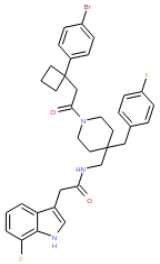
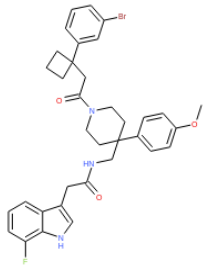
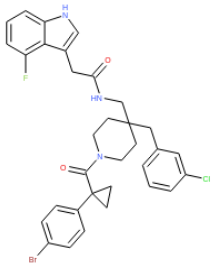
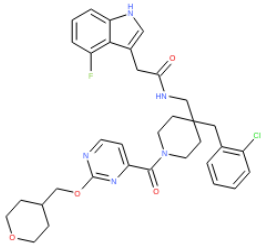
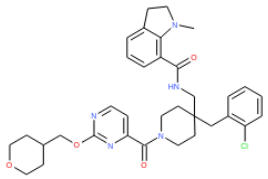
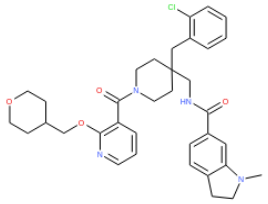
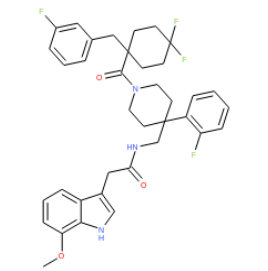
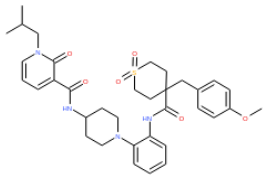
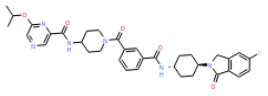
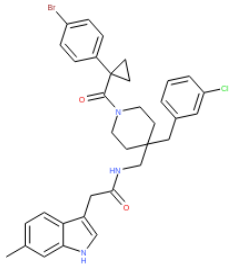
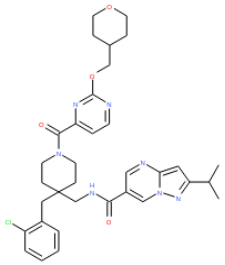
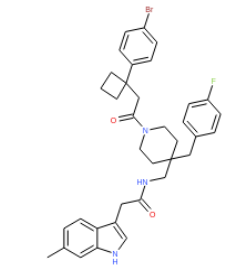
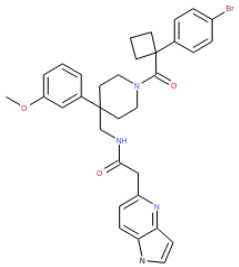
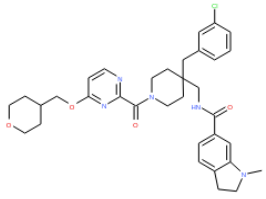
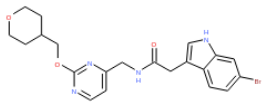
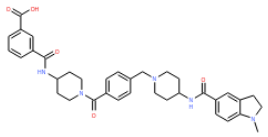
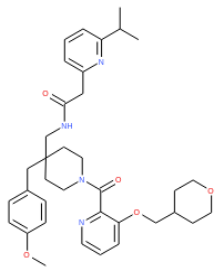
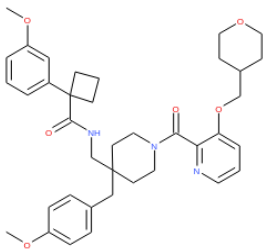
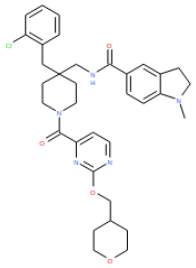
Electronic Supplementary Material (ESI) for Chemical Communications.

