

Table 1 Identification of chemical constituents of LGF

Peak (No.)	t_R /min	Molecular formula	Ion mode	Found mass (m/z)	Error / $\times 10^{-6}$	Fragment (m/z)	Compound	Attribution
P1	1.44	C ₂₁ H ₂₂ O ₈	[M+HCOO] ⁻	447.1333	8.0	225.0511	Nobiletin	g,f
P2	1.81	C ₆ H ₈ O ₇	[M-H] ⁻	191.0187	-5.4	154.9983,111.0085	Isocitric acid	c
P3	1.87	C ₁₇ H ₂₈ O ₁₄	[M-H] ⁻	455.1418	2.7	131.0345	3-Deoxy-D-ribo- γ -lactone- 3-O-gentiobioside	f
P4	1.88	C ₇ H ₁₁ NO ₅	[M-H] ⁻	188.0554	-5.5	144.0666,102.0565	N-acetyl-d-glutamic acid	h
P5	2.10	C ₁₄ H ₂₀ O ₉	[M-H] ⁻	331.1030	-1.5	153.0192	Kaoburaside	c
P6	2.17	C ₁₇ H ₂₄ O ₁₀	[M+HCOO] ⁻	433.1357	1.4	341.1074,161.0440	Swertiajaposide A	i
P7	2.30	C ₂₂ H ₃₂ O ₁₄	[M+HCOO] ⁻	565.1761	-2.2	341.1064,179.0532	Swertiapunimarin	i
P8	2.31	C ₁₀ H ₁₃ N ₅ O ₅	[M-H] ⁻	282.0831	-4.6	150.0408,133.0144	Guanosine	d,h
P9	2.42	C ₁₆ H ₂₂ O ₉	[M+H] ⁺	359.1316	-5.8	299.1103,271.1150	Sweroside	i
P10	2.66	C ₇ H ₁₂ O ₆	[M-H] ⁻	191.0552	-5.0	111.0081	Quinic acid	b,l,c,m,j,k, h
P11	2.88	C ₁₄ H ₂₀ O ₇	[M+HCOO] ⁻	345.1176	-4.4	179.0330,137.0253	Salidroside	l
P12	2.96	C ₁₇ H ₂₆ O ₁₁	[M-H] ⁻	405.1368	-8.5	179.0566,161.0437	Morrinoside	i
P13	3.43	C ₁₃ H ₂₄ O ₉	[M-H] ⁻	323.1342	-1.8	179.0566,161.0437,143.0323	Periplobiose	c
P14	3.72	C ₁₄ H ₁₈ O ₉	[M-H] ⁻	329.0888	3.0	167.0340,123.0446	Vanillic acid-4-O- β -D- glucopyranoside	l
P15	3.80	C ₁₆ H ₂₂ O ₁₀	[M-H] ⁻	373.1140	0.0	315.1066,153.0184	Swertiamarine	i
P16	3.93	C ₁₆ H ₂₄ O ₁₀	[M-H] ⁻	375.1291	-1.4	213.0753,161.0441,151.0769	Loganic acid	i
P17	4.30	C ₉ H ₁₀ O ₅	[M-H] ⁻	197.0437	-9.3	123.0445	Syringic acid	f,l,m,n,g
P18	4.34	C ₁₆ H ₂₄ O ₁₂	[M+HCOO] ⁻	453.1259	2.0	293.0877	1,2-O-di-3-O-2-deoxy-D- ribo- γ - lactonyl-glucoside	f
P19	4.68	C ₁₆ H ₂₄ O ₁₀	[M-H] ⁻	375.1288	-2.2	213.0755	8-Hydroxy-10-hydroxy- swertiamarin	i
P20	4.85	C ₉ H ₁₁ NO ₃	[M+HCOO] ⁻	226.0713	-3.4	136.0764	L-Tyrosine	e
P21	5.14	C ₁₅ H ₂₂ O ₁₀	[M+HCOO] ⁻	407.1194	-0.2	181.0523,151.0403	Catalpol	c
P22	5.38	C ₂₅ H ₃₄ O ₁₄	[M-H] ⁻	557.1835	-7.3	371.0964	Macrophylloside D	i
P23	5.60	C ₁₉ H ₂₈ O ₁₂	[M-H] ⁻	447.1494	-3.2	191.0548	Cuneataside C	l
P24	6.15	C ₁₅ H ₂₀ O ₁₀	[M-H] ⁻	359.0979	-1.3	197.0435,182.0207,166.9977,15 3.0547	4-Glucopyranosyloxy-3,5- dimethoxy benzoic acid	c
P25	6.21	C ₁₈ H ₂₂ O ₁₁	[M-H] ⁻	413.1074	-3.7	251.0591	Asperuloside	c
P26	6.34	C ₁₄ H ₁₈ O ₈	[M-H] ⁻	313.0929	0.0	151.039	Cyanoneside A	m

