Supporting Information

LC-MS Profiling of Kakkonto and Identification of Ephedrine as a Key Component for Its Anti-Glycation Activity

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Table S1. Mass and MS/MS spectrometric data of compounds identified in Kakkonto extract.

No.	t_R (min)	Molecular formula	Positive ion mode				Negative ion mode				Identification	Source
			MS		MS^2 (NCE 10 eV)	MS^2 (stepped NCE 10, 25, and 40 eV)	MS		MS^2 (stepped NCE 10, 25, 40 eV)			
			Detected mass (*m/z*)		Detected mass *m/z* (Intensity, molecular formula)	Detected mass *m/z* (Intensity, molecular formula)	Detected mass (*m/z*)		Detected mass *m/z* (Intensity, molecular formula)			
1	1.92	$C_{10}H_{15}ON$	166.1227	$[M+H]^+$	148.1120 (100, $C_{10}H_{14}N$) 117.0701 (1.9, C_9H_9)	148.1119 (100, $C_{10}H_{14}N$) 117.0701 (4.0, C_9H_9)	no detection				Ephedrine	E
2	2.32	$C_{11}H_{17}ON$	180.1383	$[M+H]^+$	180.1382 (100, $C_{11}H_{18}ON$) 162.1276 (88.8, $C_{11}H_{16}N$) 135.0804 (10.4, $C_9H_{11}O$) 117.0700 (2.4, C_9H_9)	162.1277 (100, $C_{11}H_{16}N$) 135.0804 (14.3, $C_9H_{11}O$) 117.0701 (5.6, C_9H_9)	no detection				Methylephedrine	E
3	3.51	$C_{21}H_{20}O_{10}$	433.1127	$[M+H]^+$	433.1125 (100, $C_{21}H_{21}O_{10}$) 415.1022 (1.9, $C_{21}H_{19}O_9$) 397.0922 (0.2, $C_{21}H_{17}O_8$) 367.0809 (0.4, $C_{20}H_{15}O_7$) 313.0704 (0.8, $C_{17}H_{13}O_6$)	433.1126 (100, $C_{21}H_{21}O_{10}$) 415.1018 (15.9, $C_{21}H_{19}O_9$) 397.0912 (17.3,$C_{21}H_{17}O_8$) 379.0806 (8.9, $C_{21}H_{15}O_7$) 367.0807 (11.1, $C_{20}H_{15}O_7$) 337.0701 (12.6, $C_{19}H_{13}O_6$) 313.0703 (51.9, $C_{17}H_{13}O_6$) 283.0601 (19.6, $C_{16}H_{11}O_5$)	431.0980	$[M-H]^-$	431.0984 (100, $C_{21}H_{19}O_{10}$) 311.0563 (80.1, $C_{17}H_{11}O_6$) 283.0613 (53.9, $C_{16}H_{11}O_5$)	3'-hydroxypuerarin	PU
4	5.52	$C_{21}H_{20}O_9$	417.1176	$[M+H]^+$	417.1174 (100, $C_{21}H_{21}O_9$) 399.1071 (2.4, $C_{21}H_{19}O_8$) 381.0962 (0.5, $C_{21}H_{17}O_7$) 351.0868 (0.4, $C_{20}H_{15}O_6$) 321.0761 (0.3, $C_{19}H_{13}O_5$) 297.0754 (1.6, $C_{17}H_{13}O_5$) 257.0809 (0.9, $C_{15}H_{13}O_4$)	417.1173 (100, $C_{21}H_{21}O_9$) 399.1071 (18.2, $C_{21}H_{19}O_8$) 381.0965 (4.5, $C_{21}H_{17}O_7$) 363.0858 (10.2, $C_{21}H_{15}O_6$) 351.0859 (11.6, $C_{20}H_{15}O_6$) 335.0908 (4.8, $C_{20}H_{15}O_5$) 321.0754 (12.8, $C_{19}H_{13}O_5$) 297.0755 (50.3, $C_{17}H_{13}O_5$) 281.0808 (3.0, $C_{17}H_{13}O_4$) 267.0650 (18.5, $C_{16}H_{11}O_4$) 257.0805 (26.4, $C_{15}H_{13}O_4$)	415.1031	$[M-H]^-$	415.1037 (100, $C_{21}H_{19}O_9$) 295.0612 (79.6, $C_{17}H_{11}O_5$) 267.0665 (58.9, $C_{16}H_{11}O_4$)	Puerarin	PU

