F)C | MCULE-1829062489-0-1 | -7.2 |
| 127 | O=C(C1=CC=C(C2=NOC=N2)C=C1)OCC1(C2=CC=CC=C2)CCOCC1 | MCULE-5663409575-0-1 | -7.2 |
| 128 | N1(CCCN2C(C)=C(C(C)=N2)Cl)C(=O)C2C=CC=CC=2N=C1SCN1C=CC(N(=O)=O)=N1 | MCULE-8522911125-0-1 | -7.2 |
| 129 | N1(C(=O)NC2=C(C=CC=C2)N1O)C1SC2=C(CCCC2)C=1C#N | MCULE-7140448287-0-1 | -7.2 |
| 130 | C1(SC2=C(C=C(C=C2)OC)N=1)NC1=NN=C(C2C=CC3=C(OCCO3)C=2)O1 | MCULE-2996604901-0-1 | -7.2 |
| 131 | C1C=CC(COC2C=CC(/C=C(\C#N)/C#N)=CC=2)=C(OC)C=1 | MCULE-4852353986-0-1 | -7.2 |
| 132 | C(=C(/C)\NC1C=CC(=CC=1)C)\C(=O)ONC(=O)C1=CC=C(C=C1)C | MCULE-7568708094-0-3 | -7.2 |
| 133 | C1(C2=NN=C(O2)C2C=CC(=CC=2)C)C(C(F)(F)F)=NN(C=1)C | MCULE-2660589487-0-1 | -7.2 |
| 134 | C1(SN=NC=1C1C=CC=CC=1)C(=O)N1CCN(CC1)C1C=CC(=CC=1)OC | MCULE-3254510016-0-2 | -7.2 |
| 135 | N1C(=O)S/C(=C\C2C=NN(C)C=2)/C=1NC1C=C(F)C(=C(F)C=1)F | MCULE-5530400025-0-2 | -7.2 |
| 136 | O=C(C1CCCCCC=1)NC1=CC2=C(CCS2(=O)=O)C=C1 | MCULE-6738175917-0-1 | -7.2 |
| 137 | C12N=C(C)S[C@H](C3=CC=C4C(N=CC=N4)=C3)C=1C(NN2[C@@H]1CCOC(C)(C)C1)=O | MCULE-7097410851-0-2 | -7.2 |
| 138 | C1C(C2C(Cl)=CC(Cl)=CC=2)=C2C=C(C3C=CC(C(C)C)=CC=3)N=C2NC1=O | MCULE-6871444133-0-2 | -7.2 |
| 139 | C12OC3=CC=C(C=C3CC=1C(NC(C1=CC=C(C(OC)=C1)OC)=N2)=S)Cl | MCULE-3592103656-0-1 | -7.1 |
| 140 | CN(C1=CC2N3C(=N[P@](C4OC(C)=CC=4)(=S)C=2C=C1)C1=C(C=CC=C1)C3)C | MCULE-8533406980-0-3 | -7.1 |
| 141 | C1(=CN=C(NC1=O)SCC(=O)N1CCN(CC1)C1C=CC=CC=1F)S(=O)(=O)C1=CC=C(C=C1)OCC | MCULE-7729147113-0-1 | -7.1 |
| 142 | ClC1=C(OS(CC2CCN(C(OCC3=CC=CC=C3)=O)CC2)(=O)=O)C=CC(C#N)=C1 | MCULE-3587361304-0-1 | -7.1 |
| 143 | CN1C2=C(C=C(C=C2)Cl)N=C1CN1C(=O)ON=C1C1=CC=C(N(=O)=O)C=C1 | MCULE-7389565650-0-1 | -7.1 |
| 144 | CCCN1C(COC(C2=C(NC3=CC(C(F)(F)F)=CC=C3)N=CC=C2)=O)=NN=N1 | MCULE-8253716717-0-1 | -7.1 |
| 145 | N1(C2=CC=CC=C2C2=CC=CC=C12)/N=C/C1C(O)=CC=C(C=1)N(=O)=O | MCULE-9462828033-0-1 | -7.1 |
| 146 | CCC1ON=C(C2(NC(NC3N(C4=NC(C)=CC(C)=N4)N=CC=3)=O)CCCC2)N=1 | MCULE-9736944753-0-1 | -7.1 |
| 147 | C1(=O)C2C=C(C=CC=2OC2N=CC=CC=2N1C)NC(=O)C1=CC=C(C=C1OC)OC | MCULE-7783858494-0-1 | -7.1 |
| 148 | C1(CN2C(=O)C=CC(C(F)(F)F)=C2)=NC(=NN1CC1C=CC(=CC=1)F)C | MCULE-8967752270-0-2 | -7.1 |
| 149 | C12=C(C3=CC=C(C=C3)F)NN=C1OC(N)=C(C#N)[C@@H]2C1=CC=C(C=C1)N1CCOCC1 | MCULE-2657519394-0-2 | -7.1 |
| 150 | C12(CCN(CC1)C(=O)NC1=C(OC)C=CC(OC)=C1)N=C(C(=O)N2)C1=CC=CC(Cl)=C1 | MCULE-8051959384-0-1 | -7.1 |
| 151 | C1(CO/N=C(\C)/C2=CC=C(F)C(F)=C2)C(Cl)=CC=CC=1F | MCULE-6441047230-0-2 | -7.1 |
| 152 | C1(/C=C(\C#N)/S(C2C=CC=CC=2)(=O)=O)C(=O)N2C=CC=CC2=NC=1N1CCOCC1 | MCULE-7225504290-0-2 | -7.1 |
| 153 | C12SC3=C(C(C)=CC(C)=N3)C=1N=NN(C1=CC=CC3C=CC=NC1=3)C2=O | MCULE-3154693967-0-1 | -7.1 |
| 154 | C1(C2=CC=CC=C2F)=NN=C([C@H]2CCCN(C(=O)CCC3C(C)=NOC=3C)C2)S1 | MCULE-7391624342-0-2 | -7.1 |
| 155 | CC1=NC(NNC(C2SC(S(C3=CC=CC=C3)(=O)=O)=CC=2)=O)=NC(C)=C1 | MCULE-4863536261-0-1 | -7.1 |
| 156 | O=N(C1=CN(CCNC(C2OC(C3=C(Cl)C=CC=C3)=CC=2)=O)N=C1)=O | MCULE-5098018687-0-1 | -7.1 |
| 157 | C1(N=C(N2CCCCC2)N=C(N2CCCCC2)N=1)N1C=NC(SCC(N)=O)=N1 | MCULE-4521363588-0-2 | -7.1 |
| 158 | N12ON=C(C3=C(C)C(Cl)=C(C(Cl)=C3C)C)N1C1C(=CC=CC=1)N2C(=O)C1=CC=CS1 | MCULE-3102452155-0-3 | -7.1 |
| 159 | FC(C1=CC=C(CN2CCN(C(CSC3NN=NC=3)=O)CCC2)C=C1)(F)F | MCULE-1720962177-0-1 | -7.1 |
| 160 | CN1C2=C(C=C(C=C2)NS(C2CCOC3=C(C=CC=C3)C=2)(=O)=O)OC1=O | MCULE-7241219267-0-2 | -7.1 |
| 161 | C1(=C(NCCN(C)C)SC(S(=O)(=O)C2C=CC(=CC=2)C)=N1)S(=O)(=O)C1C=CC(=CC=1)C | MCULE-9710126793-0-1 | -7.1 |
| 162 | ClC1C=CC(=CC=1)C(C1[C@@H](C2C=CC(=CC=2)Cl)C(C#N)=C(N)SC=1N)=O | MCULE-2755886321-0-3 | -7 |
| 163 | OC(C1=C(Cl)C(/C=C/C(C2N3C(SC=C3)=NC=2Cl)=O)=CC=C1)=O | MCULE-8744049005-0-1 | -7 |
| 164 | C12N=C(O)C[C@@H](C(=O)NC3C=CC=C(OC)C=3)N1N=CC=2C1=CC=C(C=C1)OC | MCULE-6060634655-0-2 | -7 |
| 165 | S(=O)(=O)(N1CCCC1)C1C(OC)=CC=C(C2=CC=C(N=N2)N2CCN(CC2)C2=CC=CC=C2F)C=1 | MCULE-4151484731-0-2 | -7 |
| 166 | CC1N(C2=CC=C(Cl)C=C2)N=C(C(NNC(NC2=NC=CC=C2)=S)=O)N=1 | MCULE-7652468581-0-1 | -7 |
| 167 | C12C(NCC3C=CC(F)=CC=3)=NC(=NC=1C1C(=CC=CC=1)O2)CC | MCULE-5439962575-1-2 | -7 |
| 168 | CC1=NN(CC2=CC(C3N=C(CSC[C@@H]4OCCCC4)ON=3)=CC=C2)C(C)=C1 | MCULE-8911493654-0-1 | -7 |
| 169 | FC(C1=C(CCOC(C2N=C(C3CCC3)OC=2)=O)C=CC=C1)(F)F | MCULE-3722512860-0-1 | -7 |
| 170 | CC1=NN(CC2=CC=CC=C2)C(NS(CC2=C(F)C=C(C)C=C2)(=O)=O)=C1 | MCULE-8830710104-0-1 | -7 |
| 171 | CC1N=C([C@H](C(C2=C(C3=CC=CC=C3)OC(C)=N2)=O)C#N)SC=1 | MCULE-1784480460-0-1 | -7 |
| 172 | N1=C(O)/C(/S/C/1=N/C1C=CC=CC=1C)=C/C1=CC=CN1C | MCULE-1888166043-0-2 | -7 |
| 173 | C12N=C3C=CC=CN3C(=O)C=1C=C(C(OCC)=O)/C(=N\C(=O)C1=CC3=C(C=CC=C3)O1)/N2CC(C)C | MCULE-3974527277-0-1 | -7 |
| 174 | CC1=NC(N/N=C2\CCCCCCCCCCC\2)=NC(C)=C1 | MCULE-9163191987-0-1 | -7 |
| 175 | C[C@@H]1C(=O)N(C2=CC=CC=C2)N=C(C(N2C[C@H](C)CSCC2)=O)N1 | MCULE-5294240948-0-1 | -7 |
| 176 | COC(C1=C(C)OC(S(N2C3=C(C=CC=C3)C=CCC2)(=O)=O)=C1)=O | MCULE-1507595130-0-1 | -7 |
| 177 | CN1C(C2C[C@H](C3=CC4=C(N=CC=N4)C=C3)N(S(C3=CC=CC=C3)(=O)=O)N=2)=CC=N1 | MCULE-3578226603-0-2 | -7 |
| 178 | CC(C1=C(OS(C2=CN=C(C3=CC=CC=C3)N=C2)(=O)=O)C=C(C)C=C1)=O | MCULE-4828152836-0-1 | -7 |
| 179 | ClC1=NC(Cl)=C(CSC2N(C3=CC4=C(OCCO4)C=C3)N=NN=2)C=C1 | MCULE-5067421403-0-1 | -7 |
| 180 | COC(C1=C(C)C=C(CN2N=C(C3=CC(C)=C(F)C=C3)N=N2)O1)=O | MCULE-5317853073-0-1 | -7 |
| 181 | N1(CC2C=CC(=CC=2)OC)C(O)=NC(C2CN(C3CCCC3)CNC1=2)=O | MCULE-4811009980-0-1 | -7 |
| 182 | C1(OC(=O)C2C=CC=CC=2N(=O)=O)N(C2=CC=CC=C2)N=C(C)C=1S(=O)(=O)C1=CC=C(C=C1)C | MCULE-1697467887-0-1 | -7 |
