Supplementary Material

Evaluation of Underutilized *Malpighia glabra* L. Fruits as a Functional Food: Nutritional Composition, Phenolic Profile, Biological Activities, and Synergistic Effects with Pharmaceutical Drugs

Table S1. Fragment ions of 24 authentic standards of phenolics using liquid chromatography-electrospray ionization-tandem mass spectrometry (LC-ESI-MS/MS) in selective reaction monitoring (SRM) mode*.

Compounds	Standards	Ion mass	Parent ions (*m/z*)	*SRM* transitions (*m/z*) and collision energy (*V*)	*RF lens (V)*
1	Epigallocatechin gallate	[M–H]	457.175	305.155 (16.84 V), 168.97 (17.59 V), 125.042 (40.30 V)	204
2	Gallic acid	[M–H]	169.05	124.988 (14.56 V), 96.917 (18.77 V), 79.185 (22.94 V)	147
3	3,4-Dihydroxybenzoic acid	[M–H]	152.95	109.113 (14.35 V), 81.042 (20.50 V), 91.042 (24.59 V)	128
4	Chlorogenic acid	[M–H]	353.075	179.042 (14.06 V), 191.000 (16.54 V), 85.095 (39.96 V)	148
5	Mangiferin	[M+H]	423.10	273.054 (23.58V), 303.113 (17.76V),327.071(16.88V)	108
6	4-Hydroxybenic acid	[M–H]	137.05	92.970 (14.86 V), 65.000 (29.39 V), 75.000 (31.96 V)	110
7	Caffeic acid	[M–H]	179.038	135.054 (15.07 V), 107.071 (22.57 V), 85.042 (31.96 V)	151
8	Syringic acid	[M–H]	197.138	182.185 (13.72 V), 167.113 (19.24 V), 123.095 (22.31 V)	130
9	Vanillic acid	[M–H]	167.000	123.042 (11.66 V), 151.97 (14.59 V), 108.042 (18.65 V)	114
10	*p*-Coumaric acid	[M+H]	165.05	147.054 (11.70 V), 119.113 (19.36 V), 91.125 (25.89 V)	90
11	Rutin	[M+H]	611.20	303.13 (20.80), 465.20 (12.71V)	198
12	Sinapic acid	[M–H]	223.25	208.125 (13.51 V), 164.024 (15.78 V), 192.970 (22.65 V)	141
13	Ferulic acid	[M–H]	192.95	149.125 (11.28 V), 177.970 (13.05 V), 134.042 (16.50 V)	124
14	Hesperidin	[M–H]	609.30	301.179 (24.50 V), 325.179 (27.83 V), 286.125 (41.60 V)	299
15	Myricetin	[M–H]	317.088	178.970 (19.53 V), 150.988 (24.50 V), 137.113 (26.86 V)	245
16	Rosmarinic acid	[M–H]	359.20	197.000 (15.70 V), 161.113 (17.38 V), 133.054 (37.81 V)	175
17	Fisetin	[M+H]	287.05	213.054(27.96V), 137.042 (30.86V), 241.125(25.09V)	244
18	Luteolin	[M–H]	285.138	197.000 (15.70 V), 161.113 (17.38 V), 133.054 (37.81 V)	241
19	Quercetin	[M–H]	301.200	178.976 (18.18 V), 273.125 (19.45 V), 151.042 (21.39 V)	237
20	Cinnamic acid	[M–H]	147.00	103.00 (11.23V), 77.083 (23.07)	107
21	Apigenin	[M–H]	269.075	116.863 (34.28 V), 149.071 (25.13 V), 151.131 (25.05 V)	244
22	Genistein	[M–H]	269.138	224.054 (25.60 V), 159.054 (29.26 V), 132.929 (30.95 V)	239
23	Naringenin	[M+H]	272.938	146.97 (21.01 V), 153.054 (24.42 V), 119.000 (31.28 V)	160
24	Kaempferol	[M–H]	285.150	184.911 (25.85 V), 239.113 (27.03 V), 186.988 (28.17 V)	260
25	Isorhamnetin	[M–H]	315.088	300.000 (21.30 V), 150.970 (29.14 V), 271.054 (30.57 V)	233
26	Galangin	[M+H]	271.088	165.042 (28.80 V), 197.125 (31.75 V), 153.113 (32.42 V)	248

*These data are from our previous study (Sirichai et al., 2022).

