

Table S1 Characterization of compounds in Qingkailing capsules by UHPLC-FT-ICR-MS

No.	RT (min)	Identification	[M+H] ⁺			[M-H] ⁻			Formula	MS/MS (<i>m/z</i>)
			Observed	Calculated	Error (ppm)	Observed	Calculated	Error (ppm)		
1	0.92	Arginine	175.11894	175.11895	0.08	-	-	-	C ₆ H ₁₄ N ₄ O ₂	(+): 158
2	0.95	Gluconic acid	-	-	-	195.05067	195.05103	1.83	C ₆ H ₁₂ O ₇	(-): 129
3	0.97	Quinic acid	-	-	-	191.05575	191.05611	1.92	C ₇ H ₁₂ O ₆	(-): 173, 127
4	0.97	D-Sorbitol	-	-	-	181.07141	181.07176	1.92	C ₆ H ₁₄ O ₆	(-): 101
5	1.01	Sucrose	343.12279	343.12349	2.03	341.10831	341.10894	1.83	C ₁₂ H ₂₂ O ₁₁	(-): 179
6	1.16	Cytidine	244.09270	244.09280	0.39	-	-	-	C ₉ H ₁₃ N ₃ O ₅	(+): 112
7	1.25	Malic acid	-	-	-	133.01398	133.01425	2.00	C ₄ H ₆ O ₅	(-): 115
8	1.36	Uridine	245.07655	245.07681	1.07	243.06188	243.06226	1.57	C ₉ H ₁₂ N ₂ O ₆	(-): 110
9	1.36	Tyrosine	182.08128	182.08117	-0.59	-	-	-	C ₉ H ₁₁ NO ₃	(+): 165, 147, 136
10	1.37	Adenosine	268.10407	268.10403	-0.14	-	-	-	C ₁₀ H ₁₃ N ₅ O ₄	(+): 136
11	1.39	Guanosine	284.09899	284.09894	-0.16	282.08428	282.08439	0.40	C ₁₀ H ₁₃ N ₅ O ₅	(+): 152
12	1.44	Leucine	132.10188	132.10191	0.18	-	-	-	C ₆ H ₁₃ NO ₂	(+): 115, 104
13	1.61	Quinic acid	337.11343	337.11292	-1.50	335.09805	335.09837	0.95	C ₁₃ H ₂₀ O ₁₀	(-): 191
		3-hydroxy-3-methylpentanedioate								
14	1.73	Gardoside	-	-	-	373.11365	373.11402	0.99	C ₁₆ H ₂₂ O ₁₀	(-): 211
15	1.98	Phenylalanine hexose	328.13925	328.13908	-0.52	326.12427	326.12453	0.78	C ₁₅ H ₂₁ NO ₇	(-): 164
16	2.00	Shanzhiside	-	-	-	391.12421	391.12459	0.97	C ₁₆ H ₂₄ O ₁₁	(-): 229
17	2.00	Phenylalanine	166.08635	166.08626	-0.56	164.07148	164.07170	1.37	C ₉ H ₁₁ NO ₂	(-): 147
18	2.02	Deacetylasperulosidic acid	391.12351	391.12349	-0.06	389.10853	389.10894	1.05	C ₁₆ H ₂₂ O ₁₁	(-): 345, 227, 209, 183, 165

19	2.23	Dihydroxybenzoic acid glucoside	-	-	-	315.07191	315.07216	0.79	C ₁₃ H ₁₆ O ₉	(-): 153, 109
20	2.25	Vanillic acid hexose	-	-	-	329.08764	329.08781	0.49	C ₁₄ H ₁₈ O ₉	(-): 167
21	2.29	Geniposidic acid	375.12932	375.12857	-1.99	373.11379	373.11402	0.60	C ₁₆ H ₂₂ O ₁₀	(-): 211, 193, 167, 149, 123
22	2.34	Ixoroside	383.13160	383.13125	-0.91 ^a	405.14001	405.14024	0.32 ^b	C ₁₆ H ₂₄ O ₉	(-): 359
23	2.48	6-oxo demethylgenipin 1- <i>O</i> -glucopyranoside	-	-	-	387.09310	387.09329	0.49	C ₁₆ H ₂₀ O ₁₁	(-): 343
24	2.63	Dihydroxybenzoic acid glucoside isomer	-	-	-	315.07180	315.07216	1.12	C ₁₃ H ₁₆ O ₉	(-): 153
25	2.73	Deacetyl asperulosidic acid methyl ester	427.12128	427.12108	-0.45 ^a	449.12961	449.13006	1.02 ^b	C ₁₇ H ₂₄ O ₁₁	(-): 403, 241
26	2.91	1- <i>O</i> -syringoyl-β- <i>D</i> -glucopyranosid e	-	-	-	359.09825	359.09837	0.32	C ₁₅ H ₂₀ O ₁₀	(-): 197
27	3.14	Gardenoside	427.12140	427.12108	-0.73 ^a	449.12985	449.13006	0.43 ^b	C ₁₇ H ₂₄ O ₁₁	(-): 241
28	3.37	Neochlorogenic acid	355.10273	355.10236	-1.06	353.08734	353.08781	1.33	C ₁₆ H ₁₈ O ₉	(-): 191, 179, 173, 135
29	3.43	Jasminoside G	347.17023	347.17004	-0.54	345.15516	345.15549	0.96	C ₁₆ H ₂₆ O ₈	(-): 165
30	3.52	Scandoside methyl ester	427.12134	427.12108	-0.60 ^a	449.12988	449.13006	0.41 ^b	C ₁₇ H ₂₄ O ₁₁	(-): 241
31	3.62	Tryptophan	205.09700	205.09715	0.74	203.08236	203.08260	1.21	C ₁₁ H ₁₂ N ₂ O ₂	(+): 188, 146
32	3.97	Shanzhiside methyl ester	-	-	-	405.13993	405.14024	0.74	C ₁₇ H ₂₆ O ₁₁	-
33	4.14	Unknown	350.18188	350.18094	-2.69	348.16748	348.16639	-3.13	C ₁₅ H ₂₇ NO ₈	-
34	4.33	Esculin	-	-	-	339.07191	339.07216	0.71	C ₁₅ H ₁₆ O ₉	(-):177
35	4.46	Jasminoside B	347.16997	347.17004	0.23	345.15519	345.15549	0.86	C ₁₆ H ₂₆ O ₈	(-): 165
36	4.54	Loganic acid	377.14408	377.14422	0.38	375.12925	375.12967	1.13	C ₁₆ H ₂₄ O ₁₀	(-): 213
37	4.82	Isaindigodione isomer	327.13379	327.13393	0.44	-	-	-	C ₁₈ H ₁₈ N ₂ O ₄	(+): 201
38	4.85	Kingside	427.12109	427.12108	-0.02 ^a	449.12946	449.13006	1.36 ^b	C ₁₇ H ₂₄ O ₁₁	(-): 403

