

Supplementary Table S1. The calculated values of descriptors for the training set and the test set

Compound	Dipole mag	Dipole Y	Jurs FNSA3	Jurs PPSA3	Jurs RASA	Jurs RNCG	Jurs TASA	Jurs WPSA3	Shadow Xlength	Shadow Ylength
1	2.78276	-1.85793	-0.05817	12.0497	0.789	0.2978	298.81	4.56342	9.37799	8.52986
2	2.5589	-1.26552	-0.04745	16.5446	0.84229	0.23384	410.865	8.07037	12.8588	9.40876
3	3.31546	-2.83955	-0.04061	14.9006	0.89471	0.24733	430.263	7.16562	13.4578	9.43588
4	4.65281	-3.82274	-0.03728	19.2707	0.89051	0.20897	480.867	10.406	14.8058	9.9906
5	3.41185	0.60589	-0.04644	20.3258	0.8804	0.1896	500.466	11.5542	14.1567	11.0177
6	2.68052	-0.09197	-0.09043	10.8268	0.91262	0.14948	527.771	6.26112	14.4093	10.303
7	2.59092	0.21141	-0.15432	15.9672	0.60909	0.15608	336.145	8.81193	14.5949	9.88243
8	3.7454	-0.37094	-0.02844	17.3717	0.91604	0.22049	531.499	10.0793	15.9051	10.6028
9	1.92571	-0.12104	-0.04388	17.2537	0.87717	0.23543	466.816	9.18205	15.6689	9.54921
10	4.41717	4.14814	-0.1079	15.8292	0.72291	0.22021	378.155	8.28024	14.7858	9.52694
11	3.1645	-0.74749	-0.04351	19.7569	0.87361	0.21326	439.863	9.94757	14.3665	9.62304
12	3.06725	-0.49263	-0.04342	14.4146	0.90355	0.24398	447.759	7.14322	13.3188	9.9803
13	7.37706	4.53465	-0.10673	16.2572	0.72684	0.21876	382.49	8.55511	15.1703	9.68291
14	6.13607	4.03917	-0.10946	23.432	0.81464	0.13901	715.551	20.5818	19.7473	15.8236
15	1.54519	1.4911	-0.03183	25.9381	0.91858	0.24776	548.678	15.493	16.042	10.8469
16	2.78591	0.24692	-0.03849	31.9212	0.89304	0.16359	666.404	23.8202	20.8062	13.9337
17	2.43796	1.35655	-0.03342	25.6676	0.94738	0.21717	612.39	16.5915	16.7607	13.6542
18	1.77607	0.47718	-0.03378	25.2616	0.94999	0.2228	621.636	16.5302	16.5068	13.8092
19	2.89826	-0.879	-0.05094	24.6934	0.95227	0.17527	652.879	16.9297	17.9965	13.8449
20	2.35497	0.85069	-0.05661	24.5922	0.95021	0.16199	730.835	18.9146	20.6951	14.507
21	2.68656	1.34334	-0.04397	25.6674	0.91821	0.21085	633.342	17.7041	20.2177	12.2305
22	1.54779	-0.54301	-0.03352	25.8542	0.97119	0.21692	704.109	18.7441	20.8512	13.3689
23	3.90607	1.49209	-0.05612	27.7189	0.94807	0.16527	725.075	21.1992	21.0786	14.4328
24	6.85898	6.02415	-0.10047	24.1036	0.85555	0.18685	626.781	17.6583	19.7113	14.1777
25	3.83066	3.57582	-0.06846	33.9028	0.80929	0.13989	605.66	25.3721	18.7472	14.6629
26	3.44031	-1.58935	-0.04878	32.2548	0.90279	0.16526	748.165	26.7302	20.953	14.6403
27	5.19194	-0.37084	-0.0782	18.9891	0.85891	0.2448	518.796	11.4697	13.9155	12.588
28	2.07557	-1.67035	-0.05583	27.6883	0.80763	0.16681	502.381	17.2231	17.2342	11.9378
29	0.55285	-0.0224	-0.04953	27.8374	0.7957	0.1816	461.852	16.1577	17.8899	10.5882
30	0.74181	0.08698	-0.04534	28.5254	0.81482	0.17159	505.58	17.6993	18.0212	10.1882
31	2.10003	-1.56202	-0.063	28.5748	0.7923	0.1674	464.588	16.7554	18.1942	10.015
32	2.34709	-2.22452	-0.06504	29.3756	0.74095	0.15866	431.723	17.116	18.0042	10.2494
33	1.23523	-0.96696	-0.06861	28.7226	0.73874	0.18109	425.853	16.5573	17.8784	10.3972
34	0.66456	-0.03668	-0.04666	30.1304	0.81832	0.16263	515.526	18.9815	17.9268	11.4818
35	2.41743	0.54271	-0.0488	27.8519	0.83252	0.15845	563.533	18.8528	17.1663	13.9436
36	0.95777	0.03678	-0.05483	28.218	0.79823	0.17319	478.098	16.901	17.9719	10.097
37	1.55824	0.76292	-0.05503	27.4262	0.80397	0.17582	471.195	16.074	17.8504	9.3711

