

Supplementary Material IV. The performance of the method based on chemical similarities, where similarity scores were computed based on 8 types of fingerprints and *k* was set to 1, 2, ..., 15, 1732.

(1) Similarity scores with fingerprint ECFP_2

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=1732
1	45.01%	48.47%	48.70%	48.12%	47.55%	46.22%	45.82%	45.41%	44.89%	44.32%	43.22%	42.47%	41.95%	41.43%	41.26%	13.10%
2	19.97%	18.87%	18.70%	18.64%	18.70%	19.45%	19.27%	19.27%	18.81%	18.93%	19.16%	18.87%	18.35%	18.18%	17.71%	16.68%
3	8.48%	7.39%	7.85%	8.31%	8.71%	9.00%	8.42%	8.08%	8.42%	7.91%	7.85%	8.19%	8.71%	7.91%	8.02%	7.56%
4	4.79%	5.83%	6.00%	5.71%	5.31%	5.14%	6.12%	6.29%	6.23%	6.35%	6.46%	6.23%	5.77%	6.58%	6.52%	9.92%
5	4.50%	4.96%	4.67%	5.71%	5.48%	4.85%	4.39%	4.04%	3.75%	3.87%	4.56%	4.56%	4.33%	4.15%	4.04%	5.37%
6	4.56%	3.40%	3.81%	3.12%	3.92%	4.15%	3.69%	3.81%	3.87%	4.33%	3.92%	3.98%	4.56%	5.14%	5.08%	4.21%
7	3.64%	3.40%	2.94%	2.54%	2.60%	2.94%	3.75%	3.69%	4.10%	3.52%	3.29%	3.58%	3.52%	3.12%	3.35%	4.15%
8	1.90%	3.12%	2.77%	3.29%	2.89%	2.77%	2.60%	2.71%	2.37%	2.65%	3.17%	3.06%	2.60%	3.06%	2.89%	3.35%
9	2.37%	2.48%	2.37%	2.31%	1.90%	2.25%	2.19%	2.19%	2.60%	2.42%	2.25%	2.19%	2.25%	2.19%	2.71%	4.33%
10	2.19%	2.02%	2.25%	1.79%	2.08%	1.67%	2.02%	2.37%	1.96%	2.19%	2.02%	2.48%	2.25%	2.31%	1.79%	2.89%

11	2.14%	1.27%	1.50%	2.02%	2.25%	2.37%	1.79%	1.79%	1.85%	1.56%	1.85%	1.62%	2.08%	1.79%	1.96%	5.48%
12	1.79%	1.67%	1.85%	1.44%	1.67%	1.44%	1.44%	1.56%	2.14%	2.31%	2.02%	2.08%	1.96%	1.67%	1.67%	4.39%
13	1.56%	0.98%	1.21%	1.38%	1.15%	1.50%	1.96%	2.25%	1.56%	1.67%	1.62%	1.44%	1.90%	2.14%	2.08%	4.21%
14	1.50%	1.21%	0.98%	1.38%	1.62%	1.56%	1.90%	1.73%	2.14%	2.08%	1.96%	1.90%	1.90%	1.56%	1.50%	2.19%
15	1.38%	1.85%	1.33%	1.50%	1.56%	1.79%	1.38%	1.44%	1.15%	0.92%	1.21%	1.27%	1.27%	1.10%	1.10%	2.08%
16	0.81%	1.15%	1.62%	1.21%	1.38%	1.44%	1.10%	0.58%	1.15%	1.38%	1.10%	1.10%	1.21%	1.38%	1.44%	1.79%
17	1.10%	1.33%	0.92%	1.15%	1.10%	0.98%	1.04%	1.33%	0.81%	0.63%	0.81%	0.98%	0.92%	1.15%	1.15%	1.96%
18	1.44%	0.75%	0.81%	1.27%	1.21%	0.81%	1.10%	0.75%	0.52%	0.69%	0.81%	0.92%	0.98%	1.27%	1.15%	2.60%
19	1.21%	0.92%	1.33%	0.98%	0.69%	0.81%	0.52%	0.87%	0.98%	0.92%	1.04%	0.98%	0.92%	0.69%	0.75%	2.25%
20	0.92%	0.75%	0.87%	0.81%	0.69%	0.63%	0.81%	0.87%	1.33%	1.21%	1.10%	0.58%	0.35%	0.87%	0.98%	2.02%
21	0.69%	1.04%	0.75%	0.63%	0.69%	0.87%	0.98%	0.81%	0.87%	0.81%	0.92%	1.10%	1.04%	0.75%	0.98%	1.67%
22	1.21%	0.75%	0.75%	0.52%	0.63%	0.98%	0.75%	1.15%	0.92%	0.92%	0.81%	0.69%	1.27%	1.15%	1.10%	1.27%
23	0.81%	0.69%	0.69%	0.35%	0.46%	0.92%	0.75%	0.63%	0.58%	0.63%	0.69%	0.87%	0.81%	0.98%	0.75%	1.85%

24	0.52%	0.63%	0.35%	0.63%	0.46%	0.52%	0.87%	0.69%	0.81%	0.81%	0.35%	0.69%	0.58%	0.58%	0.63%	1.38%
25	0.63%	1.04%	0.52%	0.81%	0.63%	0.69%	0.92%	0.63%	1.04%	0.75%	0.98%	0.81%	0.23%	0.46%	0.40%	1.27%
26	0.87%	0.69%	0.92%	0.46%	0.98%	0.46%	0.58%	0.69%	0.52%	0.69%	0.87%	0.75%	0.69%	0.40%	0.69%	0.92%
27	0.69%	0.52%	0.58%	0.35%	0.52%	0.63%	0.58%	0.63%	0.75%	0.81%	0.87%	0.58%	0.69%	0.63%	0.63%	1.04%
28	0.35%	0.69%	0.46%	0.92%	0.81%	0.63%	0.69%	0.58%	0.35%	0.35%	0.52%	0.75%	0.69%	0.63%	0.75%	0.87%
29	0.58%	0.29%	0.75%	0.98%	0.63%	0.52%	0.35%	0.87%	0.52%	0.75%	1.10%	1.10%	1.21%	1.04%	0.75%	1.15%
30	0.63%	0.52%	0.63%	0.58%	0.40%	0.46%	0.40%	0.35%	0.75%	0.98%	0.46%	0.92%	1.04%	0.69%	0.69%	1.10%
31	0.40%	0.46%	0.58%	0.52%	0.52%	0.52%	0.46%	0.52%	0.52%	0.69%	0.63%	0.40%	0.40%	0.69%	1.04%	0.75%
32	0.92%	0.40%	0.75%	0.69%	0.58%	0.58%	0.63%	0.23%	0.40%	0.29%	0.63%	0.69%	0.81%	1.15%	0.98%	0.75%
33	0.75%	0.75%	0.69%	0.63%	0.63%	0.35%	0.35%	0.52%	0.75%	0.75%	0.58%	0.81%	0.87%	0.63%	0.46%	1.62%
34	0.29%	0.81%	0.58%	0.40%	0.29%	0.46%	0.69%	0.98%	0.87%	0.58%	0.58%	0.63%	0.40%	0.69%	0.75%	0.98%
35	0.46%	0.52%	0.46%	0.52%	0.58%	0.52%	0.40%	0.46%	0.29%	0.58%	0.58%	0.29%	0.52%	0.52%	0.58%	0.75%
36	0.40%	0.23%	0.35%	0.40%	0.46%	0.35%	0.69%	0.52%	0.35%	0.35%	0.46%	0.40%	0.69%	0.52%	0.46%	0.98%

37	0.35%	0.46%	0.29%	0.35%	0.52%	0.69%	0.52%	0.52%	0.29%	0.40%	0.46%	0.35%	0.69%	0.40%	0.92%	0.75%
38	0.29%	0.63%	0.23%	0.29%	0.40%	0.58%	0.29%	0.52%	0.52%	0.58%	0.46%	0.69%	0.58%	1.04%	0.69%	0.58%
39	0.23%	0.17%	0.35%	0.63%	0.40%	0.46%	0.35%	0.17%	0.40%	0.29%	0.75%	0.63%	0.58%	0.87%	0.87%	0.69%
40	0.52%	0.35%	0.35%	0.17%	0.29%	0.40%	0.17%	0.17%	0.35%	0.69%	0.52%	0.52%	0.46%	0.40%	0.69%	0.69%
41	0.69%	0.17%	0.58%	0.40%	0.58%	0.23%	0.46%	0.29%	0.52%	0.52%	0.46%	0.58%	0.63%	0.58%	0.40%	0.46%
42	0.75%	0.17%	0.17%	0.29%	0.23%	0.35%	0.46%	0.52%	0.46%	0.40%	0.29%	0.52%	0.29%	0.46%	0.63%	0.87%
43	0.23%	0.35%	0.17%	0.23%	0.35%	0.52%	0.52%	0.69%	0.52%	0.52%	0.69%	0.75%	0.81%	0.69%	0.69%	0.75%
44	0.40%	0.29%	0.17%	0.12%	0.35%	0.46%	0.87%	0.63%	0.40%	0.52%	0.23%	0.35%	0.63%	0.69%	0.40%	0.58%
45	0.00%	0.29%	0.35%	0.52%	0.35%	0.17%	0.35%	0.29%	0.52%	0.23%	0.46%	0.23%	0.29%	0.52%	0.69%	0.58%
46	0.17%	0.40%	0.46%	0.35%	0.52%	0.52%	0.17%	0.17%	0.40%	0.52%	0.46%	0.46%	0.40%	0.17%	0.29%	0.23%
47	0.46%	0.35%	0.52%	0.46%	0.12%	0.35%	0.35%	0.52%	0.23%	0.29%	0.29%	0.35%	0.23%	0.29%	0.23%	0.35%
48	0.23%	0.35%	0.23%	0.35%	0.23%	0.17%	0.23%	0.29%	0.12%	0.23%	0.23%	0.52%	0.17%	0.23%	0.23%	0.29%
49	0.29%	0.46%	0.35%	0.23%	0.52%	0.40%	0.35%	0.35%	0.58%	0.46%	0.46%	0.17%	0.58%	0.40%	0.52%	0.35%

50	0.52%	0.35%	0.23%	0.29%	0.23%	0.29%	0.35%	0.40%	0.52%	0.46%	0.29%	0.23%	0.23%	0.46%	0.40%	0.46%
51	0.46%	0.40%	0.46%	0.40%	0.35%	0.29%	0.17%	0.29%	0.29%	0.40%	0.52%	0.52%	0.63%	0.46%	0.40%	0.40%
52	0.23%	0.35%	0.35%	0.29%	0.29%	0.23%	0.40%	0.23%	0.29%	0.17%	0.23%	0.46%	0.35%	0.40%	0.40%	0.35%
53	0.12%	0.23%	0.23%	0.29%	0.23%	0.35%	0.23%	0.29%	0.35%	0.23%	0.17%	0.17%	0.17%	0.17%	0.17%	0.23%
54	0.46%	0.29%	0.29%	0.35%	0.29%	0.23%	0.23%	0.23%	0.23%	0.29%	0.46%	0.35%	0.35%	0.35%	0.35%	0.35%
55	0.23%	0.29%	0.23%	0.17%	0.29%	0.40%	0.46%	0.46%	0.29%	0.35%	0.17%	0.23%	0.17%	0.17%	0.17%	0.17%
56	0.23%	0.12%	0.06%	0.06%	0.06%	0.00%	0.00%	0.00%	0.17%	0.17%	0.29%	0.29%	0.35%	0.35%	0.35%	0.35%

