

**Supplementary material:****Table S1: Molecular topological descriptors computed by ChemOffice software.**

N°	H°	G	IGTC	T	CT	TB	CP	KH	TVC	PC	NRB	I	SVD	TC
1	-319.40	-137.18	156.378	217.700	594.658	432.273	34.521	3.113	0.079	1.881	4	1	16	0.177
2	-360.68	-120.34	202.239	240.240	633.341	473.841	27.877	3.002	0.040	2.939	6	1	20	0.088
3	-381.32	-111.92	225.169	251.510	651.002	493.270	25.252	2.773	0.028	3.468	7	0	22	0.063
4	-324.68	-139.62	156.892	202.700	579.982	419.035	34.848	3.143	0.091	1.751	3	0	16	0.204
5	-328.15	-134.34	155.951	220.120	549.519	392.016	35.305	3.143	0.112	1.531	2	1	16	0.250
6 <sup>a</sup>	-345.32	-131.20	179.823	213.970	591.312	433.873	31.210	3.020	0.065	2.190	4	1	18	0.144
7	-365.96	-122.78	202.753	225.240	620.319	461.693	28.114	2.897	0.046	2.809	5	1	20	0.102
8	-365.96	-122.78	202.753	225.240	611.383	455.043	28.114	2.896	0.046	2.719	5	0	20	0.102
9	-412.52	-108.38	249.128	232.780	644.066	489.349	23.338	2.650	0.026	3.737	6	1	24	0.059
10	-202.18	-56.96	141.948	212.620	609.947	438.910	36.731	3.691	0.053	1.397	3	1	18	0.177
11	-222.82	-48.54	164.879	223.890	629.081	459.868	32.803	3.571	0.037	1.926	4	0	20	0.125
12	-199.25	-51.78	146.349	200.940	571.975	410.114	36.642	3.655	0.053	1.377	3	0	18	0.204
13	-258.53	-51.11	188.390	206.200	620.715	455.769	29.893	3.353	0.037	2.105	3	1	22	0.118
14	-177.85	58.85	222.766	244.400	642.828	477.226	25.820	3.662	0.013	2.749	4	0	28	0.072
15 <sup>a</sup>	-187.10	39.84	219.372	224.700	684.901	513.061	25.715	3.726	0.013	2.969	4	1	28	0.059
16 <sup>a</sup>	-252.75	-99.88	147.721	198.880	586.774	405.374	33.802	2.060	0.059	1.892	4	1	18	0.177
17	-273.39	-91.46	170.651	210.150	607.611	427.704	30.323	1.859	0.042	2.421	5	0	20	0.125
18	-294.03	-83.04	193.582	221.420	627.054	449.130	27.354	1.678	0.029	2.950	6	1	22	0.088
19 <sup>a</sup>	-258.03	-102.32	148.235	183.880	570.984	391.477	34.119	2.038	0.068	1.892	3	1	18	0.204
20	-299.31	-85.48	194.096	206.420	613.182	436.322	27.585	1.798	0.034	2.950	5	1	22	0.102
21	-328.70	-74.22	216.599	220.110	614.840	436.340	25.482	1.545	0.034	3.089	4	1	24	0.102
22 <sup>a</sup>	-135.53	-19.66	133.291	193.800	604.447	412.348	35.942	2.699	0.039	1.578	3	1	20	0.177
23	-156.17	-11.24	156.221	205.070	624.405	434.400	32.137	2.541	0.028	1.937	4	0	22	0.125
24	-124.68	-36.63	110.427	168.570	577.373	382.971	40.725	2.745	0.068	0.829	1	1	18	0.289
25	-145.32	-28.21	133.357	179.840	599.295	406.173	36.159	2.625	0.048	1.358	2	0	20	0.204
