In Silico Study of the Anti-MYC Potential of Lanostane-type Triterpenes

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SUPPORTING INFORMATION

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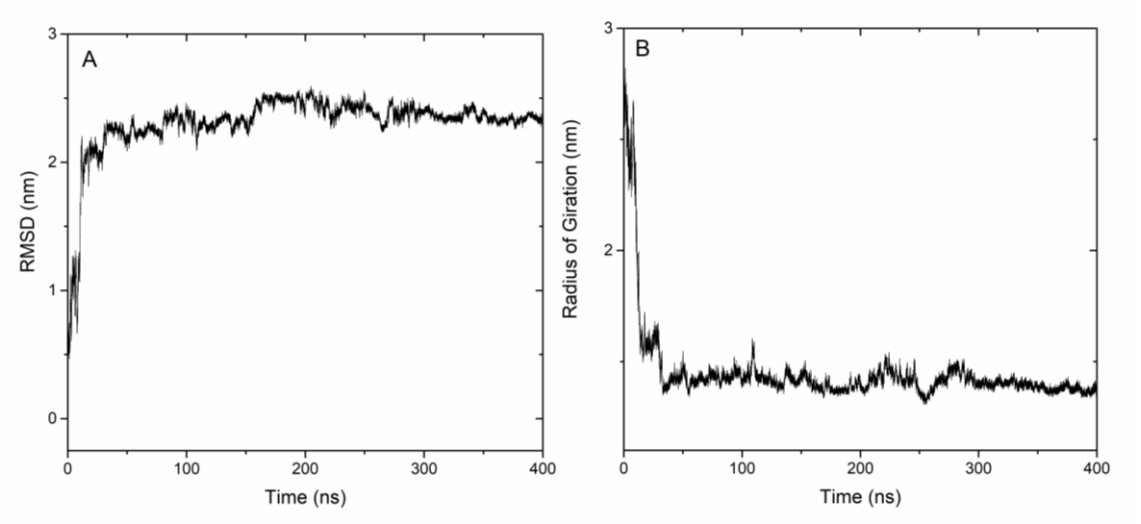


Figure S1. (A) RMSD plot for MYC protein. (B) graph of the radius of gyration for the molecular dynamics trajectory of the MYC protein.

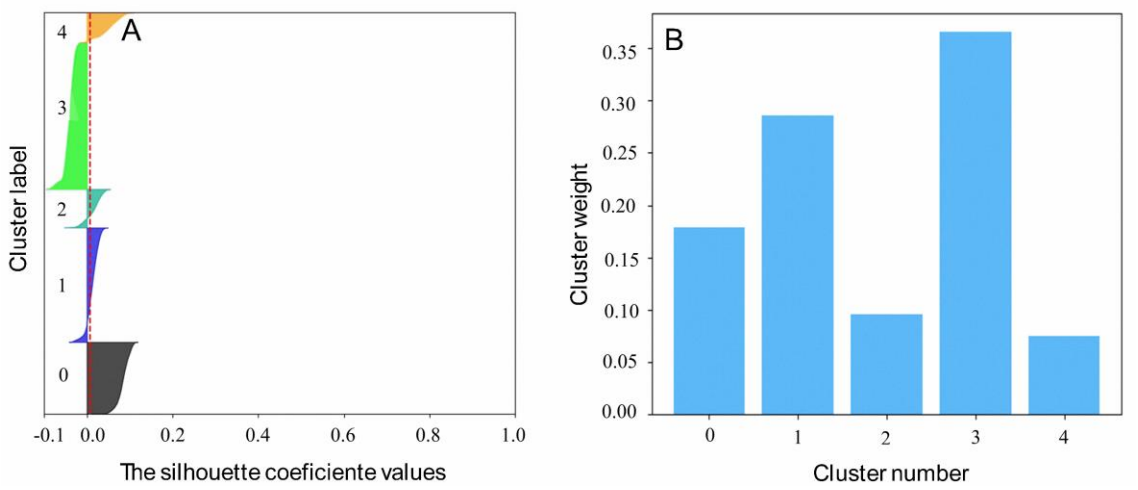


Figure S2. (A) Clusters for MYC generated by the EnGens tool. (B) Molecular weight associated with structural clusters generated by the EnGens tool.

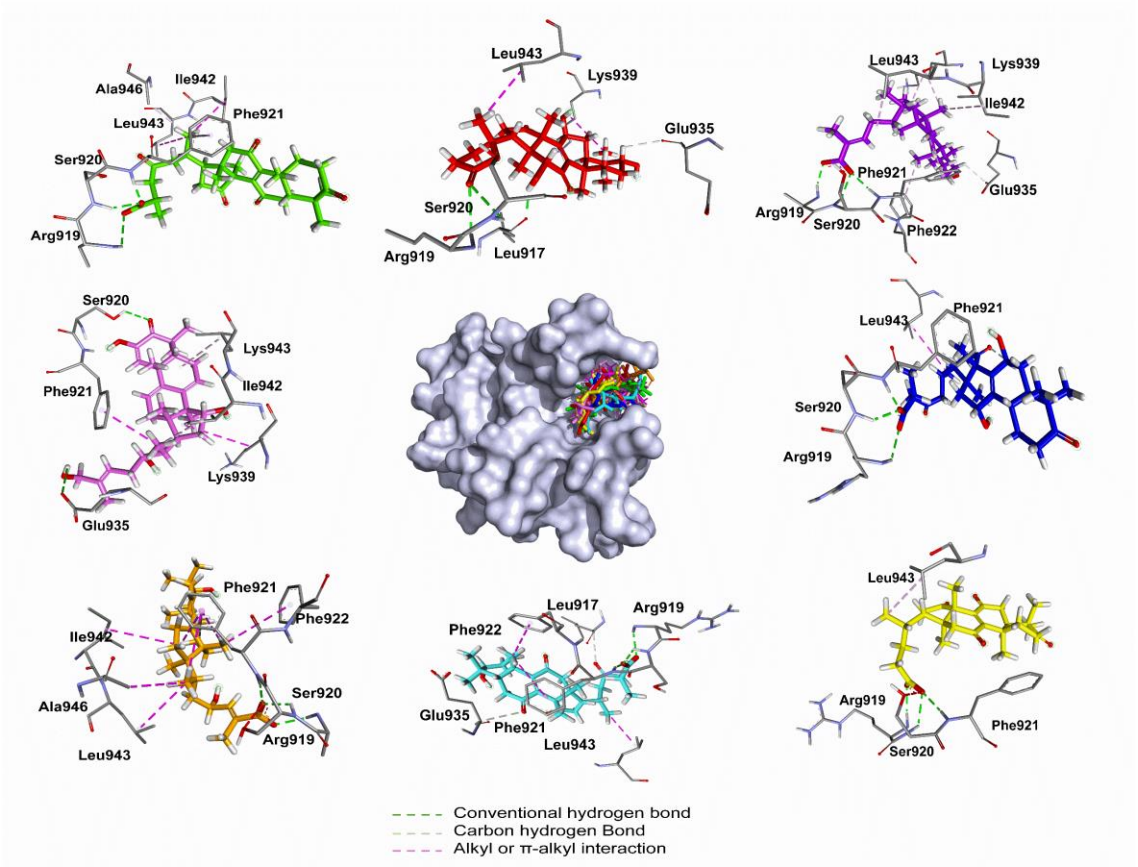


Figure S3. Result for the best molecular docking poses for the complexes MYC-**I** (green), MYC-**II** (red), MYC-**III** (violet), MYC-I**V** (blue), MYC-**V** (yellow), MYC-**VI** (cyan), MYC-**VII** (orange), and MYC-**VIII** (magent). Hydrogen bonds are represented in green, alkyl interactions in violet and salt bridges in orange.

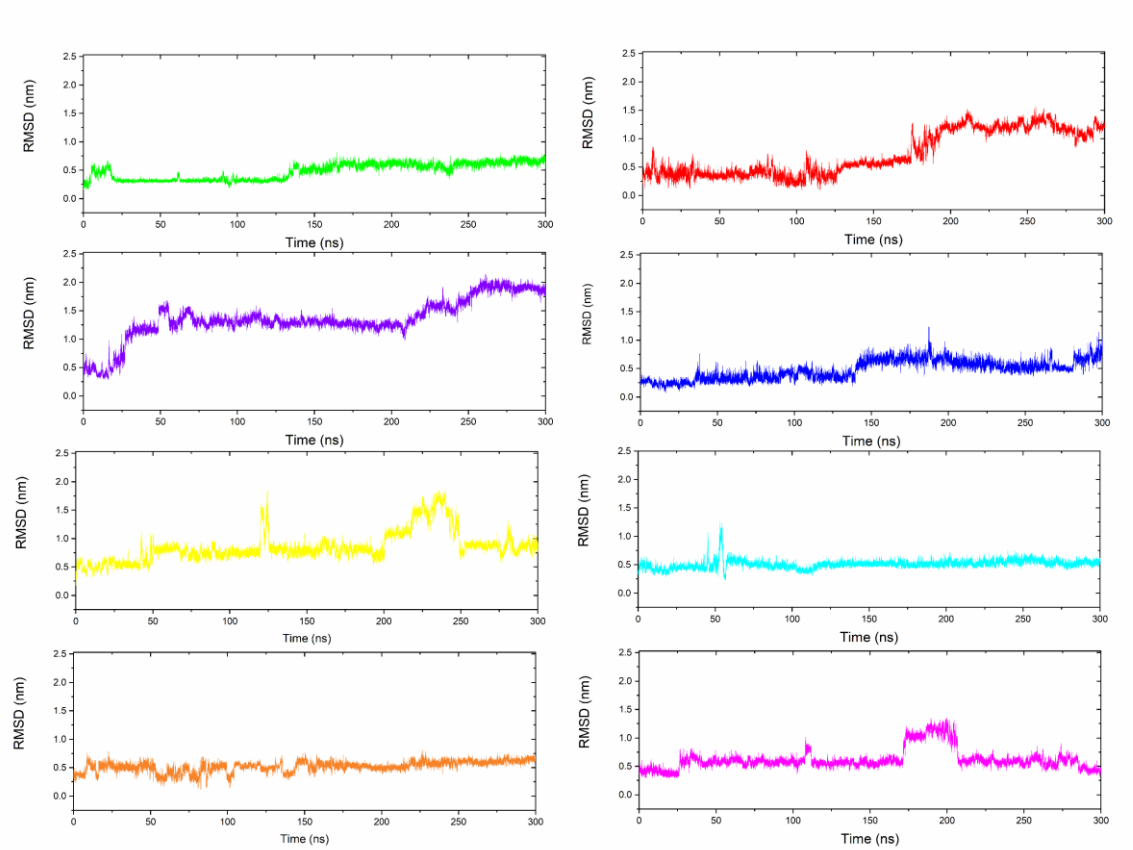


Figure S4. RMSD graph for the complexes MYC-**I** (green line), MYC-**II** (red line), MYC-**III** (violet line), MYC-**IV** (blue line), MYC-**V** (yellow line), MYC-**VI** (cyan line), MYC-**VII** (orange line), and MYC-**VIII** (magent line).