5	5.76	$C_{23}H_{28}O_{11}$	481.1699	$[M+H]^+$	319.1173 (84.0, $C_{17}H_{19}O_6$) 301.1068 (18.9, $C_{17}H_{17}O_5$) 197.0808 (100, $C_{10}H_{13}O_4$) 179.0701 (2.1, $C_{10}H_{11}O_3$) 151.0753 (3.6, $C_9H_{11}O_2$) 105.0339 (32.2, C_7H_5O)	319.1172 (23.8, $C_{17}H_{19}O_6$) 197.0807 (49.8, $C_{10}H_{13}O_4$) 179.0701 (6.6, $C_{10}H_{11}O_3$) 151.0753 (19.2, $C_9H_{11}O_2$) 133.0648 (19.6, C_9H_9O) 105.0338 (100, C_7H_5O)	525.1611	$[M+HCOO]^-$	479.1563 (13.7, $C_{23}H_{27}O_{11}$) 121.0294 (100, $C_7H_5O_2$)	Albiflorin	PA
6	6.10	$C_{22}H_{22}O_{10}$	447.1282	$[M+H]^+$	447.1280 (100, $C_{22}H_{23}O_{10}$) 429.1170 (1.4, $C_{22}H_{21}O_9$) 411.1067 (0.4, $C_{22}H_{19}O_8$) 381.0955 (0.3, $C_{21}H_{17}O_7$) 327.0858 (0.6, $C_{18}H_{15}O_6$)	447.1280 (100, $C_{22}H_{23}O_{10}$) 429.1174 (19.8, $C_{22}H_{21}O_9$) 411.1068 (18.3, $C_{22}H_{19}O_8$) 393.0963 (10.2, $C_{22}H_{17}O_7$) 381.0962 (11.8, $C_{21}H_{17}O_7$) 365.1011 (5.5, $C_{21}H_{17}O_6$) 357.0962 (3.8, $C_{19}H_{17}O_7$) 351.0856 (12.0, $C_{20}H_{15}O_6$) 337.1063 (7.3, $C_{20}H_{17}O_5$) 327.0859 (53.8, $C_{18}H_{15}O_6$) 297.0755 (20.1, $C_{17}H_{11}O_5$)	445.1137	$[M-H]^-$	445.1142(100, $C_{22}H_{21}O_{10}$) 325.0719 (82.5, $C_{18}H_{13}O_6$) 297.0770 (19.4, $C_{17}H_{13}O_5$)	3’-Methoxypuerarin	PU
7	6.35	$C_{26}H_{28}O_{13}$	549.1600	$[M+H]^+$	549.1597 (100, $C_{28}H_{29}O_{13}$) 417.1171 (5.7, $C_{21}H_{21}O_9$) 399.1067 (0.3, $C_{21}H_{19}O_8$) 297.0753 (0.4, $C_{17}H_{13}O_5$)	549.1594 (100, $C_{26}H_{29}O_{13}$) 417.1171 (60.1, $C_{21}H_{21}O_9$) 399.1067 (26.7, $C_{21}H_{19}O_8$) 381.0961 (20.8, $C_{21}H_{17}O_7$) 351.0856 (13.5, $C_{20}H_{15}O_6$) 335.0907 (6.4, $C_{20}H_{15}O_5$) 321.0751 (14.7, $C_{19}H_{13}O_5$) 297.0753 (62.7, $C_{17}H_{13}O_5$) 267.0649 (14.8, $C_{16}H_{11}O_4$)	547.1458	$[M-H]^-$	295.0612 (100, $C_{17}H_{11}O_5$) 267.0663 (53.3, $C_{16}H_{11}O_4$)	Puerarin apioside	PU
8	6.57	$C_{23}H_{28}O_{11}$	498.1966	$[M+NH_4]^+$	463.1595 (6.0, $C_{23}H_{27}O_{10}$) 341.1224 (0.8, $C_{16}H_{21}O_8$) 319.1175 (3.3, $C_{17}H_{19}O_6$) 301.1069 (13.5, $C_{17}H_{17}O_5$) 285.0966 (2.5, $C_{13}H_{17}O_7$) 197.0808 (25.2, $C_{10}H_{13}O_4$) 179.0701 (100, $C_{10}H_{11}O_3$)	197.0807 (9.4, $C_{10}H_{13}O_4$) 179.0701 (100, $C_{10}H_{11}O_3$) 151.0753 (26.7, $C_9H_{11}O_2$)	525.1613	$[M+HCOO]^-$	479.1558 (4.1, $C_{23}H_{27}O_{11}$) 449.1457 (0.5, $C_{22}H_{25}O_{10}$) 327.1088 (8.2, $C_{15}H_{19}O_8$) 165.0556 (9.5, $C_9H_9O_3$) 121.0294 (100, $C_7H_5O_2$)	Paeoniflorin	PA
9	7.20	$C_{21}H_{20}O_9$	417.1175	$[M+H]^+$	255.0650 (100, $C_{15}H_{11}O_4$)	255.0648 (100, $C_{15}H_{11}O_4$)	461.1089	$[M+HCOO]^-$	415.1037 (34.6, $C_{21}H_{19}O_9$) 253.0507 (100, $C_{16}H_9O_4$)	Daidzin	PU G
10	7.68	$C_{22}H_{22}O_{10}$	447.1284	$[M+H]^+$	285.0755 (100, $C_{16}H_{13}O_5$)	285.0755 (100, $C_{16}H_{13}O_5$)	491.1199	$[M+HCOO]^-$	445.1145 (31.2, $C_{22}H_{21}O_{10}$) 283.0613 (100, $C_{16}H_{11}O_5$)	Glycitin	PU

