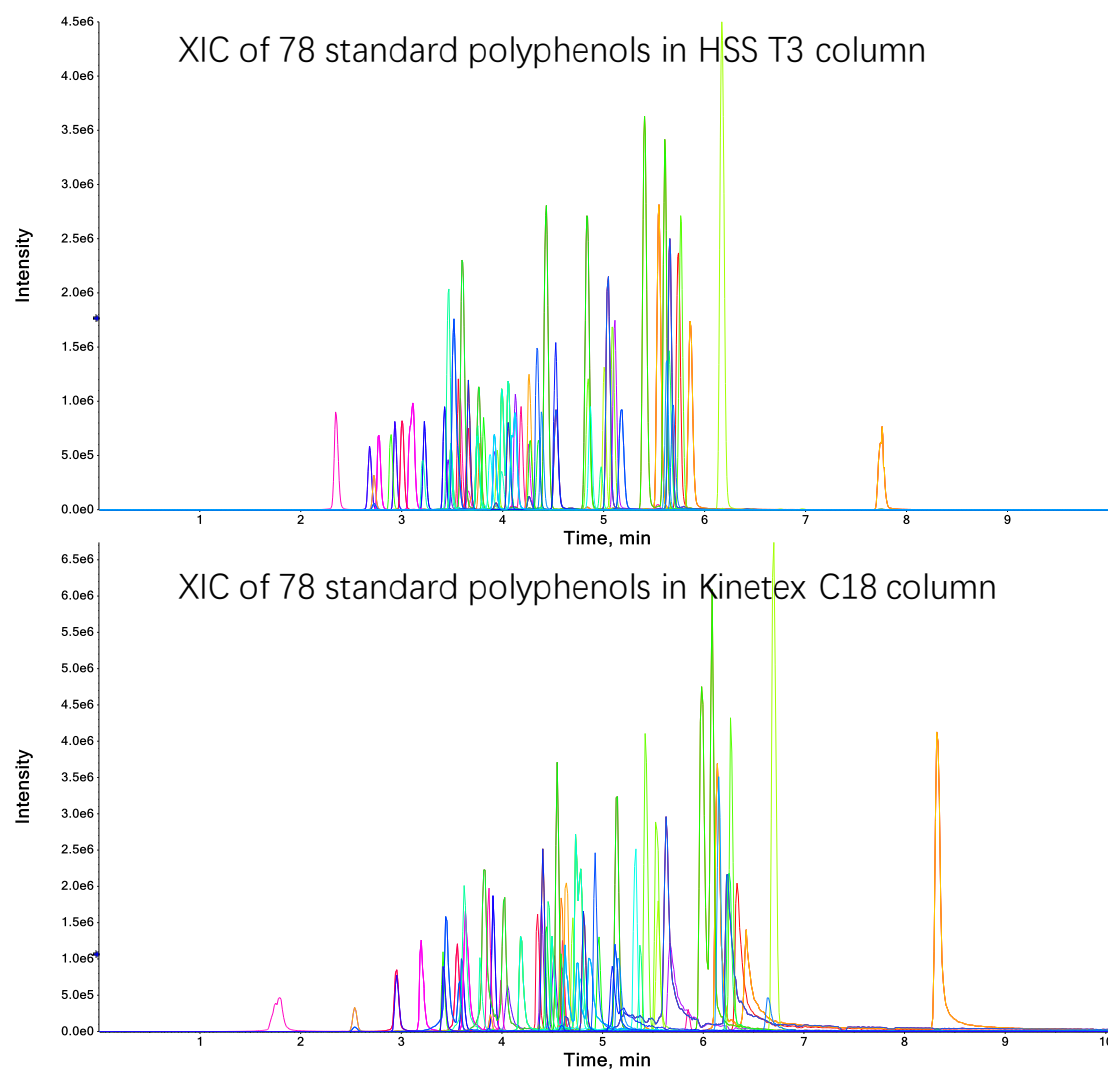


Supplementary Information

Supplementary Figure 1. XICs of polyphenol reference compounds using different columns.



Supplementary Table 1. Standard references used for quantification.

No	References	CAS registry number	Molecular Formula	Purity
1	(+)-Catechin	154-23-4	C ₁₅ H ₁₄ O ₆	99%
2	(-)-Epicatechin	490-46-0	C ₁₅ H ₁₄ O ₆	98%
3	(-)-Gallocatechin	3371-27-5	C ₁₅ H ₁₄ O ₇	98%
4	(-)-Epigallocatechin	970-74-1	C ₁₅ H ₁₄ O ₇	98%
5	(-)-Epicatechin gallate	1257-08-5	C ₂₂ H ₁₈ O ₁₀	99%
6	(-)-Epigallocatechin gallate	989-51-5	C ₂₂ H ₁₈ O ₁₁	98%
7	Kaempferol	520-18-3	C ₁₅ H ₁₀ O ₆	98%
8	trans-4-Hydroxycinnamic acid	501-98-4	C ₉ H ₈ O ₃	98%
9	Vanillic acid	121-34-6	C ₈ H ₈ O ₄	99%
10	Quercetin	117-39-5	C ₁₅ H ₁₀ O ₇	98%
11	4-Hydroxybenzoic acid	99-96-7	C ₇ H ₆ O ₃	99%
12	Ferulic acid	1135-24-6	C ₁₀ H ₁₀ O ₄	99%
13	Chlorogenic acid	327-97-9	C ₁₆ H ₁₈ O ₉	98%
14	4-O-Caffeoylquinic Acid	905-99-7	C ₁₆ H ₁₈ O ₉	98%
15	Neochlorogenic acid	906-33-2	C ₁₆ H ₁₈ O ₉	98%
16	4-Hydroxy-3,5-dimethoxybenzoic acid	530-57-4	C ₉ H ₁₀ O ₅	98%
17	Gallic acid	149-91-7	C ₇ H ₆ O ₅	99%
18	Caffeic acid	331-39-5	C ₉ H ₈ O ₄	99%
19	trans-Cinnamic acid	140-10-3	C ₉ H ₈ O ₂	99%
20	3,5-Dimethoxy-4-hydroxycinnamic acid	530-59-6	C ₁₁ H ₁₂ O ₅	98%
21	2,5-Dihydroxybenzoic acid	490-79-9	C ₇ H ₆ O ₄	99%
22	Apigenin	520-36-5	C ₁₅ H ₁₀ O ₅	98%
23	Protocatechuic acid	99-50-3	C ₇ H ₆ O ₄	99%
24	Rutin	153-18-4	C ₂₇ H ₃₀ O ₁₆	98%
25	7-Hydroxycoumarin	93-35-6	C ₉ H ₆ O ₃	98%
26	Luteolin	491-70-3	C ₁₅ H ₁₀ O ₆	96%
27	Isorhamnetin	480-19-3	C ₁₆ H ₁₂ O ₇	98%
28	6,7-Dihydroxycoumarin	305-01-1	C ₉ H ₆ O ₄	98%
29	Baicalein	491-67-8	C ₁₅ H ₁₀ O ₅	98%
30	(±)-Naringenin	67604-48-2	C ₁₅ H ₁₂ O ₅	98%
31	Apigenin 7-glucoside	578-74-5	C ₂₁ H ₂₀ O ₁₀	98%

32	Isovitexin	38953-85-4	C ₂₁ H ₂₀ O ₁₀	98%
33	Kaempferol-3-O-rutinosid	17650-84-9	C ₂₇ H ₃₀ O ₁₅	98%
34	Astragalin	480-10-4	C ₂₁ H ₂₀ O ₁₁	98%
35	Syringaldehyde	134-96-3	C ₉ H ₁₀ O ₄	98%
36	(+)-Taxifolin	480-18-2	C ₁₅ H ₁₂ O ₇	98%
37	Homogentisic Acid	451-13-8	C ₈ H ₈ O ₄	97%
38	Emodin	518-82-1	C ₁₅ H ₁₀ O ₅	95%
39	Orientin	28608-75-5	C ₂₁ H ₂₀ O ₁₁	98%
40	Glycitein	40957-83-3	C ₁₆ H ₁₂ O ₅	98%
41	Daidzin	552-66-9	C ₂₁ H ₂₀ O ₉	98%
42	Genistin	529-59-9	C ₂₁ H ₂₀ O ₁₀	99%
43	Formononetin	485-72-3	C ₁₆ H ₁₂ O ₄	98%
44	Naringin	10236-47-2	C ₂₇ H ₃₂ O ₁₄	98%
45	Eriodictyol	552-58-9	C ₁₅ H ₁₂ O ₆	98%
46	Enterodiol(P)	80226-00-2	C ₁₈ H ₂₂ O ₄	95%
47	Hesperetin	520-33-2	C ₁₆ H ₁₄ O ₆	98%
48	Nobiletin	478-01-3	C ₂₁ H ₂₂ O ₈	98%
49	Tangeretin	481-53-8	C ₂₀ H ₂₀ O ₇	98%
50	Bergenin	477-90-7	C ₁₄ H ₁₆ O ₉	99%
51	Butein	487-52-5	C ₁₅ H ₁₂ O ₅	98%
52	Phlorizin	60-81-1	C ₂₁ H ₂₄ O ₁₀	95%
53	4-Hydroxycoumarin	1076-38-6	C ₉ H ₆ O ₃	98%
54	Scopoletin	92-61-5	C ₁₀ H ₈ O ₄	98%
55	Daphnetin	486-35-1	C ₉ H ₆ O ₄	98%
56	Chrysoeriol	491-71-4	C ₁₆ H ₁₂ O ₆	95%
57	Luteolin-7-O-β-D-glucopyranoside	5373-11-5	C ₂₁ H ₂₀ O ₁₁	98%
58	Hyperoside	482-36-0	C ₂₁ H ₂₀ O ₁₂	98%
59	3,4-Dimethoxycinnamic acid	2316-26-9	C ₁₁ H ₁₂ O ₄	99%
60	Methyl gallate	99-24-1	C ₈ H ₈ O ₅	99%
61	Procyanidin B2	29106-49-8	C ₃₀ H ₂₆ O ₁₂	98%
62	Hesperidin	520-26-3	C ₂₈ H ₃₄ O ₁₅	98%
63	Quercitrin	522-12-3	C ₂₁ H ₂₀ O ₁₁	98%
64	Resveratrol	501-36-0	C ₁₄ H ₁₂ O ₃	98%
65	Ellagic acid	476-66-4	C ₁₄ H ₆ O ₈	98%
66	Salicylic acid	69-72-7	C ₇ H ₆ O ₃	99%