38	0.9003	0.4605	-0.05385	28.4752	0.78499	0.16289	487.383	17.6796	18.6799	9.44385
39	1.1439	0.39651	-0.05314	31.313	0.77623	0.15897	468.936	18.9166	18.0134	10.1944
40	0.72785	-0.26007	-0.04521	29.738	0.81858	0.16493	523.663	19.0239	19.1053	10.135
41	2.12939	-1.17769	-0.05156	32.3119	0.79374	0.15978	515.168	20.9715	20.4443	9.73426
42	0.66136	0.27894	-0.052	26.6295	0.81283	0.17174	505.37	16.5566	18.709	9.93407
43	3.04909	-1.30008	-0.05118	26.2699	0.83067	0.1613	554.984	17.5512	19.1383	10.1745
44	0.89458	0.60099	-0.04554	29.9966	0.83425	0.16128	576.348	20.7233	17.7011	10.9824
45	1.65929	-1.20962	-0.04838	32.5593	0.81315	0.15499	548.073	21.9453	20.0277	9.54898
46	1.81165	-1.25123	-0.05209	31.1867	0.80736	0.15467	538.979	20.8195	19.5698	9.43299
47	3.5703	-2.86791	-0.0558	25.6622	0.82633	0.1714	573.544	17.8117	20.0601	9.76527
48	2.34528	-1.28392	-0.05007	23.9364	0.83201	0.18014	535.002	15.3916	19.4559	9.58421
49	2.55553	-1.71448	-0.05137	25.3696	0.82831	0.17783	529.941	16.2309	19.082	9.27963
50	1.15623	-0.97088	-0.04708	25.0808	0.83515	0.18042	571.263	17.1558	18.9143	10.4893
51	3.79488	-2.93055	-0.06774	25.4094	0.76594	0.16039	479.452	15.9053	18.9844	9.90205
52*	4.76684	-4.25548	-0.04161	20.0674	0.92129	0.21012	536.638	11.689	15.7049	12.7305
53*	2.72328	0.39471	-0.06768	13.1035	0.88186	0.17177	489.167	7.26843	16.2486	9.55387
54*	4.59749	3.67342	-0.13135	16.0947	0.72571	0.20413	401.007	8.89335	14.7079	9.53877
55*	2.98662	-0.7448	-0.03827	28.6251	0.95668	0.19701	694.092	20.7681	20.3908	14.099
56*	0.88393	-0.85702	-0.03442	26.2079	0.98089	0.22002	667.619	17.8377	20.362	11.6841
57*	1.59421	-0.71937	-0.03366	28.3439	0.9683	0.19124	737.254	21.5807	20.0176	15.2617
58*	0.70933	0.05054	-0.04786	28.2216	0.8029	0.17651	483.673	17.0009	17.8769	10.3624
59*	0.73787	-0.03813	-0.06173	32.4008	0.7324	0.15005	434.353	19.2154	17.7839	9.52603
60*	0.68174	-0.23514	-0.04561	30.0019	0.8142	0.16495	519.299	19.135	19.0043	10.0527
61*	2.08849	-0.49807	-0.05448	31.4546	0.78768	0.15953	506.869	20.2408	20.0348	9.86939
62*	1.75227	0.63003	-0.04546	28.642	0.83314	0.16771	544.142	18.7065	18.3721	9.25482

*: test set compound