Supplementary Materials

The bioactive ingredients and mechanisms of Wen-Pi-Tang in treating chronic renal failure, based on UHPLC-Q-Exactive Orbitrap MS, network pharmacology, and in silico validation

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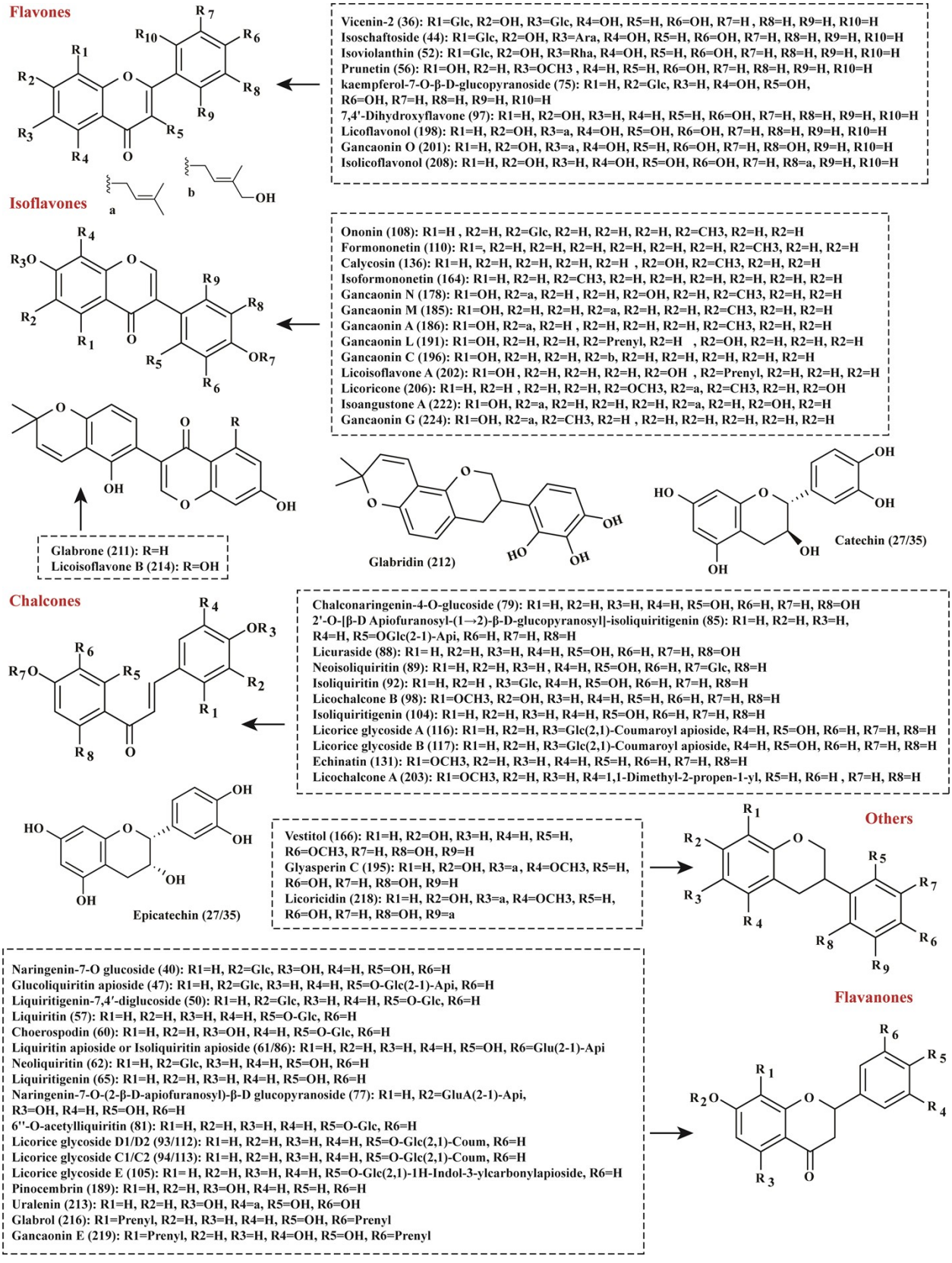
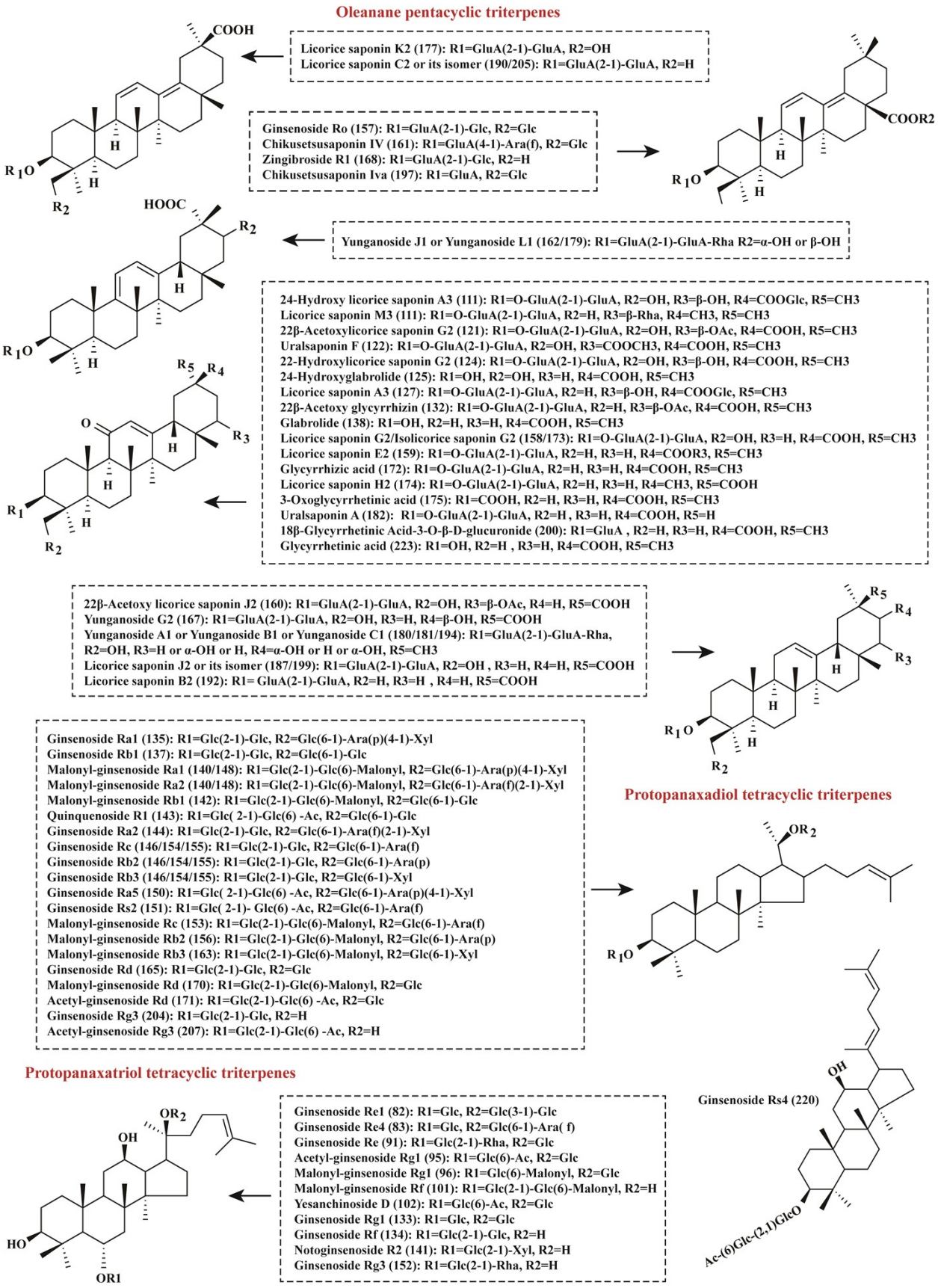
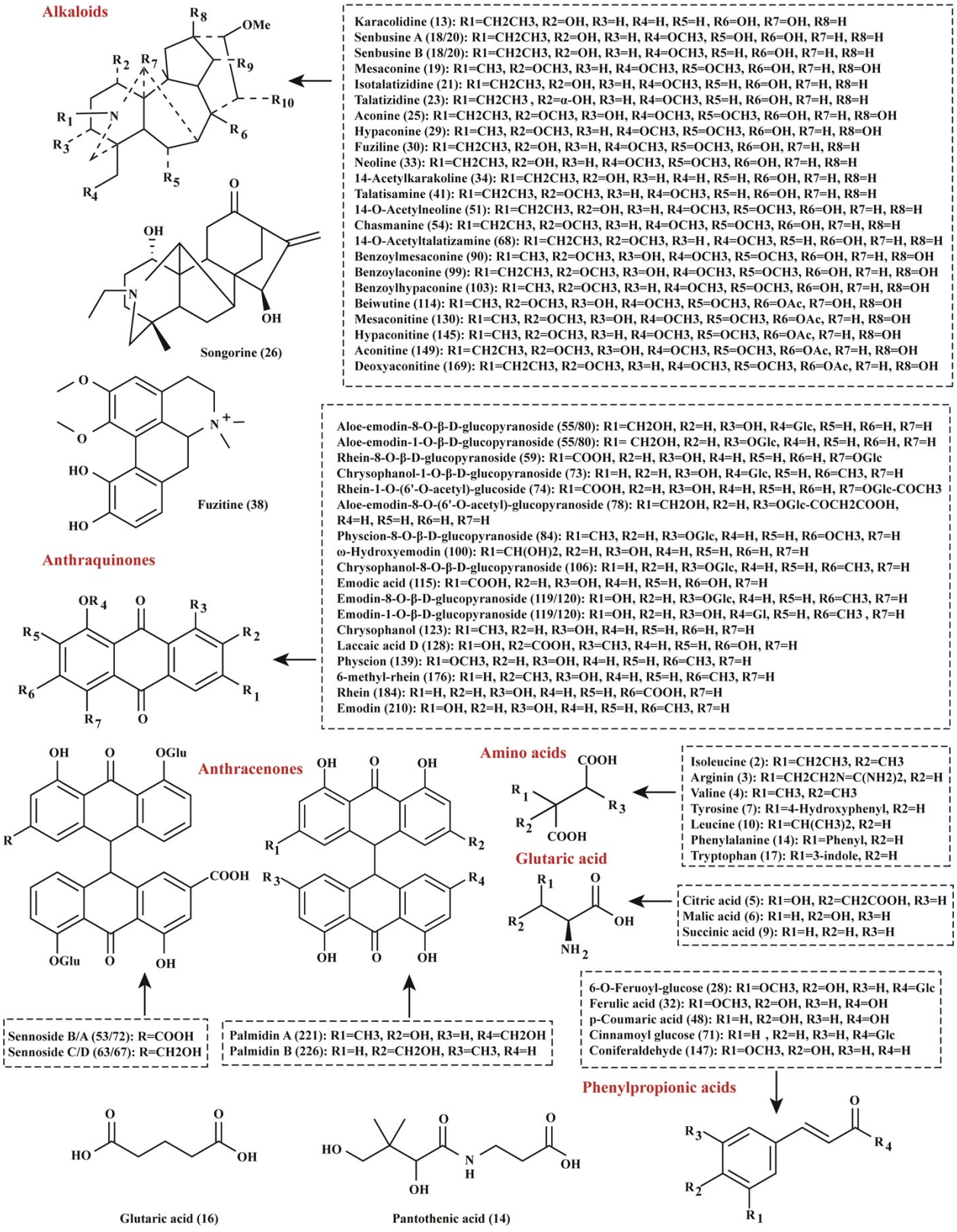