11	7.82	$C_{26}H_{28}O_{14}$	565.1550	$[M+H]^+$	565.1548 (100, $C_{26}H_{29}O_{14}$) 547.1442 (28.2, $C_{26}H_{27}O_{13}$) 433.1128 (29.1, $C_{21}H_{21}O_{10}$) 415.1024 (4.4, $C_{21}H_{19}O_9$) 313.0703 (3.1, $C_{17}H_{13}O_6$)	565.1548 (100, $C_{26}H_{29}O_{14}$) 547.1443 (33.0, $C_{26}H_{27}O_{13}$) 397.0910 (56.1, $C_{21}H_{17}O_8$) 379.0808 (34.7, $C_{21}H_{15}O_7$) 337.0703 (18.4, $C_{19}H_{13}O_6$) 325.0703 (22.8, $C_{18}H_{13}O_6$) 283.0600 (3.4, $C_{16}H_{11}O_5$)	563.1408	$[M-H]^-$	563.1407 (66.1, $C_{26}H_{27}O_{14}$) 473.1092 (5.0, $C_{23}H_{21}O_{11}$) 443.0984 (14.1, $C_{19}H_{13}O_7$) 353.0667 (5.4, $C_{18}H_{13}O_7$) 311.0565 (100, $C_{17}H_{11}O_6$) 283.0615 (24.4, $C_{16}H_{11}O_5$)	3'-Hydroxypuerarin apioside	PU
12	7.96	$C_{29}H_{34}O_{14}$	607.2022	$[M+H]^+$	571.1796 (1.7, $C_{29}H_{31}O_{12}$) 461.1437 (100, $C_{23}H_{25}O_{10}$) 299.0912 (65.4, $C_{17}H_{15}O_5$) 205.0493 (0.7, $C_{11}H_9O_4$) 107.0493 (1.9, C_7H_7O)	461.1436 (46.9, $C_{23}H_{25}O_{10}$) 299.0912 (66.0, $C_{17}H_{15}O_5$) 281.0807 (11.8, $C_{17}H_{13}O_4$) 253.0855 (11.8, $C_{16}H_{13}O_3$) 239.0700 (8.6, $C_{15}H_{11}O_3$) 107.0495 (100, C_7H_7O)	605.1884	$[M-H]^-$	297.0769 (100, $C_{17}H_{13}O_5$) 253.0871 (92.2, $C_{16}H_{13}O_3$)	Pueroside A	PU
13	8.50	$C_{21}H_{22}O_9$	436.1597	$[M+NH_4]^+$	419.1331 (4.0, $C_{21}H_{23}O_9$) 257.0806 (100, $C_{15}H_{13}O_4$) 145.0495 (1.2, $C_6H_9O_4$) 137.0233 (2.7, $C_7H_5O_3$)	257.0806 (100, $C_{15}H_{13}O_4$) 239.0698 (1.1, $C_{15}H_{11}O_3$) 147.0440 (3.5, $C_9H_7O_2$) 137.0233 (8.1, $C_7H_5O_3$) 97.0289 (1.1, $C_5H_6O_2$)	417.1187	$[M-H]^-$	255.0665 (100, $C_{15}H_{11}O_4$) 135.0087 (35.1, $C_7H_3O_3$) 119.0501 (18.1, C_8H_7O)	Liquiritin	G
14	9.43	$C_{27}H_{30}O_{13}$	563.1760	$[M+H]^+$	563.1751 (100, $C_{27}H_{31}O_{13}$) 431.1332 (4.9, $C_{22}H_{23}O_9$) 413.1228 (0.5, $C_{22}H_{21}O_8$) 311.0923 (0.4, $C_{18}H_{15}O_5$)	563.1752 (100, $C_{27}H_{31}O_{13}$) 431.1333 (57.2, $C_{22}H_{23}O_9$) 413.1226 (32.0, $C_{22}H_{21}O_8$) 395.1122 (22.3, $C_{22}H_{19}O_7$) 377.1013 (10.7, $C_{22}H_{17}O_6$) 365.1016 (13.3, $C_{21}H_{17}O_6$) 349.1064 (5.9, $C_{21}H_{17}O_5$) 335.0910 (15.5, $C_{20}H_{15}O_5$) 321.1117 (4.8, $C_{20}H_{17}O_4$) 311.0911 (71.3, $C_{18}H_{15}O_5$) 281.0808 (15.4, $C_{17}H_{13}O_4$)	561.1619	$[M-H]^-$	309.0770 (100, $C_{18}H_{13}O_5$) 281.0820 (29.7, $C_{17}H_{13}O_4$)	formononetin 8-*C*-[β-D-apiofuranosyl-(1→6)]-β-D-glucopyranoside	PU