67	Isochlorogenic acid A	2450-53-5	C ₂₅ H ₂₄ O ₁₂	98%
68	Isochlorogenic acid B	14534-61-3	C ₂₅ H ₂₄ O ₁₂	98%
69	Isochlorogenic acid C	32451-88-0	C ₂₅ H ₂₄ O ₁₂	98%
70	Engenol	97-53-0	C ₁₀ H ₁₂ O ₂	98%
71	Matairesinol	580-72-3	C ₂₀ H ₂₂ O ₆	95%
72	Baicalin	21967-41-9	C ₂₁ H ₁₈ O ₁₁	98%
73	Amentoflavone	1617-53-4	C ₃₀ H ₁₈ O ₁₀	98%
74	Polydatin	65914-17-2	C ₂₀ H ₂₂ O ₈	98%
75	Fisetin	528-48-3	C ₁₅ H ₁₀ O ₆	98%
76	Rosmarinic acid	20283-92-5	C ₁₈ H ₁₆ O ₈	99%
77	3,4-Dihydroxybenzaldehyde	139-85-5	C ₇ H ₆ O ₃	98%
78	Myricetin	529-44-2	C ₁₅ H ₁₄ O ₉	98%

Supplementary Table 2. MRM parameters used for method validation.

Compound	RT (min)	Ion mode	Parent ion(<i>m/z</i>)	Product ion 1 (<i>m/z</i>)	Product ion 2 (<i>m/z</i>)
flavonoid	2.26	ESI-	366	114	208
(+)-Catechin	5.14	ESI-	289	203	245
(-)-Epicatechin	5.46	ESI-	289	245	203
(-)-Gallocatechin	4.4	ESI-	305	125	179
(-)-Epigallocatechin	4.82	ESI-	305	125	219
(-)-Epicatechin gallate	6.12	ESI-	441	169	289
(-)-Epigallocatechin gallate	5.47	ESI-	457	125	169
Kaempferol	8.3	ESI-	285	117	93
trans-4-Hydroxycinnamic acid	6.21	ESI-	163	119	93
Vanillic acid	5.61	ESI-	167	108	123
Quercetin	7.65	ESI-	301	151	179
4-Hydroxybenzoic acid	5.33	ESI-	137	93	108
Ferulic acid	6.43	ESI-	193	134	117
Chlorogenic acid	5.06	ESI-	353	191	179
4-O-Caffeoylquinic Acid	5.1	ESI-	353	173	179
Neochlorogenic acid	4.6	ESI-	353	191	179
4-Hydroxy-3,5-dimethoxy benzoic acid	5.67	ESI-	197	121	153
Gallic acid	3.74	ESI-	169	125	79
Caffeic acid	5.52	ESI-	179	135	107

trans-Cinnamic acid	8.08	ESI-	147	103	119
3,5-Dimethoxy-4-hydroxycinnamic acid	6.39	ESI-	223	149	164
2,5-Dihydroxybenzoic acid	5.4	ESI-	153	108	109
Apigenin	8.18	ESI-	269	117	151
Protocatechuic acid	4.6	ESI-	153	109	108
Rutin	5.82	ESI-	609	300	255
7-Hydroxycoumarin	6.53	ESI-	161	133	105
Luteolin	7.58	ESI-	285	133	151
Isorhamnetin	8.4	ESI-	315	300	151
6,7-Dihydroxycoumarin	5.52	ESI-	177	133	105
Baicalein	8.53	ESI-	269	139	167
(±)-Naringenin	8.21	ESI-	271	151	119
Apigenin 7-glucoside	6.45	ESI-	431	268	240
Isovitexin	5.92	ESI-	431	311	341
Kaempferol-3-O-rutinosid	6.11	ESI-	593	285	255
Astragalin	6.35	ESI-	447	255	284
Syringaldehyde	6.46	ESI-	181	151	166
(+)-Taxifolin	6.46	ESI-	303	285	125
Homogentisic Acid	4.24	ESI-	167	123	122
Emodin	10.5	ESI-	269	245	241
Orientin	5.66	ESI-	447	327	357
Glycitein	7.55	ESI-	283	268	240
Daidzin	5.66	ESI+	417	255	
Genistin	6.24	ESI+	433	271	
Formononetin	8.84	ESI-	267	252	223
Naringin	6.33	ESI-	579	271	151
Eriodictyol	7.58	ESI-	287	135	151
Enterodiol(P)	7.37	ESI-	301	253	271

Hesperetin	8.39	ESI-	301	164	151
Sinensetin	9.07	ESI+	373	343	321
Nobiletin	9.5	ESI+	403	373	388
Tangeretin	9.99	ESI+	373	343	358
Bergenin	4.8	ESI-	327	192	207
Butein	8.02	ESI-	271	135	253
Phlorizin	6.7	ESI-	435	273	125
4-Hydroxycoumarin	7.18	ESI-	161	117	
Scopoletin	6.51	ESI-	191	176	148
Daphnetin	5.75	ESI-	177	121	93
Chrysoeriol	8.31	ESI-	299	284	256
Luteolin-7-O-β-D-glucopyranoside	6.03	ESI-	447	285	327
Hyperoside	5.99	ESI-	463	300	271
3,4-Dimethoxycinnamic acid	7.41	ESI-	207	103	163
Methyl gallate	5.31	ESI-	183	124	140
Procyanidin B2	5.18	ESI-	577	289	407
Hesperidin	6.42	ESI-	609	301	
Quercitrin	6.4	ESI-	447	300	151
Resveratrol	7.25	ESI-	227	143	185
Ellagic acid	6.04	ESI-	301	145	200
Salicylic acid	7.42	ESI-	137	93	65
Isochlorogenic acid A	6.39	ESI-	515	353	191
Isochlorogenic acid B	6.2	ESI-	515	353	173
Isochlorogenic acid C	6.47	ESI-	515	353	173
Matairesinol	8.28	ESI-	357	83	122
Baicalin	6.91	ESI-	445	269	113
Amentoflavone	8.44	ESI-	537	375	417
Polydatin	6.02	ESI-	389	227	161
Fisetin	6.89	ESI-	285	135	121
Rosmarinic acid	6.68	ESI-	359	161	197

3,4-Dihydroxybenzaldehyde	5.23	ESI-	137	108	81
Myricetin	6.85	ESI-	317	137	179

Supplementary Table 3. Summary of the method validation performance characteristics as determined in extracts from Chinese globeflower. Samples (n=5)

Compound	Calibration equation (y=)	Coefficient of determination	Dynamic range (µg L ⁻¹)	LOD (µg L ⁻¹)	LOQ (µg L ⁻¹)	Spiked (µg kg ⁻¹)	Recovery (%)	consecutive 3 days (%RSD)
(+) -Catechin	$y = 1.18980 \times 10^6 x + 15100.40088$	0.99629	5-2500	8.00	26.67	625	89.6%	8.1%
						2500	94.7%	5.3%
						6250	93.9%	9.4%
(-) -Epicatechin	$y = 4.60455 \times 10^6 x + 1.01712 \times 10^5$	0.99494	0.25-1000	6.04	20.12	625	83.5%	8.6%
						2500	97.9%	5.8%
						6250	85.8%	4.9%
(-) -Gallocatechin	$y = 3.23696 \times 10^6 x + 1.68322 \times 10^5$	0.99727	10-2500	15.87	52.91	625	96.6%	7.0%
						2500	100.0%	9.2%
						6250	85.3%	6.4%
(-) -Epigallocatechin	$y = 3.31448 \times 10^6 x + 5.31080 \times 10^5$	0.99276	100-2500	6.59	21.98	625	75.1%	8.3%
						2500	84.0%	4.1%
						6250	89.8%	6.7%
(-) -Epicatechin gallate	$y = 5.81385 \times 10^6 x + 2026.20720$	0.99864	1-1000	2.99	9.95	625	92.0%	7.8%
						2500	83.0%	7.0%
						6250	89.5%	5.5%
(-) -Epigallocatechin gallate	$y = 2.01143 \times 10^6 x + 2.31861 \times 10^5$	0.99257	5-2500	6.64	22.12	625	92.1%	8.7%
						2500	93.2%	9.7%
						6250	89.4%	6.0%