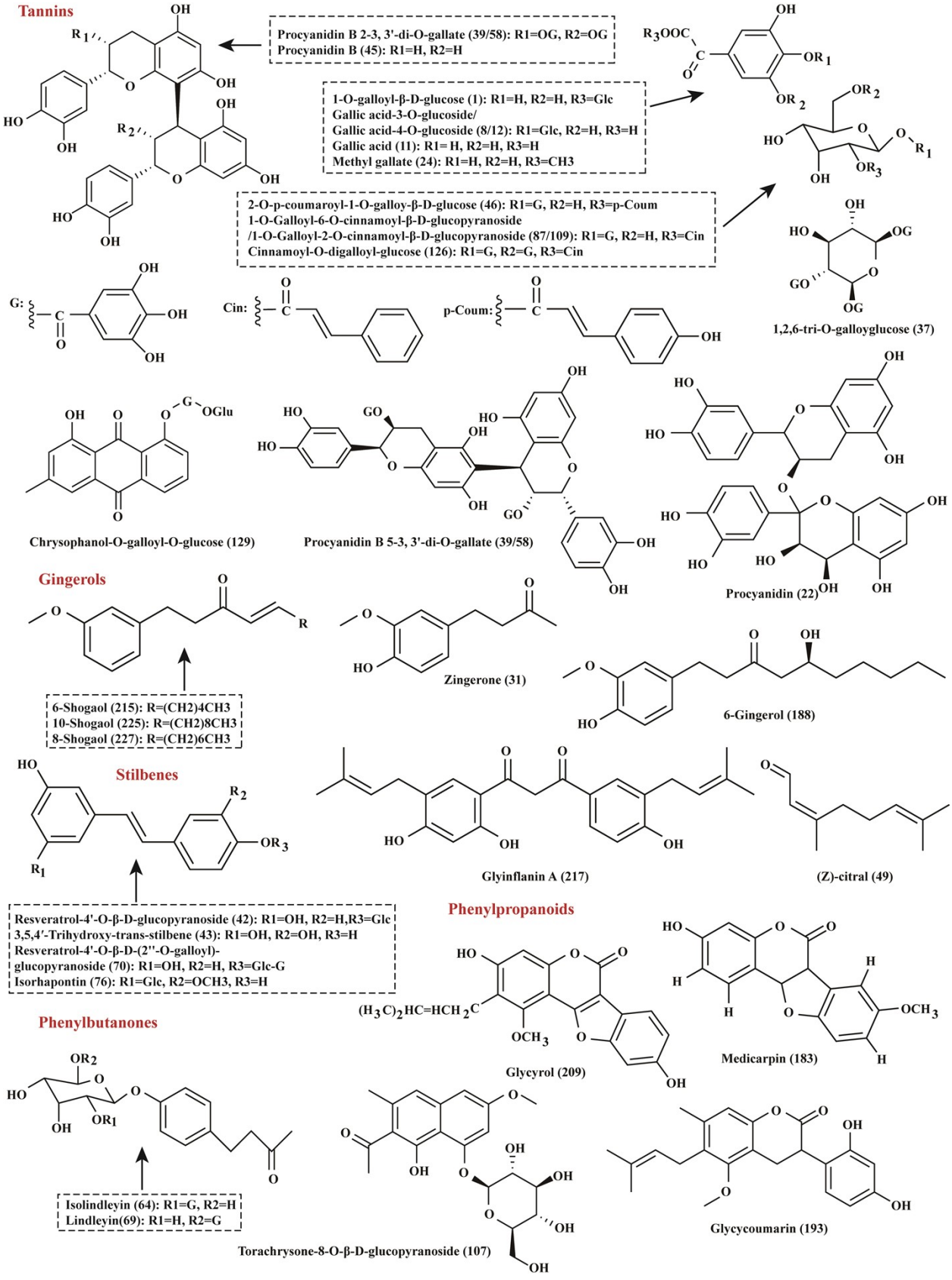
Supplementary Fig. S1. Structures of the 61 flavonoid compounds identified in the WPT.



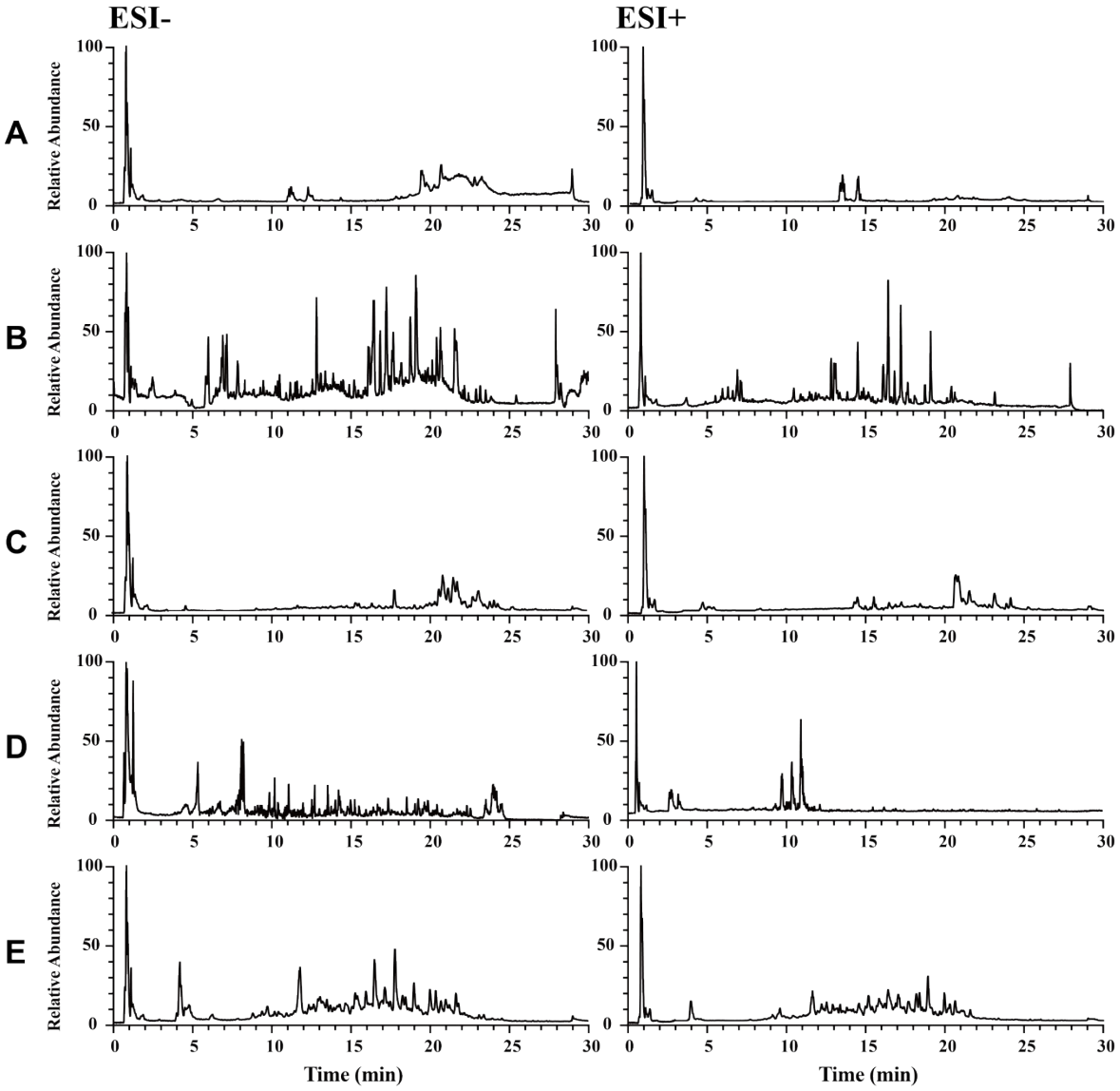
Supplementary Fig. S2. Structures of the 67 triterpenoid compounds identified in the WPT.



Supplementary Fig. S3. Structures of the 18 anthraquinone, 6 anthracenone, and 17 organic acid compounds identified in the WPT.



Supplementary Fig. S4. Structures of the 16 tannin, and 17 other-type compounds identified in the WPT.



Supplementary Fig. S5. The total ion chromatograms (TICs) of the individual herb extracts including Ganjiang**(A)**, Zhigancao **(B)**, Fuzi **(C)**, Dahuang **(D)**, and Renshen **(E)** in positive and negative ion modes.

Supplementary Table S1 Identification of chemical components in WPT by UHPLC-Q-Exactive Orbitrap-MS.

NO.	t_R (min)	Formula	MW (Da)	Detected *m/z*(+/-)	Expected	Error (ppm)	MS/MS		Identification	Source
							ESI$^-$	ESI$^+$		
1	0.82	$C_{13}H_{16}O_{10}$	332.0738	331.0676[M-H]$^-$	331.0660	4.83	271.0456,211.0243,193.0141,169.0141		1-O-galloyl-β-D-glucose[1]	DH
2	0.86	$C_6H_{13}NO_2$	131.0946	132.1017[M+H]$^+$	132.1019	-1.52		86.0970,69.0707	Isoleucine[2]	GJ
3	0.88	$C_6H_{14}N_4O_2$	174.1117	175.1182[M+H]$^+$	175.1190	-4.57		158.0923,116.0709,70.0657	Arginine[2]	GJ,RS
4	0.89	$C_5H_{11}NO_2$	117.0790	118.0861[M+H]$^+$	118.0862	-0.85		72.0813,55.0550	Valine[2]	GJ
5	1.12	$C_6H_8O_7$	192.0270	191.0190[M-H]$^-$	191.0186	2.09	111.0080,87.0077,85.0285		Citric acid[2]	GJ,ZGC,RS
6	1.17	$C_4H_6O_5$	134.0215	133.0133[M-H]$^-$	133.0131	1.50	115.0028,71.0127		Malic acid[2, 3]	GJ,ZGC,RS
7	1.18	$C_9H_{11}NO_3$	181.0738	182.0809[M+H]$^+$	182.0812	-1.65		165.0546,147.0440,136.0758,123.0443,91.0549	Tyrosine[2]	GJ,RS
8	1.22	$C_{13}H_{16}O_{10}$	332.0738	331.0673[M-H]$^-$	331.0660	3.93	271.0469,241.0796,169.0138		Gallic acid-3-O-glucoside/Gallic acid-4-O-glucoside[1]	DH
9	1.24	$C_4H_6O_4$	118.0266	117.0184[M-H]$^-$	117.0182	1.71	99.0078,73.0284		Succinic acid*	GJ
10	1.32	$C_6H_{13}NO_2$	131.0946	132.1016[M+H]$^+$	132.1019	-2.27		86.0970,69.0705	Leucine[2, 4]	GJ,RS
11	1.40	$C_7H_6O_5$	170.0215	169.0134[M-H]$^-$ 171.0288[M+H]$^+$	169.0131	1.78 2.35	125.0236,107.0128,97.0288	153.0181,135.0077,127.0392,109.0287	Gallic acid[1]	DH
12	1.54	$C_{13}H_{16}O_{10}$	332.0738	331.0672[M-H]$^-$	331.0660	3.63	271.0469,241.0365,169.0139,125.0238		Gallic acid-3-O-glucoside/Gallic acid-4-O-glucoside[1]	DH
13	1.68	$C_{22}H_{35}NO_5$	393.2515	394.2581[M+H]$^+$	394.2588	-1.78		376.2474,358.2364,328.2271,326.2105	Karacolidine[5]	FZ
14	1.91	$C_9H_{17}NO_5$	219.1107	218.1033[M-H]$^-$ 220.1175[M+H]$^+$	218.1023 220.1175	4.59 1.82	146.0815,88.0392	202.1070,184.0964,90.0555	Pantothenic acid[2]	GJ
15	1.98	$C_9H_{11}NO_2$	165.0790	164.0712[M-H]$^-$ 166.0861[M+H]$^+$	164.0706 166.0862	3.66 -0.62	147.0444,103.0541,91.0543,72.0080	149.0599,120.0810,103.0546	Phenylalanine[2, 6]	GJ,RS
16	2.35	$C_5H_8O_4$	132.0423	131.0340[M-H]$^-$	131.0339	0.76	113.0345,87.0440		Glutaric acid[2]	GJ
17	3.59	$C_{11}H_{12}N_2O_2$	204.0899	203.0824[M-H]$^-$ 205.0969[M+H]$^+$	203.0815 205.0971	4.43 -0.97	159.0921,116.0498,74.0235	188.0707,144.0806,118.0654	Tryptophan[2]	GJ