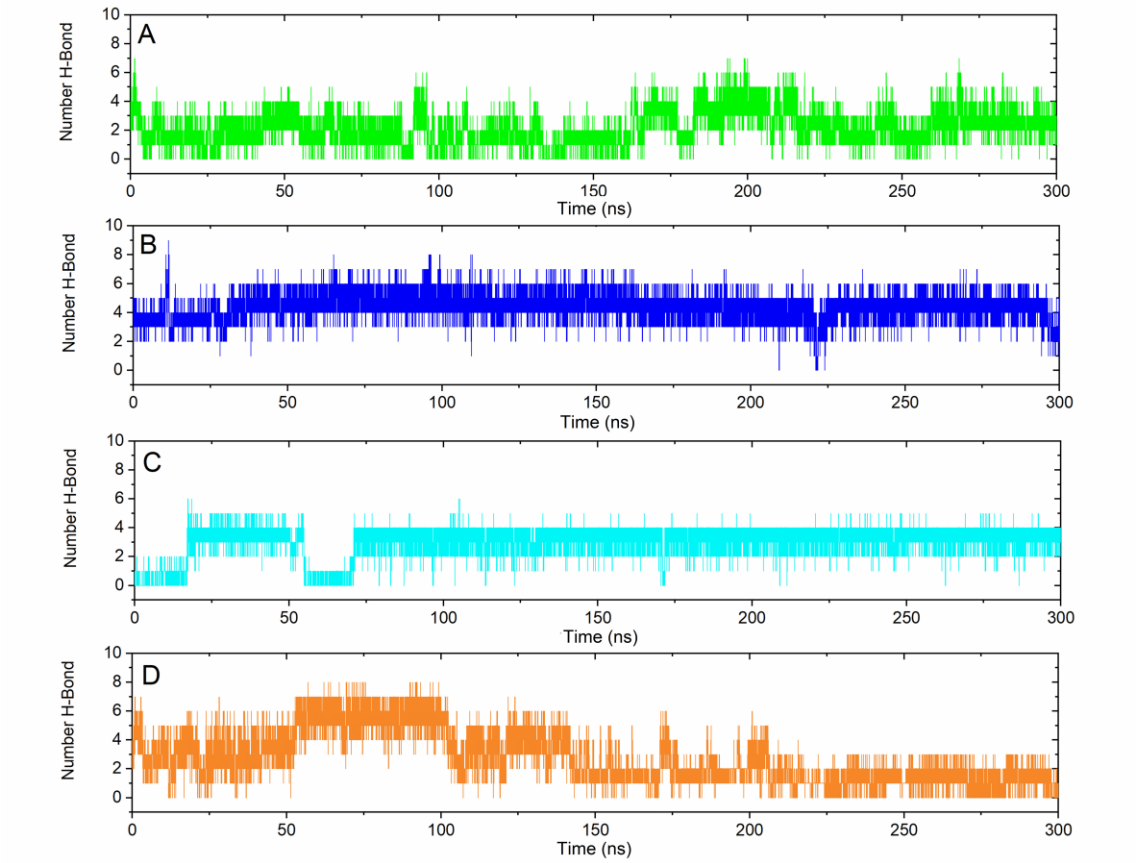


Figure S5. Hydrogen bond plots for the complex. (A) MYC-**I** (green line), (B) MYC-**IV** (blue line), (C) MYC-**VI** (cyan line), (D) MYC-**VII** (orange line)

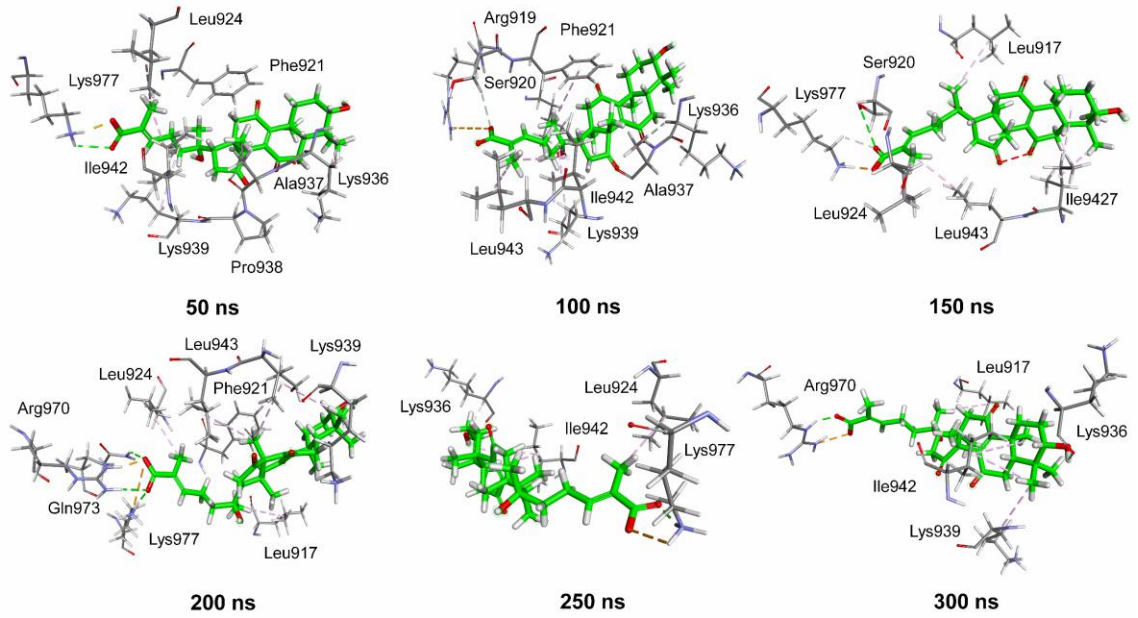


Figure S6. Interactions observed for the MYC-**I** complex during an MD trajectory at 50 ns, 100 ns, 150 ns, 200 ns, 250 ns and 300 ns. Hydrogen bonds are represented in green, alkyl interactions in violet, and salt bridges in orange.

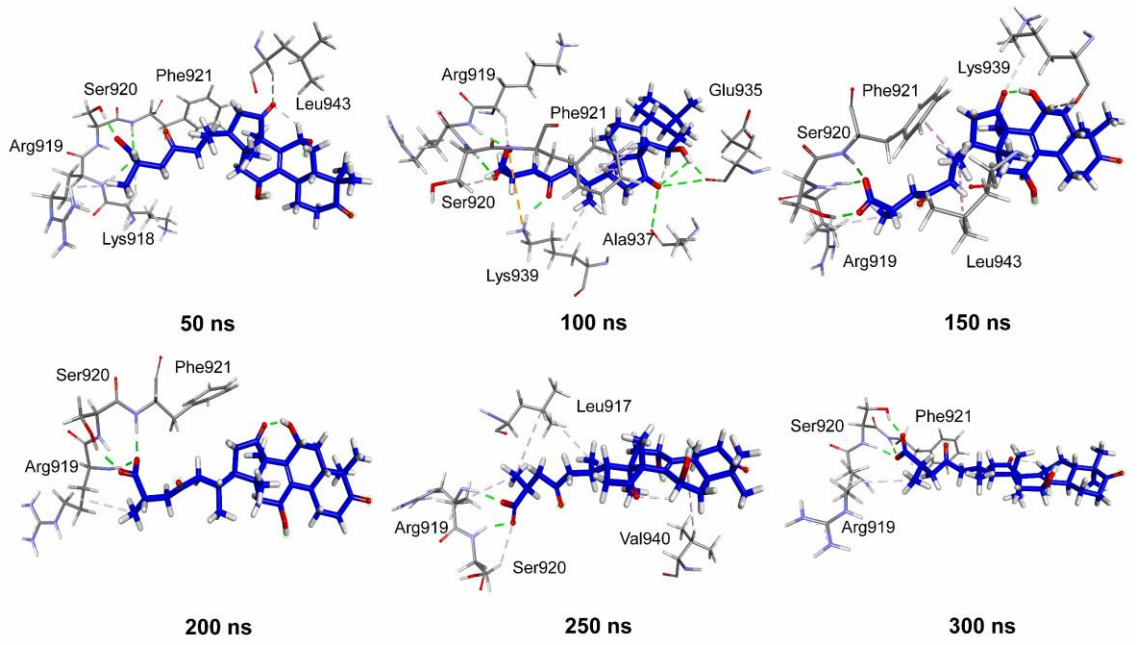


Figure S7. Interactions observed for the MYC-**IV** complex during an MD trajectory at 50 ns, 100 ns, 150 ns, 200 ns, 250 ns, and 300 ns. Hydrogen bonds are represented in green, alkyl interactions in violet and salt bridges in orange.

