

Figure S1. Standard chromatograms analyzed using GC/MS. 1, alanine; 2, valine; 3, phosphoric acid; 4, glycerol; 5, isoleucine; 6, glyceric acid; 7, serine; 8, threonine; 9, malic acid; 10, oxoproline; 11, 4-aminobutanoic acid; 12, threonic acid; 13, lyxose; 14, glutamine; 15, fructose; 16, glucose; 17, myo-inositol; 18, maltose.

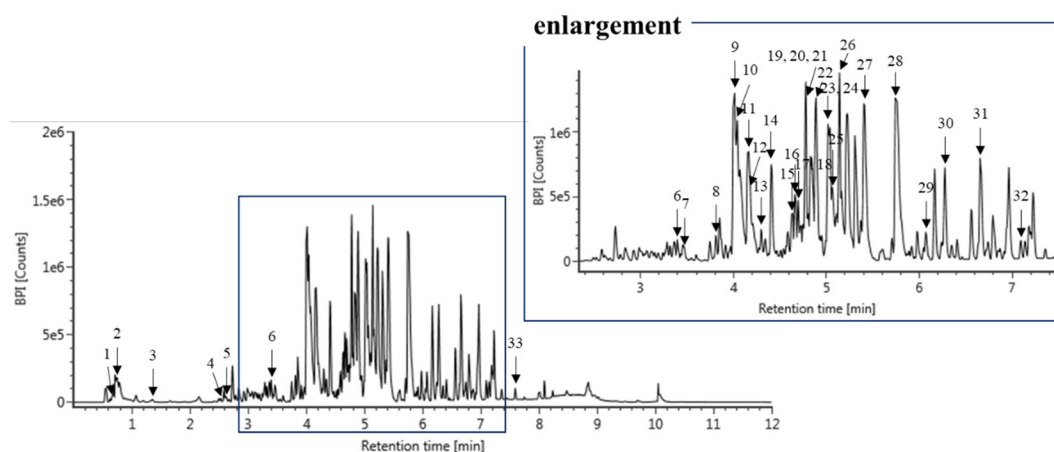


Figure S2. Standard chromatogram analyzed using UPLC/Q-TOF-MS. 1, gluconic acid / heonic acid / idonic acid / mannonic acid; 2, maltose / cellobiose / lactose; 3, uridine; 4, phenylalanine; 5, Gentisic acid 5-O-I-glucoside; 6, Kaempferol 3-O-gentiobioside / rutin / Sophoraflavonolside; 7, coumaroylquinic acid; 8, Notoginsenoside R1; 9, Ginsenoside Re; 10, ginsenoside Rg1; 11, Malonyl-Ginsenoside Re; 12, Malonyl-Ginsenoside Rg1; 13, Atractyloside A; 14, 20-glu-Ginsenoside Rf; 15, ginsenoside Rb1; 16, Malonyl-Rb1; 17, ginsenoside Rf; 18, Malonyl-ginsenoside Ra1/Ra2; 19, Malonyl-Ginsenoside Rc; 20, ginsenoside Rb2; 21, Ginsenoside F5; 22, Ginsenoside Rg2; 23, ginsenoside Rd1+Na; 24, ginsenoside Rd1; 25, Malonyl-ginsenoside Rd; 26, ginsenoside F1; 27, ginsenoside Rd2; 28, ginsenoside F2; 29, ginsenoside Rg3; 30, Gingerglycolipid A; 31, Gingerglycolipid B; 32, 9(10)-EpODE / 12(13)-EpODE; 33, Tetradecyl b-D-maltopyranoside.

