Supporting Information

LC-Q-TOF-MS Characterization of Polyphenols from White Bayberry Fruit and Its Anti-diabetic Effect in KK-A^{y} Mice

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Table S1. Polyphenols at a relative lower level identified by liquid chromatography quadrupole time-of-flight tandem mass spectrometry (LC-Q-TOF-MS) in 'Shui Jing' fruit extract (SJE).

NO.	Compound	RT [1] (min)	[M -H]$^-$ (*m*/*z*)	Molecular Formula	Fragment ions (Relative abundance)	References	Content (mg/100 g DW)
Proanthocyanidins and derivatives							
○11	(E)GC-(E)GCG isomer [2]	37.708	761.1372	$C_{37}H_{30}O_{18}$	609.1293(14), 591.1175(16), 423.0726(100), 305.0656(35), 243.0296(16)	23	30.89 ± 0.21
○12	(E)GC-(E)CG	29.922	745.1415	$C_{37}H_{30}O_{17}$	593.134(24), 575.1236(30), 423.074(100), 287.0557(29)	S1	30.47 ± 0.29
○13	Galloyl-*bis*-HHDP-*O*-hexoside [3]	28.285	935.0816	$C_{41}H_{28}O_{26}$	633.0798(100), 299.0205(53), 275.021(82)	S2	19.32 ± 0.15
●14	(E)GCG-(E)GCG isomer	43.82	913.148	$C_{44}H_{34}O_{22}$	423.0742(75), 913.1592(100), 761.1445(30), 591.1181(30)	25	17.77 ± 0.23
○15	(E)GC-(E)CG isomer	30.486	745.1415	$C_{37}H_{30}O_{17}$	593.135(37), 575.1243(29), 423.074(100), 305.067(44), 287.0568(29)	S1	15.06 ± 0.20
○16	(E)GC-(E)GCG isomer	22.999	761.1361	$C_{37}H_{30}O_{18}$	609.1296(18), 591.1189(19), 423.0736(100), 305.0669(32), 177.0199(17)	23	12.02 ± 0.09
○17	Galloyl-*bis*-HHDP-*O*-hexoside isomer	38.931	935.0818	$C_{41}H_{28}O_{26}$	633.0794(42), 300.9989(100), 275.0185(13)	S2	11.02 ± 0.41
●18	(E)GCG-(E)GC-(E)C	34.415	1049.2014	$C_{52}H_{42}O_{24}$	879.1771(34), 761.1455(76), 593.0999(36), 591.1199(54), 423.0739(100)	S3	8.56 ± 0.01
○19	Taraninin	30.668	1065.1953	$C_{52}H_{42}O_{25}$	879.1514(72), 761.1437(82), 423.0736(100)	S3	7.06 ± 0.08
○20	Taraninin isomer	30.215	1065.1953	$C_{52}H_{42}O_{25}$	897.1614(52), 879.1521(80), 761.1441(81), 727.1383(58), 423.0743(100)	S3	5.73 ± 0.08
Flavonoid glycosides							
△21	Isorhamnetin xyloside	53.297	447.0933	$C_{21}H_{20}O_{11}$	285.0402(47), 284.0327(100), 255.0298(89), 227.0345(65), 315.0144(70)	S4	26.32 ± 0.08
△22	Quercetin-3-*O*-glucoside (isoquercetrin) [a]	46.948	463.0876	$C_{21}H_{20}O_{12}$	301.0324(100), 271.0252(13), 255.0292(11)	17	24.32 ± 0.48
△23	Quercetin-3-*O*-galactoside (hyperoside)	45.932	463.0893	$C_{21}H_{20}O_{12}$	300.0279(100), 301.0353(50), 271.0249(55), 255.0301(30)	26	10.91 ± 0.19
△24	Quercetin	67.165	301.0354	$C_{15}H_{10}O_7$	151.0037(100), 178.9984(30), 301.0347 (100)	S5	0.91 ± 0.02

