

Supplementary Material VIII. The prediction accuracies obtained by methods based on chemical interactions, chemical similarities and integrated scores on $DS^{(i)}$ evaluated by jackknife test.

Prediction order	Prediction based on chemical interactions ($k=5$) (%)	Prediction based on chemical similarities (ECFP4, $k=2$) (%)	Prediction based on integrated scores (%)
1	58.48	42.52	58.82
2	22.88	18.19	23.44
3	7.92	8.59	8.37
4	5.58	6.36	5.58
5	3.79	3.35	4.46
6	2.01	4.24	2.90
7	1.90	3.46	2.46
8	2.23	3.35	2.68
9	1.56	2.46	2.23
10	1.12	1.79	1.56
11	1.00	2.46	1.00
12	0.67	1.00	1.23
13	1.45	2.12	0.78
14	0.78	1.79	1.00
15	0.45	1.45	0.45
16	0.22	2.01	1.00
17	1.23	1.34	1.23
18	0.33	1.23	0.56
19	1.00	1.12	0.33
20	1.12	1.23	0.89
21	0.56	1.45	0.56
22	1.34	1.56	0.67
23	0.89	1.00	0.56
24	0.45	1.00	0.56
25	0.78	1.23	0.67
26	0.89	0.89	0.00
27	0.45	0.89	0.22

28	0.56	0.67	0.33
29	0.33	0.22	0.11
30	0.89	0.78	0.22
31	0.11	0.56	0.22
32	0.45	1.23	0.33
33	0.67	0.11	0.22
34	0.33	0.56	0.11
35	0.33	1.12	0.56
36	0.56	0.33	0.56
37	0.78	0.33	0.56
38	0.11	0.33	0.11
39	0.45	0.33	0.11
40	0.33	0.45	0.00
41	0.33	0.33	0.11
42	0.33	0.45	0.22
43	0.33	0.78	0.22
44	0.33	0.45	0.33
45	0.56	0.56	0.45
46	0.67	0.33	0.11
47	0.11	0.33	0.33
48	0.33	0.11	0.11
49	0.00	0.22	0.22
50	0.11	0.45	0.22
51	0.56	0.78	0.45
52	0.11	0.22	0.11
53	0.33	0.78	0.45
54	0.22	0.33	0.22
55	0.00	0.11	0.11
56	0.11	0.11	0.11