| 183 | C1(=C/C2=CC(=C(SC3C=CC(=CC=3)Cl)O2)Br)\C(=O)NC(NC\1=O)=O | MCULE-6090662455-0-1 | -7 |
| 184 | O=C(N/N=C1/C2=C(C=CC=C2)O[C@@H](C2=CC=CC=C2)C/1)COC1=C(C#N)C=CC=C1 | MCULE-3442509264-0-3 | -7 |
| 185 | C1(C(F)(F)F)=NN([C@H]2OC(N)=C(C#N)[C@H](C3=CC=C(C=C3Cl)Cl)[C@H]12)C1C=CC=CC=1 | MCULE-4985703155-0-1 | -7 |
| 186 | O=C(NC[C@@H]1[C@H]2[C@@H]1CC1=C2C=CC=C1)NCCS(NCC1=CC=CC=C1)(=O)=O | MCULE-8850272549-0-1 | -7 |
| 187 | C1(=CC=C(/C(/N)=N/OC(=O)C2SC=CC=2)C=C1N(=O)=O)OC1C=C(C(Cl)=C(C)C=1)C | MCULE-2853819031-0-1 | -7 |
| 188 | N1N(C/C=C(/C)\C)C=CC=1C1C=CC=C(C2C=NC=NC=2)C=1 | MCULE-6714029607-0-1 | -6.9 |
| 189 | C1(C(=O)C2C(C)=CC(=CC=2C)C)[C@H](C2=CC=CN=C2)N(C(=O)C=1O)C1=CC=CC=N1 | MCULE-2755940955-0-1 | -6.9 |
| 190 | FC(C1=CC=C(CONC(NNC2=NC=CC=C2)=O)C=C1)(F)F | MCULE-6321801449-0-1 | -6.9 |
| 191 | CC1=C(C)C=C([C@@H](CN2C(=S)SC(N3CCCC3)=N2)O)C=C1 | MCULE-7798591154-0-3 | -6.9 |
| 192 | N12N=C(N=C1SC([C@@H](C1C=CC(=CC=1Cl)Cl)N1C[C@H](C)O[C@H](C)C1)=C2O)C1=CC=CO1 | MCULE-8690883911-0-1 | -6.9 |
| 193 | [C@]1(CC(=NO1)C1COC2C(=CC=CC=2)C=1)(CC(O)=O)C(=O)NC1C=CC(=CC=1)OC | MCULE-7883028692-0-110 | -6.9 |
| 194 | ClC1SC(C2ON=C(NC(NNC(C3=CC=NC=C3)=O)=O)C=2)=CC=1 | MCULE-7350546462-0-1 | -6.9 |
| 195 | C1([N+]2=CC=CC=C2)=C(/C=N/NC(C2C=CC=CC=2)=O)SC(=O)[N-]1 | MCULE-5972428089-0-1 | -6.9 |
| 196 | FC1=CC(C2OC(CN3C(C4SC=CC=4)=NC=C3)=NC=2)=CC=C1 | MCULE-4475983166-0-1 | -6.9 |
| 197 | CN(C1OC2=C(C=CC=C2)N=1)C(C1C[C@H](C(C)=O)N(C2=CC=CC=C2)N=1)=O | MCULE-4790677657-0-1 | -6.9 |
| 198 | CC1OC(C)=C([C@](CNC(NC2=C(C)NN=C2C)=O)(O)C)C=1 | MCULE-6972883902-0-1 | -6.9 |
| 199 | C1(C#N)=C(/C=C/NC2C=CC(O)=CC=2F)ON=C1C1=CC=CC=C1 | MCULE-3645674867-0-1 | -6.9 |
| 200 | N1(CC(=O)NC2=CC=CC(=C2)C(F)(F)F)C=CC2=C(C=C(C(OC)=C2)OC)CC1=O | MCULE-5817180883-0-1 | -6.9 |
| 201 | C[S@](C1=CC=C(C(OC[C@@H]2ON=C(C3=CC=CC=C3)NC2)=O)C=C1)=O | MCULE-4515084006-0-1 | -6.9 |
| 202 | C[C@@H](C1NC2=C(C=CC=C2)N=1)NC(C(NC1=CC(SC(F)F)=CC=C1)=O)=O | MCULE-8512440022-0-1 | -6.9 |
| 203 | OC1=C(N(=O)=O)C=CC(/C=C2\C3=C(C=CC=C3)C(=O)NC\2=O)=C1 | MCULE-4900429852-0-1 | -6.9 |
| 204 | CCCCC1NC(C(OCC)=O)=C(NC(C2=CC(C3N=C(C)ON=3)=CC=C2)=O)N=1 | MCULE-7130291437-0-1 | -6.9 |
| 205 | COC1=C(C)C=C(S(NC2=NN(CC(F)(F)F)C=N2)(=O)=O)C(C)=C1 | MCULE-4120823501-0-1 | -6.9 |
| 206 | C1(/C2=CC=CC=C2C(NC(=O)C2=CC=C(C=C2)C)=N/1)=C(/C#N)\C(NCCCCCC)=O | MCULE-8181075204-0-1 | -6.9 |
| 207 | O=C(C1=C(SCC2SC=CC=2)C=CC=C1)NC1=C2C(OCCO2)=CC=C1 | MCULE-9045755728-0-1 | -6.9 |
| 208 | C[C@@H](C1=CC(C(F)(F)F)=C(F)C=C1)OC(CN1N=C(N(=O)=O)C=C1)=O | MCULE-1382913904-0-1 | -6.9 |
| 209 | C[C@@H](C1=CC(C(F)(F)F)=CC=C1)NC[C@@H](C1=CC=CC=C1)CO | MCULE-3753544568-0-1 | -6.9 |
| 210 | N1(C(C)=CC=C1C)NC(=O)C(=O)NC1=CC=C(C(C)=C1)C | MCULE-7424094347-0-3 | -6.9 |
| 211 | N1=C(C2C=CN=CC=2)SC(C)=C1OC(C1=CC=CC=C1)=O | MCULE-4024387703-0-2 | -6.9 |
| 212 | C1(=C/C2=CC=C(C(OC)=C2)C)/C=C(OC/1=O)C1=CC=C(C(C)=C1)C | MCULE-2968565131-0-1 | -6.9 |
| 213 | BrC1C=CC2N(CC3=C(/C(/N=2)=N\C(COC2=CC4=C(C=CC=C4)C=C2)=O)C=CC=C3)C=1 | MCULE-2621699271-0-1 | -6.9 |
| 214 | C1(C=C(C=CC=1OC)Cl)NC(=O)NNC(=O)C(=O)NC1C=CC(F)=CC=1 | MCULE-1247862711-0-1 | -6.9 |
| 215 | N1(C=CC=C1/C=N/NC(=S)NC1=CC=CC=C1)C1C=CC(=CC=1)OC | MCULE-4164549318-0-1 | -6.9 |
| 216 | C1(/C(=O)ON=C/1C1C=CC=CC=1)=C/C1=CC=CC=C1OS(C1C=CC=CC=1)(=O)=O | MCULE-1808678317-0-1 | -6.9 |
| 217 | ClC1=CC=C(CC2SC(NC(NNC(C3=CC=NC=C3)=O)=O)=NN=2)C=C1 | MCULE-6218187904-0-1 | -6.9 |
| 218 | N1(C(=O)COC2=CC=CC=C2)N=C(N=C1NCC1=CC=CS1)NCC1=CC=CS1 | MCULE-9870656355-0-1 | -6.9 |
| 219 | C1[C@H](C2=CC=CC=C2)C(C(=O)OC)=C(NC2=CC=C(OC)C=C2)C=C1C | MCULE-7018196090-0-1 | -6.9 |
| 220 | C1(C(C(=O)C2C=CC=CC=2)C(C2C=CC=CC=2)=O)C(C2C=CC=CC=2)=NNC=1C1C=CC=CC=1 | MCULE-8749315588-0-1 | -6.9 |
| 221 | N1(C(C(C)C)=CC(C(=O)NCC2=CC=CO2)=N1)C1SC2=C(C=CC=C2)N=1 | MCULE-5582990861-0-1 | -6.9 |
| 222 | C1(S(=O)(=O)C2=CC=CS2)C2=NC3C=CC=CC=3N=C2N(/N=C/C2=CC=CC(OC)=C2OC)C=1N | MCULE-2747125082-0-1 | -6.9 |
| 223 | C1(C(=O)N(C)CC2ON=C(C3C=CC=CC=3)N=2)=C(C)N2C(=NCC2)S1 | MCULE-9263283905-0-1 | -6.9 |
| 224 | CN1C(=O)N(C)C(=O)C=C1CNC1=C(OC[C@@H]2OCCCC2)C=CC=C1 | MCULE-3837901520-0-1 | -6.9 |
| 225 | COC1=CC=C(C2ON=C(CSCC3=C4C(COCO4)=CC(F)=C3)N=2)C=C1 | MCULE-6142835936-0-1 | -6.9 |
| 226 | C1(/C(/C#N)=N/NC2C(Cl)=CC=C(Cl)C=2)NC2=C(C=CC=C2)N=1 | MCULE-1504975088-0-1 | -6.8 |
| 227 | N1(C2=CC=C(C(C(O)=O)=C2)Cl)N=C(/C(=C\C2C=C(OC)C3=C(SC(O3)=O)C=2)/C1=O)C | MCULE-3687316998-0-1 | -6.8 |
| 228 | C1(C(=O)NC2C=CC(=CC=2)OC)=CC2C(CO)=CN=C(C)C=2O/C/1=N\C1C=CC=CC=1 | MCULE-4551343281-0-1 | -6.8 |
| 229 | NC(CCNC(C(NC1=C(NC2=C(F)C=C(F)C=C2)C=CC=C1)=O)=O)=O | MCULE-9601786227-0-1 | -6.8 |
| 230 | CCN(S(NC(C1=CC=C(OC)C=C1)=O)(=O)=O)C1=C(F)C=CC=C1 | MCULE-6769193145-0-1 | -6.8 |
| 231 | CN1C(=O)N(C)C(=O)C(C(/C(/C#N)=C/C2=CN(C3=CC=CC=C3)N=C2)=O)=C1N | MCULE-7964645783-0-2 | -6.8 |
| 232 | N1(OC(=O)C2C=CC=CC=2OC)C(C)=NC2=C(C=CC=C2)C1=O | MCULE-2534956376-0-4 | -6.8 |
| 233 | C1(N2CCN(CC2)C(=O)[C@H]2CCC3NC(C)=NC=3C2)C2C=CC=CC=2SN=1 | MCULE-2945125495-0-1 | -6.8 |
| 234 | C1(/C(=O)C=CC2C=CC=CC/1=2)=N/NC1C=C(C=C(C(OC)=O)C=1)C(OC)=O | MCULE-2795142916-0-2 | -6.8 |
| 235 | ClC1=C(/N=C2/N(C[C@H]3OCCC3)C(C3OC=CC=3)=CS/2)C=C(S(N2CCOCC2)(=O)=O)C=C1 | MCULE-9686795830-0-2 | -6.8 |
| 236 | C1(NC(=O)C[C@H]2C(O)=NC3C(=CC=CC=3)C(=O)N2)C=NN(C)C=1C | MCULE-4693735587-0-3 | -6.8 |
| 237 | C12=NC3C=CC=CC=3C=C1C(C1=CC=C(C)C=C21)=O | MCULE-4802705854-0-21 | -6.8 |
| 238 | FC1=C(F)C=C2C(CCCN2CN2C(=O)SC=C2C2=NC=CC=C2)=C1 | MCULE-3366895979-0-1 | -6.8 |
| 239 | C[C@@H](C1ON=C(C(C)(C)C)N=1)NCC1OC(C2=CC(Cl)=CC=C2)=NN=1 | MCULE-8086905446-0-1 | -6.8 |
