Supplementary Material V. The prediction accuracies with different *k* obtained by the method based on chemical interactions on $DS^{(i)}$ evaluated by jackknife test

Order	k=1	k=2	k=3	k=4	k=5	k=6	k=7	k=8	k=9	k=10	k=11	k=12	k=13	k=14	k=15	k=895
1	47.77%	55.92%	57.59%	58.26%	58.48%	58.37%	58.15%	58.04%	58.04%	58.04%	57.81%	57.81%	57.70%	57.70%	57.70%	57.59%
2	23.55%	22.77%	21.99%	22.88%	22.88%	22.66%	23.10%	23.10%	23.21%	23.10%	23.33%	23.55%	23.66%	23.55%	23.55%	23.66%
3	12.39%	9.15%	9.60%	8.15%	7.92%	8.26%	7.92%	7.92%	7.92%	8.26%	8.37%	8.15%	8.15%	8.26%	8.26%	8.26%
4	6.36%	5.58%	5.80%	5.02%	5.58%	5.47%	5.58%	5.58%	5.58%	5.47%	5.36%	5.36%	5.36%	5.36%	5.36%	5.36%
5	5.36%	4.13%	3.24%	4.13%	3.79%	4.02%	3.91%	4.13%	3.91%	3.79%	3.79%	3.79%	3.79%	3.79%	3.79%	3.79%
6	2.46%	2.57%	2.34%	2.34%	2.01%	1.90%	2.01%	1.79%	1.90%	1.90%	1.90%	1.90%	1.90%	1.90%	1.90%	1.90%
7	2.57%	2.90%	2.46%	2.12%	1.90%	2.12%	2.12%	2.01%	2.01%	2.01%	2.01%	1.90%	1.90%	1.90%	1.90%	1.90%
8	2.34%	2.23%	2.12%	2.01%	2.23%	2.12%	2.01%	2.23%	2.23%	2.23%	2.23%	2.34%	2.34%	2.34%	2.34%	2.34%
9	2.01%	1.23%	1.12%	1.34%	1.56%	1.45%	1.34%	1.34%	1.34%	1.34%	1.34%	1.34%	1.34%	1.34%	1.34%	1.34%
10	1.00%	1.00%	1.00%	1.00%	1.12%	1.12%	1.34%	1.34%	1.34%	1.34%	1.34%	1.34%	1.34%	1.34%	1.34%	1.34%
11	1.79%	1.00%	1.12%	1.12%	1.00%	1.00%	1.00%	1.00%	1.00%	1.00%	1.00%	1.00%	1.00%	1.00%	1.00%	1.00%

12	1.34%	0.78%	0.67%	0.78%	0.67%	0.67%	0.67%	0.67%	0.67%	0.67%	0.67%	0.67%	0.67%	0.67%	0.67%	0.67%
13	1.67%	1.45%	1.56%	1.45%	1.45%	1.45%	1.45%	1.45%	1.45%	1.45%	1.45%	1.45%	1.45%	1.45%	1.45%	1.45%
14	0.78%	0.89%	0.89%	0.89%	0.78%	0.78%	0.78%	0.78%	0.78%	0.78%	0.78%	0.78%	0.78%	0.78%	0.78%	0.78%
15	0.78%	0.33%	0.33%	0.33%	0.45%	0.45%	0.45%	0.45%	0.45%	0.45%	0.45%	0.45%	0.45%	0.45%	0.45%	0.45%
16	0.22%	0.22%	0.22%	0.22%	0.22%	0.22%	0.22%	0.22%	0.22%	0.22%	0.22%	0.22%	0.22%	0.22%	0.22%	0.22%
17	1.00%	1.23%	1.23%	1.23%	1.23%	1.23%	1.23%	1.23%	1.23%	1.23%	1.23%	1.23%	1.23%	1.23%	1.23%	1.23%
18	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%
19	1.00%	1.00%	1.00%	1.00%	1.00%	1.00%	1.00%	1.00%	1.00%	1.00%	1.00%	1.00%	1.00%	1.00%	1.00%	1.00%
20	1.23%	1.12%	1.23%	1.12%	1.12%	1.12%	1.12%	1.12%	1.12%	1.12%	1.12%	1.12%	1.12%	1.12%	1.12%	1.12%
21	0.33%	0.56%	0.56%	0.67%	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%
22	1.23%	1.23%	1.23%	1.23%	1.34%	1.34%	1.34%	1.34%	1.34%	1.34%	1.34%	1.34%	1.34%	1.34%	1.34%	1.34%
23	0.89%	0.89%	0.89%	0.89%	0.89%	0.89%	0.89%	0.89%	0.89%	0.89%	0.89%	0.89%	0.89%	0.89%	0.89%	0.89%
24	0.56%	0.45%	0.45%	0.45%	0.45%	0.45%	0.45%	0.45%	0.45%	0.45%	0.45%	0.45%	0.45%	0.45%	0.45%	0.45%

25	0.78%	0.78%	0.78%	0.78%	0.78%	0.78%	0.78%	0.78%	0.78%	0.78%	0.78%	0.78%	0.78%	0.78%	0.78%	0.78%
26	0.89%	0.89%	0.89%	0.89%	0.89%	0.89%	0.89%	0.89%	0.89%	0.89%	0.89%	0.89%	0.89%	0.89%	0.89%	0.89%
27	0.45%	0.45%	0.45%	0.45%	0.45%	0.45%	0.45%	0.45%	0.45%	0.45%	0.45%	0.45%	0.45%	0.45%	0.45%	0.45%
28	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%
29	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%
30	0.89%	0.89%	0.89%	0.89%	0.89%	0.89%	0.89%	0.89%	0.89%	0.89%	0.89%	0.89%	0.89%	0.89%	0.89%	0.89%
31	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%
32	0.45%	0.45%	0.45%	0.45%	0.45%	0.45%	0.45%	0.45%	0.45%	0.45%	0.45%	0.45%	0.45%	0.45%	0.45%	0.45%
33	0.67%	0.67%	0.67%	0.67%	0.67%	0.67%	0.67%	0.67%	0.67%	0.67%	0.67%	0.67%	0.67%	0.67%	0.67%	0.67%
34	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%
35	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%
36	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%
37	0.78%	0.78%	0.78%	0.78%	0.78%	0.78%	0.78%	0.78%	0.78%	0.78%	0.78%	0.78%	0.78%	0.78%	0.78%	0.78%

38	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%
39	0.45%	0.45%	0.45%	0.45%	0.45%	0.45%	0.45%	0.45%	0.45%	0.45%	0.45%	0.45%	0.45%	0.45%	0.45%	0.45%
40	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%
41	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%
42	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%
43	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%
44	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%
45	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%
46	0.67%	0.67%	0.67%	0.67%	0.67%	0.67%	0.67%	0.67%	0.67%	0.67%	0.67%	0.67%	0.67%	0.67%	0.67%	0.67%
47	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%
48	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%
49	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
50	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%

51	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%	0.56%
52	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%
53	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%	0.33%
54	0.22%	0.22%	0.22%	0.22%	0.22%	0.22%	0.22%	0.22%	0.22%	0.22%	0.22%	0.22%	0.22%	0.22%	0.22%	0.22%
55	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
56	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%	0.11%