Table S2. The validation parameters of 24 authentic standards of phenolics using liquid chromatography-electrospray ionization-tandem mass spectrometry (LC-ESI-MS/MS) in selective reaction monitoring (SRM) mode*.

Compounds	Retention time (min)	Standards	Linear range (µg/mL)	Linear regression equation	Correlation coefficient (R^2)	LOD (µg/mL)	LOQ (µg/mL)	%RSD (Inter-day)	%Recovery		
									Low level (µg/mL)	Medium level (µg/mL)	High level (µg/mL)
1	0.44	Epigallocatechin gallate	0.125–40	y = 8533x + 1053.4	0.9985	0.067	0.230	0.023	91.84	85.36	91.37
2	0.564	Gallic acid	0.195–25	y = 3323.1x – 2100.4	0.9984	0.04	0.14	0.01	113.05	118.57	109.12
3	0.803	3,4-Dihydroxybenzoic acid	0.195–25	y = 11490x – 10877	0.9935	0.010	0.034	0.003	90.59	85.75	89.75
4	0.922	Chlorogenic acid	0.3125–40	y = 8377.5x – 3623.5	0.9934	0.017	0.055	0.006	91.94	87.50	95.02
5	1.116	Mangiferin	0.125–10	y = 7516.2x + 195.48	0.9985	0.040	0.130	3.700	102.20	91.14	91.57
6	1.16	4-Hydroxybenic acid	0.3125–40	y = 2482.6x– 3998.4	0.9917	0.027	0.090	0.009	109.67	103.60	101.28
7	1.40	Caffeic acid	0.3125–40	y = 12328x–19725	0.9918	0.010	0.035	0.003	105.36	93.98	87.41
8	1.539	Syringic acid	3.125–100	y = 68.091x + 230.43	0.9955	0.582	1.939	0.194	116.35	97.42	94.91
9	1.63	Vanillic acid	2.5–100	y = 213.67x – 975.72	0.9900	0.15	0.48	0.05	99.86	101.76	100.12
10	2.452	*p*-Coumaric acid	0.3125–40	y = 8532.4x–13559	0.9910	0.013	0.042	0.004	88.22	81.36	98.05
11	2.737	Rutin	0.009–1.25	y = 49729x – 33.064	0.9999	0.001	0.005	0.0005	94.63	114.00	108.73
12	2.772	Sinapic acid	0.39–25	y = 1592.6x – 832.22	0.9977	0.026	0.086	0.009	81.34	92.16	84.22
13	2.851	Ferulic acid	1.56–100	y = 559.03x – 1819.2	0.9947	0.155	0.518	0.052	91.51	89.24	93.10
14	3.41	Hesperidin	0.25–40	y = 838.63x – 242.2	0.9986	0.07	0.22	0.02	100.43	104.06	108.60
15	3.431	Myricetin	1.25–40	y = 303.47x – 601.81	0.9976	0.261	0.871	0.087	113.07	81.77	91.12
16	3.528	Rosmarinic acid	0.3125–40	y = 4322.4x-3744.1	0.9956	0.07	0.25	0.02	92.45	106.35	99.62
17	3.620	Fisetin	0.25–10	y = 7468.4x – 701.27	0.9979	0.150	0.490	6.900	98.01	108.94	117.51
18	4.158	Luteolin	0.195–12.5	y = 8381.9x – 5000.7	0.9945	0.015	0.050	0.0005	84.21	96.21	107.09
19	4.185	Quercetin	0.05–12.5	y = 2934x + 917.17	0.9937	0.05	0.18	0.02	83.36	115.06	95.74
20	4.522	Cinnamic acid	0.039–10	y = 6631.9x – 866.59	0.9964	0.049	0.163	0.016	101.94	98.84	95.85
21	4.689	Apigenin	0.34–11	y = 1790.7x – 287.7	0.9997	0.127	0.424	0.042	88.84	106.89	114.79
22	4.693	Genistein	0.625–40	y = 1247.2x – 1747.1	0.9977	0.049	0.163	0.016	95.33	101.49	11633
23	4.705	Naringenin	0.0008–5	y = 16755x + 443.03	0.9932	0.003	0.011	0.001	117.92	96.26	111.08
24	4.79	Kaempferol	0.25–10	y = 1006.8x – 346.28	0.9905	0.122	0.406	0.041	92.35	107.69	102.17
25	4.878	Isorhamnetin	0.0098–2.5	y = 12698x + 586.16	0.9945	0.016	0.052	0.005	113.57	105.88	111.14
26	6.146	Galangin	0.3125–40	y = 5012.1x – 9354.7	0.9879	0.010	0.035	0.003	84.01	112.92	115.80