Table S1 (*continued*)

NO.	t_R (min)	Formula	MW (Da)	Detected *m/z*(+/-)	Expected	Error (ppm)	MS/MS		Identification	Source
							ESI^-	ESI^+		
18	4.34	$C_{23}H_{37}NO_6$	423.2621	424.2685$[M+H]^+$	424.2694	-2.12		406.2578,388.2473,378.2263,374.2315,356.2204	Senbusine A /B[5]	FZ
19	4.36	$C_{24}H_{39}NO_9$	485.2625	486.2690$[M+H]^+$	486.2698	-1.65		468.2580,436.2321	Mesaconine[7]	FZ
20	4.59	$C_{23}H_{37}NO_6$	423.2621	424.2683$[M+H]^+$	424.2694	-2.59		406.2578,388.2476,378.2266,374.2339,356.2212	Senbusine A /B[5]	FZ
21	4.65	$C_{23}H_{37}NO_5$	407.2672	408.2737$[M+H]^+$	408.2744	-1.72		390.2631,372.2517,362.2317,358.2367,340.2282	Isotalatizidine[7]	FZ
22	4.75	$C_{30}H_{26}O_{13}$	594.1368	593.1317$[M-H]^-$	593.1290	4.55	467.0989,441.0848,425.0901,423.0735,407.0770,305.0671		Procyanidin[1]	DH
23	4.97	$C_{23}H_{37}NO_5$	407.2672	408.2733$[M+H]^+$	408.2744	-2.70		390.2629,372.2525,362.2323,358.2368,340.2268	Talatizidine[5]	FZ
24	5.17	$C_8H_8O_5$	184.0366	183.0294$[M-H]^-$	183.0288	3.11	168.0061,124.0159		Methyl gallate[8]	DH
25	5.34	$C_{25}H_{41}NO_9$	499.2781	500.2851$[M+H]^+$	500.2854	-0.60		482.2759,468.2577,450.2473,436.2312,418.2212	Aconine*	FZ
26	5.37	$C_{22}H_{31}NO_3$	357.2304	358.2368$[M+H]^+$	358.2377	-2.51		340.2262,322.2158,312.2324	Songorine[5]	FZ
27	5.38	$C_{15}H_{14}O_6$	290.0790	289.0723$[M-H]^-$	289.0707	5.54	245.0824,137.0239,123.0443,109.0287		Catechin or Epicatechin[2]	GJ,DH
28	5.65	$C_{16}H_{20}O_9$	356.1102	355.1036$[M-H]^-$	355.1024	3.38	193.0506,175.0399		6-O-Feruoyl-glucose[8]	DH
29	6.00	$C_{24}H_{39}NO_8$	469.2676	470.2734$[M+H]^+$	470.2748	-2.98		438.2477,406.2216,374.1949	Hypaconine*	FZ
30	6.08	$C_{24}H_{39}NO_7$	453.2721	454.2788$[M+H]^+$	454.2799	-2.42	436.2686,408.2386,404.2419,418.2574,386.2317,354.2061		Fuziline[7]	FZ
31	6.10	$C_{11}H_{14}O_3$	194.0943	193.0854$[M-H]^-$	193.0859	-2.59	178.0271,121.0283,57.3450		Zingerone[9]	GJ
32	6.11	$C_{10}H_{10}O_4$	194.0579	193.0504$[M-H]^-$ 195.0647$[M+H]^+$	193.0495 195.0651	4.66 -2.05	178.0271,149.0600,134.0367	177.0547,145.0283,117.0337	Ferulic acid*	GC
33	6.29	$C_{24}H_{39}NO_6$	437.2777	438.2840$[M+H]^+$	438.2850	-2.28		420.2735,402.2646,388.2478,370.2372,356.2210,342.2067	Neoline[5]	FZ
34	6.36	$C_{24}H_{37}NO_5$	419.2672	420.2736$[M+H]^+$	420.2744	-1.90		402.2630,388.2469,370.2364,356.2224	14-Acetylkarakoline[7]	FZ
35	6.41	$C_{15}H_{14}O_6$	290.0790	289.0714$[M-H]^-$	289.0707	2.42	245.0823,137.0237,123.0444,109.0287		Catechin/Epicatechin[2]	GJ,DH
36	6.41	$C_{27}H_{30}O_{15}$	594.1585	893.1522$[M-H]^-$ 895.1642$[M+H]^+$	893.1501 895.1657	2.35 -2.52	503.1201,473.1080,383.0788, 353.0677,325.0738,297.0776	559.1443,439.1018,409.0912 379.0805,325.0704	Vicenin-2[10]	ZGC
37	6.46	$C_{27}H_{24}O_{18}$	636.0957	635.0910$[M-H]^-$	635.0879	4.88	465.0684,466.0709		1,2,6-tri-O-galloyglucose[8]	DH
38	6.56	$C_{20}H_{23}NO_4$	341.1627	342.1687$[M+H]^+$	342.1700	-3.80	311.1278,297.1113,279.1011		Fuzitine[5]	FZ

Table S1 (*continued*)

NO.	t_R (min)	Formula	MW (Da)	Detected *m/z*(+/-)	Expected	Error (ppm)	MS/MS		Identification	Source
							ESI$^-$	ESI$^+$		
39	6.64	$C_{44}H_{34}O_{20}$	882.1638	881.1579[M-H]$^-$	881.1560	2.16	729.1497,711.1364,559.1302, 407.0782,169.0140,125.0236		Procyanidin B 2-3, 3'-di-*O*-gallate/ Procyanidin B 5-3, 3'-di-O-gallate[8]	DH
40	6.76	$C_{21}H_{22}O_{10}$	434.1213	433.1145[M-H]$^-$	433.1129	3.70	271.0621,151.0031,119.0495		Naringenin-7-O-glucoside[10]	ZGC
41	6.81	$C_{24}H_{39}NO_5$	421.2828	422.2890[M+H]$^+$	422.2901	-2.61		390.2628,372.2543,358.236,344.2210,326.2101	Talatisamine[7]	FZ
42	6.84	$C_{20}H_{22}O_8$	390.1309	389.1244[M-H]$^-$	389.1231	3.34	227.0714,185.0607,183.0811,159.0810		Resveratrol-4'-*O*-*β*-*D*-glucopyranoside[8]	DH
43	6.89	$C_{14}H_{12}O_3$	228.0781	227.0710[M-H]$^-$	227.0703	3.08	185.0608,143.0479		3,5,4′-Trihydroxy-trans-stilbene[8]	DH
44	6.94	$C_{26}H_{28}O_{14}$	564.1479	563.1405[M-H]$^-$ 565.1539[M+H]$^+$	563.1395 565.1552	1.78 -2.30	473.1119,443.0993,383.0782, 353.0678,325.0731,297.0774	547.1432,529.1327,511.1223, 433.0915,409.0907,379.0801	Isoschaftoside[10]	ZGC
45	6.98	$C_{30}H_{26}O_{12}$	578.1419	577.1361[M-H]$^-$	577.1341	3.47	559.1289,451.1051,425.0894,407.0780,289.0725,287.0559, 245.0825,137.0236,125.0237		Procyanidin B[8]	DH
46	7.03	$C_{22}H_{22}O_{12}$	478.1106	477.1051[M-H]$^-$	477.1028	4.82	331.0676,313.0575,169.0138,163.0397,125.0236		2-O-p-coumaroyl-1-O-galloy-β-D-glucose[8]	DH
47	7.12	$C_{32}H_{40}O_{18}$	712.2215	711.2160[M-H]$^-$	711.2131	4.08	549.1614,255.0668,135.0081,119.0494		Glucoliquiritinapioside	ZGC
48	7.16	$C_9H_8O_3$	164.0473	163.0397[M-H]$^-$	163.0390	4.29	119.0494,93.0335		p-Coumaric acid[2]	GJ
49	7.35	$C_{10}H_{16}O$	152.1201	153.1271[M+H]$^+$	153.1274	-1.96		93.0341,65.0392	(*Z*)-citral[2]	GJ
50	7.45	$C_{27}H_{32}O_{14}$	580.1787	581.1849[M+H]$^+$	581.1865	-2.75		239.0697,147.0439	Liquiritigenin-7,4′-diglucoside	ZGC
51	7.49	$C_{26}H_{41}NO_7$	479.2878	480.2946[M+H]$^+$	480.2956	-2.08		462.2886,430.2768	14-O-Acetylneoline[5]	FZ
52	7.52	$C_{27}H_{30}O_{14}$	578.1636	579.1696[M+H]$^+$	579.1708	-2.07		561.1597,543.1486,525.1380, 423.1063,405.0957,379.0802	Isoviolanthin[10]	ZGC
53	7.52	$C_{42}H_{38}O_{20}$	862.1951	861.1912[M-H]$^-$	861.1873	4.53	817.2036,699.1372,655.1481,537.0844,386.1014,224.0480		Sennoside B[8]	DH
54	7.57	$C_{25}H_{41}NO_6$	451.2934	452.2997[M+H]$^+$	452.3007	-2.21		420.2732,402.2635,388.2468,370.2381,356.2213	Chasmanine[7]	FZ
55	7.59	$C_{21}H_{20}O_{10}$	432.1057	431.0994[M-H]$^-$	431.0973	4.87	311.0676,269.0465,239.0351, 223.0397,211.0390		Aloe-emodin-1-O-β-D-glucopyranoside[8] /Aloe-emodin-8-O-β-D-glucopyranoside[8]	DH
56	7.60	$C_{16}H_{12}O_5$	284.0679	285.0750[M+H]$^+$	285.0758	-2.81	270.0514,253.0486,225.0540		Prunetin[10]	ZGC

Table S1 (*continued*)