P27	6.40	C ₇ H ₆ O ₄	[M-H] ⁻	153.0184	-5.9	109.0292	Gentisic acid	j
P28	6.41	C ₁₀ H ₁₄ O ₅	[M-H] ⁻	213.0765	-1.6	183.0674	Guaiacylglycerol	c
P29	6.44	C ₁₅ H ₂₂ O ₉	[M+HCOO] ⁻	391.1211	-8.8	183.0674	Aucubin	c
P30	6.58	C ₉ H ₈ O ₃	[M+HCOO] ⁻	209.0443	-5.9	135.0443	P-coumaric acid	c,g
P31	6.86	C ₁₀ H ₁₄ O ₅	[M-H] ⁻	213.0750	-8.7	139.0749	Borreriagenin	c
P32	7.16	C ₃₁ H ₄₀ O ₁₅	[M-H] ⁻	651.2244	-7.8	161.0467	Martynoside	j
P33	7.19	C ₇ H ₁₂ O ₅	[M-H] ⁻	175.0597	-8.5	115.0394	Methyl 4-acetoxy-3-hydroxybutanoate	h
P34	7.21	C ₁₆ H ₂₂ O ₁₀	[M-H] ⁻	373.1128	-3.2	193.0505,167.0726	Geniposidic acid	i,c
P35	11.47	C ₁₇ H ₂₆ O ₁₁	[M+HCOO] ⁻	451.1448	-2.1	243.0854,155.0338	Shanzhiside methylester	i
P36	11.47	C ₁₁ H ₁₆ O ₆	[M-H] ⁻	243.0861	-5.5	195.0651	5-Methoxy-guaiacylglycerol	c
P37	12.33	C ₂₇ H ₃₀ O ₁₅	[M-H] ⁻	593.1523	1.8	431.1008	Saponarin	i
P38	12.34	C ₁₆ H ₁₈ O ₉	[M-H] ⁻	353.0871	-2.1	191.0538,179.0341,135.0445,127.0393	Neochlorogenic acid	l,c,j,h
P39	12.36	C ₄₂ H ₄₆ O ₂₀	[M-H] ⁻	869.2548	4.4	675.1924	Smilaside L	n
P40	12.78	C ₂₂ H ₃₀ O ₁₄	[M+HCOO] ⁻	563.1618	0.1	193.0496	3'-O-β-D-glucopyranogentiopiecin	i
P41	13.24	C ₁₆ H ₁₈ O ₉	[M-H] ⁻	353.0868	-2.8	173.044	Cryptochlorogenic acid	l,c,d,j,h
P42	13.55	C ₁₇ H ₂₄ O ₁₁	[M+HCOO] ⁻	449.1299	-0.4	127.0393	Qinjiaoside A	i
P43	13.64	C ₁₆ H ₂₂ O ₁₁	[M-H] ⁻	389.1079	-2.7	345.1179,209.0446,183.0653	Secologanoside	i
P44	13.72	C ₂₂ H ₃₀ O ₁₄	[M+HCOO] ⁻	563.1619	0.3	341.1049,221.0650	2'-O-beta-D-Glucosylgentiopicroside	i
P45	13.72	C ₁₂ H ₂₂ O ₁₁	[M-H] ⁻	341.1077	-3.7	119.0349,113.0235	Sucrose	i,e,d
P46	14.31	C ₁₉ H ₂₈ O ₁₁	[M-H] ⁻	431.1556	-0.7	191.0544	Osmanthuside H	l
P47	14.48	C ₂₂ H ₃₄ O ₁₅	[M-H] ⁻	537.1827	0.4	375.1316	Loganine glucoside	i
P48	14.93	C ₂₁ H ₂₀ O ₉	[M-H] ⁻	415.1030	-1.1	271.0821,135.0441	Puerarin	f
P49	15.20	C ₁₆ H ₂₀ O ₉	[M+HCOO] ⁻	401.1056	-2.4	355.1036,179.0473,179.0519	Gentiopicroside	i
P50	15.32	C ₁₅ H ₁₄ O ₆	[M-H] ⁻	289.0713	-1.6	181.0523,151.0403	Catechin	n
P51	15.33	C ₃₀ H ₂₆ O ₁₂	[M-H] ⁻	577.1363	1.9	289.0706	Procyanidin B	n
P52	15.38	C ₈ H ₈ O ₃	[M-H] ⁻	151.0400	-0.7	107.0499	Vanillin	m,j,n,g
P53	15.40	C ₁₉ H ₃₀ O ₈	[M+HCOO] ⁻	431.1916	-1.6	223.0592,149.0263	Roseoside	h
P54	15.45	C ₁₆ H ₁₈ O ₈	[M-H] ⁻	337.0927	-0.5	191.0556	5-O-Coumaroylquinic acid	c
P55	15.73	C ₂₄ H ₃₉ NO ₆	[M+H] ⁺	438.2879	6.6	348.2155,105.0904	Bullatine B	a,b