(2) Similarity scores with fingerprint ECFP_4

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=1732
1	46.16%	49.39%	49.34%	49.22%	49.22%	48.47%	47.43%	46.91%	46.57%	45.99%	45.99%	45.59%	44.89%	44.37%	43.97%	16.27%
2	19.85%	18.52%	18.58%	18.98%	18.64%	18.93%	19.85%	19.91%	19.56%	19.27%	18.06%	17.89%	17.95%	18.12%	17.77%	15.18%
3	8.37%	7.91%	8.94%	8.60%	8.89%	8.77%	8.54%	8.08%	8.60%	8.94%	8.83%	8.60%	9.00%	8.71%	8.89%	7.79%
4	4.96%	5.71%	5.31%	4.79%	4.62%	4.96%	5.31%	6.17%	5.77%	5.71%	5.89%	6.23%	5.71%	5.60%	5.25%	8.94%

5	4.15%	3.52%	4.04%	4.85%	4.67%	4.50%	4.15%	3.98%	3.92%	3.58%	4.10%	3.87%	4.21%	4.27%	4.67%	6.35%
6	3.58%	4.33%	3.87%	3.81%	4.10%	3.64%	3.75%	3.29%	3.81%	4.04%	4.15%	4.39%	3.98%	4.21%	3.87%	5.08%
7	3.40%	3.40%	2.42%	2.89%	2.71%	3.00%	3.00%	3.58%	3.58%	3.75%	3.81%	3.12%	3.40%	3.46%	3.81%	2.77%
8	1.90%	1.79%	2.54%	2.48%	2.37%	2.77%	2.71%	2.65%	2.60%	2.89%	2.54%	3.06%	2.89%	2.77%	2.48%	3.12%
9	2.37%	1.96%	2.37%	2.37%	2.60%	2.71%	2.94%	2.48%	2.48%	1.90%	2.25%	1.96%	2.25%	1.67%	1.90%	4.21%
10	2.25%	2.14%	2.19%	2.19%	2.02%	1.79%	1.62%	1.90%	1.62%	1.90%	1.67%	2.25%	1.79%	2.08%	1.79%	3.06%
11	1.04%	2.08%	2.25%	1.79%	1.85%	1.50%	1.67%	1.38%	1.73%	1.67%	1.79%	1.96%	2.19%	2.25%	2.37%	6.29%
12	2.08%	1.79%	1.27%	0.87%	1.10%	0.69%	1.15%	1.73%	1.50%	2.08%	2.25%	2.31%	2.14%	2.14%	1.62%	4.79%
13	1.44%	1.27%	1.67%	1.67%	1.44%	2.08%	1.50%	1.62%	1.62%	1.04%	1.15%	0.92%	1.38%	1.44%	1.79%	3.29%
14	1.56%	1.27%	1.04%	1.33%	1.67%	1.79%	1.50%	1.62%	0.92%	1.27%	1.04%	0.98%	0.92%	1.27%	1.44%	2.02%
15	2.14%	0.98%	1.38%	1.50%	1.15%	1.62%	1.50%	1.21%	1.56%	1.33%	1.15%	1.38%	1.62%	1.33%	1.62%	2.65%
16	1.50%	1.56%	1.15%	1.10%	1.50%	0.98%	1.27%	1.38%	1.44%	1.50%	1.73%	1.27%	0.92%	1.38%	1.33%	1.85%
17	0.81%	0.92%	1.04%	1.21%	1.04%	1.04%	1.04%	0.75%	1.15%	1.15%	1.33%	1.33%	1.21%	1.10%	1.21%	2.25%

18	0.92%	1.04%	0.92%	0.92%	0.98%	0.98%	1.62%	1.04%	1.44%	1.10%	0.87%	1.10%	1.21%	1.15%	1.21%	2.14%
19	0.81%	0.81%	1.04%	0.92%	1.21%	1.04%	0.63%	0.92%	0.63%	0.87%	0.87%	0.98%	0.63%	0.69%	0.52%	2.31%
20	1.10%	0.98%	0.52%	1.04%	0.69%	0.98%	0.63%	0.75%	0.63%	0.75%	1.15%	0.58%	0.87%	0.87%	1.04%	1.67%
21	0.92%	1.27%	0.63%	0.52%	0.35%	0.63%	0.63%	0.69%	0.63%	0.81%	0.69%	0.92%	0.98%	0.98%	0.81%	1.21%
22	0.92%	0.75%	0.81%	0.81%	0.58%	0.35%	0.81%	0.81%	0.63%	0.58%	0.46%	0.52%	0.81%	0.92%	0.98%	1.33%
23	0.92%	0.98%	0.63%	0.58%	0.81%	1.04%	0.63%	0.63%	0.63%	0.87%	1.10%	1.15%	1.10%	0.63%	0.87%	1.67%
24	0.87%	0.75%	1.04%	0.52%	0.92%	0.58%	0.46%	0.58%	0.98%	0.75%	0.63%	0.75%	0.69%	0.75%	0.69%	1.96%
25	0.69%	0.46%	0.52%	0.92%	0.52%	0.58%	0.52%	0.69%	0.69%	0.58%	0.69%	0.81%	0.29%	0.46%	0.46%	0.98%
26	0.92%	0.63%	0.58%	0.17%	0.35%	0.40%	0.75%	0.81%	0.63%	0.75%	0.58%	0.69%	0.92%	0.63%	0.40%	1.04%
27	0.92%	0.52%	0.75%	0.81%	0.87%	0.98%	0.81%	0.75%	0.69%	0.75%	0.58%	0.40%	0.40%	0.63%	0.52%	0.81%
28	0.23%	0.58%	0.87%	0.69%	0.75%	0.29%	0.63%	0.69%	0.58%	0.69%	0.75%	0.75%	0.75%	0.69%	0.81%	1.10%
29	0.87%	0.92%	0.63%	0.87%	0.58%	0.87%	0.46%	0.35%	0.35%	0.46%	0.63%	0.75%	0.46%	0.75%	0.46%	1.04%
30	0.52%	0.58%	0.81%	0.23%	0.40%	0.52%	0.69%	0.75%	0.69%	0.46%	0.58%	0.58%	0.98%	0.46%	0.75%	1.04%

31	0.40%	0.46%	0.46%	0.63%	0.69%	0.58%	0.52%	0.63%	0.75%	0.52%	0.46%	0.52%	0.81%	0.98%	0.58%	0.52%
32	0.40%	0.46%	0.46%	0.81%	0.69%	0.46%	0.63%	0.63%	0.40%	0.58%	0.63%	0.46%	0.81%	0.81%	1.04%	0.69%
33	0.81%	0.63%	0.35%	0.81%	0.46%	0.81%	0.69%	0.46%	0.52%	0.63%	0.63%	0.63%	0.52%	0.75%	1.04%	1.04%
34	0.63%	0.58%	0.35%	0.29%	0.29%	0.29%	0.17%	0.29%	0.46%	0.58%	0.63%	0.92%	0.40%	0.40%	0.40%	0.87%
35	0.46%	0.46%	0.87%	0.23%	0.52%	0.46%	0.81%	0.75%	0.46%	0.69%	0.58%	0.40%	0.35%	0.58%	0.87%	1.27%
36	0.75%	0.12%	0.29%	0.52%	0.52%	0.81%	0.69%	0.63%	0.75%	0.46%	0.52%	0.46%	0.40%	0.52%	0.46%	0.63%
37	0.29%	0.52%	0.35%	0.63%	0.75%	0.46%	0.40%	0.46%	0.46%	0.23%	0.23%	0.12%	0.63%	0.81%	0.69%	0.87%
38	0.46%	0.29%	0.75%	0.40%	0.40%	0.35%	0.46%	0.52%	0.69%	0.35%	0.52%	0.46%	0.75%	0.40%	0.75%	0.81%
39	0.35%	0.46%	0.17%	0.17%	0.17%	0.40%	0.23%	0.17%	0.29%	0.46%	0.35%	0.87%	0.52%	0.63%	0.52%	0.63%
40	0.12%	0.35%	0.23%	0.35%	0.35%	0.23%	0.23%	0.46%	0.29%	0.69%	0.58%	0.40%	0.69%	0.75%	0.58%	0.63%
41	0.40%	0.35%	0.35%	0.29%	0.40%	0.12%	0.23%	0.29%	0.52%	0.63%	0.46%	0.75%	0.46%	0.40%	0.46%	0.46%
42	0.40%	0.52%	0.12%	0.40%	0.17%	0.29%	0.58%	0.46%	0.29%	0.40%	0.46%	0.35%	0.17%	0.40%	0.52%	0.69%
43	0.58%	0.35%	0.63%	0.29%	0.23%	0.63%	0.46%	0.40%	0.46%	0.40%	0.69%	0.40%	0.40%	0.29%	0.40%	0.29%

44	0.40%	0.40%	0.40%	0.63%	0.98%	0.58%	0.40%	0.46%	0.40%	0.46%	0.40%	0.46%	0.58%	0.35%	0.46%	0.29%
45	0.12%	0.40%	0.29%	0.40%	0.29%	0.52%	0.46%	0.46%	0.63%	0.40%	0.23%	0.40%	0.52%	0.69%	0.46%	0.63%
46	0.52%	0.52%	0.52%	0.35%	0.29%	0.29%	0.58%	0.35%	0.29%	0.46%	0.46%	0.46%	0.23%	0.46%	0.52%	0.58%
47	0.58%	0.12%	0.23%	0.29%	0.35%	0.29%	0.29%	0.00%	0.35%	0.40%	0.46%	0.35%	0.52%	0.40%	0.35%	0.35%
48	0.29%	0.29%	0.35%	0.23%	0.23%	0.35%	0.29%	0.63%	0.40%	0.17%	0.35%	0.52%	0.46%	0.35%	0.46%	0.40%
49	0.17%	0.35%	0.17%	0.17%	0.12%	0.12%	0.23%	0.58%	0.35%	0.35%	0.23%	0.17%	0.40%	0.46%	0.35%	0.29%
50	0.23%	0.52%	0.35%	0.23%	0.17%	0.35%	0.35%	0.23%	0.40%	0.23%	0.23%	0.29%	0.35%	0.35%	0.40%	0.46%
51	0.58%	0.12%	0.17%	0.29%	0.29%	0.35%	0.23%	0.12%	0.35%	0.63%	0.58%	0.46%	0.46%	0.40%	0.40%	0.35%
52	0.17%	0.35%	0.46%	0.35%	0.35%	0.17%	0.17%	0.29%	0.17%	0.17%	0.29%	0.40%	0.35%	0.35%	0.35%	0.40%
53	0.35%	0.29%	0.17%	0.35%	0.46%	0.29%	0.40%	0.35%	0.29%	0.23%	0.35%	0.29%	0.29%	0.29%	0.29%	0.29%
54	0.23%	0.23%	0.23%	0.23%	0.17%	0.23%	0.06%	0.12%	0.23%	0.23%	0.23%	0.23%	0.23%	0.23%	0.23%	0.23%
55	0.29%	0.29%	0.35%	0.29%	0.35%	0.40%	0.52%	0.40%	0.29%	0.35%	0.23%	0.17%	0.17%	0.17%	0.17%	0.17%
56	0.17%	0.12%	0.12%	0.06%	0.06%	0.06%	0.00%	0.06%	0.17%	0.17%	0.23%	0.29%	0.29%	0.29%	0.29%	0.29%