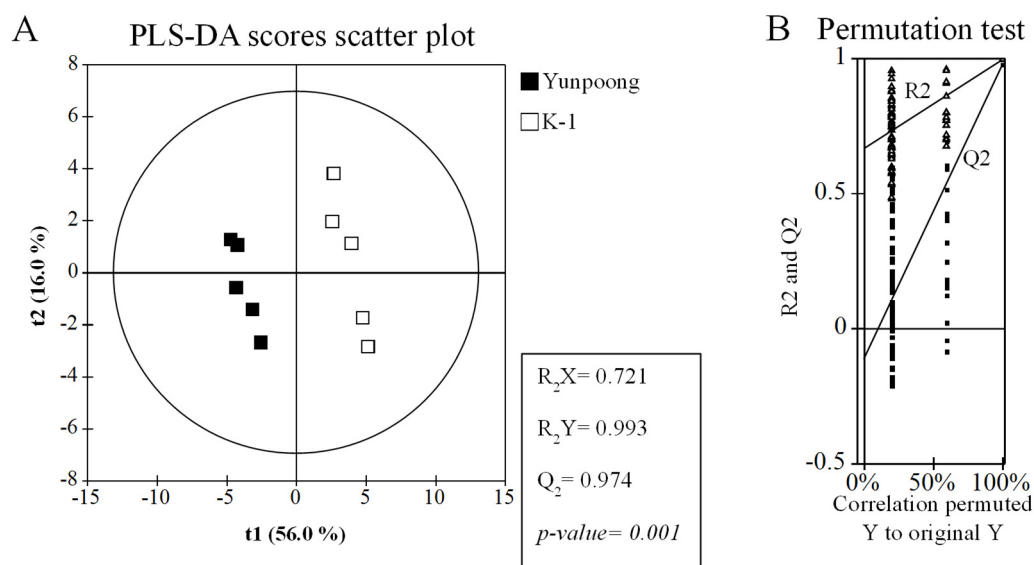


Figure S3. Partial least-squares discriminant analysis and Permutation in ‘Yunpoong’ and ‘K-1’ of primary metabolites. Metabolites were analyzed using GC-MS. The qualification of the PLS-DA model was evaluated using R^2X , R^2Y , Q^2 , and p -value and validated using cross-validation with a permutation test ($n = 5$).

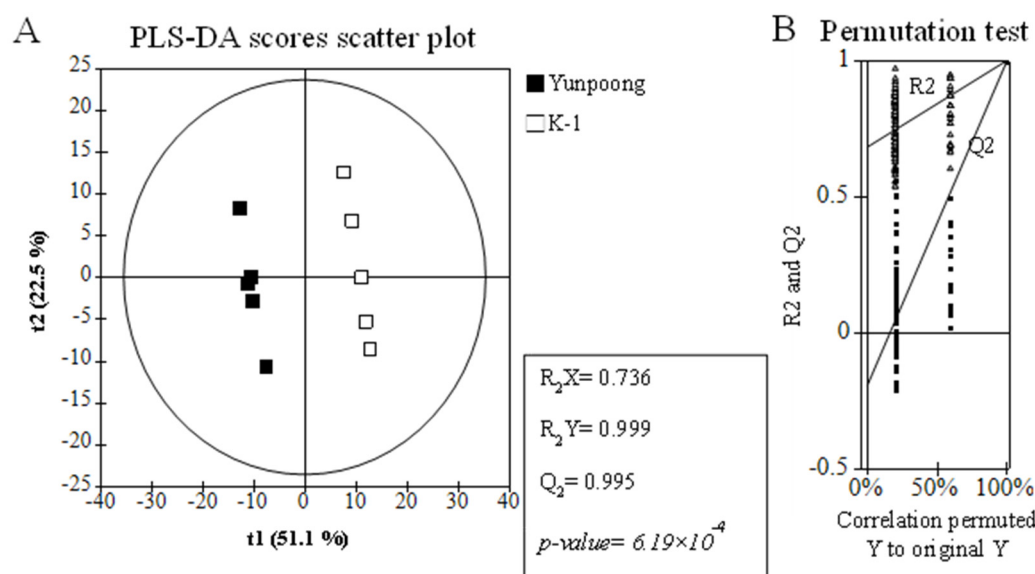


Figure S4. Partial least-squares discriminant analysis and Permutation in ‘Yunpoong’ and ‘K-1’ of secondary metabolites. Metabolites were analyzed using UPLC/Q-TOF-MS. The qualification of the PLS-DA model was evaluated using R^2_X , R^2_Y , Q^2 , and p -value and validated using cross-validation with a permutation test ($n = 5$).

Table S1. Identification of significant primary metabolites contributing to the separation among sample groups.

No.	RT (min)	Compound	RI ^(a)	VIP	<i>p</i> -value
1	6.84	alanine	1090	1.03	0.015
2	8.68	valine	1202	1.21	4.37E-04
3	9.52	phosphoric acid	1256	1.18	8.78E-04
4	9.56	glycerol	1259	1.12	3.16E-03
5	9.88	isoleucine	1279	1.10	4.10E-03
6	10.40	glyceric acid	1314	1.33	2.40E-07
7	10.85	serine	1344	1.01	0.020
8	11.22	threonine	1368	0.86	0.049
9	12.63	malic acid	1467	1.27	1.22E-03
10	13.09	oxoproline	1500	1.01	0.014
11	13.21	4-aminobutanoic acid	1510	1.22	3.77E-04
12	13.55	threonic acid	1536	1.31	4.04E-04
13	14.74	lyxose	1634	1.34	1.74E-08
14	16.17	glutamine	1755	1.10	4.20E-03
15	17.23/17.33	fructose	1849	1.24	2.01E-04
16	17.51/17.73	glucose	1875	1.35	2.82E-09
17	19.55	myo-inositol	2070	1.22	3.65E-04
18	25.12	maltose	2710	1.04	9.84E-03

Table S2. Identification of major secondary metabolites contributing to the separation among sample groups.

