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Electronic Supplementary Information

Table S1. The detailed information of the training sets and test sets

No.	Molecule ChEMBL ID	Molecular Weight	AlogP	Smiles	IC50	Assay ChEMBL ID	Target ChEMBL ID	Type
1	CHEMBL3896829	427.4	4.51	Cc1sc(NC(=O)C2=C(CCC2)C(=O)O)c(c3onc(n3)C(F)(F)F)c1C4CC4	10 nM	CHEMBL3888563	CHEMBL2083	Training Set
2	CHEMBL3905766	345.38	3.18	OC(=O)C1=C(CCC1)C(=O)Nc2sccc2c3onc(n3)C4CC4	10 nM	CHEMBL3888563	CHEMBL2083	Training Set
3	CHEMBL3919426	373.43	3.8	Cc1sc(NC(=O)C2=C(CCC2)C(=O)O)c(c1C)c3onc(n3)C4CC4	10 nM	CHEMBL3888563	CHEMBL2083	Training Set
4	CHEMBL3915309	389.5	4.26	Cc1sc(NC(=O)C2=C(CCC2)C(=O)O)c(c1C)c3nc(ns3)C4CC4	11 nM	CHEMBL3888563	CHEMBL2083	Training Set
5	CHEMBL3923099	455.61	5.47	Cc1c(sc(NC(=O)C2=C(C3CCC2CC3)C(=O)O)c1c4nc(ns4)C5CC5)C6CC6	13 nM	CHEMBL3888563	CHEMBL2083	Training Set
6	CHEMBL3914116	415.54	4.83	Cc1c(sc(NC(=O)C2=C(CCC2)C(=O)O)c1c3nc(ns3)C4CC4)C5CC5	13 nM	CHEMBL3888563	CHEMBL2083	Training Set
7	CHEMBL3964149	359.41	3.49	Cc1csc(NC(=O)C2=C(CCC2)C(=O)O)c1c3onc(n3)C4CC4	15 nM	CHEMBL3888563	CHEMBL2083	Training Set
8	CHEMBL3920664	429.57	5.22	Cc1c(sc(NC(=O)C2=C(CCCC2)C(=O)O)c1c3nc(ns3)C4CC4)C5CC5	19 nM	CHEMBL3888563	CHEMBL2083	Training Set
9	CHEMBL3903803	385.45	4.06	OC(=O)C1=C(CCC1)C(=O)Nc2scc(C3CC3)c2c4onc(n4)C5CC5	19.2 nM	CHEMBL3888563	CHEMBL2083	Training Set
10	CHEMBL3979971	387.46	4.19	Cc1sc(NC(=O)C2=C(CCCC2)C(=O)O)c(c1C)c3onc(n3)C4CC4	20 nM	CHEMBL3888563	CHEMBL2083	Training Set
11	CHEMBL3896498	399.47	4.36	Cc1sc(NC(=O)C2=C(CCC2)C(=O)O)c(c3onc(n3)C4CC4)c1C5CC5	20 nM	CHEMBL3888563	CHEMBL2083	Training Set
12	CHEMBL3897486	413.38	4.2	OC(=O)C1=C(CCC1)C(=O)Nc2scc(c2c3onc(n3)C4CC4)C(F)(F)F	20.5 nM	CHEMBL3888563	CHEMBL2083	Training Set
13	CHEMBL3919746	389.43	3.03	Cc1sc(NC(=O)C2=C(COCC2)C(=O)O)c(c1C)c3onc(n3)C4CC4	21 nM	CHEMBL3888563	CHEMBL2083	Training Set
14	CHEMBL3986878	377.49	4.09	Cc1nsc(n1)c2c(C)c(C)sc2NC(=O)C3=C(CCCC3)C(=O)O	23 nM	CHEMBL3888563	CHEMBL2083	Training Set
15	CHEMBL3950827	363.46	3.7	Cc1nsc(n1)c2c(C)c(C)sc2NC(=O)C3=C(CCC3)C(=O)O	25 nM	CHEMBL3888563	CHEMBL2083	Training Set
16	CHEMBL3920801	429.57	4.9	Cc1sc(NC(=O)C2=C(C3CCC2CC3)C(=O)O)c(c1C)c4nc(ns4)C5CC5	27 nM	CHEMBL3888563	CHEMBL2083	Training Set
17	CHEMBL3938613	429.57	4.9	Cc1nsc(n1)c2c(C)c(sc2NC(=O)C3=C(C4CCC3CC4)C(=O)O)C5CC5	29 nM	CHEMBL3888563	CHEMBL2083	Training Set
18	CHEMBL3891355	413.5	4.43	Cc1sc(NC(=O)C2=C(C3CCC2CC3)C(=O)O)c(c1C)c4onc(n4)C5CC5	40 nM	CHEMBL3888563	CHEMBL2083	Training Set
19	CHEMBL3981828	385.45	4.06	OC(=O)C1=C(CCC1)C(=O)Nc2sc(cc2c3onc(n3)C4CC4)C5CC5	40.8 nM	CHEMBL3888563	CHEMBL2083	Training Set
20	CHEMBL460750	387.4	5.68	OC(=O)c1cccc2c3CCCCCc3n(Cc4ccccc4C(F)(F)F)c12	49 nM	CHEMBL964127	CHEMBL2083	Training Set
21	CHEMBL3953175	393.27	5.18	OC(=O)C1(CCCC1)NC(=O)Nc2cc(Cl)cc(Cl)c2c3ccccc3	50 nM	CHEMBL3888115	CHEMBL2083	Training Set
22	CHEMBL3969505	348.76	3.88	OC(=O)C1(CC1)NC(=O)Nc2cc(Cl)c(F)cc2c3ccccc3	60 nM	CHEMBL3888115	CHEMBL2083	Training Set
23	CHEMBL516023	362.43	3.76	NC(=O)c1cccc(Cn2c3CCCCCc3c4cccc(C(=O)O)c24)c1	69 nM	CHEMBL964127	CHEMBL2083	Training Set
24	CHEMBL3975095	373.43	3.8	Cc1noc(n1)c2c(NC(=O)C3=C(CCC3)C(=O)O)sc(C)c2C4CC4	70 nM	CHEMBL3888563	CHEMBL2083	Training Set
25	CHEMBL3916530	365.22	4.4	OC(=O)C1(CC1)NC(=O)Nc2cc(Cl)cc(Cl)c2c3ccccc3	80 nM	CHEMBL3888115	CHEMBL2083	Training Set
26	CHEMBL3933786	415.47	3.6	Cc1c(sc(NC(=O)C2=C(CCC2)C(=O)O)c1c3onc(n3)C4CC4)C5COC5	90 nM	CHEMBL3888563	CHEMBL2083	Training Set
27	CHEMBL514969	319.4	4.66	OC(=O)c1cccc2c3CCCCCc3n(Cc4ccccc4)c12	96 nM	CHEMBL964127	CHEMBL2083	Training Set
28	CHEMBL474944	362.43	3.76	NC(=O)c1ccccc1Cn2c3CCCCCc3c4cccc(C(=O)O)c24	98 nM	CHEMBL964127	CHEMBL2083	Training Set
29	CHEMBL3944468	376.82	4.67	OC(=O)C1(CCCC1)NC(=O)Nc2cc(Cl)c(F)cc2c3ccccc3	100 nM	CHEMBL3888115	CHEMBL2083	Training Set
30	CHEMBL3890150	429.5	3.99	Cc1c(sc(NC(=O)C2=C(CCCC2)C(=O)O)c1c3onc(n3)C4CC4)C5COC5	105 nM	CHEMBL3888563	CHEMBL2083	Training Set
31	CHEMBL3919746	389.43	3.03	Cc1sc(NC(=O)C2=C(COCC2)C(=O)O)c(c1C)c3onc(n3)C4CC4	107 nM	CHEMBL3888563	CHEMBL2083	Training Set
32	CHEMBL3903176	413.5	4.43	Cc1noc(n1)c2c(NC(=O)C3=C(C4CCC3CC4)C(=O)O)sc(C)c2C5CC5	140 nM	CHEMBL3888563	CHEMBL2083	Training Set
33	CHEMBL3967738	330.77	3.75	OC(=O)C1(CC1)NC(=O)Nc2cc(Cl)ccc2c3ccccc3	140 nM	CHEMBL3888115	CHEMBL2083	Training Set
34	CHEMBL3930938	376.82	4.67	OC(=O)C1(CCCC1)NC(=O)Nc2cc(Cl)ccc2c3ccc(F)cc3	140 nM	CHEMBL3888115	CHEMBL2083	Training Set
35	CHEMBL3958926	358.83	4.53	OC(=O)C1(CCCC1)NC(=O)Nc2cc(Cl)ccc2c3ccccc3	150 nM	CHEMBL3888115	CHEMBL2083	Training Set
36	CHEMBL3890665	439.54	5	Cc1c(sc(NC(=O)C2=C(C3CCC2CC3)C(=O)O)c1c4onc(n4)C5CC5)C6CC6	210 nM	CHEMBL3888563	CHEMBL2083	Training Set
37	CHEMBL4113722	404.37	3.51	Cc1sc(NC(=O)N2CCC[C@@H]2C(=O)O)c(c1C)c3onc(n3)C(F)(F)F	217 nM	CHEMBL3888563	CHEMBL2083	Training Set
38	CHEMBL3980900	348.76	3.88	OC(=O)C1(CC1)NC(=O)Nc2ccc(Cl)cc2c3ccc(F)cc3	290 nM	CHEMBL3888115	CHEMBL2083	Training Set
39	CHEMBL3927654	387.46	4.19	Cc1noc(n1)c2c(NC(=O)C3=C(CCCC3)C(=O)O)sc(C)c2C4CC4	310 nM	CHEMBL3888563	CHEMBL2083	Training Set