Kaempferol	$y = 8.42601e5 x + -14668.82708$	0.99941	1-2500	5.88	19.61	625	91.0%	11.7%
						2500	89.0%	3.1%
						6250	99.0%	5.3%
trans-4-Hydroxycinnamic acid	$y = 1.48341e7 x + 1.91271e5$	0.9971	10-250	7.26	24.21	625	103.1%	6.0%
						2500	90.7%	3.8%
						6250	94.3%	6.3%
Vanillic acid	$y = 3.12050e6 x + 6743.12295$	0.99966	0.5-500	6.90	22.99	625	89.6%	7.6%
						2500	90.9%	6.3%
						6250	89.8%	4.4%
Quercetin	$y = 8.28497e6 x + -4.57391e5$	0.99036	25-2500	1.93	6.42	625	97.8%	8.2%
						2500	90.8%	7.1%
						6250	97.6%	4.5%
4-Hydroxybenzoic acid	$y = 3.33790e7 x + 3.57807e5$	0.99645	0.25-250	4.48	14.95	625	97.8%	8.0%
						2500	94.5%	6.5%
						6250	86.1%	5.2%
Ferulic acid	$y = 1.32026e7 x + 9.76408e4$	0.99582	0.1-500	3.44	11.48	625	104.8%	5.5%
						2500	99.9%	5.6%
						6250	99.5%	5.2%
Chlorogenic acid	$y = 1.56478e7 x + 4.10184e5$	0.99934	1-2500	1.79	5.98	625	94.1%	5.8%
						2500	93.4%	5.3%
						6250	91.9%	5.3%
4-O-Caffeoylquinic Acid	$y = 8.48070e6 x + 1.29841e5$	0.99943	0.25-2500	2.32	7.73	625	96.6%	5.9%
						2500	99.6%	4.7%
						6250	91.4%	3.6%
Neochlorogenic acid		0.99814	0.5-500	6.32	21.05	625	118.6%	6.1%

	$y = 1.07471e7 x + 8.06889e4$					2500	102.8%	5.4%
						6250	92.2%	5.1%
4-Hydroxy-3,5-dimethoxybenzoic acid	$y = 6.16434e5 x + 2182.63860$	0.99848	5-2500	33.33	111.11	625	86.2%	6.4%
						2500	104.3%	7.3%
						6250	93.2%	6.3%
Gallic acid	$y = 2.09978e7 x + 25636.96090$	0.99328	2.5-1000	1.24	4.12	625	104.7%	6.2%
						2500	96.3%	6.2%
						6250	98.6%	3.2%
Caffeic acid	$y = 3.17533e7 x + 4.91710e5$	0.99793	2.5-500	4.34	14.47	625	99.0%	4.3%
						2500	93.5%	4.0%
						6250	102.1%	3.3%
trans-Cinnamic acid	$y = 1.67166e6 x + 2.56305e5$	0.99632	2.5-2500	8.13	27.10	625	82.3%	9.2%
						2500	98.6%	5.4%
						6250	106.9%	6.2%
3,5-Dimethoxy-4-hydroxycinnamic acid	$y = 3.34826e6 x + 3.71588e4$	0.99788	2.5-1000	5.61	18.69	625	106.2%	2.1%
						2500	102.7%	3.7%
						6250	102.8%	3.0%
2,5-Dihydroxybenzoic acid	$y = 2.05251e7 x + 3.03349e5$	0.99702	0.25-1000	5.22	17.39	625	87.2%	5.7%
						2500	95.6%	7.5%
						6250	94.0%	6.0%
Apigenin	$y = 1.52282e7 x + 2.26293e5$	0.99718	0.1-1000	2.33	7.78	625	102.5%	8.4%
						2500	103.4%	6.4%
						6250	103.4%	6.7%
Protocatechuic acid	$y = 4.81725e7 x + 8.56361e4$	0.99897	1-100	3.81	12.69	625	100.4%	5.3%
						2500	95.5%	6.8%

						6250	97.2%	6.1%
						625	96.5%	6.5%
Rutin	$y = 2.14215e7 x + 1.00955e5$	0.99886	0.1-500	5.08	16.95	2500	94.3%	6.3%
						6250	93.1%	5.6%
						625	99.8%	6.3%
7-Hydroxycoumarin	$y = 3.44335e7 x + 2.02994e5$	0.9942	0.25-250	7.32	24.39	2500	92.1%	4.5%
						6250	102.1%	5.2%
						625	95.4%	6.1%
Luteolin	$y = 1.08559e7 x + 2.45213e5$	0.99892	0.25-2500	2.02	6.73	2500	95.0%	6.4%
						6250	97.5%	3.5%
						625	102.7%	3.6%
Isorhamnetin	$y = 1.80843e7 x + 1.25728e6$	0.99734	10-2500	6.06	20.20	2500	99.4%	5.1%
						6250	105.3%	5.3%
						625	98.0%	4.9%
6,7-Dihydroxycoumarin	$y = 2.70960e7 x + 5.88233e4$	0.99776	1-100	4.27	14.22	2500	101.8%	2.7%
						6250	100.8%	2.5%
						625	101.9%	3.1%
Baicalein	$y = 1.87874e6 x + 7.85865e4$	0.99087	0.5-2500	5.41	18.02	2500	96.3%	8.0%
						6250	98.3%	2.8%
						625	95.6%	4.7%
(±)-Naringenin	$y = 2.53540e7 x + 5.40825e4$	0.99956	0.5-250	1.43	4.77	2500	79.4%	11.2%
						6250	90.2%	3.2%
						625	92.4%	3.3%
Apigenin 7-glucoside	$y = 1.77909e7 x + 1.62807e5$	0.99892	0.1-1000	2.36	7.87	2500	95.8%	2.1%
						6250	98.9%	4.6%

Isovitexin	$y = 1.31684e7 x + 1.73428e5$	0.99775	0.5-1000	1.85	6.17	625	93.7%	3.0%
						2500	101.4%	2.8%
						6250	101.0%	2.2%
Kaempferol-3-O-rutinosid	$y = 1.48482e7 x + 10799.21249$	0.99982	0.25-500	3.42	11.39	625	94.0%	8.6%
						2500	99.3%	8.5%
						6250	103.8%	4.7%
Astragalin	$y = 2.50862e7 x + 6.04243e4$	0.99904	0.1-500	2.61	8.70	625	97.2%	4.8%
						2500	97.4%	3.8%
						6250	106.7%	3.7%
Syringaldehyde	$y = 2.39685e6 x + 22827.46439$	0.99876	2.5-1000	2.05	6.85	625	94.1%	9.5%
						2500	109.5%	3.8%
						6250	94.3%	7.2%
(+) -Taxifolin	$y = 1.76750e7 x + 1.24435e5$	0.99971	2.5-500	2.08	6.93	625	95.1%	9.7%
						2500	92.4%	6.3%
						6250	95.6%	5.3%
Homogentisic Acid	$y = 1.12228e7 x + 1.99863e5$	0.998	1-1000	6.04	20.12	625	105.2%	4.7%
						2500	101.6%	4.5%
						6250	102.2%	6.5%
Orientin	$y = 2.25705e7 x + 2308.97107$	0.99967	0.1-250	3.24	10.80	625	101.9%	2.0%
						2500	100.4%	2.4%
						6250	101.3%	2.6%
Glycitein	$y = 2.16660e7 x + 4.31584e4$	0.99863	0.1-250	3.65	12.18	625	87.1%	5.7%
						2500	100.2%	7.1%
						6250	93.8%	6.0%
Daidzin		0.99953	0.1-1000	4.64	15.46	625	100.6%	2.8%

		$y = 2.72009e6 x + 19544.37945$	0.9998	0.1-1000	26.55	88.50	2500	101.0%	2.6%
							6250	100.6%	1.4%
							625	87.2%	4.5%
Genistin		$y = 9.15247e6 x + 22598.15980$	0.9998	0.1-1000	26.55	88.50	2500	98.7%	4.2%
							6250	86.8%	3.5%
							625	117.6%	7.7%
Formononetin		$1.42034e8 x + 3.10931e5$	0.9965	0.1-100	0.12	0.40	2500	91.4%	5.1%
							6250	101.0%	5.6%
							625	81.2%	7.1%
Naringin		$y = 7.82169e6 x + 3.65724e4$	0.99878	0.5-500	4.67	15.55	2500	93.7%	6.7%
							6250	102.8%	6.9%
							625	94.6%	4.1%
Eriodictyol		$y = 3.10832e7 x + 1.03703e5$	0.99884	0.5-250	1.86	6.19	2500	92.5%	6.4%
							6250	98.1%	6.6%
							625	91.4%	8.5%
Enterodiol(P)		$y = 2.62915e7 x + -611.72541$	0.99913	0.25-100	3.32	11.07	2500	95.9%	6.5%
							6250	96.1%	3.8%
							625	95.3%	9.5%
Hesperetin		$1.81795e7 x + 3.23384e4$	0.99979	0.5-250	1.20	4.00	2500	95.9%	7.1%
							6250	105.3%	4.0%
							625	97.9%	8.6%
Bergenin		$y = 5.68259e6 x + 11045.65442$	0.99931	0.1-500	8.29	27.62	2500	95.5%	5.0%
							6250	113.1%	4.4%
							625	112.4%	5.5%
Butein		$y = 2.17637e7 x + -1.57406e6$	0.99582	5-2500	0.92	3.06	2500	100.8%	4.8%