15	10.38	$C_{23}H_{28}O_{11}$	481.1704	$[M+H]^+$	319.11743 (32.2, $C_{17}H_{19}O_6$) 301.1070 (7.0, $C_{17}H_{17}O_5$) 285.1126 (0.6, $C_{17}H_{17}O_4$) 267.0864 (3.1, $C_{13}H_{15}O_6$) 257.1378 (1.5, $C_{13}H_{21}O_{15}$) 249.0751 (0.8, $C_{13}H_{13}O_5$) 215.0910 (0.9, $C_{10}H_{15}O_5$) 197.0808 (100, $C_{10}H_{13}O_4$) 179.0701 (1.8, $C_{10}H_{11}O_3$) 161.0597 (0.6, $C_{10}H_9O_2$) 151.0753 (1.6, $C_9H_{11}O_2$) 145.0495 (0.7, $C_6H_9O_4$) 133.0650 (0.4, C_9H_9O) 105.0339 (10.3, C_7H_5O)	319.1173 (18.9, $C_{17}H_{19}O_6$) 197.0808 (100, $C_{10}H_{13}O_4$) 179.0702 (29.6, $C_{10}H_{11}O_3$) 161.0596 (14.0, $C_{10}H_9O_2$) 151.0753 (14.0, $C_9H_{11}O_2$) 133.0648 (27.9, C_9H_9O) 105.0338 (71.4, C_7H_5O)	525.1616	$[M+HCOO]^-$	479.1563 (13.4, $C_{23}H_{27}O_{11}$) 121.0294 (100, $C_7H_6O_2$)	4-epi-albiflorin	PA
16	11.19	$C_{24}H_{26}O_{10}$	475.1598	$[M+H]^+$	313.1067 (100, $C_{18}H_{17}O_5$) 295.0968 (1.3, $C_{18}H_{15}O_4$) 267.1026 (0.1, $C_{17}H_{15}O_3$) 253.0864 (0.2, $C_{16}H_{13}O_3$) 219.0650 (4.2, $C_{12}H_{11}O_4$) 207.0651 (0.8, $C_{11}H_{11}O_4$) 145.0496 (0.8, $C_6H_9O_4$) 107.0495 (14.1, C_7H_7O)	313.1066 (64.2, $C_{18}H_{17}O_5$) 295.0963 (10.3, $C_{18}H_{15}O_4$) 267.1014 (12.7, $C_{17}H_{15}O_3$) 253.0857 (7.3, $C_{16}H_{13}O_3$) 219.0650 (6.9, $C_{12}H_{11}O_4$) 207.0651 (6.5, $C_{11}H_{11}O_4$) 189.0546 (1.8, $C_{11}H_9O_3$) 175.0754 (2.6, $C_{11}H_{11}O_2$) 161.0596 (1.0, $C_{10}H_9O_2$) 145.0646 (2.0, $C_{10}H_9O$) 127.0391 (2.3, $C_6H_7O_3$) 107.0495 (100, C_7H_7O)	519.1508	$[M+HCOO]^-$	473.1453 (2.5, $C_{24}H_{25}O_{10}$) 311.0927 (100, $C_{18}H_{15}O_5$) 267.1021 (62.5, $C_{17}H_{15}O_3$)	Sophoraside A	PU