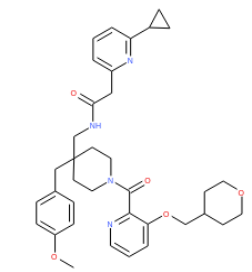
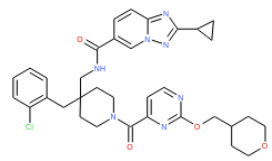
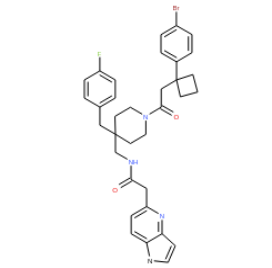
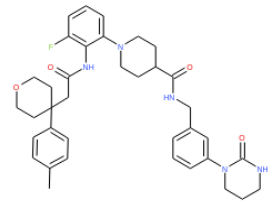
Compound	Image	TR-FRET (Keap1/Nrf2) (%)	TR-FRET (Bcl6/F1325) (%)	Max similarity to 1st assay actives	Max similarity to DB actives	SMILES	cluster ID	DNN-hybrid	DNN-hybrid-PI	RF-PA	RF-DB-PI	RF-DB-TI	LF dG
1		36.1	NI	0.44	0.19	Fc1ccc(CC2(CNC(=O)Cc3c[nH]c4c(F)cccc34)CCN(CC2)C(=O)CC5(CCC5)c6ccc(Br)cc6)cc1	28	45	NS	4	NS	NS	-13.03
2		32.9	NI	0.43	0.20	COc1ccc(cc1)C2(CNC(=O)Cc3c[nH]c4c(F)cccc34)CCN(CC2)C(=O)CC5(CCC5)c6cccc(Br)c6	28	3	11	11	36	NS	-12.32
3		32.1	NI	0.50	0.17	Fc1cccc2[nH]cc(CC(=O)NCC3(Cc4cccc(Cl)c4)CCN(CC3)C(=O)C5(CC5)c6ccc(Br)cc6)c12	4	NS	NS	9	NS	NS	-12.55

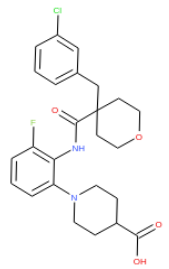
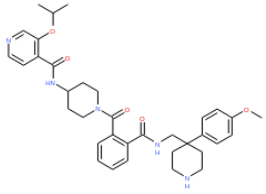
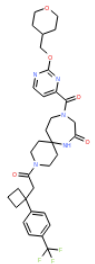
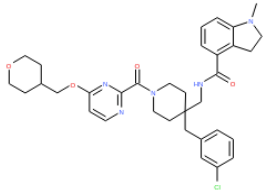
4		30.4	NI	0.36	0.12	Fc1cccc2[nH]cc(CC(=O)NCC3(Cc4ccccc4Cl)CCN(CC3)C(=O)c5ccnc(OCC6CCOCC6)n5)c12	17	2	3	7	NS	NS	-12.44
5		28.2	NI	0.29	0.12	CN1CCc2cccc(C(=O)NCC3(Cc4ccccc4Cl)CCN(CC3)C(=O)c5ccnc(OCC6CCOCC6)n5)c12	17	11	5	100	NS	NS	-12.31
6		28.1	NI	0.23	0.13	CN1CCc2ccc(cc12)C(=O)NCC3(Cc4ccccc4Cl)CCN(CC3)C(=O)c5cccnc5OCC6CCOCC6	20	39	27	NS	NS	NS	NA
7		28.0	NI	0.40	0.15	COc1cccc2c(CC(=O)NCC3(CCN(CC3)C(=O)C4(Cc5ccccc(F)c5)CCC(F)(F)CC4)c6ccccc6F)c[nH]c12	28	72	53	12	82	NS	NA

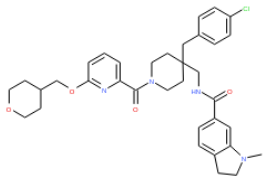
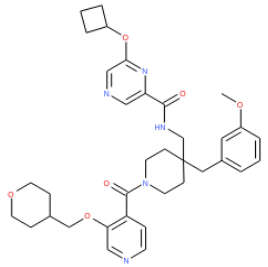
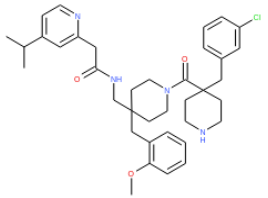
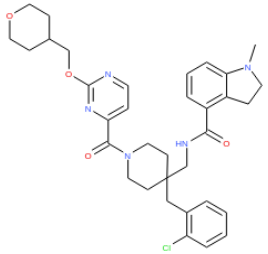
8		26.7	NI	0.50	0.19	COc1ccc(CC2(CCS(=O)(=O)CC2)C(=O)Nc3ccccc3N4CCC(CC4)NC(=O)C5=CC=CN(CC(C)C)C5=O)cc1	12	52	56	46	12	77	NA
9		26.6	NI	0.46	0.13	CC(C)Oc1cncc(n1)C(=O)NC2CCN(CC2)C(=O)c3ccc(c3)C(=O)N[C@@H]4CC[C@H](CC4)N5Cc6cc(F)ccc6C5=O	25	76	52	NS	NS	NS	NA
10		25.5	NI	0.66	0.18	Cc1ccc2c(CC(=O)NCC3(Cc4cccc(Cl)c4)CCN(CC3)C(=O)C5(CC5)c6ccc(Br)cc6)c[nH]c2c1	4	82	NS	2	NS	NS	NA
11		22.6	NI	0.28	0.12	CC(C)c1cc2ncc(cn2n1)C(=O)NCC3(Cc4ccccc4Cl)CCN(CC3)C(=O)c5ccnc(OCC6CCOCC6)n5	17	8	4	47	NS	NS	NA