Phlorizin	$y = 2.13330e7 x + 7.42339e4$	0.99916	0.1-500	3.31	11.03	6250	106.3%	2.6%
						625	95.8%	7.6%
						2500	97.9%	6.6%
						6250	99.5%	3.2%
4-Hydroxycoumarin	$y = 1.12737e8 x + 8.96716e4$	0.99682	0.1-50	4.86	16.21	625	43.8%	8.8%
						2500	42.9%	11.3%
						6250	46.4%	6.7%
Scopoletin	$y = 3.82756e7 x + 4.67278e4$	0.99817	0.1-100	12.05	40.16	625	84.5%	7.8%
						2500	99.1%	8.0%
						6250	94.1%	7.7%
Daphnetin	$y = 7.58185e6 x + 1.14556e5$	0.99744	2.5-1000	4.43	14.77	625	89.0%	9.0%
						2500	98.8%	4.5%
						6250	95.7%	5.3%
Chrysoeriol	$y = 6.04170e7 x + 6.70617e4$	0.99885	0.1-100	8.24	27.47	625	104.9%	4.8%
						2500	98.6%	4.5%
						6250	93.8%	4.6%
Luteolin-7-O-β-D-glucopyranoside	$y = 1.88754e7 x + 1.29246e5$	0.99938	0.1-1000	26.55	88.50	625	98.5%	3.4%
						2500	103.2%	4.3%
						6250	101.6%	2.6%
Hyperoside	$y = 1.37714e7 x + 9.61943e4$	0.99908	0.25-1000	3.17	10.56	625	100.2%	4.0%
						2500	109.0%	3.5%
						6250	109.1%	2.5%
3,4-Dimethoxycinnamic acid	$y = 2.04161e6 x + -13303.63319$	0.99831	1-500	22.39	74.63	625	90.4%	4.9%
						2500	95.0%	8.8%
						6250	102.4%	8.6%

Methyl gallate	$y = 3.67764e7 x + 29514.26391$	0.99913	1-100	3.95	13.18	625	107.0%	7.6%
						2500	94.3%	9.1%
						6250	94.4%	6.4%
Procyanidin B2	$y = 3.42078e6 x + -8.03870e4$	0.99614	1-1000	12.77	42.55	625	72.4%	23.9%
						2500	86.7%	7.6%
						6250	79.9%	7.1%
Hesperidin	$y = 1.51841e7 x + 4913.09960$	0.99972	0.1-250	6.40	21.32	625	94.5%	4.8%
						2500	90.9%	6.0%
						6250	92.6%	4.9%
Quercitrin	$y = 1.98496e7 x + 8.57720e4$	0.99885	0.25-500	2.35	7.84	625	103.8%	5.2%
						2500	99.4%	4.3%
						6250	98.1%	4.5%
Resveratrol	$y = 5.69155e6 x + 27911.01407$	0.9994	0.5-1000	6.70	22.32	625	78.5%	16.9%
						2500	87.8%	13.8%
						6250	87.8%	13.8%
Ellagic acid	$y = 1.67751e6 x + -4.18737e5$	0.9638	50-2500	1.72	5.75	625	83.0%	6.4%
						2500	79.8%	4.1%
						6250	101.7%	7.4%
Salicylic acid	$y = 6.04396e7 x + 4.42332e5$	0.99657	0.5-250	1.78	5.92	625	79.7%	4.8%
						2500	75.9%	5.7%
						6250	92.2%	4.6%
Isochlorogenic acid A	$y = 8.85809e6 x + -14750.74487$	0.99909	0.1-1000	0.53	1.77	625	77.8%	5.1%
						2500	97.3%	2.1%
						6250	83.5%	5.8%
Isochlorogenic acid B		0.9992	0.1-2500	1.71	5.70	625	71.2%	4.9%

	$y = 5.89359e6 x + 1.05944e5$	0.99843	0.1-2500	3.72	12.39	2500	104.4%	8.1%
						6250	93.1%	4.4%
						625	101.0%	6.5%
Isochlorogenic acid C	$y = 9.89023e6 x + 1.14082e5$	0.99843	0.1-2500	3.72	12.39	2500	104.5%	5.5%
						6250	108.1%	9.5%
						625	107.0%	10.3%
Matairesinol	$y = 5.54232e6 x + 2.60055e5$	0.99344	10-1000	3.57	11.89	2500	94.2%	5.3%
						6250	101.5%	6.9%
						625	88.6%	4.1%
Baicalin	$y = 1.67040e7 x + 7.22858e4$	0.99924	1-500	5.41	18.02	2500	84.2%	5.2%
						6250	89.0%	4.7%
						625	92.0%	5.9%
Polydatin	$y = 1.13366e7 x + 27670.68243$	0.99929	0.25-500	4.59	15.29	2500	99.2%	4.8%
						6250	99.1%	6.8%
						625	102.6%	7.8%
Fisetin	$y = 5.50156e6 x + -1.56017e5$	0.99449	10-2500	4.17	13.91	2500	80.1%	4.3%
						6250	92.8%	7.8%
						625	97.8%	8.7%
Rosmarinic acid	$y = 1.20570e7 x + -3.66961e4$	0.99972	0.5-1000	2.07	6.89	2500	84.2%	5.0%
						6250	94.7%	5.5%
						625	85.2%	7.6%
3,4-Dihydroxybenzaldehyde	$y = 1.78216e7 x + 25896.86562$	0.99843	0.25-100	2.35	7.83	2500	93.7%	11.9%
						6250	94.6%	8.7%
						625	113.3%	6.9%
Myricetin	$y = 2.66264e6 x + -2.60900e5$	0.98196	0.1-2500	5.29	17.64	2500	102.0%	7.1%

	6250	102.0%	4.5%
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Supplementary Table 4. Absolute quantification results of *T. chinensis* and *T. ledebouri* by QqQ-MS. Samples (n=5),

SampleID	<i>T. chinensis</i> (µg/g)					<i>T. ledebouri</i> (µg/g)					p value	Fold changes(<i>T. chinensis</i> / <i>T. ledebouri</i>)
	1	2	3	4	5	1	2	3	4	5		
(-)-Gallocatechin	1.51	1.71	1.53	1.78	1.48	1.73	1.81	1.96	1.65	1.80	4.62E-02	0.90
(-)-Epigallocatechin	4.20	4.23	4.18	4.27	4.17	4.19	4.42	4.18	4.15	4.34	4.32E-01	0.99
(-)-Epigallocatechin gallate	3.12	3.16	3.21	3.16	3.21	3.13	3.35	3.25	3.24	3.13	3.17E-01	0.98
Kaempferol	1.55	1.54	1.68	1.31	1.50	1.11	0.98	0.93	1.12	0.75	3.34E-04	1.55
trans-4-Hydroxycinnamic acid	3.53	2.48	3.97	2.30	2.55	3.72	5.27	3.65	3.90	4.15	2.95E-02	0.72
Vanillic acid	13.53	11.71	12.81	13.60	13.87	15.81	18.30	13.85	18.29	18.18	4.70E-03	0.78
Quercetin	6.05	5.68	5.26	5.60	5.41	9.16	10.37	9.99	9.31	12.14	3.20E-05	0.55
4-Hydroxybenzoic acid	2.15	2.03	2.05	2.03	1.48	2.99	2.29	2.83	2.44	3.13	4.25E-03	0.71
Ferulic acid	3.32	3.50	3.09	2.83	3.07	2.38	2.18	1.81	2.10	2.55	4.94E-04	1.43
Chlorogenic acid	22.33	2.13	18.10	17.78	9.67	ND	ND	ND	ND	ND		
Neochlorogenic acid	5.47	0.18	3.68	3.06	1.76	ND	ND	ND	ND	ND		
4-Hydroxy-3,5-dimethoxy benzoic acid	0.36	0.57	0.73	1.22	0.64	0.14	0.22	0.63	0.34	1.14	3.90E-01	1.42
Gallic acid	0.37	0.44	0.40	0.40	0.54	0.23	0.34	0.11	0.20	0.26	2.71E-03	1.92
Caffeic acid	0.83	0.92	0.93	0.94	0.71	1.43	1.51	1.41	1.77	1.53	2.86E-05	0.56
trans-Cinnamic acid	1.27	4.13	2.53	1.91	1.28	ND	ND	ND	ND	ND		
3,5-Dimethoxy-4-hydroxycinnamic acid	198.93	208.90	237.40	223.28	236.80	94.98	98.28	103.83	79.45	95.13	4.50E-07	2.34
Apigenin	0.37	0.56	0.50	0.49	0.36	1.14	1.67	1.30	1.26	1.28	1.94E-05	0.34