40	CHEMBL3986323	389.48	4.12	Cc1sc(NC(=O)C2CCCCC2C(=O)O)c(c1C)c3onc(n3)C4CC4	345 nM	CHEMBL3888563	CHEMBL2083	Training Set
41	CHEMBL474744	323.37	4.41	OC(=O)c1cccc2c3CCCCc3n(Cc4cccc(F)c4)c12	400 nM	CHEMBL964125	CHEMBL2083	Training Set
42	CHEMBL474743	323.37	4.41	OC(=O)c1cccc2c3CCCCc3n(Cc4ccccc4F)c12	400 nM	CHEMBL964125	CHEMBL2083	Training Set
43	CHEMBL474944	362.43	3.76	NC(=O)c1ccccc1Cn2c3CCCCCc3c4cccc(C(=O)O)c24	400 nM	CHEMBL964125	CHEMBL2083	Training Set
44	CHEMBL474942	373.37	5.29	OC(=O)c1cccc2c3CCCCc3n(Cc4ccccc4C(F)(F)F)c12	400 nM	CHEMBL964125	CHEMBL2083	Training Set
45	CHEMBL516469	271.36	4.02	CCCn1c2CCCCCc2c3cccc(C(=O)O)c13	430 nM	CHEMBL964125	CHEMBL2083	Training Set
46	CHEMBL516023	362.43	3.76	NC(=O)c1cccc(Cn2c3CCCCCc3c4cccc(C(=O)O)c24)c1	450 nM	CHEMBL964125	CHEMBL2083	Training Set
47	CHEMBL3922017	392.38	4.89	OC(=O)C1(CCCC1)NC(=O)Nc2cc(ccc2c3ccccc3)C(F)(F)F	520 nM	CHEMBL3888115	CHEMBL2083	Training Set
48	CHEMBL514666	335.4	4.28	COc1cccc(Cn2c3CCCCc3c4cccc(C(=O)O)c24)c1	550 nM	CHEMBL964125	CHEMBL2083	Training Set
49	CHEMBL185595	253.3	3.66	OC(=O)CCCn1c2ccccc2c3ccccc13	570 nM	CHEMBL832621	CHEMBL2083	Training Set
50	CHEMBL516469	271.36	4.02	CCCn1c2CCCCCc2c3cccc(C(=O)O)c13	580 nM	CHEMBL964127	CHEMBL2083	Training Set
51	CHEMBL514969	319.4	4.66	OC(=O)c1cccc2c3CCCCCc3n(Cc4ccccc4)c12	590 nM	CHEMBL964125	CHEMBL2083	Training Set
52	CHEMBL184136	316.3	3.5	COc1ccc(CSc2nc(O)cc(n2)C(F)(F)F)cc1	600 nM	CHEMBL833473	CHEMBL2083	Training Set
53	CHEMBL475549	335.4	4.28	COc1ccccc1Cn2c3CCCCc3c4cccc(C(=O)O)c24	600 nM	CHEMBL964125	CHEMBL2083	Training Set
54	CHEMBL460750	387.4	5.68	OC(=O)c1cccc2c3CCCCCc3n(Cc4ccccc4C(F)(F)F)c12	650 nM	CHEMBL964125	CHEMBL2083	Training Set
55	CHEMBL501361	257.33	3.63	CCCn1c2CCCCc2c3cccc(C(=O)O)c13	670 nM	CHEMBL964127	CHEMBL2083	Training Set
56	CHEMBL518180	337.39	4.8	OC(=O)c1cccc2c3CCCCCc3n(Cc4ccccc4F)c12	710 nM	CHEMBL964125	CHEMBL2083	Training Set
57	CHEMBL501361	257.33	3.63	CCCn1c2CCCCc2c3cccc(C(=O)O)c13	730 nM	CHEMBL964125	CHEMBL2083	Training Set
58	CHEMBL459901	305.38	4.27	OC(=O)c1ccc2c3CCCCc3n(Cc4ccccc4)c2c1	750 nM	CHEMBL964125	CHEMBL2083	Training Set
59	CHEMBL3938704	376.82	4.67	OC(=O)C1(CCCC1)NC(=O)Nc2ccc(Cl)cc2c3ccc(F)cc3	750 nM	CHEMBL3888115	CHEMBL2083	Training Set
60	CHEMBL184795	267.33	4.05	OC(=O)CCCCn1c2ccccc2c3ccccc13	800 nM	CHEMBL832621	CHEMBL2083	Training Set
61	CHEMBL3893057	344.8	4.14	OC(=O)C1(CCC1)NC(=O)Nc2cc(Cl)ccc2c3ccccc3	810 nM	CHEMBL3888115	CHEMBL2083	Training Set
62	CHEMBL3943391	330.77	3.75	OC(=O)C1(CC1)NC(=O)Nc2ccc(Cl)cc2c3ccccc3	890 nM	CHEMBL3888115	CHEMBL2083	Training Set
63	CHEMBL82293	256.43	5.55	CCCCCCCCCCCCCCCC(=O)O	930 nM	CHEMBL832621	CHEMBL2083	Training Set
64	CHEMBL3968270	364.32	4.11	OC(=O)C1(CC1)NC(=O)Nc2cc(ccc2c3ccccc3)C(F)(F)F	950 nM	CHEMBL3888115	CHEMBL2083	Training Set
65	CHEMBL459902	291.35	3.88	OC(=O)c1cccc2c3CCCc3n(Cc4ccccc4)c12	970 nM	CHEMBL964125	CHEMBL2083	Training Set
66	CHEMBL267476	280.45	5.88	CCCCC\C=C/C\C=C/CCCCCCCC(=O)O	1000 nM	CHEMBL1120075	CHEMBL2083	Training Set
67	CHEMBL1085570	294.16	2.75	OC(=O)CSCC(=O)Nc1cc(Cl)cc(Cl)c1	1000 nM	CHEMBL1120075	CHEMBL2083	Training Set
68	CHEMBL360376	321.32	2.31	Oc1cc(nc(SCC(=O)N2CCCCC2)n1)C(F)(F)F	1000 nM	CHEMBL833473	CHEMBL2083	Training Set
69	CHEMBL474943	387.4	5.68	OC(=O)c1cccc2c3CCCCCc3n(Cc4cccc(c4)C(F)(F)F)c12	1040 nM	CHEMBL964125	CHEMBL2083	Training Set
70	CHEMBL454404	319.4	4.58	Cc1ccc(Cn2c3CCCCc3c4cccc(C(=O)O)c24)cc1	1090 nM	CHEMBL964125	CHEMBL2083	Training Set
71	CHEMBL363032	357.41	3.79	OC(=O)c1sccc1S(=O)(=O)n2c3ccccc3c4ccccc24	1100 nM	CHEMBL832621	CHEMBL2083	Training Set
72	CHEMBL472747	282.34	3.24	OC(=O)CC\C=C/c1nn(c2CCCc12)c3ccccc3	1100 nM	CHEMBL964125	CHEMBL2083	Training Set
73	CHEMBL184605	321.38	2.95	Cc1ccc2ccn(c2c1)S(=O)(=O)c3ccsc3C(=O)O	1300 nM	CHEMBL832621	CHEMBL2083	Training Set
74	CHEMBL427320	386.25	3.4	OC(=O)c1sccc1S(=O)(=O)n2ccc3cc(Br)ccc23	1300 nM	CHEMBL832621	CHEMBL2083	Training Set
75	CHEMBL3914457	358.83	4.53	OC(=O)C1(CCCC1)NC(=O)Nc2ccc(Cl)cc2c3ccccc3	1350 nM	CHEMBL3888115	CHEMBL2083	Training Set
76	CHEMBL183802	321.38	2.95	Cc1cn(c2ccccc12)S(=O)(=O)c3ccsc3C(=O)O	1500 nM	CHEMBL832621	CHEMBL2083	Training Set
77	CHEMBL510638	373.37	5.29	OC(=O)c1cccc2c3CCCCc3n(Cc4cccc(c4)C(F)(F)F)c12	1660 nM	CHEMBL964125	CHEMBL2083	Training Set
78	CHEMBL508994	391.36	5.42	OC(=O)c1cccc2c3CCCCc3n(Cc4c(F)cccc4C(F)(F)F)c12	1810 nM	CHEMBL964125	CHEMBL2083	Training Set
79	CHEMBL452160	373.37	5.29	OC(=O)c1cccc2c3CCCCc3n(Cc4ccc(cc4)C(F)(F)F)c12	2390 nM	CHEMBL964125	CHEMBL2083	Training Set
80	CHEMBL185553	337.38	2.65	COc1ccc2ccn(c2c1)S(=O)(=O)c3ccsc3C(=O)O	2600 nM	CHEMBL832621	CHEMBL2083	Training Set
81	CHEMBL185362	337.38	2.65	COc1cccc2ccn(c12)S(=O)(=O)c3ccsc3C(=O)O	2600 nM	CHEMBL832621	CHEMBL2083	Training Set
82	CHEMBL2334251	398.46	5.45	OC(=O)CCCOc1ccccc1c2cc(c3ccccc3)n(n2)c4ccccc4	3020 nM	CHEMBL2339128	CHEMBL2083	Training Set
83	CHEMBL1085571	365.84	3.57	OC(=O)CSCC(=O)NCc1c(Cl)cccc1Oc2ccccc2	3100 nM	CHEMBL1120075	CHEMBL2083	Training Set

84	CHEMBL3927133	430.49	3.19	CN(C)C(=O)c1sc(NC(=O)C2=C(CCC2)C(=O)O)c(c1C)c3onc(n3)C4CC4	3325.9 nM	CHEMBL3888563	CHEMBL2083	Training Set
85	CHEMBL475548	334.38	3.9	O\N=C/1\CCCc2c1c3cccc(C(=O)O)c3n2Cc4ccccc4	3500 nM	CHEMBL964125	CHEMBL2083	Training Set
86	CHEMBL365476	325.34	2.78	OC(=O)c1sccc1S(=O)(=O)n2ccc3cc(F)ccc23	3500 nM	CHEMBL832621	CHEMBL2083	Training Set
87	CHEMBL515599	279.34	4	Cc1c(C)n(Cc2ccccc2)c3c(cccc13)C(=O)O	3600 nM	CHEMBL964125	CHEMBL2083	Training Set
88	CHEMBL182801	299.25	2.82	COc1ccc(CNc2nc(O)cc(n2)C(F)(F)F)cc1	3900 nM	CHEMBL833473	CHEMBL2083	Training Set
89	CHEMBL184142	317.7	3.49	CN(Cc1ccc(Cl)cc1)c2nc(O)cc(n2)C(F)(F)F	4000 nM	CHEMBL833473	CHEMBL2083	Training Set
90	CHEMBL3400905	248.37	4.76	CC(C)c1cc(C(C)C)c(C(=O)O)c(c1)C(C)C	4000 nM	CHEMBL3404792	CHEMBL2083	Training Set
91	CHEMBL1085797	322.43	2.11	OC(=O)CSCC(=O)NCc1ccccc1N2CCCCC2	4100 nM	CHEMBL1120075	CHEMBL2083	Training Set
92	CHEMBL3931426	310.35	3.43	CN(C(=O)Nc1ccccc1c2ccccc2)C3(CC3)C(=O)O	4260 nM	CHEMBL3888115	CHEMBL2083	Training Set
93	CHEMBL2334259	432.91	6.1	OC(=O)CCCOc1ccccc1c2cc(c3ccccc3)n(n2)c4ccccc4Cl	4270 nM	CHEMBL2339128	CHEMBL2083	Training Set
94	CHEMBL364141	351.38	3.73	OC(=O)c1ccccc1S(=O)(=O)n2c3ccccc3c4ccccc24	4300 nM	CHEMBL832621	CHEMBL2083	Training Set
95	CHEMBL2334256	432.91	6.1	OC(=O)CCCOc1ccccc1c2cc(c3ccccc3)n(n2)c4ccc(Cl)cc4	4320 nM	CHEMBL2339128	CHEMBL2083	Training Set
96	CHEMBL1086224	277.7	2.24	OC(=O)CSCC(=O)Nc1ccc(F)c(Cl)c1	4400 nM	CHEMBL1120075	CHEMBL2083	Training Set
97	CHEMBL2334249	412.49	5.76	Cc1ccc(cc1)c2cc(nn2c3ccccc3)c4ccccc4OCCCC(=O)O	5410 nM	CHEMBL2339128	CHEMBL2083	Training Set
98	CHEMBL2334255	477.36	6.21	OC(=O)CCCOc1ccccc1c2cc(c3ccccc3)n(n2)c4ccc(Br)cc4	5640 nM	CHEMBL2339128	CHEMBL2083	Training Set
99	CHEMBL365508	331.35	2.59	COc1ccc2ccn(c2c1)S(=O)(=O)c3ccccc3C(=O)O	6100 nM	CHEMBL832621	CHEMBL2083	Training Set
100	CHEMBL2334246	432.91	6.1	OC(=O)CCCOc1ccccc1c2cc(c3ccc(Cl)cc3)n(n2)c4ccccc4	6130 nM	CHEMBL2339128	CHEMBL2083	Training Set
101	CHEMBL3964559	446.55	4.41	COC(=O)c1sc(NC(=O)C2=C(C3CCC2CC3)C(=O)O)c(c1C)c4nc(C)cs4	6160 nM	CHEMBL3888563	CHEMBL2083	Training Set
102	CHEMBL2334252	412.49	5.84	OC(=O)CCCCOc1ccccc1c2cc(c3ccccc3)n(n2)c4ccccc4	6390 nM	CHEMBL2339128	CHEMBL2083	Training Set
103	CHEMBL360007	321.38	2.95	Cc1ccc2c(ccn2S(=O)(=O)c3ccsc3C(=O)O)c1	7100 nM	CHEMBL832621	CHEMBL2083	Training Set
104	CHEMBL361037	321.38	2.95	Cc1cccc2c1ccn2S(=O)(=O)c3ccsc3C(=O)O	7400 nM	CHEMBL832621	CHEMBL2083	Training Set
105	CHEMBL3400157	284.42	4.3	CC(C)c1cc(C(C)C)c(c(c1)C(C)C)S(=O)(=O)O	7900 nM	CHEMBL3404792	CHEMBL2083	Training Set
106	CHEMBL361251	315.35	2.88	Cc1cn(c2ccccc12)S(=O)(=O)c3ccccc3C(=O)O	8500 nM	CHEMBL832621	CHEMBL2083	Training Set
107	CHEMBL184817	239.27	3.27	OC(=O)CCn1c2ccccc2c3ccccc13	9400 nM	CHEMBL832621	CHEMBL2083	Training Set
108	CHEMBL2334250	477.36	6.21	OC(=O)CCCOc1ccccc1c2cc(c3ccc(Br)cc3)n(n2)c4ccccc4	9510 nM	CHEMBL2339128	CHEMBL2083	Training Set
109	CHEMBL3918729	399.47	4.36	Cc1c(sc(NC(=O)C2=C(CCC2)C(=O)O)c1c3onc(n3)C4CC4)C5CC5	10 nM	CHEMBL3888563	CHEMBL2083	Test Set
110	CHEMBL3928329	359.41	3.49	Cc1cc(c(NC(=O)C2=C(CCC2)C(=O)O)s1)c3onc(n3)C4CC4	20 nM	CHEMBL3888563	CHEMBL2083	Test Set
111	CHEMBL3967672	439.54	5	Cc1sc(NC(=O)C2=C(C3CCC2CC3)C(=O)O)c(c4onc(n4)C5CC5)c1C6CC6	20 nM	CHEMBL3888563	CHEMBL2083	Test Set
112	CHEMBL3914622	427.4	4.51	Cc1sc(NC(=O)C2=C(CCC2)C(=O)O)c(c3onc(n3)C4CC4)c1C(F)(F)F	20 nM	CHEMBL3888563	CHEMBL2083	Test Set
113	CHEMBL3957282	389.5	4.26	Cc1nsc(n1)c2c(C)c(sc2NC(=O)C3=C(CCC3)C(=O)O)C4CC4	22 nM	CHEMBL3888563	CHEMBL2083	Test Set
114	CHEMBL3913234	467.47	5.14	Cc1sc(NC(=O)C2=C(C3CCC2CC3)C(=O)O)c(c4onc(n4)C(F)(F)F)c1C5CC5	30 nM	CHEMBL3888563	CHEMBL2083	Test Set
115	CHEMBL3929717	403.53	4.65	Cc1nsc(n1)c2c(C)c(sc2NC(=O)C3=C(CCCC3)C(=O)O)C4CC4	31 nM	CHEMBL3888563	CHEMBL2083	Test Set
116	CHEMBL3943278	403.53	4.33	Cc1nsc(n1)c2c(C)c(C)sc2NC(=O)C3=C(C4CCC3CC4)C(=O)O	44 nM	CHEMBL3888563	CHEMBL2083	Test Set
117	CHEMBL3962973	486.58	4.07	CN(C)c1nc(ns1)c2sc(NC(=O)C3=C(CCC3)C(=O)O)c(c2C)c4onc(n4)C5CC5	58.1 nM	CHEMBL3888563	CHEMBL2083	Test Set
118	CHEMBL3952008	403.53	4.65	Cc1sc(NC(=O)C2=C(CCCC2)C(=O)O)c(c1C)c3nc(ns3)C4CC4	85 nM	CHEMBL3888563	CHEMBL2083	Test Set
119	CHEMBL3972884	313.38	3.92	OC(=O)C1=C(CCC1)C(=O)Nc2sccc2c3ccccc3	200 nM	CHEMBL3888563	CHEMBL2083	Test Set
120	CHEMBL247920	474.56	6.9	CCc1c(c2ccccc2)c(nn1c3ccccc3c4cccc(OCC(=O)O)c4)c5ccccc5	221 nM	CHEMBL2339128	CHEMBL2083	Test Set
121	CHEMBL3986323	389.48	4.12	Cc1sc(NC(=O)C2CCCCC2C(=O)O)c(c1C)c3onc(n3)C4CC4	244 nM	CHEMBL3888563	CHEMBL2083	Test Set
122	CHEMBL3973942	427.4	4.28	OC(=O)C1=C(CCC1)C(=O)Nc2sc(CC(F)(F)F)cc2c3onc(n3)C4CC4	247.6 nM	CHEMBL3888563	CHEMBL2083	Test Set
123	CHEMBL3899095	431.47	3.66	CCOC(=O)c1sc(NC(=O)C2=C(CCC2)C(=O)O)c(c1C)c3onc(n3)C4CC4	250 nM	CHEMBL3888563	CHEMBL2083	Test Set
124	CHEMBL3958454	348.76	3.88	OC(=O)C1(CC1)NC(=O)Nc2cc(Cl)ccc2c3ccc(F)cc3	330 nM	CHEMBL3888115	CHEMBL2083	Test Set
125	CHEMBL452596	305.38	4.27	OC(=O)c1cccc2c3CCCCc3n(Cc4ccccc4)c12	590 nM	CHEMBL964125	CHEMBL2083	Test Set
126	CHEMBL460749	337.39	4.8	OC(=O)c1cccc2c3CCCCCc3n(Cc4cccc(F)c4)c12	720 nM	CHEMBL964125	CHEMBL2083	Test Set
127	CHEMBL518181	337.39	4.8	OC(=O)c1cccc2c3CCCCCc3n(Cc4ccc(F)cc4)c12	780 nM	CHEMBL964125	CHEMBL2083	Test Set