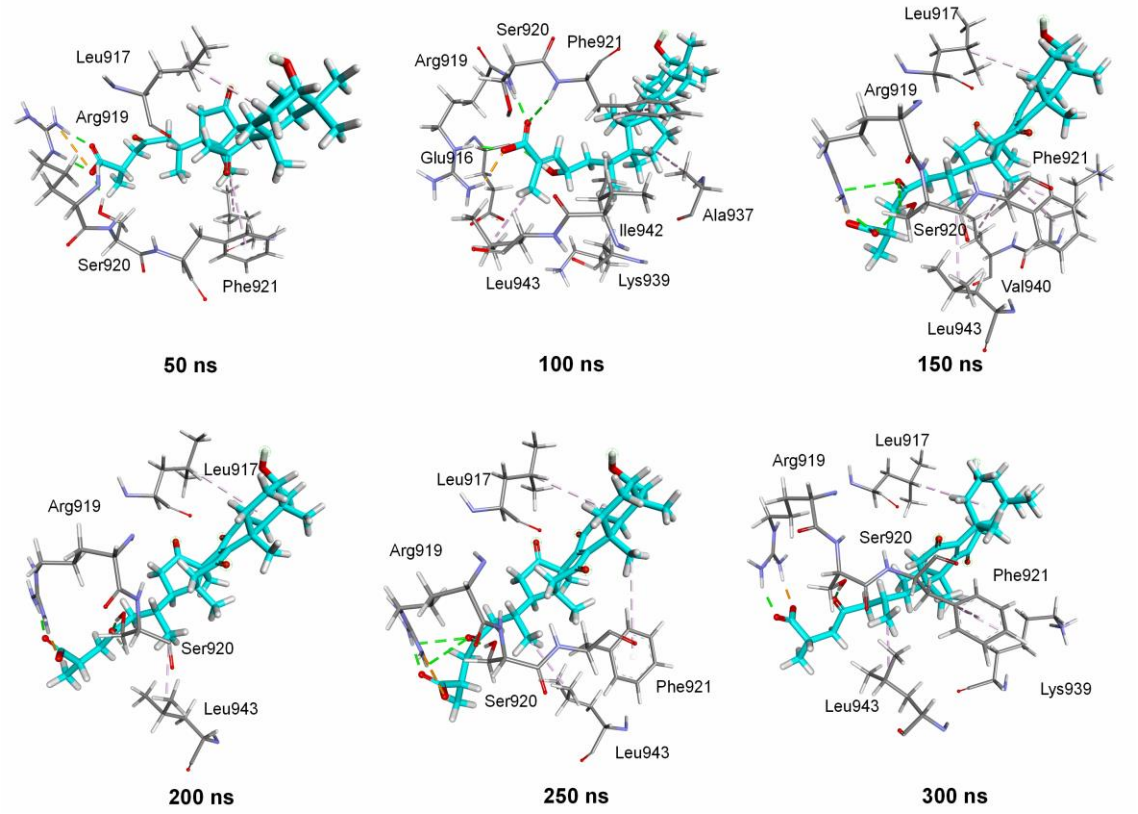


Figure S8. Interactions observed for the MYC-**VI** complex during an MD trajectory at 50 ns, 100 ns, 150 ns, 200 ns, 250 ns, and 300 ns. Hydrogen bonds are represented in green, alkyl interactions in violet, and salt bridges in orange.

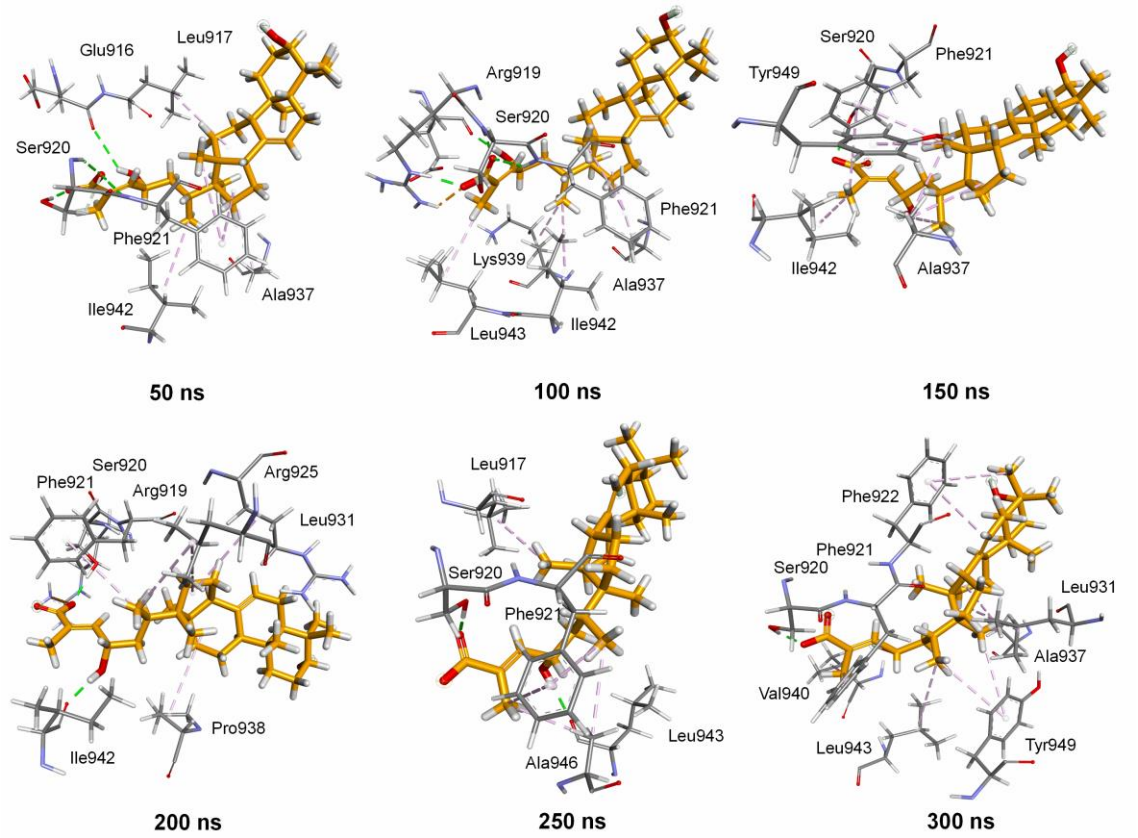


Figure S9. Interactions observed for the MYC-**VII** complex during an MD trajectory at 50 ns, 100 ns, 150 ns, 200 ns, 250 ns, and 300 ns. Hydrogen bonds are represented in green, alkyl interactions in violet and salt bridges in orange.

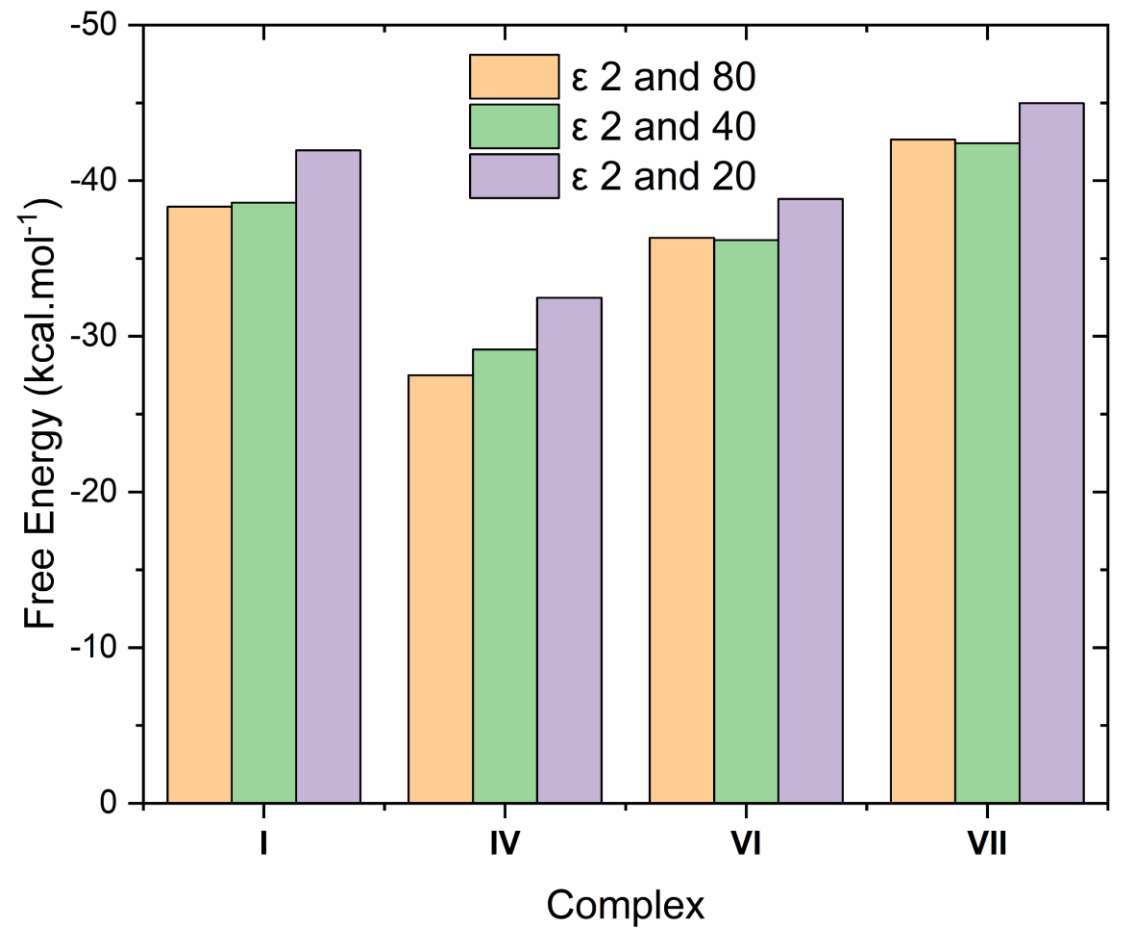
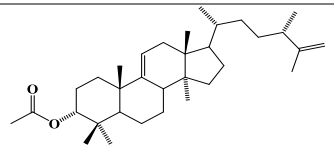
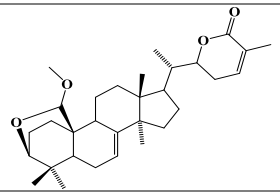
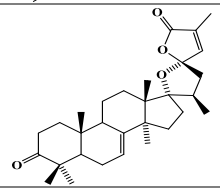
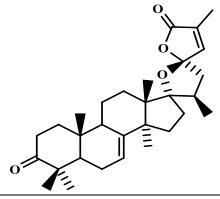


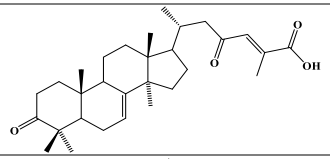
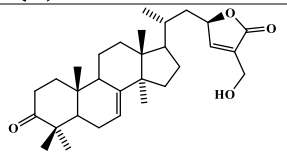
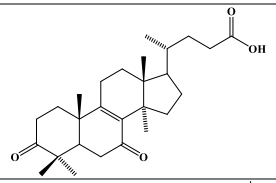
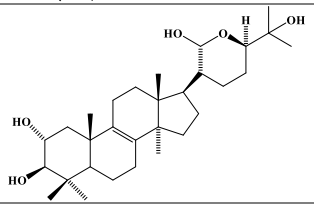
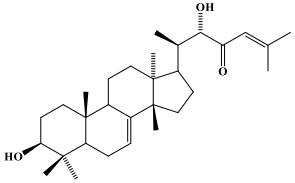
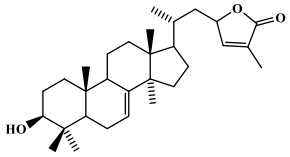
Figure S10. Influence of the external dielectric constant of the solvent on the calculation of free energy for values 20, 40, and 80.