Protocatechuic acid	1.91	2.04	2.26	2.17	2.05	1.45	1.66	1.23	1.12	1.37	1.89E-04	1.53
Rutin	ND	ND	ND	ND	ND	0.03	0.09	0.11	0.10	0.06		
7-Hydroxycoumarin	0.34	0.21	0.04	0.25	0.13	0.86	0.27	0.26	0.15	0.25	2.70E-01	0.55
Luteolin	5.08	5.38	4.61	4.99	5.33	7.42	8.00	9.31	7.30	8.83	7.35E-05	0.62
Isorhamnetin	5.21	3.16	3.09	4.25	4.33	2.17	2.07	2.06	2.15	2.12	1.47E-03	1.90
6,7-Dihydroxycoumarin	4.89	4.44	4.80	4.74	4.60	3.18	2.99	2.52	2.82	3.01	1.08E-06	1.62
Baicalein	1.06	1.05	1.08	1.05	1.05	1.05	1.06	1.05	1.05	1.08	7.93E-01	1.00
Apigenin 7-glucoside	8.36	8.41	7.90	7.73	7.75	7.79	9.28	8.45	8.79	8.47	1.02E-01	0.94
Isovitexin	57.08	53.15	55.55	51.75	54.18	24.49	25.40	24.21	25.63	25.68	1.63E-09	2.17
Kaempferol-3-O-rutinosid	0.38	0.14	0.17	0.19	0.15	0.76	0.86	1.08	0.97	0.82	1.21E-05	0.23
Astragalin	2.00	1.73	1.63	1.70	1.50	10.67	10.32	8.90	8.80	10.07	3.17E-08	0.18
Syringaldehyde	15.93	15.56	12.99	15.87	17.05	6.12	5.84	5.58	4.29	4.94	8.58E-07	2.89
Homogentisic Acid	4.39	5.52	5.19	5.11	5.31	4.65	4.50	4.67	3.47	4.63	4.36E-02	1.16
Orientin	68.50	77.53	71.23	73.20	79.65	88.73	139.63	120.43	85.68	119.28	8.03E-03	0.67
Glycitein	0.21	0.48	0.45	0.29	0.19	17.73	17.16	14.65	13.75	15.90	3.04E-08	0.02
Genistin	0.08	0.08	0.18	0.07	0.20	0.81	0.80	0.75	0.32	ND	1.48E-03	0.18
Naringin	1.93	2.20	1.96	2.07	1.66	29.28	28.80	26.23	22.59	27.85	3.18E-08	0.07
Eriodictyol	0.11	0.13	0.08	0.11	0.13	0.11	0.10	0.11	0.12	0.13	6.43E-01	0.95
Scopoletin	0.02	0.01	0.01	0.03	0.02	0.05	0.02	0.01	0.04	0.02	3.27E-01	0.70
Chrysoeriol	12.88	11.88	10.42	12.10	11.20	5.01	4.29	5.53	8.89	4.61	1.91E-04	2.07
Luteolin-7-O-β-D-glucopyranoside	12.03	12.46	13.18	13.64	12.88	31.83	35.63	32.00	30.35	34.10	3.28E-08	0.39
Hyperoside	60.18	52.05	58.53	58.13	57.95	82.60	82.13	78.75	75.10	80.83	2.85E-06	0.72
3,4-Dimethoxycinnamic acid	7.85	6.57	6.55	7.04	8.02	7.02	8.55	7.06	5.68	7.17	8.45E-01	1.02

Ellagic acid	8.05	6.63	7.20	7.57	7.26	6.36	6.62	6.39	6.39	6.52	5.71E-03	1.14
Salicylic acid	0.53	0.66	0.41	0.72	0.88	0.26	0.39	0.39	0.39	0.34	8.82E-03	1.82
Isochlorogenic acid A	48.70	14.88	33.83	30.88	27.30	1.33	1.59	1.01	0.90	1.13	5.83E-04	26.14
Isochlorogenic acid B	2.86	18.07	1.94	1.57	29.48	ND	1.98	1.21	0.97	1.48	1.84E-01	7.66
Isochlorogenic acid C	53.88	14.96	37.40	33.80	27.40	ND	ND	ND	ND	ND		
Polydatin	0.19	0.20	0.13	0.18	0.27	0.15	0.21	0.15	0.13	0.17	2.29E-01	1.20
3,4-												
Dihydroxybenzaldehyde	1.16	1.67	1.12	1.38	1.74	0.59	0.85	0.92	0.71	1.02	4.14E-03	1.72
myricetin	3.26	3.29	3.87	3.64	3.61	3.01	3.07	3.38	2.95	3.41	3.83E-02	1.12

Supplementary Table 5. Absolute/relative quantitative results of 154 polyphenols in *T. chinensis* and *T. ledebouri* extracts.

No	Identification methods	Class	Absolute/relative quantification methods	Code for heatmaps	Metabolite name	Formula	Average contents of <i>T. chinensis</i> (µg/g)	Average contents of <i>T. ledebouri</i> (µg/g)	Fold (<i>T. chinensis</i> / <i>T. ledebouri</i>)	p value
1	QqQ	Flavonoid aglycones	A	Flavonoid aglycone1	Daidzin	C ₂₁ H ₂₀ O ₉	9.23	2.303	4.01	3.80E-11
2	QqQ	Flavonoid aglycones	A	Flavonoid aglycone2	Glycitein	C ₁₆ H ₁₂ O ₅	0.32	15.84	0.02	3.04E-08
3	QqQ	Flavonoid aglycones	A	Flavonoid aglycone3	Quercetin	C ₁₅ H ₁₀ O ₇	8.14	16.51	0.49	4.39E-06
4	QqQ	Flavonoid aglycones	A	Flavonoid aglycone4	Luteolin	C ₁₅ H ₁₀ O ₆	5.08	8.17	0.62	7.35E-05
5	QqQ	Flavonoid aglycones	A	Flavonoid aglycone5	Chrysoeriol	C ₁₆ H ₁₂ O ₆	11.70	5.66	2.07	1.91E-04
6	QqQ	Flavonoid aglycones	A	Flavonoid aglycone6	Kaempferol	C ₁₅ H ₁₀ O ₆	1.52	0.98	1.55	3.34E-04
7	QqQ	Flavonoid aglycones	A	Flavonoid aglycone7	Myricetin	C ₁₅ H ₁₄ O ₉	3.53	3.16	1.12	3.83E-02
8	QqQ	Flavonoid aglycones	A	Flavonoid aglycone8	(-)-Gallocatechin	C ₁₅ H ₁₄ O ₇	1.60	1.79	0.90	4.62E-02
9	QqQ	Flavonoid aglycones	A	Flavonoid aglycone9	(-)-Epigallocatechin	C ₁₅ H ₁₄ O ₇	4.21	4.25	0.99	0.43
10	QqQ	Flavonoid aglycones	A	Flavonoid aglycone10	Eriodictyol	C ₁₅ H ₁₂ O ₆	0.11	0.12	0.96	0.64

11	IDA	Flavonoid aglycones	R	Flavonoid aglycone11	5-Hydroxy-4',7,8-trimethoxyflavone	C ₁₈ H ₁₆ O ₆	24.32	4.13	5.89	1.57E-10
12	DIA	Flavonoid aglycones	R	Flavonoid aglycone12	Daidzein	C ₁₅ H ₁₀ O ₄	24.32	4.13	5.89	1.57E-10
13	IDA	Flavonoid aglycones	R	Flavonoid aglycone13	4',5-Dihydroxy-3',7- dimethoxyisoflavone	C ₁₇ H ₁₄ O ₆	174.51	51.05	3.42	3.59E-08
14	DIA	Flavonoid aglycones	R	Flavonoid aglycone14	Farnisin	C ₁₆ H ₁₂ O ₅	2.13	101.85	0.02	6.89E-08
15	IDA	Flavonoid aglycones	R	Flavonoid aglycone15	Diosmetin	C ₁₆ H ₁₂ O ₆	100.58	26.50	3.80	1.95E-06
16	IDA	Flavonoid aglycones	R	Flavonoid aglycone16	4',5-Dihydroxy-7,8-dimethoxyflavone	C ₁₇ H ₁₄ O ₆	66.62	20.65	3.23	5.17E-06
17	QqQ	Flavonoid aglycones	A	Flavonoid aglycone17	Apigenin	C ₁₅ H ₁₀ O ₅	0.45	1.33	0.34	1.95E-05
18	QqQ	Flavonoid aglycones	A	Flavonoid aglycone18	Isorhamnetin	C ₁₆ H ₁₂ O ₇	4.01	2.11	1.90	1.48E-03
19	QqQ	Flavonoid aglycones	A	Flavonoid aglycone19	Baicalein	C ₁₅ H ₁₀ O ₅	1.06	1.06	1.00	0.79
20	QqQ	Flavonoid glycosides	A	Flavonoid glycoside1	^a Astragalin	C ₂₁ H ₂₀ O ₁₁	1.71	9.75	0.176	3.17E-08
21	QqQ	Flavonoid glycosides	A	Flavonoid glycoside2	^a Naringin	C ₂₇ H ₃₂ O ₁₄	1.97	26.95	0.07	3.18E-08
22	QqQ	Flavonoid glycosides	A	Flavonoid glycoside3	^a Luteolin-7-O-β-D-glucopyranoside	C ₂₁ H ₂₀ O ₁₁	12.84	32.78	0.39	3.284E-08
23	QqQ	Flavonoid glycosides	A	Flavonoid glycoside4	^c Vitexin	C ₂₁ H ₂₀ O ₁₀	86.12	49.73	1.73	8.18E-07