NO.	t_R (min)	Formula	MW (Da)	Detected *m/z*(+/-)	Expected	Error (ppm)	MS/MS		Identification	Source
							ESI$^-$	ESI$^+$		
57	7.66	$C_{21}H_{22}O_9$	418.1264	419.1323[M+H]$^+$ 417.1198[M-H]$^-$	419.1337 417.1180	-3.34 4.32	255.0607,135.0082,119.0494	257.0802,239.0697,137.0232	Isoliquiritin[10]	ZGC
58	7.69	$C_{44}H_{34}O_{20}$	882.1638	881.1597[M-H]$^-$	881.1560	4.20	729.1483,711.1392,559.1292, 407.0781,169.0138,125.0236		Procyanidin B 2-3,3'-di-*O*-gallate/Procyanidin B 5-3,3'- *O*-gallate[11]	DH
59	7.74	$C_{21}H_{18}O_{11}$	446.0844	445.0782[M-H]$^-$	445.0765	3.82	283.0255,269.0461,239.0354		Rhein-8-*O*-*β*-*D*-glucopyranoside[11]	DH
60	7.75	$C_{21}H_{22}O_{10}$	434.1213	433.1147[M-H]$^-$	433.1129	4.16	271.0620,151.0030,119.0494		Choerospodin[10]	ZGC
61	7.78	$C_{26}H_{30}O_{13}$	550.1686	549.1623[M-H]$^-$ 551.1743[M+H]$^+$	549.1603 551.1759	3.64 -2.90	417.1214,255.0668,135.0081, 119.0494	257.0803,239.0692,137.0232	Liquiritin apioside or Isoliquiritin apioside[10]	ZGC
62	7.82	$C_{21}H_{22}O_9$	418.1264	417.1197[M-H]$^-$	417.1180	4.08	255.0669,135.0180,119.0494		Liquiritin*	ZGC
63	7.86	$C_{42}H_{40}O_{19}$	848.2164	847.2107[M-H]$^-$	847.2080	3.19	803.2122,685.1588,667.1528,641.1688,479.1140,389.0887,386.0990		Sennoside C[11]	DH
64	7.87	$C_{23}H_{26}O_{11}$	478.1470	477.1407[M-H]$^-$	477.1391	3.35	313.0569,211.0245,169.0139,125.0237		Lindleyin or Isolindleyin[11]	DH
65	7.88	$C_{15}H_{12}O_4$	256.2534	255.0665[M-H]$^-$ 257.0801[M+H]$^+$	255.0652 257.0808	1.18 -2.72	213.0559,135.0082,119.0495	239.0696,211.0752,165.0702	Liquiritigenin[10]	ZGC
66	7.95	$C_{22}H_{18}O_{10}$	442.0894	441.0835[M-H]$^-$	441.0816	-1.36	331.0467,289.0725,271.0621,193.0143,169.0135		(Epi)catechin -3-*O*-gallate[11]	DH
67	8.09	$C_{42}H_{40}O_{19}$	848.2164	847.2118[M-H]$^-$	847.2080	4.49	803.2209,685.1591,667.1395,641.1707,386.1017		Sennoside D[11]	DH
68	8.10	$C_{26}H_{41}NO_6$	463.2928	464.2990[M+H]$^+$	464.3007	-3.66	432.2736,414.2629,400.2455,382.2355,372.2535		14-O-Acetyltalatizamine[7]	FZ
69	8.11	$C_{23}H_{26}O_{11}$	478.1470	477.1409[M-H]$^-$	477.1391	3.77	313.0576,211.0247,169.0139,125.0237		Lindleyin or Isolindleyin[12]	DH
70	8.16	$C_{27}H_{26}O_{12}$	542.1419	541.1366[M-H]$^-$	541.1341	4.62	313.0556,169.0138,125.0237		Resveratrol-4'-*O*-*β*-*D*-(2''-*O*-galloyl)-[illegible][12]	DH
71	8.22	$C_{15}H_{18}O_7$	310.1047	309.0980[M-H]$^-$	309.0969	3.56	147.0444,131.0498,103.0551		Cinnamoyl glucose[12]	DH
72	8.32	$C_{42}H_{38}O_{20}$	862.1951	861.1912[M-H]$^-$	861.1873	4.53	817.2048,699.1364,655.1516,537.0831,386.1015,224.04		Sennoside A[12]	DH
73	8.48	$C_{21}H_{20}O_9$	416.1102	415.1041[M-H]$^-$	415.1024	4.10	295.0622,267.0661,253.0512,225.05		Chrysophanol-1-*O*-*β*-D-glucopyranoside[12]	DH
74	8.58	$C_{23}H_{20}O_{12}$	488.0949	487.0889[M-H]$^-$	487.0871	3.70	283.0254,269.0467,239.0353,211.04		Rhein-1-O-(6'-O-acetyl)-glucoside[12]	DH

Table S1 (*continued*)

NO.	t_R (min)	Formula	MW (Da)	Detected *m/z*(+/-)	Expected	Error (ppm)	MS/MS ESI$^-$	Identification	Source
75	8.61	$C_{21}H_{20}O_{11}$	448.1000	447.0940[M-H]$^-$	447.0922	4.03	327.0500,285.0396,284.0316	kaempferol-7-O-β-D-glucopyranoside[12]	DH
76	8.70	$C_{21}H_{24}O_9$	420.1415	419.1349[M-H]$^-$	419.1337	2.86	401.1253,257.0823,239.0713	Isorhapontin[12]	DH
77	8.79	$C_{26}H_{30}O_{14}$	566.1636	565.1578[M-H]$^-$	565.1552	4.60	271.0619,227.0710,151.0031,119.0494	Naringenin-7-O-(2-β-D-apiofuranosyl)-β-D-glucopyranoside[10]	ZGC
78	8.86	$C_{23}H_{22}O_{11}$	474.1157	473.1098[M-H]$^-$	473.1078	4.23	413.0866,269.0464,239.0354, 223.0397,211.0401,195.0455	Aloe-emodin-8-*O*-(6'-*O*-acetyl)-glucopyranoside[12]	DH
79	8.93	$C_{21}H_{22}O_{10}$	434.1213	433.1149[M-H]$^-$	433.1129	4.62	271.0620,151.0031,119.0494	Chalconaringenin-4-O-glucoside[10]	ZGC
80	9.02	$C_{21}H_{20}O_{10}$	432.1057	431.0993[M-H]$^-$	431.0973	4.64	311.0568,269.0463,239.0349, 223.0393,211.0398	Aloe-emodin-1-O-β-D-glucopyranoside / Aloe-emodin-8-O-β-D-glucopyranoside[12]	DH
81	9.05	$C_{23}H_{24}O_{10}$	460.1364	459.1292[M-H]$^-$	459.1286	1.31	417.1207,255.0669,135.0082,119.0495	6"-O-acetylliquiritin[10]	ZGC
82	9.05	$C_{48}H_{82}O_{19}$	962.5445	961.5390[M-H]$^-$	961.5367	3.02	799.4871,637.4335,475.3799	Ginsenoside Re1[6]	RS
83	9.21	$C_{47}H_{80}O_{18}$	932.5345	931.5297[M-H]$^-$	931.5261	3.89	799.4847,637.4335,475.3802	Ginsenoside Re4[6]	RS
84	9.25	$C_{22}H_{22}O_{10}$	446.1207	445.1153[M-H]$^-$	445.1150	0.67	283.0617,325.0725	Physcion 8-*O*-*β*-*D*-glucopyranoside[12]	DH
85	9.27	$C_{26}H_{30}O_{13}$	550.1686	551.1746[M+H]$^+$	551.1759	-2.36	257.0803,137.0233	2'-O-[β-D-Apiofuranosyl-(1→2)-β-D-	ZGC
86	9.32	$C_{26}H_{30}O_{13}$	550.1686	549.1628[M-H]$^-$ 551.1746[M+H]$^+$	549.1603 551.1759	4.55 -2.36	417.1201,255.0669,135.0082, 119.0494	257.0804,239.0704, 137.0233	Liquiritin apioside / Isoliquiritin apioside[10]	ZGC
87	9.5	$C_{22}H_{22}O_{11}$	462.1157	461.1099[M-H]$^-$	461.1078	4.56	313.0575,169.0139,125.0237	1-*O*-Galloyl-6-*O*-cinnamoyl-*β*-*D*-glucopyranoside/1-O-Galloyl-2-O-cinnamoyl-β-D-	DH
88	9.51	$C_{26}H_{30}O_{13}$	550.1686	549.1623[M-H]$^-$ 551.1734[M+H]$^+$	549.1603 551.1759	3.64 -4.54	429.1045,417.1176,255.0669, 135.0082,119.0495	257.0804,137.0233	Licuraside[10]	ZGC
89	9.57	$C_{21}H_{22}O_9$	418.1264	417.1200[M-H]$^-$ 419.1327[M+H]$^+$	417.1180 419.1337	4.80 -2.39	255.0668,213.0558,135.0081, 119.0439	257.0803,239.0695,147.0439, 137.0232,119.0494	Neoisoliquiritin[10]	ZGC
90	9.57	$C_{31}H_{43}NO_{10}$	589.2881	590.2941[M+H]$^+$	590.2960	-3.22	572.2839,558.2693,540.2570,508.2319,476.2078,105.0338	Benzoylmesaconine[7]	FZ

Table S1 (*continued*)

NO.	t_R (min)	Formula	MW (Da)	Detected *m/z*(+/-)	Expected	Error (ppm)	MS/MS		Identification	Source
							ESI$^-$	ESI$^+$		
91	9.61	$C_{48}H_{82}O_{18}$	946.5501	945.5432[M-H]$^-$	945.5417	1.59	765.4805,637.4343,475.3809		Ginsenoside Re*	RS
92	9.61	$C_{21}H_{22}O_9$	418.1264	419.1325[M+H]$^+$ 417.1199[M-H]$^-$	419.1337 417.1180	-2.86 4.56	255.0668,135.0081,119.0493	257.0803,239.0694,137.0232	Neoliquiritin[10]	ZGC
93	9.85	$C_{35}H_{36}O_{15}$	696.2054	695.1999[M-H]$^-$	695.1970	4.12	549.1629,531.1525,255.0668,135.0082,119.0494		Licorice glycoside D1/D2[10]	ZGC
94	9.89	$C_{36}H_{38}O_{16}$	726.2160	725.2112[M-H]$^-$	725.2076	4.97	549.1629,531.1526,399.1091,255.0669,135.0082		Licorice glycoside C1/C2[10]	ZGC
95	9.91	$C_{44}H_{74}O_{15}$	842.5022	841.4980[M-H]$^-$	841.4944	4.28	637.4337,475.3810		Acetyl-ginsenoside Rg1[6]	RS
96	9.91	$C_{45}H_{74}O_{17}$	886.4921	885.4886[M-H]$^-$	885.4842	4.97	637.4315,475.3835	Malonyl-ginsenoside Rg1/Acetyl-ginsenoside Rg1[M+COOH]$^-$ [6]		RS
97	9.94	$C_{15}H_{10}O_4$	254.0574	299.0645[M+H]$^+$	255.0652	-2.75	237.0548,227.0698,209.0580,145.0284, 137.0234,119.0497,109.1013		7,4'-Dihydroxyflavne[10]	ZGC
98	9.98	$C_{16}H_{14}O_5$	286.0841	285.0776[M-H]$^-$ 287.0907[M+H]$^+$	285.0758 287.0914	2.22 -2.44	270.0526,177.0179, 150.0306	245.0804,193.0495, 121.0287	Licochalcone B[10]	ZGC
99	10.03	$C_{32}H_{45}NO_{10}$	603.3043	604.3108[M+H]$^+$	604.3116	-1.32	586.3002,572.2838,554.2739,540.2593,496.2328,105.0339		Benzoylaconitine[7]	FZ
100	10.24	$C_{15}H_{10}O_6$	286.0472	285.0402[M-H]$^-$	285.0394	2.81	255.0305,239.0325		ω-Hydroxyemodin	DH
101	10.24	$C_{45}H_{74}O_{17}$	886.4921	885.4871[M-H]$^-$	885.4842	3.28	637.4315,475.3788		Malonyl-ginsenoside Rf[6]	RS
102	10.28	$C_{44}H_{74}O_{15}$	842.5022	841.4983[M-H]$^-$	841.4944	4.64	799.4892,637.4333,475.3790		Yesanchinoside D[13]	RS
103	10.31	$C_{31}H_{43}NO_9$	573.2932	574.2997[M+H]$^+$	574.3011	-2.44	542.2737,524.2643,510.2477,478.2232,105.0338		Benzoylhypaconine[14]	FZ
104	10.39	$C_{15}H_{12}O_4$	256.2534	257.0801[M+H]$^+$	257.0808	-2.72		239.0700,211.0751,165.0699, 137.0233	Isoliquiritigenin[10]	ZGC
105	10.65	$C_{35}H_{35}NO_{14}$	693.2058	692.2007[M-H]$^-$	692.1974	4.78	255.0668,135.0081,119.0495		Licorice glycoside E[10]	ZGC
106	10.66	$C_{21}H_{20}O_9$	416.1102	415.1047[M-H]$^-$	415.1024	1.20	295.0633,267.0660,253.0512,225.0560		Chrysophanol-8-*O*-*β*-D-glucopyranoside[12]	DH
107	10.67	$C_{20}H_{24}O_9$	408.1414	407.1350[M-H]$^-$	407.1337	3.19	245.0824,230.0586,215.0352,187.0389,159.0446		Torachrysone-8-*O*-*β*-*D*-glucopyranoside[12]	DH