P56	15.74	C ₃₂ H ₄₂ O ₁₆	[M+HCOO] ⁻	727.2450	-0.7	327.1231	Pinoresinol Di-O-β-D-glucopyranoside	c
P57	15.76	C ₂₆ H ₃₄ O ₁₂	[M+HCOO] ⁻	583.2032	-0.1	375.1349	Olivil 4''-O-glucoside	c
P58	15.85	C ₈ H ₁₄ O ₅	[M-H] ⁻	189.0758	-5.7	153.0548,129.0553,107.0501	3-Hydroxysuberic acid	l

P59	15.88	C ₁₀ H ₁₂ O ₄	[M-H] ⁻	195.0654	-4.6	147.0443	Methyl 3-(3,4-dihydroxyphenyl)propanoate	c
P60	15.88	C ₁₇ H ₂₆ O ₁₀	[M+HCOO] ⁻	435.1489	-4.3	185.0846,167.0723,149.0564,141.0519	Reptoside	c
P61	15.97	C ₁₆ H ₁₆ O ₈	[M-H] ⁻	335.0762	-3.2	179.0338,135.0436	5-O-Caffeoylshikimic Acid	n
P62	16.01	C ₁₅ H ₁₄ O ₆	[M-H] ⁻	289.0708	-3.2	245.0797,205.0505,179.0338,137.0236	Epicatechin	l,n
P63	16.18	C ₂₆ H ₃₂ O ₁₃	[M-H] ⁻	551.1777	1.2	165.0545	Glehlinside C	l
P64	16.29	C ₂₂ H ₂₀ O ₁₂	[M+HCOO] ⁻	521.0972	6.7	299.0555,284.0348	Takakin-8-glucuronide	j
P65	16.32	C ₁₂ H ₁₃ NO ₅	[M-H] ⁻	250.0724	1.3	164.0705	5-Acetamido-2-(2-carboxyethyl) benzoic acid	h
P66	16.47	C ₉ H ₁₀ O ₃	[M-H] ⁻	165.0553	-2.5	147.0438	1-(4-Hydroxy-2-methoxyphenyl)ethanone	m
P67	16.51	C ₂₇ H ₃₀ O ₁₅	[M-H] ⁻	593.1524	2.0	285.0425	Kaempferol-3-O-rutinoside	j
P68	16.60	C ₁₆ H ₁₆ O ₈	[M-H] ⁻	335.0764	-2.6	179.0335,135.0436	4-O-Caffeoylshikimic Acid	n
P69	16.69	C ₃₂ H ₄₂ O ₁₆	[M+HCOO] ⁻	727.2476	2.9	519.1876,339.1218	Dehydrodiconiferyl alcohol 4,γ'-di-O-β-D-glucopyranoside	c
P70	16.73	C ₁₇ H ₂₀ O ₉	[M-H] ⁻	367.1038	0.9	173.0454	5-O-feruloylquinic acid	c
P71	17.12	C ₁₇ H ₂₄ O ₁₀	[M+HCOO] ⁻	433.1321	-7.0	355.1008,175.0394	Geniposide	c
P72	17.73	C ₁₅ H ₁₆ O ₉	[M-H] ⁻	339.0721	-0.1	193.0130	Smiglanin	n
P73	17.93	C ₂₁ H ₂₀ O ₁₁	[M-H] ⁻	447.0959	5.9	285.0423	Kaempferol 3-O-glucoside	j
P74	17.93	C ₃₃ H ₄₄ O ₁₇	[M-H] ⁻	711.2501	-0.7	549.1968,387.1438	Mediresinol Di-O-β-D-glucopyranoside	c
P75	18.18	C ₂₁ H ₂₀ O ₁₁	[M-H] ⁻	447.0947	3.1	357.0600	Luteolin-6-C-glucoside	i
P76	18.21	C ₂₈ H ₃₈ O ₁₃	[M-H] ⁻	581.2233	-1.1	419.1697,404.1474,401.1606	Lyoniresin-4-yl-β-D-glucopyranoside	l
P77	18.60	C ₁₁ H ₁₂ O ₅	[M-H] ⁻	223.0613	0.5	193.0130,149.0220,135.0420,121.0291	Sinapic acid	g
P78	18.61	C ₃₄ H ₄₆ O ₁₈	[M+HCOO] ⁻	787.2677	1.4	579.2079,417.1544	Liriodendrin	c
P79	18.82	C ₇ H ₆ O ₃	[M-H] ⁻	137.0236	-6.1	121.0290	4-Hydroxybenzoic acid	m,e
P80	18.98	C ₂₁ H ₂₀ O ₁₀	[M-H] ⁻	431.1003	4.4	178.0266	Scutellarein-7-O-rhamnoside	j
P81	19.15	C ₂₅ H ₄₁ NO ₆	[M+H] ⁺	452.3027	4.5	363.2038,265.1697	Chasmanine	a,b