128	CHEMBL515905	323.37	4.41	OC(=O)c1cccc2c3CCCCc3n(Cc4ccc(F)cc4)c12	830 nM	CHEMBL964125	CHEMBL2083	Test Set
129	CHEMBL1782963	446.51	6.34	OC(=O)COc1cccc(c1)c2ccccc2c3cc(c4ccccc4)n(n3)c5ccccc5	987 nM	CHEMBL2339128	CHEMBL2083	Test Set
130	CHEMBL514654	387.4	5.68	OC(=O)c1cccc2c3CCCCCc3n(Cc4ccc(cc4)C(F)(F)F)c12	2030 nM	CHEMBL964125	CHEMBL2083	Test Set
131	CHEMBL2334261	432.91	6.1	OC(=O)CCCOc1ccccc1c2cc(c3ccccc3)n(n2)c4cccc(Cl)c4	2500 nM	CHEMBL2339128	CHEMBL2083	Test Set
132	CHEMBL442621	335.4	4.28	COc1ccc(Cn2c3CCCCc3c4cccc(C(=O)O)c24)cc1	2680 nM	CHEMBL964125	CHEMBL2083	Test Set
133	CHEMBL184852	303.67	3.47	Oc1cc(nc(NCc2ccc(Cl)cc2)n1)C(F)(F)F	2900 nM	CHEMBL833473	CHEMBL2083	Test Set
134	CHEMBL181645	325.34	2.78	OC(=O)c1sccc1S(=O)(=O)n2ccc3cccc(F)c23	4500 nM	CHEMBL832621	CHEMBL2083	Test Set
135	CHEMBL184846	325.34	2.78	OC(=O)c1sccc1S(=O)(=O)n2ccc3ccc(F)cc23	4700 nM	CHEMBL832621	CHEMBL2083	Test Set

Electronic Supplementary Information

Table S2. The detailed information of the predicted compounds

No.	DRUGBANK_ID	GENERIC_NAME	Bayesian #EstPGood	Bayesian #Prediction	SMILE
1	DB06803	Niclosamide	0.997166	TRUE	OC1=C(C=C(Cl)C=C1)C(=O)NC1=C(Cl)C=C(C=C1)[N+]([O-])=O
2	DB00824	Enprofylline	0.996349	TRUE	CCCN1C2=C(NC=N2)C(=O)NC1=O
3	DB12332	Rucaparib	0.995734	TRUE	CNCC1=CC=C(C=C1)C1=C2CCNC(=O)C3=C2C(N1)=CC(F)=C3
4	DB00900	Didanosine	0.995393	TRUE	OC[C@@H]1CC[C@@H](O1)N1C=NC2=C1NC=NC2=O
5	DB03585	Oxyphenbutazone	0.992165	TRUE	CCCCC1C(=O)N(N(C1=O)C1=CC=C(O)C=C1)C1=CC=CC=C1
6	DB00670	Pirenzepine	0.987449	TRUE	CN1CCN(CC(=O)N2C3=CC=CC=C3C(=O)NC3=C2N=CC=C3)CC1
7	DB01392	Yohimbine	0.986557	TRUE	[H][C@@]12CC[C@H](O)[C@H](C(=O)OC)[C@@]1([H])C[C@]1([H])N(CCC3=C1NC1=CC=CC=C31)C2
8	DB08826	Deferiprone	0.978131	TRUE	CN1C=CC(=O)C(O)=C1C
9	DB00697	Tizanidine	0.974106	TRUE	ClC1=C(NC2=NCCN2)C2=NSN=C2C=C1
10	DB06193	Pixantrone	0.97331	TRUE	NCCNC1=CC=C(NCCN)C2=C1C(=O)C1=C(C=NC=C1)C2=O
11	DB04876	Vildagliptin	0.971999	TRUE	OC12CC3CC(C1)CC(C3)(C2)NCC(=O)N1CCC[C@H]1C#N
12	DB00998	Frovatriptan	0.971266	TRUE	CN[C@@H]1CCC2=C(C1)C1=C(N2)C=CC(=C1)C(N)=O
13	DB00993	Azathioprine	0.958691	TRUE	CN1C=NC(=C1SC1=NC=NC2=C1NC=N2)[N+]([O-])=O
14	DB00507	Nitazoxanide	0.958246	TRUE	CC(=O)OC1=CC=CC=C1C(=O)NC1=NC=C(S1)[N+]([O-])=O
15	DB00457	Prazosin	0.954689	TRUE	COC1=C(OC)C=C2C(N)=NC(=NC2=C1)N1CCN(CC1)C(=O)C1=CC=C
16	DB00889	Granisetron	0.948685	TRUE	CN1N=C(C(=O)N[C@@H]2C[C@@H]3CCC[C@H](C2)N3C)C2=C1C=CC=C2
17	DB09282	Molsidomine	0.946336	TRUE	CCOC(=O)[N-]C1=C[N+](=NO1)N1CCOCC1
18	DB00213	Pantoprazole	0.945318	TRUE	COC1=C(OC)C(CS(=O)C2=NC3=C(N2)C=C(OC(F)F)C=C3)=NC=C1
19	DB00315	Zolmitriptan	0.935964	TRUE	CN(C)CCC1=CNC2=CC=C(C[C@H]3COC(=O)N3)C=C12
20	DB11071	Phenyl salicylate	0.930295	TRUE	OC1=CC=CC=C1C(=O)OC1=CC=CC=C1
21	DB05239	Cobimetinib	0.928284	TRUE	OC1(CN(C1)C(=O)C1=C(NC2=C(F)C=C(I)C=C2)C(F)=C(F)C=C1)[C@@H]1CCCCN1
22	DB00310	Chlorthalidone	0.92612	TRUE	NS(=O)(=O)C1=C(Cl)C=CC(=C1)C1(O)NC(=O)C2=CC=CC=C12
23	DB09343	Tipiracil	0.92233	TRUE	ClC1=C(CN2CCCC2=N)NC(=O)NC1=O
24	DB09151	Flutemetamol (18F)	0.919838	TRUE	CNC1=C([18F])C=C(C=C1)C1=NC2=CC=C(O)C=C2S1
25	DB04816	Dantron	0.916411	TRUE	OC1=CC=CC2=C1C(=O)C1=C(C=CC=C1O)C2=O
26	DB04880	Enoximone	0.913778	TRUE	CSC1=CC=C(C=C1)C(=O)C1=C(C)NC(=O)N1
27	DB00744	Zileuton	0.913352	TRUE	CC(N(O)C(N)=O)C1=CC2=CC=CC=C2S1
28	DB00819	Acetazolamide	0.912074	TRUE	CC(=O)NC1=NN=C(S1)S(N)(=O)=O

29	DB14723	Larotrectinib	0.909175	TRUE	O[C@H]1CCN(C1)C(=O)NC1=C2N=C(C=CN2N=C1)N1CCC[C@@H]1C1=C(F)C=CC(F)=C1
30	DB00277	Theophylline	0.906245	TRUE	CN1C2=C(NC=N2)C(=O)N(C)C1=O
31	DB09210	Piracetam	0.899645	TRUE	OC(=N)CN1CCCC1=O
32	DB11994	Diacerein	0.895923	TRUE	CC(=O)OC1=CC=CC2=C1C(=O)C1=C(OC(C)=O)C=C(C=C1C2=O)C(O)=O
33	DB00791	Uracil mustard	0.895759	TRUE	ClCCN(CCCl)C1=CNC(=O)NC1=O
34	DB00692	Phentolamine	0.895674	TRUE	CC1=CC=C(C=C1)N(CC1=NCCN1)C1=CC(O)=CC=C1
35	DB14176	Benzylparaben	0.894131	TRUE	OC1=CC=C(C=C1)C(=O)OCC1=CC=CC=C1
36	DB00432	Trifluridine	0.891466	TRUE	OC[C@H]1O[C@H](C[C@@H]1O)N1C=C(C(=O)NC1=O)C(F)(F)F
37	DB00544	Fluorouracil	0.890239	TRUE	FC1=CNC(=O)NC1=O
38	DB00252	Phenytoin	0.888466	TRUE	O=C1NC(=O)C(N1)(C1=CC=CC=C1)C1=CC=CC=C1
39	DB14569	Tedizolid	0.885363	TRUE	CN1N=NC(=N1)C1=NC=C(C=C1)C1=C(F)C=C(C=C1)N1C[C@H](CO)OC1=O
40	DB00353	Methylergometrine	0.873171	TRUE	[H][C@@]12CC3=CNC4=CC=CC(=C34)C1=C[C@H](CN2C)C(=O)N[C@@H](CC)CO
41	DB12867	Benperidol	0.855388	TRUE	OC1=NC2=CC=CC=C2N1C1CCN(CCCC(=O)C2=CC=C(F)C=C2)CC1
42	DB00316	Acetaminophen	0.855119	TRUE	CC(=O)NC1=CC=C(O)C=C1
43	DB01253	Ergometrine	0.851646	TRUE	[H][C@@]12CC3=CNC4=CC=CC(=C34)C1=C[C@H](CN2C)C(=O)N[C@@H](C)CO
44	DB01205	Flumazenil	0.845882	TRUE	CCOC(=O)C1=C2CN(C)C(=O)C3=C(C=CC(F)=C3)N2C=N1
45	DB00323	Tolcapone	0.83873	TRUE	CC1=CC=C(C=C1)C(=O)C1=CC(=C(O)C(O)=C1)[N+]([O-])=O
46	DB00909	Zonisamide	0.817339	TRUE	NS(=O)(=O)CC1=NOC2=CC=CC=C12
47	DB06807	Phenyl aminosalicylate	0.802597	TRUE	NC1=CC(O)=C(C=C1)C(=O)OC1=CC=CC=C1
48	DB00442	Entecavir	0.795359	TRUE	NC1=NC(=O)C2=C(N1)N(C=N2)[C@H]1C[C@H](O)[C@@H](CO)C1
49	DB00960	Pindolol	0.794436	TRUE	CC(C)NCC(O)COC1=CC=CC2=C1C=CN2
50	DB00246	Ziprasidone	0.788525	TRUE	ClC1=C(CCN2CCN(CC2)C2=NSC3=CC=CC=C23)C=C2CC(=O)NC2=
51	DB00247	Methysergide	0.786938	TRUE	[H][C@@]12CC3=CN(C)C4=C3C(=CC=C4)C1=C[C@H](CN2C)C(=O)NC(CC)CO
52	DB02959	Oxitriptan	0.78627	TRUE	N[C@@H](CC1=CNC2=C1C=C(O)C=C2)C(O)=O
53	DB12015	Alpelisib	0.781161	TRUE	CC1=C(SC(NC(=O)N2CCC[C@H]2C(N)=O)=N1)C1=CC(=NC=C1)C(C)(C)C(F)(F)F
54	DB01048	Abacavir	0.777855	TRUE	NC1=NC2=C(N=CN2[C@@H]2C[C@H](CO)C=C2)C(NC2CC2)=N1
55	DB11793	Niraparib	0.767727	TRUE	NC(=O)C1=CC=CC2=CN(N=C12)C1=CC=C(C=C1)[C@@H]1CCCNC
56	DB06335	Saxagliptin	0.7654	TRUE	N[C@H](C(=O)N1[C@H]2C[C@H]2C[C@H]1C#N)C12CC3CC(CC(O)(C3)C1)C2
57	DB04908	Flibanserin	0.760944	TRUE	FC(F)(F)C1=CC(=CC=C1)N1CCN(CCN2C(=O)NC3=CC=CC=C23)CC1