Table S1 (*continued*)

NO.	t_R (min)	Formula	MW (Da)	Detected *m/z*(+/-)	Expected	Error (ppm)	MS/MS ESI$^-$	MS/MS ESI$^+$	Identification	Source
108	10.70	$C_{22}H_{22}O_9$	430.1264	431.1324[M+H]$^+$	431.1337	-3.02		269.0779,254.0574,237.0519	Ononin[10]	ZGC
109	10.70	$C_{22}H_{22}O_{11}$	462.1157	461.1091[M-H]$^-$	461.1078	2.82	401.0918,313.0575,211.0251, 193.0148,169.0140	1-*O*-Galloyl-6-*O*-cinnamoyl-*β*-*D*-glucopyranoside/1-O-Galloyl-2-O-cinnamoyl-β-D-glucopyranoside[12]		DH
110	10.73	$C_{16}H_{12}O_4$	268.0736	267.0661[M-H]$^-$ 269.0800[M+H]$^+$	267.0652 269.0808	3.37 -2.97	252.0432,223.0402,208.0538, 195.0455,135.0081,132.0209	254.0565,237.0541,226.0621,213.0908, 181.0649,137.0233	Formononetin /Isoformononeti	ZGC
111	10.74	$C_{48}H_{72}O_{22}$	1000.4515	999.4476[M-H]$^-$ 1001.4561[M+H]$^+$	999.4431 1001.4588	4.50 -2.70	837.3940,351.0576,193.0354, 113.0237	487.3410,469.3306,451.3193,439.3192	24-Hydroxy-licorice saponin	ZGC
112	10.75	$C_{35}H_{36}O_{15}$	696.2054	695.2001[M-H]$^-$	695.1970	4.46	549.1630,531.1523,255.0670,135.0081,119.0494		Licorice glycoside D1/D2[10]	ZGC
113	10.75	$C_{36}H_{38}O_{16}$	726.2160	725.2110[M-H]$^-$	725.2076	4.69	549.1631,531.1525,399.1098,255.0669,135.0081,119.0494		Licorice glycoside C1/C2[10]	ZGC
114	10.79	$C_{33}H_{45}NO_{12}$	647.2936	648.3001[M+H]$^+$	648.3015	-2.16	630.2943,616.2699,598.2641,588.2786,556.2535,538.2420,506.2179		Beiwutine[7]	FZ
115	10.80	$C_{15}H_8O_7$	300.0265	299.0193[M-H]$^-$	299.0186	2.34	255.0305,239.3029		Emodic acid[12]	DH
116	10.82	$C_{36}H_{38}O_{16}$	726.2160	725.2104[M-H]$^-$	725.2076	3.86	549.1624,531.1521,399.1127,255.0668,135.0082,119.0494		Licorice glycoside A[10]	ZGC
117	10.83	$C_{35}H_{36}O_{15}$	696.2054	695.2002[M-H]$^-$	695.1970	4.60	549.1628,531.1527,255.0669,135.0082,119.0495		Licorice glycoside B[10]	ZGC
118	10.83	$C_{48}H_{74}O_{19}$	954.4824	953.4773[M-H]$^-$	953.4740	3.46	351.0576,193.0355,175.0250,113.0236		Licorice saponin M3[10]	ZGC
119	10.87	$C_{21}H_{20}O_{10}$	432.1057	431.0993[M-H]$^-$	431.0973	4.64	311.0579,269.0464,241.0507, 225.0559,213.0553,197.0607	Emodin-1-O-β-D-glucopyranoside/ Emodin-8-O-β-D-glucopyranoside[12]		DH
120	10.92	$C_{21}H_{20}O_{10}$	432.1057	431.0988[M-H]$^-$	431.0973	3.48	311.0566,269.0464,241.0487,225.0559, 213.0547,197.0612	Emodin-1-O-β-D-glucopyranoside / Emodin-8-O-β-D-glucopyranoside[12]		DH
121	10.98	$C_{44}H_{64}O_{19}$	896.4042	895.3997[M-H]$^-$ 897.4100[M+H]$^+$	895.3958 897.4115	4.36 -1.67	351.0558,193.0342, 175.0232,113.0228	545.3433,527.3336,509.3240, 467.3145,449.3026	22β-Acetoxylicoricesaponin G2[15]	ZGC
122	10.98	$C_{44}H_{64}O_{19}$	896.4041	895.3997[M-H]$^-$ 897.4100[M+H]$^+$	895.3958 897.4115	4.36 -1.67	659.3447,351.0579	545.3461,527.3357,497.3257	Uralsaponin F[15]	ZGC
123	10.69	$C_{15}H_{10}O_4$	254.0574	253.0501[M-H]$^-$	253.0495	2.37	225.0558,210.0322		Chrysophanol[12]	DH

Table S1 (*continued*)

NO.	t_R (min)	Formula	MW (Da)	Detected *m/z*(+/-)	Expected	Error (ppm)	MS/MS		Identification	Source
							ESI$^-$	ESI$^+$		
124	11.13	$C_{42}H_{62}O_{18}$	854.3936	853.3855[M-H]$^-$ 855.4019[M+H]$^+$	853.3852 855.4009	0.32 1.17	677.3553,501.3225,351.0577, 193.0355,113.0236	503.3356,485.3251,467.3148	22-Hydroxylicorice saponin G2[15]	ZGC
125	11.13	$C_{30}H_{44}O_5$	484.3183	485.3255[M+H]+	485.3262	-1.44	409.3136,315.1994,261.1479,187.1483,173.1326		24-	ZGC
126	11.26	$C_{29}H_{26}O_{15}$	614.1266	613.1213[M-H]$^-$	613.1188	4.08	569.1310,461.1111,443.0991		Cinnamoyl-O-digalloyl-glucose[16]	DH
127	11.31	$C_{48}H_{72}O_{21}$	984.4566	983.4525[M-H]$^-$ 985.4620[M+H]$^+$	983.4482 985.4639	4.37 -1.92	821.3976,803.3820, 645.3718,469.3368	615.3876,471.3462,453.3356	Licorice saponin A3[15]	ZGC
128	11.39	$C_{16}H_{10}O_7$	314.0427	313.0344[M-H]$^-$	313.0343	0.32	269.0464,197.0606		Laccaic acid D[16]	DH
129	11.49	$C_{28}H_{24}O_{13}$	568.1211	567.1161[M-H]$^-$	567.1133	4.94	313.0576,271.0470		Chrysophanol-*O*-galloyl-*O*-glucose[16]	DH
130	11.50	$C_{33}H_{45}NO$	631.2987	632.3054[M+H]$^+$	632.3065	-1.74	572.2842,540.2588,512.2623,496.2309,390.2269,105.0339		Mesaconitine[14]	FZ
131	11.52	$C_{16}H_{14}O_4$	270.0892	271.0957[M+H]$^+$	271.0965	-2.95		253.0489,229.0855,177.0546, 123.0443,121.0287	Echinatin[15]	ZGC
132	11.66	$C_{44}H_{64}O_{18}$	880.4093	879.4036[M-H]$^-$	879.4009	3.07	351.0577,193.0358,175.0242,113.0236		22β-Acetoxyglycyrrhizin[15]	ZGC
133	11.69	$C_{42}H_{72}O_{14}$	800.4922	799.4869[M-H]$^-$	799.4838	3.88	637.4338,475.3799		Ginsenoside Rg1/Ginsenoside Rf[13]	RS
134	11.78	$C_{42}H_{72}O_{14}$	800.4922	799.4876[M-H]$^-$	799.4838	4.76	637.4347,475.3801		Ginsenoside Rg1/Ginsenoside Rf[13]	RS
135	11.79	$C_{58}H_{98}O_{26}$	1210.634	1209.6306[M-H]$^-$	1209.626	3.56	1077.5878,945.5449,783.4905,621.4406,459.3844		Ginsenoside Ra1[13]	RS
136	11.86	$C_{16}H_{12}O_5$	284.0685	285.0748[M+H]$^+$	285.0758	-3.51		270.0515,253.0484,242.0569, 229.0854,225.0541,137.0234	Calycosin[15]	ZGC
137	11.92	$C_{54}H_{92}O_{23}$	1108.6029	1107.5977[M-H]$^-$	1107.5946	2.80	945.5433,783.4944,621.4376,459.3845		Ginsenoside Rb1*	RS
138	11.92	$C_{30}H_{44}O_4$	468.3234	469.3300[M+H]$^+$	469.3312	-2.56	451.3196,285.1864,261.1485,237.1461,233.1531		Glabrolide[15]	ZGC
139	11.93	$C_{16}H_{12}O_5$	284.0685	283.0611[M-H]$^-$	283.0623	-4.24	268.0319,240.0431,212.0478		Physcion[16]	DH
140	11.95	$C_{61}H_{100}O_{29}$	1296.6345	1295.6304[M-H]$^-$	1295.6267	2.86	1209.6298,1077.5853,945.5468, 783.4932,621.4357,459.3863		Malonyl-ginsenoside Ra1/ Malonyl-ginsenoside Ra2[13]	RS

Table S1 (*continued*)