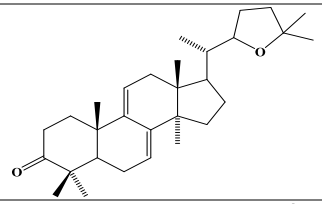
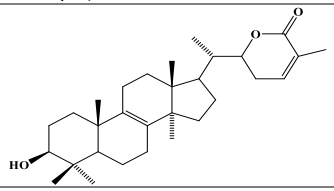
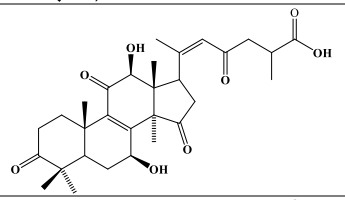
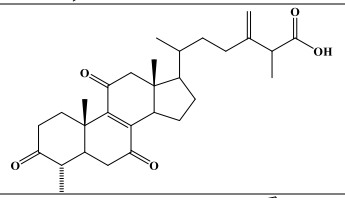
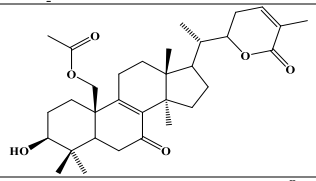
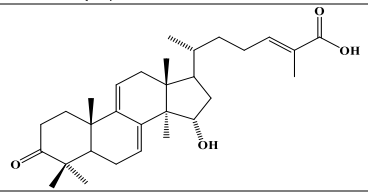
Table S1. Binding site identified by the cavityplus server for clusters 0-4.

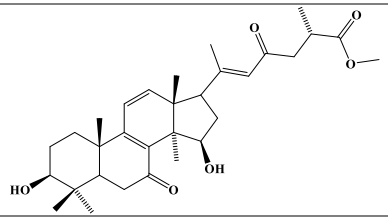
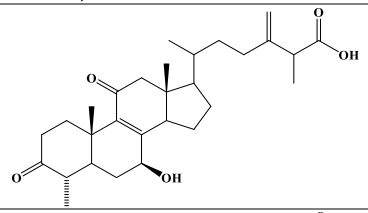
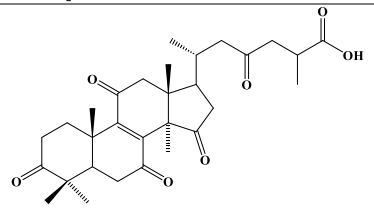
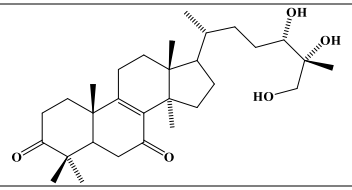
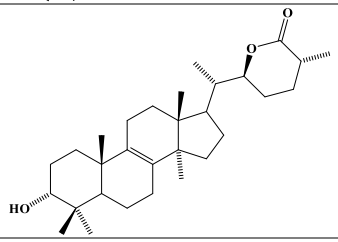
Cluster	DrugScore	Druggabilitty	Residues
0	1092.00	Strong	Gly982, Arg919, Leu943, Lys936, Gly983, Ala946, Gln912, Ile942, Lys918, Thr947, Arg925, Leu931, Val940, Leu924, Ser920, Cys984, Ala937, Phe921, Val941, Lys939, Lys944, Leu917, Glu916, Pro938, Phe922, Asn915, Asn934, Gln980, Glu935
1	175.00	Medium	Val908, Leu943, Lys936, Leu909, Gln912, Ile942, Lys918, Arg925, Leu931, Val940, Arg904, Ala937, Thr905, Phe921, Val941, Lys939, Leu917, Glu916, Pro938, Phe922, Asn915, Asn934, Val901, Glu935
2	-699.00	Weak	Leu931, Val940, Lys918, Pro938, Phe922, Asn933, Leu943, Asn915, Glu932, Asn934, Ala937, Ile942, Phe921, Lys939, Glu935, Val941, Arg925
3	-560,00	Weak	Leu966, Ile928, Arg919, Ile961, Glu932, Glu910, His906, Ser952, Asp965, Arg903, Leu909, Gln958, Glu964, Gln973, His976, Ser962, Pro929, Arg925, Lys902, Arg971, Glu972, Asn907, Val953, Met899, Leu924, Ser920, Gln954, Arg904, Lys969, Leu978, Arg913, Cys984, Thr905, Lys975, Glu979, Asn900, Ala923, asp926, Leu974, Gln927, Phe922, Glu930, Arg968, Lys977, Val901, Gln980
4	-780.00	Weak	His898, Gly897, Ile928, Val908, Arg919, Glu932, Glu910, His906, Arg903, Leu909, Gln973, His976, Glu972, Arg925, Lys902, Arg971, Leu931, Asn907, Met899, Leu924, Arg904, Lys969, Arg913, Thr905, Phe921, Lys975, Ala923, Asp926, Leu974, Gln927, Phe922, Asn933, Arg968, Asn934, Val901

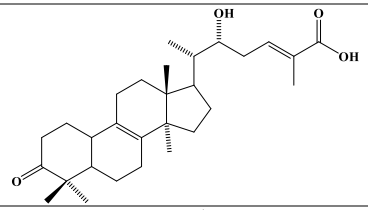
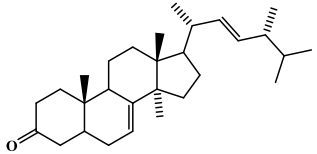
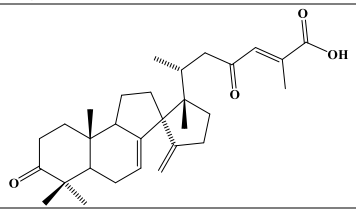
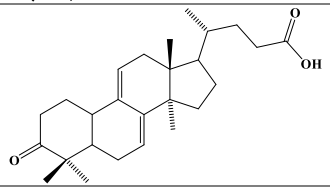
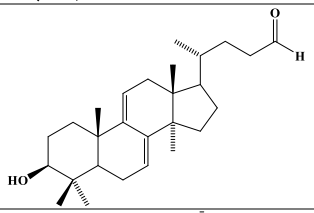
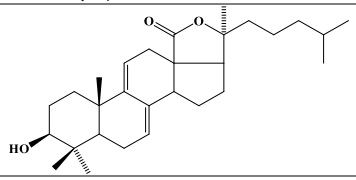
Table S2. Interaction energy results for the 82 ligands selected by induced coupling and inhibitors described in the literature.

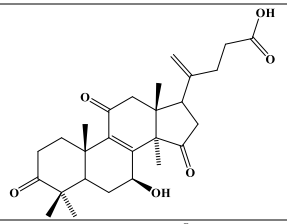
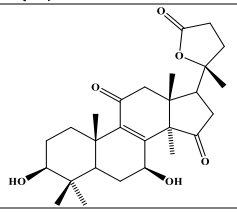
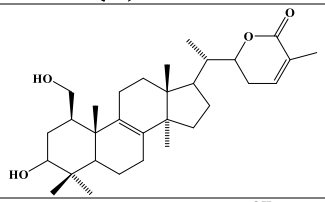
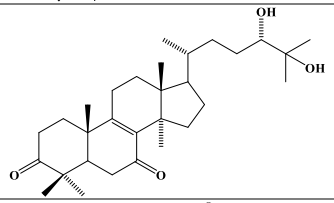
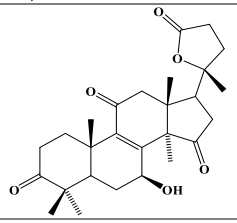
Ligand	Energy (kcal.mol^{-1})	Cluster	Chemical structure	Reference
9-ene-C16	-10.1	1		1
8-ene-epoxy-new-C2	-9.4	0		2
7(8)-ene-C16	-9.1	0		3
7(8)-ene-C15	-9.0	0		3

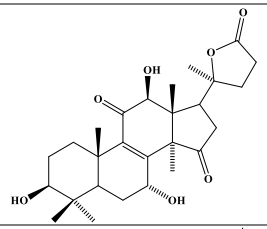
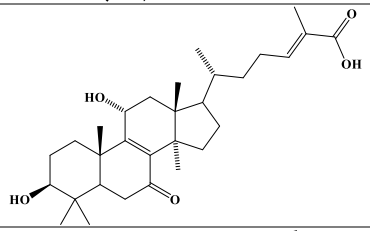
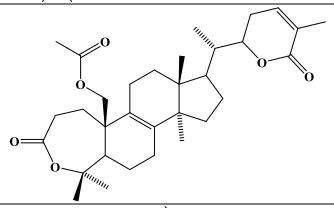
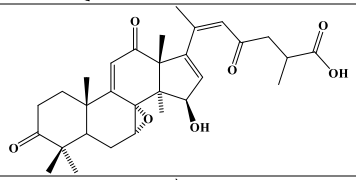
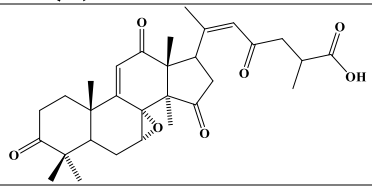
7(8)-ene-C11	-8.9	0		3
7(8)-ene-C3	-8.9	0		4
8-ene-C60	-8.9	0		5
8-ene-C179	-8.8	0		6
7(8)-ene-C27	-8.7	0		7
7(8)-ene-C4	-8.7	0		8