58	DB01097	Leflunomide	0.748518	TRUE	CC1=C(C=NO1)C(=O)NC1=CC=C(C=C1)C(F)(F)F
59	DB00322	Floxuridine	0.746043	TRUE	OC[C@H]1O[C@H](C[C@@H]1O)N1C=C(F)C(=O)NC1=O
60	DB00749	Etodolac	0.715893	TRUE	CCC1=C2NC3=C(CCOC3(CC)CC(O)=O)C2=CC=C1
61	DB00649	Stavudine	0.714929	TRUE	CC1=CN([C@@H]2O[C@H](CO)C=C2)C(=O)NC1=O
62	DB00601	Linezolid	0.712955	TRUE	CC(=O)NC[C@H]1CN(C(=O)O1)C1=CC(F)=C(C=C1)N1CCOCC1
63	DB01437	Glutethimide	0.703624	TRUE	CCC1(CCC(=O)NC1=O)C1=CC=CC=C1
64	DB05016	Ataluren	0.691258	TRUE	OC(=O)C1=CC=CC(=C1)C1=NOC(=N1)C1=CC=CC=C1F
65	DB00969	Alosetron	0.690017	TRUE	CN1C2=C(C3=CC=CC=C13)C(=O)N(CC1=C(C)NC=N1)CC2
66	DB13253	Proxibarbal	0.68991	TRUE	CC(O)CC1(CC=C)C(=O)NC(=O)NC1=O
67	DB00494	Entacapone	0.68354	TRUE	CCN(CC)C(=O)C(=C\C1=CC(=C(O)C(O)=C1)[N+]([O-])=O)\C#N
68	DB00249	Idoxuridine	0.672712	TRUE	OC[C@H]1O[C@H](C[C@@H]1O)N1C=C(I)C(=O)NC1=O
69	DB01020	Isosorbide Mononitrate	0.671196	TRUE	[H][C@]12OC[C@@H](O[N+]([O-])=O)[C@@]1([H])OC[C@@H]2O
70	DB00879	Emtricitabine	0.653477	TRUE	NC1=NC(=O)N(C=C1F)[C@@H]1CS[C@H](CO)O1
71	DB00225	Gadodiamide	0.642425	TRUE	O=C1[O-][Gd+3]234567[O]=C(C[N]2(CC[N]3(CC([O-]4)=O)CC[N]5(CC(=[O]6)NC)CC(=O)[O-]7)C1)NC
72	DB06795	Mafenide	0.635063	TRUE	NCC1=CC=C(C=C1)S(N)(=O)=O
73	DB06203	Alogliptin	0.628567	TRUE	CN1C(=O)C=C(N2CCC[C@@H](N)C2)N(CC2=C(C=CC=C2)C#N)C1=
74	DB02266	Flufenamic Acid	0.627966	TRUE	OC(=O)C1=CC=CC=C1NC1=CC(=CC=C1)C(F)(F)F
75	DB01096	Oxamniquine	0.622147	TRUE	CC(C)NCC1CCC2=CC(CO)=C(C=C2N1)[N+]([O-])=O
76	DB09219	Bisoxatin	0.617603	TRUE	OC1=CC=C(C=C1)C1(OC2=CC=CC=C2NC1=O)C1=CC=C(O)C=C1
77	DB00186	Lorazepam	0.615966	TRUE	OC1N=C(C2=CC=CC=C2Cl)C2=C(NC1=O)C=CC(Cl)=C2
78	DB09421	Protirelin	0.611068	TRUE	[H][C@@](CC1=CN=CN1)(NC(=O)[C@]1([H])CCC(=O)N1)C(=O)N1C CC[C@@]1([H])C(N)=O
79	DB09256	Tegafur	0.57836	TRUE	FC1=CN(C2CCCO2)C(=O)NC1=O
80	DB09327	Tegafur-uracil	0.57836	TRUE	O=C1NC=CC(=O)N1.FC1=CN(C2CCCO2)C(=O)NC1=O
81	DB00580	Valdecoxib	0.574496	TRUE	CC1=C(C(=NO1)C1=CC=CC=C1)C1=CC=C(C=C1)S(N)(=O)=O
82	DB00655	Estrone	0.560934	TRUE	[H][C@@]12CCC(=O)[C@@]1(C)CC[C@]1([H])C3=C(CC[C@@]21[H])C=C(O)C=C3
83	DB13211	Guanoxan	0.559394	TRUE	NC(=N)NCC1COC2=CC=CC=C2O1
84	DB00299	Penciclovir	0.556805	TRUE	NC1=NC(=O)C2=C(N1)N(CCC(CO)CO)C=N2
85	DB09220	Nicorandil	0.55631	TRUE	[O-][N+](=O)OCCNC(=O)C1=CC=CN=C1
86	DB14018	Bromotheophylline	0.55545	TRUE	CN1C2=C(NC(Br)=N2)C(=O)N(C)C1=O
87	DB00943	Zalcitabine	0.553894	TRUE	NC1=NC(=O)N(C=C1)[C@H]1CC[C@@H](CO)O1
88	DB00357	Aminoglutethimide	0.550852	TRUE	CCC1(CCC(=O)NC1=O)C1=CC=C(N)C=C1
89	DB08797	Salicylamide	0.542737	TRUE	NC(=O)C1=CC=CC=C1O
90	DB00495	Zidovudine	0.532211	TRUE	CC1=CN([C@H]2C[C@H](N=[N+]=[N-

91	DB13381	Sodium feredetate	0.527626	TRUE	[Na+].[O-]C(=O)C[N+]12CC[N+]34CC(=O)O[Fe--]13(OC(=O)C2)OC(=O)C4
92	DB13421	Edoxudine	0.523614	TRUE	CCC1=CN([C@H]2C[C@H](O)[C@@H](CO)O2)C(=O)NC1=O
93	DB00698	Nitrofurantoin	0.513255	TRUE	[O-][N+](=O)C1=CC=C(O1)\C=N\N1CC(=O)NC1=O
94	DB12301	Doravirine	0.513143	TRUE	CN1C(O)=NN=C1CN1C=CC(=C(OC2=CC(=CC(Cl)=C2)C#N)C1=O)C(F)(F)F
95	DB09074	Olaparib	0.502972	TRUE	OC1=NN=C(CC2=CC(C(=O)N3CCN(CC3)C(=O)C3CC3)=C(F)C=C2)C2=CC=CC=C12
96	DB01656	Roflumilast	0.500744	TRUE	FC(F)OC1=C(OCC2CC2)C=C(C=C1)C(=O)NC1=C(Cl)C=NC=C1Cl
97	DB00302	Tranexamic acid	0.498838	TRUE	NC[C@H]1CC[C@@H](CC1)C(O)=O
98	DB00174	Asparagine	0.49537	TRUE	N[C@@H](CC(N)=O)C(O)=O
99	DB00651	Dyphylline	0.491929	TRUE	CN1C2=C(N(CC(O)CO)C=N2)C(=O)N(C)C1=O
100	DB01265	Telbivudine	0.487204	TRUE	CC1=CN([C@@H]2C[C@@H](O)[C@H](CO)O2)C(=O)NC1=O
101	DB11080	Silver nitrate	0.484313	TRUE	[O-][N+](=O)O[Ag]
102	DB00551	Acetohydroxamic acid	0.48136	TRUE	CC(=O)NO
103	DB13628	Ethyl hydroxybenzoate	0.480988	TRUE	CCOC(=O)C1=CC=C(O)C=C1
104	DB00916	Metronidazole	0.480005	TRUE	CC1=NC=C(N1CCO)[N+]([O-])=O
105	DB11629	Laropiprant	0.477431	TRUE	CS(=O)(=O)C1=C2N(CC3=CC=C(Cl)C=C3)C3=C(CC[C@@H]3CC(O)=O)C2=CC(F)=C1
106	DB14084	Butylparaben	0.473428	TRUE	CCCCOC(=O)C1=CC=C(O)C=C1
107	DB00130	L-Glutamine	0.471525	TRUE	N[C@@H](CCC(N)=O)C(O)=O
108	DB00231	Temazepam	0.464912	TRUE	CN1C2=C(C=C(Cl)C=C2)C(=NC(O)C1=O)C1=CC=CC=C1
109	DB00619	Imatinib	0.460717	TRUE	CN1CCN(CC2=CC=C(C=C2)C(=O)NC2=CC(NC3=NC=CC(=N3)C3=CN=CC=C3)=C(C)C=C2)CC1
110	DB00484	Brimonidine	0.456721	TRUE	BrC1=C(NC2=NCCN2)C=CC2=NC=CN=C12
111	DB01005	Hydroxyurea	0.451656	TRUE	NC(=O)NO
112	DB00499	Flutamide	0.444897	TRUE	CC(C)C(=O)NC1=CC(=C(C=C1)[N+]([O-])=O)C(F)(F)F
113	DB00643	Mebendazole	0.442305	TRUE	COC(=O)NC1=NC2=C(N1)C=C(C=C2)C(=O)C1=CC=CC=C1
114	DB00787	Acyclovir	0.438616	TRUE	NC1=NC(=O)C2=C(N1)N(COCCO)C=N2
115	DB00576	Sulfamethizole	0.436126	TRUE	CC1=NN=C(NS(=O)(=O)C2=CC=C(N)C=C2)S1
116	DB00201	Caffeine	0.435799	TRUE	CN1C=NC2=C1C(=O)N(C)C(=O)N2C
117	DB01015	Sulfamethoxazole	0.429954	TRUE	CC1=CC(NS(=O)(=O)C2=CC=C(N)C=C2)=NO1
118	DB12834	Secnidazole	0.428307	TRUE	CC(O)CN1C(C)=NC=C1N(=O)=O
119	DB14177	Propylparaben	0.423761	TRUE	CCCOC(=O)C1=CC=C(O)C=C1
120	DB00552	Pentostatin	0.419358	TRUE	OC[C@H]1O[C@H](C[C@@H]1O)N1C=NC2=C1N=CNC[C@H]2O
121	DB11637	Delamanid	0.417527	TRUE	C[C@]1(COC2=CC=C(C=C2)N2CCC(CC2)OC2=CC=C(OC(F)(F)F)C=C2)CN2C=C(N=C2O1)[N+]([O-])=O