| 240 | CC(C1C(C)=C(C(CN2C(=O)ON=C2C2=NC=CN=C2)=O)NC=1C)=O | MCULE-2261453164-0-1 | -6.8 |
| 241 | C1C=C(C=CC=1C)C(/N=C1/SN2C=CC(C)=CC2=N/1)=O | MCULE-9395006562-0-4 | -6.8 |
| 242 | O=C([C@@H]1[C@H](C2CC2)C1)NC1=CN=C(N2C=CC(=O)C=C2)C=C1 | MCULE-3680751741-0-1 | -6.8 |
| 243 | C(/C#N)(\C(=S)NC1=CC=C(C=C1)Cl)=C(\N)/N1CCN(CC1)C1C=CC(=CC=1)OC | MCULE-6871632280-0-2 | -6.8 |
| 244 | [C@]1(C)(C(=O)NC2=CC=C(C=C2)N2C=CC=N2)OC2C=CC=CC=2N=C1O | MCULE-2957406201-0-1 | -6.8 |
| 245 | C1(C#N)C(/C(/C#N)=C/C2C=C(Br)C=CC=2OCC2C=CC=CC=2)=NN(C2C=CC=CC=2)C=1N | MCULE-1462969051-0-1 | -6.8 |
| 246 | N1(CC2=CC=C(C#N)C=C2)C2C(C=C1)=C(C1C=C(F)C=C(F)C=1)C(OC(=O)N(CC)CC)=CC=2 | MCULE-2706492531-0-1 | -6.8 |
| 247 | C12=NC3C(=CC=CC=3)N1C(N[C@](C1C=CC=CC=1)(C(F)(F)F)S2)=O | MCULE-3639101791-0-57 | -6.8 |
| 248 | S(=O)(=O)(N1CCN(CC1)C1=CC=CC=N1)C1SC=C(C2=NN=C(C(=O)N3CCCCC3)O2)C=1 | MCULE-6755388701-0-38 | -6.8 |
| 249 | C1(=C(SCC2=CC=C(C=C2)F)OC(C2C=CC(=CC=2)F)=N1)S(C1=CC=CC=C1)(=O)=O | MCULE-6669918192-0-1 | -6.8 |
| 250 | C/C(/C(NNC(COCC1=CC=CC=C1)=O)=O)=C/C1=CC=C(N(=O)=O)C=C1 | MCULE-9633151779-0-1 | -6.8 |
| 251 | N(=O)(=O)C1C(/C=C/C2=CC=CC=C2N)=CC(/C=C/C2=CC=CC=C2)=C(N(=O)=O)C=1 | MCULE-8018651487-0-1 | -6.8 |
| 252 | C1(=NNC(=S)N1C1CCCCC1)C1C=C(SC=1N)C1=CC=CC=C1 | MCULE-9994160358-0-6 | -6.8 |
| 253 | C1(=N/O)/C2=CC=CC=C2C2=C(C=CC=C/12)C#N | MCULE-9439145031-0-2 | -6.8 |
| 254 | CS(C1=CC(N(=O)=O)=CC(C(O[C@H](C2=CC=CC=C2)CC=C)=O)=C1)(=O)=O | MCULE-5492028466-0-1 | -6.8 |
| 255 | C1(OCC(=O)C2C=CC(=CC=2)NC(C)=O)=COC(=CC1=O)CN1CCSCC1 | MCULE-7864331116-0-2 | -6.8 |
| 256 | O=C([C@H](C(C1=CC(S(CC2=CC=CC=C2)(=O)=O)=CC=C1)=O)C#N)NC1CC1 | MCULE-2915794201-0-1 | -6.8 |
| 257 | O=C(C1[C@@H]2C3C([C@@H](O2)C=1)=C(C(F)(F)F)C=CC=3)O | MCULE-8473086369-0-1 | -6.7 |
| 258 | C1([C@H](C2C=CC=NC=2)CC(OC)=O)OC(CSC2C=CC=CC=2Cl)=CC(=O)C=1O | MCULE-8614176832-0-1 | -6.7 |
| 259 | CCOC1=CC(C)=C(NC(C2=NN(C3NC(C(F)(F)F)=NN=3)C(C)=N2)=O)C=C1 | MCULE-3616534106-0-2 | -6.7 |
| 260 | C1(C(=O)C(C)(C)C)C(=O)O[C@](OC=1C(C)(C)C)(C)C1=CC=CC=C1 | MCULE-7224913632-0-2 | -6.7 |
| 261 | CCC1=CC2=C(C(=CC(O2)=O)CSC2=CC(O)=CC=C2)C=C1 | MCULE-9163001537-0-1 | -6.7 |
| 262 | O=S(NCC1(C2=CC3=C(OCCO3)C=C2)CCCC1)(CC1(C#N)CC1)=O | MCULE-1813270980-0-1 | -6.7 |
| 263 | COC1=C2C(C=C(C3ON=C(C4=CC=C(S(C)(=O)=O)C=C4)N=3)CO2)=CC=C1 | MCULE-4038937678-0-1 | -6.7 |
| 264 | S(=O)(=O)(CCN1C=C(N=N1)C1=CNN=C1C1=CC=CC=C1)N1CCCC1 | MCULE-7118416248-0-58 | -6.7 |
| 265 | CC([C@@H]1[C@@H](C2N=C([C@H]3[C@@H](C(N4CCOCC4)=O)CC=CC3)ON=2)CCO1)(C)C | MCULE-9630168745-0-1 | -6.7 |
| 266 | C1(=NN=CN1C)SC1=CC=C(CN(C)CC2NC3C(=CC=C(F)C=3)N=2)O1 | MCULE-5359141248-0-1 | -6.7 |
| 267 | N1([C@H](CC)C(=O)NCC2C=CC(=CC=2)OCC)SC2C(=CC=CC=2)C1=O | MCULE-2925331688-0-1 | -6.7 |
| 268 | COC(C1C=C(C(NC2N=NN(CC3=CC=CC=C3)C=2)=O)OC=1)=O | MCULE-7443692022-0-1 | -6.7 |
| 269 | C12C(=O)CC(CC=1C(C1CC(C)(C)CC(=O)C=1O2)C1=CC=C(C=C1)OC)(C)C | MCULE-8155828073-0-1 | -6.7 |
| 270 | O=C(/C=C/C1=NC2=C(C=CC=C2)N=C1)NC1=CN2C(=NN=C2)C=C1 | MCULE-8537163720-0-1 | -6.7 |
| 271 | C[C@H](C(N(CC(NC1CC1)=O)C)=O)OC1=CC2=C(C(CCC2)=O)C=C1 | MCULE-2816421792-0-1 | -6.7 |
| 272 | O=N(C1=CC(OC2OC3=C(C=C(C=C3)F)N=2)=CC=C1)=O | MCULE-2567166678-0-1 | -6.7 |
| 273 | CC1OC(C(NNC(NCCC2=CC=C(Cl)C=C2)=S)=O)=C(C)C=1 | MCULE-8828810687-0-1 | -6.7 |
| 274 | N1NC2C(=NC=C(C=2)C2C=CC(=C3C=CC=NC=23)F)N=1 | MCULE-2941724860-0-1 | -6.7 |
| 275 | O=C1/C(=C/NCC2=CC=CC=C2)/C(=O)CCC1 | MCULE-5841209623-0-1 | -6.7 |
| 276 | CC1OC(N2CCC(C(N[C@@H]3[C@@H]4[C@H]5C[C@@H]([C@H]34)CC5)=O)CC2)=C(C#N)N=1 | MCULE-6319616478-0-1 | -6.7 |
| 277 | CCC1C(NS(C2CCC3=C(C=CC=C3)C=2)(=O)=O)=C(C)ON=1 | MCULE-1940225449-0-2 | -6.7 |
| 278 | CC1=C(S(NCCN2N=CC(N(=O)=O)=C2)(=O)=O)C=C(F)C=C1 | MCULE-6735551471-0-1 | -6.7 |
| 279 | C[C@H](C1SC(Cl)=CC=1)OC(C1=C(F)C=C(C2=CN=CN=C2)C=C1)=O | MCULE-3692062182-0-1 | -6.7 |
| 280 | C1(C2C=C(C3=CC=CN3)N=C(N)C=2C#N)=C(Cl)N(N=C1C1C=C(ON=1)C)C | MCULE-6225812798-0-1 | -6.7 |
| 281 | C1(C(=O)NC2=CC=C(C=C2)F)=NN=C(SCC(=O)N2CCOCC2)S1 | MCULE-9037497465-0-1 | -6.7 |
| 282 | N1C(C)=NC(=CC=1O)CCNC(=O)[C@@H](O)C1C=CC=C(Cl)C=1 | MCULE-8218697399-0-1 | -6.7 |
| 283 | C(F)(F)(F)C1=CC(C2C=CC3=C(OCO3)C=2)=NC(SCCC(NCCC)=O)=N1 | MCULE-8829300092-0-1 | -6.7 |
| 284 | C1(NC(=S)NC(=O)/C=C/C2=CC=CO2)SC2=C(CCCC2)C=1C#N | MCULE-3862754959-0-1 | -6.7 |
| 285 | S1(=O)(=O)C2=CC=CC=C2C(=C(C(C2=CC=CC=C2)=O)N1CCC)OC(=O)C(C)(C)C | MCULE-4849167936-0-3 | -6.7 |
| 286 | N1(/N=C/C2C=CC(=CC=2)OCCOC2C=CC(=CC=2)C)C=NN=C1 | MCULE-1027147080-0-1 | -6.7 |
| 287 | COC(C1SC(C)=C(CSC2OC(C3C4=C(C=CC=C4)NC=3)=NN=2)C=1)=O | MCULE-7810806769-0-1 | -6.7 |
| 288 | C1(/S/C(/C(=O)N/1C1=CC=CC=C1)=C/C1=CC=C(C=C1)N(=O)=O)=C(\C#N)/C(=O)NCC1=CC=CO1 | MCULE-9471839242-0-1 | -6.7 |
| 289 | N12[C@H](C3=CC=CC=C3)N=C(SCC(N)=O)N1[C@@H](N=C2SCC(N)=O)C1C=CC=CC=1 | MCULE-3413204661-0-3 | -6.7 |
| 290 | C12/C(/C3=C(SC=C3)SCC1=CC=CC=2)=C1/CCN(C)CC/1 | MCULE-1684680854-0-1 | -6.7 |
| 291 | C1(C=CC(Cl)=CC=1)S(=O)(=O)CC1SC=C(C2=CC=CC=C2)N=1 | MCULE-3889383039-0-1 | -6.7 |
| 292 | C1(S[C@@H]2[C@H](CCCCC2)C=1C(OCC)=O)NC(=S)NC(=O)C1C=CC(=CC=1Cl)Cl | MCULE-1474039735-0-1 | -6.7 |
| 293 | CC(NS(C1=CC=C(C2O/C(=C3\N(C)C=CC=C\3)/C(=O)N=2)C=C1)(=O)=O)C | MCULE-1365034658-0-3 | -6.7 |
| 294 | ClC1=CC=C(CNC(CON2C3=C(C=CC=C3)N=N2)=O)C=C1 | MCULE-4104171675-0-1 | -6.7 |
| 295 | C1CCCC/[N+](=C/C=C(\Cl)/C2C=CC(F)=CC=2)/C1 | MCULE-2818035187-0-1 | -6.7 |
| 296 | C1(CCCC=1NNC(C1C=CN=CC=1)=O)C(=O)C(F)(F)F | MCULE-5319850747-0-1 | -6.7 |