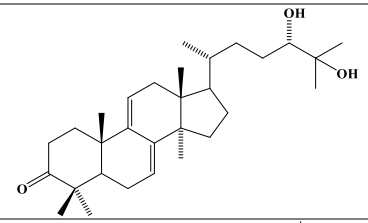
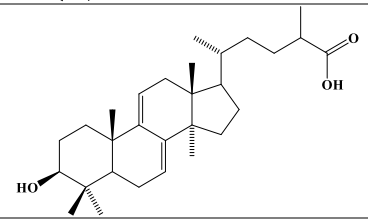
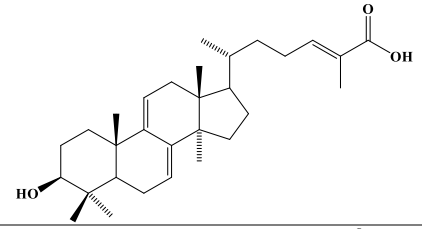
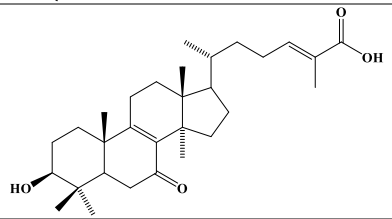
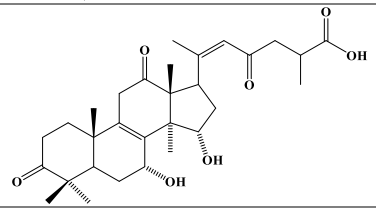
7,9-diene-C120	-8.7	0		9
8-ene-C137	-8.7	0		2
8-ene-C157	-8.7	0		10
8-ene-C186	-8.7	0		11
8-ene-C353	-8.7	0		12
7,9-diene-C22	-8.6	0		13

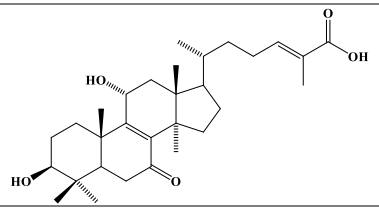
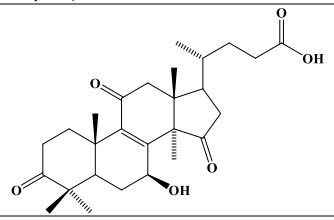
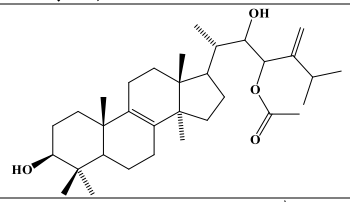
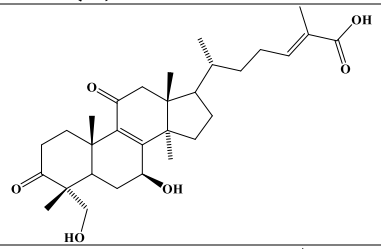
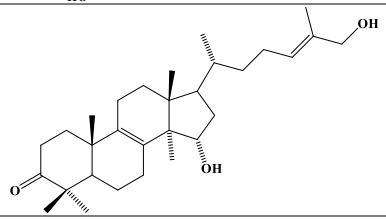
8,11(12)-diene-C2	-8.6	0		14
8-ene-C188	-8.6	0		11
8-ene-C287	-8.6	0		15
8-ene-C344	-8.6	0		16
8-ene-C434	-8.6	0		17

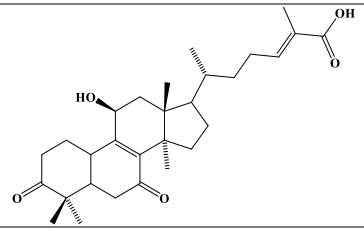
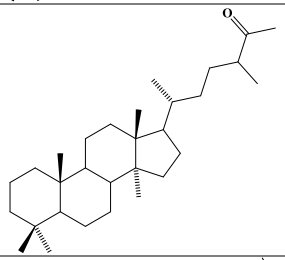
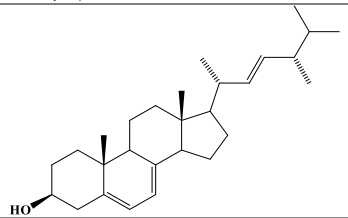
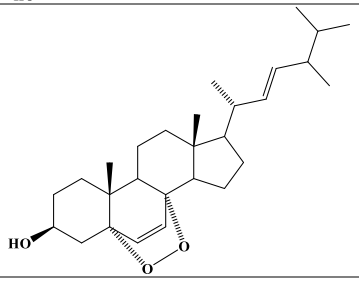
8-ene-C47	-8.6	0		17
7(8)-ene-C19	-8.5	0		18
7,14-diene-exo-C3	-8.5	0		3
7,9-diene-C125	-8.5	0		19
7,9-diene-C91	-8.5	0		20
7,9-diene-lactone-C1	-8.5	0		21

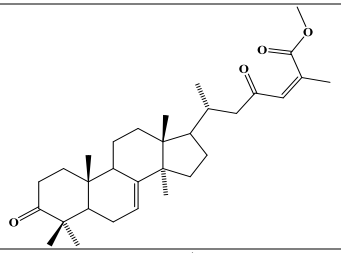
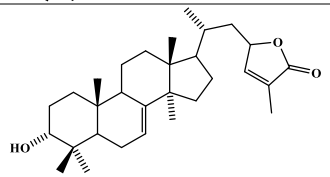
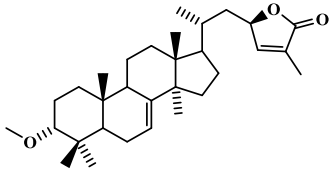
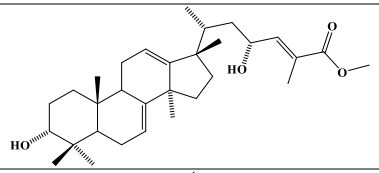
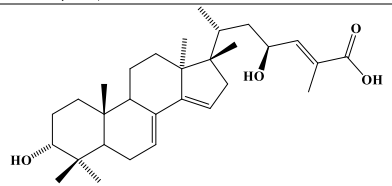
8-ene-C114	-8.5	0		22
8-ene-C135	-8.5	0		23
8-ene-C138	-8.5	0		2
8-ene-C163	-8.5	0		24
8-ene-C284	-8.5	0		23

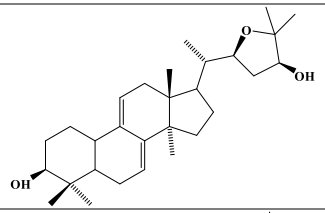
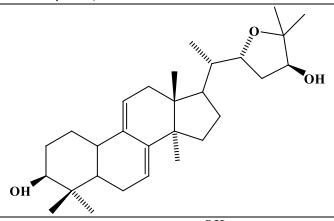
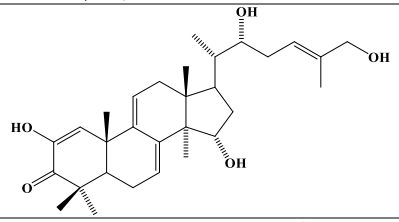
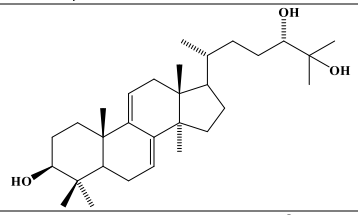
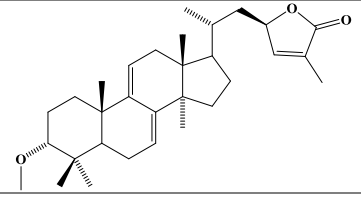
8-ene-C314	-8.5	0		25
8-ene-C382	-8.5	0		26
8-ene-new-C1	-8.5	0		27
9,16-diene-epoxy-C6	-8.5	0		28
9-ene-epoxy-C4	-8.5	0		29

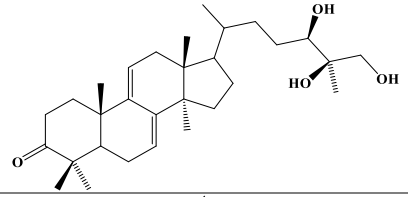
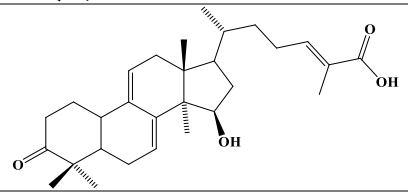
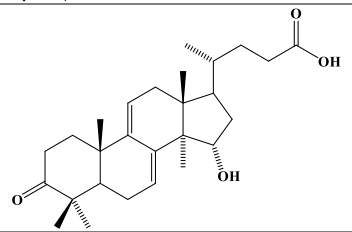
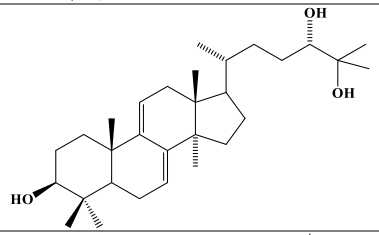
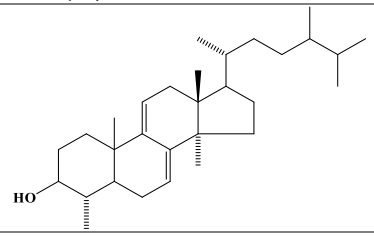
7,9-diene-C113	-8.4	0		30
7,9-diene-C14	-8.4	0		31
7,9-diene-C20	-8.4	0		32
8-ene-C107	-8.4	0		33
8-ene-C219	-8.4	0		34