39	4.90	Jasminoside C	-	-	-	327.14454	327.14493	1.18	C ₁₆ H ₂₄ O ₇	-
40	4.95	Coniferin	365.12070	365.12069	-0.03 ^a	387.12949	387.12967	0.48 ^b	C ₁₆ H ₂₂ O ₈	(-): 341, 179
41	5.28	3-p-coumaroylquinic acid	339.10742	339.10744	0.07	337.09270	337.09289	0.58	C ₁₆ H ₁₈ O ₈	(-): 191, 163
42	5.33	Shanzhiside methyl ester	-	-	-	405.13994	405.14024	0.73	C ₁₇ H ₂₆ O ₁₁	(-): 243
43	5.34	Isaindigodione	327.13403	327.13393	-0.30	-	-	-	C ₁₈ H ₁₈ N ₂ O ₄	(+): 201
44	5.36	7-epiloganin	-	-	-	389.14515	389.14532	0.44	C ₁₇ H ₂₆ O ₁₀	-
45	5.43	Indole-3-acetonitrile-6-O-β-D-glucopyranoside	335.12460	335.12376	-2.50	379.11432	379.11469	0.97 ^b	C ₁₆ H ₁₈ N ₂ O ₆	(-): 333, 306, 144
46	5.59	Chlorogenic acid*	355.10242	355.10236	-0.17	353.08719	353.08781	1.76	C ₁₆ H ₁₈ O ₉	(-): 191, 179, 173, 135
47	5.59	Syringin	390.17740	390.17586	-3.95 ^c	417.13993	417.14024	0.72 ^b	C ₁₇ H ₂₄ O ₉	(-): 209
48	5.59	Secologanoside	391.12351	391.12349	-0.06	389.10805	389.10894	2.28	C ₁₆ H ₂₂ O ₁₁	(-): 345, 209, 183, 165, 121
49	5.65	Indican	296.11279	296.11286	0.25	340.10361	340.10379	0.54 ^b	C ₁₄ H ₁₇ NO ₆	(-): 294, 161, 132
50	5.65	Unknown	-	-	-	743.20247	743.20402	2.08	C ₃₂ H ₄₀ O ₂₀	(-): 191
51	5.66	2,3-dihydro-1H-pyrrolo[2,1-c][1,4]benzodiazepine-5,11(10H,11ah)-dione	217.09707	217.09715	0.39	-	-	-	C ₁₂ H ₁₂ N ₂ O ₂	(+): 144
52	5.72	8-Epiapodantheroside	389.14473	389.14422	-1.31	-	-	-	C ₁₇ H ₂₄ O ₁₀	-
53	5.76	Genipin-1-O-β-D-gentiobioside	551.19816	551.19705	-2.02	595.18640	595.18797	2.65 ^b	C ₂₃ H ₃₄ O ₁₅	(-): 549, 225, 207
54	5.83	Cryptochlorogenic acid	355.10258	355.10236	-0.63	353.08710	353.08781	1.99	C ₁₆ H ₁₈ O ₉	(-): 191, 179, 173, 135
55	5.90	5-O-feruloylquinic acid	369.11849	369.11801	-1.30	367.10279	367.10346	1.82	C ₁₇ H ₂₀ O ₉	(-): 193, 191, 173, 149, 134

56	5.90	Secoxyloganin	-	-	-	449.12947	449.13006	1.32	C ₁₈ H ₂₆ O ₁₃	-
57	6.00	Unknown	350.18133	350.18094	-1.09	348.16693	348.16639	-1.55	C ₁₅ H ₂₇ NO ₈	(+): 333
58	6.04	4-sinapoylquinic acid	-	-	-	397.11337	397.11402	1.64	C ₁₈ H ₂₂ O ₁₀	(-): 223, 191, 169, 146
59	6.04	Genameside C	551.19731	551.19705	-0.48	595.18690	595.18797	1.81 ^b	C ₂₃ H ₃₄ O ₁₅	(-): 549, 225
60	6.12	Jasminoside I	493.22942	493.22795	-2.97	537.21744	537.21888	2.68 ^b	C ₂₂ H ₃₆ O ₁₂	-
61	6.19	8-epiloganin	-	-	-	435.15027	435.15080	1.22 ^b	C ₁₇ H ₂₆ O ₁₀	-
62	6.20	Clemastanin B	685.27192	685.27021	-2.49	729.26019	729.26114	1.30 ^b	C ₃₂ H ₄₄ O ₁₆	(-): 683, 521, 359, 329
63	6.23	Genipin 1- <i>O</i> -apiofuranosyl glucopyranoside	-	-	-	565.17717	565.17741	0.43 ^b	C ₂₂ H ₃₂ O ₁₄	(-): 519, 225
64	6.30	Geniposide	411.12650	411.12617	-0.80 ^a	433.13404	433.13515	2.57 ^b	C ₁₇ H ₂₄ O ₁₀	(-): 225, 207, 175, 147, 123, 101
65	6.37	Lariciresinol-4'- <i>O</i> -β-D-glucoside	-	-	-	521.20174	521.20284	2.10	C ₂₆ H ₃₄ O ₁₁	(-): 359
66	6.39	Loganin	-	-	-	435.15037	435.15080	0.99 ^b	C ₁₇ H ₂₆ O ₁₀	(-): 389, 227
67	6.40	Genameside D	551.19810	551.19705	-1.92	595.18761	595.18797	0.62 ^b	C ₂₃ H ₃₄ O ₁₅	(-): 549, 387, 225
68	6.45	Genipin 1- <i>O</i> -xylopyranosyl glucopyranoside	-	-	-	565.17714	565.17741	0.47 ^b	C ₂₂ H ₃₂ O ₁₄	(-): 519, 225
69	6.56	4- <i>p</i> -coumaroylquinic acid	339.10760	339.10744	-0.46	337.09252	337.09289	1.10	C ₁₆ H ₁₈ O ₈	(-): 191, 163
70	6.57	Dihydrogeniposide	-	-	-	435.15039	435.15080	0.94 ^b	C ₁₇ H ₂₆ O ₁₀	-
71	6.64	3,4-dicaffeoyl quinic acid isomer	-	-	-	515.11893	515.11950	1.10	C ₂₅ H ₂₄ O ₁₂	(-): 353, 191, 179, 135
72	6.66	2-hydroxy-1,4-phthalic acid	-	-	-	181.01393	181.01425	1.77	C ₈ H ₆ O ₅	(-): 137
73	6.69	Sinapoyl glucose	409.11081	409.11052	-0.71 ^a	385.11377	385.11402	0.65	C ₁₇ H ₂₂ O ₁₀	(-): 205