| 297 | C1(OCC(C2=CC=C(C=C2)Br)=NN=1)C(=O)SC1=CC=C(Cl)C=C1 | MCULE-2579653131-0-6 | -6.7 |
| 298 | CC1=C(C)C=C(S(NC2=C(CS(C)(=O)=O)C=C(F)C=C2)(=O)=O)C=C1 | MCULE-5324459990-0-1 | -6.7 |
| 299 | CCOCC1C2=C(C=CC=C2)OC=1C(N[C@H]1C2=C(C=CC=C2)SCC1)=O | MCULE-6431756243-0-1 | -6.7 |
| 300 | CC(C1=NC(SCCCC(N2CCN(S(C3=CC=C(Cl)C=C3)(=O)=O)CC2)=O)=CC(C)=N1)C | MCULE-2642719953-0-1 | -6.7 |
| 301 | N1(C2C=CC=CC=2)CCC2N=C(NCCNC3=NC(C)=CC(=O)N3)N=CC1=2 | MCULE-4408605808-0-2 | -6.7 |
| 302 | C1(C(OC)=O)C(C2C=CC(=CC=2)Cl)=NOC=1N1CCC(=CC1)C1=CC=CC=C1 | MCULE-5893857120-0-3 | -6.7 |
| 303 | CCOC1=CC=C(C2=NN(CN3CC4=C(C=NC(=N4)CC)CC3)N=N2)C=C1 | MCULE-4746034410-0-1 | -6.7 |
| 304 | CC(C(/C=C1\N(CC(NC2=CC3=C(OCCCO3)C=C2)=O)C(=O)CS\1)=O)(C)C | MCULE-9184792839-0-2 | -6.6 |
| 305 | OC([C@H](NC(C1SC2C3C=CC=CC=3OCC=2C=1)=O)CC1CC1)=O | MCULE-7468081041-0-1 | -6.6 |
| 306 | COC1=CC=C(N2C3=C(C=CC=C3)N=C2NC(C2N=NSC=2)=O)C=C1 | MCULE-7721831218-0-1 | -6.6 |
| 307 | CC1=C([C@@H]2[C@H](C(OCCN3C(=O)C4=C(C=CS4)N=C3)=O)C2)SC=C1 | MCULE-9430434307-0-1 | -6.6 |
| 308 | CCOC(/C(/C#N)=C/NC1NC(SCC2=CC=CC=C2)=NN=1)=O | MCULE-9796399071-0-1 | -6.6 |
| 309 | COC1=CC(OCNC(NNC(C2=CC=NC=C2)=O)=O)=CC=C1 | MCULE-8771260560-0-4 | -6.6 |
| 310 | O=C(NN1C(=O)C2=C(C=CC=C2)C1)CCC1=COC=C1 | MCULE-7713197141-0-1 | -6.6 |
| 311 | CC1=CC=C(C2=CN(CN3CCC(=O)NCC3)N=C2)C=C1 | MCULE-2958339299-0-2 | -6.6 |
| 312 | CCN(C(NCCC1N=C(C2=CC=C(C)C=C2)OC=1)=O)[C@@H]1CS(=O)(=O)CC1 | MCULE-8722000380-0-1 | -6.6 |
| 313 | CC(CO[C@@H](C1N=C(COC2=CC3=C(C(C(C)C)=CC(O3)=O)C=C2)ON=1)C)C | MCULE-2835635969-0-1 | -6.6 |
| 314 | COC(C1=C(CSC2=C(C(/N=C3/N(C)C=CS/3)=O)C=CC=C2)OC=C1)=O | MCULE-9580950999-0-1 | -6.6 |
| 315 | FC1=CC=C(N2C(=O)C=CC(C(NC3=C(C#N)N4C(SCC4)=N3)=O)=N2)C=C1 | MCULE-2364659757-0-1 | -6.6 |
| 316 | CCC1NN=C(CN2N=C(C3=CC=CC=C3)N=N2)N=1 | MCULE-5793424308-0-1 | -6.6 |
| 317 | C12NC(=O)N(C(=O)C1=NSC=2C(=O)N1CCN(CC1)CC1C=CC=CC=1)CC(C)C | MCULE-4446795983-0-1 | -6.6 |
| 318 | O=N(C1=CC(/C=C2/C(=O)C3=C(C=CC(=C3)Cl)SC/2)=CC=C1)=O | MCULE-1427145242-0-1 | -6.6 |
| 319 | C(=S)(NC1C=CC(=CC=1)C(OC)=O)NC1=CC=C2C(N=CC=N2)=C1 | MCULE-8430594715-0-1 | -6.6 |
| 320 | C1(C=CSC=1NC(=O)C1=CC2=CC=CC(OC)=C2O1)C1ON=C(C)N=1 | MCULE-8457081425-0-1 | -6.6 |
| 321 | COC(C1=C(OCC(N([C@H](C2=CC(F)=C(F)C=C2)C)C)=O)C=C(C)S1)=O | MCULE-6692323756-0-1 | -6.6 |
| 322 | FC(C1=CC(NC(N2CC=C(C3SC=CC=3)CC2)=O)=NC=C1)(F)F | MCULE-8262305285-0-1 | -6.6 |
| 323 | CC(C1=NC(N(C)C)=NC(NCC2=CC(COCC(F)(F)F)=CC=C2)=N1)C | MCULE-9778954660-0-1 | -6.6 |
| 324 | N1([C@@H](COC)C2C=CC=CN=2)C=C(N=N1)C1C=CC(=C(Cl)C=1)F | MCULE-4541815416-0-56 | -6.6 |
| 325 | COC1=CC(/C=C(/N2C(C)=NN=N2)\C(N[C@@H]2CC=CCC2)=O)=CC=C1 | MCULE-8180845229-0-1 | -6.6 |
| 326 | S=C1N(CN2CCN(C3=NC=CC=N3)CC2)N=C(CCCC2=CC=CC=C2)O1 | MCULE-5643792264-0-1 | -6.6 |
| 327 | CC1=C(C(NNC(/C=C/C2SC(Cl)=CC=2)=O)=O)SC=N1 | MCULE-1842094701-0-1 | -6.6 |
| 328 | N1(C/C(/C)=N/NC(C2C(N(=O)=O)=CC=CC=2)=O)N=C(N(=O)=O)N=C1 | MCULE-7902071456-0-1 | -6.6 |
| 329 | O=C([C@@H]1CN(CC2=CC=CC=C2)CCC1)NNC1=NC=CN=C1 | MCULE-8857776431-0-1 | -6.6 |
| 330 | N(=O)(=O)C1C=CC=C(C(=O)O/N=C2\C=CC(C=C\2C)=O)C=1Br | MCULE-4032706815-0-1 | -6.6 |
| 331 | S(=O)(=O)(NCC1C=CC2=C(OCO2)C=1)C1=CC=C2C(=C1)SC(N2CCC(=O)N1CCOCC1)=O | MCULE-6523790570-0-1 | -6.6 |
| 332 | C12/C(/CCCC1=NON=2)=N/OCC(=O)NC1C=CC(=CC=1)OC | MCULE-1627366430-0-5 | -6.6 |
| 333 | CC(C1OC([C@H]2OCCN(C([C@@H]3C4=C(SC=C4)CCC3)=O)C2)=NN=1)C | MCULE-6142777612-0-1 | -6.6 |
| 334 | C12=CC3=CC(CCCCCC)=C(C=C3OC1=NN(C1=CC=C(C=C1)CC)C2=O)O | MCULE-1704183301-0-3 | -6.6 |
| 335 | C1(=NN(C=C1Cl)C)/C=C(\C#N)/S(=O)(=O)C1=CC=CC=C1 | MCULE-8888457491-0-1 | -6.6 |
| 336 | CN(C1N=C(CNS(C2=C(Cl)C=CC(C#N)=C2)(=O)=O)ON=1)C | MCULE-8686666860-0-1 | -6.6 |
| 337 | N1(C=C(C=N1)C)C1N=CN=C(N/N=C(\C)/C2=CC=C(C=C2)I)C=1 | MCULE-7449730414-0-3 | -6.6 |
| 338 | BrC1=CC(CC(NO[C@@H]2OCCCC2)=O)=CC=C1 | MCULE-1598936579-0-1 | -6.6 |
| 339 | CC1=C(CC2=CC=CC=C2)NC(S(CCO)(=O)=O)=N1 | MCULE-5779853217-0-1 | -6.6 |
| 340 | N1N=C(N(C=1S)C1=CC(OC)=CC=C1OC)CCN1C(=O)C2C=CC=CC=2C=N1 | MCULE-6488956276-0-1 | -6.6 |
| 341 | CN1N=CC(N2C(=O)[C@@H](ONC(CCC3CCCCC3)=O)CC2)=C1 | MCULE-7817364475-0-1 | -6.6 |
| 342 | S(=O)(=O)(C1C=CC(=CC=1)Br)N1CCN=C1SCC1C=CC=CC=1Cl | MCULE-9906778654-0-2 | -6.6 |
| 343 | C(#C[C@]1(O)[C@@H]2CCCC([C@@H]2CCC1)=O)C1=CC=CC(OC)=C1 | MCULE-4213160941-0-19 | -6.6 |
| 344 | FC1=CC2=C(C(N(C=N2)CC2=C(Cl)C3=C(C=CC=C3)S2)=O)C=C1 | MCULE-2053488436-0-2 | -6.5 |
| 345 | C1(C(O)=O)C2C=C(C)C=CC=2OC2=CC=CC=C2C=1 | MCULE-6814640820-0-68 | -6.5 |
| 346 | N1(CC(F)(F)F)N=C(N=C1C1=CN=C(N=C1)N1CCOCC1)CC1CC1 | MCULE-9975635910-0-3 | -6.5 |
| 347 | FC(C1SC(NS(/C=C/C2=CC(Br)=CC=C2)(=O)=O)=NN=1)F | MCULE-6766414712-0-1 | -6.5 |
| 348 | CCN1C(/C=N/N2/C(=N\C3=NC=CC=C3)/SC=C2C2=C(C)ON=C2C)=CC=N1 | MCULE-1725154351-0-1 | -6.5 |
| 349 | ClC1=CC=C(S(CCNC2C(=O)N(C3CC3)C=CN=2)(=O)=O)C=C1 | MCULE-8579411959-0-1 | -6.5 |
| 350 | N12C=CN=CC1=NC(C1C=CC=C(C)C=1)=C2NCCC(=O)N(C)C | MCULE-9912215111-0-1 | -6.5 |
| 351 | COC(C1=CC(F)=C(CN2C3=C(C=C(S(N)(=O)=O)C=C3)CC2)C=C1)=O | MCULE-7550420408-0-1 | -6.5 |
| 352 | CCOC(C1=C(C)N=C(NS(C2=C(Cl)C(Cl)=CC=C2)(=O)=O)O1)=O | MCULE-1576861740-0-1 | -6.5 |
| 353 | C12N(C)N=C(C)C=1SC(N(CCCO)CC1C=CC(=CC=1)F)=N2 | MCULE-3967046882-0-1 | -6.5 |
| 354 | C12C(=CC=C3C=1C(=CC=C2N(=O)=O)C(=O)OC3=O)N(=O)=O | MCULE-1818576173-0-1 | -6.5 |
| 355 | CC1C(C([C@@H](C2OC3=C(C=CC=C3)N=2)C#N)=O)=C(N2N=CC=C2)N(C)N=1 | MCULE-9602125558-0-1 | -6.5 |
| 356 | C/C(/C1=CC=C(N2CCCCCC2)C=C1)=N/NS(CC1=CC=CC=C1)(=O)=O | MCULE-6704157967-0-1 | -6.5 |