24	QqQ	Flavonoid glycosides	A	Flavonoid glycoside5	^a Hyperoside	C ₂₁ H ₂₀ O ₁₂	57.37	79.88	0.72	2.85E-06
25	QqQ	Flavonoid glycosides	A	Flavonoid glycoside6	^b Isovitexin	C ₂₁ H ₂₀ O ₁₀	54.34	25.08	2.167	1.63E-09
26	QqQ	Flavonoid glycosides	A	Flavonoid glycoside7	^a Quercitrin	C ₂₁ H ₂₀ O ₁₁	0.49	0.40	1.23	3.76E-05
27	QqQ	Flavonoid glycosides	A	Flavonoid glycoside8	^a Apigenin 7-glucoside	C ₂₁ H ₂₀ O ₁₀	0.53	0.91	0.58	1.11E-04
28	QqQ	Flavonoid glycosides	A	Flavonoid glycoside9	^d Orientin	C ₂₁ H ₂₀ O ₁₁	74.02	110.75	0.67	8.03E-03
29	QqQ	Flavonoid glycosides	A	Flavonoid glycoside10	^a (-)-Epigallocatechin gallate	C ₂₂ H ₁₈ O ₁₁	3.17	3.22	0.99	0.32
30	DIA	Flavonoid glycosides	R	Flavonoid glycoside11	^a Kaempferol 3-[6''-(3-hydroxy-3-methylglutaryl) hexoside]-7-hexoside	C ₃₃ H ₃₈ O ₂₀	1224.00	1.09	1120.86	8.57E-13
31	IDA	Flavonoid glycosides	R	Flavonoid glycoside12	^b Neocarlinoside	C ₂₆ H ₂₈ O ₁₅	19.43	1.30	14.90	1.16E-12
32	DIA	Flavonoid glycosides	R	Flavonoid glycoside13	^c Kaempferol 3-(6''-ethylglucuronide)	C ₂₃ H ₂₂ O ₁₂	6.58	441.73	0.02	3.37E-12
33	DIA	Flavonoid glycosides	R	Flavonoid glycoside14	^a Unidentified22	C ₃₃ H ₃₈ O ₂₀	41.92	0.02	1925.96	5.03E-12
34	IDA	Flavonoid glycosides	R	Flavonoid glycoside15	^b Unidentified2	C ₃₂ H ₃₀ O ₁₅	2.23	30.02	0.072	2.27E-11
35	IDA	Flavonoid glycosides	R	Flavonoid glycoside16	^d 2''-O-beta-L-galactopyranosylorientin (OGA)	C ₂₇ H ₃₀ O ₁₆	645.34	100.23	6.44	5.77E-11
36	DIA	Flavonoid glycosides	R	Flavonoid glycoside17	^c Kaempferol 7- dihexanoside	C ₂₇ H ₃₀ O ₁₆	0.93	9.67	0.10	8.98E-11

37	IDA	Flavonoid glycosides	R	Flavonoid glycoside18	^a Kaempferol 3-(6''-sinapylglucosyl)-(1->2)- hexoside	C ₃₈ H ₄₀ O ₂₀	84.07	4.64	18.14	1.04E-10
38	DIA	Flavonoid glycosides	R	Flavonoid glycoside19	^b Unidentified19	C ₂₃ H ₂₂ O ₁₂	0.14	12.84	0.01	1.05E-10
39	IDA	Flavonoid glycosides	R	Flavonoid glycoside20	^a 6''-Malonylastragalin	C ₂₄ H ₂₂ O ₁₄	430.68	1016.92	0.42	1.66E-10
40	IDA	Flavonoid glycosides	R	Flavonoid glycoside21	^b Unidentified6	C ₃₃ H ₃₈ O ₁₉	186.59	1.59	117.31	1.91E-10
41	DIA	Flavonoid glycosides	R	Flavonoid glycoside22	^a Quercetin 3-(2'''-feruloyldihexanoside)	C ₃₇ H ₃₈ O ₂₀	0.43	0.05	8.06	3.10E-10
42	IDA	Flavonoid glycosides	R	Flavonoid glycoside23	^d Astragalin 7-deoxyhexoside	C ₂₇ H ₃₀ O ₁₅	0.29	7.88	0.04	3.47E-10
43	IDA	Flavonoid glycosides	R	Flavonoid glycoside24	^a 6''-Malonylcosmosiin	C ₂₄ H ₂₂ O ₁₃	109.80	328.81	0.33	4.72E-10
44	IDA	Flavonoid glycosides	R	Flavonoid glycoside25	^d Kaempferol 3-(6-acetylhexoside)	C ₂₃ H ₂₂ O ₁₂	182.01	467.34	0.39	5.52E-10
45	IDA	Flavonoid glycosides	R	Flavonoid glycoside26	^a Isoorientin 2''-[p-coumaroyl(->6)-hexoside]	C ₃₆ H ₃₆ O ₁₈	23.34	2.57	9.07	7.04E-10
46	DIA	Flavonoid glycosides	R	Flavonoid glycoside27	^a Delphinidin-3-O-(6-O-feruloyl)-5-dihexanoside	C ₃₇ H ₃₈ O ₂₀	9.10	0.59	15.53	7.94E-10
47	IDA	Flavonoid glycosides	R	Flavonoid glycoside28	^a Betavulgarin hexoside	C ₂₃ H ₂₂ O ₁₁	1.32	40.21	0.03	8.30E-10
48	IDA	Flavonoid glycosides	R	Flavonoid glycoside29	^d Glucosylvitexin	C ₂₇ H ₃₀ O ₁₅	103.79	39.16	2.65	3.67E-09
49	IDA	Flavonoid glycosides	R	Flavonoid glycoside30	^a Quercetin 3-(2'''-caffeyldihexanoside)	C ₃₆ H ₃₆ O ₂₀	1.08	11.24	0.10	4.08E-09

50	DIA	Flavonoid glycosides	R	Flavonoid glycoside31	^a 6'''-O-Sinapoylsaponarin	C ₃₈ H ₄₀ O ₁₉	0.039	1.37	0.03	4.68E-09
51	DIA	Flavonoid glycosides	R	Flavonoid glycoside32	^b Isovitexin 2''-O-(6'''-feruloyl) hexoside	C ₃₇ H ₃₈ O ₁₈	0.07	0.81	0.09	5.88E-09
52	IDA	Flavonoid glycosides	R	Flavonoid glycoside33	^a Quercetin 3-xylosyl-(1->6)- hexoside	C ₂₆ H ₂₈ O ₁₆	39.44	142.69	0.28	6.21E-09
53	IDA	Flavonoid glycosides	R	Flavonoid glycoside34	^a Unidentified7	C ₅₆ H ₉₄ O ₂₈	57.53	105.44	0.55	6.69E-09
54	IDA	Flavonoid glycosides	R	Flavonoid glycoside35	^b Unidentified18	C ₃₆ H ₃₈ O ₁₉	78.58	4.52	17.38	9.89E-09
55	DIA	Flavonoid glycosides	R	Flavonoid glycoside36	^d Kaempferol 3-(6''-acetylhexoside)	C ₂₃ H ₂₂ O ₁₂	1.80	0.50	3.61	1.59E-08
56	IDA	Flavonoid glycosides	R	Flavonoid glycoside37	^a Quercetin 3-(6''-.malonylneohesperidoside)	C ₃₀ H ₃₂ O ₁₉	215.32	72.74	2.96	1.88E-08
57	IDA	Flavonoid glycosides	R	Flavonoid glycoside38	^b 2''-O-D-Arabinopyranosylvitexin 7-methyl ether	C ₂₇ H ₃₀ O ₁₄	2.62	9.69	0.27	2.30E-08
58	IDA	Flavonoid glycosides	R	Flavonoid glycoside39	^a Unidentified5	C ₃₅ H ₅₆ O ₁₆	119.76	44.22	2.71	2.33E-08
59	IDA	Flavonoid glycosides	R	Flavonoid glycoside40	^b Isotectorigenin 4'-hexoside 7-deoxyhexoside	C ₂₈ H ₃₂ O ₁₅	0.09	2.06	0.04	3.06E-08
60	DIA	Flavonoid glycosides	R	Flavonoid glycoside41	^b Isoscoparin 2''-(6-(E)-ferulylhexoside)	C ₃₈ H ₄₁ O ₁₉	6.82	0.28	24.05	3.54E-08
61	IDA	Flavonoid glycosides	R	Flavonoid glycoside42	^a Isorhamnetin 3-(3'''-ferulylrobinobioside)	C ₃₈ H ₄₀ O ₁₉	19.51	7.17	2.72	4.28E-08
62	IDA	Flavonoid glycosides	R	Flavonoid glycoside43	^b Unidentified4	C ₂₉ H ₃₄ O ₁₆	2.35	139.26	0.02	4.99E-08