(3) Similarity scores with fingerprint ECFP₆

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=1732
1	45.82%	48.87%	48.87%	49.05%	49.11%	48.76%	48.24%	47.09%	46.86%	46.57%	46.45%	45.93%	45.35%	44.78%	44.26%	17.14%
2	19.27%	18.98%	19.62%	19.33%	18.75%	18.93%	18.93%	19.97%	19.73%	19.16%	18.64%	18.12%	18.06%	17.54%	17.54%	15.06%
3	9.35%	7.96%	8.08%	8.02%	8.25%	8.31%	8.60%	8.54%	8.89%	8.83%	8.37%	9.12%	8.89%	9.12%	9.06%	7.73%
4	4.85%	5.14%	5.42%	5.71%	5.42%	5.08%	4.96%	5.02%	4.73%	5.19%	5.37%	5.02%	5.25%	5.77%	6.06%	8.71%
5	4.04%	3.87%	4.67%	4.67%	4.90%	4.73%	4.50%	4.27%	4.50%	4.21%	4.50%	4.44%	4.39%	4.10%	3.98%	6.41%
6	3.06%	3.98%	2.77%	3.23%	3.12%	3.40%	3.52%	3.40%	3.17%	3.81%	4.04%	4.10%	4.15%	4.39%	4.15%	5.14%
7	2.65%	2.31%	3.06%	2.42%	2.77%	2.60%	3.06%	3.75%	3.87%	3.46%	3.75%	3.87%	4.39%	4.10%	4.04%	3.06%
8	2.31%	2.83%	2.42%	2.25%	2.77%	3.40%	3.40%	2.94%	3.23%	3.06%	2.71%	3.12%	2.71%	2.77%	3.06%	2.60%
9	3.06%	2.42%	2.37%	2.60%	2.65%	2.08%	2.65%	2.48%	1.79%	2.19%	2.25%	2.19%	1.90%	1.96%	1.67%	4.44%
10	1.73%	1.96%	2.14%	2.25%	2.31%	2.65%	1.56%	1.56%	2.08%	2.25%	2.31%	1.79%	1.73%	1.44%	1.50%	3.64%
11	1.50%	2.08%	2.08%	2.19%	1.62%	1.15%	1.38%	1.44%	1.56%	1.67%	1.56%	1.85%	1.90%	1.96%	1.79%	6.00%

12	1.33%	1.62%	2.02%	1.79%	1.33%	0.98%	1.38%	2.02%	1.90%	1.44%	1.56%	1.44%	1.73%	1.79%	2.02%	4.62%
13	2.19%	1.56%	1.44%	1.10%	1.10%	1.27%	1.15%	1.50%	1.21%	1.38%	1.10%	1.73%	1.62%	1.56%	1.85%	2.94%
14	2.02%	1.38%	1.10%	1.62%	1.56%	1.96%	1.96%	1.33%	1.10%	1.27%	1.62%	1.33%	1.50%	1.67%	1.21%	2.54%
15	1.27%	1.15%	0.92%	1.44%	1.44%	1.79%	1.38%	1.27%	1.67%	0.92%	1.33%	0.87%	0.81%	1.15%	1.21%	2.60%
16	1.33%	1.21%	1.38%	1.10%	1.50%	1.10%	0.92%	0.92%	1.04%	1.56%	1.50%	1.33%	1.33%	1.33%	1.56%	1.73%
17	1.15%	1.10%	0.63%	1.04%	0.81%	1.04%	1.04%	0.92%	1.04%	1.21%	0.52%	1.38%	1.44%	1.15%	0.98%	2.42%
18	1.27%	1.15%	1.15%	0.46%	0.69%	0.63%	1.21%	1.10%	0.92%	0.98%	0.98%	0.58%	0.87%	0.98%	1.27%	2.31%
19	1.27%	0.87%	0.81%	0.81%	0.75%	0.81%	1.10%	0.98%	1.04%	0.75%	0.69%	0.75%	0.75%	0.81%	0.81%	1.96%
20	0.87%	0.69%	0.69%	0.69%	1.33%	1.15%	0.69%	0.75%	0.75%	0.98%	1.33%	1.21%	1.21%	0.87%	0.98%	1.56%
21	1.10%	0.98%	0.63%	0.58%	0.40%	0.52%	0.46%	0.46%	0.63%	0.75%	0.69%	0.58%	0.81%	1.15%	0.81%	0.87%
22	0.75%	0.81%	0.40%	0.69%	0.58%	0.40%	0.29%	0.81%	0.63%	0.75%	0.69%	0.81%	0.52%	0.69%	0.87%	1.15%
23	0.75%	0.58%	0.75%	0.69%	0.40%	0.75%	0.87%	0.75%	0.98%	0.63%	0.63%	0.63%	0.87%	0.75%	0.69%	2.37%
24	0.92%	0.69%	0.63%	0.52%	0.63%	0.63%	0.69%	0.58%	0.23%	0.52%	0.63%	0.81%	0.46%	0.52%	0.81%	1.44%

25	0.81%	0.58%	0.69%	0.63%	1.04%	0.92%	0.87%	0.63%	0.69%	0.92%	0.92%	1.04%	0.69%	0.69%	0.58%	1.21%
26	0.81%	0.63%	0.87%	0.87%	0.40%	0.63%	0.75%	0.98%	0.98%	0.58%	0.63%	0.75%	0.81%	0.63%	0.63%	1.27%
27	0.58%	0.81%	0.87%	0.69%	0.92%	0.63%	0.81%	0.75%	0.75%	0.69%	0.63%	0.46%	0.52%	0.46%	0.35%	0.87%
28	0.69%	0.58%	0.81%	0.87%	0.63%	0.63%	0.75%	0.63%	0.40%	0.69%	0.52%	0.46%	0.58%	0.87%	0.52%	0.81%
29	0.69%	1.04%	0.58%	0.87%	0.87%	0.81%	0.46%	0.52%	0.69%	0.40%	0.52%	0.52%	0.58%	0.46%	0.75%	1.38%
30	0.52%	0.69%	0.81%	0.58%	0.58%	0.63%	0.52%	0.46%	0.40%	0.63%	1.10%	0.75%	0.63%	0.63%	0.29%	0.46%
31	0.52%	0.58%	0.63%	0.46%	0.63%	0.63%	0.87%	0.69%	0.63%	0.46%	0.12%	0.58%	0.63%	0.63%	1.04%	0.63%
32	0.81%	0.46%	0.63%	0.63%	0.46%	0.52%	0.63%	0.81%	0.58%	0.40%	0.69%	0.46%	0.63%	0.52%	0.63%	0.69%
33	0.23%	0.46%	0.46%	0.69%	0.46%	0.58%	0.35%	0.40%	0.58%	0.35%	0.52%	0.58%	0.75%	0.58%	0.63%	1.04%
34	0.58%	0.40%	0.23%	0.35%	0.69%	0.40%	0.35%	0.46%	0.35%	0.81%	0.46%	0.87%	0.69%	0.87%	0.75%	0.81%
35	0.46%	0.63%	0.23%	0.29%	0.46%	0.58%	0.58%	0.35%	0.75%	0.63%	0.98%	0.58%	0.29%	0.52%	0.58%	0.87%
36	0.46%	0.58%	0.63%	0.75%	0.46%	0.69%	0.69%	0.69%	0.63%	0.63%	0.52%	0.35%	0.46%	0.29%	0.58%	0.81%
37	0.46%	0.35%	0.69%	0.40%	0.23%	0.52%	0.40%	0.58%	0.52%	0.46%	0.29%	0.40%	0.52%	0.98%	0.81%	0.98%

38	0.75%	0.12%	0.35%	0.40%	0.63%	0.29%	0.52%	0.75%	0.52%	0.46%	0.29%	0.46%	0.75%	0.63%	0.69%	0.81%
39	0.12%	0.75%	0.40%	0.35%	0.35%	0.23%	0.35%	0.35%	0.40%	0.35%	0.40%	0.29%	0.58%	0.52%	0.63%	0.75%
40	0.46%	0.29%	0.69%	0.35%	0.35%	0.46%	0.23%	0.12%	0.23%	0.35%	0.46%	0.63%	0.40%	0.52%	0.58%	0.35%
41	0.46%	0.81%	0.23%	0.35%	0.17%	0.12%	0.23%	0.29%	0.46%	0.52%	0.63%	0.63%	0.46%	0.52%	0.46%	0.35%
42	0.46%	0.23%	0.29%	0.35%	0.29%	0.46%	0.46%	0.35%	0.35%	0.52%	0.40%	0.35%	0.58%	0.46%	0.35%	0.58%
43	0.23%	0.29%	0.40%	0.23%	0.69%	0.29%	0.29%	0.58%	0.58%	0.58%	0.40%	0.46%	0.23%	0.40%	0.35%	0.46%
44	0.52%	0.29%	0.46%	0.58%	0.35%	0.58%	0.40%	0.40%	0.35%	0.40%	0.58%	0.35%	0.35%	0.12%	0.52%	0.23%
45	0.35%	0.46%	0.29%	0.58%	0.52%	0.58%	0.58%	0.40%	0.58%	0.35%	0.58%	0.58%	0.63%	0.69%	0.46%	0.69%
46	0.52%	0.23%	0.29%	0.23%	0.35%	0.29%	0.58%	0.40%	0.35%	0.58%	0.23%	0.63%	0.52%	0.69%	0.69%	0.58%
47	0.52%	0.40%	0.35%	0.23%	0.35%	0.46%	0.23%	0.23%	0.29%	0.29%	0.46%	0.52%	0.40%	0.29%	0.29%	0.35%
48	0.23%	0.23%	0.35%	0.35%	0.29%	0.35%	0.58%	0.58%	0.46%	0.35%	0.40%	0.29%	0.52%	0.52%	0.52%	0.46%
49	0.23%	0.29%	0.29%	0.23%	0.12%	0.12%	0.17%	0.46%	0.23%	0.35%	0.23%	0.29%	0.29%	0.29%	0.35%	0.29%
50	0.52%	0.35%	0.17%	0.29%	0.12%	0.23%	0.29%	0.23%	0.40%	0.23%	0.40%	0.29%	0.40%	0.46%	0.35%	0.40%

51	0.12%	0.29%	0.12%	0.23%	0.40%	0.35%	0.35%	0.29%	0.35%	0.46%	0.40%	0.58%	0.63%	0.58%	0.63%	0.58%
52	0.29%	0.23%	0.29%	0.23%	0.29%	0.29%	0.23%	0.06%	0.29%	0.35%	0.29%	0.35%	0.29%	0.29%	0.29%	0.35%
53	0.23%	0.35%	0.40%	0.29%	0.29%	0.17%	0.17%	0.40%	0.17%	0.23%	0.23%	0.12%	0.12%	0.12%	0.12%	0.12%
54	0.35%	0.23%	0.23%	0.35%	0.35%	0.23%	0.17%	0.06%	0.29%	0.23%	0.35%	0.29%	0.29%	0.29%	0.29%	0.29%
55	0.40%	0.40%	0.40%	0.35%	0.35%	0.40%	0.40%	0.40%	0.35%	0.35%	0.17%	0.17%	0.17%	0.17%	0.17%	0.17%
56	0.12%	0.12%	0.12%	0.06%	0.06%	0.12%	0.12%	0.17%	0.17%	0.17%	0.29%	0.29%	0.29%	0.29%	0.29%	0.29%