| 357 | CCN1C2=C(C=C(S(N3CCOCC3)(=O)=O)C=C2)N=C1CN1N=C(C2=CSC=C2)N=N1 | MCULE-3715053770-0-1 | -6.5 |
| 358 | O=N(C1=C(NCC2=C3C(OCO3)=CC=C2)C=CC(F)=C1)=O | MCULE-4253408503-0-1 | -6.5 |
| 359 | COCCN1C(C)=C(C(/C=C/C2C3=C(C=CC=C3)OC=2C)=O)C(C)=N1 | MCULE-2297626912-0-1 | -6.5 |
| 360 | CC1=CC(S(NC2SN=C(C3SC=CC=3)N=2)(=O)=O)=C(Cl)C=C1 | MCULE-3326325871-0-2 | -6.5 |
| 361 | CCCC1=NN(C)C(NC(NNC2=C(Cl)C=CC=C2F)=O)=C1 | MCULE-4651996177-0-2 | -6.5 |
| 362 | N1=C(O)[C@@H](S/C/1=N\N=C(/C)\C(C)(C)C)CC(=O)NC1C=CC=C(C(C)=O)C=1 | MCULE-5877517361-0-1 | -6.5 |
| 363 | N12C3=CC=CC=C3N=C1SC(C(=O)NC1C=CC(=CC=1)NC(C)=O)=CC2=O | MCULE-6966863269-0-1 | -6.5 |
| 364 | CC1C(N(=O)=O)=C(SC2=NN(C3=CC=CC=C3)C=N2)N(C)N=1 | MCULE-5697898608-0-1 | -6.5 |
| 365 | CC1=C(C(NC2=CC(S(NC3CCCN=3)(=O)=O)=CC=C2)=O)N(C)C=C1 | MCULE-8196602112-0-1 | -6.5 |
| 366 | FC1=CC(Br)=C(CONC(C2NC=C(Cl)C=2)=O)C=C1 | MCULE-3462709102-0-1 | -6.5 |
| 367 | CCS(NCC(NC1=CC=C(SC2=C(Cl)C=CC=C2)C=C1)=O)(=O)=O | MCULE-2096929584-0-1 | -6.5 |
| 368 | CC1=C(C)N=NC(OCC(C2=CC=C(F)C=C2)=O)=C1 | MCULE-3149814568-0-1 | -6.5 |
| 369 | N12C(=O)CCSC1=NC(C)=C(C(OCC=C)=O)[C@@H]2C1C=CC=C(OC)C=1 | MCULE-2950279940-0-1 | -6.5 |
| 370 | CC(N(C1=CC=CC=C1)C1SC=C(CSC2N(C3=NC=C(C)C=C3)C(=O)C3=C(C=CC=C3)N=2)N=1)=O | MCULE-6463964094-0-1 | -6.5 |
| 371 | CCNS(N1[C@H](C2OC(C)=NN=2)CC2=C(C=CC=C2)C1)(=O)=O | MCULE-2578539026-0-1 | -6.5 |
| 372 | C1(=N/C2C=CC(=CC=2)C)\C2=CC=CC=C2OC(C2C=C(OC)C(=C(OC)C=2)OC)=C\1 | MCULE-5662070044-0-1 | -6.5 |
| 373 | CCC1=CC=C(C(NNC(C(NC2N(C(C)C)N=CC=2)=O)=O)=O)C=C1 | MCULE-1478963969-0-1 | -6.5 |
| 374 | BrC1=CC(C(NC2NC(C#N)=C(C#N)N=2)=O)=C(Br)C=C1 | MCULE-6773723308-0-1 | -6.5 |
| 375 | CCC1=NN(CCS(C2=CC(C#N)=CC=C2)(=O)=O)C(CC)=N1 | MCULE-4644630646-0-1 | -6.5 |
| 376 | C1=CC=C(C=C1)C1=CSC(/N=C/C2C(O)=CC=CC=2)=N1 | MCULE-3452208485-0-1 | -6.5 |
| 377 | CC1N(CCNC(CN2C3=C(C=CC(=C3)Cl)C=C2)=O)C=NN=1 | MCULE-5942754570-0-1 | -6.5 |
| 378 | N1C2=CC(Cl)=CC=C2C(OC=1C1=CC=CC(Br)=C1)=O | MCULE-2763957088-0-1 | -6.5 |
| 379 | C12=CN(NC(=O)C3C=CC(=C(OC)C=3)O)C=C(C(OC)=O)C1=NNC2=O | MCULE-7955807557-0-1 | -6.5 |
| 380 | N1(C2=CC=C(C=C2C)C)C(C)=C(C=C1C)/C=C1/C(=O)C(=C(C)N/1)C(OCC)=O | MCULE-2762085902-0-1 | -6.5 |
| 381 | CCOC(/C(/C1N(CC2C=CC=CC=2)C=CN=1)=C/C1C=CC(C(=O)O)=CC=1)=O | MCULE-9983029169-0-1 | -6.5 |
| 382 | CC(C(NNC(C#CC1=CC=CC=C1)=O)=O)(C)C | MCULE-8538831765-0-2 | -6.5 |
| 383 | CC1=CC(CS(NC2SC=C(CN3CCOCC3)N=2)(=O)=O)=CC=C1 | MCULE-3427700127-0-1 | -6.5 |
| 384 | C1(C(OCC)=O)C(C)=C(SC=1N/C=C(/C#N)\C1SC=C(C2=CC=CC(OC)=C2)N=1)C | MCULE-5075371223-0-1 | -6.5 |
| 385 | CC1=CC=C(OCCOC(CCN2C3=C(C=CC=C3)SC3=C2C=CC=C3)=O)C=C1 | MCULE-6598990978-0-1 | -6.5 |
| 386 | C1(C#N)C(SCC2=CC=C(C=C2)C)=NSC=1SCC1=CC=C(C=C1)C | MCULE-3785523591-0-13 | -6.5 |
| 387 | COC1=C(SCC2OC(C3=CC=C(Cl)C=C3)=NN=2)C=CC(C(C)=O)=C1 | MCULE-4952057983-0-1 | -6.5 |
| 388 | CC1(CC2=C(SC(=N2)NS(C2SC(Cl)=CC=2)(=O)=O)C(=O)C1)C | MCULE-1223857882-0-1 | -6.5 |
| 389 | COC(C1=CC2=C(C(NC(C3=C(C)OC(C)=C3)=N2)=O)C=C1)=O | MCULE-5244333113-0-1 | -6.5 |
| 390 | N1(CCC[C@@H](C(O)=O)C1)C(=O)CCN1C=CC2C=CC(Br)=CC1=2 | MCULE-7049070654-0-1 | -6.5 |
| 391 | O[C@@H](C1=C(F)C=C(F)C=C1)CS(CC1=C(C(F)(F)F)C=CC=C1)(=O)=O | MCULE-4438900815-0-1 | -6.4 |
| 392 | C1(CS/C(=N\C2=CC=CC=C2Cl)/N(C)N=1)C1C=CC=CC=1 | MCULE-9390013149-0-1 | -6.4 |
| 393 | CC1C(CN2CCN(C3=C(F)C4=C(C(=CC=N4)Cl)C=C3)CC2)=C(C)N(C)N=1 | MCULE-2442520377-0-1 | -6.4 |
| 394 | CC[C@@]1(CN(C2N(CC3OC=CC=3)C(C3N=CC=CC=3)=NN=2)CCC1)C | MCULE-6669733715-0-1 | -6.4 |
| 395 | CN1C2=C(C(=NC=N2)SCC(NN2C(=O)C3(CCCCC3)NC2=O)=O)C=N1 | MCULE-9795571504-0-1 | -6.4 |
| 396 | FC1=NC=CC(NNC(C2(C#N)CCCCC2)=O)=C1 | MCULE-5293534540-0-1 | -6.4 |
| 397 | [N+]1(C2C=CC=CC=2C)C[C@@](N2CCCCC2=1)(O)C1=CC=CS1 | MCULE-6227732929-0-1 | -6.4 |
| 398 | C(N1N=C(C2=CC=CC=C2)N=C1)N1C[C@H](C2SC=CC=2)OCC1 | MCULE-6488492152-0-1 | -6.4 |
| 399 | C1(=C(C)N(C(C)=C1C1ON=C(CC)N=1)C)S(=O)(=O)NC1C=CC(=C(Cl)C=1)F | MCULE-4788901100-0-1 | -6.4 |
| 400 | O[C@@H](CN1N=C(C2CC2)N=N1)COCC1=CC=CC=C1 | MCULE-1009966632-0-1 | -6.4 |
| 401 | C1(S)=C(C#N)C(=O)N[C@H](C2=CC=C(C(OC)=C2)OCC)N1C1C=CC(=CC=1)F | MCULE-6610621151-0-1 | -6.4 |
| 402 | CC1N(C2CC2)C(CSC2OC3=C(C=C(C=C3C)Cl)N=2)=NN=1 | MCULE-4909762252-0-2 | -6.4 |
| 403 | C1([C@@H]2CCCN2C(=O)OC(C)(C)C)=NN=C(SCC2C=CC(=CC=2Cl)Cl)O1 | MCULE-9991558968-0-1 | -6.4 |
| 404 | S(C1C=CC=CC=1)(=O)(=O)[C@H]1CC2=C(C=CC=C2)[C@H]1Cl | MCULE-1100270561-0-20 | -6.4 |
| 405 | FC(C1=CC(C#N)=C(NCCS(NCC2CCC2)(=O)=O)C=C1)(F)F | MCULE-7582646122-0-1 | -6.4 |
| 406 | CC[C@H](OC1=C(CNS(CC2C3=C(C=CC=C3)ON=2)(=O)=O)C=CC(C)=C1)C | MCULE-1577432606-0-1 | -6.4 |
| 407 | CN(C(C1=CC=CC=C1)=O)CC1=NN(CC2=C(Cl)C=CC=C2Cl)N=N1 | MCULE-1697358457-0-1 | -6.4 |
| 408 | O=C(/C(/C#N)=C/C1SC(C2=CC=CC=C2)=CN=1)NC1CCCC1 | MCULE-9315498104-0-1 | -6.4 |
| 409 | CC(CCNC(C[C@H]1C(=O)N=C(C2C(=O)OC3=C(C=CC=C3)C=2)S1)=O)C | MCULE-4508966819-0-3 | -6.4 |
| 410 | IC(C(C(C1=CC=CC=C1)=O)=O)=P(C1=CC=CC=C1)(C1=CC=CC=C1)C1=CC=CC=C1 | MCULE-1248945032-0-5 | -6.4 |
| 411 | CCOC(C1C(C)=C(C(/C(/C#N)=C/C2=C3C(OCO3)=CC=C2)=O)NC=1C)=O | MCULE-4460062773-0-1 | -6.4 |
| 412 | O=N(C1=CC(OS(CC2=C(F)C=CC(Cl)=C2)(=O)=O)=CC=C1)=O | MCULE-9238629216-0-1 | -6.4 |
| 413 | CCOCCONC(CCC1C2=C(C(=CC=C2)C)NC=1)=O | MCULE-3556834577-0-1 | -6.4 |
| 414 | NS(C1=CC(N(=O)=O)=C(NNC(NC2=CC=C(OC(F)F)C=C2)=S)C=C1)(=O)=O | MCULE-5553238710-0-1 | -6.4 |
| 415 | COCCOC1=C(OC)C=C(C(/C=C/C2N=C(C3=CC=C(C)C=C3)OC=2)=O)C=C1 | MCULE-2376983022-0-1 | -6.4 |
| 416 | NC(CC1(NC(CSCC(C2=CC=CC=C2)=O)=O)CCOCC1)=O | MCULE-5911843506-0-1 | -6.4 |