63	DIA	Flavonoid glycosides	R	Flavonoid glycoside44	^c Margaritene	C ₂₈ H ₃₂ O ₁₄	0.22	8.52	0.03	1.12E-07
64	IDA	Flavonoid glycosides	R	Flavonoid glycoside45	^a Glucosylorientin	C ₂₇ H ₃₀ O ₁₇	21.35	33.465	0.64	1.53E-07
65	IDA	Flavonoid glycosides	R	Flavonoid glycoside46	^b 2''-O-feruloylorientin	C ₃₁ H ₂₈ O ₁₄	5.80	23.47	0.25	1.56E-07
66	IDA	Flavonoid glycosides	R	Flavonoid glycoside47	^b 2''-O-feruloylisoswertiajaponin	C ₃₂ H ₃₀ O ₁₄	7.13	29.20	0.24	1.69E-07
67	IDA	Flavonoid glycosides	R	Flavonoid glycoside48	^d 2''-O-(2''-methylbutyryl)isowertiajaponin	C ₂₇ H ₃₀ O ₁₂	114.64	254.99	0.45	2.31E-07
68	IDA	Flavonoid glycosides	R	Flavonoid glycoside49	^b 2''-O-feruloylvitexin	C ₃₁ H ₂₈ O ₁₃	11.54	38.88	0.30	2.41E-07
69	DIA	Flavonoid glycosides	R	Flavonoid glycoside50	^d Isoswertisin 2''-O-(2'''-methylbutyrate)	C ₂₇ H ₃₀ O ₁₁	276.39	517.20	0.53	3.66E-07
70	DIA	Flavonoid glycosides	R	Flavonoid glycoside51	^a Quercetin 3-(6''-malonylhexoside)-7-deoxyhexoside	C ₃₀ H ₃₂ O ₁₉	0.11	0.34	0.33	1.15E-06
71	DIA	Flavonoid glycosides	R	Flavonoid glycoside52	^a Luteone 7-hexoside	C ₂₆ H ₂₈ O ₁₁	1.55	2.78	0.56	2.35E-06
72	IDA	Flavonoid glycosides	R	Flavonoid glycoside53	^b 2''-O-(2'''-methylbutyryl)orientin	C ₂₆ H ₂₈ O ₁₂	38.66	85.76	0.45	2.49E-06
73	IDA	Flavonoid glycosides	R	Flavonoid glycoside54	^b Unidentified3	C ₂₁ H ₂₀ O ₁₁	33.95	73.45	0.46	2.81E-06
74	IDA	Flavonoid glycosides	R	Flavonoid glycoside55	^d Isoswertiajaponin	C ₂₂ H ₂₂ O ₁₁	45.09	25.44	1.77	3.52E-06
75	DIA	Flavonoid glycosides	R	Flavonoid glycoside56	^b 4''-Hydroxy-3'-methoxymaysin	C ₂₈ H ₃₂ O ₁₄	1.71	3.76	0.45	4.34E-06

76	DIA	Flavonoid glycosides	R	Flavonoid glycoside57	^b Unidentified14	C ₉₄ H ₁₁₀ O ₂₃	1.38	2.98	0.46	6.21E-06
77	DIA	Flavonoid glycosides	R	Flavonoid glycoside58	^b Unidentified21	C ₂₆ H ₂₈ O ₁₂	0.76	1.46	0.53	6.67E-06
78	IDA	Flavonoid glycosides	R	Flavonoid glycoside59	^d Orientin 7-deoxyhexoside	C ₂₇ H ₃₀ O ₁₅	0.14	0.47	0.29	4.95E-06
79	IDA	Flavonoid glycosides	R	Flavonoid glycoside60	^b Isoscoparin 2''-(6-(E)-p-coumaroylhexoside)	C ₃₇ H ₃₈ O ₁₈	8.68	4.44	1.96	2.07E-05
80	IDA	Flavonoid glycosides	R	Flavonoid glycoside61	^d Vitexin 2''-O-(2'''-methylbutyryl)	C ₂₆ H ₂₈ O ₁₁	191.82	290.35	0.66	2.67E-05
81	IDA	Flavonoid glycosides	R	Flavonoid glycoside62	^b 2''-O-vanilloylvitexin	C ₂₉ H ₂₆ O ₁₃	9.96	14.66	0.68	2.16E-04
82	DIA	Flavonoid glycosides	R	Flavonoid glycoside63	^b 2''-O-vanilloylorientin	C ₂₉ H ₂₆ O ₁₄	6.43	9.79	0.67	5.02E-04
83	IDA	Flavonoid glycosides	R	Flavonoid glycoside64	^b 2''-O-(3''',4'''-dimethoxybenzoyl)isoswertiajaponin	C ₃₁ H ₃₀ O ₁₄	23.23	15.48	1.50	1.24E-03
84	IDA	Flavonoid glycosides	R	Flavonoid glycoside65	^a Kaempferol 3- α -L-arabinofuranoside	C ₂₀ H ₁₈ O ₁₀	0.36	0.68	0.53	2.43E-03
85	DIA	Flavonoid glycosides	R	Flavonoid glycoside66	^a Quercetin 3-pentoside	C ₂₀ H ₁₈ O ₁₁	0.22	0.35	0.62	8.35E-03
86	IDA	Flavonoid glycosides	R	Flavonoid glycoside67	^b 2''-O-(3''',4'''-dimethoxybenzoyl)orientin	C ₃₀ H ₂₈ O ₁₄	32.05	41.48	0.77	8.77E-03
87	DIA	Flavonoid glycosides	R	Flavonoid glycoside68	^a Kaempferide 7- hexoside	C ₂₂ H ₂₂ O ₁₁	0.79	0.95	0.83	0.01
88	IDA	Flavonoid glycosides	R	Flavonoid glycoside69	^b Unidentified1	C ₃₄ H ₄₂ O ₁₈	9.65	13.78	0.70	0.02

89	DIA	Flavonoid glycosides	R	Flavonoid glycoside70	^a Unidentified17	C ₂₀ H ₁₈ O ₁₀	0.62	0.80	0.77	0.04
90	DIA	Flavonoid glycosides	R	Flavonoid glycoside71	^b Isoswertisin 3''-O-(2'''-methylbutyrate)	C ₂₇ H ₃₀ O ₁₁	0.19	0.25	0.74	4.98E-02
91	DIA	Flavonoid glycosides	R	Flavonoid glycoside72	^a Unidentified16	C ₂₀ H ₁₈ O ₁₀	1.37	1.62	0.85	0.16
92	IDA	Flavonoid glycosides	R	Flavonoid glycoside73	^a 3',8-Dimethoxyapigenin 7-hexoside	C ₂₃ H ₂₄ O ₁₂	7.97	8.68	0.92	0.20
93	IDA	Flavonoid glycosides	R	Flavonoid glycoside74	^b Unidentified15	C ₃₀ H ₂₈ O ₁₃	52.75	57.79	0.91	0.21
94	IDA	Flavonoid glycosides	R	Flavonoid glycoside75	^a 2''-O-(3''',4'''-dimethoxybenzoyl)isoswertisin	C ₃₁ H ₃₀ O ₁₃	25.60	26.06	0.98	0.78
95	QqQ	Phenolic acids	A	Phenolic acid1	Phlorizin	C ₂₁ H ₂₄ O ₁₀	7.36	0.37	19.69	3.52E-10
96	QqQ	Phenolic acids	A	Phenolic acid2	3,5-Dimethoxy-4-hydroxycinnamic acid	C ₁₁ H ₁₂ O ₅	221.06	94.33	2.34	4.50E-07
97	QqQ	Phenolic acids	A	Phenolic acid3	Syringaldehyde	C ₉ H ₁₀ O ₄	15.48	5.35	2.89	8.58E-07
98	QqQ	Phenolic acids	A	Phenolic acid4	6,7-Dihydroxycoumarin	C ₉ H ₆ O ₄	4.69	2.90	1.62	1.09E-06
99	QqQ	Phenolic acids	A	Phenolic acid5	Caffeic acid	C ₉ H ₈ O ₄	0.86	1.53	0.57	2.86E-05
100	QqQ	Phenolic acids	A	Phenolic acid6	Protocatechuic acid	C ₇ H ₆ O ₄	2.09	1.37	1.53	1.89E-04
101	QqQ	Phenolic acids	A	Phenolic acid7	Ferulic acid	C ₁₀ H ₁₀ O ₄	3.16	2.20	1.43	4.94E-04