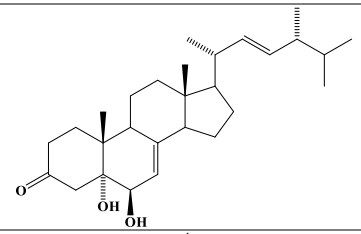
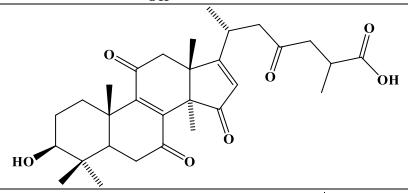
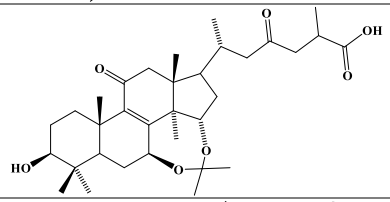
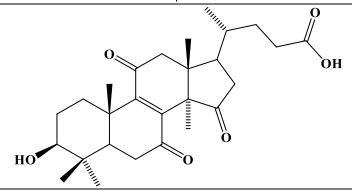
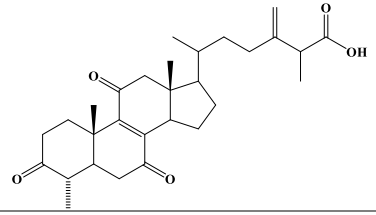
8-ene-C295	-8.4	0		26
8-ene-C300	-8.4	0		35
8-ene-C342	-8.4	0		36
8-ene-C368	-8.4	0		37
8-ene-C375	-8.4	0		38

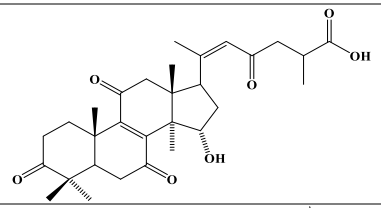
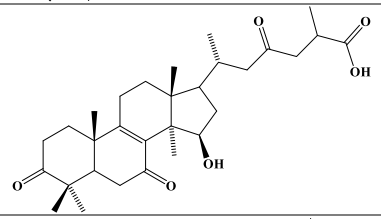
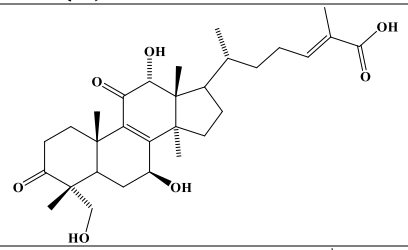
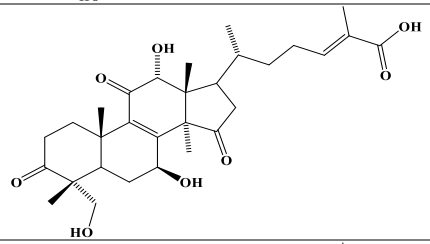
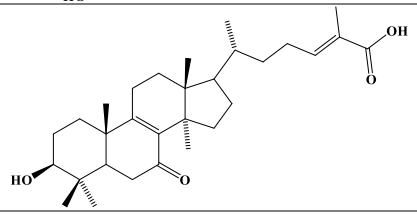
8-ene-C68	-8.4	0		5
saturated-C6	-8.4	0		39
5,7-diene-demethylated-C1	-8.3	0		17
6-ene-peroxy-C1	-8.3	0		40

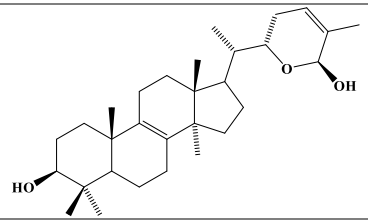
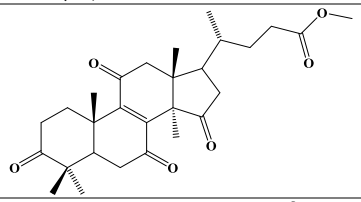
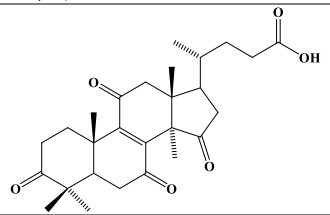
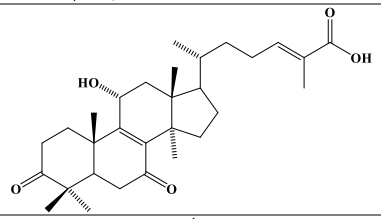
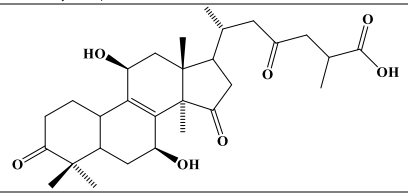
7(8)-ene-C18	-8.3	0		3
7(8)-ene-C6	-8.3	0		8
7(8)-ene-C7	-8.3	0		8
7,12-diene-C4	-8.3	0		3
7,14-diene-C1	-8.3	0		3

7,9-diene-C132	-8.3	0		41
7,9-diene-C133	-8.3	0		41
1,7,9-triene-C4	-8.3	0		42
7,9-diene-C43	-8.3	0		43
7,9-diene-C57	-8.3	0		8

7,9-diene-C6	-8.3	0		44
7,9-diene-C76	-8.3	0		45
7,9-diene-C92	-8.3	0		31
7,9-diene-C96	-8.3	0		30
7,9-diene-demethylated-C3	-8.3	0		46

7-ene-demethylated-C4	-8.3	0		47
8,16-diene-C6	-8.3	0		26
8-ene-7,15-epoxy-C2	-8.3	0		48
8-ene-C104	-8.3	0		49
8-ene-C187	-8.3	0		11

8-ene-C223	-8.3	0		50
8-ene-C325	-8.3	0		16
8-ene-C369	-8.3	0		37
8-ene-C370	-8.3	0		37
8-ene-C420	-8.3	0		33

8-ene-C421	-8.3	0		51
8-ene-C439	-8.3	0		15
8-ene-C58	-8.3	0		15
8-ene-C69	-8.3	0		5
8-ene-C72	-8.3	0		52

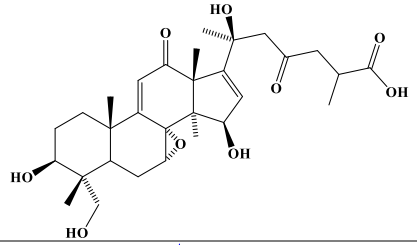
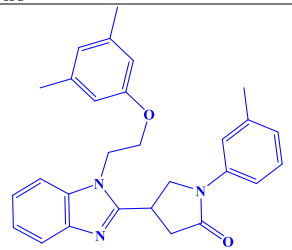
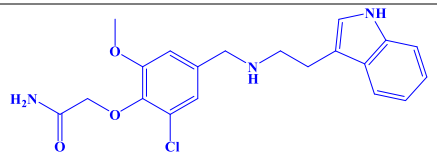
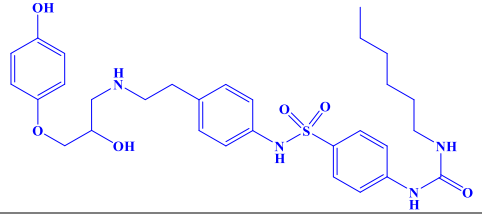
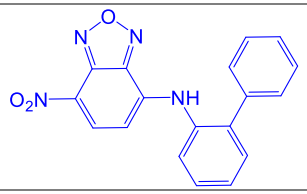
9,16-diene-epoxy-C15	-8.3	0		53
D347-2761	-7.6	-		54
7594-0037	-6.8	-		55
L755507	-5.6	-		56
10074-65	-8.3	-		57

Table S3. Druglikeness and physiochemical properties for the 82 selected ligands.

Ligand	MF	MW	cLog P	HBA	HBD	TPSA	RB	Log S	Log $D_{7.4}$	Lipinski	Veber
7(8)-ene-C11	$C_{30}H_{44}O_4$	468.678	6.787	4	1	71.44	5	-5.91	2.01	Yes	Yes
7(8)-ene-C15	$C_{30}H_{42}O_4$	466.662	6.539	4	0	52.60	0	-6.17	4.08	Yes	Yes
7(8)-ene-C16	$C_{30}H_{42}O_4$	466.662	6.539	4	0	52.60	0	-6.17	4.08	Yes	Yes
7(8)-ene-C19	$C_{29}H_{46}O$	410.686	8.009	1	0	17.07	4	-6.98	5.02	Yes	Yes
7(8)-ene-C27	$C_{30}H_{48}O_3$	456.711	6.485	3	2	57.53	4	-6.19	4.36	Yes	Yes
7(8)-ene-C3	$C_{30}H_{44}O_4$	468.678	6.031	4	1	63.60	4	-6.04	3.92	Yes	Yes
7(8)-ene-C4	$C_{30}H_{46}O_3$	454.695	6.852	3	1	46,53	3	-6.25	4.16	Yes	Yes
7(8)-ene-C6	$C_{30}H_{46}O_3$	454.695	6.852	3	1	46,53	3	-6.25	4.16	Yes	Yes
7,12-diene-C4	$C_{31}H_{48}O_4$	484.721	6.379	4	2	66.76	6	-5.84	3.76	Yes	Yes
7,14-diene-exo-C3	$C_{30}H_{42}O_4$	466.662	6.707	4	1	71.44	3	-5.85	1.99	Yes	Yes
7,9-diene-C113	$C_{30}H_{48}O_3$	456.711	6.629	3	2	57.53	5	-6.17	4.53	Yes	Yes
7,9-diene-C120	$C_{30}H_{46}O_2$	438696	7.675	2	0	26.30	2	-6.33	5.04	Yes	Yes
7,9-diene-C125	$C_{26}H_{38}O_3$	398.587	6.192	3	1	54.37	4	-6.03	2.04	Yes	Yes
7,9-diene-C132	$C_{29}H_{46}O_3$	442.684	6.047	3	2	49.69	2	-6.44	4.30	Yes	Yes
7,9-diene-C133	$C_{29}H_{46}O_3$	442.684	6.047	3	2	49.69	2	-6.44	4.30	Yes	Yes
7,9-diene-C20	$C_{30}H_{46}O_3$	454.695	7.320	3	2	57.53	5	-6.16	2.09	Yes	Yes
7,9-diene-C43	$C_{30}H_{50}O_3$	458.727	6421	3	3	60.69	5	-6.18	4.34	Yes	Yes
7,9-diene-C76	$C_{29}H_{42}O_4$	454.651	6.109	4	2	74.60	5	-5.95	1.97	Yes	Yes
7,9-diene-C91	$C_{27}H_{42}O_2$	398.631	6.488	3	1	37.30	4	-5.99	4.55	Yes	Yes
7,9-diene-C92	$C_{27}H_{40}O_4$	428.613	5.553	4	2	74.60	4	-6.04	2.02	Yes	Yes
7,9-diene-C96	$C_{30}H_{50}O_3$	458.727	6.421	3	3	60.69	4	-6.18	4.34	Yes	Yes
7,9-diene-demethylated-C3	$C_{30}H_{50}O$	426.729	8.191	1	1	20.23	5	-6.61	4.64	Yes	Yes
7,9-diene-lactone-C1	$C_{29}H_{44}O_3$	440.668	6.604	3	1	46.53	4	-6.19	4.21	Yes	Yes
8-ene-C107	$C_{30}H_{46}O_4$	470.694	6.723	4	2	74.60	5	-5.91	2.00	Yes	Yes
8-ene-C135	$C_{27}H_{38}O_6$	458.595	3.521	6	2	100.90	1	-4.95	3.30	Yes	Yes
8-ene-C137	$C_{30}H_{46}O_3$	454.695	6.995	3	1	46.53	2	-6.38	4.19	Yes	Yes
8-ene-C138	$C_{31}H_{48}O_4$	484.721	6.213	4	2	66.76	3	-5.82	3.92	Yes	Yes
8-ene-C163	$C_{30}H_{48}O_4$	472.710	6.032	4	2	74.60	5	-5.89	4.23	Yes	Yes
8-ene-C284	$C_{27}H_{36}O_6$	456.579	3.729	6	1	97.74	1	-4.95	3.26	Yes	Yes