| 417 | [C@@]12(C)ON=C(C)[C@@H]1[C@H](C1=CC=CC=C1)N1C(=NC=N1)N2 | MCULE-1808990004-0-1 | -6.4 |
| 418 | CO[C@@H](C1=CC(N[C@H](C2=CC3=C(C=CS3)N=C2)C)=CC=C1)C | MCULE-9438572745-0-1 | -6.4 |
| 419 | S1C(C2=CC=C(C=C2)OCC)=NN/C/1=N/C(=O)NC1C=CC(=CC=1)C | MCULE-4553959228-0-1 | -6.4 |
| 420 | C1(C(O)=NNC=1CC1=CC(F)=C(C=C1F)F)[C@@H](C1=CC=NC=C1)CC(OC)=O | MCULE-6794480236-0-1 | -6.4 |
| 421 | CC1=C(SCC#N)SC(NC(C[C@@H]2C3=C(C=CC=C3)CCO2)=O)=N1 | MCULE-4999792323-0-1 | -6.4 |
| 422 | O=C(NOCC1=CC=CC=C1)CN1C(=O)SCC1 | MCULE-9347303807-0-1 | -6.4 |
| 423 | C1(/C(=O)SC(N/N=C\C2C=CC(OC)=C(OC)C=2)=N/1)=C/C1C=CC(Br)=CC=1 | MCULE-5365063497-0-1 | -6.4 |
| 424 | FC(OC1=CC=C(/C=C/C(NC2=NC=C(Br)N=C2)=O)C=C1)F | MCULE-6363224384-0-1 | -6.4 |
| 425 | COC(NC1=CC=C(OC(/C(/C)=C2\CCCC\2)=O)C=C1)=O | MCULE-1932313855-0-1 | -6.4 |
| 426 | N1(C2=CC=CC(Cl)=C2)C(C)=C(/C(/C)=N\OCC2=CC=C(C=C2)C)C=C1C1=CC=C(C=C1)F | MCULE-8593730222-0-1 | -6.4 |
| 427 | C12SSC(=S)C=1C1=C(C=C(C(C)=C1)C)N(C(=O)C1=CC=CC=C1Cl)C2(C)C | MCULE-1615178629-0-2 | -6.4 |
| 428 | C[C@H](C1N(C2CC2)N=NN=1)NS(C1N2C(C=CC=C2)=NC=1Cl)(=O)=O | MCULE-5651768861-0-1 | -6.4 |
| 429 | CN1C(C2CCC2)=NN=C1CSC1=C2C(SC3=C2CCC3)=NC=N1 | MCULE-2777365590-0-1 | -6.4 |
| 430 | COC(C1C=C(C2ON=C(C3=CC(Br)=CC=C3)N=2)OC=1)=O | MCULE-2773877388-0-1 | -6.4 |
| 431 | CC1C2=C(C=CC(=C2)Br)OC(=O)C=1C(NC1SC=CN=1)=O | MCULE-9658834728-0-1 | -6.4 |
| 432 | FC(OC1=C(S(NNC2=C3C(C=CS3)=NC=N2)(=O)=O)C=CC=C1)(F)F | MCULE-4118501063-0-1 | -6.4 |
| 433 | COCC1=CC=C(NCC2NN=C(C3SC=CC=3)N=2)C=C1 | MCULE-7683226056-0-1 | -6.4 |
| 434 | N12N=C(SC1=NC(C)=C2S(=O)(=O)NC1C=CC(=C(C)C=1)C)C | MCULE-3533943806-0-1 | -6.4 |
| 435 | C(NC1C=C(Cl)C(Cl)=CC=1)(=O)N(C1C=CC(F)=CC=1)C1=NC[C@H](C)S1 | MCULE-2528182695-0-2 | -6.3 |
| 436 | C1(C(OCC)=O)SC(=CC=1NC(=S)N1CCCN(C)CC1)C1=CC=C(C=C1)C | MCULE-7674495319-0-1 | -6.3 |
| 437 | C[C@H](CCNC(NCCC1SC(C2N=C(C)SC=2)=CC=1)=O)O | MCULE-4486616491-0-1 | -6.3 |
| 438 | C[S@](C1=CC=C(NC(C2C(C3SC(C)=CC=3)=CNC=2)=O)C=C1)=O | MCULE-1948713893-0-1 | -6.3 |
| 439 | C(=S)(NC1C=CC(=CC=1)Br)N1CCN(CC1)C1C=CC(=CC=1)F | MCULE-4532816028-0-1 | -6.3 |
| 440 | C(C1OC(OC2=CC=CC=C2)=CC=1)NC1N(C[C@@H]2COCC2)N=CC=1 | MCULE-2583392627-0-1 | -6.3 |
| 441 | COC1=C(CSC2CC3=C(C=CC=C3)N=2)C=CC=N1 | MCULE-8132532595-0-1 | -6.3 |
| 442 | COC1=CC=C([C@@H](N(C)C)CN/C=C2\C(=O)NC(=S)NC\2=O)C=C1 | MCULE-5814498063-0-1 | -6.3 |
| 443 | CO[C@@H](CCC(NNC1ON=C(C2=CC=NC=C2)N=1)=O)C | MCULE-8762767483-0-1 | -6.3 |
| 444 | N1=C(NC2C(C)=CC=CC=2C)[C@](N(C2C=CC=CC=2OC)C1=S)(C)CC | MCULE-7838354605-0-2 | -6.3 |
| 445 | C1(/CCC/C(=C\C2=CC=C(C=C2)Br)/C/1=O)=C/C1=CC=CO1 | MCULE-9368204550-0-3 | -6.3 |
| 446 | CC[C@H](CCNC(N[C@H](C1=CC=C(Cl)C=C1)C1=CSC=C1)=O)O | MCULE-2468600190-0-1 | -6.3 |
| 447 | O=N(C1=CC=C(S(N2C3=C(C=CC=C3)COCC2)(=O)=O)C=C1)=O | MCULE-1174966688-0-1 | -6.3 |
| 448 | C1(OC)C=CC(C(=O)C2=C(N)C3C=CC(C4SC=CC=4)=NC=3S2)=CC=1OC | MCULE-6359190188-0-1 | -6.3 |
| 449 | CC1SC(C(NNC(CCC2=NC(OC(C)(C)C)=CC=C2)=O)=O)=CC=1 | MCULE-1023884502-0-1 | -6.3 |
| 450 | O=C(C1=CN(CC2=CC=CC=C2)N=C1)OCC1SC=NC=1 | MCULE-5369758990-0-1 | -6.3 |
| 451 | CC(/C(/C(NC1=CC=C(N(=O)=O)C=C1)=O)=C\C1=CSC=C1)=O | MCULE-5085740276-0-1 | -6.3 |
| 452 | O=C(N1CCN(C2=NC=CC=C2)CC1)NC1SC(/C=C/C2OC=CC=2)=NN=1 | MCULE-5984093393-0-1 | -6.3 |
| 453 | BrC1=CC(S(NC(/C=C/C2=NC=NC=C2)=O)(=O)=O)=CC(C#N)=C1 | MCULE-7711596997-0-1 | -6.3 |
| 454 | CC1C(C)=NC(NCCNS(C2SC(Cl)=CC=2)(=O)=O)=NN=1 | MCULE-8093555008-0-1 | -6.3 |
| 455 | C1(C(=CC=C(S(O)(=O)=O)C=1)SC1SC2C=CC=CC=2N=1)N(=O)=O | MCULE-2963583666-0-1 | -6.3 |
| 456 | COC1=CC(OC)=C(/C=N/NC2=C(Cl)C=C(C(F)(F)F)C=N2)C=C1 | MCULE-7707074929-0-1 | -6.3 |
| 457 | C[C@H](C1=NC=CN=C1)[S@](CCC(NC1=CC(Br)=CC=C1)=O)=O | MCULE-3628718982-0-1 | -6.3 |
| 458 | C12CN(CCCN1N=C(C#N)C=2)C(=O)C1=CC=C([C@H]2CCCO2)S1 | MCULE-4634895338-0-2 | -6.3 |
| 459 | COC1=C(OCC2=C(Cl)C=C(Cl)C=C2)C=CC(CNCC2=NNC=C2)=C1 | MCULE-7440433579-0-1 | -6.3 |
| 460 | COC1=CC=C(OCCCC(NC2=CC(C3=C4C(C(NNC4=O)=O)=C4N3CCC4)=CC=C2)=O)C=C1 | MCULE-6471874370-0-1 | -6.3 |
| 461 | O=C(C1CCCOC=1)OC1=CC(N2N=CC=C2)=CC=C1 | MCULE-3377862534-0-1 | -6.3 |
| 462 | CC1=CC(C)=C(CNC(NNC(OC(C)(C)C)=O)=O)C=C1 | MCULE-2241376197-0-1 | -6.3 |
| 463 | CC1C(NC(CSCC2=C3C(C=CC=N3)=C(Cl)C=C2)=O)=C(C)NN=1 | MCULE-9268288481-0-1 | -6.3 |
| 464 | S1(=O)(=O)C2C=C(C=CC=2C(OC2=CC=C(C=C2)N(=O)=O)=N1)N(=O)=O | MCULE-5640238683-0-10 | -6.3 |
| 465 | CC1SC(COC([C@H]2N(C(C3CCCC3)=O)CSC2)=O)=C(C)N=1 | MCULE-6548199967-0-1 | -6.3 |
| 466 | C1(C2=CN=CC=N2)OC(=NN=1)CC[C@H]1CCCN(C(NCCC)=O)C1 | MCULE-3733260902-0-1 | -6.3 |
| 467 | S(=O)(=O)(N1CCOCC1)C1=CC=C(O1)C1=NN=C(C(C)C)O1 | MCULE-3364512165-0-2 | -6.3 |
| 468 | ClC1=C2C(OCCO2)=CC(C[S@](CC2N=C([C@@H]3OCCC3)SC=2)=O)=C1 | MCULE-3382783288-0-1 | -6.3 |
| 469 | C1(CP(O)(CCC2C=CC=CC=2)=O)NC2C(=CC=CC=2)N=1 | MCULE-1333556608-0-7 | -6.3 |
| 470 | C1=C(SC=C1)N(C1C=CC(OC)=CC=1)C1=CC=CC=C1 | MCULE-6683778472-0-2 | -6.3 |
| 471 | C1(C2C=C(F)C=CC=2C)N=C(OC)N=C(OC)N=1 | MCULE-6822831411-0-22 | -6.3 |
| 472 | FC1=C(Cl)C=C(N2N=NC(CSC3SC(NC4CC4)=NN=3)=C2)C=C1 | MCULE-5558575435-0-2 | -6.3 |
| 473 | C(CC1C=CC=CC=1)(CC1=CC=CC=C1)(C(OC)=O)P(C1=CC=CC=C1)(C1=CC=CC=C1)=O | MCULE-9578646806-0-2 | -6.3 |
| 474 | C1=CC2C(=NSC=2/N=N/C2C=CC(O)=C(Cl)C=2Cl)C=C1N(=O)=O | MCULE-3135414099-0-2 | -6.3 |
| 475 | C(=O)(NC1=CC=C2C(OCO2)=C1)N1CCOC2C=CC=CC1=2 | MCULE-9496267476-0-1 | -6.3 |
| 476 | C(=O)(O)[C@@H](C1NN=NN=1)CC1C=CC=CC=1 | MCULE-3743099769-0-20 | -6.3 |