P82	19.63	C ₁₆ H ₁₂ O ₅	[M-H] ⁻	283.0597	-5.1	268.0364	Calycosin	d,m
P83	19.78	C ₂₀ H ₂₄ O ₆	[M-H] ⁻	359.1498	-0.6	297.0784,109.0291	Isolariciresinol	f
P84	19.89	C ₂₂ H ₂₂ O ₁₀	[M+HCOO] ⁻	491.1192	-0.5	445.1248,283.0597,268.0363	Calycosin-7-O-β-D-glucoside	d
P85	19.98	C ₂₄ H ₃₉ NO ₇	[M+H] ⁺	454.2767	-7.2	364.1545,336.1594	Fuziline	a,b
P86	20.17	C ₃₄ H ₄₇ NO ₁₁	[M+H] ⁺	646.3237	2.3	599.2765,495.2221,369.1753	Aconitine	a,b
P87	20.21	C ₂₉ H ₄₀ O ₉	[M+HCOO] ⁻	577.2604	-8.8	167.0342	12-O-vanilloyl-sarcostin	m

P88	20.29	C ₂₇ H ₃₀ O ₁₆	[M-H] ⁻	609.1471	1.5	301.0313,273.0421,255.0306,15 1.0011	Rutin	c,d,j,h
P89	20.32	C ₂₁ H ₂₀ O ₁₀	[M-H] ⁻	431.1003	4.4	283.0600	Isovitexin	i
P90	20.47	C ₂₈ H ₃₈ O ₁₃	[M-H] ⁻	581.2233	-1.2	389.1581	Lyoni-resinol-3 α -O- β -D- glucopyranoside	e
P91	20.54	C ₂₀ H ₁₈ O ₁₁	[M-H] ⁻	433.0814	8.7	300.0275	Quercetin 3-O-beta-D- xylopyranoside	c
P92	20.56	C ₂₈ H ₃₂ O ₁₄	[M-H] ⁻	591.1728	1.4	459.1159,339.0732	Linarin	f
P93	20.60	C ₂₁ H ₂₀ O ₁₂	[M-H] ⁻	463.0893	2.5	300.0283	Quercetin-7-O- β -D- glucopyranoside	j
P94	20.69	C ₂₁ H ₂₂ O ₁₁	[M-H] ⁻	449.1100	-0.4	303.0504,285.0384,178.9953,15 1.0011	Astilbin	n
P95	20.71	C ₄₀ H ₄₂ O ₁₈	[M+HCOO] ⁻	855.2383	3.4	217.0497	Smilaside G	n
P96	20.82	C ₂₂ H ₂₂ O ₁₁	[M-H] ⁻	461.1126	7.9	179.0350,135.0441	2-O-Cinnamoyl glucogallin	j
P97	20.94	C ₁₅ H ₁₀ O ₆	[M-H] ⁻	285.0395	-3.3	267.0255,257.0416,151.0011,13 3.0286	Luteolin	j,n,f,g
P98	21.03	C ₃₃ H ₄₀ O ₁₉	[M-H] ⁻	739.2104	1.8	693.2061,499.1518	Clitorin	j
P99	21.05	C ₂₅ H ₂₄ O ₁₂	[M-H] ⁻	515.1215	3.9	191.0545,179.0363,137.0241	4,5-Dicaffeoylquinic acid	j
P100	21.08	C ₂₂ H ₂₂ O ₁₁	[M-H] ⁻	461.1126	7.9	284.0327	5-Hydroxy-calycosin-7-O- β - D-glucoside	d
P101	21.16	C ₁₅ H ₁₂ O ₇	[M-H] ⁻	303.0501	-3.1	285.0392	Taxifolin	n
P102	21.59	C ₂₆ H ₃₂ O ₁₁	[M-H] ⁻	519.1865	-1.4	357.1311	Pinoresinol- β -D-glucoside	c
P103	21.75	C ₂₅ H ₃₉ NO ₇	[M+H] ⁺	466.2805	1.3	379.2333,281.1762,173.1414	Delbruine	a
P104	21.75	C ₂₅ H ₂₄ O ₁₂	[M-H] ⁻	515.1203	1.6	191.0539,179.0349,173.0452,13 5.0437	3,4-Dicaffeoylquinic acid	j
P105	21.78	C ₂₆ H ₃₂ O ₁₁	[M-H] ⁻	519.1866	-1.2	357.1317,151.0381,113.0242	6'-O-beta-D- Glucosylswertiamarine	i
P106	21.78	C ₃₅ H ₄₉ NO ₉	[M+H] ⁺	628.3465	-2.5	563.2879,491.2502,197.1402	Vilmorrianine C	a
P107	21.84	C ₂₁ H ₂₀ O ₇	[M+HCOO] ⁻	429.1203	2.9	119.0454	1,2-O-di-p-Coumaroylglycerol	n
