

Supplementary Material IX. The prediction accuracies obtained by three methods on $DS^{(i)}$, $DS^{(s)}$, DS_2 , evaluated by jackknife test.

Order	The integrated method on DS_2 (%)	The method based on chemical interactions on $DS^{(i)}$ (%)	The method based on chemical similarities on $DS^{(s)}$ (%)
1	53.66	58.48	47.27
2	18.69	22.88	13.15
3	7.44	7.92	6.79
4	5.40	5.58	5.17
5	3.69	3.79	3.55
6	3.05	2.01	4.43
7	2.54	1.90	3.40
8	1.84	2.23	1.33
9	2.10	1.56	2.81
10	1.34	1.12	1.62
11	1.53	1.00	2.22
12	1.02	0.67	1.48
13	1.40	1.45	1.33
14	1.21	0.78	1.77
15	1.08	0.45	1.92
16	1.02	0.22	2.07
17	1.21	1.23	1.18
18	0.45	0.33	0.59
19	0.64	1.00	0.15
20	0.89	1.12	0.59

21	1.08	0.56	1.77
22	1.34	1.34	1.33
23	1.02	0.89	1.18
24	0.38	0.45	0.30
25	0.64	0.78	0.44
26	0.95	0.89	1.03
27	0.76	0.45	1.18
28	0.57	0.56	0.59
29	0.51	0.33	0.74
30	0.64	0.89	0.30
31	0.19	0.11	0.30
32	0.70	0.45	1.03
33	0.57	0.67	0.44
34	0.25	0.33	0.15
35	0.32	0.33	0.30
36	0.45	0.56	0.30
37	0.76	0.78	0.74
38	0.25	0.11	0.44
39	0.45	0.45	0.44
40	0.25	0.33	0.15
41	0.51	0.33	0.74
42	0.32	0.33	0.30

43	0.38	0.33	0.44
44	0.64	0.33	1.03
45	0.57	0.56	0.59
46	0.45	0.67	0.15
47	0.06	0.11	0.00
48	0.25	0.33	0.15
49	0.25	0.00	0.59
50	0.25	0.11	0.44
51	0.38	0.56	0.15
52	0.06	0.11	0.00
53	0.38	0.33	0.44
54	0.38	0.22	0.59
55	0.13	0.00	0.30
56	0.19	0.11	0.30