NO.	t_R (min)	Formula	MW (Da)	Detected *m/z*(+/-)	Expected	Error (ppm)	MS/MS		Identification	Source
							ESI$^-$	ESI$^+$		
141	12.00	$C_{41}H_{70}O_{13}$	770.4811	769.4761[M-H]$^-$	769.4733	3.64	637.4340,475.3803		Notoginsenoside	RS
142	12.04	$C_{57}H_{94}O_{26}$	1194.6028	1193.6008[M-H]$^-$	1193.5950	4.86	1107.5988,945.5446,783.4938,621.4384,459.3856		Malonyl-ginsenoside Rb1/Quinquenoside	RS
143	12.05	$C_{56}H_{94}O_{24}$	1150.6130	1149.6095[M-H]$^-$	1149.6051	3.83	1107.5985,945.5456,783.4929,621.4385,459.3850		Quinquenoside R1[13]	RS
144	12.15	$C_{58}H_{98}O_{26}$	1210.6341	1209.6298[M-H]$^-$	1209.6263	2.89	1077.5864,945.5434,783.4925,621.4410,459.3859		Ginsenoside Ra2[13]	RS
145	12.23	$C_{33}H_{45}NO_{10}$	615.3043	616.3091[M+H]$^+$	616.3116	-1.57	584.2834,556.2892,524.2432,496.2744,105.0338		Hypaconitine[17]	FZ
146	12.23	$C_{53}H_{90}O_{22}$	1078.5924	1077.5884[M-H]$^-$	1077.5840	4.09	945.5457,783.4927,621.4385,459.3861		Ginsenoside Rc /Rb2 / Rb3[13]	RS
147	12.27	$C_{10}H_{10}O_3$	178.0630	179.0698[M+H]$^+$	179.0702	-2.23	161.0602,147.0439,119.0494,55.0181		Coniferaldehyde	GJ
148	12.27	$C_{61}H_{100}O_{29}$	1296.6345	1295.6321[M-H]$^-$	1295.6267	4.17	1209.6303,1077.5865,945.5455, 783.4958,621.4397,459.3870		Malonyl-ginsenoside Ra1/ Malonyl-ginsenoside Ra2[13]	RS
149	12.29	$C_{34}H_{47}NO_{11}$	645.3146	646.3201[M+H]$^+$	646.3222	-3.25	586.2996,554.2744,526.2791,522.2488,404.2410,105.0338		Aconitine[17]	FZ
150	12.29	$C_{60}H_{100}O_{27}$	1252.6446	1251.6412[M-H]$^-$	1251.6368	3.52	1209.6202,1077.5837,945.5429,783.4920,621.4395,459.3865		Ginsenoside Ra5[18]	RS
151	12.3	$C_{55}H_{92}O_{23}$	1120.6029	1119.5991[M-H]$^-$	1119.5946	4.02	1077.5806,945.5352,783.4962,621.4344,459.3892		Ginsenoside Rs2[18]	RS
152	12.31	$C_{42}H_{72}O_{13}$	784.4973	783.4919[M-H]$^-$	783.4889	3.83	637.4345,475.3805		Ginsenoside Rg2[18]	RS
153	12.36	$C_{56}H_{92}O_{25}$	1164.5922	1163.5895[M-H]$^-$	1163.5844	4.39	1077.5883,945.5498,783.4932,621.4417,459.3850		Malonyl-ginsenoside Rc[18]	RS
154	12.42	$C_{53}H_{90}O_{22}$	1078.5924	1077.5874[M-H]$^-$	1077.5840	3.16	945.5457,783.4922,621.4415,459.3838		Ginsenoside Rc / Rb2 /Rb3[18]	RS
155	12.51	$C_{53}H_{90}O_{22}$	1078.5924	1077.5873[M-H]$^-$	1077.5840	3.06	945.5443,783.4905,621.4412,459.3858		Ginsenoside Rc / Rb2 /Rb3[18]	RS
156	12.56	$C_{56}H_{92}O_{25}$	1164.5922	1163.5900[M-H]$^-$	1163.5844	4.82	1077.5878,945.5460,783.4984,621.4395,459.3837		Malonyl-ginsenoside Rb2[18]	RS
157	12.59	$C_{48}H_{76}O_{19}$	956.4975	955.4941[M-H]$^-$	955.4897	4.61	793.4373,731.4409,613.3781,569.3878,455.3558		Ginsenoside Ro[18]	RS
158	12.67	$C_{42}H_{62}O_{17}$	838.3987	839.4044[M+H]$^+$	839.4060	-1.91		663.3789,487.3405, 469.3304,451.3200	Licorice saponin G2/ Isolicorice saponin[15]	ZGC

Table S1 (*continued*)

NO.	t_R (min)	Formula	MW (Da)	Detected *m/z*(+/-)	Expected	Error (ppm)	MS/MS		Identification	Source
							ESI$^-$	ESI$^+$		
159	12.74	$C_{42}H_{60}O_{16}$	820.3876	819.3837[M-H]$^-$	819.3798	4.76	643.3491,351.0576,193.0356,113.0236		Licorice saponin E2[15]	ZGC
160	12.77	$C_{44}H_{66}O_{18}$	882.4249	881.4202[M-H]$^-$	881.4165	4.20	351.0580,193.0355,175.0247,113.0236		22β-Acetoxy licorice[15]	ZGC
161	12.81	$C_{47}H_{74}O_{18}$	926.4870	925.4838[M-H]$^-$	925.4792	4.97	613.3762,569.3862		Chikusetsusaponin IV[18]	RS
162	12.82	$C_{48}H_{72}O_{20}$	968.4617	967.4583[M-H]$^-$	967.4575	0.83	497.1156,339.0949,321.0838		Yunganoside J1/L1[15]	ZGC
163	12.92	$C_{56}H_{92}O_{25}$	1164.592	1163.5900[M-	1163.584	4.82	1077.5879,945.5488,783.4902,621.4374,459.3850		Malonyl-ginsenoside[18]	RS
164	12.97	$C_{16}H_{12}O_4$	268.0736	269.0803[M+H]$^+$	269.0808	-1.86		254.0564,237.0542,226.062, 213.0908,181.0616,137.0234	Formononetin or Isoformononetin[15]	ZGC
165	13.04	$C_{48}H_{82}O_{18}$	946.5501	945.5440[M-H]$^-$	945.5417	2.43	783.4935,621.4406,459.3864		Ginsenoside Rd[18]	RS
166	13.12	$C_{16}H_{16}O_4$	272.1043	273.1110[M+H]$^+$	273.1121	-4.03		163.0752,148.0521,137.0597,123.0443	Vestitol[15]	ZGC
167	13.14	$C_{42}H_{64}O_{17}$	840.4144	839.4101[M-H]$^-$	839.4060	4.89	351.0579,193.0358,175.0246,113.0236		Yunganoside G2[15]	ZGC
168	13.14	$C_{42}H_{66}O_{14}$	794.4447	793.4405[M-H]$^-$	793.4369	4.54	631.3832,569.3848,455.3564		Zingibroside R1[18]	RS,GJ
169	13.15	$C_{34}H_{47}NO_{10}$	629.3194	630.3262[M+H]$^+$	630.3272	-1.59	598.3008,570.3047,538.2792,510.2877,478.2614,416.2430		Deoxyaconitine[17]	FZ
170	13.18	$C_{51}H_{84}O_{21}$	1032.5491	1031.5470[M-H]$^-$	1031.5421	4.75	945.5458,783.4910,621.4408,459.3864		Malonyl-ginsenoside Rd/Acetyl-ginsenoside[M+COOH]$^-$ [19]	RS
171	13.19	$C_{50}H_{84}O_{19}$	988.5601	987.5572[M-H]$^-$	987.5523	4.96	945.5456,783.4932,621.4384,459.3857		Acetyl-ginsenoside[19]	RS
172	13.30	$C_{42}H_{62}O_{16}$	822.4038	821.3987[M-H]$^-$	821.3954	4.02	627.3561,469.3340,351.0577,	647.3771,471.3453,453.3355	Glycyrrhizic acid*	ZGC
				823.4088[M+H]$^+$	823.4111	-2.79	193.0355.113.0236			
173	13.33	$C_{42}H_{62}O_{17}$	838.3987	837.3918[M-H]$^-$	837.3903	1.79	661.3646,351.0576,	663.3759,487.3412,469.3305	Licorice saponiG2/ Isolicorice saponin G2[15]	ZGC
				839.4039[M+H]$^+$	839.4060	-2.50	193.0356,113.0236	,451.3201,439.3207		
174	13.33	$C_{42}H_{62}O_{16}$	822.4038	821.3994[M-H]$^-$	821.3954	4.87	627.3561,469.3340,351.0577,193.0355,175.0264,113.0236		Licorice saponin H2[15]	ZGC
175	13.34	$C_{30}H_{44}O_4$	468.3234	469.3296[M+H]$^+$	469.3312	-3.41	423.3243,313.2171,299.2001,235.1689,217.1582		3-Oxoglycyrrhetinic acid[15]	ZGC
176	13.47	$C_{16}H_{10}O_6$	298.0472	297.0408[M-H]$^-$	297.0394	4.71	253.0512,225.0557		6-methyl-rhein[16]	DH

Table S1 (*continued*)

NO.	t_R (min)	Formula	MW (Da)	Detected *m/z*(+/-)	Expected	Error (ppm)	MS/MS		Identification	Source
							ESI$^-$	ESI$^+$		
177	13.49	$C_{42}H_{62}O_{16}$	822.4038	821.3994[M-H]$^-$	821.3954	4.87	627.3468,469.3340,351.0574,193.0353,175.0249,113.0236		Licorice saponin	ZGC
178	13.85	$C_{21}H_{20}O_6$	368.1260	367.1194[M-H]$^-$	367.1176	4.90	309.0414,281.0464,269.0455		Gancaonin N[20]	ZGC
179	13.87	$C_{48}H_{72}O_{20}$	968.4617	967.4581[M-H]$^-$	967.4575	0.62	497.1163,339.0945,321.0838		Yunganoside	ZGC
180	14.01	$C_{48}H_{76}O_{19}$	956.4981	955.4923[M-H]$^-$	955.4897	2.72	497.1154,339.0956,321.0836		Yunganoside A1/B1/C1[20]	ZGC
181	14.09	$C_{48}H_{76}O_{19}$	956.4981	955.4921[M-H]$^-$	955.4897	2.51	497.1158,339.0925,321.0831		Yunganoside A1/B1/C1[20]	ZGC
182	14.14	$C_{42}H_{62}O_{16}$	822.4038	823.4099[M+H]$^+$	823.4111	-1.46		647.3782,453.3352	Uralsaponin A[20]	ZGC
183	14.23	$C_{16}H_{14}O_4$	270.0892	271.0960[M+H]$^+$	271.0965	-1.85	213.0537,161.0596,147.0439,137.0597,123.0443		Medicarpin[20]	ZGC
184	14.26	$C_{15}H_8O_6$	284.0321	283.0245[M-H]$^-$	283.0237	2.83	255.0305,257.0416,239.0353,227.0356,211.0404		Rhein*	DH
185	14.27	$C_{21}H_{20}O_5$	352.1305	353.1378[M+H]$^+$	353.1384	-1.70	321.1111,283.0588,267.0645,199.0754,181.0646		Gancaonin M[20]	ZGC
186	14.35	$C_{21}H_{20}O_5$	352.1305	353.1377[M+H]$^+$	353.1384	-1.98	323.0919,297.0752,282.0519,267.0645,181.0646		Gancaonin A[20]	ZGC
187	14.38	$C_{42}H_{64}O_{16}$	824.4194	823.4152[M-H]$^-$ 825.4255[M+H]$^+$	823.4111 825.4267	4.98 -1.45	471.3495,351.0577, 193.0354	455.3505,437.3399,315.2 314,301.2158,287.1995	Licorice saponin J2 or its isomer[20]	ZGC
188	14.53	$C_{17}H_{26}O_4$	294.1831	293.1753[M-H]$^-$	293.1747	-2.05	193.0508,99.0806,57.0334		6-Gingerol*	GJ
189	14.67	$C_{15}H_{12}O_4$	256.0736	257.0805[M+H]$^+$	257.0808	-1.17	213.0561,151.0031	153.0182,131.0493,103.0548	Pinocembrin[20]	GJ,ZGC
190	14.84	$C_{42}H_{62}O_{15}$	806.4088	805.4036[M-H]$^-$	805.4005	3.85	351.0573,193.0355,175.0238		Licorice saponin C2 or its isomer[20]	ZGC
191	14.99	$C_{20}H_{18}O_6$	354.1103	355.1168[M+H]$^+$	355.1176	-2.25		299.0544,165.0181	Gancaonin L[20]	ZGC
192	15	$C_{42}H_{64}O_{15}$	808.4245	807.4171[M-H]$^-$	807.4205	-4.21	631.3821,351.0580,193.0353,113.0236		Licorice saponin B2[20]	ZGC

Table S1 (*continued*)