74	6.75	Jasminoside O	463.21815	463.21739	-1.64	507.20775	507.20831	1.12 ^b	C ₂₁ H ₃₄ O ₁₁	(-): 461
75	6.83	Epijasminoside A or Jasminoside A/E/K	331.17531	331.17513	-0.53	375.16576	375.16606	0.80 ^b	C ₁₆ H ₂₆ O ₇	(+): 169
76	6.91	Epijasminoside A or Jasminoside A/E/K	331.17535	331.17513	-0.66	375.16562	375.16606	1.16 ^b	C ₁₆ H ₂₆ O ₇	(+): 169
77	6.91	Acetylchlorogenic acid isomer	-	-	-	395.09796	395.09837	1.05	C ₁₈ H ₂₀ O ₁₀	(-): 161
78	6.95	3- <i>O</i> -feruloylquinic acid	369.11863	369.11801	-1.68	367.10320	367.10346	0.69	C ₁₇ H ₂₀ O ₉	(-): 193, 191, 173, 134
79	7.04	3-sinapoylquinic acid	399.12832	399.12857	0.63	397.11372	397.11402	0.75	C ₁₈ H ₂₂ O ₁₀	(-): 223, 191, 169, 146
80	7.05	Acetylchlorogenic acid isomer	-	-	-	395.09788	395.09837	1.25	C ₁₈ H ₂₀ O ₁₀	(-): 161
81	7.10	Epijasminoside A or Jasminoside A/E/K	331.17587	331.17513	-2.24	375.16571	375.16606	0.92 ^b	C ₁₆ H ₂₆ O ₇	-
82	7.10	Liriodendrin	-	-	-	787.26423	787.26662	3.04 ^b	C ₃₄ H ₄₆ O ₁₈	(-): 741
83	7.18	3- <i>O</i> -caffeoylshikimic acid	337.09182	337.09179	-0.08	335.07689	335.07724	1.05	C ₁₆ H ₁₆ O ₈	(-): 179, 161, 135
84	7.25	5,5'-dimethoxy lariciresinol-4'- <i>O</i> -glucoside isomer	605.22142	605.22046	-1.58 ^a	581.22327	581.22396	1.20	C ₂₈ H ₃₈ O ₁₃	(-): 415
85	7.26	Deoxyvasicinone	187.08655	187.08659	0.23	-	-	-	C ₁₁ H ₁₀ N ₂ O	-
86	7.33	4- <i>O</i> -caffeoylshikimic acid	337.09196	337.09179	-0.49	335.07695	335.07724	0.87	C ₁₆ H ₁₆ O ₈	(-): 179, 161, 135
87	7.34	Jasminoside C	329.15958	329.15948	-0.30	373.15012	373.15041	0.77 ^b	C ₁₆ H ₂₄ O ₇	(-): 165
88	7.40	Secoisolariciresinol 4- <i>O</i> -β-D-glucopyranoside	-	-	-	523.21806	523.21849	0.81	C ₂₆ H ₃₆ O ₁₁	(-): 361, 346, 165
89	7.42	3,4-dicaffeoyl quinic acid isomer	-	-	-	515.11917	515.11950	0.64	C ₂₅ H ₂₄ O ₁₂	(-): 353, 191, 179, 135

90	7.43	Darendroside B	-	-	-	475.18152	475.18210	1.22	C ₂₁ H ₃₂ O ₁₂	-
91	7.46	1- <i>O</i> -feruloyl heptopyranose	409.11085	409.11052	-0.80 ^a	385.11379	385.11402	0.59	C ₁₇ H ₂₂ O ₁₀	(+): 387
92	7.49	5- <i>O</i> -caffeoylshikimic acid	337.09182	337.09179	-0.08	335.07697	335.07724	0.80	C ₁₆ H ₁₆ O ₈	(-): 179, 161, 135
93	7.53	4- <i>O</i> -feruloylquinic acid	369.11834	369.11801	-0.91	367.10318	367.10346	0.76	C ₁₇ H ₂₀ O ₉	(-): 193, 191, 173
94	7.53	Methyl 5- <i>O</i> -feruloylquininate	383.13395	383.13366	-0.75	381.11878	381.11911	0.85	C ₁₈ H ₂₂ O ₉	(-): 179, 135
95	7.55	Acetylchlorogenic acid isomer	397.11398	397.11292	-2.66	395.09797	395.09837	1.01	C ₁₈ H ₂₀ O ₁₀	(-): 161
96	7.67	6''- <i>O</i> -trans- <i>p</i> -coumaroylgenipin gentiobioside isomer	-	-	-	695.21845	695.21927	1.19	C ₃₂ H ₄₀ O ₁₇	(-): 163
97	7.84	10- <i>O</i> -succinoylgeniposide isomer	-	-	-	487.14520	487.14571	1.06	C ₂₁ H ₂₈ O ₁₃	(-): 207
98	7.85	Rutin	611.16194	611.16066	-2.09	609.14541	609.14611	1.15	C ₂₇ H ₃₀ O ₁₆	(+): 465, 303
99	7.93	Kaempferol- <i>O</i> -rutinoside	595.16659	595.16575	-1.42	593.15034	593.15119	1.43	C ₂₇ H ₃₀ O ₁₅	(+): 449, 287
100	7.97	3,3',4-trihydroxy-4-methoxy-7,7'-epoxylignan or isomer	331.15398	331.15400	0.06	329.13936	329.13945	0.27	C ₁₉ H ₂₂ O ₅	-
101	7.97	Isovitexin	433.11320	433.11292	-0.63	431.09794	431.09837	0.99	C ₂₁ H ₂₀ O ₁₀	(+): 397, 379, 367, 361, 351, 349, 337, 323, 313, 309, 295, 283
102	7.98	Ferulic acid	-	-	-	193.05030	193.05063	1.75	C ₁₀ H ₁₀ O ₄	(-): 149
103	7.99	Lariciresinol-4- <i>O</i> -β- <i>D</i> -glucoside	545.20030	545.19933	-1.78 ^a	521.20208	521.20284	1.45	C ₂₆ H ₃₄ O ₁₁	(-): 359
104	8.06	Isoquercitrin	465.10324	465.10275	-1.05	463.08825	463.08820	-0.11	C ₂₁ H ₂₀ O ₁₂	(-): 301
105	8.08	5,5'-dimethoxy lariciresinol-4'- <i>O</i> -glucoside	-	-	-	581.22278	581.22396	2.04	C ₂₈ H ₃₈ O ₁₃	(-): 419
106	8.14	Neoamygdalin	458.16622	458.16569	-1.17	456.15052	456.15113	1.34	C ₂₀ H ₂₇ NO ₁₁	(+): 296, 278,