(4) Similarity scores with fingerprint FCFP_2

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=1732
1	38.78%	42.87%	42.87%	42.07%	41.26%	41.49%	41.14%	39.76%	38.89%	38.03%	37.39%	36.70%	36.41%	36.18%	35.89%	12.98%
2	19.97%	19.39%	18.81%	18.47%	18.98%	17.89%	17.54%	17.60%	18.18%	18.58%	18.41%	18.00%	18.06%	17.71%	17.14%	14.71%
3	10.39%	8.14%	8.94%	9.98%	9.17%	8.83%	9.06%	9.00%	8.66%	8.02%	8.48%	8.77%	8.66%	8.48%	8.83%	7.91%
4	5.37%	7.33%	7.33%	6.87%	7.39%	7.21%	6.87%	7.56%	7.16%	7.56%	6.92%	6.75%	6.52%	6.87%	7.04%	9.87%
5	4.44%	4.85%	4.15%	4.44%	4.85%	5.65%	5.25%	4.44%	4.39%	4.79%	5.02%	4.90%	5.02%	4.67%	4.62%	6.98%

6	4.39%	3.29%	3.75%	4.15%	3.92%	4.21%	4.73%	4.56%	4.33%	4.04%	4.10%	4.10%	3.64%	3.69%	3.29%	4.56%
7	3.75%	3.12%	3.23%	3.12%	3.29%	3.17%	3.12%	3.52%	3.46%	3.64%	3.69%	4.04%	3.98%	4.27%	4.27%	3.23%
8	3.46%	2.77%	2.77%	2.42%	2.25%	2.48%	2.65%	3.00%	3.17%	3.29%	3.46%	3.29%	3.46%	3.00%	3.12%	3.46%
9	2.42%	2.31%	2.60%	2.25%	2.37%	1.96%	2.19%	2.71%	2.42%	2.48%	2.71%	2.83%	2.83%	2.89%	2.94%	4.21%
10	1.90%	2.31%	2.71%	2.60%	2.08%	2.08%	2.60%	2.48%	2.94%	1.90%	1.85%	2.42%	2.54%	2.31%	2.42%	3.75%
11	1.62%	2.31%	2.19%	2.19%	2.25%	2.19%	1.79%	1.79%	2.37%	2.42%	2.14%	1.73%	1.73%	2.54%	1.73%	3.64%
12	1.90%	2.25%	1.50%	1.79%	1.96%	1.62%	1.85%	1.96%	1.85%	2.08%	1.79%	2.31%	2.25%	1.85%	2.19%	4.67%
13	2.08%	1.79%	2.02%	1.15%	1.90%	1.79%	1.44%	1.85%	1.67%	2.14%	2.37%	2.14%	2.42%	2.19%	2.60%	3.92%
14	1.79%	1.67%	1.04%	1.67%	1.56%	1.85%	1.62%	1.90%	1.90%	1.79%	2.02%	1.96%	1.79%	2.42%	2.31%	2.19%
15	1.38%	1.38%	1.10%	1.33%	1.50%	1.44%	2.02%	1.21%	1.62%	1.67%	1.90%	2.08%	2.25%	1.96%	1.96%	2.65%
16	1.21%	0.40%	1.79%	1.67%	1.56%	1.96%	1.50%	1.79%	1.67%	1.67%	1.44%	1.62%	1.56%	1.62%	1.56%	2.31%
17	1.33%	1.50%	1.04%	1.56%	1.44%	1.44%	1.85%	1.56%	1.15%	1.62%	1.73%	1.73%	1.50%	1.44%	1.33%	1.44%
18	1.15%	0.98%	0.98%	1.33%	0.98%	1.62%	1.33%	1.15%	1.85%	1.67%	1.27%	1.04%	1.21%	1.04%	1.33%	2.42%

19	1.44%	0.92%	1.38%	1.44%	1.33%	1.21%	1.21%	1.56%	1.50%	0.75%	0.69%	0.63%	0.98%	0.87%	1.04%	1.73%
20	1.04%	1.21%	1.04%	0.92%	1.62%	1.21%	1.10%	1.33%	0.98%	0.92%	0.63%	0.75%	0.81%	1.04%	0.87%	1.79%
21	1.10%	0.98%	1.33%	1.73%	1.21%	1.21%	0.81%	0.75%	0.75%	0.98%	1.04%	0.52%	0.75%	0.98%	0.81%	1.67%
22	0.81%	1.10%	0.98%	0.81%	1.04%	0.92%	0.87%	0.52%	0.58%	0.75%	0.69%	1.10%	0.58%	0.81%	0.63%	1.50%
23	0.87%	1.21%	0.98%	0.69%	0.87%	0.69%	0.92%	0.81%	0.58%	0.58%	0.98%	0.98%	0.81%	0.63%	0.81%	1.67%
24	0.69%	0.98%	0.63%	0.69%	0.69%	0.81%	0.52%	0.58%	0.63%	0.81%	1.04%	0.63%	0.58%	0.46%	1.04%	1.79%
25	0.63%	0.29%	0.63%	0.58%	0.46%	0.46%	0.87%	0.75%	0.92%	0.87%	0.81%	1.04%	0.75%	0.46%	0.29%	1.73%
26	0.81%	0.63%	0.40%	0.58%	0.52%	0.69%	0.92%	0.87%	0.87%	0.75%	0.52%	0.46%	0.52%	0.75%	0.69%	1.27%
27	1.04%	0.40%	0.46%	0.46%	0.29%	0.58%	0.63%	0.87%	0.75%	0.92%	0.81%	0.81%	0.63%	0.63%	0.98%	1.21%
28	0.92%	0.52%	0.46%	0.46%	0.58%	0.75%	0.75%	0.63%	0.58%	0.63%	0.81%	0.81%	0.81%	1.04%	1.04%	0.75%
29	0.63%	0.69%	0.75%	0.46%	0.52%	0.52%	0.46%	0.52%	0.87%	0.63%	0.46%	0.87%	1.15%	1.04%	0.98%	1.04%
30	1.21%	0.81%	0.58%	0.52%	0.46%	0.46%	0.40%	0.35%	0.23%	0.75%	0.92%	0.75%	0.81%	0.75%	0.52%	1.56%
31	0.63%	0.58%	0.29%	0.69%	0.69%	0.69%	0.69%	0.69%	0.52%	0.58%	0.75%	0.69%	0.69%	0.75%	0.98%	1.04%

32	0.58%	0.75%	0.75%	0.63%	0.92%	0.40%	0.35%	0.75%	0.52%	0.81%	0.75%	0.58%	0.92%	0.87%	0.52%	0.98%
33	0.46%	0.29%	0.58%	0.46%	0.23%	0.46%	0.75%	0.58%	0.98%	0.63%	0.58%	0.87%	0.63%	0.63%	0.81%	1.10%
34	0.17%	0.58%	0.58%	0.75%	0.58%	0.46%	0.35%	0.69%	0.46%	0.58%	0.46%	0.81%	0.87%	0.52%	0.58%	0.92%
35	0.63%	0.29%	0.52%	0.35%	0.29%	0.58%	0.63%	0.52%	0.63%	0.46%	0.75%	0.52%	0.58%	0.87%	0.81%	0.52%
36	0.29%	0.63%	0.63%	0.40%	0.69%	0.35%	0.58%	0.46%	0.63%	0.52%	0.63%	0.58%	0.63%	0.17%	0.69%	0.58%
37	0.58%	0.40%	0.29%	0.29%	0.35%	0.63%	0.29%	0.58%	0.69%	0.46%	0.52%	0.35%	0.35%	0.87%	0.52%	0.81%
38	0.29%	0.58%	0.46%	0.35%	0.29%	0.40%	0.52%	0.29%	0.23%	0.52%	0.35%	0.46%	0.63%	0.63%	0.69%	1.15%
39	0.12%	0.52%	0.40%	0.52%	0.52%	0.29%	0.58%	0.29%	0.58%	0.58%	0.69%	0.87%	0.69%	0.98%	0.69%	0.46%
40	0.35%	0.23%	0.29%	0.58%	0.52%	0.58%	0.29%	0.75%	0.58%	0.58%	0.63%	0.69%	0.87%	0.92%	0.69%	0.81%
41	0.58%	0.35%	0.46%	0.63%	0.40%	0.35%	0.35%	0.69%	0.87%	1.10%	0.81%	0.63%	1.15%	0.98%	1.21%	0.92%
42	0.40%	0.35%	0.46%	0.17%	0.17%	0.35%	0.58%	0.35%	0.35%	0.40%	0.58%	0.75%	0.35%	0.46%	0.63%	0.98%
43	0.40%	0.40%	0.35%	0.35%	0.46%	0.29%	0.52%	0.35%	0.35%	0.35%	0.63%	0.46%	0.17%	0.29%	0.29%	0.58%
44	0.29%	0.40%	0.17%	0.17%	0.29%	0.35%	0.17%	0.17%	0.29%	0.35%	0.46%	0.52%	0.46%	0.40%	0.40%	0.29%

45	0.58%	0.12%	0.40%	0.35%	0.58%	0.63%	0.46%	0.58%	0.40%	0.35%	0.40%	0.29%	0.75%	0.58%	0.58%	0.46%
46	0.40%	0.29%	0.29%	0.52%	0.40%	0.46%	0.40%	0.52%	0.40%	0.46%	0.29%	0.35%	0.23%	0.35%	0.46%	0.29%
47	0.46%	0.29%	0.40%	0.46%	0.46%	0.46%	0.52%	0.29%	0.23%	0.40%	0.17%	0.23%	0.23%	0.40%	0.29%	0.58%
48	0.46%	0.69%	0.52%	0.17%	0.23%	0.29%	0.40%	0.29%	0.35%	0.06%	0.23%	0.35%	0.40%	0.40%	0.52%	0.52%
49	0.29%	0.40%	0.35%	0.52%	0.46%	0.23%	0.23%	0.23%	0.17%	0.00%	0.23%	0.23%	0.46%	0.35%	0.29%	0.23%
50	0.46%	0.35%	0.29%	0.29%	0.12%	0.29%	0.06%	0.17%	0.12%	0.23%	0.17%	0.35%	0.46%	0.46%	0.46%	0.52%
51	0.17%	0.35%	0.40%	0.23%	0.12%	0.12%	0.23%	0.23%	0.29%	0.35%	0.58%	0.52%	0.35%	0.40%	0.35%	0.35%
52	0.40%	0.35%	0.17%	0.29%	0.35%	0.29%	0.23%	0.23%	0.29%	0.35%	0.29%	0.23%	0.17%	0.17%	0.35%	0.29%
53	0.12%	0.17%	0.17%	0.12%	0.29%	0.29%	0.29%	0.40%	0.69%	0.58%	0.40%	0.40%	0.40%	0.40%	0.40%	0.46%
54	0.29%	0.23%	0.17%	0.23%	0.23%	0.35%	0.58%	0.63%	0.46%	0.46%	0.23%	0.23%	0.23%	0.23%	0.23%	0.17%
55	0.29%	0.17%	0.40%	0.35%	0.40%	0.29%	0.23%	0.17%	0.17%	0.29%	0.40%	0.40%	0.40%	0.40%	0.40%	0.46%
56	0.12%	0.17%	0.06%	0.06%	0.00%	0.06%	0.06%	0.06%	0.17%	0.17%	0.23%	0.23%	0.23%	0.23%	0.23%	0.23%