NO.	t_R (min)	Formula	MW (Da)	Detected *m/z*(+/-)	Expected	Error (ppm)	MS/MS		Identification	Source
							ESI$^-$	ESI$^+$		
193	15.15	$C_{21}H_{20}O_6$	368.1260	367.1194[M-H]$^-$ 369.1325[M+H]$^+$	367.1176 369.1333	4.90 -2.17	337.0723,324.1021,309.0414,2	313.0697,285.0751 97.0412,281.0460,173.0237,16	Glycycoumarin[20]	ZGC
194	15.4	$C_{48}H_{76}O_{19}$	956.4981	955.4943[M-H]$^-$	955.4897	4.82	497.1154,339.0933,321.0837		Yunganoside A1/B1/C1[20]	ZGC
195	15.45	$C_{21}H_{24}O_5$	356.1624	357.1688[M+H]$^+$	357.1697	-2.52		301.1065,165.0545,137.0597, 123.0443	Glyasperin C[20]	ZGC
196	15.47	$C_{20}H_{18}O_6$	354.1103	355.1170[M+H]$^+$	355.1176	-1.69		299.0547,281.0438,243.0655,165.0182	Gancaonin C[20]	ZGC
197	15.56	$C_{42}H_{66}O_{14}$	794.4447	793.4400[M-H]$^-$	793.4369	3.91	613.3773,569.3842,455.3530		ChikusetsusaponinIva[19]	RS
198	15.66	$C_{20}H_{18}O_6$	354.1103	355.1171[M+H]$^+$	355.1176	-1.41		299.0544,269.0441,243.0649,231.0651	Licoflavonol	ZGC
199	15.66	$C_{42}H_{64}O_{16}$	824.4194	825.4258[M+H]$^+$	825.4267	-1.09		455.3511,437.3399, 315.2320,301.2169	Licorice saponin J2 or its isomer[20]	ZGC
200	15.83	$C_{36}H_{54}O_{10}$	646.3717	647.3781[M+H]$^+$	647.3790	-1.39		471.3474,453.3353, 435.3239,407.3304	18β-Glycyrrhetinic acid-3-O-β-D-glucuronide[20]	ZGC
201	16	$C_{20}H_{18}O_6$	354.1103	355.1169[M+H]$^+$	355.1176	-1.97		299.0543,281.0440,245.0440,153.0181	Gancaonin O[20]	ZGC
202	16.04	$C_{20}H_{18}O_6$	354.1103	353.1036[M-H]$^-$ 355.1169[M+H]$^+$	353.1020 355.1176	4.53 -1.97	298.0472,285.1140,284.0334, 267.1036,266.0580,201.0923	337.1062,299.0545,201.0909	Licoisoflavone A[20]	ZGC
203	16.08	$C_{21}H_{22}O_4$	338.1518	339.1584[M+H]$^+$	339.1591	-2.06		297.1479,271.0959,121.0287	Licochalcone A[20]	ZGC
204	16.08	$C_{42}H_{72}O_{13}$	784.4973	783.4912[M-H]$^-$	783.4889	2.94	621.4396,459.3815		Ginsenoside Rg3[19]	RS
205	16.15	$C_{42}H_{62}O_{15}$	806.4088	805.4032[M-H]$^-$	805.4005	3.35	351.0579,193.0356,175.0249,113.0237		Licorice-Saponin C2 or its isomer[20]	ZGC
206	16.20	$C_{22}H_{22}O_6$	382.1416	381.1351[M-H]$^-$	381.1333	4.72	351.0884,323.0564,308.0333,201.0197		Licoricone[20]	ZGC
207	16.20	$C_{44}H_{74}O_{14}$	826.5073	825.5041[M-H]$^-$	825.4995	2.30	783.4927,621.4399,459.3858		Acetyl-ginsenoside Rg3[19]	RS

Table S1 (*continued*)

NO.	t_R (min)	Formula	MW (Da)	Detected *m/z*(+/-)	Expected	Error (ppm)	MS/MS		Identification	Source
							ESI^-	ESI^+		
208	16.24	$C_{20}H_{18}O_6$	354.1103	355.1169[M+H]$^+$	355.1176	-1.97		299.0541,229.0856,215.0696,153.0544	Isolicoflavonol[21]	ZGC
209	16.35	$C_{21}H_{18}O_6$	366.1103	365.1036[M-H]$^-$	365.1020	4.38	335.0575,307.0256,295.0253,282.0178,267.0304		Glycyrol[21]	ZGC
210	16.74	$C_{15}H_{10}O_5$	270.0528	269.0453[M-H]$^-$	269.0444	3.35	241.0510,225.0559,213.0553,197.0609,185.0608		Emodin*	DH
211	16.93	$C_{20}H_{16}O_5$	336.0998	337.1064[M+H]$^+$	337.1070	-1.78		295.0598,283.0594,137.0234	Glabrone[21]	ZGC
212	17.04	$C_{20}H_{20}O_4$	324.1362	325.1429[M+H]$^+$	325.1434	-1.54		189.0911,149.0597,123.0443	Glabridin[21]	ZGC
213	17.21	$C_{20}H_{18}O_6$	354.1103	355.1164[M+H]$^+$	355.1176	-3.38		299.0554,243.0650,215.0699	Uralenin[21]	ZGC
214	17.57	$C_{20}H_{16}O_6$	352.0947	351.0874[M-H]$^-$ 353.1014[M+H]$^+$	351.0863 353.1020	3.13 -1.70	336.0652,335.0578,283.0984,265.0877,241.0871, 199.0764,175.0339,151.0031	311.0546	Licoisoflavone B[21]	ZGC
215	17.76	$C_{17}H_{24}O_3$	276.1725	277.1794[M+H]$^+$	277.1798	-1.44		137.0596,122.0364,94.0417	6-Shogaol*	GJ
216	17.87	$C_{25}H_{28}O_4$	392.1988	393.2054[M+H]$^+$	393.2060	-1.53		337.1427,205.0861,149.0233	Glabrol[2]	ZGC
217	18.13	$C_{25}H_{28}O_5$	408.1937	409.2004[M+H]$^+$	409.2010	-1.47		353.1375,297.0752,279.0645, 205.0859,189.0910,175.0388	Glyinflanin A[1,21]	ZGC
218	18.34	$C_{26}H_{32}O_5$	424.2244	425.2305[M+H]$^+$	425.2322	-4.00		313.0701,221.1158,177.0548,135.0441	Licoricidin[21]	ZGC
219	18.35	$C_{25}H_{28}O_6$	424.1886	423.1823[M-H]$^-$ 425.1952[M+H]$^+$	423.1802 425.1959	4.96 -1.65	229.0872,193.0872	369.1321,313.0701, 175.0390,139.0388	Gancaonin E[21]	ZGC
220	18.37	$C_{44}H_{72}O_{13}$	808.4973	807.4921[M-H]$^-$	807.4889	3.66	765.4818,603.4274		Ginsenoside Rs4[19]	RS
221	18.61	$C_{30}H_{22}O_8$	510.1309	509.1235[M-H]$^-$	509.1231	0.79	254.0591,225.0554		Palmidin A[16]	DH
222	18.79	$C_{25}H_{26}O_6$	422.1724	423.1797[M+H]$^+$	423.1802	-1.18		367.1168,311.0544,299.0594	Isoangustone A[21]	ZGC

Table S1 (*continued*)

NO.	t_R (min)	Formula	MW (Da)	Detected *m/z*(+/-)	Expected	Error (ppm)	MS/MS		Identification	Source
							ESI^-	ESI^+		
223	19.16	$C_{30}H_{46}O_4$	470.3396	471.3462[M+H]$^+$ 469.3332[M-H]$^-$	471.3469 469.3312	-1.49 4.26	425.3441,355.2646	453.3357,425.3403,407.3316, 235.1688,189.1641	18-β-Glycyrrhetinic acid*	ZGC
224	19.24	$C_{21}H_{20}O_5$	352.1305	353.1376[M+H]$^+$	353.1384	-2.67		297.0757,267.0647,165.0700	Gancaonin G[21]	ZGC
225	19.53	$C_{19}H_{28}O_3$	304.4238	305.2105[M+H]$^+$	305.2111	-1.96		137.0597,122.0366,94.0417	8-Shogaol[9]	GJ
226	19.60	$C_{30}H_{22}O_7$	494.1360	493.1301[M-H]$^-$	493.1282	4.06	254.0591,225.0559		Palmidin B[16]	DH
227	20.84	$C_{21}H_{32}O_3$	332.2351	333.2417[M+H]$^+$	333.2424	-2.10	137.0596,122.0365,94.0416		10-Shogaol[9]	GJ

FZ:*Radix Aconiti Lateralis Preparata*;DH:*Radix et Rhizoma Rhei*;GJ:*Zingiber offcinale Rosc*;RS:*Ginseng Radix Et Rhizoma*;ZGC: *Glycyrrhizae radix et rhizome Praeparata Cum Melle*

* :Compared with reference standards

Glc: Glucosyl; GluA: Glucuronic acid residue; Rha: Rhamnosyl; Api: Apiosyl；Cin: Cinnamoyl

AC:Acetyl;Ph:Phenol;Coum: Coumaroyl;Fer: feruloyl;Xyl:Xylose;Ara:Arabinose.

Supplementary Table S2 Identification of prototype components in rat plasma after oral administration of WPT.

NO.	Name	t_R (min)	Detected *m/z*(+/-)	Expected	Error (ppm)	MS/MS		Formula	Identification	Source
						ESI^-	ESI^+			
3	P1	0.98	175.1189[M+H]$^+$	175.1190	-0.51		158.0925,116.0711,70.0658	$C_6H_{14}N_4O_2$	Arginine	GJ,RS
5	P2	1.10	191.0193[M-H]$^-$	191.0186	3.66	111.0079,87.0077,85.0284		$C_6H_8O_7$	Citric acid	GJ,ZGC,RS
7	P3	1.17	182.0809[M+H]$^+$	182.0812	-1.65		165.0548,147.0441,136.0758, 123.0444,91.0550	$C_9H_{11}NO_3$	Tyrosine	GJ,RS
10	P4	1.35	132.1018[M+H]$^+$	132.1019	-0.08		86.0971,69.0706	$C_6H_{13}NO_2$	Leucine	GJ,RS
13	P5	1.66	394.2586[M+H]$^+$	394.2588	-0.51		376.2477	$C_{22}H_{35}NO_5$	Karacolidine	FZ
14	P6	1.88	220.1178[M+H]$^+$	220.1175	1.36		202.1076,184.0971,90.0557	$C_9H_{17}NO_5$	Pantothenic acid	GJ
15	P7	1.97	166.0860[M+H]$^+$	166.0862	-1.20		149.0596,120.0812,103.0547	$C_9H_{11}NO_2$	Phenylalanine	GJ,RS
17	P8	3.62	205.0968[M+H]$^+$	205.0971	-1.46		188.0709,144.0809,118.0655	$C_{11}H_{12}N_2O_2$	Tryptophan	GJ
33	P9	6.32	438.2852[M+H]$^+$	438.2850	0.46		420.2757,388.2473,356.2233	$C_{24}H_{39}NO_6$	Neoline	FZ
41	P10	6.94	422.2901[M+H]$^+$	422.2901	0.00		390.2628,372.2533	$C_{24}H_{39}NO_5$	Talatisamine	FZ
48	P11	7.14	163.0393[M-H]$^-$	163.0390	1.80	119.0493,93.0335		$C_9H_8O_3$	p-Coumaric acid	GJ
56	P12	7.58	285.0750[M+H]$^+$	285.0758	2.81		270.0515,253.0500,225.0542	$C_{16}H_{12}O_5$	Prunetin	ZGC
59	P13	7.70	445.0789[M-H]$^-$	445.0765	5.39	269.0463,239.0347		$C_{21}H_{18}O_{11}$	Rhein-8-*O*-*β*-*D*-glucopyranoside	DH
61	P14	7.79	549.1633[M-H]$^-$	549.1603	5.46	255.0671,135.0075,119.0491		$C_{26}H_{30}O_{13}$	Liquiritin apioside or Isoliquiritin apioside	ZGC
62	P15	7.81	417.1203[M-H]$^-$	417.1180	5.52	255.0668,135.0081,119.0493		$C_{21}H_{22}O_9$	Liquiritin*	ZGC

Table S2 (*continued*)