P108	21.85	C ₂₇ H ₂₈ O ₁₄	[M-H] ⁻	575.1435	5.0	267.0658	Rhamnosyl-glucosyl-apigenin	e
P109	21.89	C ₂₂ H ₂₆ O ₈	[M-H] ⁻	417.1550	-1.1	181.0488,166.0256	Syringaresinol	i,n
P110	21.95	C ₂₅ H ₂₄ O ₁₂	[M-H] ⁻	515.1208	2.6	353.0872,135.0442	1,5-Dicaffeoylquinic acid	j
P111	22.02	C ₁₅ H ₁₀ O ₆	[M-H] ⁻	285.0407	0.8	257.0470,229.0501,169.0141,15 1.0019	Kaempferol	c,j,e,i,g
P112	22.06	C ₁₆ H ₁₄ O ₆	[M-H] ⁻	301.0728	3.4	283.0604,268.0387,259.0606,24 1.0504,151.0382	Baishouwuhenzophenone	m
P113	22.18	C ₄₇ H ₅₀ O ₂₂	[M-H] ⁻	965.2711	-1.0	279.0164,189.0570	Smiglaside D	n
P114	22.33	C ₂₇ H ₃₀ O ₁₄	[M-H] ⁻	577.1575	2.2	459.1163,313.0719	Rhoifolin	e
P115	22.33	C ₂₁ H ₂₀ O ₁₁	[M-H] ⁻	447.0933	0.1	300.0267,255.0302	Quercitrin	c,j,e,h
P116	22.36	C ₁₆ H ₁₄ O ₆	[M-H] ⁻	301.0722	1.4	255.0302,241.0512	Hesperitin	g

P117	22.77	C ₁₈ H ₂₄ O ₁₂	[M+HCOO] ⁻	477.1283	6.9	251.0570	Asperulosidic acid	c
P118	22.97	C ₃₁ H ₄₃ NO ₁₀	[M+HCOO] ⁻	634.2873	0.7	515.1875,395.1612,229.0503	Benzoylmesaconine	a
P119	23.21	C ₁₆ H ₁₂ O ₆	[M-H] ⁻	299.0561	0.0	151.0021	Chrysoeriol	g
P120	23.32	C ₅₁ H ₈₄ O ₂₃	[M+H] ⁺	1065.5419	-5.4	979.5174,912.4721,693.3352	Protogracillin	k
P121	23.34	C ₂₁ H ₁₈ O ₁₁	[M-H] ⁻	445.0816	9.0	269.0449,223.0592,195.0629	Baicalin	d,j
P122	23.44	C ₂₇ H ₃₀ O ₁₄	[M+HCOO] ⁻	623.1659	6.7	577.1571,431.0995	Kaempferitrin	e
P123	23.47	C ₂₁ H ₂₀ O ₁₀	[M-H] ⁻	431.0983	-0.2	285.0397	Afzelin	h
P124	23.64	C ₂₁ H ₂₂ O ₁₀	[M-H] ⁻	433.1136	-1.0	269.0434,259.0604,178.9966	Isoengeletin	n
P125	23.70	C ₂₄ H ₂₄ O ₁₁	[M+HCOO] ⁻	533.1319	3.4	283.0608	3'-Acetyl-calycosin-7-O-β-D-glucoside	d
P126	23.88	C ₂₁ H ₂₂ O ₁₂	[M-H] ⁻	465.1015	-5.1	341.0693,313.0928,209.0450	Taxifolin-3-glucoside	n
P127	23.88	C ₂₆ H ₄₁ NO ₇	[M+H] ⁺	480.2929	-5.6	393.2121,349.1867	14-Acetylneoline	a
P128	23.88	C ₂₀ H ₂₀ O ₇	[M+HCOO] ⁻	417.1196	1.2	325.0746,181.0497,177.0183	Tangeretin	f
P129	23.90	C ₂₂ H ₂₂ O ₉	[M+HCOO] ⁻	475.1248	0.4	267.0647,252.0424	Formononetin-7-O-β-D-glucoside	d
P130	23.92	C ₂₄ H ₂₀ O ₉	[M-H] ⁻	451.1033	-0.2	341.0717	Cinchonain	n
P131	23.93	C ₁₆ H ₁₄ O ₅	[M+HCOO] ⁻	331.0827	1.0	271.0604	Sakuranetin	n
P132	23.99	C ₃₃ H ₂₆ O ₁₂	[M-H] ⁻	613.1388	6.0	189.0172	Cinchonain caffeate	n
P133	24.13	C ₁₀ H ₁₀ O ₄	[M-H] ⁻	193.0496	-5.4	179.0566,149.0564,135.0440	Ferulic acid	m,d,e,n,g
P134	24.13	C ₄₅ H ₇₂ O ₁₆	[M+H] ⁺	869.4848	-5.1	821.4331,737.3733,591.3396,269.0879	Dioscin	k
