

Table S1. Statistical parameters of CoMFA and CoMSIA models based on non-covalent proteasome inhibitors

PLS	Q ²	r ²	SEE	F	ONC	CONTRIBUTIONS (%)				
						S	E	H	D	A
COMFA-S	0.234	0.883	0.230	24.165	5	100	-	-	-	-
COMFA-E	0.376	0.882	0.231	23.842	5	-	100	-	-	-
COMFA-SE	0.574	0.999	0.026	1084.404	10	47.1	52.9	-	-	-
COMSIA-SE	0.43	0.954	0.144	66.227	5	28.1	71.9	-	-	-
COMSIA-SH	0.136	0.604	0.388	14.510	2	30.6	-	69.4	-	-
COMSIA-SD	0.095	0.578	0.412	8.221	3	50.7	-	-	49.3	-
COMSIA-SA	0.529	0.915	0.190	45.843	4	37.5	-	-	-	62.5
COMSIA-EH	0.383	0.966	0.121	119.568	4	-	60.3	39.7	-	-
COMSIA-ED	0.156	0.825	0.281	15.100	5	-	80.7	-	19.3	-
COMSIA-EA	0.24	0.620	0.381	15.477	2	-	42.0	-	-	58.0
COMSIA-HD	0.09	0.384	0.484	5.932	2	-	-	44.2	55.8	-
COMSIA-HA	0.681	0.973	0.117	73.434	7	-	-	55.8	-	44.2
COMSIA-DA	0.302	0.712	0.400	4.027	8	-	-	-	30.6	69.4
COMSIA-SEH	0.366	0.984	0.087	157.972	6	14.4	53.8	31.8	-	-
COMSIA-SED	0.409	0.949	0.153	58.972	5	23.2	61.4	-	15.5	-
COMSIA-SEA	0.49	0.975	0.109	98.647	6	25.9	40.9	-	-	33.2
COMSIA-SHD	0.105	0.408	0.475	6.550	2	15.4	-	37.1	47.5	-
COMSIA-SHA	0.591	0.967	0.126	74.103	6	17.7	-	39.1	-	43.3
COMSIA-SDA	0.506	0.939	0.167	48.895	5	33.8	-	-	17.9	48.3
COMSIA-EHD	0.314	0.969	0.118	100.121	5	-	52.9	33.9	13.1	-
COMSIA-EHA	0.591	0.987	0.083	149.958	7	-	38.8	35.4	-	25.8
COMSIA-EDA	0.219	0.820	0.285	14.597	5	-	49.4	-	13.5	37.2
COMSIA-HDA	0.647	0.984	0.095	97.915	8	-	-	50.4	10.9	38.8
COMSIA-SEHD	0.285	0.982	0.094	134.530	6	12.2	48.4	27.5	11.8	-
COMSIA-SEHA	0.584	0.989	0.077	172.183	7	12.6	35.2	27.6	-	24.5
COMSIA-SEDA	0.474	0.974	0.112	94.143	6	23.3	36.8	-	8.9	31.0
COMSIA-SHDA	0.573	0.986	0.088	114.800	8	15.6	-	38.0	12.0	34.4
COMSIA-EHDA	0.566	0.986	0.085	142.024	7	-	35.7	31.9	8.5	23.9
COMSIA-SEHDA	0.558	0.988	0.080	159.753	7	11.5	32.3	25.0	8.1	23.1