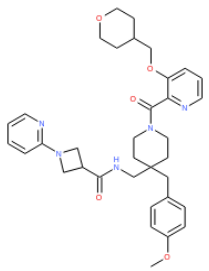
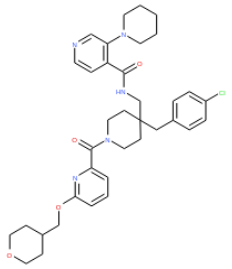
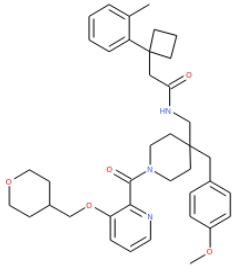
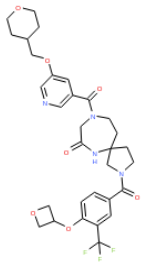
12		21.1	NI	0.56	0.17	Cc1ccc2c(CC(=O)NCC3(Cc4ccc(F)cc4)CCN(CC3)C(=O)CC5(CCC5)c6ccc(Br)cc6)c[nH]c2c1	4	41	NS	1	NS	NS	NA
13		20.0	NI	0.31	0.17	COc1cccc(c1)C2(CNC(=O)Cc3ccc4[nH]ccc4n3)CCN(CC2)C(=O)C5(CCC5)c6ccc(Br)cc6	16	15	47	NS	NS	NS	NA
14		20.0	NI	0.26	0.13	CN1CCc2ccc(cc12)C(=O)NCC3(Cc4cccc(Cl)c4)CCN(CC3)C(=O)c5nccc(OCC6CCOCC6)n5	20	35	42	NS	NS	NS	NA
15		19.7	NI	0.30	0.14	Brc1ccc2c(CC(=O)NCc3ccnc(OCC4CCOCC4)n3)c[nH]c2c1	19	NS	NS	8	NS	NS	NA

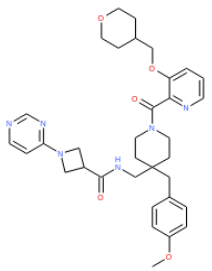
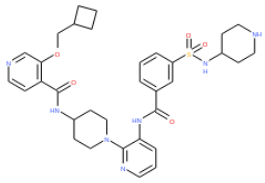
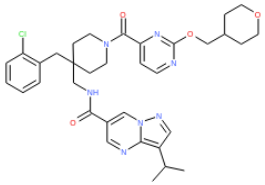
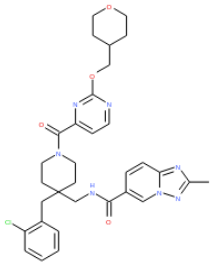
16		19.5	4.6	0.23	0.16	CN1CCc2cc(ccc12)C(=O)NC3CCN(Cc4ccc(cc4)C(=O)N5CCC(CC5)NC(=O)c6ccccc6)C(=O)O)CC3	13	NS	NS	NS	21	8	NA
17		19.4	5.8	0.25	0.17	COc1ccc(CC2(CNC(=O)Cc3cccc(n3)C(C)C)CCN(CC2)C(=O)c4ncccc4OCC5CCOCC5)cc1	11	NS	NS	NS	87	NS	NA
18		18.9	5.8	0.26	0.19	COc1ccc(CC2(CNC(=O)C3(CCC3)c4cccc(OC)c4)CCN(CC2)C(=O)c5ncccc5OCC6CCOCC6)cc1	11	NS	NS	NS	83	NS	NA
19		18.7	NI	0.29	0.13	CN1CCc2cc(ccc12)C(=O)NCC3(Cc4ccccc4Cl)CCN(CC3)C(=O)c5ccnc(OCC6CCOCC6)n5	17	10	13	80	NS	NS	NA