P135	24.20	C ₉ H ₈ O ₃	[M+HCOO] ⁻	209.0442	-6.3	147.0445,107.0499	2-Coumaric acid	j
P136	24.49	C ₂₉ H ₃₈ O ₁₅	[M-H] ⁻	625.2132	-0.9	286.0936	Isomucronulatol-7,2'-di-O-glucoside	d
P137	24.50	C ₂₆ H ₂₆ O ₁₀	[M+HCOO] ⁻	543.1542	6.2	289.0715	Hydrogenated smiglabrone A	n
P138	24.58	C ₂₉ H ₃₇ NO ₅	[M+H] ⁺	480.2791	9.8	417.2440,209.1416	Cytochalasin B	a
P139	24.70	C ₂₆ H ₄₄ O ₉	[M+HCOO] ⁻	545.2951	-3.0	337.2378	2-Deoxy-1,3,4,6-tetra-O-pivaloyl-glucopyranose	j
P140	24.75	C ₅₈ H ₈₆ O ₁₉	[M+H] ⁺	1087.5738	-9.0	1019.5758,739.3743	Wilfoside K1N	m
P141	24.76	C ₂₂ H ₂₄ O ₁₀	[M+HCOO] ⁻	493.1367	3.1	178.9963	10-Demethyl-9,10-dimethoxypterocarpan-3-O-β-D-glucoside	d
P142	24.81	C ₁₅ H ₁₂ O ₄	[M-H] ⁻	255.0646	-6.7	135.0077,109.0286	Liquiritigenin	f
P143	24.92	C ₂₃ H ₂₈ O ₁₀	[M-H] ⁻	463.1613	0.6	301.1057,271.0606	Isomucronulatol-7-O-β-D-glucoside	d
P144	25.06	C ₁₆ H ₁₂ O ₄	[M-H] ⁻	267.0663	-0.1	252.0448	Formononetin	d,f
P145	25.17	C ₁₅ H ₁₀ O ₇	[M-H] ⁻	301.0356	0.7	199.0376,178.9972,151.0024	Quercetin	j,i,n,f
P146	25.24	C ₈₂ H ₁₃₄ O ₄₃	[M+HCOO] ⁻	1851.8357	4.1	469.1554	Clematichinenoside AR	f

P147	25.31	C ₂₉ H ₃₉ NO ₆	[M+H] ⁺	498.2849	-0.3	305.2345,293.1355,201.0556	Delavaconitine	a
P148	25.32	C ₂₁ H ₂₀ O ₁₀	[M-H] ⁻	431.0998	3.4	269.0458	4'-Demethylcalycosin-7-O-β-D-glucoside	d
P149	25.34	C ₄₇ H ₇₈ O ₁₉	[M+HCOO] ⁻	991.5108	-1.1	945.5071	Astragaloside VI	d
P150	25.35	C ₇₆ H ₁₂₄ O ₃₉	[M+HCOO] ⁻	1705.7765	3.7	1689.7808,1189.6034	Clematiunicinoside E	f
P151	25.44	C ₂₈ H ₄₂ O ₇	[M+H] ⁺	491.3013	1.9	103.0747	Caudatin	m
P152	25.47	C ₇₀ H ₁₁₄ O ₃₄	[M+HCOO] ⁻	1543.7212	2.5	865.4920,733.4459	Clematichinenoside C	f
P153	25.52	C ₂₈ H ₃₆ O ₈	[M-H] ⁻	499.2327	-2.1	361.1530,343.2103,325.1977,283.0566,259.0606	Qingyangshengenin	m
P154	25.55	C ₂₃ H ₃₇ NO ₆	[M+H] ⁺	424.2697	0.7	335.2247,247.1209	Senbusine A	a,b
P155	25.55	C ₃₆ H ₄₂ O ₁₉	[M-H] ⁻	777.2280	4.2	735.2130,481.1231	Smilaside A	n
P156	25.67	C ₂₈ H ₃₆ O ₇	[M-H] ⁻	483.2368	-4.2	121.0293	12-O-benzoyl-deacymetaplexigenin	m
P157	25.81	C ₉₂ H ₁₄₂ O ₄₆	[M-H] ⁻	1981.8740	2.1	990.4320,469.1560	Clematomandshurica saponin B	f
P158	25.85	C ₅₉ H ₉₆ O ₂₆	[M+HCOO] ⁻	1265.6161	-0.8	749.4457,469.1560	Herderacoside C	f
P159	25.91	C ₈₆ H ₁₃₂ O ₄₂	[M-H] ⁻	1835.8137	0.9	733.4488	Clematochinenoside F	f
P160	25.95	C ₆₄ H ₁₀₄ O ₂₉	[M+HCOO] ⁻	1381.6670	1.8	865.4954,733.4488	Huzhangoside B	f