										250, 226
107	8.16	Prinsepiol	-	-	-	389.12433	389.12419	-0.36	C ₂₀ H ₂₂ O ₈	(-): 374
108	8.21	Kaempferol-3- <i>O</i> -rhamnose-7- <i>O</i> -glucose	595.16685	595.16575	-1.85	593.15013	593.15119	1.80	C ₂₇ H ₃₀ O ₁₅	(-): 285
109	8.22	Conicaoside	-	-	-	551.21258	551.21340	1.49	C ₂₇ H ₃₆ O ₁₂	-
110	8.23	(1R,7R,8S,10R)-7,8,11-trihydroxyguai-4-en-3-one-8-β-D-glucopyranoside	431.22802	431.22756	-1.07	429.21220	429.21301	1.88	C ₂₁ H ₃₄ O ₉	-
111	8.25	Scutellarin*	-	-	-	461.07177	461.07255	1.69	C ₂₁ H ₁₈ O ₁₂	(-): 285, 267, 239
112	8.26	Hyperoside	-	-	-	463.08806	463.08820	0.31	C ₂₁ H ₂₀ O ₁₂	(-): 301
113	8.28	Cynaroside	449.10858	449.10784	-1.66	-	-	-	C ₂₁ H ₂₀ O ₁₁	(+): 287
114	8.28	10- <i>O</i> -acetylgeniposide	453.13749	453.13673	-1.68 ^a	475.14518	475.14571	1.14 ^b	C ₁₉ H ₂₆ O ₁₁	(-): 209
115	8.33	Ferulic acid isomer	-	-	-	193.05025	193.05063	1.96	C ₁₀ H ₁₀ O ₄	(-): 149
116	8.40	2'- <i>O</i> -trans-p-coumaroylgardoside	-	-	-	519.15056	519.15080	0.46	C ₂₅ H ₂₈ O ₁₂	(-): 163, 145, 123
117	8.46	Methyl 3- <i>O</i> -feruloylquininate	383.13392	383.13366	-0.69	381.11872	381.11911	1.02	C ₁₈ H ₂₂ O ₉	(-): 179, 135
118	8.49	Quercetin 7- <i>O</i> -glucoside	-	-	-	463.08803	463.08820	0.37	C ₂₁ H ₂₀ O ₁₂	-
119	8.50	Isaindigodione isomer	327.13404	327.13393	-0.33	-	-	-	C ₁₈ H ₁₈ N ₂ O ₄	(+): 201
120	8.50	Acetylchlorogenic acid	397.11323	397.11292	-0.77	395.09803	395.09837	0.86	C ₁₈ H ₂₀ O ₁₀	(-): 161
121	8.55	3,4-dicaffeoyl quinic acid isomer	517.13394	517.13405	0.22	515.11892	515.11950	1.12	C ₂₅ H ₂₄ O ₁₂	(-): 353, 191, 179, 135
122	8.64	6'- <i>O</i> -trans-sinapoylgardoside	581.18735	581.18648	-1.49	579.17096	579.17193	1.68	C ₂₇ H ₃₂ O ₁₄	(-): 325, 223, 205
123	8.67	6''- <i>O</i> -trans-caffeoylgenipin gentiobioside	-	-	-	711.21302	711.21419	1.64	C ₃₂ H ₄₀ O ₁₈	(-): 179, 123

124	8.73	Nicotiflorin	595.16702	595.16575	-2.14	593.15055	593.15119	1.08	C ₂₇ H ₃₀ O ₁₅	(+): 287
125	8.74	Jasminoside T	463.21777	463.21739	-0.83	507.20763	507.20831	1.34 ^b	C ₂₁ H ₃₄ O ₁₁	(-): 461
126	8.77	3,4-dicaffeoyl quinic acid	517.13444	517.13405	-0.76	515.11880	515.11950	1.36	C ₂₅ H ₂₄ O ₁₂	(-): 353, 191, 179, 135
127	8.82	6'-O-trans-p-coumaroylgeniposidic acid	-	-	-	519.15034	519.15080	0.89	C ₂₅ H ₂₈ O ₁₂	(-): 211, 163, 145, 123
128	8.87	Methyl 4-O-feruloylquinic acid	383.13383	383.13366	-0.45	381.11868	381.11911	1.12	C ₁₈ H ₂₂ O ₉	(-): 179, 135
129	8.87	Isolariciresinol	-	-	-	405.15511	405.15549	0.93 ^b	C ₂₀ H ₂₄ O ₆	(-): 359, 344, 313
130	8.88	Acteoside	-	-	-	623.19687	623.19814	2.04	C ₂₉ H ₃₆ O ₁₅	(-): 461, 179, 161
131	8.89	10-O-succinoylgeniposide	-	-	-	487.14508	487.14571	1.31	C ₂₁ H ₂₈ O ₁₃	(-): 207
132	8.93	Chrysin-6,8-di-C-glucoside isomer	579.17083	579.17083	0.00	-	-	-	C ₂₇ H ₃₀ O ₁₄	-
133	8.94	Pinoresinol-4-O-glucoside	-	-	-	519.18678	519.18719	0.78	C ₂₆ H ₃₂ O ₁₁	(-): 357, 342, 151, 136
134	8.95	Kaempferol-3-O-rhamnose-7-O-glucose isomer	595.16702	595.16575	-2.14	593.15033	593.15119	1.46	C ₂₇ H ₃₀ O ₁₅	(-): 285
135	8.98	11-(6-O-trans-sinapoylglucopyranosyl)-gardendiol	-	-	-	565.19196	565.19266	1.25	C ₂₇ H ₃₄ O ₁₃	(-): 325, 295, 265, 223
136	9.01	6'-O-trans-sinapoylgardoside isomer	581.18696	581.18648	-0.82	579.17113	579.17193	1.39	C ₂₇ H ₃₂ O ₁₄	(-): 325, 223, 205
137	9.12	6''-O-trans-p-coumaroylgenipin gentiobioside isomer	697.23441	697.23383	-0.83	695.21800	695.21927	1.83	C ₃₂ H ₄₀ O ₁₇	(-): 469, 163
138	9.13	3,5-dicaffeoyl quinic acid	517.13446	517.13405	-0.78	515.11891	515.11950	1.14	C ₂₅ H ₂₄ O ₁₂	(-): 353, 191, 179, 135
139	9.13	Jasminoside R	-	-	-	535.20321	535.20323	0.04 ^b	C ₂₂ H ₃₄ O ₁₂	-