| 477 | OC1NC(SCC2SC(C3=CC=CC=C3)=NN=2)=NN=1 | MCULE-1506633541-0-1 | -6.3 |
| 478 | S(=O)(=O)(C1=CC=CC(OCC)=C1)/N=C1/C=C(C(C)(C)C)C(C(C(C)(C)C)=C/1)=O | MCULE-3651324127-0-2 | -6.3 |
| 479 | CN(C1=CC=CC=C1)N/C(/C1=CC=CC=C1)=N/S(C1=CC=CC=C1)(=O)=O | MCULE-2695865728-0-1 | -6.3 |
| 480 | N1C2C=CC=CC=2NC(CC(OCC)=O)=CC=1SCC(=O)NC1=CC=CC(SC)=C1 | MCULE-6488747060-0-1 | -6.3 |
| 481 | CC1=CC(C)=C(NC2SCC(C3NC=CC=3)=NN=2)C=C1 | MCULE-3558153691-0-3 | -6.3 |
| 482 | C12[C@@H](C3=CC=C(C=C3)C)C3SC(NC=3SC=1C(C1C=CC=CC=1C2=O)=O)=O | MCULE-5197209275-0-2 | -6.3 |
| 483 | CS(C1SC(Cl)=C(S(NC2=CC3=C(C=CN3)C=C2)(=O)=O)C=1)(=O)=O | MCULE-3696328886-0-1 | -6.3 |
| 484 | CC1SC2N(CCS(N=2)(=O)=O)C=1C1=CC=C(F)C=C1 | MCULE-6730278979-0-2 | -6.3 |
| 485 | ClC1=NC=C(Cl)C(C(OC2=CC3=C(OCO3)C=C2)=O)=C1 | MCULE-7243649928-0-1 | -6.3 |
| 486 | N1(N=NN=C1N(C)C)S(=O)(=O)C1C=CC=C(C=1)C(F)(F)F | MCULE-2061937224-0-1 | -6.2 |
| 487 | S(=O)(=O)(C(C)(C)C)/C(/C#N)=C/C1=C(C)C2=CC=CC=C2S1 | MCULE-3556031411-0-1 | -6.2 |
| 488 | BrC1=CC=C(NC(CN2C(=O)C3=C(OC=C3)C=C2)=O)C=C1 | MCULE-8953371655-0-1 | -6.2 |
| 489 | CC1=C(Cl)C(C)=CC(OS(N2CCN(C=O)CC2)(=O)=O)=C1 | MCULE-9762223605-0-1 | -6.2 |
| 490 | CS(C1=C(F)C=CC(S(OC2=C(Cl)C=CC=C2F)(=O)=O)=C1)(=O)=O | MCULE-7887566026-0-1 | -6.2 |
| 491 | CC1=C(C)OC(CN2CCN(C(CC3N=C(C4=CN=CC=C4)SC=3)=O)CC2)=N1 | MCULE-4323490082-0-1 | -6.2 |
| 492 | NC(CCC1N(CC2OC=CC=2)C(S[C@@H]2C=CCCC2)=NN=1)=O | MCULE-4780205922-0-1 | -6.2 |
| 493 | C1C(C2SC(N3C[C@H](N4C5CCCCC=5N=C4)CC3)=NN=2)C1 | MCULE-6644155293-0-1 | -6.2 |
| 494 | CS([C@@H]1N(C(/C=C/C2CCCCC2)=O)CCSC1)(=O)=O | MCULE-4830244626-0-1 | -6.2 |
| 495 | N1(CC(O)=NC2=CC=CC=C12)C(=O)N[C@@H](CC(C)C)C(OC)=O | MCULE-8354073463-0-1 | -6.2 |
| 496 | CC1SC(CN2CCN(CN3C(=O)C4C(=C(ON=4)C)C(C)=N3)CC2)=CN=1 | MCULE-8363928213-0-1 | -6.2 |
| 497 | C(/C1C=CN=CC=1)(\C1=CC=CC=C1)=N/O | MCULE-8138038847-0-1 | -6.2 |
| 498 | C1(=C(O)C=C(N(C)C1=O)C)C(C1=CC=CO1)C1=C(O)C=C(N(C)C1=O)C | MCULE-9897331668-0-1 | -6.2 |
| 499 | CC(OC(N1C[C@H](CCNC(C2C=C(Br)OC=2)=O)CC1)=O)(C)C | MCULE-7084763412-0-1 | -6.2 |
| 500 | CCN(C1=C(S(CC)(=O)=O)C=CC=C1)C(CN1C(C(C)C)=NN=N1)=O | MCULE-5055487564-0-1 | -6.2 |

**Table S2:** The docking results using CLCDDW

|  |  |  |
| --- | --- | --- |
| **S/N** | **MCULE ID** | **SCORE** |
| 1 | MCULE-2706492531-0-1 | -66.95 |
| 2 | MCULE-2635982406-0-1 | -64.9 |
| 3 | MCULE-8443281251-0-1 | -64.6 |
| 4 | MCULE-2173184013-0-1 | -63.42 |
| 5 | MCULE-6523790570-0-1 | -62.72 |
| 6 | MCULE-2819757532-0-4 | -62.41 |
| 7 | MCULE-5942754570-0-1 | -62.23 |
| 8 | MCULE-6669918192-0-1 | -61.9 |
| 9 | MCULE-7389565650-0-1 | -61.85 |
| 10 | MCULE-4741178768-0-1 | -61.16 |
| 11 | MCULE-1558157577-0-1 | -60.91 |
| 12 | MCULE-8969405481-0-1 | -60.58 |
| 13 | MCULE-3254184720-0-1 | -60.53 |
| 14 | MCULE-3753544568-0-1 | -60.32 |
| 15 | MCULE-3967046882-0-1 | -60.23 |
| 16 | MCULE-3715053770-0-1 | -60.19 |
| 17 | MCULE-1018045960-0-1 | -60.11 |
| 18 | MCULE-6471874370-0-1 | -60.07 |
| 19 | MCULE-1549237209-0-3 | -59.98 |
| 20 | MCULE-8828810687-0-1 | -59.86 |
| 21 | MCULE-4164549318-0-1 | -59.81 |
| 22 | MCULE-2114638567-0-2 | -59.66 |
| 23 | MCULE-6122270640-0-2 | -59.49 |
| 24 | MCULE-1509614166-0-3 | -59.25 |
| 25 | MCULE-8041377389-0-1 | -59.25 |
| 26 | MCULE-7049070654-0-1 | -59.23 |
| 27 | MCULE-9870656355-0-1 | -59.04 |
| 28 | MCULE-8279910233-0-1 | -58.54 |
| 29 | MCULE-4765178291-0-1 | -58.29 |
| 30 | MCULE-8522911125-0-1 | -58.22 |
| 31 | MCULE-8850272549-0-1 | -58.21 |
| 32 | MCULE-6463964094-0-1 | -58.21 |
| 33 | MCULE-2639921006-0-1 | -58.05 |
| 34 | MCULE-7246818590-0-1 | -58.04 |
| 35 | MCULE-9998470483-0-1 | -57.91 |
| 36 | MCULE-5273153078-0-1 | -57.68 |
| 37 | MCULE-7391624342-0-2 | -57.61 |
| 38 | MCULE-5929541522-0-41 | -57.48 |
| 39 | MCULE-8593730222-0-1 | -57.46 |
| 40 | MCULE-9462828033-0-1 | -57.3 |
| 41 | MCULE-9430434307-0-1 | -57.28 |
| 42 | MCULE-9565740349-0-1 | -57.27 |
| 43 | MCULE-3128059000-0-1 | -57.21 |
| 44 | MCULE-7539618691-0-2 | -57.21 |
| 45 | MCULE-6598990978-0-1 | -56.94 |
| 46 | MCULE-1343386283-0-3 | -56.86 |
| 47 | MCULE-2987506470-0-1 | -56.8 |
| 48 | MCULE-9346699773-0-1 | -56.78 |
| 49 | MCULE-6794480236-0-1 | -56.74 |
| 50 | MCULE-2254917819-0-1 | -56.68 |
| 51 | MCULE-6431756243-0-1 | -56.56 |
| 52 | MCULE-7674495319-0-1 | -56.55 |
| 53 | MCULE-4788901100-0-1 | -56.53 |
| 54 | MCULE-3389288402-0-1 | -56.37 |
| 55 | MCULE-7731866337-0-1 | -56.35 |
| 56 | MCULE-6887869192-0-1 | -56.34 |
| 57 | MCULE-3289368793-0-1 | -56.29 |
| 58 | MCULE-1486436428-0-1 | -56.29 |
| 59 | MCULE-6084272273-0-1 | -56.26 |
| 60 | MCULE-7247419279-0-1 | -56.22 |
| 61 | MCULE-4438900815-0-1 | -56.21 |
| 62 | MCULE-7798591154-0-3 | -56.11 |
| 63 | MCULE-5199506278-0-1 | -56.09 |
| 64 | MCULE-1940225449-0-2 | -55.98 |
| 65 | MCULE-1626453876-0-1 | -55.97 |
| 66 | MCULE-9045755728-0-1 | -55.93 |
| 67 | MCULE-4718215784-0-1 | -55.86 |
| 68 | MCULE-8690883911-0-1 | -55.85 |
| 69 | MCULE-9912215111-0-1 | -55.82 |
| 70 | MCULE-6470395655-0-1 | -55.81 |
| 71 | MCULE-3413204661-0-3 | -55.8 |
| 72 | MCULE-6277098690-0-1 | -55.72 |
| 73 | MCULE-4323490082-0-1 | -55.62 |
| 74 | MCULE-5530400025-0-2 | -55.61 |
| 75 | MCULE-9207274769-0-1 | -55.59 |
| 76 | MCULE-4521363588-0-2 | -55.59 |
| 77 | MCULE-5067421403-0-1 | -55.55 |
| 78 | MCULE-7560305677-0-1 | -55.52 |
| 79 | MCULE-2442520377-0-1 | -55.36 |
| 80 | MCULE-9778954660-0-1 | -55.35 |
| 81 | MCULE-6217345482-0-1 | -55.32 |
| 82 | MCULE-1603455942-0-1 | -55.28 |
| 83 | MCULE-4151484731-0-2 | -55.27 |