122	DB00349	Clobazam	0.410195	TRUE	CN1C2=C(C=C(Cl)C=C2)N(C2=CC=CC=C2)C(=O)CC1=O
123	DB05219	Crisaborole	0.404005	TRUE	OB1OCC2=C1C=CC(OC1=CC=C(C=C1)C#N)=C2
124	DB00441	Gemcitabine	0.397512	TRUE	NC1=NC(=O)N(C=C1)[C@@H]1O[C@H](CO)[C@@H](O)C1(F)F
125	DB14203	Disperse Blue 106	0.392736	TRUE	CCN(CCO)C1=CC=C(\N=N\C2=NC=C(S2)N(=O)=O)C(C)=C1
126	DB09355	Sulfabenzamide	0.390343	TRUE	NC1=CC=C(C=C1)S(=O)(=O)NC(=O)C1=CC=CC=C1
127	DB00812	Phenylbutazone	0.384726	TRUE	CCCCC1C(=O)N(N(C1=O)C1=CC=CC=C1)C1=CC=CC=C1
128	DB00809	Tropicamide	0.383871	TRUE	CCN(CC1=CC=NC=C1)C(=O)C(CO)C1=CC=CC=C1
129	DB00398	Sorafenib	0.377385	TRUE	CNC(=O)C1=NC=CC(OC2=CC=C(NC(=O)NC3=CC(=C(Cl)C=C3)C(F)(F)F)C=C2)=C1
130	DB00348	Nitisinone	0.376824	TRUE	[O-][N+](=O)C1=C(C=CC(=C1)C(F)(F)F)C(=O)C1C(=O)CCCC1=O
131	DB00260	Cycloserine	0.373351	TRUE	N[C@@H]1CONC1=O
132	DB00664	Sulfametopyrazine	0.372733	TRUE	COC1=NC=CN=C1NS(=O)(=O)C1=CC=C(N)C=C1
133	DB00820	Tadalafil	0.372115	TRUE	[H][C@]12CC3=C(NC4=CC=CC=C34)[C@H](N1C(=O)CN(C)C2=O)C1=CC2=C(OCO2)C=C1
134	DB12300	P-nitrobiphenyl	0.37202	TRUE	O=N(=O)C1=CC=C(C=C1)C1=CC=CC=C1
135	DB13248	Phthalylsulfathiazole	0.371702	TRUE	OC(=O)C1=CC=CC=C1C(=O)NC1=CC=C(C=C1)S(=O)(=O)NC1=NC=CS1
136	DB01606	Tazobactam	0.362611	TRUE	[H][C@@]12CC(=O)N1[C@@H](C(O)=O)[C@](C)(CN1C=CN=N1)S2(=O)=O
137	DB12938	Isoxaflutole	0.361905	TRUE	[H]C1=NOC(=C1C(=O)C1=C(C([H])=C(C([H])=C1[H])C(F)(F)F)S(=O)(=O)C([H])([H])[H])C1([H])C([H])([H])C1([H])[H]
138	DB11157	Anthralin	0.360101	TRUE	OC1=CC=CC2=C1C(=O)C1=C(O)C=CC=C1C2
139	DB00853	Temozolomide	0.354813	TRUE	CN1N=NC2=C(N=CN2C1=O)C(N)=O
140	DB00424	Hyoscyamine	0.351755	TRUE	CN1[C@H]2CC[C@@H]1C[C@@H](C2)OC(=O)[C@H](CO)C1=CC=CC=C1
141	DB00572	Atropine	0.351755	TRUE	CN1[C@H]2CC[C@@H]1C[C@@H](C2)OC(=O)C(CO)C1=CC=CC=C
142	DB01000	Cyclacillin	0.346679	TRUE	[H][C@]12SC(C)(C)[C@@H](N1C(=O)[C@H]2NC(=O)C1(N)CCCCC1)C(O)=O
143	DB00928	Azacitidine	0.344651	TRUE	NC1=NC(=O)N(C=N1)[C@@H]1O[C@H](CO)[C@@H](O)[C@H]1O
144	DB01084	Emedastine	0.34091	TRUE	CCOCCN1C(=NC2=CC=CC=C12)N1CCCN(C)CC1
145	DB11644	Tafamidis	0.338799	TRUE	OC(=O)C1=CC2=C(C=C1)N=C(O2)C1=CC(Cl)=CC(Cl)=C1
146	DB00242	Cladribine	0.332049	TRUE	NC1=C2N=CN([C@H]3C[C@H](O)[C@@H](CO)O3)C2=NC(Cl)=N1
147	DB11978	Glasdegib	0.329698	TRUE	CN1CC[C@H](C[C@@H]1C1=NC2=CC=CC=C2N1)NC(=O)NC1=CC=C(C=C1)C#N
148	DB01262	Decitabine	0.326834	TRUE	NC1=NC(=O)N(C=N1)[C@H]1C[C@H](O)[C@@H](CO)O1
149	DB04812	Benoxaprofen	0.324659	TRUE	CC(C(O)=O)C1=CC2=C(OC(=N2)C2=CC=C(Cl)C=C2)C=C1
150	DB00842	Oxazepam	0.323044	TRUE	OC1N=C(C2=CC=CC=C2)C2=C(NC1=O)C=CC(Cl)=C2

151	DB01219	Dantrolene	0.318712	TRUE	[O-][N+](=O)C1=CC=C(C=C1)C1=CC=C(O1)C=NN1CC(=O)NC1=O
152	DB04896	Milnacipran	0.317151	TRUE	CCN(CC)C(=O)C1(CC1CN)C1=CC=CC=C1
153	DB08918	Levomilnacipran	0.317151	TRUE	CCN(CC)C(=O)[C@]1(C[C@H]1CN)C1=CC=CC=C1
154	DB00518	Albendazole	0.313128	TRUE	CCCSC1=CC2=C(C=C1)N=C(NC(=O)OC)N2
155	DB13180	Gluconic Acid	0.309798	TRUE	OC[C@@H](O)[C@@H](O)[C@H](O)[C@@H](O)C(O)=O
156	DB13620	Potassium gluconate	0.309798	TRUE	[K+].[H][C@@](O)(CO)[C@@]([H])(O)[C@]([H])(O)[C@@]([H])(O)C([O-])=O
157	DB00356	Chlorzoxazone	0.304636	TRUE	ClC1=CC2=C(OC(=O)N2)C=C1
158	DB11100	Allantoin	0.300526	TRUE	NC(=O)NC1NC(=O)NC1=O
159	DB01004	Ganciclovir	0.293844	TRUE	NC1=NC2=C(N=CN2COC(CO)CO)C(=O)N1
160	DB00276	Amsacrine	0.293215	TRUE	COC1=C(NC2=C3C=CC=CC3=NC3=CC=CC=C23)C=CC(NS(C)(=O)=O)=C1
161	DB11285	Ethyl ferulate	0.292436	TRUE	[H]\C(=C(\[H])C1=CC(OC)=C(O)C=C1)C(=O)OCC
162	DB00933	Mesoridazine	0.291757	TRUE	CN1CCCCC1CCN1C2=C(SC3=C1C=C(C=C3)S(C)=O)C=CC=C2
163	DB01087	Primaquine	0.287904	TRUE	COC1=CC(NC(C)CCCN)=C2N=CC=CC2=C1
164	DB00709	Lamivudine	0.287517	TRUE	NC1=NC(=O)N(C=C1)[C@@H]1CS[C@H](CO)O1
165	DB00435	Nitric Oxide	0.28066	TRUE	[N]=O
166	DB00188	Bortezomib	0.266979	TRUE	CC(C)C[C@H](NC(=O)[C@H](CC1=CC=CC=C1)NC(=O)C1=CN=CC=N1)B(O)O
167	DB01303	Oxtriphylline	0.263443	TRUE	C[N+](C)(C)CCO.CN1C2=C([N-]C=N2)C(=O)N(C)C1=O
168	DB01068	Clonazepam	0.261108	TRUE	[O-][N+](=O)C1=CC2=C(NC(=O)CN=C2C2=CC=CC=C2Cl)C=C1
169	DB00270	Isradipine	0.25936	TRUE	COC(=O)C1=C(C)NC(C)=C(C1C1=CC=CC2=NON=C12)C(=O)OC(C)C
170	DB06605	Apixaban	0.258625	TRUE	COC1=CC=C(C=C1)N1N=C(C(N)=O)C2=C1C(=O)N(CC2)C1=CC=C(C=C1)N1CCCCC1=O
171	DB02701	Nicotinamide	0.257052	TRUE	NC(=O)C1=CC=CN=C1
172	DB11730	Ribociclib	0.25026	TRUE	CN(C)C(=O)C1=CC2=CN=C(NC3=CC=C(C=N3)N3CCNCC3)N=C2N1C1CCCC1
173	DB00360	Sapropterin	0.248805	TRUE	[H][C@@]1(CNC2=C(N1)C(=O)NC(N)=N2)[C@@H](O)[C@H](C)O
174	DB01558	Bromazepam	0.246194	TRUE	BrC1=CC2=C(NC(=O)CN=C2C2=CC=CC=N2)C=C1
175	DB11145	Oxyquinoline	0.243848	TRUE	OC1=CC=CC2=C1N=CC=C2
176	DB00150	L-Tryptophan	0.24049	TRUE	N[C@@H](CC1=CNC2=CC=CC=C12)C(O)=O
177	DB00383	Oxyphencyclimine	0.2404	TRUE	CN1CCCN=C1COC(=O)C(O)(C1CCCCC1)C1=CC=CC=C1
178	DB09510	Urea C-13	0.23199	TRUE	N[13C](O)=N
179	DB11129	Carbamide peroxide	0.23199	TRUE	OO.NC(O)=N
180	DB00593	Ethosuximide	0.23014	TRUE	CCC1(C)CC(=O)NC1=O
181	DB08931	Riociguat	0.227183	TRUE	COC(=O)N(C)C1=C(N)N=C(N=C1N)C1=NN(CC2=C(F)C=CC=C2)C2=C1C=CC=N2

182	DB11901	Apalutamide	0.227026	TRUE	CNC(=O)C1=CC=C(C=C1F)N1C(=S)N(C(=O)C11CCC1)C1=CC(=C(N=C1)C#N)C(F)(F)F
183	DB09009	Articaine	0.221224	TRUE	CCCNC(C)C(O)=NC1=C(SC=C1C)C(=O)OC
184	DB02546	Vorinostat	0.220316	TRUE	ONC(=O)CCCCCCC(=O)NC1=CC=CC=C1
185	DB00987	Cytarabine	0.214746	TRUE	NC1=NC(=O)N(C=C1)[C@@H]1O[C@H](CO)[C@@H](O)[C@@H]1
186	DB00238	Nevirapine	0.211619	TRUE	CC1=C2NC(=O)C3=C(N=CC=C3)N(C3CC3)C2=NC=C1
187	DB01065	Melatonin	0.210605	TRUE	COC1=CC=C2NC=C(CCNC(C)=O)C2=C1
188	DB08882	Linagliptin	0.210477	TRUE	[H][C@@]1(N)CCCN(C1)C1=NC2=C(N1CC#CC)C(=O)N(CC1=NC3=CC=CC=C3C(C)=N1)C(=O)N2C
189	DB01202	Levetiracetam	0.208106	TRUE	CC[C@H](N1CCCC1=O)C(N)=O
190	DB00740	Riluzole	0.207843	TRUE	NC1=NC2=C(S1)C=C(OC(F)(F)F)C=C2
191	DB01261	Sitagliptin	0.206751	TRUE	N[C@@H](CC(=O)N1CCN2C(C1)=NN=C2C(F)(F)F)CC1=CC(F)=C(F)C=C1F
192	DB00575	Clonidine	0.206347	TRUE	ClC1=CC=CC(Cl)=C1NC1=NCCN1
193	DB00469	Tenoxicam	0.199837	TRUE	CN1C(C(=O)NC2=CC=CC=N2)=C(O)C2=C(C=CS2)S1(=O)=O
194	DB01162	Terazosin	0.198153	TRUE	COC1=C(OC)C=C2C(N)=NC(=NC2=C1)N1CCN(CC1)C(=O)C1CCCO1
195	DB01595	Nitrazepam	0.192314	TRUE	[O-][N+](=O)C1=CC2=C(NC(=O)CN=C2C2=CC=CC=C2)C=C1
196	DB00730	Thiabendazole	0.182823	TRUE	N1C2=CC=CC=C2N=C1C1=CSC=N1
197	DB04824	Phenolphthalein	0.182337	TRUE	OC1=CC=C(C=C1)C1(OC(=O)C2=CC=CC=C12)C1=CC=C(O)C=C1
198	DB11221	Dioxybenzone	0.180699	TRUE	COC1=CC(O)=C(C=C1)C(=O)C1=CC=CC=C1O
199	DB01188	Ciclopirox	0.179486	TRUE	CC1=CC(=O)N(O)C(=C1)C1CCCCC1
200	DB00883	Isosorbide dinitrate	0.178845	TRUE	[H][C@]12OC[C@H](O[N+]([O-])=O)[C@@]1([H])OC[C@H]2O[N+]([O-])=O
201	DB00331	Metformin	0.173193	TRUE	CN(C)C(=N)NC(N)=N
202	DB06729	Sulfaphenazole	0.173156	TRUE	NC1=CC=C(C=C1)S(=O)(=O)NC1=CC=NN1C1=CC=CC=C1
203	DB06268	Sitaxentan	0.171189	TRUE	CC1=NOC(NS(=O)(=O)C2=C(SC=C2)C(=O)CC2=CC3=C(OCO3)C=C2C)=C1Cl
204	DB00920	Ketotifen	0.169119	TRUE	CN1CCC(CC1)=C1C2=C(SC=C2)C(=O)CC2=CC=CC=C12
205	DB01268	Sunitinib	0.167044	TRUE	CCN(CC)CCNC(=O)C1=C(C)NC(\C=C2/C(=O)NC3=C2C=C(F)C=C3)=C1C
206	DB00915	Amantadine	0.166891	TRUE	NC12CC3CC(CC(C3)C1)C2
207	DB00128	Aspartic acid	0.163596	TRUE	N[C@@H](CC(O)=O)C(O)=O
208	DB00808	Indapamide	0.157879	TRUE	CC1CC2=CC=CC=C2N1NC(=O)C1=CC(=C(Cl)C=C1)S(N)(=O)=O
209	DB00358	Mefloquine	0.157699	TRUE	OC(C1CCCCN1)C1=CC(=NC2=C1C=CC=C2C(F)(F)F)C(F)(F)F
210	DB00261	Anagrelide	0.153479	TRUE	ClC1=CC=C2N=C3NC(=O)CN3CC2=C1Cl
211	DB05381	Histamine	0.151711	TRUE	NCCC1=CNC=N1
212	DB14212	Methylparaben	0.145667	TRUE	COC(=O)C1=CC=C(O)C=C1