(5) Similarity scores with fingerprint FCFP_4

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=1732
1	45.35%	47.95%	48.07%	47.78%	47.55%	46.97%	46.80%	45.70%	45.07%	44.43%	43.97%	43.05%	42.41%	42.12%	41.37%	16.04%
2	19.73%	19.56%	19.16%	19.56%	19.10%	18.93%	18.35%	18.58%	18.75%	18.70%	18.12%	18.75%	18.41%	17.95%	17.95%	13.85%
3	8.02%	8.14%	8.83%	8.02%	8.54%	8.71%	9.23%	9.35%	8.77%	9.00%	9.23%	8.31%	8.02%	7.96%	7.67%	8.37%
4	6.06%	4.96%	5.42%	5.83%	5.37%	5.77%	5.65%	5.89%	5.42%	4.90%	5.42%	6.00%	6.17%	6.23%	6.46%	8.77%
5	3.87%	4.27%	4.27%	4.44%	4.39%	3.98%	3.64%	3.64%	4.10%	4.33%	3.58%	3.64%	4.62%	4.67%	4.56%	6.92%
6	2.42%	3.69%	3.17%	2.48%	3.17%	3.12%	3.40%	3.29%	3.64%	4.15%	3.87%	3.81%	3.52%	3.64%	3.75%	4.50%
7	2.71%	2.89%	2.65%	3.17%	2.77%	3.23%	3.52%	3.75%	3.40%	3.06%	3.40%	3.69%	3.87%	3.87%	4.33%	3.58%
8	3.17%	2.25%	2.37%	2.60%	3.00%	2.89%	3.35%	3.64%	3.81%	3.46%	3.75%	3.12%	2.71%	2.77%	2.42%	2.83%
9	2.37%	1.96%	2.25%	2.19%	2.77%	2.77%	2.08%	2.14%	2.48%	2.77%	2.60%	3.06%	2.83%	2.77%	2.89%	3.87%
10	1.44%	2.19%	2.19%	2.31%	2.08%	2.08%	2.19%	2.25%	2.25%	2.14%	2.48%	2.31%	1.79%	1.79%	1.67%	3.64%
11	1.85%	1.44%	2.14%	2.65%	2.19%	2.42%	2.25%	1.96%	1.67%	1.90%	1.96%	1.90%	1.73%	1.96%	1.90%	4.85%
12	2.31%	1.04%	1.79%	1.67%	1.73%	1.67%	1.79%	1.62%	1.56%	1.33%	1.50%	1.90%	2.42%	2.08%	2.25%	3.87%

13	1.96%	2.25%	1.73%	1.67%	1.50%	1.10%	1.15%	1.27%	1.62%	1.56%	1.33%	1.21%	1.73%	1.73%	1.50%	4.39%
14	1.21%	2.31%	1.79%	1.50%	1.85%	1.62%	1.79%	1.50%	1.85%	1.62%	1.38%	1.56%	1.38%	1.56%	1.73%	2.54%
15	1.73%	1.67%	1.10%	1.21%	1.62%	1.96%	1.33%	1.44%	1.15%	1.44%	1.33%	1.21%	1.56%	1.50%	1.67%	2.25%
16	1.33%	1.44%	1.44%	1.27%	0.69%	0.63%	0.92%	0.98%	1.27%	1.44%	1.79%	1.33%	1.27%	1.44%	1.56%	2.02%
17	0.92%	1.44%	1.27%	1.38%	0.87%	1.15%	1.33%	1.44%	1.21%	1.04%	1.27%	1.67%	1.67%	1.27%	0.98%	2.42%
18	1.50%	0.58%	0.75%	0.92%	1.38%	1.04%	1.04%	1.67%	1.50%	1.33%	1.21%	1.04%	0.98%	1.33%	1.85%	2.48%
19	1.38%	1.04%	1.04%	0.81%	0.87%	1.15%	1.33%	0.92%	1.10%	1.33%	1.15%	0.87%	0.92%	0.98%	0.46%	1.79%
20	0.75%	0.75%	0.58%	0.75%	0.69%	1.10%	1.15%	0.58%	0.75%	0.81%	0.81%	1.15%	0.63%	0.75%	0.98%	1.56%
21	1.62%	0.87%	0.98%	0.92%	1.15%	0.69%	0.58%	0.46%	0.52%	0.46%	0.46%	0.92%	1.10%	0.92%	1.10%	0.98%
22	0.92%	0.81%	0.69%	0.63%	0.87%	0.40%	0.58%	0.98%	0.52%	0.98%	0.98%	0.98%	0.58%	0.87%	0.52%	1.27%
23	0.87%	0.81%	0.63%	0.75%	0.52%	0.58%	0.81%	0.75%	0.87%	0.75%	0.63%	0.40%	1.04%	0.75%	0.75%	1.90%
24	0.92%	0.63%	0.58%	0.75%	0.46%	1.04%	0.46%	0.81%	0.81%	0.58%	0.69%	0.81%	0.87%	0.92%	1.10%	2.14%
25	0.58%	0.63%	0.75%	0.81%	0.92%	0.69%	0.46%	0.52%	0.52%	0.69%	0.69%	0.46%	0.58%	0.40%	0.63%	1.96%

26	0.46%	0.63%	0.81%	0.58%	0.52%	0.40%	0.63%	0.52%	0.98%	0.92%	1.04%	0.87%	0.81%	0.87%	0.75%	0.63%
27	0.46%	0.46%	0.52%	0.46%	0.46%	0.58%	0.87%	0.87%	0.40%	0.75%	0.69%	0.98%	0.81%	1.04%	0.92%	1.21%
28	0.75%	0.63%	0.46%	0.69%	0.46%	0.92%	0.75%	0.52%	0.63%	0.52%	0.69%	0.69%	0.63%	0.58%	0.35%	0.92%
29	0.46%	0.58%	0.58%	0.35%	0.75%	0.35%	0.35%	0.75%	0.40%	0.58%	0.58%	0.69%	0.58%	0.46%	0.40%	1.10%
30	0.81%	0.75%	0.87%	0.46%	0.75%	0.52%	0.58%	0.46%	0.69%	0.69%	0.69%	0.63%	0.98%	0.98%	0.92%	1.10%
31	0.69%	0.46%	0.35%	0.69%	0.29%	0.63%	0.52%	0.58%	0.87%	0.75%	0.35%	0.46%	0.40%	0.46%	0.98%	1.15%
32	0.58%	0.69%	0.63%	0.63%	0.81%	0.58%	0.75%	0.58%	0.58%	0.58%	1.10%	0.81%	0.81%	0.69%	0.69%	0.81%
33	0.52%	0.46%	1.04%	0.52%	0.40%	0.87%	0.58%	0.40%	0.35%	0.40%	0.46%	0.52%	0.69%	0.58%	0.63%	1.15%
34	0.40%	0.52%	0.29%	0.52%	0.40%	0.40%	0.29%	0.40%	0.35%	0.46%	0.52%	0.58%	0.58%	0.52%	0.35%	0.87%
35	0.58%	0.63%	0.52%	0.58%	0.52%	0.58%	0.29%	0.52%	0.58%	0.46%	0.52%	0.58%	0.40%	0.81%	0.63%	0.58%
36	0.46%	0.63%	0.52%	0.52%	0.52%	0.40%	0.75%	0.46%	0.75%	0.52%	0.58%	0.35%	0.40%	0.58%	0.92%	0.69%
37	0.35%	0.35%	0.35%	0.46%	0.46%	0.40%	0.35%	0.35%	0.52%	0.69%	0.23%	0.58%	0.52%	0.69%	0.63%	0.75%
38	0.81%	0.40%	0.52%	0.52%	0.52%	0.40%	0.63%	0.46%	0.23%	0.12%	0.40%	0.40%	0.52%	0.35%	0.58%	0.40%

39	0.29%	0.52%	0.35%	0.29%	0.29%	0.29%	0.40%	0.63%	0.35%	0.52%	0.35%	0.40%	0.69%	0.75%	0.46%	0.75%
40	0.87%	0.35%	0.40%	0.52%	0.52%	0.52%	0.40%	0.23%	0.35%	0.46%	0.81%	0.98%	0.75%	0.52%	0.63%	0.58%
41	0.40%	0.35%	0.23%	0.17%	0.29%	0.40%	0.63%	0.35%	0.58%	0.87%	0.52%	0.75%	0.75%	1.04%	0.92%	0.98%
42	0.35%	0.23%	0.17%	0.35%	0.35%	0.23%	0.12%	0.81%	0.52%	0.35%	0.63%	0.35%	0.46%	0.52%	0.81%	0.92%
43	0.29%	0.29%	0.40%	0.40%	0.23%	0.17%	0.58%	0.35%	0.46%	0.46%	0.63%	0.46%	0.52%	0.29%	0.40%	0.69%
44	0.29%	0.17%	0.23%	0.06%	0.40%	0.75%	0.40%	0.75%	0.63%	0.29%	0.23%	0.40%	0.23%	0.29%	0.23%	0.29%
45	0.23%	0.52%	0.23%	0.35%	0.17%	0.17%	0.29%	0.23%	0.46%	0.69%	0.58%	0.35%	0.40%	0.29%	0.17%	0.17%
46	0.52%	0.29%	0.46%	0.58%	0.35%	0.46%	0.52%	0.58%	0.40%	0.23%	0.17%	0.35%	0.58%	0.58%	0.46%	0.17%
47	0.17%	0.23%	0.23%	0.17%	0.63%	0.35%	0.17%	0.06%	0.23%	0.29%	0.23%	0.17%	0.23%	0.52%	0.58%	0.75%
48	0.35%	0.40%	0.35%	0.17%	0.06%	0.17%	0.17%	0.17%	0.17%	0.06%	0.17%	0.29%	0.40%	0.46%	0.52%	0.52%
49	0.35%	0.52%	0.58%	0.40%	0.29%	0.17%	0.12%	0.17%	0.23%	0.35%	0.29%	0.40%	0.12%	0.12%	0.17%	0.23%
50	0.29%	0.23%	0.00%	0.17%	0.35%	0.17%	0.46%	0.29%	0.12%	0.35%	0.46%	0.35%	0.40%	0.35%	0.23%	0.23%
51	0.40%	0.23%	0.35%	0.35%	0.12%	0.35%	0.23%	0.29%	0.40%	0.23%	0.40%	0.40%	0.52%	0.46%	0.52%	0.46%

52	0.17%	0.23%	0.35%	0.40%	0.40%	0.46%	0.35%	0.52%	0.58%	0.52%	0.29%	0.35%	0.23%	0.23%	0.29%	0.35%
53	0.29%	0.52%	0.29%	0.23%	0.35%	0.29%	0.35%	0.23%	0.17%	0.23%	0.23%	0.17%	0.23%	0.23%	0.23%	0.23%
54	0.58%	0.23%	0.35%	0.29%	0.35%	0.29%	0.17%	0.17%	0.17%	0.29%	0.29%	0.29%	0.29%	0.29%	0.29%	0.29%
55	0.06%	0.12%	0.17%	0.29%	0.23%	0.29%	0.35%	0.35%	0.35%	0.23%	0.23%	0.23%	0.17%	0.17%	0.17%	0.17%
56	0.12%	0.12%	0.12%	0.06%	0.06%	0.06%	0.12%	0.17%	0.23%	0.29%	0.35%	0.35%	0.40%	0.40%	0.40%	0.40%