Table S1. *Cont.*

NO.	Compound	RT [1] (min)	[M -H]$^-$ (*m*/*z*)	Molecular Formula	Fragment ions (Relative abundance)	References	Content (mg/100 g DW)
Phenolic acid and derivatives							
■25	Methylellagic acid glucuronide	48.620	491.0467	$C_{21}H_{16}O_{14}$	315.0179(5), 300.9939(7)	S6	42.07 ± 0.22
■26	Ellagic acid [a]	45.489	300.9992	$C_{14}H_6O_8$	283.9960(20), 229.0141(10), 245.0080(10)	S7	36.66 ± 0.90
■27	Dimethyl-ellagic acid-glucuronide	66.060	505.0617	$C_{22}H_{18}O_{14}$	329.0312(100), 314.0071(51), 298.9835(24), 285.0034(7), 270.988(7)	S8	28.55 ± 0.02
■28	Ellagic acid 3,3'-dimethyl ether-*O*-*β*-D-glucopyranoside	59.239	491.0822	$C_{22}H_{20}O_{13}$	329.0303(100), 314.0067(42), 298.9832(18), 285.0028(10)	S9,S10	21.81 ± 0.29
■29	4-*O*-[*β*-D-xylopyranosyl]-3,3′-di-*O*-methyl ellagic acid	66.787	461.072	$C_{21}H_{18}O_{12}$	329.0314(100), 328.0233(11.572), 314.0076(43), 298.9832(25), 270.9867(11)	S11	20.61 ± 0.06
□30	*p*-Coumaric acid [a]	38.642	163.0395	$C_9H_8O_3$	119.0509(100), 163.0395(15)	S12	11.80 ± 0.03
□31	Coumaric acid hexoside	22.210	325.0928	$C_{15}H_{18}O_9$	119.0508(100), 163.0399(70)	S13	11.18 ± 0.04
□32	Caffeic acid hexoside	22.469	341.0881	$C_{15}H_{18}O_9$	135.0459(100), 179.0357(64)	S14	10.58 ± 0.04
□33	Vanillic acid 1-*O*-*β*-D-glucopyranosyl ester	32.458	329.0882	$C_{14}H_{18}O_9$	221.045(5), 209.0449(12), 191.0356(23), 167.0356(100), 125.0248(7), 123.0459(36)	S15,S16	8.56 ± 0.02
□34	Caffeic acid hexoside isomer	17.837	341.0883	$C_{15}H_{18}O_9$	179.0360(100), 135.0462(81)	S14	6.79 ± 0.01
□35	Caffeic acid hexoside isomer	28.049	341.0880	$C_{15}H_{18}O_9$	179.0355(70), 135.0457(100)	S14	5.28 ± 0.04
□36	Ferulic acid hexoside	21.063	355.1034	$C_{16}H_{20}O_9$	134.0378(100), 193.0506(65), 149.0603(30), 178.0264(20)	S17,S18	3.90 ± 0.08
□37	Ferulic acid hexoside isomer	27.161	355.1039	$C_{16}H_{20}O_9$	193.0499(100), 178.0267(61), 149.0606(30), 134.0377(91)	S17,S18	3.83 ± 0.08
□38	Coumaric acid hexoside isomer	17.579	325.0934	$C_{15}H_{18}O_8$	119.0504(100), 163.0403(39)	S13	3.72 ± 0.04

[1] RT: Retention time; [2] EGC: Epigallocatechin, EGCG: Epigallocatechin gallate; [3] HHDP: Hexahydroxydiphenoyl.

[a] Further confirmed in comparison with authentic standard and its quantitative analysis was on absolute.

Among proanthocyanidins (PAs) and derivatives (○), (E)GCG-(E)GCG was relatively quantified based on EGCG content (●), and others were relatively quantified based on EGC content.

Flavonoid glycosides (△) were relatively quantified based on isoquercetrin content.

Among phenolic acid and derivatives (□), ellagic acid derivatives were relatively quantified based on ellagic acid content (■) and others were relatively quantified according to the content of *p*-coumaric acid.

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