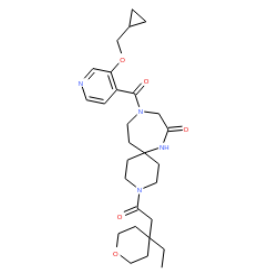
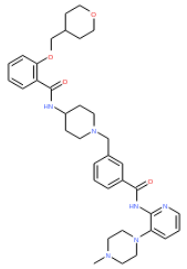
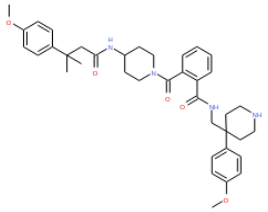
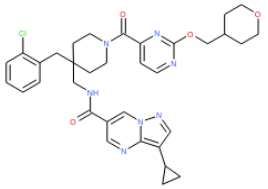
20		17.8	5.2	0.25	0.17	COc1ccc(CC2(CNC(=O)Cc3cccc(n3)C4CC4)CCN(CC2)C(=O)c5ncccc5OCC6CCOCC6)cc1	11	NS	NS	NS	84	NS	NA
21		17.8	NI	0.27	0.12	Clc1ccccc1CC2(CNC(=O)c3ccc4nc(nn4c3)C5CC5)CCN(CC2)C(=O)c6ccnc(OCC7CCOCC7)n6	17	53	NS	55	NS	NS	NA
22		17.8	NI	0.35	0.14	Fc1ccc(CC2(CNC(=O)Cc3ccc4[nH]ccc4n3)CCN(CC2)C(=O)CC5(CCC5)c6ccc(Br)cc6)cc1	16	73	NS	45	NS	NS	NA
23		17.7	11.3	0.39	0.16	Cc1ccc(cc1)C2(CC(=O)Nc3c(F)cccc3N4CCC(CC4)C(=O)NCc5cccc(c5)N6CCCNC6=O)CCOCC2	6	101	NS	66	NS	NS	NA

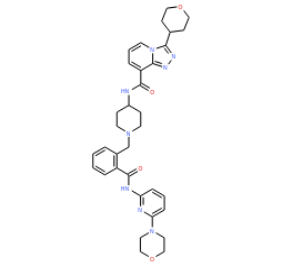
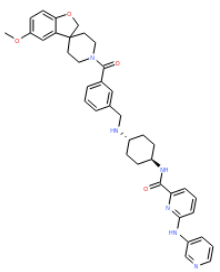
24		17.6	0.8	0.67	0.22	OC(=O)C1CCN(CC1)c2ccccc(F)c2NC(=O)C3(Cc4ccccc(Cl)c4)CCOCC3	6	81	NS	32	58	NS	NA
25		17.2	5.7	0.25	0.17	COc1ccc(cc1)C2(CNC(=O)c3ccccc3C(=O)N4CCC(CC4)NC(=O)c5ccncc5OC(C)C)CCNCC2	10	56	NS	NS	30	NS	NA
26		16.7	9.2	0.24	0.13	FC(F)(F)c1ccc(cc1)C2(CC(=O)N3CCC4(CC3)CCN(CC(=O)N4)C(=O)c5ccnc(OCC6CCOCC6)n5)CCC2	21	NS	NS	58	NS	NS	NA
27		16.6	NI	0.26	0.14	CN1CCc2c1cccc2C(=O)NCC3(Cc4cccc(Cl)c4)CCN(CC3)C(=O)c5nccc(OCC6CCOCC6)n5	20	33	41	NS	NS	NS	NA

28		16.4	NI	0.31	0.15	CN1CCc2ccc(cc12)C(=O)NCC3(Cc4ccc(Cl)cc4)CCN(CC3)C(=O)c5cccc(OCC6CCOCC6)n5	20	37	26	NS	NS	NS	NA
29		16.4	13.0	0.24	0.16	COc1cccc(CC2(CNC(=O)c3cncc(OC4CCC4)n3)CCN(CC2)C(=O)c5ccncc5OCC6CCOCC6)c1	26	91	NS	NS	NS	69	NA
30		16.3	1.3	0.40	0.15	COc1ccccc1CC2(CNC(=O)Cc3cc(ccn3)C(C)C)CCN(CC2)C(=O)C4(Cc5cccc(Cl)c5)CCNCC4	24	NS	NS	59	NS	NS	NA
31		16.2	3.0	0.28	0.13	CN1CCc2c1cccc2C(=O)NCC3(Cc4ccccc4Cl)CCN(CC3)C(=O)c5ccnc(OCC6CCOCC6)n5	17	7	8	NS	NS	NS	NA