102	QqQ	Phenolic acids	A	Phenolic acid8	Isochlorogenic acid A	C ₂₅ H ₂₄ O ₁₂	31.12	1.19	26.14	1.79E-06
103	QqQ	Phenolic acids	A	Phenolic acid9	3,4-Dihydroxybenzaldehyde	C ₇ H ₆ O ₃	1.41	0.82	1.72	4.14E-03
104	QqQ	Phenolic acids	A	Phenolic acid10	4-Hydroxybenzoic acid	C ₇ H ₆ O ₃	1.95	2.74	0.71	4.25E-03
105	QqQ	Phenolic acids	A	Phenolic acid11	Chlorogenic acid	C ₁₆ H ₁₈ O ₉	0.73	0.02	29.87	4.44E-03
106	QqQ	Phenolic acids	A	Phenolic acid12	Vanillic acid	C ₈ H ₈ O ₄	13.10	16.89	0.78	4.70E-03
107	QqQ	Phenolic acids	A	Phenolic acid13	Ellagic acid	C ₁₄ H ₆ O ₈	7.34	6.46	1.14	5.71E-03
108	QqQ	Phenolic acids	A	Phenolic acid14	Salicylic acid	C ₇ H ₆ O ₃	0.64	0.35	1.82	8.82E-03
109	QqQ	Phenolic acids	A	Phenolic acid15	trans-Cinnamic acid	C ₉ H ₈ O ₂	2.22	0.47	4.77	0.02
110	QqQ	Phenolic acids	A	Phenolic acid16	trans-4-Hydroxycinnamic acid	C ₉ H ₈ O ₃	2.97	4.14	0.72	0.03
111	QqQ	Phenolic acids	A	Phenolic acid17	4-O-Caffeoylquinic acid	C ₁₆ H ₁₈ O ₉	0.89	0		0.03
112	QqQ	Phenolic acids	A	Phenolic acid18	Homogentisic acid	C ₈ H ₈ O ₄	5.10	4.38	1.16	0.04
113	QqQ	Phenolic acids	A	Phenolic acid19	Isochlorogenic acid B	C ₂₅ H ₂₄ O ₁₂	10.78	1.41	7.66	0.13
114	QqQ	Phenolic acids	A	Phenolic acid20	Polydatin	C ₂₀ H ₂₂ O ₈	0.20	0.16	1.20	0.23

115	QqQ	Phenolic acids	A	Phenolic acid21	7-Hydroxycoumarin	C ₉ H ₆ O ₃	0.20	0.36	0.55	0.27
116	QqQ	Phenolic acids	A	Phenolic acid22	Scopoletin	C ₁₀ H ₈ O ₄	0.02	0.03	0.70	0.33
117	QqQ	Phenolic acids	A	Phenolic acid23	4-Hydroxy-3,5-dimethoxy benzoic acid	C ₉ H ₁₀ O ₅	0.71	0.50	1.42	0.39
118	QqQ	Phenolic acids	A	Phenolic acid24	3,4-Dimethoxycinnamic acid	C ₁₁ H ₁₂ O ₄	7.21	7.09	1.02	0.85
119	QqQ	Phenolic acids	A	Phenolic acid25	Butein	C ₁₅ H ₁₂ O ₅	0.04	0.04	0.97	0.92
120	QqQ	Phenolic acids	A	Phenolic acid26	Isochlorogenic acid C	C ₂₅ H ₂₄ O ₁₂	35.49	0.15	240.63	8.19E-11
121	IDA	Phenolic acids	R	Phenolic acid27	Trollioside	C ₁₉ H ₂₆ O ₉	264.36	10.02	26.39	3.26E-11
122	IDA	Phenolic acids	R	Phenolic acid28	Vanillylmandelic acid	C ₉ H ₁₀ O ₅	5.08	27.95	0.18	5.81E-11
123	IDA	Phenolic acids	R	Phenolic acid29	Unidentified13	C ₁₉ H ₂₆ O ₁₀	58.65	3.40	17.27	7.15E-11
124	DIA	Phenolic acids	R	Phenolic acid30	cis-Sinapic acid	C ₁₁ H ₁₂ O ₅	7.77	1.20	3.89	1.61E-10
125	IDA	Phenolic acids	R	Phenolic acid31	Salviaflaside	C ₂₄ H ₂₆ O ₁₃	17.01	3.350	5.08	2.64E-10
126	IDA	Phenolic acids	R	Phenolic acid32	Sinaptic acid	C ₁₁ H ₁₂ O ₅	78.95	16.04	4.9209	2.17E-09
127	IDA	Phenolic acids	R	Phenolic acid33	Veratric acid	C ₉ H ₁₀ O ₄	19.67	5.05	3.90	6.00E-09

128	IDA	Phenolic acids	R	Phenolic acid34	Unidentified11	C ₃₆ H ₃₈ O ₁₈	35.87	2.11	16.98	1.01E-08
129	IDA	Phenolic acids	R	Phenolic acid35	Hydroxytyrosol 1-O- hexoside	C ₁₄ H ₂₀ O ₈	149.34	231.19	0.65	3.00E-08
130	IDA	Phenolic acids	R	Phenolic acid36	Vanillic acid 4-O-glucuronide	C ₁₄ H ₁₆ O ₁₀	1.24	3.23	0.38	1.37E-07
131	DIA	Phenolic acids	R	Phenolic acid37	4-Hydroxy-3,5-dimethoxybenzaldehyde	C ₉ H ₁₀ O ₄	0.75	0.10	7.47	1.46E-07
132	IDA	Phenolic acids	R	Phenolic acid38	Vanillylamine	C ₈ H ₁₁ NO ₂	110.06	58.77	1.87	1.51E-07
133	IDA	Phenolic acids	R	Phenolic acid39	3-(6-hydroxy-7-methoxy-2H-1,3-benzodioxol-5-yl)propanoic acid	C ₁₁ H ₁₂ O ₆	232.04	120.46	1.93	6.02E-07
134	IDA	Phenolic acids	R	Phenolic acid40	4-Hydroxycinnamic acid	C ₉ H ₈ O ₃	0.32	0.13	2.47	1.16E-06
135	DIA	Phenolic acids	R	Phenolic acid41	(2R,3S)-Piscidic acid	C ₁₁ H ₁₂ O ₇	8.70	21.79	0.40	3.68E-06
136	IDA	Phenolic acids	R	Phenolic acid42	Fukiic acid	C ₁₁ H ₁₂ O ₈	14.99	38.51	0.39	4.93E-06
137	IDA	Phenolic acids	R	Phenolic acid43	Hydroxytyrosol 3'-glucuronide	C ₁₄ H ₁₈ O ₉	28.97	57.96	0.50	9.02E-06
138	IDA	Phenolic acids	R	Phenolic acid44	Unidentified20	C ₁₉ H ₂₆ O ₁₀	1.54	0.26	5.84	9.13E-06
139	IDA	Phenolic acids	R	Phenolic acid45	Monotropein	C ₁₆ H ₂₂ O ₁₁	90.61	158.44	0.57	6.13E-05
140	IDA	Phenolic acids	R	Phenolic acid46	Glucobtusifolin	C ₂₂ H ₂₂ O ₁₀	10.85	6.90	1.57	9.66E-05

141	IDA	Phenolic acids	R	Phenolic acid47	Unidentified23	C ₁₁ H ₁₂ O ₇	328.84	230.78	1.43	1.24E-04
142	DIA	Phenolic acids	R	Phenolic acid48	4,5-Di-O-caffeoylquinic acid	C ₂₅ H ₂₄ O ₁₂	0.07	0.02	4.32	2.40E-03
143	IDA	Phenolic acids	R	Phenolic acid49	Unidentified12	C ₂₂ H ₃₈ O ₁₂	18.19	23.37	0.78	2.47E-03
144	QqQ	Phenolic acids	A	Phenolic acid50	Gallic acid	C ₇ H ₆ O ₅	0.43	0.22	1.92	2.71E-03
145	IDA	Phenolic acids	R	Phenolic acid51	3,5-Di-O-caffeoylquinic acid	C ₂₅ H ₂₄ O ₁₂	1.43	0.21	6.97	3.55E-03
146	DIA	Phenolic acids	R	Phenolic acid52	Vanillin	C ₈ H ₈ O ₃	0.43	0.32	1.36	7.21E-03
147	DIA	Phenolic acids	R	Phenolic acid53	Unidentified10	C ₂₇ H ₂₄ O ₁₈	1.01	0.79	1.29	1.71E-02
148	IDA	Phenolic acids	R	Phenolic acid54	2-Pyrocatechuic acid	C ₇ H ₆ O ₄	0.46	0.59	0.79	2.46E-02
149	IDA	Phenolic acids	R	Phenolic acid55	Ascorbic acid	C ₆ H ₈ O ₆	17.87	20.76	0.86	0.10
150	IDA	Phenolic acids	R	Phenolic acid56	Quercetin 3-lathyroside	C ₂₆ H ₂₈ O ₁₆	0.85	0.94	0.904	0.17
151	DIA	Phenolic acids	R	Phenolic acid57	Shikimic acid	C ₇ H ₁₀ O ₅	5.14	4.06	1.27	0.43
152	IDA	Phenolic acids	R	Phenolic acid58	Unidentified9	C ₅₈ H ₉₄ O ₂₉	25.09	25.80	0.97	0.59

153	IDA	Phenolic acids	R	Phenolic acid59	(±)-threo-1-(p-Hydroxyphenyl)propylene glycol 4'-hexoside	C ₁₅ H ₂₂ O ₈	118.85	32.96	3.61	1.74E-10
154	IDA	Phenolic acids	R	Phenolic acid60	Unidentified8	C ₁₆ H ₂₄ O ₁₀	196.01	56.64	3.46	2.82E-10

Note: A, absolute quantification; R, relative quantification

Compared with reference 31, newly detected in this work, ^a flavone O-glycosides, ^b flavone C-glycosides; detected in both work for ^c flavone O-glycosides and ^d flavone C-glycosides