17	11.60	$C_{22}H_{22}O_9$	431.1334	$[M+H]^+$	269.0806 (100, $C_{16}H_{13}O_4$)	269.0807 (100, $C_{16}H_{13}O_4$)	475.1247	$[M+HCOO]^-$	267.0665 (100, $C_{16}H_{11}O_4$)	Ononin	PU, G
18	11.88	$C_{21}H_{22}O_9$	419.1333	$[M+H]^+$	257.0806 (100, $C_{15}H_{13}O_4$) 137.0233 (0.4, $C_7H_5O_3$)	257.0806 (100, $C_{15}H_{13}O_4$) 147.0440 (7.4, $C_9H_7O_2$) 137.0233 (12.7, $C_7H_5O_3$)	417.1192	$[M-H]^-$	255.0664 (100, $C_{15}H_{11}O_4$) 135.0088 (30.1, $C_7H_3O_3$) 119.0501 (11.6, C_8H_7O)	Isoliquiritin	G
19	12.47	$C_{15}H_{10}O_4$	255.0649	$[M+H]^+$	255.0649 (100, $C_{15}H_{11}O_4$)	255.0650 (100, $C_{15}H_{11}O_4$)	253.0506	$[M-H]^-$	253.0506 (100, $C_{15}H_9O_4$)	Daidzein	PU G
20	12.71	$C_{15}H_{12}O_4$	257.0807	$[M+H]^+$	257.0805 (100, $C_{15}H_{13}O_4$) 239.0703 (1.5, $C_{15}H_{11}O_3$) 211.0755 (0.3, $C_{14}H_{11}O_2$) 147.0439 (3.2, $C_9H_7O_2$) 137.0233 (4.6, $C_7H_5O_3$)	257.0806 (100, $C_{15}H_{13}O_4$) 211.0753 (3.2, $C_{14}H_{11}O_2$) 163.0389 (1.6, $C_9H_7O_3$) 147.0440 (19.3, $C_9H_7O_2$) 137.0233 (35.9, $C_7H_5O_3$)	255.1663	$[M-H]^-$	255.0665 (90.9, $C_{15}H_{11}O_4$) 135.0088 (90.2, $C_7H_3O_3$) 119.0502 (100, C_8H_7O) 91.0189 (11.3, C_6H_3O)	Liquiritigenin	G
21	12.99	$C_{16}H_{12}O_5$	285.0754	$[M+H]^+$		285.0755 (100, $C_{16}H_{13}O_5$)[a]	283.0612	$[M-H]^-$	283.0613 (100, $C_{16}H_{11}O_5$)	Glycitein	PU