(6) Similarity scores with fingerprint FCFP_6

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=1732
1	45.99%	48.70%	48.99%	48.64%	48.41%	48.01%	47.43%	46.91%	46.39%	46.11%	45.12%	44.55%	43.97%	43.34%	42.76%	17.31%
2	19.22%	18.75%	18.81%	19.10%	19.27%	19.79%	19.45%	19.27%	19.33%	18.70%	18.58%	18.06%	17.95%	17.83%	17.66%	13.50%
3	7.85%	7.56%	8.48%	8.71%	8.37%	7.67%	8.54%	8.71%	8.54%	8.66%	9.64%	9.64%	9.29%	9.00%	9.17%	8.66%
4	5.25%	5.42%	5.42%	5.14%	5.48%	5.77%	5.48%	4.96%	5.31%	5.31%	4.67%	5.14%	5.48%	5.89%	5.54%	9.00%
5	4.56%	4.56%	3.64%	4.39%	4.21%	4.15%	4.21%	4.50%	3.87%	4.56%	4.33%	4.79%	4.44%	4.27%	4.44%	6.87%
6	2.42%	3.12%	3.69%	3.52%	3.40%	3.40%	3.12%	3.69%	4.04%	3.69%	3.98%	3.87%	3.87%	3.87%	3.64%	3.81%

7	2.65%	3.12%	3.23%	2.89%	2.94%	3.06%	3.40%	3.29%	3.64%	3.58%	3.52%	2.83%	3.12%	3.23%	3.29%	3.17%
8	2.48%	2.48%	2.25%	2.48%	2.25%	2.60%	2.71%	2.54%	2.83%	2.94%	3.12%	3.52%	3.23%	3.12%	3.12%	3.12%
9	2.25%	2.25%	2.37%	2.37%	2.94%	2.65%	2.65%	2.42%	1.79%	2.08%	2.14%	2.14%	1.85%	1.96%	2.60%	4.33%
10	2.54%	1.85%	1.73%	1.67%	1.67%	1.79%	1.67%	1.96%	1.79%	1.62%	1.85%	1.85%	2.25%	2.83%	2.42%	3.35%
11	2.02%	1.56%	1.79%	1.73%	1.67%	1.73%	1.79%	1.44%	1.79%	1.67%	1.85%	1.85%	1.90%	1.79%	1.90%	4.96%
12	2.08%	2.14%	1.73%	1.38%	1.73%	1.56%	1.79%	1.96%	1.85%	2.08%	1.85%	1.96%	2.19%	1.44%	1.62%	4.56%
13	2.19%	1.44%	1.67%	1.67%	1.27%	1.50%	1.15%	1.73%	1.62%	1.27%	1.44%	1.44%	1.38%	1.62%	1.67%	4.21%
14	1.27%	1.38%	1.21%	1.33%	1.44%	1.79%	1.44%	1.44%	1.79%	1.56%	1.10%	1.04%	1.50%	1.50%	1.27%	2.48%
15	1.56%	1.27%	1.15%	1.44%	1.56%	1.15%	1.67%	1.38%	0.98%	1.33%	1.44%	1.56%	1.15%	1.15%	1.21%	2.54%
16	1.21%	1.44%	1.21%	1.56%	0.92%	0.75%	0.98%	0.92%	1.56%	1.50%	1.73%	1.38%	1.33%	1.44%	1.56%	2.31%
17	1.15%	1.50%	1.15%	0.81%	1.10%	1.62%	1.10%	1.33%	0.98%	1.04%	1.10%	1.73%	1.79%	2.14%	1.96%	2.31%
18	1.10%	1.04%	1.04%	1.44%	1.27%	0.87%	0.98%	1.27%	1.21%	1.21%	1.15%	1.04%	1.44%	1.15%	1.38%	1.96%
19	0.92%	0.98%	1.27%	1.04%	1.10%	0.81%	1.15%	0.81%	1.10%	1.21%	1.21%	1.33%	0.81%	0.98%	0.92%	0.98%

20	0.98%	0.81%	1.27%	0.92%	1.15%	0.69%	0.69%	0.87%	0.98%	1.04%	0.81%	0.46%	0.69%	0.87%	0.92%	1.56%
21	1.67%	0.87%	0.81%	0.81%	0.52%	1.27%	0.81%	0.87%	0.58%	0.63%	0.63%	0.75%	1.10%	1.15%	0.63%	0.87%
22	0.58%	1.15%	0.98%	0.81%	0.75%	1.21%	1.04%	0.98%	1.15%	1.10%	0.87%	0.98%	0.69%	0.69%	1.33%	1.73%
23	0.92%	1.04%	0.63%	0.87%	0.98%	0.69%	0.58%	0.87%	0.58%	0.75%	0.75%	0.92%	0.46%	0.52%	0.75%	2.25%
24	1.21%	0.58%	0.81%	0.52%	0.81%	0.69%	0.92%	0.35%	0.63%	0.81%	1.04%	0.58%	0.98%	0.87%	0.63%	1.73%
25	0.92%	0.75%	0.75%	0.46%	0.69%	0.29%	0.75%	0.63%	0.29%	0.46%	0.58%	0.52%	0.63%	0.58%	0.63%	1.90%
26	0.81%	0.63%	0.63%	0.92%	0.69%	0.92%	0.46%	0.63%	0.69%	0.35%	0.46%	0.52%	0.87%	0.69%	0.52%	0.87%
27	0.58%	0.46%	0.23%	0.69%	0.58%	0.69%	0.81%	0.63%	0.58%	0.29%	0.40%	0.81%	0.69%	0.75%	0.63%	1.21%
28	0.75%	0.35%	0.46%	0.40%	0.92%	0.69%	0.63%	0.69%	0.75%	0.63%	0.58%	0.29%	0.40%	0.58%	0.58%	0.98%
29	0.63%	0.81%	0.17%	0.46%	0.35%	0.46%	0.52%	0.58%	0.63%	0.69%	0.75%	1.04%	0.81%	0.35%	0.75%	0.98%
30	0.52%	0.58%	0.75%	0.58%	0.46%	0.40%	0.35%	0.46%	0.46%	0.69%	0.81%	0.58%	0.58%	0.92%	0.75%	1.04%
31	0.52%	0.58%	0.46%	0.35%	0.46%	0.40%	0.52%	0.40%	0.69%	0.87%	0.58%	0.69%	0.58%	0.40%	0.46%	1.10%
32	0.58%	0.46%	1.04%	0.75%	0.52%	0.40%	0.81%	0.69%	0.58%	0.58%	0.58%	0.81%	0.46%	0.69%	0.63%	0.75%

33	0.35%	0.52%	0.63%	0.40%	0.29%	0.40%	0.17%	0.58%	0.40%	0.40%	0.63%	0.23%	0.69%	0.98%	0.63%	0.92%
34	0.46%	0.58%	0.52%	0.63%	0.46%	0.52%	0.29%	0.52%	0.29%	0.58%	0.40%	0.69%	0.46%	0.52%	0.69%	0.52%
35	0.58%	0.75%	0.40%	0.40%	0.52%	0.52%	0.63%	0.58%	0.92%	0.23%	0.35%	0.23%	0.63%	0.52%	0.40%	0.75%
36	0.52%	0.58%	0.40%	0.40%	0.40%	0.40%	0.35%	0.40%	0.17%	0.40%	0.29%	0.75%	0.35%	0.46%	0.75%	0.58%
37	0.63%	0.29%	0.63%	0.87%	0.58%	0.58%	0.69%	0.23%	0.40%	0.52%	0.58%	0.35%	0.52%	0.40%	0.46%	0.87%
38	0.69%	0.40%	0.69%	0.06%	0.63%	0.52%	0.58%	0.29%	0.46%	0.46%	0.69%	0.35%	0.40%	0.40%	0.52%	0.35%
39	0.52%	0.58%	0.58%	0.58%	0.17%	0.58%	0.35%	0.63%	0.58%	0.52%	0.46%	0.58%	0.75%	0.87%	0.52%	0.92%
40	0.46%	0.23%	0.12%	0.75%	0.58%	0.58%	0.63%	0.35%	0.35%	0.46%	0.63%	0.35%	0.46%	0.52%	0.52%	0.52%
41	0.35%	0.69%	0.40%	0.35%	0.52%	0.29%	0.69%	0.63%	0.63%	0.58%	0.40%	1.04%	0.87%	0.81%	1.10%	0.69%
42	0.29%	0.12%	0.35%	0.17%	0.23%	0.23%	0.12%	0.52%	0.35%	0.58%	0.52%	0.46%	0.58%	0.40%	0.52%	0.81%
43	0.35%	0.29%	0.17%	0.17%	0.17%	0.46%	0.40%	0.40%	0.58%	0.52%	0.58%	0.29%	0.40%	0.46%	0.58%	0.58%
44	0.40%	0.29%	0.17%	0.17%	0.35%	0.29%	0.35%	0.40%	0.46%	0.40%	0.40%	0.40%	0.29%	0.46%	0.35%	0.46%
45	0.17%	0.17%	0.23%	0.29%	0.40%	0.29%	0.40%	0.63%	0.63%	0.58%	0.46%	0.40%	0.17%	0.17%	0.17%	0.17%

46	0.23%	0.06%	0.17%	0.29%	0.23%	0.46%	0.58%	0.29%	0.23%	0.29%	0.35%	0.40%	0.46%	0.29%	0.23%	0.23%
47	0.23%	0.35%	0.40%	0.58%	0.52%	0.17%	0.12%	0.29%	0.29%	0.35%	0.29%	0.29%	0.46%	0.58%	0.63%	0.69%
48	0.35%	0.69%	0.46%	0.35%	0.35%	0.35%	0.29%	0.29%	0.23%	0.23%	0.29%	0.46%	0.52%	0.58%	0.46%	0.46%
49	0.35%	0.23%	0.52%	0.29%	0.29%	0.35%	0.12%	0.12%	0.35%	0.17%	0.35%	0.29%	0.23%	0.17%	0.29%	0.29%
50	0.58%	0.40%	0.12%	0.40%	0.17%	0.23%	0.29%	0.06%	0.23%	0.40%	0.40%	0.63%	0.63%	0.52%	0.46%	0.46%
51	0.17%	0.23%	0.17%	0.12%	0.35%	0.23%	0.23%	0.40%	0.17%	0.17%	0.29%	0.29%	0.29%	0.29%	0.35%	0.29%
52	0.40%	0.23%	0.29%	0.29%	0.29%	0.46%	0.52%	0.46%	0.58%	0.35%	0.17%	0.06%	0.12%	0.17%	0.17%	0.23%
53	0.00%	0.29%	0.35%	0.17%	0.12%	0.17%	0.23%	0.29%	0.23%	0.40%	0.35%	0.35%	0.35%	0.35%	0.35%	0.35%
54	0.69%	0.52%	0.40%	0.40%	0.40%	0.29%	0.17%	0.23%	0.12%	0.12%	0.12%	0.12%	0.12%	0.12%	0.12%	0.12%
55	0.06%	0.12%	0.17%	0.23%	0.23%	0.29%	0.35%	0.29%	0.46%	0.29%	0.29%	0.29%	0.29%	0.29%	0.29%	0.29%
56	0.12%	0.12%	0.12%	0.12%	0.17%	0.17%	0.17%	0.23%	0.23%	0.35%	0.40%	0.40%	0.40%	0.40%	0.40%	0.40%