P161	25.98	C ₅₁ H ₈₂ O ₂₁	[M+HCOO] ⁻	1075.5353	2.1	1029.5296,987.5175	Agroastragaloside I	d
P162	26.01	C ₃₅ H ₄₂ O ₂₁	[M-H] ⁻	797.2179	4.2	755.2088,593.1550,451.1275	Rindoside	i
P163	26.02	C ₄₉ H ₈₀ O ₂₀	[M+HCOO] ⁻	1033.5243	1.7	987.5175,927.4967	Agroastragaloside III	d
P164	26.14	C ₁₅ H ₁₂ O ₅	[M-H] ⁻	271.0599	-4.9	151.0011,119.0503,107.0137	Naringenin	f,n
P165	26.25	C ₄₁ H ₆₆ O ₁₅	[M+HCOO] ⁻	843.4371	-1.5	761.4067,743.4058	Cynsaccatol C	m
P166	26.29	C ₄₁ H ₆₄ O ₁₃	[M+HCOO] ⁻	809.4322	-0.8	635.3401	Wallicoside D	m
P167	26.59	C ₁₇ H ₁₆ O ₆	[M-H] ⁻	315.0865	-2.9	109.0298	2,3-Dihydroxy-9,10-dimethoxypterocarpan	d
P168	26.67	C ₄₃ H ₇₀ O ₁₅	[M+HCOO] ⁻	871.4663	-3.8	765.4362	Astragaloside II	d
P169	26.80	C ₄₉ H ₇₆ O ₂₀	[M-H] ⁻	983.4848	-0.9	113.0244	Achyranthoside C dimethyl ester	e
P170	26.83	C ₄₁ H ₆₈ O ₁₄	[M+HCOO] ⁻	829.4554	0.2	783.4509,621.4067,489.3512,329.2288	Astragaloside A	d
P171	26.87	C ₁₈ H ₃₄ O ₅	[M-H] ⁻	329.2322	-3.6	293.2114	Pinellie acid	e
P172	26.97	C ₃₈ H ₄₄ O ₂₀	[M-H] ⁻	819.2376	2.7	583.1594,559.1649,513.1378	Smiglaside C	n
P173	27.02	C ₄₇ H ₇₄ O ₁₈	[M+HCOO] ⁻	971.4869	1.2	925.4781	Pseudoginsenoside RT1	e
P174	27.31	C ₅₆ H ₈₄ O ₂₀	[M+HCOO] ⁻	1121.5454	-7.5	137.0253	Otophyllsode O	m
P175	27.37	C ₄₂ H ₆₈ O ₁₅	[M+HCOO] ⁻	857.4526	-1.7	775.4244,757.4132,739.4021	Cynawilfoside E	m
P176	27.63	C ₄₉ H ₇₂ O ₁₇	[M-H] ⁻	931.4647	-5.4	343.2115	Cynanchin C	m
P177	27.69	C ₄₇ H ₇₄ O ₁₇	[M+HCOO] ⁻	955.4916	0.8	867.4757	Acetytastragaloside	d

P178	27.74	C ₄₈ H ₇₈ O ₁₈	[M+HCOO] ⁻	987.5203	3.4	941.5137	Soyasaponin I methyl ester	d
P179	27.84	C ₆₄ H ₁₀₄ O ₃₀	[M-H] ⁻	1351.6560	1.5	979.4596,779.4289	Huzhangoside D	f
P180	27.85	C ₄₀ H ₄₆ O ₂₁	[M-H] ⁻	861.2507	5.6	583.1612	Acetylated smiglaside C	n
P181	27.98	C ₂₂ H ₂₉ NO ₃	[M+H] ⁺	356.2211	-2.7	295.1349,265.1071	Songoramine	a
P182	28.12	C ₄₃ H ₇₀ O ₁₅	[M+HCOO] ⁻	871.4696	-0.1	765.4387	Isoastragaloside II	d
P183	28.44	C ₄₇ H ₇₀ O ₂₀	[M-H] ⁻	953.4467	8.3	793.4337	Achyranthoside B	e
P184	28.56	C ₄₈ H ₇₆ O ₁₈	[M+HCOO] ⁻	985.5083	7.1	615.3835,455.3538	Momordin IIa	e
P185	28.74	C ₄₂ H ₆₀ O ₁₄	[M-H] ⁻	787.3956	5.9	137.0239	Cynanauriculoside C	m
P186	28.79	C ₄₈ H ₇₀ O ₁₇	[M-H] ⁻	917.4597	6.2	137.0239	Wallicoside H	m
P187	29.09	C ₄₅ H ₇₂ O ₁₆	[M+HCOO] ⁻	913.4808	0.6	867.4766,825.4636,765.4450	Astragaloside I	d
P188	29.22	C ₃₀ H ₄₆ O ₅	[M-H] ⁻	485.3256	-3.4	441.3325,365.2860	Quillaic acid	e
