

Supplementary Table 1. Outcome of the docking analysis for all the molecules considered for this study. Molecules are represented based on their energy values. The Compound ID column represents the CID according to PubChem nomenclature. The end part of the Compound ID after the underscore (“_”) represents the different conformation number.

Compound ID	Cluster	Cluster Rank	deltaG	deltaG vdw	deltaG ligsolvnonpol	deltaG ligsolvpol	deltaG protsolvnonpol	deltaG protsolvpol	deltaG compsolvnonpol	deltaG compsolvpol	Surf Full	Solv Full	Intra Full	Inter Full	Full Fitness	Simple Fitness	Energy
CID70675472	7	1	-6.95	-35.35	8.89	-9.45	416.47	-3170.96	414.61	-3157.44	414.61	-3157.44	-4.58	-35.35	-2782.76	-20.88	-20.88
CID11068499	0	2	-8.05	-49.35	9.72	-12.12	416.47	-3170.96	413.87	-3154.07	413.87	-3154.07	24.16	-49.35	-2765.39	-20.02	-20.02
CID57417072_1	2	0	-7.29	-40.58	9.89	-11.55	416.47	-3170.96	414.12	-3154.75	414.12	-3154.75	14.98	-40.58	-2766.24	-18.61	-18.61
CID88293	0	0	-7.88	-49.78	9.31	-11.44	416.47	-3170.96	414.31	-3151.24	414.31	-3151.24	19.07	-49.78	-2767.64	-18.39	-18.39
CID56945244	1	5	-7.86	-49.59	9.37	-9.01	416.47	-3170.96	414.22	-3148.65	414.22	-3148.65	21.00	-49.59	-2763.03	-18.37	-18.37
CID10904578_1	4	0	-7.52	-43.19	9.60	-11.95	416.47	-3170.96	413.85	-3154.95	413.85	-3154.95	20.83	-43.19	-2763.47	-17.54	-17.54
CID153711_3	2	5	-7.88	-50.04	9.72	-10.90	416.47	-3170.96	413.63	-3148.69	413.63	-3148.69	22.73	-50.04	-2762.37	-17.44	-17.44
CID11100577_1	1	0	-8.00	-53.63	9.79	-10.74	416.47	-3170.96	413.97	-3145.36	413.97	-3145.36	23.46	-53.63	-2761.57	-17.40	-17.40
CID153711_12	8	0	-7.11	-42.45	9.98	-12.09	416.47	-3170.96	413.46	-3148.32	413.46	-3148.32	18.10	-42.45	-2759.21	-17.00	-17.00
CID153711	14	0	-7.20	-47.93	9.89	-11.39	416.47	-3170.96	413.76	-3141.16	413.76	-3141.16	17.77	-47.93	-2757.57	-16.51	-16.51
CID57417072	3	0	-7.24	-39.61	10.08	-10.09	416.47	-3170.96	413.99	-3153.49	413.99	-3153.49	13.53	-39.61	-2765.57	-16.31	-16.31
CID23238908	1	1	-7.19	-36.70	9.10	-9.20	416.47	-3170.96	413.94	-3157.69	413.94	-3157.69	18.58	-36.70	-2761.87	-15.25	-15.25
CID153711_1	20	0	-6.91	-40.17	10.02	-11.83	416.47	-3170.96	413.77	-3148.8	413.77	-3148.8	20.20	-40.17	-2755.00	-13.88	-13.88
CID10904578	13	0	-6.80	-34.87	10.03	-11.33	416.47	-3170.96	414.15	-3155.17	414.15	-3155.17	18.55	-34.87	-2757.34	-13.72	-13.72
CID153711_11	0	0	-7.47	-42.37	9.67	-11.03	416.47	-3170.96	414.41	-3155.23	414.41	-3155.23	18.61	-42.37	-2764.58	-13.64	-13.64
CID56945244_1	18	1	-6.71	-39.65	9.12	-9.87	416.47	-3170.96	413.75	-3145.68	413.75	-3145.68	17.02	-39.65	-2754.56	-13.54	-13.54
CID153711_10	3	0	-7.52	-46.86	9.73	-11.23	416.47	-3170.96	414.26	-3148.97	414.26	-3148.97	19.29	-46.86	-2762.28	-13.50	-13.50
CID153711_4	0	0	-7.89	-35.69	9.78	-11.85	416.47	-3170.96	415.78	-3175.1	415.78	-3175.1	20.03	-35.69	-2774.98	-13.42	-13.42
CID153711_5	14	0	-6.91	-43.19	9.85	-10.74	416.47	-3170.96	413.76	-3143.23	413.76	-3143.23	18.52	-43.19	-2754.14	-13.22	-13.22
CID88293_5	1	0	-7.26	-35.66	9.54	-11.60	416.47	-3170.96	414.77	-3163.55	414.77	-3163.55	19.11	-35.66	-2765.33	-13.16	-13.16
CID88293_1	12	0	-7.21	-44.04	9.30	-12.20	416.47	-3170.96	414.44	-3150.27	414.44	-3150.27	21.15	-44.04	-2758.72	-13.16	-13.16
CID153711_6	2	0	-6.99	-35.09	9.87	-11.35	416.47	-3170.96	414.32	-3158.56	414.32	-3158.56	17.38	-35.09	-2761.95	-13.07	-13.07
CID153711_7	9	0	-7.48	-50.69	9.79	-11.48	416.47	-3170.96	414.09	-3142.22	414.09	-3142.22	20.42	-50.69	-2758.41	-13.05	-13.05
CID153711_2	10	1	-7.10	-42.52	9.72	-11.54	416.47	-3170.96	414.06	-3148.91	414.06	-3148.91	19.89	-42.52	-2757.47	-12.71	-12.71
CID88293_2	1	0	-6.86	-29.35	9.62	-10.76	416.47	-3170.96	415.11	-3166.28	415.11	-3166.28	16.98	-29.35	-2763.54	-12.61	-12.61
CID88293_4	9	1	-7.13	-43.03	9.66	-11.52	416.47	-3170.96	413.71	-3148.03	413.71	-3148.03	21.82	-43.03	-2755.52	-12.59	-12.59
CID153711_9	0	0	-7.54	-42.64	9.54	-11.51	416.47	-3170.96	414.92	-3157.5	414.92	-3157.5	20.08	-42.64	-2765.14	-12.46	-12.46
CID153711_8	0	0	-7.89	-38.13	9.61	-11.28	416.47	-3170.96	415.42	-3170.53	415.42	-3170.53	23.16	-38.13	-2770.07	-11.73	-11.73
CID10372383	8	0	-7.22	-43.46	9.10	-11.11	416.47	-3170.96	414.44	-3150.55	414.44	-3150.55	19.57	-43.46	-2759.99	-11.71	-11.71
CID88293_3	26	0	-6.97	-39.20	9.62	-10.78	416.47	-3170.96	413.94	-3151	413.94	-3151	19.94	-39.20	-2756.32	-11.71	-11.71
CID11100577	10	1	-6.94	-40.06	9.53	-11.22	416.47	-3170.96	414.18	-3150.2	414.18	-3150.2	19.05	-40.06	-2757.03	-11.09	-11.09
CID303996	0	0	-8.30	-50.00	10.07	-12.53	416.47	-3170.96	414.50	-3157.99	414.50	-3157.99	188.04	-50.00	-2605.45	142.08	142.08
ID303994	6	0	-7.40	-40.91	10.04	-10.00	416.47	-3170.96	413.61	-3153.45	413.61	-3153.45	188.51	-40.91	-2592.24	144.29	144.29