(7) Similarity scores with fingerprint FP2

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=1732
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1	41.78%	43.45%	43.91%	43.62%	42.82%	42.12%	41.32%	40.74%	40.05%	39.70%	39.01%	38.14%	37.39%	36.87%	36.24%	12.98%
2	19.62%	19.10%	17.54%	17.31%	17.71%	18.35%	17.83%	17.37%	18.06%	17.66%	17.66%	17.83%	17.89%	17.66%	18.06%	13.73%
3	8.31%	7.21%	8.94%	8.71%	9.06%	8.54%	8.83%	9.29%	8.54%	8.37%	8.48%	8.89%	8.94%	8.66%	7.85%	6.58%
4	5.65%	6.46%	6.17%	6.23%	6.00%	5.37%	5.71%	5.94%	6.00%	5.54%	5.60%	5.14%	5.48%	5.83%	6.46%	13.16%
5	4.33%	5.37%	4.62%	5.08%	4.96%	5.48%	5.77%	5.83%	5.77%	6.35%	5.94%	6.06%	5.54%	5.48%	5.77%	6.06%
6	3.00%	3.58%	3.64%	3.81%	3.52%	4.44%	5.54%	4.96%	5.02%	4.67%	4.39%	4.39%	4.50%	4.44%	3.92%	4.33%
7	2.94%	2.89%	4.10%	3.35%	3.64%	3.46%	2.42%	3.23%	3.17%	3.23%	3.40%	3.46%	3.69%	3.69%	3.75%	2.60%
8	2.94%	3.12%	2.94%	3.23%	3.00%	2.94%	2.71%	2.71%	2.77%	3.12%	3.52%	3.46%	3.40%	3.58%	3.87%	3.64%
9	2.31%	1.79%	2.77%	2.31%	2.60%	2.25%	2.42%	2.48%	2.71%	3.06%	2.65%	2.65%	2.08%	2.31%	2.31%	4.44%
10	1.73%	2.65%	2.31%	2.08%	2.83%	2.77%	3.06%	2.54%	2.31%	1.85%	2.19%	2.37%	2.48%	2.08%	2.08%	3.58%
11	1.79%	1.79%	1.79%	2.19%	1.56%	1.44%	1.38%	1.10%	1.62%	1.90%	1.85%	1.85%	2.25%	2.60%	2.19%	5.54%
12	1.90%	1.56%	1.04%	1.67%	2.02%	1.56%	1.79%	1.73%	1.79%	1.67%	1.44%	1.67%	2.02%	1.90%	1.79%	4.90%
13	1.90%	1.62%	1.79%	1.56%	1.27%	1.67%	1.38%	1.90%	1.90%	1.67%	1.85%	1.73%	1.85%	1.96%	1.96%	3.12%

14	1.96%	1.50%	1.21%	1.33%	0.98%	1.04%	1.21%	1.38%	1.33%	1.96%	2.02%	1.73%	1.50%	1.50%	1.73%	2.19%
15	1.33%	0.98%	0.81%	1.44%	1.33%	1.27%	1.21%	0.81%	0.81%	1.27%	1.67%	1.67%	1.67%	1.62%	1.73%	1.85%
16	1.50%	1.38%	1.38%	1.73%	1.04%	1.15%	1.10%	1.62%	1.90%	1.38%	1.38%	1.33%	1.04%	1.04%	1.21%	1.90%
17	1.44%	0.87%	1.27%	0.87%	1.44%	1.38%	1.21%	1.33%	0.98%	1.10%	0.92%	1.15%	1.27%	1.21%	1.10%	2.37%
18	1.79%	1.33%	1.04%	0.69%	1.38%	1.44%	1.62%	1.27%	0.92%	1.15%	0.87%	1.04%	1.15%	1.27%	1.56%	2.31%
19	0.75%	1.50%	0.92%	1.38%	1.21%	1.15%	1.04%	0.75%	1.04%	1.15%	1.38%	1.27%	1.44%	1.10%	1.04%	2.02%
20	1.04%	0.98%	1.10%	1.27%	1.15%	0.92%	0.92%	1.10%	1.21%	1.15%	1.21%	0.98%	1.38%	1.56%	1.50%	1.56%
21	0.98%	0.81%	1.15%	0.69%	0.81%	1.33%	1.21%	1.15%	0.75%	0.92%	1.38%	1.56%	0.75%	1.21%	1.38%	1.44%
22	1.50%	1.27%	0.92%	0.75%	1.15%	0.87%	0.98%	0.75%	0.69%	0.81%	0.69%	0.69%	1.15%	1.10%	0.87%	2.08%
23	0.92%	1.27%	0.87%	1.15%	0.87%	1.15%	0.92%	1.21%	1.33%	0.75%	0.92%	1.04%	1.15%	0.69%	0.63%	1.73%
24	0.75%	0.75%	1.04%	0.87%	1.10%	1.15%	1.21%	1.10%	1.27%	1.10%	0.63%	0.92%	0.46%	1.04%	0.92%	2.02%
25	1.10%	0.63%	1.10%	0.87%	0.69%	0.75%	1.15%	1.38%	1.15%	1.10%	1.04%	0.46%	0.87%	0.75%	1.33%	1.67%
26	0.81%	1.04%	0.69%	0.52%	0.98%	0.81%	0.75%	0.69%	0.87%	0.98%	0.98%	1.15%	1.15%	1.15%	0.87%	1.44%

27	0.92%	0.35%	0.75%	1.10%	0.58%	0.69%	0.69%	0.63%	1.04%	0.58%	0.75%	1.21%	0.98%	0.98%	0.92%	1.50%
28	1.10%	0.75%	0.63%	0.75%	0.58%	0.92%	0.58%	0.58%	0.29%	0.87%	0.98%	0.69%	0.75%	0.63%	0.58%	0.81%
29	0.81%	0.87%	0.69%	0.58%	0.81%	0.40%	0.69%	0.69%	0.81%	0.92%	0.69%	0.81%	0.63%	0.52%	0.52%	1.56%
30	0.58%	0.52%	0.52%	0.75%	0.81%	0.52%	0.40%	0.46%	0.58%	0.58%	0.58%	0.40%	0.69%	0.81%	0.69%	0.92%
31	1.04%	0.98%	0.52%	0.52%	0.69%	0.69%	0.46%	0.69%	0.63%	0.75%	0.63%	0.69%	0.63%	0.35%	0.75%	0.81%
32	0.46%	0.29%	0.75%	0.40%	0.29%	0.46%	0.75%	0.75%	0.69%	0.35%	0.35%	0.40%	0.40%	0.98%	0.46%	0.81%
33	0.46%	0.92%	0.81%	0.40%	0.40%	0.46%	0.69%	0.58%	0.52%	0.40%	0.46%	0.40%	0.35%	0.52%	1.15%	0.52%
34	0.23%	0.58%	0.40%	0.52%	0.29%	0.81%	0.46%	0.69%	0.69%	0.69%	0.58%	0.35%	0.46%	0.46%	0.52%	0.52%
35	0.75%	0.58%	0.52%	0.35%	0.40%	0.58%	0.46%	0.52%	0.35%	0.52%	0.52%	0.75%	0.58%	0.52%	0.29%	0.63%
36	0.46%	0.69%	0.69%	0.81%	0.81%	0.52%	0.69%	0.46%	0.58%	0.58%	0.75%	0.63%	0.63%	0.40%	0.29%	1.10%
37	0.58%	0.63%	0.58%	0.46%	0.40%	0.23%	0.29%	0.35%	0.69%	0.81%	0.58%	0.75%	0.46%	0.58%	0.52%	0.52%
38	0.52%	0.52%	0.46%	0.81%	0.63%	0.52%	0.69%	0.46%	0.46%	0.58%	0.75%	0.87%	0.81%	0.46%	0.63%	0.52%
39	0.81%	0.35%	0.40%	0.52%	0.35%	0.52%	0.63%	0.46%	0.35%	0.46%	0.69%	0.81%	0.92%	0.75%	0.75%	0.63%

40	0.46%	0.35%	0.92%	0.63%	0.92%	0.63%	0.40%	0.52%	0.52%	0.52%	0.40%	0.40%	0.35%	0.63%	0.58%	0.81%
41	0.17%	0.40%	0.35%	0.58%	0.75%	0.58%	0.40%	0.40%	0.40%	0.29%	0.46%	0.35%	0.87%	0.92%	0.75%	0.58%
42	0.23%	0.40%	0.17%	0.52%	0.23%	0.29%	0.58%	0.52%	0.29%	0.40%	0.58%	0.40%	0.75%	0.58%	0.69%	0.75%
43	0.40%	0.12%	0.17%	0.12%	0.40%	0.52%	0.40%	0.40%	0.35%	0.63%	0.52%	0.87%	0.46%	0.92%	1.10%	0.81%
44	0.29%	0.40%	0.29%	0.23%	0.23%	0.35%	0.35%	0.52%	0.52%	0.40%	0.69%	0.40%	0.69%	0.58%	0.52%	0.69%
45	0.23%	0.29%	0.40%	0.35%	0.29%	0.17%	0.23%	0.63%	0.81%	0.69%	0.46%	0.69%	0.52%	0.46%	0.52%	0.46%
46	0.29%	0.23%	0.23%	0.35%	0.23%	0.40%	0.35%	0.46%	0.40%	0.35%	0.63%	0.52%	0.46%	0.46%	0.40%	0.46%
47	0.40%	0.52%	0.29%	0.12%	0.29%	0.29%	0.69%	0.52%	0.52%	0.23%	0.12%	0.17%	0.29%	0.35%	0.29%	0.40%
48	0.40%	0.17%	0.06%	0.12%	0.46%	0.52%	0.23%	0.23%	0.29%	0.40%	0.23%	0.58%	0.58%	0.52%	0.58%	0.58%
49	0.29%	0.35%	0.35%	0.23%	0.29%	0.29%	0.40%	0.58%	0.40%	0.29%	0.52%	0.35%	0.29%	0.46%	0.46%	0.46%
50	0.23%	0.23%	0.46%	0.69%	0.35%	0.40%	0.46%	0.23%	0.29%	0.35%	0.23%	0.17%	0.17%	0.17%	0.23%	0.23%
51	0.63%	0.23%	0.35%	0.46%	0.40%	0.40%	0.29%	0.12%	0.35%	0.40%	0.29%	0.35%	0.40%	0.29%	0.29%	0.23%
52	0.06%	0.23%	0.17%	0.23%	0.17%	0.29%	0.17%	0.29%	0.29%	0.23%	0.23%	0.12%	0.17%	0.23%	0.23%	0.29%

53	0.52%	0.35%	0.40%	0.17%	0.35%	0.12%	0.17%	0.35%	0.23%	0.40%	0.46%	0.35%	0.29%	0.23%	0.17%	0.17%
54	0.29%	0.58%	0.46%	0.46%	0.35%	0.46%	0.63%	0.40%	0.46%	0.40%	0.40%	0.46%	0.52%	0.58%	0.63%	0.63%
55	0.46%	0.52%	0.17%	0.17%	0.29%	0.29%	0.17%	0.29%	0.23%	0.29%	0.23%	0.23%	0.17%	0.17%	0.17%	0.17%
56	0.17%	0.06%	0.29%	0.23%	0.17%	0.17%	0.17%	0.17%	0.35%	0.35%	0.46%	0.52%	0.52%	0.52%	0.52%	0.52%