140	9.13	Acanthoside B	603.20543	603.20481	-1.02 ^a	579.20755	579.20831	1.31	C ₂₈ H ₃₆ O ₁₃	(-): 417, 402
141	9.16	Aschantin	401.15937	401.15948	0.27	-	-	-	C ₂₂ H ₂₄ O ₇	-
142	9.28	Rhoifolin	579.17148	579.17083	-1.11	577.15535	577.15628	1.61	C ₂₇ H ₃₀ O ₁₄	(+): 271
143	9.42	Isorhamnetin-3- <i>O</i> -glucoside	-	-	-	477.10445	477.10385	-1.26	C ₂₂ H ₂₂ O ₁₂	-
144	9.43	10- <i>O</i> -acetylgeniposide isomer	453.13697	453.13673	-0.53 ^a	475.14511	475.14571	1.28 ^b	C ₁₉ H ₂₆ O ₁₁	(-): 209
145	9.50	Apigenin-7- <i>O</i> -glucoside	433.11322	433.11292	-0.69	431.09786	431.09837	1.17	C ₂₁ H ₂₀ O ₁₀	(-): 269
146	9.58	Hesperidin	-	-	-	609.18270	609.18249	-0.34	C ₂₈ H ₃₄ O ₁₅	(-): 301
147	9.68	Indole-3-acetonitrile-2- <i>S</i> -β- <i>D</i> -glucopyranoside	351.10091	351.10092	0.03	349.08600	349.08637	1.05	C ₁₆ H ₁₈ N ₂ O ₅ S	(-): 187, 160
148	9.70	4,5-dicaffeoyl quinic acid	517.13420	517.13405	-0.29	515.11855	515.11950	1.85	C ₂₅ H ₂₄ O ₁₂	(-): 353, 191, 179, 135
149	9.77	6''- <i>O</i> -trans- <i>p</i> -coumaroylgenipin gentiobioside	697.23462	697.23383	-1.14	695.21785	695.21927	2.04	C ₃₂ H ₄₀ O ₁₇	(-): 469, 367, 349, 307, 265, 235, 207, 163, 145, 123
150	9.87	Salicylic acid	-	-	-	137.02415	137.02442	1.97	C ₇ H ₆ O ₃	-
151	9.93	6''- <i>O</i> -trans-sinapoylgenipin gentiobioside	757.25583	757.25496	-1.15	755.23836	755.24040	2.71	C ₃₄ H ₄₄ O ₁₉	(-): 427, 325, 265, 223, 205
152	10.03	3- <i>O</i> -caffeoyl-4- <i>O</i> -sinapoylquinic acid	561.16064	561.16027	-0.67	559.14498	559.14571	1.31	C ₂₇ H ₂₈ O ₁₃	(-): 397, 379, 353, 335, 223, 205, 191, 179, 173
153	10.05	Chrysoeriol-5- <i>O</i> -β- <i>D</i> -glucuronide	477.10278	477.10275	-0.06	475.08767	475.08820	1.11	C ₂₂ H ₂₀ O ₁₂	(-): 299, 284
154	10.07	6''- <i>O</i> -trans-feruloylgenipin gentiobioside	727.24492	727.24439	-0.72	725.22797	725.22984	2.57	C ₃₃ H ₄₂ O ₁₈	(-): 397, 295, 235, 225, 207, 193, 175, 123

155	10.10	3-(2'-carboxyphenyl)-4(3 <i>H</i>)-quinazolinone	267.07650	267.07642	-0.29	265.06144	265.06187	1.62	C ₁₅ H ₁₀ N ₂ O ₃	(+): 249
156	10.18	Scutellarein-4'-methyl ether- <i>O</i> -glucuronide	477.10276	477.10275	-0.02	475.08762	475.08820	1.22	C ₂₂ H ₂₀ O ₁₂	(-): 299, 284, 267
157	10.20	3,5-di- <i>O</i> -caffeoyl-4- <i>O</i> -(3-hydroxy-3-methyl) glutarylquinic acid	661.17685	661.17631	-0.82	659.16082	659.16176	1.42	C ₃₁ H ₃₂ O ₁₆	(-): 353, 191
158	10.27	8-hydroxypinoresinol	-	-	-	373.12859	373.12928	1.84	C ₂₀ H ₂₂ O ₇	(-): 313
159	10.33	Crocin I	-	-	-	975.37050	975.37148	1.00	C ₄₄ H ₆₄ O ₂₄	(-): 651
160	10.39	8-hydroxysyringaresinol	435.16490	435.16496	0.14	433.15006	433.15041	0.80	C ₂₂ H ₂₆ O ₉	(-): 403, 385, 373, 358, 343, 325
161	10.38	Pinoresinol-4- <i>O</i> -glucoside isomer	-	-	-	519.18682	519.18719	0.71	C ₂₆ H ₃₂ O ₁₁	(-): 357, 342
162	10.40	Methyl caffeate	-	-	-	193.05033	193.05063	1.57	C ₁₀ H ₁₀ O ₄	(-): 161
163	10.43	Secoisolariciresinol	-	-	-	361.16517	361.16566	1.35	C ₂₀ H ₂₆ O ₆	(-): 346, 165
164	10.63	Hydroxymedioresinol	405.15380	405.15439	1.47	403.13953	403.13984	0.77	C ₂₁ H ₂₄ O ₈	(-): 343
165	10.71	Indole-3-acetonitrile-4-methoxy-2- <i>S</i> -β-D-glucopyranoside or <i>N</i> -methoxyindole-3-acetonitrile-2- <i>S</i> -β-D-glucopyranoside	381.11170	381.11148	-0.57	379.09650	379.09693	1.13	C ₁₇ H ₂₀ N ₂ O ₆ S	(+): 219
166	10.73	6'-trans-sinapoylgeniposide isomer	-	-	-	593.18666	593.18758	1.56	C ₂₈ H ₃₄ O ₁₄	-
167	10.78	6'- <i>O</i> -trans-sinapoyl jasminoside L	553.22815	553.22795	-0.35	551.21256	551.21340	1.52	C ₂₇ H ₃₆ O ₁₂	(-): 223
168	10.83	5- <i>O</i> -caffeoyl-4- <i>O</i> -sinapoylquinic acid	561.16062	561.16027	-0.63	559.14497	559.14571	1.33	C ₂₇ H ₂₈ O ₁₃	(-): 397, 379, 353, 335, 223, 205, 191, 179, 173