| 84 | MCULE-5420487886-0-1 | -55.27 |
| 85 | MCULE-5643792264-0-1 | -55.19 |
| 86 | MCULE-1309971741-0-1 | -55.17 |
| 87 | MCULE-2925331688-0-1 | -55.03 |
| 88 | MCULE-2915794201-0-1 | -55.02 |
| 89 | MCULE-3680751741-0-1 | -55.01 |
| 90 | MCULE-9995974956-0-1 | -54.87 |
| 91 | MCULE-3439413100-0-1 | -54.8 |
| 92 | MCULE-4182318424-0-38 | -54.77 |
| 93 | MCULE-7962068695-0-1 | -54.68 |
| 94 | MCULE-9960939319-0-1 | -54.55 |
| 95 | MCULE-5830645399-0-1 | -54.53 |
| 96 | MCULE-4475983166-0-1 | -54.49 |
| 97 | MCULE-8830710104-0-1 | -54.46 |
| 98 | MCULE-7834508649-0-1 | -54.38 |
| 99 | MCULE-2894347504-0-1 | -54.36 |
| 100 | MCULE-8857776431-0-1 | -54.29 |
| 101 | MCULE-2602756469-0-1 | -54.28 |
| 102 | MCULE-8912229689-0-1 | -54.26 |
| 103 | MCULE-6488747060-0-1 | -54.21 |
| 104 | MCULE-2945125495-0-1 | -54.18 |
| 105 | MCULE-6441047230-0-2 | -54.12 |
| 106 | MCULE-6714029607-0-1 | -54.11 |
| 107 | MCULE-2642719953-0-1 | -54.09 |
| 108 | MCULE-9633151779-0-1 | -54.01 |
| 109 | MCULE-6762395817-0-1 | -53.99 |
| 110 | MCULE-5886489196-0-1 | -53.93 |
| 111 | MCULE-9578646806-0-2 | -53.93 |
| 112 | MCULE-1784480460-0-1 | -53.88 |
| 113 | MCULE-3427700127-0-1 | -53.87 |
| 114 | MCULE-3785523591-0-13 | -53.87 |
| 115 | MCULE-1382913904-0-1 | -53.83 |
| 116 | MCULE-3587361304-0-1 | -53.78 |
| 117 | MCULE-5439962575-1-2 | -53.72 |
| 118 | MCULE-4860195799-0-2 | -53.72 |
| 119 | MCULE-7683226056-0-1 | -53.67 |
| 120 | MCULE-8614176832-0-1 | -53.66 |
| 121 | MCULE-8994798017-0-1 | -53.58 |
| 122 | MCULE-8533406980-0-3 | -53.57 |
| 123 | MCULE-1478963969-0-1 | -53.55 |
| 124 | MCULE-9630168745-0-1 | -53.47 |
| 125 | MCULE-3578226603-0-2 | -53.46 |
| 126 | MCULE-2004433404-0-1 | -53.39 |
| 127 | MCULE-1720962177-0-1 | -53.36 |
| 128 | MCULE-4644630646-0-1 | -53.32 |
| 129 | MCULE-9602125558-0-1 | -53.29 |
| 130 | MCULE-4590635244-0-1 | -53.25 |
| 131 | MCULE-8372782252-0-1 | -53.21 |
| 132 | MCULE-8663107798-0-1 | -53.19 |
| 133 | MCULE-7578904639-0-1 | -53.17 |
| 134 | MCULE-3366895979-0-1 | -53.15 |
| 135 | MCULE-4790677657-0-1 | -53.15 |
| 136 | MCULE-2621699271-0-1 | -53.1 |
| 137 | MCULE-6488492152-0-1 | -53.09 |
| 138 | MCULE-8967752270-0-2 | -53.03 |
| 139 | MCULE-8491581618-0-1 | -53.03 |
| 140 | MCULE-2755886321-0-3 | -53.03 |
| 141 | MCULE-5883354014-0-1 | -53 |
| 142 | MCULE-2747125082-0-1 | -52.92 |
| 143 | MCULE-5817180883-0-1 | -52.88 |
| 144 | MCULE-4408605808-0-2 | -52.85 |
| 145 | MCULE-9410581573-0-1 | -52.8 |
| 146 | MCULE-5359141248-0-1 | -52.73 |
| 147 | MCULE-8440683563-0-1 | -52.59 |
| 148 | MCULE-7550420408-0-1 | -52.54 |
| 149 | MCULE-3967939030-0-1 | -52.48 |
| 150 | MCULE-7810806769-0-1 | -52.47 |
| 151 | MCULE-7817364475-0-1 | -52.46 |
| 152 | MCULE-8749315588-0-1 | -52.37 |
| 153 | MCULE-1333556608-0-7 | -52.35 |
| 154 | MCULE-9438572745-0-1 | -52.25 |
| 155 | MCULE-7097410851-0-2 | -52.17 |
| 156 | MCULE-9976836886-0-1 | -52.15 |
| 157 | MCULE-9991558968-0-1 | -52.14 |
| 158 | MCULE-5624146770-0-1 | -52.13 |
| 159 | MCULE-5663409575-0-1 | -52.02 |
| 160 | MCULE-6692323756-0-1 | -51.99 |
| 161 | MCULE-2634744591-0-1 | -51.99 |
| 162 | MCULE-7424094347-0-3 | -51.96 |
| 163 | MCULE-6060634655-0-2 | -51.93 |
| 164 | MCULE-3144366771-0-1 | -51.91 |
| 165 | MCULE-2636033371-0-2 | -51.89 |
| 166 | MCULE-7826929160-0-1 | -51.88 |
| 167 | MCULE-7130291437-0-1 | -51.82 |
| 168 | MCULE-8744049005-0-1 | -51.76 |
| 169 | MCULE-5877517361-0-1 | -51.75 |
| 170 | MCULE-2821431762-0-1 | -51.74 |
| 171 | MCULE-6142777612-0-1 | -51.66 |
| 172 | MCULE-3837901520-0-1 | -51.65 |
| 173 | MCULE-5098018687-0-1 | -51.58 |
| 174 | MCULE-6644155293-0-1 | -51.58 |
| 175 | MCULE-2777365590-0-1 | -51.57 |
| 176 | MCULE-8911493654-0-1 | -51.54 |
| 177 | MCULE-9710126793-0-1 | -51.5 |
| 178 | MCULE-3722512860-0-1 | -51.49 |
| 179 | MCULE-7241219267-0-2 | -51.46 |
| 180 | MCULE-9007015866-0-1 | -51.46 |
| 181 | MCULE-4104171675-0-1 | -51.45 |
| 182 | MCULE-7308674377-0-4 | -51.42 |
| 183 | MCULE-7231722824-0-1 | -51.37 |
| 184 | MCULE-9268288481-0-1 | -51.33 |
| 185 | MCULE-3663386420-0-1 | -51.32 |
| 186 | MCULE-9087873656-0-1 | -51.31 |
| 187 | MCULE-9601786227-0-1 | -51.31 |
| 188 | MCULE-8953371655-0-1 | -51.21 |
| 189 | MCULE-1697358457-0-1 | -51.21 |
| 190 | MCULE-8226146640-0-1 | -51.2 |
| 191 | MCULE-2853819031-0-1 | -51.18 |
| 192 | MCULE-9163001537-0-1 | -51.17 |
| 193 | MCULE-2053488436-0-2 | -51.17 |
| 194 | MCULE-1522865047-0-1 | -51.14 |
| 195 | MCULE-2795142916-0-2 | -51.11 |
| 196 | MCULE-4746034410-0-1 | -51.08 |
| 197 | MCULE-9994160358-0-6 | -51.01 |
| 198 | MCULE-4828152836-0-1 | -50.97 |
| 199 | MCULE-1054176167-0-1 | -50.95 |
| 200 | MCULE-6142835936-0-1 | -50.95 |
| 201 | MCULE-6669733715-0-1 | -50.91 |
| 202 | MCULE-1365034658-0-3 | -50.86 |
| 203 | MCULE-2695865728-0-1 | -50.76 |
| 204 | MCULE-9263283905-0-1 | -50.72 |
| 205 | MCULE-4651996177-0-2 | -50.71 |
| 206 | MCULE-1704183301-0-3 | -50.69 |
| 207 | MCULE-8714561085-0-1 | -50.66 |
| 208 | MCULE-9906778654-0-2 | -50.65 |
| 209 | MCULE-7729147113-0-1 | -50.62 |
| 210 | MCULE-4985703155-0-1 | -50.61 |
| 211 | MCULE-8253716717-0-1 | -50.61 |
| 212 | MCULE-6256273847-0-2 | -50.55 |
| 213 | MCULE-2096929584-0-1 | -50.53 |
| 214 | MCULE-6169724363-0-1 | -50.53 |
| 215 | MCULE-2583392627-0-1 | -50.51 |
| 216 | MCULE-9606225094-0-1 | -50.48 |
| 217 | MCULE-8658699071-0-1 | -50.44 |
| 218 | MCULE-6871444133-0-2 | -50.41 |
| 219 | MCULE-5689264030-0-1 | -50.3 |
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