

**Supporting Information**

**A novel ion mobility separation-enabled and precursor ions list-included high-definition data-dependent acquisition (HDDDA) approach: Method development and its application to the comprehensive multicomponent characterization of Fangji Huangqi Decoction**

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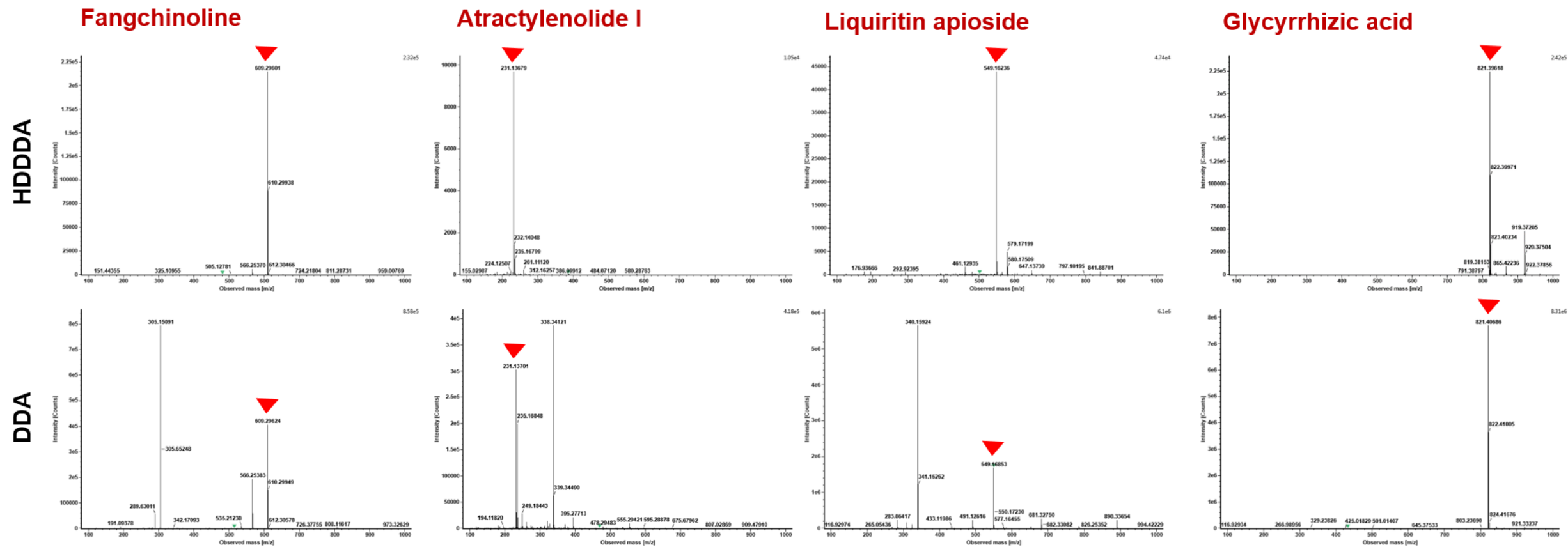


Fig. S1 Comparison of the MS<sup>1</sup> spectra of four representative components acquired by HDDDA and DDA.