8-ene-C314	$C_{27}H_{38}O_7$	474.594	2.482	7	3	121.13	1	-4.43	2.35	Yes	Yes
8-ene-C344	$C_{30}H_{48}O_5$	488.709	5.004	5	3	94.83	6	-5.61	4.03	Yes	Yes
8-ene-C420	$C_{30}H_{46}O_4$	470.694	6.723	4	2	74.60	5	-5.91	2.07	Yes	Yes
8-ene-C421	$C_{30}H_{48}O_3$	456.711	6.786	3	2	49.69	2	-6.44	4.47	Yes	Yes
8-ene-C434	$C_{30}H_{48}O_3$	456.711	7.074	3	1	46.53	2	-6.37	4.47	Yes	Yes
8-ene-C47	$C_{29}H_{44}O_4$	456.667	6.333	4	2	74.60	5	-6.03	1.96	Yes	Yes
8-ene-C69	$C_{30}H_{44}O_5$	484.677	5.902	5	2	91.67	5	-5.68	1.95	Yes	Yes
5,7-diene-demethylated-C1	$C_{28}H_{44}O$	396.659	7.331	1	1	20.23	4	-654	4.12	Yes	Yes
6-ene-peroxy-C1	$C_{28}H_{44}O_3$	442.684	6.864	3	1	36.69	4	-6.54	4.57	Yes	Yes
7(8)-ene-C18	$C_{31}H_{46}O_4$	482.705	6.875	4	0	60.44	6	-6.98	5.02	Yes	Yes
7(8)-ene-C7	$C_{31}H_{48}O_3$	468.722	7.505	3	0	35.53	3	-6.35	4.52	Yes	Yes
7,14-diene-C1	$C_{30}H_{46}O_4$	470.694	6.291	4	3	77.76	5	-5.88	2.04	Yes	Yes
7,9-diene-C14	$C_{29}H_{46}O_3$	442.684	7.010	3	2	57.53	5	-6.09	2.12	Yes	Yes
7,9-diene-C22	$C_{30}H_{44}O_4$	468.678	6.499	4	2	74.60	5	-5.80	1.98	Yes	Yes
1,7,9-triene-C4	$C_{30}H_{44}O_5$	484.677	5.039	5	4	97.99	5	-5.56	2.11	Yes	Yes
7,9-diene-C57	$C_{31}H_{46}O_3$	466.706	7.425	3	0	35.53	4	-6.30	4.32	Yes	Yes
7,9-diene-C6	$C_{30}H_{48}O_4$	472.710	5.601	4	3	77.76	6	-5.88	4.29	Yes	Yes
7-ene-demethylated-C4	$C_{28}H_{44}O$	396.659	7.331	1	1	20.23	4	-6.29	4.39	Yes	Yes
8,11(12)-diene-C2	$C_{31}H_{44}O_6$	512.687	4.737	6	2	100.90	6	-5.19	2.79	Yes	Yes
8,16-diene-C6	$C_{32}H_{44}O_9$	512.643	4.260	7	2	125.81	6	-5.05	1.44	Yes	Yes
8-ene-7,15-epoxy-C2	$C_{33}H_{50}O_7$	558.756	5.722	7	2	110.13	6	-5.46	2.39	No	Yes
8-ene-C104	$C_{27}H_{38}O_6$	458.595	4.135	6	2	108.74	4	-5.13	1.44	Yes	Yes
8-ene-C114	$C_{27}H36O_6$	456.579	4.055	6	2	108.74	4	-5.09	1.42	Yes	Yes
8-ene-C157	$C_{30}H_{40}O_8$	528.642	3.231	8	3	146.04	5	-4.33	0.99	Yes	No
8-ene-C179	$C_{30}H_{50}O_5$	490.725	4.952	5	4	90.15	2	-5.65	3.94	Yes	Yes
8-ene-C186	$C_{29}H_{42}O_4$	454.651	6.397	4	1	71.44	6	-5.90	1.95	Yes	Yes
8-ene-C187	$C_{29}H_{40}O_5$	468.634	5.576	5	1	88.51	6	-5.91	1.84	Yes	Yes
8-ene-C188	$C_{29}H_{42}O_5$	470.650	5.368	5	2	91.67	6	-5.88	1.86	Yes	Yes
8-ene-C219	$C_{30}H_{42}O_7$	514.659	4.052	7	3	128.97	5	-4.98	1.52	Yes	Yes
8-ene-C223	$C_{30}H_{40}O_7$	512.643	4.260	7	2	125.81	5	-5.07	1.59	Yes	Yes
8-ene-C287	$C_{30}H_{40}O_7$	512.643	4.548	7	1	122.65	6	-5.20	1.30	Yes	Yes
8-ene-C295	$C_{30}H_{46}O_5$	486.693	5.694	5	3	94.83	5	-5.75	2.03	Yes	Yes
8-ene-C300	$C_{27}H_{38}O_6$	458.595	4.135	6	2	108.74	4	-5.09	1.52	Yes	Yes
8-ene-C325	$C_{30}H_{44}O_6$	500.676	5.161	6	2	108.74	5	-5.59	1.93	No	Yes
8-ene-C342	$C_{33}H_{54}O_4$	514.791	7.238	4	2	66.76	6	-5.83	4.25	No	Yes

8-ene-C353	$C_{32}H_{46}O_6$	526.714	5.717	6	1	89.90	5	-5.77	3.92	No	Yes
8-ene-C368	$C_{30}H_{44}O_6$	500.676	4.874	6	3	111.90	6	-5.41	1.81	Yes	Yes
8-ene-C369	$C_{30}H_{44}O_7$	516.675	3.845	7	4	132.13	6	-4.89	1.35	Yes	Yes
8-ene-C370	$C_{30}H_{42}O_8$	530.658	3.024	8	4	149.20	6	-4.10	0.63	Yes	No
8-ene-C375	$C_{30}H_{48}O_3$	456.711	6.631	3	2	57.53	5	-6.20	4.48	Yes	Yes
8-ene-C382	$C_{30}H_{46}O_5$	486.693	5.694	5	3	94.83	5	-5.75	2.03	Yes	Yes
8-ene-C439	$C_{28}H_{38}O_6$	470.606	4.431	6	0	94.58	5	-5.21	2.46	No	Yes
8-ene-C58	$C_{27}H_{36}O_6$	456.579	4.343	6	1	105.58	4	-5.11	1.42	Yes	Yes
8-ene-C60	$C_{27}H_{40}O_4$	428.613	5.985	4	1	71.44	4	-6.04	2.00	Yes	Yes
8-ene-C68	$C_{24}H_{49}O_5$	470.650	5.512	5	2	91.67	5	-5.84	1.86	Yes	Yes
8-ene-C72	$C_{29}H_{42}O_7$	502.648	3.741	7	3	128.97	6	-4.97	1.37	Yes	Yes
8-ene-epoxy-new-C2	$C_{31}H_{46}O_4$	482.705	6.841	4	0	44.76	3	-6.15	4.30	Yes	Yes
8-ene-new-C1	$C_{32}H_{46}O_6$	526.714	6.472	6	0	78.90	5	-5.56	3.83	No	Yes
9,16-diene-epoxy-C6	$C_{30}H_{38}O_7$	510.627	3.988	7	2	121.27	5	-4.88	1.64	Yes	Yes
9-ene-epoxy-C4	$C_{30}H_{38}O_7$	510.627	4.276	7	1	118.11	5	-5.08	1.74	Yes	Yes
saturated-C6	$C_{30}H_{52}O$	428.745	8.703	1	0	17.07	5	-7.05	5.21	Yes	Yes
9-ene-C16	$C_{33}H_{54}O_2$	482.793	9.152	2	0	26.30	7	-6.47	4.68	Yes	Yes
9,16-diene-epoxy-C15	$C_{30}H_{42}O_9$	546.657	1.947	9	5	164.89	6	-3.68	0.57	Yes	No

Molecular formula (MF), partition coefficient (cLog P), molecular weight (MW, Daltons), hydrogen bond acceptors (HBA), hydrogen bond donors (HBD), topological polar surface area (TPSA, $Å^2$), number of rotatable bonds (RB), solubility (Log S, log $mol.L^{-1}$), and distribution coefficient (Log $D_{7.4}$).

