

Supplementary Tables

Table S1. Full factorial design (n=81) of quaternary mixtures of corn, cane, beet, and rice syrup adulterants using Manuka honey as the standard matrices used in the training set.

Mixture	Corn (% w/w)	Cane (% w/w)	Beet (% w/w)	Rice (% w/w)	Manuka honey (% w/w)
1	9.52	0.00	10.54	5.37	74.57
2	13.36	0.00	13.30	0.00	73.34
3	9.13	5.91	0.00	11.04	73.92
4	3.66	4.75	8.10	8.80	74.69
5	0.00	9.30	0.00	15.98	0.00
6	5.24	0.00	7.03	14.01	73.72
7	0.00	9.25	15.77	0.00	74.98
8	10.90	7.57	0.00	6.72	74.81
9	7.35	2.36	8.49	8.06	73.74
10	16.36	10.37	0.00	0.00	73.27
11	0.00	13.44	0.00	11.66	74.90
12	0.00	3.54	10.80	10.94	74.71
13	11.47	0.00	0.00	13.56	74.97
14	11.08	7.65	6.46	0.00	74.81
15	7.28	4.97	4.33	8.51	74.92
16	4.87	3.27	5.84	11.27	74.75
17	8.92	6.04	10.19	0.00	74.85
18	5.21	7.12	6.22	6.64	74.81
19	4.28	5.86	10.02	5.02	74.82
20	5.39	7.24	12.35	0.00	75.01
21	15.66	0.00	0.00	9.43	74.92
22	0.00	0.00	16.62	8.47	74.91
23	24.97	0.00	0.00	0.00	75.03
24	7.43	0.00	17.60	0.00	74.97
25	7.97	2.95	9.38	4.88	74.83
26	0.00	25.00	0.00	0.00	75.00
27	7.05	9.62	8.29	0.00	75.04
28	0.00	0.00	24.99	0.00	75.01
29	0.00	4.00	13.90	7.05	75.05
30	0.00	0.00	12.38	12.62	75.00
31	0.00	13.46	11.73	0.00	74.81
32	15.84	0.00	9.19	0.00	74.98
33	0.00	7.08	11.97	6.05	74.90

34	6.25	4.24	7.21	7.45	74.84
35	14.88	10.28	0.00	0.00	74.84
36	5.75	0.00	12.93	6.55	74.77
37	0.00	5.71	9.66	9.90	74.73
38	0.00	9.19	7.83	7.99	75.00
39	0.00	0.00	12.40	12.57	75.03
40	7.21	5.08	8.58	4.42	74.72
41	6.34	4.25	7.18	7.40	74.84
42	0.00	25.06	0.00	0.00	74.94
43	4.20	6.17	4.99	10.01	74.63
44	4.46	0.00	10.31	10.47	74.76
45	0.00	0.00	0.00	25.06	74.94
46	25.05	0.00	0.00	0.00	74.95
47	7.05	9.63	0.00	8.41	74.91
48	8.94	0.00	5.25	11.46	74.35
49	0.00	0.00	0.00	25.05	74.95
50	10.65	14.44	0.00	0.00	74.91
51	0.00	0.00	24.97	0.00	75.03
52	6.24	4.19	0.00	14.70	74.87
53	0.00	0.00	8.16	17.35	74.49
54	7.49	0.00	8.61	8.79	75.12
55	11.43	0.00	6.80	6.92	74.85
56	0.00	5.61	0.00	19.48	74.91
57	0.00	4.08	6.83	14.03	75.06
58	0.00	5.58	19.42	0.00	75.00
59	11.73	0.00	13.41	0.00	74.86
60	7.49	0.00	8.64	8.92	74.95
61	8.82	6.14	5.18	5.24	74.62
62	9.88	3.56	0.00	11.79	74.77
63	10.02	3.40	11.60	0.00	74.99
64	7.44	0.00	0.00	17.59	74.98
65	12.97	4.47	7.60	0.00	74.96
66	0.00	9.54	15.73	0.00	74.73
67	9.99	3.54	5.85	5.95	74.66
68	0.00	7.21	6.04	12.16	74.59
69	0.00	5.60	9.61	9.85	74.94
70	12.83	4.62	0.00	7.83	74.73
71	8.10	2.77	4.61	9.61	74.92
72	18.63	6.36	0.00	0.00	75.01

73	0.00	0.00	0.00	0.00	100.00
74	8.58	6.09	0.00	10.48	74.85
75	3.83	2.69	9.25	9.41	74.83
76	8.88	6.03	10.20	0.00	74.89
77	11.43	0.00	0.00	13.60	74.97
78	0.00	9.37	0.00	16.00	74.63
79	5.20	7.20	0.00	12.60	75.00
80	4.87	3.17	11.24	5.81	74.92
81	6.29	4.34	14.62	0.00	74.75

Table S2. Central composite design (n=32) of quaternary mixtures of corn, cane, beet, and rice syrup adulterants using Manuka honey as the standard matrices used in the testing set.