22	14.86	$C_{30}H_{32}O_{12}$	602.2230	$[M+NH_4]^+$	567.1841 (7.1, $C_{30}H_{31}O_{11}$) 463.1586 (3.1, $C_{23}H_{27}O_{10}$) 445.1489 (22.3, $C_{23}H_{25}O_9$) 427.1385 (23.1, $C_{23}H_{23}O_8$) 301.1068 (18.5, $C_{17}H_{17}O_5$) 267.0863 (93.9, $C_{13}H_{15}O_6$) 249.0755 (28.4, $C_{13}H_{13}O_5$) 197.0809 (1.8, $C_{10}H_{13}O_4$) 179.0702 (100, $C_{10}H_{11}O_3$) 151.0753 (1.8, $C_9H_{11}O_2$) 105.0338 (3.0, C_7H_5O)	267.0862 (62.7, $C_{13}H_{15}O_6$) 249.0755 (45.3, $C_{13}H_{13}O_5$) 179.0702 (88.6, $C_{10}H_{11}O_3$) 151.0753 (30.6, $C_9H_{11}O_2$) 105.0338 (100, C_7H_5O)	629.1881	$[M+HCOO]^-$	583.1821 (5.6, $C_{30}H_{31}O_{12}$) 121.0294 (100, $C_7H_5O_2$)	Benzoylpaeoniflorin	PA
23	15.20	$C_{30}H_{32}O_{12}$	585.1966	$[M+H]^+$	319.1174 (100, $C_{17}H_{19}O_6$) 301.1069 (16.1, $C_{17}H_{17}O_5$) 267.0863 (28.7, $C_{13}H_{15}O_6$) 249.0756 (6.4, $C_{13}H_{13}O_5$) 197.0808 (25.3, $C_{10}H_{13}O_4$) 151.0753 (1.5, $C_9H_{11}O_2$) 105.0339 (18.6, C_7H_5O)	319.1174 (32.3, $C_{17}H_{19}O_6$) 301.1069 (6.1, $C_{17}H_{17}O_5$) 267.0863 (10.0, $C_{13}H_{15}O_6$) 249.0756 (9.6, $C_{13}H_{13}O_5$) 197.0808 (18.2, $C_{10}H_{13}O_4$) 151.0753 (12.2, $C_9H_{11}O_2$) 105.0339 (100, C_7H_5O)	629.1880	$[M+HCOO]^-$	583.1825 (10.4, $C_{30}H_{31}O_{12}$) 121.0294 (100, $C_7H_5O_2$)	Paeonivayin	PA
24	15.24	$C_{48}H_{72}O_{21}$	985.4637	$[M+H]^+$	985.4625 (100, $C_{48}H_{73}O_{21}$) 809.4303 (13.5, $C_{42}H_{65}O_{15}$) 615.3882 (26.2, $C_{36}H_{55}O_8$) 453.3357 (14.6, $C_{30}H_{45}O_3$)	809.4305 (7.6, $C_{42}H_{65}O_{15}$) 647.3774 (3.4, $C_{36}H_{55}O_{10}$) 633.3985 (2.1, $C_{36}H_{57}O_9$) 615.3884 (30.9, $C_{36}H_{55}O_8$) 471.3465 (8.0, $C_{30}H_{47}O_4$) 453.3358 (100, $C_{30}H_{45}O_3$) 435.3253 (7.4, $C_{30}H_{43}O_2$) 407.3302 (6.3, $C_{29}H_{43}O$) 389.3197 (2.6, $C_{29}H_{41}$) 357.2418 (3.6, $C_{23}H_{33}O_3$) 217.1586 (6.3, $C_{15}H_{21}O$) 189.1637 (5.7, $C_{14}H_{21}$)	983.4503	$[M-H]^-$	983.4498 (100, $C_{48}H_{71}O_{21}$) 821.3972 (24.1, $C_{42}H_{61}O_{16}$) 645.3640 (3.5, $C_{36}H_{53}O_{10}$) 351.0569 (36.5, $C_{12}H_{15}O_{12}$) 289.0569 (2.6, $C_{11}H_{13}O_9$) 193.0353 (19.5, $C_6H_9O_7$) 175.0247 (9.4, $C_6H_7O_6$) 157.0142 (4.0, $C_6H_5O_5$) 113.0243 (34.6, $C_5H_5O_3$)	Licorice saponin A_3	G
25	16.09	$C_{44}H_{64}O_{18}$	881.4155	$[M+H]^+$	705.3835 (91.6, $C_{38}H_{57}O_{12}$) 529.3523 (2.2, $C_{32}H_{49}O_6$) 511.3415 (100, $C_{32}H_{47}O_5$)	705.3832 (11.7, $C_{38}H_{57}O_{12}$) 529.3522 (5.1, $C_{32}H_{49}O_6$) 511.3414 (100, $C_{32}H_{47}O_5$) 451.3202 (5.1, $C_{30}H_{43}O_3$) 433.3096 (2.3, $C_{30}H_{41}O_2$) 405.3148 (3.1, $C_{29}H_{41}O$) 233.1536 (1.3, $C_{15}H_{21}O_2$) 217.1585 (2.5, $C_{15}H_{21}O$) 215.1433 (1.3, $C_{15}H_{19}O$) 189.1636 (2.1, $C_{14}H_{21}$) 187.1481 (2.5, $C_{14}H_{19}$)	879.4023	$[M-H]^-$	351.0570 (95.6, $C_{12}H_{15}O_{12}$) 289.0562 (7.0, $C_{11}H_{13}O_9$) 193.0353 (49.9, $C_6H_9O_7$) 175.0247 (25.8, $C_6H_7O_6$) 157.0140 (5.8, $C_6H_5O_5$) 113.0243 (100, $C_5H_5O_3$)	22β-acetoxyglycyrrhizic acid	G