Table S4. Pharmacokinetic parameters for the 82 ligands selected by induced coupling.

Ligand	Pgpi (%)	Pgps (%)	GI-A (%)	F30 (%)	BBB (%)	T1/2 (h)	CL (h)	hERG (%)	H-HT (%)
7(8)-ene-C11	76.30	6.10	76.70	36.30	80.10	1.86	1.17	40.80	57.00
7(8)-ene-C15	81.20	6.20	73.80	39.20	88.60	2.00	1.40	55.10	49.40
7(8)-ene-C16	81.20	6.20	73.80	39.20	88.60	2.00	1.40	55.10	49.40
7(8)-ene-C19	92.30	10.40	89.30	43.50	97.90	2.00	0.93	47.30	7.00
7(8)-ene-C27	54.00	11.10	83.30	41.50	75.80	1.79	1.22	55.20	41.80
7(8)-ene-C3	79.90	12.20	71.30	32.60	87.70	1.99	1.38	48.8	57.20
7(8)-ene-C4	80.60	16.40	81.70	39.20	85.50	1.91	1.16	50.7	45.00
7(8)-ene-C6	80.60	16.40	81.70	39.20	85.50	1.91	1.16	50.7	45.00
7,12-diene-C4	89.90	8.70	70.50	32.60	35.20	1.92	1.29	41.90	46.60
7,14-diene-exo-C3	77.40	1.60	76.30	38.00	76.00	2.03	1.17	44.40	54.80
7,9-diene-C113	75.80	7.60	77.80	42.80	84.40	1.95	1.12	41.70	43.80
7,9-diene-C120	70.30	8.60	89.00	42.40	94.30	2.01	1.03	47.50	29.00
7,9-diene-C125	63.90	12.70	82.20	47.90	87.80	1.98	1.13	45.80	62.20
7,9-diene-C132	60.90	39.30	80.00	47.90	95.20	2.01	1.17	47.40	49.80
7,9-diene-C133	60.90	39.30	80.00	47.90	95.20	2.01	1.17	47.40	49.80
7,9-diene-C20	84.10	8.70	80.8	40.90	65.90	1.96	1.16	44.20	48.40
7,9-diene-C43	61.7	23.10	77.90	47.80	76.60	1.90	1.12	42.00	32.00
7,9-diene-C76	85.20	15.70	72.10	41.30	64.60	1.94	1.42	44.30	68.60
7,9-diene-C91	84.30	8.00	93.50	48.80	85.90	1.99	1.29	47.70	59.20
7,9-diene-C92	52.30	12.80	71.60	35.20	88.80	2.02	1.59	37.60	70.80
7,9-diene-C96	61.70	23.10	77.90	47.80	76.60	1.90	1.12	42.00	32.00
7,9-diene-demethylated-C3	78.70	34.40	93.10	49.00	87.50	1.93	1.11	47.20	4.20
7,9-diene-lactone-C1	74.90	18.60	81.70	35.30	81.50	1.79	1.38	53.40	52.80
8-ene-C107	91.10	5.50	71.60	40.80	58.50	1.69	1.36	42.50	65.20
8-ene-C135	51.60	2.50	70.80	41.90	96.60	1.47	1.95	38.00	58.40
8-ene-C137	81.10	4.30	82.20	44.90	90.30	1.79	1.23	50.70	50.60
8-ene-C138	87.90	8.60	68.40	41.20	87.40	1.27	1.75	47.30	53.60
8-ene-C163	85.50	6.10	71.60	41.10	77.60	1.67	1.29	44.60	51.20
8-ene-C284	51.70	3.40	73.80	39.00	97.50	1.59	1.87	38.80	54.20
8-ene-C314	58.80	2.80	70.00	45.00	93.90	1.54	1.87	36.50	43.00
8-ene-C344	79.90	7.90	65.00	39.90	60.40	1.84	1.83	60.00	37.00
8-ene-C420	91.10	5.50	71.60	40.80	58.50	1.69	1.36	42.50	65.20
8-ene-C421	62.90	7.10	79.60	44.20	83.60	1.81	1.21	47.80	46.80
8-ene-C434	74.50	4.40	82.20	42.80	74.70	1.65	1.27	49.90	40.60
8-ene-C47	89.90	5.10	72.10	45.70	33.10	1.74	1.34	40.00	65.00
8-ene-C69	90.30	7.10	72.10	35.50	57.90	1.61	1.54	33.80	65.20
5,7-diene-demethylated-C1	90.10	11.20	92.10	46.30	92.90	1.98	1.05	53.10	11.00
6-ene-peroxy-C1	75.00	31.60	80.30	48.30	91.20	1.91	1.22	48.80	21.20
7(8)-ene-C18	92.30	10.04	89.30	43.50	97.90	2.03	0.93	47.30	7.00
7(8)-ene-C7	92.80	28.10	79.30	40.80	74.20	1.85	1.18	50.50	39.40
7,14-diene-C1	71.60	11.40	71.70	40.50	35.60	1.94	1.27	38.90	44.60
7,9-diene-C14	57.80	10.40	80.80	43.10	88.70	1.89	1.11	40.20	51.60
7,9-diene-C22	84.30	8.90	72.10	32.70	77.90	1.98	1.39	41.20	69.40
1,7,9-triene-C4	47.50	34.50	78.90	39.20	22.90	1.69	1.61	38.00	35.80
7,9-diene-C57	93.00	34.50	79.30	48.40	82.22	1.95	1.29	51.50	42.40
7,9-diene-C6	68.20	9.80	65.00	41.50	69.90	1.97	1.23	41.40	47.40
7-ene-demethylated-C4	93.10	5.80	76.00	47.80	82.50	2.07	1.07	45.90	41.40

8,11(12)-diene-C2	81.50	26.40	70.30	30.10	86.40	1.82	1.58	38.70	70.20
8,16-diene-C6	41.20	7.00	71.60	31.80	89.80	1.74	1.64	34.70	43.60
8-ene-7,15-epoxy-C2	44.80	9.40	67.40	28.70	82.10	1.61	1.72	39.90	58.00
8-ene-C104	29.50	4.40	71.60	36.40	76.10	1.63	1.83	32.90	54.60
8-ene-C114	45.50	6.80	70.90	37.70	89.30	1.65	1.88	31.70	56.60
8-ene-C157	72.00	15.80	72.20	37.70	85.60	1.86	1.59	35.50	55.20
8-ene-C179	69.60	3.30	62.30	40.70	81.70	1.74	1.31	48.00	45.20
8-ene-C186	88.30	1.50	75.50	40.30	81.20	1.71	1.26	49.70	57.40
8-ene-C187	85.00	2.40	75.50	42.30	85.00	1.59	1.33	40.90	56.80
8-ene-C188	83.50	4.60	71.50	41.50	78.70	1.52	1.49	36.80	62.00
8-ene-C219	71.50	10.10	71.60	34.60	80.60	1.73	1.72	32.90	67.00
8-ene-C223	78.70	12.30	71.60	34.50	93.20	1.75	1.66	35.10	50.20
8-ene-C287	27.00	3.70	76.30	34.60	95.30	1.72	1.45	37.80	17.40
8-ene-C295	85.40	7.50	71.60	39.40	58.30	1.68	1.59	35.60	72.40
8-ene-C300	51.90	8.10	71.30	36.80	88.60	1.63	1.86	32.90	55.60
8-ene-C325	58.40	8.50	71.60	31.00	88.40	1.66	1.63	35.20	55.60
8-ene-C342	81.90	1.70	72.50	38.10	39.80	1.70	1.20	45.60	42.20
8-ene-C353	89.40	7.10	67.20	31.80	75.10	1.60	1.57	41.30	55.60
8-ene-C368	84.70	8.30	74.00	34.70	53.90	1.64	1.68	34.50	64.80
8-ene-C369	88.40	10.00	74.80	35.70	41.20	1.59	1.73	33.50	65.60
8-ene-C370	87.90	12.00	74.80	34.60	54.60	1.73	1.64	34.10	51.60
8-ene-C375	91.40	4.10	85.00	39.60	52.50	1.83	1.23	55.20	45.40
8-ene-C382	85.40	7.50	71.60	39.40	58.30	1.68	1.59	35.60	72.40
8-ene-C439	75.00	3.50	77.60	31.40	95.70	1.71	1.47	38.30	33.20
8-ene-C58	40.90	4.00	74.70	33.30	93.30	1.67	1.57	36.90	29.80
8-ene-C60	78.60	6.50	74.70	39.00	83.30	1.68	1.40	43.30	64.60
8-ene-C68	88.10	11.70	72.10	48.80	55.30	1.60	1.54	37.00	81.20
8-ene-C72	38.70	17.50	71.60	46.00	86.00	1.62	1.75	34.50	46.00
8-ene-epoxy-new-C2	83.80	16.60	72.00	41.30	74.80	1.68	1.33	52.20	38.80
8-ene-new-C1	93.90	5.00	66.00	35.00	79.50	1.58	1.43	46.00	61.20
9,16-diene-epoxy-C6	76.20	23.60	68.30	34.20	77.20	1.92	1.72	38.20	66.20
9-ene-epoxy-C4	79.20	13.20	70.60	39.40	93.50	1.92	1.94	39.70	62.00
Saturated-C6	83.20	4.40	88.80	47.80	95.50	1.96	1.15	45.50	5.20
9-ene-C16	89.30	2.80	84.60	34.40	77.70	1.78	0.96	45.51	19.80
9,16-diene-epoxy-C15	46.40	17.90	60.02	29.50	46.90	1.89	1.54	40.60	62.20

P-glycoprotein inhibitor (Pgpi), P-glycoprotein substrate (Pgps), gastrointestinal absorption (GI-A), bioavailability (F30%), probability of crossing the blood-brain barrier (BBB), Half lifetime (T1/2), clearance rate (CL), hERG channel blocker (hERG), and human hepatotoxicity (H-HT).

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