26 <sup>a</sup>	-238.44	0.59	226.107	194.920	647.950	466.216	24.243	2.065	0.016	3.214	4	1	28	0.068
27	-300.39	-120.86	166.665	218.080	591.988	414.823	29.959	2.210	0.051	1.908	4	1	20	0.144
28	-285.03	-131.72	144.249	191.810	553.736	377.753	33.684	2.324	0.083	1.379	2	1	18	0.236
29	-285.03	-131.72	144.249	191.810	553.736	377.753	33.684	2.249	0.083	1.249	2	1	18	0.236
30 <sup>a</sup>	-305.67	-123.30	167.179	203.080	576.617	401.154	30.223	2.201	0.059	1.778	3	0	20	0.167
31	-326.31	-114.88	190.109	214.350	597.955	423.651	27.269	2.078	0.042	2.437	4	1	22	0.118
32	-326.31	-114.88	190.109	214.350	597.955	423.651	27.269	2.078	0.042	2.307	4	1	22	0.118
33	-352.23	-108.90	213.554	210.620	603.820	432.335	24.925	1.955	0.034	2.706	4	1	24	0.096
34	-154.32	-41.44	133.191	205.050	572.941	390.223	35.054	2.942	0.042	0.895	3	0	20	0.204
35 <sup>a</sup>	-172.32	-57.61	129.371	187.770	582.573	392.785	35.685	2.893	0.059	0.915	1	1	20	0.236
36 <sup>a</sup>	-463.81	-319.15	136.346	187.940	551.301	375.484	34.889	1.986	0.042	1.240	3	0	22	0.204
37 <sup>a</sup>	-484.45	-310.73	159.276	199.210	574.343	398.971	31.245	1.766	0.029	1.769	4	1	24	0.144
38	-505.09	-302.31	182.206	210.480	595.827	421.553	28.143	1.848	0.021	2.298	5	0	26	0.102
39	-525.73	-293.89	205.137	221.750	615.900	443.232	25.482	1.529	0.015	2.827	6	1	28	0.072
40 <sup>a</sup>	-546.37	-285.47	228.067	233.020	634.691	464.006	23.181	1.406	0.010	3.356	7	0	30	0.051
41	-546.37	-285.47	228.067	233.020	634.691	464.006	23.181	1.700	0.010	3.356	7	0	30	0.051
42 <sup>a</sup>	-489.73	-313.17	159.790	184.210	558.261	384.921	31.526	1.775	0.034	1.549	3	0	24	0.167
43	-510.37	-304.75	182.721	195.480	580.745	408.049	28.384	1.708	0.024	2.168	4	1	26	0.118
44	-556.93	-290.35	229.096	203.020	607.561	438.848	23.542	1.406	0.014	3.096	5	0	30	0.068
45	-577.57	-281.93	252.026	214.290	626.806	459.809	21.493	1.283	0.010	3.535	6	1	32	0.048
46 <sup>a</sup>	-367.23	-230.51	144.846	194.130	591.763	406.023	33.144	2.405	0.020	1.855	3	1	26	0.144
47	-423.58	-224.66	191.287	187.710	612.931	431.036	27.240	2.085	0.014	2.473	3	1	30	0.096
48	-418.30	-222.22	190.773	202.710	626.993	443.976	27.014	2.134	0.012	2.693	4	0	30	0.083
49 <sup>a</sup>	-444.22	-216.24	214.218	198.980	632.073	452.323	24.703	1.965	0.010	3.092	4	0	32	0.068
50	-464.86	-207.82	237.148	210.250	649.961	472.707	22.504	1.845	0.007	3.621	5	1	34	0.048
51	-480.22	-196.96	259.564	236.520	678.309	503.493	20.438	1.774	0.004	4.280	7	1	36	0.029