Mixture	Corn (% w/w)	Cane (% w/w)	Beet (% w/w)	Rice (% w/w)	Manuka honey (% w/w)
1	7.66	5.30	9.00	3.00	75.04
2	9.03	2.04	10.40	3.61	74.92
3	6.22	4.25	7.20	7.46	74.87
4	3.23	6.64	3.79	11.41	74.93
5	2.44	5.23	8.59	8.81	74.93
6	8.81	2.02	3.54	10.72	74.92
7	6.23	4.27	7.19	7.37	74.95
8	7.11	1.73	8.16	8.48	74.53
9	3.19	6.65	11.44	3.77	74.95
10	6.22	4.35	7.22	7.38	74.83
11	7.67	5.21	2.98	9.23	74.91
12	6.28	4.30	7.16	7.50	74.77
13	3.80	2.75	4.68	13.94	74.83
14	2.87	2.02	9.98	10.20	74.93
15	6.18	4.30	7.17	7.47	74.87
16	12.40	2.81	4.87	5.07	74.85
17	4.03	2.59	13.81	4.62	74.95
18	4.70	9.41	5.49	5.69	74.71
19	10.15	7.10	4.06	4.04	74.64
20	6.19	4.31	7.36	7.38	74.76
21	4.86	3.29	11.22	5.80	74.84
22	4.77	3.25	5.67	11.39	74.93
23	5.24	7.23	6.28	6.38	74.87
24	10.05	3.48	5.79	6.01	74.66
25	6.23	4.32	7.23	7.39	74.83
26	0.00	5.66	9.69	9.81	74.84
27	7.46	0.00	8.63	8.77	75.13
28	6.18	4.29	7.26	7.42	74.85
29	8.60	6.14	0.00	10.43	74.83
30	6.22	4.36	7.16	7.43	74.83
31	6.21	4.26	7.17	7.41	74.95
32	8.80	6.05	10.20	0.00	74.96

Table S3. Description of samples used in the exploratory principal component analysis (FFD = full factorial design, CCD = central composite design, UNK = unknown dataset) and their respective PCA clusters.

Sample ID	Dataset	Description	PCA cluster
1	FFD	Training set	8
2	FFD	Training set	8
3	FFD	Training set	8
4	FFD	Training set	8
5	FFD	Training set	4
6	FFD	Training set	4
7	FFD	Training set	8
8	FFD	Training set	4
9	FFD	Training set	8
10	FFD	Training set	4
11	FFD	Training set	6
12	FFD	Training set	8
13	FFD	Training set	8
14	FFD	Training set	8
15	FFD	Training set	4
16	FFD	Training set	8
17	FFD	Training set	8
18	FFD	Training set	4
19	FFD	Training set	6
20	FFD	Training set	8
21	FFD	Training set	8
22	FFD	Training set	8
23	FFD	Training set	8
24	FFD	Training set	8
25	FFD	Training set	8
26	FFD	Training set	6
27	FFD	Training set	8
28	FFD	Training set	8
29	FFD	Training set	8
30	FFD	Training set	4
31	FFD	Training set	3
32	FFD	Training set	4
33	FFD	Training set	8
34	FFD	Training set	6
35	FFD	Training set	6
36	FFD	Training set	6
37	FFD	Training set	6
38	FFD	Training set	6
39	FFD	Training set	6
40	FFD	Training set	4
41	FFD	Training set	6
42	FFD	Training set	6

43	FFD	Training set	4
44	FFD	Training set	8
45	FFD	Training set	4
46	FFD	Training set	8
47	FFD	Training set	4
48	FFD	Training set	8
49	FFD	Training set	8
50	FFD	Training set	4
51	FFD	Training set	8
52	FFD	Training set	4
53	FFD	Training set	4
54	FFD	Training set	8
55	FFD	Training set	8
56	FFD	Training set	4
57	FFD	Training set	4
58	FFD	Training set	8
59	FFD	Training set	8
60	FFD	Training set	8
61	FFD	Training set	4
62	FFD	Training set	8
63	FFD	Training set	8
64	FFD	Training set	4
65	FFD	Training set	8
66	FFD	Training set	8
67	FFD	Training set	8
68	FFD	Training set	8
69	FFD	Training set	8
70	FFD	Training set	8
71	FFD	Training set	8
72	FFD	Training set	4
73	FFD	Training set	1
74	FFD	Training set	4
75	FFD	Training set	8
76	FFD	Training set	8
77	FFD	Training set	4
78	FFD	Training set	4
79	FFD	Training set	4
80	FFD	Training set	8
81	FFD	Training set	8
82	CCD	Testing set	8
83	CCD	Testing set	8
84	CCD	Testing set	8
85	CCD	Testing set	4
86	CCD	Testing set	8
87	CCD	Testing set	8
88	CCD	Testing set	8

89	CCD	Testing set	8
90	CCD	Testing set	4
91	CCD	Testing set	8
92	CCD	Testing set	8
93	CCD	Testing set	8
94	CCD	Testing set	8
95	CCD	Testing set	8
96	CCD	Testing set	8
97	CCD	Testing set	8
98	CCD	Testing set	8
99	CCD	Testing set	4
100	CCD	Testing set	3
101	CCD	Testing set	8
102	CCD	Testing set	8
103	CCD	Testing set	8
104	CCD	Testing set	8
105	CCD	Testing set	8
106	CCD	Testing set	8
107	CCD	Testing set	8
108	CCD	Testing set	8
109	CCD	Testing set	4
110	CCD	Testing set	4
111	CCD	Testing set	4
112	CCD	Testing set	8
113	CCD	Testing set	8
114	UNK	Pure beet syrup	5
115	UNK	Pure cane syrup 1	2
116	UNK	Pure corn syrup	7
117	UNK	Pure rice syrup 1	7
118	UNK	Pure cane syrup 2	7
119	UNK	Manuka honey 1	1
120	UNK	Manuka honey 2	1
121	UNK	Manuka honey 3	1
122	UNK	Pure rice syrup 2	7
123	UNK	Manuka honey 4	1
124	UNK	Manuka honey 5	1