No.	RT (min)	Compound	m/z	Adduct	MS Fragments	VIP	p-value
1	0.69	gluconic acid / heonic acid / idonic acid / mannonic acid	195.0392	[M-H] ⁻	75, 165	1.37	1.49E-06
2	0.72	maltose / cellobiose / lactose	341.1001	[M-H] ⁻	89, 105, 161, 179, 281	1.38	5.53E-07
3	1.40	uridine	243.0517	[M-H] ⁻	200	1.26	4.23E-04
4	2.53	phenylalanine	164.0594	[M-H] ⁻	147	1.26	5.31E-04
5	2.63	Gentisic acid 5-O-I-glucoside	315.0628	[M-H] ⁻	71, 108, 152	1.39	1.20E-05
6	3.37	Kaempferol 3-O-gentiobioside / rutin / Sophoraflavonolside	609.1482	[M-H] ⁻	89, 173, 191	1.41	2.11E-11
7	3.45	coumaroylquinic acid	337.0845	[M-H] ⁻	163, 191	1.41	3.07E-11
8	3.82	Notoginsenoside R1	977.5509	[M+Na] ⁻	475, 637, 783, 799	0.86	0.086
9	3.99	Ginsenoside Re	991.5670	[M+Na] ⁻	475, 619, 783	0.73	0.126
10	4.01	ginsenoside Rg1	845.5022	[M+Na] ⁻	637, 799	0.30	0.977
11	4.14	Malonyl-Ginsenoside Re	1031.5648	[M+Na] ⁻	475, 637, 783, 927, 945	1.19	2.29E-03
12	4.17	Malonyl-Ginsenoside Rg1	885.4996	[M-H] ⁻	781, 799, 841	0.33	0.945
13	4.28	Atractyloside A	493.2258	[M+Na] ⁻	161, 225, 251, 315	0.99	0.027
14	4.38	20-glu-Ginsenoside Rf	1007.5625	[M+Na] ⁻	475, 637, 799	1.35	8.64E-06
15	4.61	ginsenoside Rb1	1153.6286	[M+Na] ⁻	553, 783, 945	0.36	0.775
16	4.65	Malonyl-Rb1	1193.6264	[M-H] ⁻	783, 945, 1089, 1107, 1149	1.11	6.98E-03
17	4.67	ginsenoside Rf	845.5020	[M+Na] ⁻	475, 637	1.18	2.92E-03
18	4.71	Malonyl-ginsenoside Ra1/Ra2	1295.6660	[M-H] ⁻	621, 1077, 1191, 1251	0.95	0.037
19	4.77	Malonyl-Ginsenoside Rc	1163.6141	[M-H] ⁻	459, 621, 783, 1059, 1120	1.17	0.004
20	4.78	ginsenoside Rb2	1123.6164	[M+Na] ⁻	538, 783, 945	0.85	0.088
21	4.78	Ginsenoside F5	815.4901	[M+Na] ⁻	475, 637, 769	0.62	0.207
22	4.86	Ginsenoside Rg2	829.5063	[M+Na] ⁻	391, 457, 475, 637	0.71	0.173

23	5.00	ginsenoside Rd1	991.5670	[M+Na] ⁻	621, 783	0.51	0.390
24	5.00	ginsenoside Rd1	945.5635	[M-H] ⁻	161, 459, 621, 783	0.32	0.984
25	5.05	Malonyl-ginsenoside Rd	1031.5638	[M+HCOO] ⁻	927	0.45	0.416
26	5.11	ginsenoside F1	683.4417	[M+Na] ⁻	475	0.32	0.884
27	5.38	ginsenoside Rd2	961.5545	[M+Na] ⁻	621, 783	1.25	5.84E-04
28	5.72	ginsenoside F2	829.5060	[M+Na] ⁻	459, 621	1.32	5.57E-05
29	6.04	ginsenoside Rg3	829.5067	[M+Na] ⁻	459, 621	0.74	0.154
30	6.25	Gingerglycolipid A	721.3714	[M+Na] ⁻	249, 277, 397, 415	1.24	7.65E-04
31	6.63	Gingerglycolipid B	723.3867	[M+Na] ⁻	277, 279, 397, 415	1.25	6.55E-04
32	7.07	9(10)-EpODE / 12(13)-EpODE	293.2025	[M-H] ⁻	113, 195, 249, 279	1.34	2.44E-05
33	7.58	Tetradecyl b-D-maltopyranoside	537.3277	[M-H] ⁻	253, 255, 341, 491	1.35	1.42E-05