213	DB01428	Oxybenzone	0.145642	TRUE	COC1=CC(O)=C(C=C1)C(=O)C1=CC=CC=C1
214	DB00328	Indometacin	0.144258	TRUE	COC1=CC2=C(C=C1)N(C(=O)C1=CC=C(Cl)C=C1)C(C)=C2CC(O)=O
215	DB00589	Lisuride	0.143884	TRUE	[H][C@@]12CC3=CNC4=CC=CC(=C34)C1=C[C@@H](CN2C)NC(=O)N(CC)CC
216	DB00758	Clopidogrel	0.143045	TRUE	[H][C@@](N1CCC2=C(C1)C=CS2)(C(=O)OC)C1=CC=CC=C1Cl
217	DB00703	Methazolamide	0.139892	TRUE	CN1N=C(SC1=NC(C)=O)S(N)(=O)=O
218	DB01353	Butobarbital	0.136221	TRUE	CCCCC1(CC)C(=O)NC(=O)NC1=O
219	DB00693	Fluorescein	0.135618	TRUE	OC1=CC=C2C(OC3=CC(O)=CC=C3C22OC(=O)C3=C2C=CC=C3)=C1
220	DB00465	Ketorolac	0.133132	TRUE	OC(=O)C1CCN2C1=CC=C2C(=O)C1=CC=CC=C1
221	DB00437	Allopurinol	0.131456	TRUE	O=C1N=CN=C2NNC=C12
222	DB00236	Pipobroman	0.122589	TRUE	BrCCC(=O)N1CCN(CC1)C(=O)CCBr
223	DB01426	Ajmaline	0.120893	TRUE	CC[C@H]1[C@@H]2C[C@H]3[C@@H]4N(C)C5=CC=CC=C5[C@]44C[C@@H](C2[C@H]4O)N3[C@@H]1O
224	DB11989	Benznidazole	0.120474	TRUE	OC(CN1C=CN=C1N(=O)=O)=NCC1=CC=CC=C1
225	DB08905	Formestane	0.120293	TRUE	[H][C@@]12CCC(=O)[C@@]1(C)CC[C@@]1([H])[C@@]2([H])CCC2=C(O)C(=O)CC[C@]12C
226	DB00747	Scopolamine	0.119647	TRUE	CN1[C@H]2C[C@@H](C[C@@H]1[C@H]1O[C@@H]21)OC(=O)[C@H](CO)C1=CC=CC=C1
227	DB00226	Guanadrel	0.11889	TRUE	NC(N)=NCC1COC2(CCCCC2)O1
228	DB00338	Omeprazole	0.117756	TRUE	COC1=CC2=C(C=C1)N=C(N2)S(=O)CC1=NC=C(C)C(OC)=C1C
229	DB00736	Esomeprazole	0.117756	TRUE	COC1=CC2=C(NC(=N2)[S@@](=O)CC2=NC=C(C)C(OC)=C2C)C=C1
230	DB11967	Binimetinib	0.117167	TRUE	CN1C=NC2=C(F)C(NC3=CC=C(Br)C=C3F)=C(C=C12)C(=O)NOCCO
231	DB00194	Vidarabine	0.11686	TRUE	NC1=NC=NC2=C1N=CN2[C@@H]1O[C@H](CO)[C@@H](O)[C@@H]1O
232	DB00640	Adenosine	0.11686	TRUE	NC1=C2N=CN([C@@H]3O[C@H](CO)[C@@H](O)[C@H]3O)C2=NC=N1
233	DB13221	Apronalide	0.116311	TRUE	CC(C)C(CC=C)C(=O)NC(N)=O
234	DB11738	Rilmenidine	0.115686	TRUE	C1CC1C(NC1=NCCO1)C1CC1
235	DB00359	Sulfadiazine	0.115208	TRUE	NC1=CC=C(C=C1)S(=O)(=O)NC1=NC=CC=N1
236	DB00600	Monobenzone	0.114168	TRUE	OC1=CC=C(OCC2=CC=CC=C2)C=C1
237	DB08875	Cabozantinib	0.114167	TRUE	COC1=CC2=C(C=C1OC)C(OC1=CC=C(NC(=O)C3(CC3)C(=O)NC3=CC=C(F)C=C3)C=C1)=CC=N2
238	DB04743	Nimesulide	0.113606	TRUE	CS(=O)(=O)NC1=C(OC2=CC=CC=C2)C=C(C=C1)[N+]([O-])=O
239	DB00263	Sulfisoxazole	0.112683	TRUE	CC1=NOC(NS(=O)(=O)C2=CC=C(N)C=C2)=C1C
240	DB09543	Methyl salicylate	0.111671	TRUE	COC(=O)C1=CC=CC=C1O
241	DB00754	Ethotoin	0.11138	TRUE	CCN1C(=O)NC(C1=O)C1=CC=CC=C1
242	DB02925	Piretanide	0.110852	TRUE	NS(=O)(=O)C1=CC(=CC(N2CCCC2)=C1OC1=CC=CC=C1)C(O)=O

243	DB08883	Perampanel	0.110195	TRUE	O=C1N(C=C(C=C1C1=CC=CC=C1C#N)C1=NC=CC=C1)C1=CC=CC=
244	DB13278	Bucetin	0.109591	TRUE	CCOC1=CC=C(NC(=O)CC(C)O)C=C1
245	DB00794	Primidone	0.104656	TRUE	CCC1(C(=O)NCNC1=O)C1=CC=CC=C1
246	DB01331	Cefoxitin	0.104526	TRUE	[H][C@]12SCC(COC(N)=O)=C(N1C(=O)[C@]2(NC(=O)CC1=CC=CS1)OC)C(O)=O
247	DB09034	Suvorexant	0.103634	TRUE	[H][C@@]1(C)CCN(CCN1C(=O)C1=C(C=CC(C)=C1)N1N=CC=N1)C1 =NC2=C(O1)C=CC(Cl)=C2
248	DB00625	Efavirenz	0.101847	TRUE	FC(F)(F)[C@]1(OC(=O)NC2=C1C=C(Cl)C=C2)C#CC1CC1
249	DB06201	Rufinamide	0.0995199	TRUE	NC(=O)C1=CN(CC2=C(F)C=CC=C2F)N=N1
250	DB13235	Perboric acid	0.0977367	TRUE	OOB=O
251	DB00145	Glycine	0.0963813	TRUE	NCC(O)=O
252	DB11189	Magnesium glycinate	0.0963813	TRUE	[Mg++].NCC([O-])=O.NCC([O-])=O
253	DB11200	Aluminum zirconium octachlorohydrex gly	0.0963813	TRUE	O.O.[Al+3].[Cl-].[Zr+4].NCC([O-])=O
254	DB11210	Ferrous bisglycinate	0.0963813	TRUE	[Fe++].NCC([O-])=O.NCC([O-])=O
255	DB11699	Tropisetron	0.0935824	TRUE	[H][C@]12CC[C@]([H])(C[C@@]([H])(C1)OC(=O)C1=CNC3=CC=CC =C13)N2C
256	DB00339	Pyrazinamide	0.0934215	TRUE	NC(=O)C1=NC=CN=C1
257	DB00211	Midodrine	0.0930224	TRUE	COC1=CC(C(O)CNC(=O)CN)=C(OC)C=C1
258	DB09060	Avibactam	0.0925319	TRUE	[H]OS(=O)(=O)ON1C(=O)N2C([H])([H])[C@@]1([H])C([H])([H])C([H])([H])[C@@]2([H])C(=O)N([H])[H]
259	DB01544	Flunitrazepam	0.0914111	TRUE	CN1C2=C(C=C(C=C2)[N+]([O-])=O)C(=NCC1=O)C1=CC=CC=C1F
260	DB00271	Diatrizoate	0.0913417	TRUE	CC(=O)NC1=C(I)C(C(O)=O)=C(I)C(NC(C)=O)=C1I
261	DB00811	Ribavirin	0.0895423	TRUE	NC(=O)C1=NN(C=N1)[C@@H]1O[C@H](CO)[C@@H](O)[C@H]1O
262	DB01609	Deferasirox	0.0889495	TRUE	OC(=O)C1=CC=C(C=C1)N1N=C(N=C1C1=CC=CC=C1O)C1=CC=CC= C1O
263	DB01063	Acetophenazine	0.0888546	TRUE	CC(=O)C1=CC=C2SC3=C(C=CC=C3)N(CCCN3CCN(CCO)CC3)C2=C
264	DB05245	Silver sulfadiazine	0.0886943	TRUE	[Ag+].NC1=CC=C(C=C1)S(=O)(=O)[N-]C1=NC=CC=N1
265	DB00305	Mitomycin	0.0874806	TRUE	CO[C@]12[C@H]3N[C@H]3CN1C1=C([C@H]2COC(N)=O)C(=O)C(N)=C(C)C1=O
266	DB00951	Isoniazid	0.0872446	TRUE	NNC(=O)C1=CC=NC=C1
267	DB00402	Eszopiclone	0.0868553	TRUE	CN1CCN(CC1)C(=O)O[C@@H]1N(C(=O)C2=NC=CN=C12)C1=NC=C (Cl)C=C1
268	DB01198	Zopiclone	0.0868553	TRUE	CN1CCN(CC1)C(=O)OC1N(C(=O)C2=NC=CN=C12)C1=NC=C(Cl)C=
269	DB05541	Brivaracetam	0.0856979	TRUE	CCC[C@H]1CN([C@@H](CC)C(N)=O)C(=O)C1
270	DB01041	Thalidomide	0.0845614	TRUE	O=C1N(C2CCC(=O)NC2=O)C(=O)C2=CC=CC=C12
271	DB00155	L-Citrulline	0.0833195	TRUE	N[C@@H](CCCNC(N)=O)C(O)=O

272	DB14763	Cycloguanil	0.0833136	TRUE	CC1(C)N=C(N)N=C(N)N1C1=CC=C(Cl)C=C1
273	DB00680	Moricizine	0.0830163	TRUE	CCOC(=O)NC1=CC2=C(SC3=CC=CC=C3N2C(=O)CCN2CCOCC2)C=
274	DB01250	Olsalazine	0.0829222	TRUE	OC(=O)C1=CC(=CC=C1O)\N=N\C1=CC=C(O)C(=C1)C(O)=O
275	DB11346	Rubidium	0.0815577	TRUE	[Rb]
276	DB04571	Trioxsalen	0.0810232	TRUE	CC1=CC2=CC3=C(OC(=O)C=C3C)C(C)=C2O1
277	DB00123	L-Lysine	0.0804925	TRUE	NCCCC[C@H](N)C(O)=O
278	DB13146	Fluciclovine (18F)	0.0795394	TRUE	N[C@]1(C[C@H]([18F])C1)C(O)=O
279	DB06766	Alcaftadine	0.0783772	TRUE	CN1CCC(CC1)=C1C2=NC=C(C=O)N2CCC2=CC=CC=C12
280	DB04272	Citric acid	0.0781864	TRUE	OC(=O)CC(O)(CC(O)=O)C(O)=O
281	DB06784	Gallium citrate Ga 67	0.0781864	TRUE	[67Ga+3].OC(CC([O-])=O)(CC([O-])=O)C([O-])=O
282	DB09125	Potassium Citrate	0.0781864	TRUE	[K+].[K+].[K+].OC(CC([O-])=O)(CC([O-])=O)C([O-])=O
283	DB09154	Sodium citrate	0.0781864	TRUE	[Na+].[Na+].[Na+].OC(CC([O-])=O)(CC([O-])=O)C([O-])=O
284	DB14507	Lithium citrate	0.0781864	TRUE	[Li+].[Li+].[Li+].OC(CC([O-])=O)(CC([O-])=O)C([O-])=O
285	DB06713	Norelgestromin	0.0781516	TRUE	[H][C@@]12CC[C@@](O)(C#C)[C@@]1(CC)CC[C@]1([H])[C@@]3([H])CCC(C=C3CC[C@@]21[H])=NO
286	DB00347	Trimethadione	0.078127	TRUE	CN1C(=O)OC(C)(C)C1=O
287	DB11115	Ensulizole	0.0771652	TRUE	OS(=O)(=O)C1=CC2=C(C=C1)N=C(N2)C1=CC=CC=C1
288	DB01333	Cefradine	0.0769813	TRUE	[H][C@]12SCC(C)=C(N1C(=O)[C@H]2NC(=O)[C@H](N)C1=CCC=CC1)C(O)=O
289	DB06711	Naphazoline	0.0769542	TRUE	C(C1=NCCN1)C1=CC=CC2=CC=CC=C12
290	DB11268	Protocatechualdehyde	0.0758732	TRUE	OC1=CC=C(C=O)C=C1O
291	DB01112	Cefuroxime	0.0754888	TRUE	[H][C@]12SCC(COC(N)=O)=C(N1C(=O)[C@H]2NC(=O)C(=N/OC)\C1=CC=CO1)C(O)=O
292	DB00217	Bethanidine	0.074771	TRUE	CN\C(NCC1=CC=CC=C1)=N/C
293	DB00480	Lenalidomide	0.0746258	TRUE	NC1=CC=CC2=C1CN(C1CCC(=O)NC1=O)C2=O
294	DB08896	Regorafenib	0.0732597	TRUE	CNC(=O)C1=CC(OC2=CC(F)=C(NC(=O)NC3=CC=C(Cl)C(=C3)C(F)(F)F)C=C2)=CC=N1
295	DB00165	Pyridoxine	0.0731211	TRUE	CC1=C(O)C(CO)=C(CO)C=N1
296	DB13222	Tilbroquinol	0.0730644	TRUE	CC1=C2C=CC=NC2=C(O)C(Br)=C1
297	DB00784	Mefenamic acid	0.0728386	TRUE	CC1=C(C)C(NC2=CC=CC=C2C(O)=O)=CC=C1
298	DB11274	Dihydro-alpha-ergocryptine	0.0725382	TRUE	[H][C@@]12CCCN1C(=O)[C@H](CC(C)C)N1C(=O)[C@](NC(=O)[C@H]3CN(C)[C@]4([H])CC5=CNC6=CC=CC(=C56)[C@@]4([H])C3)(O[C@@]21O)C(C)C
299	DB11275	Epicriptine	0.0725382	TRUE	[H][C@@]12CCCN1C(=O)[C@]([H])([C@H](C)CC)N1C(=O)[C@](NC(=O)[C@H]3CN(C)[C@]4([H])CC5=CNC6=CC=CC(=C56)[C@@]4([H])C3)(O[C@@]21O)C(C)C
300	DB01129	Rabeprazole	0.0718749	TRUE	COCCCOC1=C(C)C(CS(=O)C2=NC3=CC=CC=C3N2)=NC=C1