169	11.04	Baicalin*	447.09147	447.09219	1.61	445.07661	445.07763	2.31	C ₂₁ H ₁₈ O ₁₁	(-): 269, 251, 241, 223
170	11.12	Fisetin	287.05482	287.05501	0.68	285.03979	285.04046	2.36	C ₁₅ H ₁₀ O ₆	(+): 137
171	11.18	Oroxin A	433.11293	433.11292	-0.01	431.09763	431.09837	1.73	C ₂₁ H ₂₀ O ₁₀	(+): 271
172	11.21	5- <i>O</i> -caffeoyl-4- <i>O</i> -sinapoylquinic acid isomer	561.16119	561.16027	-1.65	559.14468	559.14571	1.85	C ₂₇ H ₂₈ O ₁₃	(-): 223
173	11.24	3-(2'-hydroxyphenyl)-4-(3 <i>H</i>)-quinazolinone	239.08141	239.08150	0.38	-	-	-	C ₁₄ H ₁₀ N ₂ O ₂	(+): 221
174	11.41	6'-trans-sinapoylgeniposide	595.20212	595.20213	0.02	593.18659	593.18758	1.67	C ₂₈ H ₃₄ O ₁₄	(-): 367, 223, 205, 123
175	11.49	6''- <i>O</i> -trans-coumaroylgeniposide	535.18076	535.18100	0.45	533.16588	533.16645	1.07	C ₂₆ H ₃₀ O ₁₂	(-): 307, 145
176	11.49	6'- <i>O</i> -trans-sinapoyljasminoside L isomer	553.22812	553.22795	-0.30	551.21263	551.21340	1.39	C ₂₇ H ₃₆ O ₁₂	(-): 265
177	11.78	Chrysoeriol-7- <i>O</i> -β-D-glucuronide	477.10243	477.10275	0.67	475.08770	475.08820	1.06	C ₂₂ H ₂₀ O ₁₂	(-): 299, 284
178	11.92	5,6-dihydroxyl flavanone-7- <i>O</i> -glucuronide	-	-	-	447.09274	447.09329	1.21	C ₂₁ H ₂₀ O ₁₁	(-): 271
179	12.14	Oroxylin A-7- <i>O</i> -glucuronide isomer	461.10757	461.10784	0.59	459.09264	459.09329	1.40	C ₂₂ H ₂₀ O ₁₁	-
180	12.21	Norwogonin-7- <i>O</i> -glucuronide	447.09176	447.09219	0.95	445.07686	445.07763	1.73	C ₂₁ H ₁₈ O ₁₁	(-): 269
181	12.42	Fisetin isomer	287.05465	287.05501	1.27	285.04016	285.04046	1.04	C ₁₅ H ₁₀ O ₆	(-): 241
182	12.51	Hydroxyl oroxylin-A-7- <i>O</i> -glucuronide	477.10233	477.10275	0.88	475.08769	475.08820	1.08	C ₂₂ H ₂₀ O ₁₂	(-): 299
183	12.55	Phellinsin A	-	-	-	357.06119	357.06159	1.11	C ₁₈ H ₁₄ O ₈	-
184	12.72	Dihydroxyflavone- <i>O</i> -glucopyranoside	417.11788	417.11801	0.30	-	-	-	C ₂₁ H ₂₀ O ₉	(+): 255
185	12.73	Norwogonin-8- <i>O</i> -glucuronide	447.09171	447.09219	1.07	445.07691	445.07763	1.63	C ₂₁ H ₁₈ O ₁₁	(-): 269

		isomer								
186	12.81	Luteolin*	287.05489	287.05501	0.43	285.04015	285.04046	1.09	C ₁₅ H ₁₀ O ₆	(-): 241, 217, 199, 175, 151, 133
187	12.81	Tricin 7- <i>O</i> -glucoside	-	-	-	491.11918	491.11950	0.65	C ₂₃ H ₂₄ O ₁₂	(-): 329, 313
188	12.83	Quercetin	-	-	-	301.03481	301.03538	1.88	C ₁₅ H ₁₀ O ₇	-
189	12.89	Oroxylin A-7- <i>O</i> -glucuronide*	461.10720	461.10784	1.39	459.09243	459.09329	1.87	C ₂₂ H ₂₀ O ₁₁	(+): 285, 270
190	13.00	Chrysin-7- <i>O</i> -glucuronide	431.09730	431.09727	-0.07	429.08197	429.08272	1.75	C ₂₁ H ₁₈ O ₁₀	(-): 253
191	13.09	Hydroxyl wogonoside	477.10274	477.10275	0.02	475.08787	475.08820	0.70	C ₂₂ H ₂₀ O ₁₂	(-): 299
192	13.29	6''- <i>O</i> -trans- <i>p</i> -cinnamoylgenipin gentiobioside	703.22056	703.22086	0.43 ^a	725.22860	725.22984	1.71 ^b	C ₃₂ H ₄₀ O ₁₆	(-): 531, 355, 225, 207, 147, 123
193	13.35	Norwogonin-8- <i>O</i> -glucuronide	447.09160	447.09219	1.32	445.07686	445.07763	1.74	C ₂₁ H ₁₈ O ₁₁	(-): 269
194	13.46	Oroxin A isomer	433.11242	433.11292	1.16	431.09801	431.09837	0.84	C ₂₁ H ₂₀ O ₁₀	(+): 271
195	13.61	Wogonoside*	461.10741	461.10784	0.93	459.09240	459.09329	1.93	C ₂₂ H ₂₀ O ₁₁	(-): 283, 268
196	13.87	Baicalin isomer	447.09155	447.09219	1.44	445.07707	445.07763	1.26	C ₂₁ H ₁₈ O ₁₁	(-): 269
197	13.99	6'- <i>O</i> -trans-sinapoyl jasminoside A	537.23257	537.23304	0.87	535.21786	535.21849	1.18	C ₂₇ H ₃₆ O ₁₁	-
198	13.99	5,7-dihydroxy-6,8-dimethoxyflavo ne-7- <i>O</i> -glucuronide	491.11798	491.11840	0.86	489.10346	489.10385	0.80	C ₂₃ H ₂₂ O ₁₂	(+): 315, 285
199	14.09	Baicalin ethyl ester or isomer	475.12292	475.12349	1.19	473.10849	473.10894	0.95	C ₂₃ H ₂₂ O ₁₁	(+): 271
200	14.11	Fisetin isomer	287.05497	287.05501	0.15	285.04011	285.04046	1.23	C ₁₅ H ₁₀ O ₆	(-): 241
201	14.66	6'-trans-sinapoylgeniposide isomer	617.18321	617.18408	1.40 ^a	593.18695	593.18758	1.06	C ₂₈ H ₃₄ O ₁₄	(-): 367, 223, 205, 123
202	14.75	6'- <i>O</i> -trans-sinapoyljasminoside C	535.21673	535.21739	1.22	533.20211	533.20284	1.36	C ₂₇ H ₃₄ O ₁₁	(-): 223, 205
203	14.77	Baicalin ethyl ester or isomer	475.12276	475.12349	1.53	473.10828	473.10894	1.38	C ₂₃ H ₂₂ O ₁₁	(-): 269
204	15.09	Apigenin*	271.06019	271.06010	-0.33	269.04512	269.04555	1.59	C ₁₅ H ₁₀ O ₅	(-): 237, 227,