*These data are from our previous study (Sirichai et al., 2022)

Table S3. A liquid chromatography-electrospray ionization-tandem mass spectrometry (LC-ESI-MS/MS) integration result of *Malpighia glabra* L. extract.

No	Peak Name	Retention time (min)	Quantitation ion	Area (counts*min)	Height (counts)	Overall ion ratio Confirmation
1	ECG	0.462	168.97	7	109	Not confirmed
2	Gallic acid	0.470	124.99	12	1430	Not confirmed
3	Chlorogenic acid	0.679	191.00	81	912	Not confirmed
4	3,4-Dihydroxybenzoic acid	0.781	109.11	2032	11557	Not confirmed
5	Mangiferin	1.162	273.05	20	1291	Not confirmed
6	4-Hydroxybenzoic acid	1.262	92.97	122	3265	Not confirmed
7	Syringic acid	1.499	182.18	10	207	Not confirmed
8	Caffeic acid	1.564	135.00	492	5342	Not confirmed
9	Vanillic acid	n.a.	151.97	n.a.	n.a.	Not confirmed
10	p-Coumaric acid	2.520	147.05	26	2850	Not confirmed
11	Rutin	2.719	303.13	2336	52101	Confirmed
12	Ferulic acid	2.843	134.04	3	389	Not confirmed
13	Sinapic acid	2.858	208.13	17	1030	Not confirmed
14	Hesperidin	3.378	301.18	28	535	Not confirmed
15	Myricetin	n.a.	150.99	n.a.	n.a.	Not confirmed
16	Rosmarinic acid	3.534	161.11	12	442	Not confirmed
17	Fisetin	3.649	213.05	1012	26042	Not confirmed
18	Quercetin	n.a.	151.04	n.a.	n.a.	Not confirmed
19	Luteolin	4.204	133.07	113	1861	Not confirmed
20	Cinnamic acid	4.571	103.00	31	2492	Not confirmed
21	Genistein	n.a.	132.93	n.a.	n.a.	Not confirmed
22	Apigenin	4.714	116.86	2	65	Not confirmed
23	Naringenin	4.749	153.05	503	10747	Not confirmed
24	Kaempferol	4.822	239.11	595	6300	Not confirmed
25	Isorhamnetin	4.931	300.00	243	4878	Not confirmed
26	Galangin	6.180	153.11	4	290	Not confirmed

Reference

Sirichai, P., Kittibunchakul, S., Thangsiri, S., On-Nom, N., Chupeerach, C., Temviriyanukul, P., Inthachat, W., Nuchuchua, O., Aursalung, A., Sahasakul, Y., Charoenkiatkul, S., Suttisansanee, U., Impact of drying processes on phenolics and in vitro health-related activities of indigenous plants in Thailand, Plants (Basel). 11(3) (2022), doi: 10.3390/plants11030294.