301	DB00508	Triflupromazine	0.0718005	TRUE	CN(C)CCCN1C2=CC=CC=C2SC2=C1C=C(C=C2)C(F)(F)F
302	DB00891	Sulfapyridine	0.0711981	TRUE	NC1=CC=C(C=C1)S(=O)(=O)NC1=CC=CC=N1
303	DB09348	Propiolactone	0.0708797	TRUE	O=C1CCO1
304	DB00536	Guanidine	0.0706807	TRUE	NC(N)=N
305	DB14189	Ethylenediamine	0.0697482	TRUE	NCCN
306	DB01243	Chloroxine	0.0696971	TRUE	OC1=C(Cl)C=C(Cl)C2=C1N=CC=C2
307	DB04864	Huperzine A	0.0695212	TRUE	[H][C@@]12CC3=C(C=CC(=O)N3)[C@@](N)(CC(C)=C1)\C2=C\C
308	DB00571	Propranolol	0.0688609	TRUE	CC(C)NCC(O)COC1=CC=CC2=C1C=CC=C2
309	DB01419	Antrafenine	0.0687457	TRUE	FC(F)(F)C1=CC(=CC=C1)N1CCN(CCOC(=O)C2=CC=CC=C2NC2=C3C=CC(=CC3=NC=C2)C(F)(F)F)CC1
310	DB00209	Trospium	0.0686243	TRUE	[H][C@]12CC[C@]([H])(C[C@@H](C1)OC(=O)C(O)(C1=CC=CC=C1)C1=CC=CC=C1)[N+]21CCCC1
311	DB00996	Gabapentin	0.0676154	TRUE	NCC1(CC(O)=O)CCCCC1
312	DB11323	Glycol salicylate	0.0674483	TRUE	OCCOC(=O)C1=CC=CC=C1O
313	DB12328	Cantharidin	0.0655448	TRUE	[H][C@]12CC[C@]([H])(O1)[C@]1(C)C(=O)OC(=O)[C@]21C
314	DB00911	Tinidazole	0.0653416	TRUE	CCS(=O)(=O)CCN1C(C)=NC=C1[N+]([O-])=O
315	DB06147	Sulfathiazole	0.062849	TRUE	NC1=CC=C(C=C1)S(=O)(=O)NC1=NC=CS1
316	DB00423	Methocarbamol	0.0626494	TRUE	COC1=C(OCC(O)COC(N)=O)C=CC=C1
317	DB00156	L-Threonine	0.0623263	TRUE	C[C@@H](O)[C@H](N)C(O)=O

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Table S3. The docking score of the 30 compounds

No.	DRUGBANK_ID	GENERIC_NAME	S	No.	DRUGBANK_ID	GENERIC_NAME	S
1	DB05239	Cobimetinib	-6.9310613	70	DB00900	Didanosine	-5.0609403
2	DB14723	Larotrectinib	-6.8676357	71	DB04876	Vildagliptin	-5.0533996
3	DB00213	Pantoprazole	-6.7913752	72	DB00744	Zileuton	-5.0380626
4	DB00213	Pantoprazole	-6.7520752	73	DB00998	Frovatriptan	-5.0302234
5	DB00213	Pantoprazole	-6.6503758	74	DB04880	Enoximone	-5.0110369
6	DB04876	Vildagliptin	-6.4164033	75	DB09282	Molsidomine	-5.0015845
7	DB00213	Pantoprazole	-6.4119277	76	DB04880	Enoximone	-4.9902353
8	DB00213	Pantoprazole	-6.3987718	77	DB03585	Oxyphenbutazone	-4.9828973
9	DB00213	Pantoprazole	-6.3169456	78	DB00819	Acetazolamide	-4.9660068
10	DB00213	Pantoprazole	-6.2566361	79	DB04880	Enoximone	-4.9610066
11	DB00213	Pantoprazole	-6.2308168	80	DB00819	Acetazolamide	-4.9598055
12	DB04876	Vildagliptin	-6.1883755	81	DB00819	Acetazolamide	-4.9260912
13	DB05239	Cobimetinib	-6.1456776	82	DB00998	Frovatriptan	-4.9125171
14	DB00213	Pantoprazole	-6.1377616	83	DB00819	Acetazolamide	-4.9092851
15	DB00213	Pantoprazole	-6.0704384	84	DB04880	Enoximone	-4.8812084
16	DB00310	Chlorthalidone	-5.9882131	85	DB00310	Chlorthalidone	-4.8554726
17	DB09282	Molsidomine	-5.9811907	86	DB00900	Didanosine	-4.8495426
18	DB00507	Nitazoxanide	-5.9355636	87	DB00819	Acetazolamide	-4.8384676
19	DB00310	Chlorthalidone	-5.9206076	88	DB04880	Enoximone	-4.8022776
20	DB00315	Zolmitriptan	-5.9201198	89	DB00819	Acetazolamide	-4.7723927
21	DB04876	Vildagliptin	-5.9064178	90	DB00744	Zileuton	-4.7609982
22	DB00310	Chlorthalidone	-5.8500347	91	DB00900	Didanosine	-4.7413168
23	DB09282	Molsidomine	-5.8116651	92	DB09343	Tipiracil	-4.7008104
24	DB00507	Nitazoxanide	-5.80197	93	DB04880	Enoximone	-4.6996794
25	DB09282	Molsidomine	-5.7635555	94	DB00900	Didanosine	-4.6848683
26	DB00670	Pirenzepine	-5.7619653	95	DB00744	Zileuton	-4.6568017
27	DB00507	Nitazoxanide	-5.7578802	96	DB00744	Zileuton	-4.6483922
28	DB04876	Vildagliptin	-5.7227197	97	DB04876	Vildagliptin	-4.62394
29	DB00507	Nitazoxanide	-5.7087951	98	DB00900	Didanosine	-4.6178613
30	DB00315	Zolmitriptan	-5.7006006	99	DB11071	Phenyl salicylate	-4.60466
31	DB09282	Molsidomine	-5.6945457	100	DB00819	Acetazolamide	-4.6022539
32	DB04876	Vildagliptin	-5.6750097	101	DB00819	Acetazolamide	-4.5971136
33	DB00310	Chlorthalidone	-5.6692777	102	DB00744	Zileuton	-4.5873461
34	DB09282	Molsidomine	-5.649694	103	DB00900	Didanosine	-4.5755157
35	DB00507	Nitazoxanide	-5.6490493	104	DB09343	Tipiracil	-4.5649681
36	DB00315	Zolmitriptan	-5.6438961	105	DB00744	Zileuton	-4.5559154
37	DB00315	Zolmitriptan	-5.6402564	106	DB00900	Didanosine	-4.5550489
38	DB00315	Zolmitriptan	-5.57125	107	DB00900	Didanosine	-4.5194349
39	DB00315	Zolmitriptan	-5.5673938	108	DB09343	Tipiracil	-4.5189333
40	DB00507	Nitazoxanide	-5.5527329	109	DB00744	Zileuton	-4.4812813
41	DB06803	Niclosamide	-5.5374866	110	DB09343	Tipiracil	-4.4812746
42	DB09282	Molsidomine	-5.4974127	111	DB00900	Didanosine	-4.4752998
43	DB00315	Zolmitriptan	-5.4557352	112	DB00824	Enprofylline	-4.4344225
44	DB00310	Chlorthalidone	-5.454011	113	DB00744	Zileuton	-4.3904948
45	DB00998	Frovatriptan	-5.4325595	114	DB00744	Zileuton	-4.3821363
46	DB09282	Molsidomine	-5.4288454	115	DB00744	Zileuton	-4.3412452
47	DB00310	Chlorthalidone	-5.4204068	116	DB00824	Enprofylline	-4.3327179
48	DB00507	Nitazoxanide	-5.4191132	117	DB11071	Phenyl salicylate	-4.3224015
49	DB09282	Molsidomine	-5.4189315	118	DB04876	Vildagliptin	-4.3051376
50	DB00310	Chlorthalidone	-5.4050231	119	DB00824	Enprofylline	-4.3013377
51	DB09282	Molsidomine	-5.3831968	120	DB00824	Enprofylline	-4.281477
52	DB06803	Niclosamide	-5.3375182	121	DB00819	Acetazolamide	-4.2222891
53	DB04876	Vildagliptin	-5.3273134	122	DB00819	Acetazolamide	-4.1852341
54	DB00315	Zolmitriptan	-5.3225026	123	DB00824	Enprofylline	-4.1829643
55	DB00998	Frovatriptan	-5.3047891	124	DB00824	Enprofylline	-4.1712618
56	DB00315	Zolmitriptan	-5.2804046	125	DB00824	Enprofylline	-4.1663761
57	DB00998	Frovatriptan	-5.259182	126	DB01392	Yohimbine	-4.0634894
58	DB14723	Larotrectinib	-5.2465992	127	DB00824	Enprofylline	-4.0518947
59	DB00998	Frovatriptan	-5.2332926	128	DB09343	Tipiracil	-4.0467296

60	DB04880	Enoximone	-5.2275014	129	DB00824	Enprofylline	-4.0120158
61	DB00900	Didanosine	-5.2228055	130	DB01392	Yohimbine	-3.9413302
62	DB00315	Zolmitriptan	-5.2075071	131	DB00824	Enprofylline	-3.8031516
63	DB00310	Chlorthalidone	-5.1740584	132	DB01392	Yohimbine	-3.3361256
64	DB04880	Enoximone	-5.1681366	133	DB00670	Pirenzepine	25.356607
65	DB00670	Pirenzepine	-5.1599541	134	DB03585	Oxyphenbutazone	26.837795
66	DB04880	Enoximone	-5.130342	135	DB12332	Rucaparib	37.265541
67	DB00507	Nitazoxanide	-5.1014695	136	DB00457	Prazosin	82.314819
68	DB00310	Chlorthalidone	-5.0798001	137	DB14723	Larotrectinib	123.47587
69	DB04880	Enoximone	-5.0775814	138	DB00670	Pirenzepine	125.87755