P189	29.46	C ₄₁ H ₆₄ O ₁₃	[M-H] ⁻	763.4247	-3.5	763.4270	Tarasaponin VI	e
P190	30.20	C ₁₈ H ₃₄ O ₄	[M-H] ⁻	313.2376	-2.8	295.2270,183.1389	12DiHOME	k
P191	30.51	C ₃₀ H ₄₆ O ₆	[M-H] ⁻	501.3227	1.1	439.3175	26-Hydroxypticolic acid G	e
P192	31.31	C ₁₇ H ₃₄ O ₂	[M+HCOO] ⁻	315.2530	-3.4	116.9280	Margaric acid	e
P193	32.70	C ₂₈ H ₄₆ O ₇	[M-H] ⁻	493.3210	7.9	319.1944	Makisterone B	e
P194	33.25	C ₃₂ H ₄₅ NO ₁₀	[M+H] ⁺	604.3119	0.4	586.2984,572.2898,554.2755,54 0.2563,522.2509	Benzoylaconine	a,b
P195	33.71	C ₁₈ H ₃₀ O ₃	[M-H] ⁻	293.2114	-2.8	277.2169	13-Keto-9Z,11E- octadecadienoic acid	e
P196	34.67	C ₁₈ H ₃₂ O ₃	[M-H] ⁻	295.2279	0.0	277.2168	13S-hydroxyoctadecadienoic acid	e
P197	34.68	C ₃₀ H ₄₈ O ₆	[M-H] ⁻	503.3393	3.0	485.327	23-Hydroxytormentic acid	e
P198	39.42	C ₂₃ H ₄₆ O ₃	[M+HCOO] ⁻	415.3429	0.1	369.3371	2-Hydroxytricosanoic acid	c
P199	39.46	C ₁₆ H ₃₂ O ₃	[M-H] ⁻	271.2278	-0.1	225.2224	16-Hydroxyhexadecanoic acid	k
P200	40.87	C ₂₇ H ₄₁ NO ₃	[M-H] ⁻	426.3009	-1.2	120.0897	Peimisine	e
P201	41.10	C ₁₈ H ₃₂ O ₂	[M-H] ⁻	279.2319	-3.7	261.2297,221.1546	Linoleic acid	a,j,k,e,n,g
P202	41.10	C ₃₀ H ₄₆ O ₃	[M-H] ⁻	453.3403	6.4	353.2127,191.1074	Oleanonic acid	f
P203	41.34	C ₃₀ H ₄₈ O ₄	[M-H] ⁻	471.3473	-1.5	409.3465	Hederagenin	j,f
P204	42.32	C ₂₉ H ₄₈ O	[M+HCOO] ⁻	457.3677	-2.1	341.2882,125.0972	Stigmasterol	i,n,f
P205	42.33	C ₃₂ H ₅₀ O ₄	[M-H] ⁻	497.3653	3.4	483.3574	Oleanolic acid 3-acetate	m
P206	42.36	C ₃₀ H ₄₈ O ₃	[M-H] ⁻	455.3504	-5.8	371.3302,179.1091,111.0811	Oleanolic acid	e,i,f
P207	42.38	C ₁₆ H ₃₂ O ₂	[M-H] ⁻	255.2321	-3.2	227.2009,169.1242	Palmic acid	k
P208	42.84	C ₁₈ H ₃₄ O ₂	[M-H] ⁻	281.2477	-3.0	241.2180	Oleic acid	k,e,n,g

Notes: a. *Aconiti radix cocta* (Zhichuanwu, 制川乌); b. *Aconiti kusnezoffii radix cocta* (Zhicao Wu, 制草乌); c. *Eucommia ulmoides*

Oliv. (Yanduzhong, 盐杜仲); d. *Astragalus mongholicus* Bunge (Huangqi, 黄芪); e. *Achyranthes bidentata* Blume (Niuxi, 牛膝); f.

Clematis chinensis Osbeck (Weilingxian, 威灵仙); g. *Coix lacryma-jobi* L. (Yiyiren, 薏苡仁); h. *Houttuynia cordata* Thunb. (Yuxingcao, 鱼腥草); i. *Gentiana macrophylla* Pall. (Qinjiao, 秦艽); j. *Aster indicus* L. (Malancao, 马兰草); k. *Dioscorea septemloba* Thunb. (Mianbixie, 绵萆薢); l. *Sargentodoxa cuneata* (Oliv.) Rehder & E.H.Wilson (Daxueteng, 大血藤); m. *Cynanchum wilfordii* (Maxim.) Hook.f. (Geshanxiao, 隔山消); n. *Smilax glabra* Roxb. (Tufuling, 土茯苓)