NO.	Name	t_R (min)	Detected *m/z*(+/-)	Expected	Error (ppm)	MS/MS		Formula	Identification	Source
						ESI$^-$	ESI$^+$			
77	P16	8.79	565.1580[M-H]$^-$	566.1552	4.56	271.0619,227.0710, 151.0031,119.0494		$C_{26}H_{30}O_{14}$	Naringenin-7-O-(2-β-D-apiofuranosyl)-β-D-glucopyranoside	ZGC
123	P17	10.52	253.0513[M-H]$^-$	253.0495	7.11	225.0558		$C_{15}H_{10}O_4$	Chrysophanol	DH
136	P18	12.03	285.0755[M+H]$^+$	285.0758	-1.05		270.0518,253.0488,242.0570	$C_{16}H_{12}O_5$	Calycosin	ZGC
176	P19	13.68	297.0408[M-H]$^-$	297.0394	4.71	253.0511,225.0557		$C_{16}H_{10}O_6$	6-methyl-rhein	DH
184	P20	14.29	283.0255[M-H]$^-$	283.0237	6.36	257.0462,239.0354 211.0403,183.0451		$C_{15}H_8O_6$	Rhein*	DH
185	P21	14.33	353.1378[M+H]$^+$	353.1384	-1.70		199.1478,147.1166	$C_{21}H_{20}O_5$	Gancaonin M	ZGC
186	P22	14.44	353.1377[M+H]$^+$	353.1384	-1.98		297.1851,267.1749, 181.1010,147.1171	$C_{21}H_{20}O_5$	Gancaonin A	ZGC
210	P23	16.72	269.0461[M-H]$^-$	269.0444	6.32	241.0506,225.0561,197.0605		$C_{15}H_{10}O_5$	Emodin*	DH
223	P24	19.15	471.3465[M+H]$^+$ 469.3332[M-H]$^-$	471.3469 469.3312	-0.85 4.26	425.3438,355.2652	453.3355,425.3409, 407.3302,235.1690	$C_{30}H_{46}O_4$	18-β-Glycyrrhetinic acid*	ZGC

FZ:*Radix Aconiti Lateralis Preparata*;DH:*Radix et Rhizoma Rhei*;GJ:*Zingiber offcinale Rosc*;RS:*Ginseng Radix Et Rhizoma*;ZGC: *Glycyrrhizae radix et rhizome Praeparata Cum Melle*

* :Compared with reference standards

Supplementary Table S3 Identification of metabolic components in rat plasma after oral administration of WPT.

NO.	t_R (min)	Detected *m/z*(+/-)	Expected	Error (ppm)	MS/MS		Formula	Identification	Source
					ESI$^-$	ESI$^+$			
M1	6.00	593.1531[M-H]$^-$	593.1501	5.06	255.0673,175.0240,119.0489		$C_{27}H_{30}O_{15}$	Liquiritin-7-O-glucuronide	ZGC
M2	6.73	621.1121[M-H]$^-$	621.1086	5.64	445.0769,269.0464		$C_{27}H_{26}O_{17}$	Emodin-O-diglucuronide	DH
M3	6.98	511.0566[M-H]$^-$	511.0541	4.89	431.0978,335.0241,255.0670,119.0490		$C_{21}H_{20}O_{13}S$	Liquiritigenin-O-glucuronide-O-sulfate	ZGC
M4	7.37	525.0360[M-H]$^-$	525.0334	4.95	445.0796,269.0464,241.0504,225.0556		$C_{21}H_{18}O_{14}S$	Emodin-O-sulfate-O-glucuronide	DH
M5	7.54	497.0776[M-H]$^-$	497.0748	5.63	417.1222,135.0439		$C_{21}H_{22}O_{12}S$	Liquiritin-7-O-sulfate	ZGC
M6	7.76	389.1288[M-H]$^-$	389.1265	5.91	273.0446,259.0287		$C_{17}H_{26}O_8S$	6-Gingerol+ OH + Sul	GJ
M7	7.90	431.0996[M-H]$^-$ 433.1132[M+H]$^+$	431.0973 433.1129	5.34	255.0669,175.0246,135.0081, 119.0494	257.0807,239.0701, 137.0235	$C_{21}H_{20}O_{10}$	Liquiritigenin-O-glucuronide	ZGC
M8	8.72	461.0740[M-H]$^-$	461.0715	6.93	285.0411,257.0451,241.0514		$C_{21}H_{18}O_{12}$	Hydroxyemodin-O-glucuronide	DH
M9	8.87	355.0242[M-H]$^-$	355.0220	6.20	255.0668,135.0080,119.0493		$C_{15}H_{12}O_7S$	Isoliquiritigenin-O-sulfate	ZGC
M10	8.94	621.1118[M-H]$^-$	621.1086	5.15	445.0792,269.0463		$C_{27}H_{26}O_{17}$	Emodin-O-diglucuronide	DH
M11	8.95	355.0240[M-H]$^-$	355.0220	5.63	255.0667,135.0082,119.0493		$C_{15}H_{12}O_7S$	Liquiritigenin-O-sulfate	ZGC
M12	9.23	299.0204[M-H]$^-$	299.0186	6.02	255.0303,227.0348,211.0392		$C_{15}H_8O_7$	Emodic acid	DH
M13	9.32	445.0791[M-H]$^-$	445.0765	5.71	269.0463,241.0525,225.0554		$C_{21}H_{18}O_{11}$	Emodin-O-glucuronide	DH
M14	9.63	337.0398[M-H]$^-$	337.0376	6.53	257.0825,151.0399		$C_{15}H_{14}O_7S$	Davidigenin-O-sulfate	ZGC
M15	9.87	443.0997[M-H]$^-$ 445.1128[M+H]$^+$	443.0973 445.1129	5.42 0.22	267.0669,252.0431	269.0807,254.0566	$C_{22}H_{20}O_{10}$	Formononetin-7-O- glucuronide	ZGC

Table S3 (*continued*)

NO.	t_R (min)	Detected *m/z*(+/-)	Expected	Error (ppm)	MS/MS		Formula	Identification	Source
					ESI$^-$	ESI$^+$			
M16	9.97	431.0739[M-H]$^-$ 433.1126[M+H]$^+$	431.0773 433.1129	-7.89	255.0667,175.0249, 135.0081,119.0493	257.0806,239.0701, 137.0235	$C_{21}H_{20}O_{10}$	isoliquiritigenin-O-glucuronide	ZGC
M17	10.07	275.1670[M+H-H_2O]$^+$	275.1641	10.50		177.0910,179.0702,137.0598	$C_{17}H_{24}O_4$	6-Gingerdione	GJ
M18	10.12	451.1987[M-H]$^-$	451.1963	5.32	275.1665,175.0237,113.0235		$C_{23}H_{32}O_9$	6-Shogaol+GluA	GJ
M19	10.18	433.1151[M-H]$^-$	433.1129	5.08	257.0824,113.0235		$C_{21}H_{22}O_{10}$	Davidigenin-O-glucuronide	ZGC
M20	10.38	447.1308[M-H]$^-$	447.0922	8.64	271.0990,135.0448		$C_{21}H_{20}O_{11}$	Hydroxyliquiritigenin(Bring)-O-glucuronide	ZGC
M21	10.38	357.1022[M-H]$^-$	357.1003	5.32	277.1449,163.0760		$C_{23}H_{32}O_9$	6-Shogaol − CH_2 +OH + Sul	GJ
M22	10.73	351.0153[M-H]$^-$	351.0169	-4.56	271.0983,135.0447		$C_{15}H_{12}O_8S$	Hydroxyliquiritigenin(Bring)-O-sulfate	ZGC
M23	10.87	445.0789[M-H]$^-$	445.0765	5.39	269.0464,241.0494,225.0557		$C_{21}H_{18}O_{11}$	Emodin-O-glucuronide	DH
M24	11.30	347.0240[M-H]$^-$	347.0220	5.76	267.0671,252.0433		$C_{16}H_{12}O_7S$	Formononetin-7-O-sulfate	ZGC
M25	12.03	445.0789[M-H]$^-$	445.0765	5.39	269.0463,241.0508,225.0558		$C_{21}H_{18}O_{11}$	Emodin-O-glucuronide	DH
M26	12.18	373.1332[M-H]$^-$	373.1316	4.29	293.1768,259.0445		$C_{17}H_{25}O_7S$	6-Gingerol+Sul	GJ
M27	12.93	349.0033[M-H]$^-$	349.0013	5.73	269.0464,241.0517		$C_{15}H_{10}O_8S$	Emodin-O-sulfate	DH
M28	14.06	455.2300[M-H]$^-$	455.2276	5.27	279.1976,175.0246,113.0236		$C_{23}H_{36}O_9$	6-Shogaol+4H + GluA	GJ
M29	14.74	467.1934[M-H]$^-$	467.1912	4.71	291.1604,175.0245,117.0183		$C_{23}H_{32}O_{10}$	6-Gingerol− 2H + GluA	GJ

Table S3 (*continued*)

NO.	t_R (min)	Detected *m/z*(+/-)	Expected	Error (ppm)	MS/MS		Formula	Identification	Source
					ESI$^-$	ESI$^+$			
M30	14.97	453.2143[M-H]$^-$	453.2119	5.30	277.1821,175.0249,113.0235		$C_{23}H_{34}O_9$	6-Shogaol+2H + GluA	GJ
M31	15.07	469.3341[M+H]$^+$	469.3312	6.18		451.2390,423.2059	$C_{30}H_{44}O_4$	3-keto-18α/β-Glycyrrhetinicacid	ZGC
M32	16.79	485.3285[M-H]$^-$	485.3262	4.74	441.3416,355.2637		$C_{30}H_{46}O_5$	22-hydroxy-18α/β-Glycyrrhetinic acid	ZGC

DH:*Radix et Rhizoma Rhei*;GJ:*Zingiber offcinale Rosc*;ZGC: *Glycyrrhizae radix et rhizome Praeparata Cum Melle*

* :Compared with reference standards

Glc: Glucosyl; GluA: Glucuronic acid residue;Sul:Sulfation

Supplementary Table S4 Binding energy of molecular docking between key components and core targets (kcal/mol).

COMPONNETS	AKT1	BCL2	EGFR	STAT3	ESR1	SRC	MAPK3	ERBB2	MTOR
Davidigenin-O-sulfate	-6.5	-4.9	-7.7	-7.2	-6.2	-6.4	-6.4	-4.1	-6.8
6-Gingerol-O-sulfate	-6.1	-3.7	-6.3	-6.6	-6.1	-5.3	-5.5	-3.0	-5.9
Liquiritin-7-O-sulfate	-8.1	-4.7	-8	-8.2	-7.8	-6.3	-8.2	-3.9	-7.1
6-Shogaol−CH2+OH+Sul	-6.2	-3.8	-7.2	-7.0	-6.3	-5.9	-6.0	-3.5	-6.6
3-keto-18β-Glycyrrhetinic acid	-7.8	-5.8	-8.4	-9.4	-8.1	-7.0	-8.4	-4.6	-7.4
6-Gingerdione	-5.4	-3.5	-5.4	-6.0	-5.6	-4.8	-5.2	-2.8	-5.9
Liquiritigenin-O-sulfate	-6.5	-5.4	-7.0	-7.1	-6.8	-6.1	-6.8	-4.1	-7.4
22-hydroxy-18β-Glycyrrhetinic acid	-7.4	-5.7	-8.4	-7.9	-8.2	-7.0	-8.2	-4.5	-7.0
Hydroxyliquiritigenin (B ring)-O-sulfate	-6.8	-5.6	-7.3	-8.0	-7.1	-6.3	-7.3	-4.2	-7.9
Isoliquiritigenin-O-sulfate	-6.8	-5.0	-7.1	-7.1	-6.7	-6.4	-7.3	-4.0	-7.8

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