										225, 209, 201,183, 181, 175, 151, 149
205	15.09	Tenaxin II	301.07030	301.07066	1.22	299.05570	299.05611	1.39	C ₁₆ H ₁₂ O ₆	(-): 284
206	15.49	Tectorigenin	301.07033	301.07066	1.10	299.05569	299.05611	1.40	C ₁₆ H ₁₂ O ₆	(-): 284
207	15.61	9,12-dihydroxy-13-oxooctadec-14- enoic acid	329.23259	329.23225	-1.03	327.21728	327.21770	1.27	C ₁₈ H ₃₂ O ₅	(-): 291, 273, 247, 239, 229, 211, 209, 203, 197, 193, 183, 171
208	15.73	Norwogonin	271.05982	271.06010	1.02	269.04515	269.04555	1.49	C ₁₅ H ₁₀ O ₅	(+): 253, 225
209	15.85	Baicalin ethyl ester or isomer	475.12266	475.12349	1.74	473.10820	473.10894	1.55	C ₂₃ H ₂₂ O ₁₁	(-): 269
210	15.91	9,12-dihydroxy-13-oxooctadec-14- enoic acid isomer	329.23156	329.23225	2.10	327.21722	327.21770	1.44	C ₁₈ H ₃₂ O ₅	(-): 229, 211, 183, 171
211	16.08	4'-hydroxyl wogonin	301.07023	301.07066	1.45	299.05566	299.05611	1.52	C ₁₆ H ₁₂ O ₆	(+): 286
212	16.34	Baicalein*	271.05970	271.06010	1.49	269.04510	269.04555	1.65	C ₁₅ H ₁₀ O ₅	(+): 253, 225
213	16.35	Fisetin isomer	287.05504	287.05501	-0.09	285.03999	285.04046	1.67	C ₁₅ H ₁₀ O ₆	(+): 241
214	16.41	Kaempferide isomer	301.07062	301.07066	0.15	299.05556	299.05611	1.86	C ₁₆ H ₁₂ O ₆	(+): 286, 258
215	16.57	Neocrocin E	-	-	-	975.36982	975.37148	1.70	C ₄₄ H ₆₄ O ₂₄	(-): 651
216	16.77	Tricin	331.08103	331.08123	0.60	329.06627	329.06668	1.23	C ₁₇ H ₁₄ O ₇	(-): 314, 299
217	16.88	Crocin-III or 13-cis-croctin-8'-O-β-D-gentiobio side or isomer	653.28018	653.28038	0.31	651.26341	651.26583	3.72	C ₃₂ H ₄₄ O ₁₄	(-): 327
218	17.06	9,12-dihydroxy-13-oxooctadecanoi c acid	-	-	-	329.23281	329.23335	1.63	C ₁₈ H ₃₄ O ₅	(-): 311, 229, 211, 183, 171
219	17.13	4'-hydroxyl wogonin isomer	-	-	-	299.05571	299.05611	1.35	C ₁₆ H ₁₂ O ₆	-

220	17.62	Dehydrodeoxycholic acid or isomer	389.26791	389.26864	1.87	-	-	-	C ₂₄ H ₃₆ O ₄	(+): 353
221	17.86	Tetrahydroxycholan-24-oic acid	-	-	-	423.27447	423.27521	1.76	C ₂₄ H ₄₀ O ₆	(-): 405
222	18.35	Glycodeoxycholate	450.32058	450.32140	1.81	448.30582	448.30685	2.30	C ₂₆ H ₄₃ NO ₅	(-): 404, 403
223	18.37	6'-O-trans-sinapoyljasminoside A	-	-	-	535.21818	535.21849	0.57	C ₂₇ H ₃₆ O ₁₁	-
224	18.69	Trihydroxy-dimethoxyflavone	331.08050	331.08123	2.20	329.06615	329.06668	1.59	C ₁₇ H ₁₄ O ₇	(-): 314, 299
225	18.71	9,12-dihydroxy-13-oxooctadecanoic acid isomer	-	-	-	329.23279	329.23335	1.69	C ₁₈ H ₃₄ O ₅	(-): 311, 229, 211
226	18.94	9,12-dihydroxy-13-oxooctadecanoic acid isomer	-	-	-	329.23287	329.23335	1.46	C ₁₈ H ₃₄ O ₅	(-): 311, 229, 211
227	18.98	Dehydrodeoxycholic acid or isomer	389.26815	389.26864	1.25	-	-	-	C ₂₄ H ₃₆ O ₄	(+): 353, 335
228	19.17	3,12-dihydroxy-7-oxo-5-cholan-24-oic acid isomer	407.27837	407.27920	2.04	405.26388	405.26465	1.90	C ₂₄ H ₃₈ O ₅	(-): 387, 369, 361, 343, 289
229	19.61	9,12-dihydroxy-13-oxooctadecanoic acid isomer	-	-	-	329.23276	329.23335	1.80	C ₁₈ H ₃₄ O ₅	(-): 311, 229, 211
230	19.69	5,7,3'-trihydroxy-6,4',5'-trimethoxyflavone	-	-	-	359.07639	359.07724	2.36	C ₁₈ H ₁₆ O ₈	-
231	20.14	5,2'-dihydroxy-6,7,8-trimethoxyflavone	345.09644	345.09688	1.27	343.08168	343.08233	1.88	C ₁₈ H ₁₆ O ₇	(-): 328, 313, 298, 285, 270
232	20.42	3-hydroxy-6-oxo-cholan-24-oic acid isomer	391.28418	391.28429	0.28	-	-	-	C ₂₄ H ₃₈ O ₄	(+): 355, 337, 319
233	20.42	Hyocholic acid	409.29450	409.29485	0.85	407.27999	407.28030	0.75	C ₂₄ H ₄₀ O ₅	(+): 373, 355, 337
234	20.50	Wogonin*	285.07532	285.07575	1.52	283.06082	283.06120	1.34	C ₁₆ H ₁₂ O ₅	(+): 270
235	20.50	Dehydrodeoxycholic acid or isomer	389.26794	389.26864	1.78	-	-	-	C ₂₄ H ₃₆ O ₄	(+): 371, 353,