(8) Similarity scores with fingerprint MACCS

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=1732
1	39.99%	43.39%	43.39%	42.53%	41.32%	40.05%	38.78%	37.74%	37.28%	37.10%	35.72%	35.31%	34.05%	33.70%	33.53%	12.46%
2	18.35%	17.14%	18.23%	17.48%	16.85%	17.20%	17.43%	17.60%	16.91%	16.04%	16.10%	15.46%	16.56%	16.68%	16.68%	12.64%
3	9.17%	8.83%	8.14%	9.06%	9.35%	8.94%	9.06%	9.12%	8.94%	9.06%	9.52%	9.75%	8.66%	8.37%	8.25%	9.75%
4	6.92%	5.37%	5.25%	5.14%	5.65%	6.46%	6.41%	6.35%	6.35%	6.00%	6.23%	5.94%	6.35%	6.06%	6.17%	8.66%
5	4.21%	5.60%	4.96%	5.08%	5.14%	5.02%	5.14%	4.85%	4.79%	5.37%	4.90%	5.60%	5.42%	5.37%	5.42%	8.66%
6	3.17%	3.81%	3.64%	3.92%	4.56%	4.04%	4.96%	4.96%	5.14%	4.56%	5.08%	4.44%	4.39%	4.21%	4.10%	4.79%
7	3.29%	3.40%	3.87%	3.81%	4.33%	4.62%	3.64%	4.15%	4.56%	4.39%	3.52%	3.87%	4.27%	4.44%	3.81%	2.60%

8	3.75%	3.23%	4.10%	3.69%	3.64%	3.06%	2.94%	3.00%	3.29%	4.33%	4.79%	4.10%	3.58%	3.81%	3.52%	2.14%
9	2.71%	2.94%	2.83%	2.89%	2.60%	2.65%	3.00%	2.77%	3.46%	3.23%	3.40%	4.10%	4.50%	4.04%	3.87%	5.14%
10	2.19%	2.48%	2.19%	2.83%	2.60%	2.94%	3.29%	3.81%	2.89%	2.48%	2.89%	3.12%	3.29%	3.46%	3.87%	3.58%
11	2.71%	2.83%	2.48%	2.02%	2.31%	2.37%	2.42%	2.37%	2.54%	2.31%	1.96%	1.73%	1.73%	1.67%	1.96%	4.73%
12	1.79%	2.08%	1.90%	2.31%	2.08%	2.08%	1.96%	1.73%	1.73%	1.67%	1.67%	1.73%	2.14%	1.85%	1.67%	2.94%
13	2.08%	1.56%	2.14%	1.85%	1.67%	2.02%	1.56%	1.56%	1.50%	1.85%	2.19%	2.31%	2.02%	2.25%	2.37%	3.35%
14	1.90%	1.90%	1.67%	1.96%	1.67%	1.79%	1.44%	1.85%	1.27%	1.79%	1.90%	1.90%	1.85%	2.25%	2.02%	3.06%
15	1.50%	1.27%	0.92%	1.38%	1.44%	1.04%	1.79%	1.27%	1.90%	1.67%	1.27%	1.62%	1.67%	1.67%	1.73%	2.54%
16	1.38%	1.27%	1.50%	1.79%	1.73%	1.96%	1.44%	1.38%	1.62%	1.56%	1.38%	0.98%	0.69%	1.21%	1.21%	2.83%
17	1.33%	0.63%	1.90%	1.33%	1.10%	1.73%	1.50%	1.50%	0.81%	1.33%	1.27%	1.67%	1.79%	1.33%	1.33%	2.31%
18	1.27%	1.15%	0.69%	1.27%	1.79%	1.38%	1.50%	1.79%	1.56%	1.44%	1.62%	1.38%	1.15%	1.33%	1.56%	1.73%
19	0.87%	1.27%	1.21%	0.75%	1.21%	1.10%	1.62%	1.33%	1.96%	1.15%	1.27%	0.98%	1.10%	0.98%	1.10%	2.02%
20	0.92%	1.10%	0.58%	1.10%	0.81%	1.27%	1.04%	0.81%	0.81%	1.04%	1.04%	1.44%	1.62%	1.15%	0.92%	1.90%

21	1.27%	0.75%	0.87%	0.75%	1.27%	0.75%	1.04%	1.10%	0.98%	1.15%	1.21%	1.15%	0.87%	1.44%	1.27%	1.38%
22	0.75%	0.81%	0.87%	0.69%	0.63%	0.98%	0.98%	1.10%	0.87%	0.98%	0.69%	0.58%	0.98%	0.87%	0.92%	1.62%
23	1.10%	0.63%	0.92%	0.46%	0.69%	0.58%	0.81%	0.98%	0.81%	1.10%	0.92%	1.04%	0.98%	1.10%	1.38%	1.38%
24	0.87%	1.15%	0.46%	1.04%	0.69%	0.75%	0.98%	0.92%	1.15%	0.98%	1.10%	0.92%	1.15%	0.75%	1.33%	1.38%
25	0.92%	0.58%	0.75%	0.58%	0.81%	0.81%	0.63%	0.87%	1.10%	0.81%	1.10%	1.33%	0.75%	0.92%	0.40%	1.90%
26	1.21%	0.75%	0.69%	0.69%	0.46%	1.10%	0.98%	1.04%	0.75%	0.69%	1.04%	0.98%	0.58%	0.46%	0.40%	1.56%
27	0.69%	0.69%	1.04%	0.69%	0.87%	0.69%	0.81%	0.92%	0.63%	0.81%	0.29%	0.40%	0.63%	0.52%	0.69%	1.38%
28	0.92%	0.58%	0.69%	0.46%	0.52%	0.46%	0.75%	0.35%	0.69%	0.69%	0.52%	0.58%	0.35%	0.63%	0.58%	1.38%
29	0.69%	0.81%	0.63%	0.69%	0.75%	0.40%	0.12%	0.35%	0.40%	0.52%	0.75%	0.46%	0.92%	0.58%	0.35%	1.27%
30	0.69%	0.69%	0.46%	0.29%	0.40%	0.23%	0.35%	0.40%	0.63%	0.63%	0.63%	0.69%	0.58%	0.69%	0.87%	0.58%
31	0.63%	1.21%	0.46%	0.81%	0.29%	0.12%	0.12%	0.23%	0.58%	0.40%	0.58%	0.75%	0.81%	0.92%	0.87%	0.81%
32	0.69%	0.35%	0.46%	0.40%	0.17%	0.40%	0.17%	0.46%	0.35%	0.23%	0.46%	0.23%	0.69%	0.63%	1.10%	1.04%
33	0.69%	0.69%	0.40%	0.35%	0.17%	0.46%	0.52%	0.35%	0.35%	0.40%	0.40%	0.46%	0.40%	0.58%	0.46%	1.04%

34	0.29%	0.35%	0.58%	0.29%	0.52%	0.46%	0.40%	0.29%	0.35%	0.69%	0.69%	0.58%	0.52%	0.81%	0.46%	1.27%
35	0.35%	0.52%	0.63%	0.52%	0.46%	0.46%	0.58%	0.63%	0.58%	0.58%	0.29%	0.81%	1.10%	0.81%	1.15%	1.15%
36	0.52%	0.40%	0.40%	0.40%	0.23%	0.35%	0.35%	0.69%	0.58%	0.40%	0.63%	0.92%	0.35%	0.75%	0.75%	0.35%
37	0.63%	0.29%	0.35%	0.40%	0.58%	0.58%	0.81%	0.17%	0.29%	0.75%	0.75%	0.52%	0.52%	0.75%	0.81%	1.10%
38	0.52%	0.29%	0.40%	0.46%	0.40%	0.52%	0.40%	0.75%	0.69%	0.92%	0.46%	0.52%	1.44%	0.92%	1.10%	1.10%
39	0.46%	0.35%	0.23%	0.58%	0.75%	0.23%	0.40%	0.58%	0.92%	0.63%	0.63%	0.46%	0.52%	0.81%	0.63%	0.52%
40	0.52%	0.52%	0.69%	0.40%	0.58%	0.63%	0.63%	0.46%	0.23%	0.58%	1.21%	0.92%	0.52%	0.69%	0.58%	0.75%
41	0.23%	0.35%	0.35%	0.63%	0.29%	0.63%	0.35%	0.17%	0.52%	0.52%	0.40%	0.29%	0.40%	0.29%	0.58%	0.81%
42	0.00%	0.17%	0.35%	0.52%	0.40%	0.35%	0.40%	0.81%	0.58%	0.23%	0.40%	0.58%	0.40%	0.35%	0.40%	0.35%
43	0.29%	0.29%	0.46%	0.40%	0.40%	0.52%	0.58%	0.35%	0.12%	0.46%	0.52%	0.58%	0.52%	0.52%	0.35%	0.46%
44	0.40%	0.29%	0.23%	0.17%	0.52%	0.40%	0.29%	0.29%	0.40%	0.29%	0.52%	0.40%	0.46%	0.52%	0.58%	0.63%
45	0.35%	0.35%	0.12%	0.35%	0.40%	0.40%	0.52%	0.46%	0.40%	0.29%	0.23%	0.58%	0.58%	0.58%	0.58%	0.46%
46	0.23%	0.29%	0.23%	0.35%	0.40%	0.35%	0.46%	0.40%	0.35%	0.23%	0.23%	0.35%	0.58%	0.52%	0.40%	0.35%

47	0.35%	0.17%	0.17%	0.06%	0.29%	0.46%	0.35%	0.35%	0.52%	0.29%	0.23%	0.35%	0.40%	0.63%	0.52%	0.58%
48	0.23%	0.35%	0.40%	0.52%	0.29%	0.23%	0.29%	0.35%	0.06%	0.46%	0.40%	0.29%	0.40%	0.35%	0.75%	0.87%
49	0.40%	0.12%	0.23%	0.12%	0.17%	0.12%	0.17%	0.29%	0.46%	0.46%	0.52%	0.29%	0.35%	0.46%	0.23%	0.23%
50	0.23%	0.58%	0.52%	0.23%	0.29%	0.40%	0.23%	0.29%	0.46%	0.69%	0.69%	0.69%	0.40%	0.17%	0.23%	0.23%
51	0.29%	0.40%	0.29%	0.52%	0.46%	0.35%	0.52%	0.52%	0.46%	0.17%	0.40%	0.46%	0.46%	0.29%	0.29%	0.29%
52	0.35%	0.35%	0.35%	0.23%	0.29%	0.40%	0.35%	0.40%	0.29%	0.35%	0.12%	0.12%	0.29%	0.52%	0.52%	0.46%
53	0.52%	0.46%	0.12%	0.35%	0.23%	0.29%	0.35%	0.12%	0.23%	0.40%	0.40%	0.52%	0.29%	0.29%	0.35%	0.46%
54	0.12%	0.06%	0.52%	0.29%	0.23%	0.23%	0.17%	0.23%	0.63%	0.58%	0.52%	0.29%	0.46%	0.52%	0.52%	0.52%
55	0.23%	0.29%	0.29%	0.35%	0.46%	0.46%	0.52%	0.63%	0.40%	0.40%	0.40%	0.58%	0.52%	0.52%	0.52%	0.52%
56	0.17%	0.17%	0.12%	0.12%	0.12%	0.06%	0.06%	0.12%	0.23%	0.17%	0.23%	0.23%	0.35%	0.35%	0.35%	0.35%