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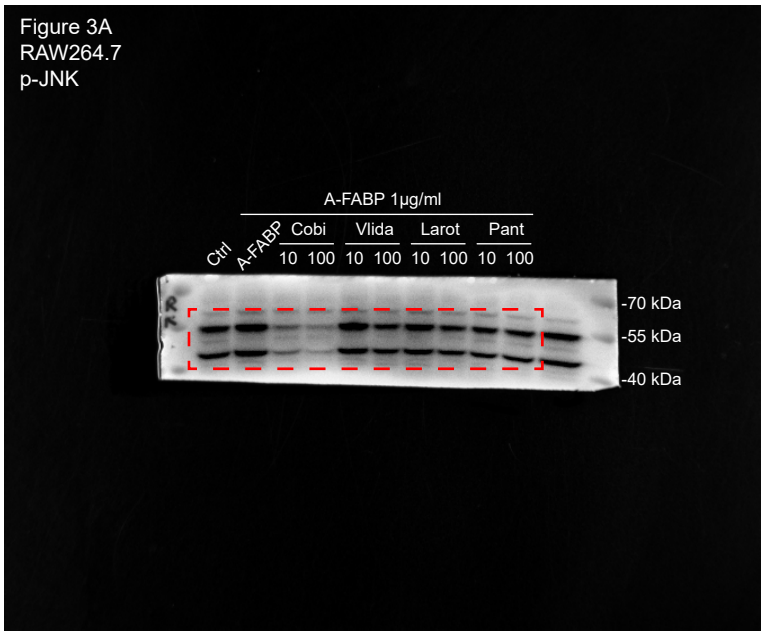
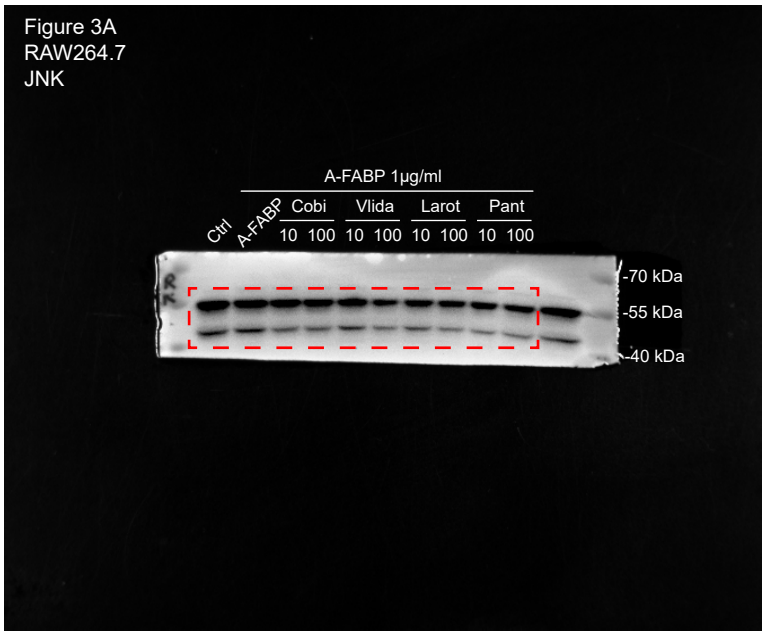
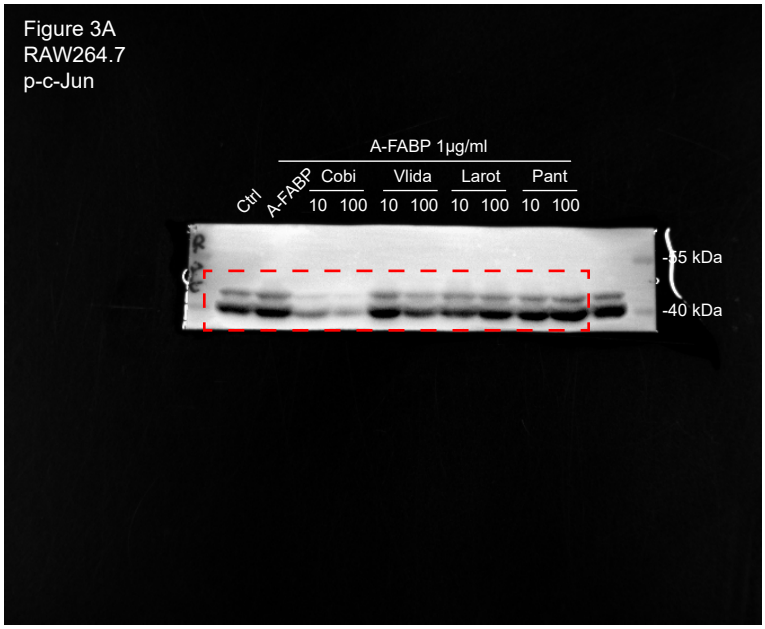
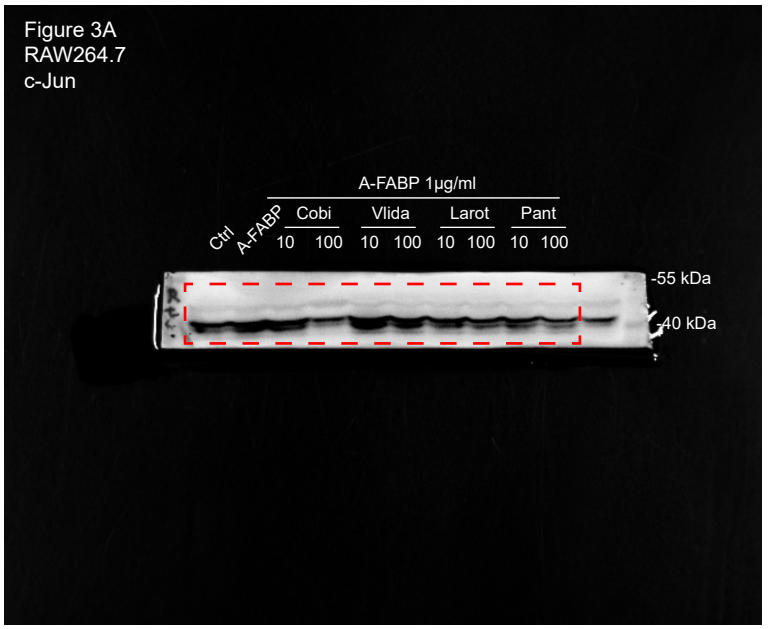
Figure 3A-The uncropped and unprocessed image of the full blot









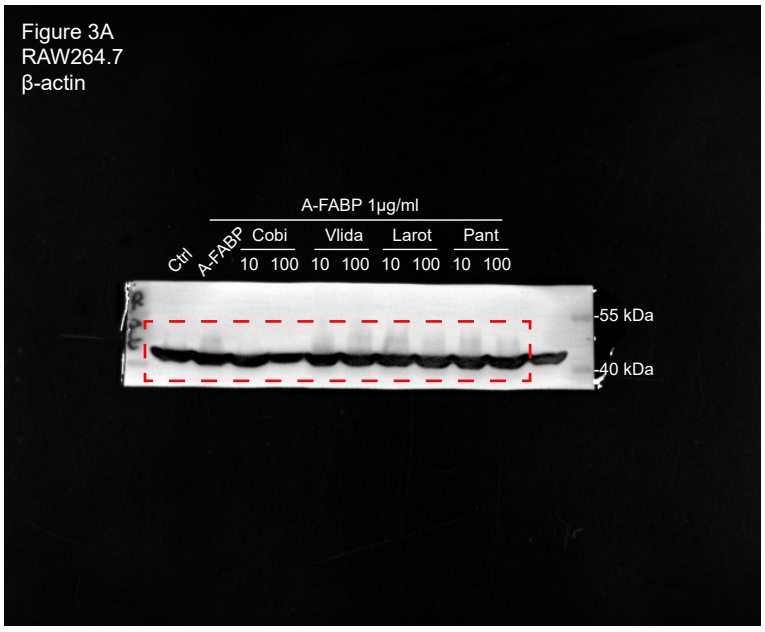


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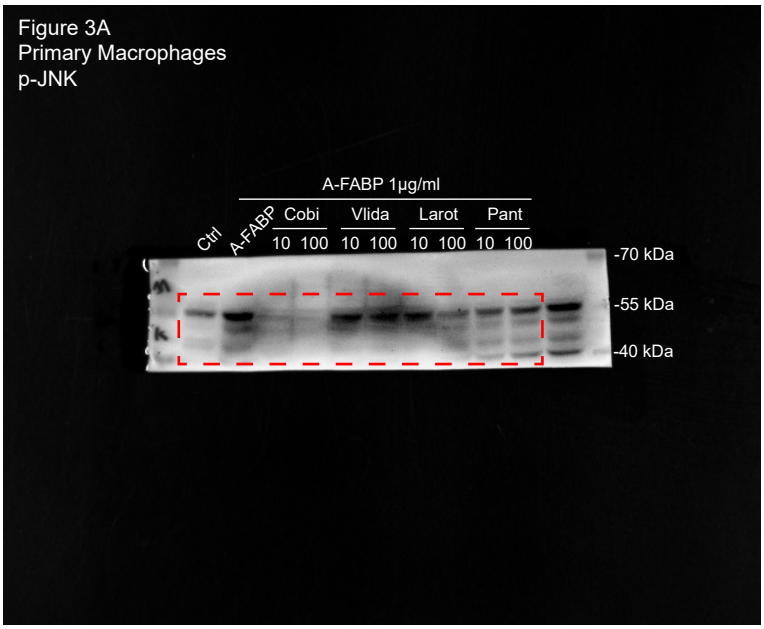
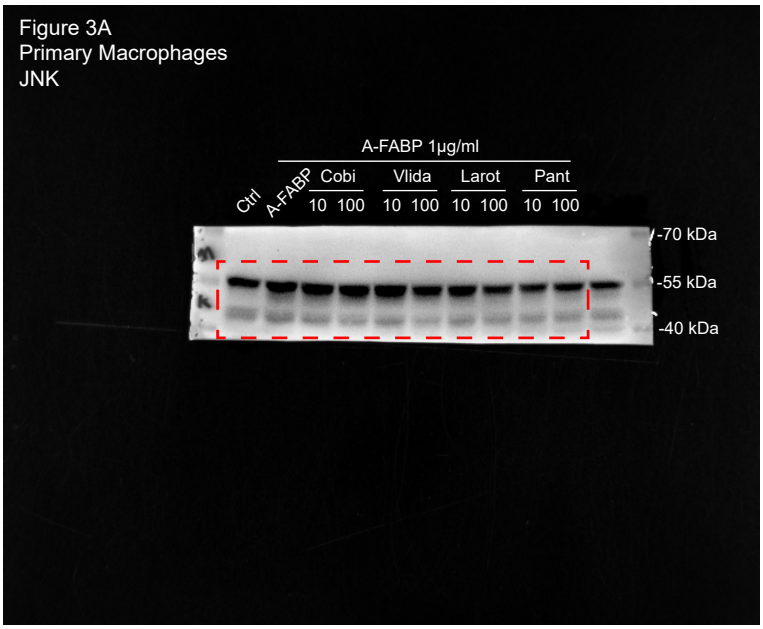
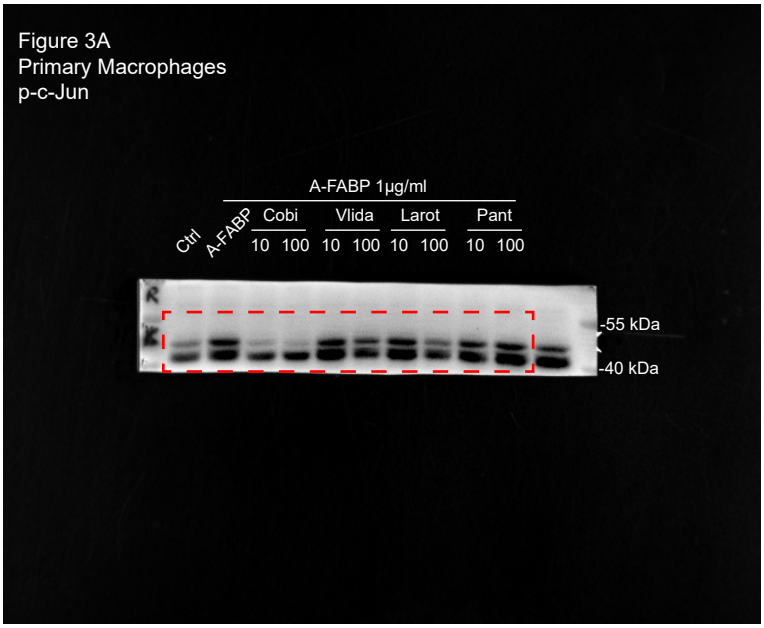
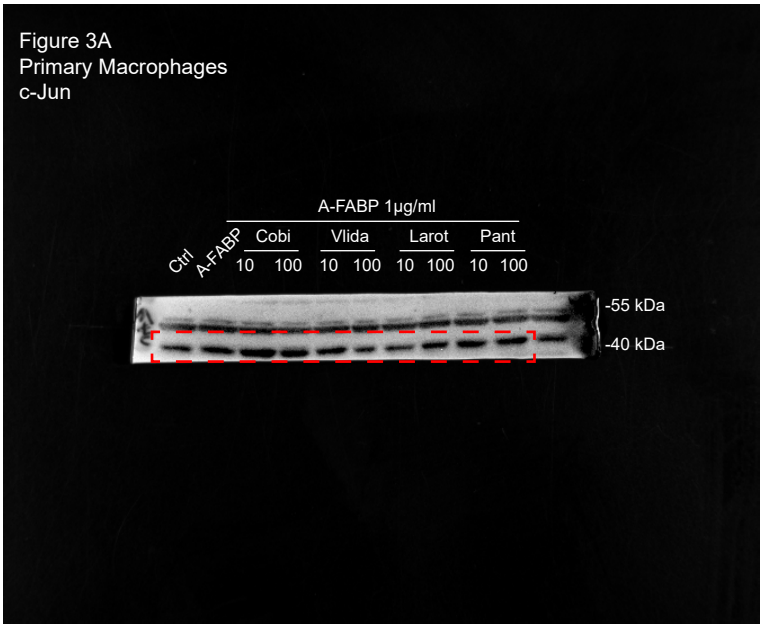
Figure 3A-The uncropped and unprocessed image of the full blot









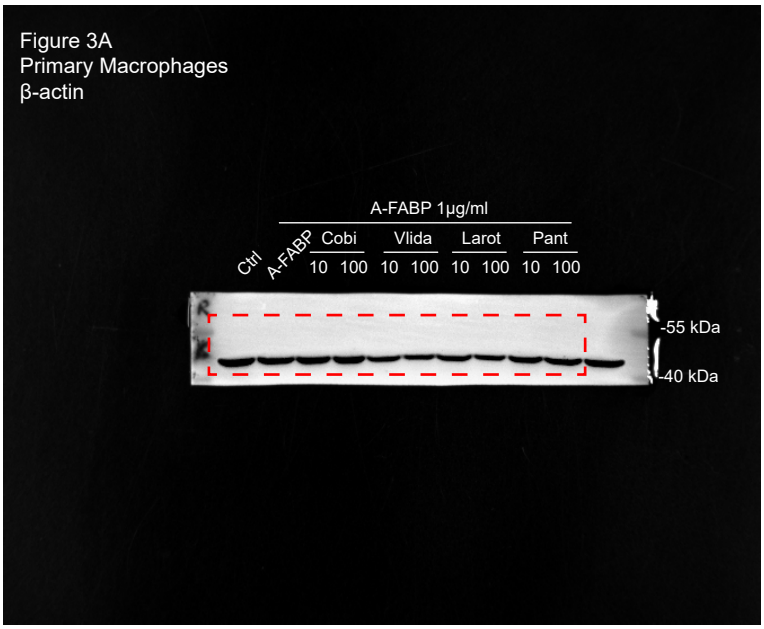


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Figure 4A-The uncropped and unprocessed image of the full blot