26	17.08	$C_{42}H_{62}O_{17}$	839.4055	$[M+H]^+$	663.3727 (21.4, $C_{36}H_{55}O_{11}$) 645.3621 (12.9, $C_{36}H_{53}O_{10}$) 487.3414 (81.2, $C_{30}H_{47}O_5$) 469.3309 (100, $C_{30}H_{45}O_4$) 451.3203 (12.5, $C_{30}H_{43}O_3$)	645.3633 (5.7, $C_{36}H_{53}O_{10}$) 487.3415 (54.5, $C_{36}H_{53}O_{10}$) 469.3311 (100, $C_{30}H_{45}O_4$) 451.3203 (23.5, $C_{30}H_{43}O_3$) 439.3205 (4.8, $C_{29}H_{43}O_3$) 217.1581 (2.5, $C_{15}H_{21}O$) 205.1588 (1.4, $C_{14}H_{21}O$) 189.1637 (4.5, $C_{14}H_{21}$) 175.1482 (3.9, $C_{13}H_{19}$) 159.0287 (7.2, $C_6H_7O_5$) 141.0181 (20.2, $C_6H_5O_4$)	837.3918	$[M-H]^-$	837.3921 (100, $C_{42}H_{61}O_{17}$) 351.0571 (65.6, $C_{12}H_{15}O_{12}$) 289.0564 (4.2, $C_{11}H_{13}O_9$) 193.0353 (39.6, $C_6H_9O_7$) 175.0248 (17.2, $C_6H_7O_6$) 157.0141 (4.8, $C_6H_5O_5$) 113.0244 (65.4, $C_5H_5O_3$)	Licorice saponin G_2	G
27	17.77	$C_{42}H_{62}O_{16}$	823.4097	$[M+H]^+$	647.3777 (31.0, $C_{36}H_{55}O_{10}$) 471.3463 (5.4, $C_{30}H_{47}O_4$) 453.3356 (100, $C_{30}H_{45}O_3$)	647.3784 (13.8, $C_{36}H_{55}O_{10}$) 471.3468 (6.0, $C_{30}H_{47}O_4$) 453.3359 (100, $C_{30}H_{45}O_3$) 407.3302 (3.2, $C_{29}H_{43}O$) 217.1587 (3.2, $C_{15}H_{21}O$) 189.1638 (3.3, $C_{14}H_{21}$)	821.3966	$[M-H]^-$	821.3975 (100, $C_{42}H_{61}O_{16}$) 351.0572 (65.6, $C_{12}H_{15}O_{12}$) 193.0353 (39.6, $C_6H_9O_7$) 175.0248 (17.02, $C_6H_7O_6$) 157.0141 (4.8, $C_6H_5O_5$) 113.0244 (65.4, $C_5H_5O_3$)	Glycyrrhizin	G