		isomer								335, 317
236	20.58	9,12-dihydroxy-13-oxooctadecanoic acid isomer	-	-	-	329.23281	329.23335	1.64	C ₁₈ H ₃₄ O ₅	(-): 311, 229, 211
237	20.63	Amentoflavone isomer	539.09618	539.09727	2.03	537.08230	537.08272	0.79	C ₃₀ H ₁₈ O ₁₀	(-): 375
238	20.66	Chrysin	255.06477	255.06519	1.63	253.05015	253.05063	1.90	C ₁₅ H ₁₀ O ₄	(-): 209, 181
239	20.71	Crocin-III or 13-cis-crocetin-8'-O-β-D-gentiobioside or isomer	-	-	-	651.26416	651.26583	2.56	C ₃₂ H ₄₄ O ₁₄	(-): 327
240	20.92	Skullcapflavone I	315.08580	315.08631	1.65	313.07119	313.07176	1.83	C ₁₇ H ₁₄ O ₆	(-): 298, 283, 255, 239, 211, 201, 199, 183, 173, 155
241	20.99	Hyodeoxycholic acid isomer	-	-	-	437.28983	437.29086	2.36 ^b	C ₂₄ H ₄₀ O ₄	(-): 391
242	21.00	Crocin-III or 13-cis-crocetin-8'-O-β-D-gentiobioside or isomer	-	-	-	651.26419	651.26583	2.52	C ₃₂ H ₄₄ O ₁₄	(-): 327
243	21.20	Skullcapflavone II	375.10666	375.10744	2.09	373.09218	373.09289	1.89	C ₁₉ H ₁₈ O ₈	(-): 358, 343, 328, 315, 300, 285, 272, 269, 257, 213
244	21.30	Dehydrodeoxycholic acid or isomer	389.26796	389.26864	1.73	-	-	-	C ₂₄ H ₃₆ O ₄	(+): 371, 353, 335, 317
245	21.34	3,12-dihydroxy-7-oxo-5-cholan-24-oic acid	407.27833	407.27920	2.15	405.26380	405.26465	2.09	C ₂₄ H ₃₈ O ₅	(-): 361
246	21.38	Oroxylin A	285.07527	285.07575	1.67	283.06069	283.06120	1.78	C ₁₆ H ₁₂ O ₅	(+): 270
247	21.50	3-hydroxy-6-oxo-cholan-24-oic	391.28467	391.28429	-0.98	435.27447	435.27521	1.70 ^b	C ₂₄ H ₃₈ O ₄	(-): 389, 371

		acid isomer								
248	21.65	Cholic acid*	409.29494	409.29485	-0.22	407.28006	407.28030	0.59	C ₂₄ H ₄₀ O ₅	(-): 343
249	22.01	Crocin-III or 13-cis-croctetin-8'-O-β-D-gentiobio side or isomer	653.27815	653.28038	3.42	651.26426	651.26583	2.42	C ₃₂ H ₄₄ O ₁₄	(-): 327
250	22.42	Chenodeoxycholic acid	393.29839	393.29994	3.93	391.28502	391.28538	0.93	C ₂₄ H ₄₀ O ₄	(-): 373
251	22.65	Rivularin	345.09644	345.09688	1.27	343.08198	343.08233	1.01	C ₁₈ H ₁₆ O ₇	(-): 328, 313, 298, 270
252	23.29	3-hydroxy-6-oxo-cholan-24-oic acid isomer	391.28343	391.28429	2.20	435.27436	435.27521	1.97 ^b	C ₂₄ H ₃₈ O ₄	(-): 389
253	23.66	3-hydroxy-6-oxo-cholan-24-oic acid isomer	-	-	-	435.27434	435.27521	2.00 ^b	C ₂₄ H ₃₈ O ₄	(-): 389
254	23.72	7-O-methylscutellarein-O-baicalei n	553.11192	553.11292	1.81	551.09743	551.09837	1.71	C ₃₁ H ₂₀ O ₁₀	(-): 281, 269
255	24.22	3-hydroxy-6-oxo-cholan-24-oic acid	391.28342	391.28429	2.22	435.27418	435.27521	2.36 ^b	C ₂₄ H ₃₈ O ₄	(-): 389, 345
256	24.56	Bis(2-ethylhexyl) phthalate	391.28345	391.28429	2.13	435.27442	435.27521	1.81 ^b	C ₂₄ H ₃₈ O ₄	(-): 389
257	24.77	Moslosooflavone	299.09125	299.09140	0.50	-	-	-	C ₁₇ H ₁₄ O ₅	(+): 284, 266, 238
258	24.98	9/12-Octadecanedioic acid or isomer	337.23498	337.23493	-0.16 ^a	313.23850	313.23843	-0.22	C ₁₈ H ₃₄ O ₄	(-): 295, 277
259	25.08	Croctetin	329.17413	329.17474	1.85	327.16015	327.16018	0.09	C ₂₀ H ₂₄ O ₄	(-): 283
260	25.25	3-hydroxy-6-oxo-cholan-24-oic acid	391.28324	391.28429	2.69	435.27450	435.27521	1.63 ^b	C ₂₄ H ₃₈ O ₄	(-): 389
261	25.30	9/12-Octadecanedioic acid or isomer	337.23499	337.23493	-0.19 ^a	313.23829	313.23843	0.45	C ₁₈ H ₃₄ O ₄	(-): 295

262	25.30	Croctetin isomer	329.17438	329.17474	1.08	327.15998	327.16018	0.63	C ₂₀ H ₂₄ O ₄	(-): 283
263	25.46	Mosloflavone	299.09101	299.09140	1.30	-	-	-	C ₁₇ H ₁₄ O ₅	(+): 284, 255
264	25.50	3-hydroxy-6-oxo-cholan-24-oic acid isomer	-	-	-	435.27457	435.27521	1.47 ^b	C ₂₄ H ₃₈ O ₄	(-): 389
265	25.80	Croctetin isomer	-	-	-	327.16003	327.16018	0.45	C ₂₀ H ₂₄ O ₄	(-): 283
266	25.85	Deoxycholic acid	-	-	-	391.28482	391.28538	1.44	C ₂₄ H ₄₀ O ₄	(-): 355
267	26.25	Hyodeoxycholic acid*	-	-	-	391.28527	391.28538	0.30	C ₂₄ H ₄₀ O ₄	(-): 355, 347, 345, 329, 327
268	26.34	3-hydroxy-6-oxo-cholan-24-oic acid isomer	-	-	-	435.27474	435.27521	1.09 ^b	C ₂₄ H ₃₈ O ₄	(-): 389
269	26.59	Croctetin isomer	329.17417	329.17474	1.70	327.16009	327.16018	0.28	C ₂₀ H ₂₄ O ₄	(-): 283
270	26.66	3-hydroxy-6-oxo-cholan-24-oic acid	-	-	-	435.27444	435.27521	1.77 ^b	C ₂₄ H ₃₈ O ₄	(-): 389
271	27.18	Croctetin isomer	329.17422	329.17474	1.57	327.15996	327.16018	0.68	C ₂₀ H ₂₄ O ₄	(-): 283
272	27.92	Croctetin isomer	-	-	-	327.16014	327.16018	0.12	C ₂₀ H ₂₄ O ₄	(-): 283
273	29.03	9-hydroxyoctadecanoic acid	-	-	-	299.25865	299.25917	1.74	C ₁₈ H ₃₆ O ₃	-
274	29.96	γ-Linolenic acid	-	-	-	277.21672	277.21730	2.09	C ₁₈ H ₃₀ O ₂	(-): 233
275	30.73	Linoleic acid	-	-	-	279.23226	279.23295	2.47	C ₁₈ H ₃₂ O ₂	-
276	31.60	Oleic acid	-	-	-	281.24785	281.24860	2.69	C ₁₈ H ₃₄ O ₂	-

^a: [M+Na]⁺ ; ^b: [M+HCOO]⁻; ^c: [M+NH₄]⁺. -: not detected. *Compared with a reference standard.