32		16.1	10.2	0.26	0.18	COc1ccc(CC2(CNC(=O)C3CN(C3)c4ccccn4)CCN(CC2)C(=O)c5ncccc5OCC6CCOCC6)cc1	11	NS	NS	NS	39	NS	NA
33		16.0	NI	0.32	0.15	Clc1ccc(CC2(CNC(=O)c3ccncc3N4CCCCC4)CCN(CC2)C(=O)c5cccc(OCC6CCOCC6)n5)cc1	17	108	NS	NS	NS	NS	NA
34		15.9	8.7	0.26	0.17	COc1ccc(CC2(CNC(=O)CC3(CCC3)c4ccccc4C)CCN(CC2)C(=O)c5ncccc5OCC6CCOCC6)cc1	11	NS	NS	NS	68	NS	NA
35		15.9	2.4	0.19	0.13	FC(F)(F)c1cc(ccc1OC2COC2)C(=O)N3CCC4(CCN(CC(=O)N4)C(=O)c5cncc(OCC6CCOCC6)c5)C3	3	NS	NS	NS	NS	51	NA

36		15.6	NI	0.28	0.17	COc1ccc(CC2(CNC(=O)C3CN(C3)c4ccncn4)CCN(CC2)C(=O)c5ncccc5OCC6CCOCC6)cc1	11	NS	NS	NS	48	NS	NA
37		15.5	4.5	0.30	0.16	O=C(Nc1cccnc1N2CCC(CC2)NC(=O)c3ccncc3OCC4CCC4)c5cccc(c5)S(=O)(=O)NC6CCNCC6	23	66	NS	NS	32	75	NA
38		15.3	7.2	0.28	0.12	CC(C)c1cnn2cc(cnc12)C(=O)NCC3(Cc4ccccc4Cl)CCN(CC3)C(=O)c5ccnc(OCC6CCOCC6)n5	17	31	28	49	NS	NS	NA
39		15.3	0.8	0.27	0.11	Cc1nc2ccc(cn2n1)C(=O)NCC3(Cc4ccccc4Cl)CCN(CC3)C(=O)c5ccnc(OCC6CCOCC6)n5	17	47	25	NS	NS	NS	NA

40		15.2	3.9	0.16	0.13	CCC1(CC(=O)N2CCC3(CC2)CCN(CC(=O)N3)C(=O)c4ccncc4OCC5CC5)CCOCC1	27	NS	NS	NS	NS	57	NA
41		51.9	63.2	0.18	0.15	CN1CCN(CC1)c2cccnc2NC(=O)c3cccc(CN4CCC(CC4)NC(=O)c5ccccc5OCC6CCOCC6)c3	8	NS	NS	NS	NS	74	NA
42		19.1	23.5	0.25	0.20	COc1ccc(cc1)C(C)(C)CC(=O)NC2CCN(CC2)C(=O)c3ccccc3C(=O)NCC4(CCNCC4)c5ccc(OC)cc5	10	12	NS	NS	15	NS	NA
43		17.0	17.1	0.27	0.12	Clc1ccccc1CC2(CNC(=O)c3cnc4c(cnn4c3)C5CC5)CCN(CC2)C(=O)c6ccnc(OCC7CCOCC7)n6	17	51	NS	53	NS	NS	NA

44		15.9	23.7	0.39	0.11	O=C(NC1CCN(Cc2ccccc2C(=O)Nc3cccc(n3)N4CCOCC4)CC1)c5cccn6c(nnc56)C7CCOCC7	29	NS	NS	NS	NS	79	NA
45		15.6	33.2	0.25	0.19	COc1ccc2OCC3(CCN(CC3)C(=O)c4cccc(CN[C@@H]5CC[C@H](CC5)NC(=O)c6cccc(Nc7cccnc7)n6)c4)c2c1	15	87	NS	NS	NS	NS	NA