<sup>a</sup>Test Set.

**Table S2: Molecular topological descriptors computed by ChemSketch and MarvinSketch.**

No	H%	O%	C%	$\gamma$	n	D	log P	W	NHA	NHD	J	PSA
1	13.81	15.66	70.53	27.9	1.415	0.816	1.69	56	1	1	2.45	20.23
2	13.93	12.29	73.78	29.0	1.427	0.823	2.58	120	1	1	2.60	20.23
3	13.97	11.09	74.94	29.5	1.431	0.826	3.03	165	1	1	2.65	20.23
4	13.81	15.66	70.53	26.6	1.413	0.814	1.61	50	1	1	2.83	20.23
5	13.81	15.66	70.53	26.0	1.415	0.816	1.58	44	1	1	3.36	20.23
6 <sup>a</sup>	13.88	13.77	72.35	27.3	1.420	0.818	2.11	79	1	1	2.72	20.23
7	13.93	12.29	73.78	28.0	1.426	0.821	2.50	104	1	1	3.09	20.23
8	13.93	12.29	73.78	28.0	1.426	0.821	2.63	110	1	1	2.88	20.23
9	14.01	10.11	75.88	28.0	1.432	0.824	3.16	194	1	1	3.10	20.23
10	12.08	15.97	71.95	28.7	1.442	0.843	1.33	56	1	1	2.45	20.23
11	12.36	14.01	73.63	29.3	1.446	0.844	1.78	84	1	1	2.53	20.23
12	12.08	15.97	71.95	26.6	1.428	0.830	1.60	50	1	1	2.83	20.23
13	12.58	12.48	74.94	27.5	1.446	0.844	1.99	108	1	1	2.91	20.23
14	11.76	10.37	77.87	28.2	1.463	0.858	2.65	180	1	1	3.38	20.23
15 <sup>a</sup>	11.76	10.37	77.87	29.1	1.470	0.866	2.50	194	1	1	3.10	20.23
16 <sup>a</sup>	12.08	15.97	71.95	25.1	1.396	0.800	1.65	56	1	0	2.45	17.07
17	12.36	14.01	73.63	26.0	1.405	0.807	2.10	84	1	0	2.53	17.07
18	12.58	12.48	74.94	26.8	1.412	0.811	2.54	120	1	0	2.60	17.07
19 <sup>a</sup>	12.08	15.97	71.95	23.9	1.394	0.799	1.75	48	1	0	2.99	17.07
20	12.58	12.48	74.94	25.7	1.410	0.809	2.64	104	1	0	3.09	17.07
21	12.76	11.25	75.99	25.1	1.415	0.813	2.53	131	1	0	3.47	17.07
22 <sup>a</sup>	10.27	16.30	73.43	25.7	1.421	0.828	1.65	56	1	0	2.45	17.07
23	10.78	14.26	74.96	26.6	1.427	0.830	1.73	84	1	0	2.53	17.07
24	9.59	19.02	71.39	23.1	1.411	0.826	1.16	31	1	0	2.75	17.07
25	10.27	16.30	73.43	24.4	1.419	0.829	1.60	50	1	0	2.83	17.07
26 <sup>a</sup>	11.76	10.37	77.87	25.7	1.435	0.833	3.06	174	1	0	3.52	17.07
27	12.36	14.01	73.63	24.9	1.403	0.808	2.14	79	1	0	2.72	17.07
28	12.08	15.97	71.95	22.8	1.392	0.800	1.79	46	1	0	3.14	17.07
29	12.08	15.97	71.95	22.8	1.392	0.800	1.54	48	1	0	2.95	17.07
30 <sup>a</sup>	12.36	14.01	73.63	23.9	1.401	0.806	1.98	74	1	0	2.93	17.07
31	12.58	12.48	74.94	24.8	1.409	0.811	2.94	102	1	0	3.16	17.07
32	12.58	12.48	74.94	24.8	1.409	0.811	2.68	100	1	0	3.22	17.07
33	12.76	11.25	75.99	24.6	1.413	0.812	2.97	135	1	0	3.34	17.07
34	10.27	16.30	73.43	23.9	1.408	0.819	1.39	52	1	0	2.68	17.07
35 <sup>a</sup>	10.27	16.30	73.43	23.2	1.418	0.830	1.49	48	1	0	2.95	17.07
36 <sup>a</sup>	9.87	31.33	58.80	24.8	1.387	0.891	0.98	50	1	0	2.83	26.30
37 <sup>a</sup>	10.41	27.55	62.04	25.8	1.397	0.886	1.42	75	1	0	2.92	26.30
38	10.84	24.58	64.58	26.6	1.406	0.882	1.87	108	1	0	2.95	26.30
39	11.18	22.19	66.63	27.3	1.412	0.878	2.31	150	1	0	2.97	26.30
40 <sup>a</sup>	11.47	20.22	68.31	27.8	1.418	0.876	2.84	200	1	0	3.02	26.30
41	11.47	20.22	68.31	27.8	1.418	0.876	2.76	202	1	0	2.79	26.30
42 <sup>a</sup>	10.41	27.55	62.04	24.6	1.395	0.883	1.52	70	1	0	3.17	26.30
43	10.84	24.58	64.58	25.5	1.404	0.879	1.53	108	1	0	2.91	26.30
44	11.47	20.22	68.31	26.0	1.415	0.872	2.60	184	1	0	3.29	26.30
45	11.70	18.58	69.72	26.6	1.420	0.870	3.30	230	1	0	3.49	26.30
46 <sup>a</sup>	8.83	28.03	63.14	26.4	1.421	0.915	1.66	75	1	0	2.92	26.30
47	9.92	22.50	67.58	25.8	1.429	0.900	2.47	130	1	0	3.50	26.30
48	9.92	22.50	67.58	26.8	1.431	0.902	2.57	137	1	0	3.31	26.30
49 <sup>a</sup>	10.32	20.48	69.20	26.5	1.433	0.895	2.94	178	1	0	3.43	26.30
50	10.66	18.80	70.54	27.1	1.437	0.891	3.31	237	1	0	3.37	26.30
51	10.94	17.36	71.70	28.4	1.441	0.890	3.91	318	1	0	3.21	26.30

<sup>a</sup>Test Set.