PU: PUERARIAE RADIX (*Pueraria lobata*)

E: EPHEDRAE HERBA (*Ephedra sinica*; *Ephedra intermedia*; *Ephedra equisetina*)

PA: PAEONIAE RADIX (*Paenonia lactiflora*)

G: GLYCYRRHIZAE RADIX (*Glycyrrhiza uralensis*; *Glycyrrhiza glabra*)

[a] Normalized collision energy at 30 eV

Table S2. Mass spectrometric data of products detected in Kakkonto extract reacted with glyceraldehyde (GA).

No.	t_R (min)	Molecular formula	Positive ion mode		MS/MS (30 eV)
			Detected mass (*m/z*)		Detected mass *m/z* (Intensity, molecular formula)
EM1	1.80	$C_{12}H_{18}O_3N$	224.1281	[M+H]+	206.1174 (100.0, $C_{12}H_{16}O_2N$)
					188.1068 (6.6, $C_{12}H_{14}ON$)
					170.0962 (5.2, $C_{12}H_{12}N$)
					158.0962 (5.5, $C_{11}H_{12}N$)
					134.0963 (5.2, $C_9H_{12}N$)
					117.0699 (0.6, C_9H_9)
EM2	2.42	$C_{12}H_{18}O_3N$	224.1280	[M+H]+	206.1174 (100.0, $C_{12}H_{16}O_2N$)
					188.1068 (1.0, $C_{12}H_{14}ON$)
					135.0804 (11.4, $C_9H_{11}O$)
					117.0700 (4.5, C_9H_9)
EM3	2.60	$C_{13}H_{20}O_3N$	238.1438	[M+H]+	220.1330 (100.0, $C_{13}H_{18}O_2N$)
					202.1226 (3.0, $C_{13}H_{16}ON$)
					184.1119 (0.9, $C_{13}H_{14}N$)
					172.1119 (1.4, $C_{12}H_{14}N$)
					148.1120 (21.3, $C_{10}H_{14}N$)
					135.0803 (0.6, $C_9H_{11}O$)
					117.0702 (0.4, C_9H_9)
					114.0915 (0.8, $C_6H_{12}ON$)
					104.0709 (4.3, $C_4H_{10}O_2N$)

Table S3. Mass spectrometric data of products detected in Kakkonto extract reacted with methylglyoxal (MGO).

No.	t_R (min)	Molecular formula	Positive ion mode		MS/MS (30 eV)
			Detected mass *m/z*		Detected mass *m/z* (Intensity, molecular formula)
EM4	3.07	$C_{13}H_{19}O_3N$	238.1436	[M+H]+	220.1330 (49.2, $C_{13}H_{18}O_2N$) 202.1226 (0.6, $C_{13}H_{16}ON$) 192.1381 (2.5, $C_{12}H_{18}ON$) 174.1274 (0.8, $C_{12}H_{16}N$) 135.0804 (17.2, $C_9H_{11}O$) 117.0700 (4.6, C_9H_9) 104.0709 (100.0, $C_4H_{10}O_2N$)
EM5	3.59	$C_{13}H_{19}O_3N$	238.1436	[M+H]+	220.1329 (68.3, $C_{13}H_{18}O_2N$) 202.1223 (0.7, $C_{13}H_{16}ON$) 192.1380 (3.8, $C_{12}H_{18}ON$) 174.1276 (0.9, $C_{12}H_{16}N$) 135.0803 (18.6, $C_9H_{11}O$) 117.0700 (5.7, C_9H_9) 104.0709 (100, $C_4H_{10}O_2N$)