

Additional File 3: Molprobit score of the best *Bhageerath*-H prediction

<b>S.No.</b>	<b>Target</b>	<b>Molprobit score of best <i>Bhageerath</i>-H prediction</b>
1	T0644	1.8
2	T0645	1.54
3	T0649	2.44
4	T0650	1.31
5	T0651	3.59
6	T0652	1.25
7	T0653	1.82
8	T0654	1.75
9	T0655	1.61
10	T0657	1.46
11	T0658	2.05
12	T0659	1.11
13	T0661	1.07
14	T0662	0.93
15	T0663	2.07
16	T0664	1.64
17	T0666	1.7
18	T0667	1.5
19	T0669	1.38
20	T0671	0.85
21	T0672	1.82
22	T0673	1.44
23	T0674	1.68
24	T0675	1.32
25	T0676	2.2
26	T0678	1.39
27	T0679	2.52
28	T0680	1.59
29	T0681	1.79
30	T0682	1.61
31	T0683	1.65
32	T0684	1.91
33	T0685	2.51
34	T0686	2.27
35	T0687	1.97
36	T0688	1.22
37	T0689	2.53

38	T0690	2.6
39	T0691	1.73
40	T0692	1.56
41	T0699	1.59
42	T0700	1.08
43	T0703	1.67
44	T0704	2.79
45	T0705	2.56
46	T0707	2.66
47	T0708	1.2
48	T0712	1.5
49	T0713	1
50	T0714	1.03
51	T0715	1.83
52	T0716	1.53
53	T0717	2.93
54	T0719	2.74
55	T0720	2.11
56	T0721	1
57	T0724	2.98
58	T0726	2.27
59	T0731	3.12
60	T0733	1.32
61	T0735	2.49
62	T0736	1.65
63	T0737	1.95
64	T0738	0.96
65	T0742	2.53
66	T0743	2.36
67	T0744	2.81
68	T0746	2.05
69	T0747	0.85
70	T0749	1.25
71	T0752	2.12
72	T0753	1.34
73	T0755	3.71
74	T0756	1.85
75	T0757	1.31
<b>Average</b>		<b>1.84</b>