**Table S1** Detailed information of 62 reference compounds used in this work.

NO.	Trivial name	M.F.	Exact Mass	Type
1	Liquiritin	C <sub>21</sub> H <sub>22</sub> O <sub>9</sub>	418.1264	<b>Flavonoid</b>
2	Liquiritigenin	C <sub>15</sub> H <sub>12</sub> O <sub>4</sub>	256.0736	
3	Neoliquiritin	C <sub>21</sub> H <sub>22</sub> O <sub>9</sub>	418.1264	
4	(+/-)-Naringenin	C <sub>15</sub> H <sub>12</sub> O <sub>5</sub>	272.0685	
5	Liquiritin apioside	C <sub>26</sub> H <sub>30</sub> O <sub>13</sub>	550.1686	
6	Naringin	C <sub>27</sub> H <sub>32</sub> O <sub>14</sub>	580.1792	
7	Complanatoside	C <sub>28</sub> H <sub>32</sub> O <sub>16</sub>	624.1690	
8	Astragalin	C <sub>21</sub> H <sub>20</sub> O <sub>11</sub>	448.1006	
9	Neoisoliquiritin	C <sub>21</sub> H <sub>22</sub> O <sub>9</sub>	418.1264	
10	Formononetin glucoside	C <sub>22</sub> H <sub>22</sub> O <sub>9</sub>	430.1264	
11	Calycosin	C <sub>16</sub> H <sub>12</sub> O <sub>5</sub>	284.0685	
12	Formononetin	C <sub>16</sub> H <sub>12</sub> O <sub>4</sub>	268.0736	
13	Daidzein	C <sub>15</sub> H <sub>10</sub> O <sub>4</sub>	254.0579	
14	Calycosin-7- <i>O</i> - $\beta$ -D-glucoside	C <sub>22</sub> H <sub>22</sub> O <sub>10</sub>	446.1213	
15	Glycyrrhisoflavone	C <sub>20</sub> H <sub>18</sub> O <sub>6</sub>	354.1103	
16	Semilicoisoflavone B	C <sub>20</sub> H <sub>16</sub> O <sub>6</sub>	352.0947	
17	Fangchinoline	C <sub>37</sub> H <sub>40</sub> N <sub>2</sub> O <sub>6</sub>	608.2886	<b>Alkaloid</b>
18	Tetrandrine	C <sub>38</sub> H <sub>42</sub> N <sub>2</sub> O <sub>6</sub>	622.3043	
19	Cepharanthine	C <sub>37</sub> H <sub>38</sub> N <sub>2</sub> O <sub>6</sub>	606.2730	
20	Neferine	C <sub>38</sub> H <sub>44</sub> N <sub>2</sub> O <sub>6</sub>	624.3199	
21	Daurisoline	C <sub>37</sub> H <sub>42</sub> N <sub>2</sub> O <sub>6</sub>	610.3043	
22	(+)-Norisoboldine	C <sub>18</sub> H <sub>19</sub> NO <sub>4</sub>	313.1314	
23	Magnoflorine	C <sub>20</sub> H <sub>24</sub> NO <sub>4</sub> <sup>+</sup>	342.1700	
24	Sinomenine	C <sub>19</sub> H <sub>23</sub> NO <sub>4</sub>	329.1627	
25	Berberine	C <sub>20</sub> H <sub>18</sub> NO <sub>4</sub> <sup>+</sup>	336.1230	
26	Protopine	C <sub>20</sub> H <sub>19</sub> NO <sub>5</sub>	353.1263	
27	Palmatine	C <sub>21</sub> H <sub>22</sub> NO <sub>4</sub> <sup>+</sup>	352.1543	
28	Tetrahydroberberine	C <sub>20</sub> H <sub>21</sub> NO <sub>4</sub>	339.1471	
29	( <i>R</i> )-(+)-Corypalmine	C <sub>20</sub> H <sub>23</sub> NO <sub>4</sub>	341.1627	
30	Rotundine	C <sub>21</sub> H <sub>25</sub> NO <sub>4</sub>	355.1784	
31	Glycyrrhizic acid	C <sub>42</sub> H <sub>62</sub> O <sub>16</sub>	822.4038	<b>Triterpene/ Saponin</b>
32	Astragaloside IV	C <sub>41</sub> H <sub>68</sub> O <sub>14</sub>	784.4609	
33	Astragaloside II	C <sub>43</sub> H <sub>70</sub> O <sub>15</sub>	826.4715	
34	Isoastragaloside I	C <sub>45</sub> H <sub>72</sub> O <sub>16</sub>	868.4820	
35	Astragaloside III	C <sub>41</sub> H <sub>68</sub> O <sub>14</sub>	784.4609	
36	Isoastragaloside IV	C <sub>41</sub> H <sub>68</sub> O <sub>12</sub>	784.4609	
37	Isoastragaloside II	C <sub>43</sub> H <sub>70</sub> O <sub>15</sub>	826.4715	

38	Astragaloside I	C <sub>45</sub> H <sub>72</sub> O <sub>16</sub>	868.4820	
39	Glycyrrhizic acid ammonium salt	C <sub>42</sub> H <sub>65</sub> NO <sub>16</sub>	839.4303	
40	Lupeol	C <sub>30</sub> H <sub>50</sub> O	426.3862	
41	Betulinic acid	C <sub>30</sub> H <sub>48</sub> O <sub>3</sub>	456.3603	
42	Glycyrrhetic acid	C <sub>30</sub> H <sub>46</sub> O <sub>4</sub>	470.3396	
43	Cycloastragenol	C <sub>30</sub> H <sub>50</sub> O <sub>5</sub>	490.3658	
44	Glabridin	C <sub>20</sub> H <sub>20</sub> O <sub>4</sub>	324.1362	
45	Astraisoflavan-7- <i>O</i> - $\beta$ -D-glucoside (6aR, 11aR)9,10-	C <sub>23</sub> H <sub>28</sub> O <sub>10</sub>	464.1682	
46	Dimethoxypterocarpan-3- <i>O</i> - $\beta$ -D- glycoside	C <sub>23</sub> H <sub>26</sub> O <sub>10</sub>	462.1526	
47	Aristolochic acid I	C <sub>17</sub> H <sub>11</sub> NO <sub>7</sub>	341.0536	
48	Syringin	C <sub>17</sub> H <sub>24</sub> O <sub>9</sub>	372.1420	
49	Echinatin	C <sub>16</sub> H <sub>14</sub> O <sub>4</sub>	270.0892	
50	Isoliquiritigenin	C <sub>15</sub> H <sub>12</sub> O <sub>4</sub>	256.0736	
51	Licochalcone A	C <sub>21</sub> H <sub>22</sub> O <sub>4</sub>	338.1518	
52	Corylifolinin	C <sub>20</sub> H <sub>20</sub> O <sub>4</sub>	324.1362	<b>Others</b>
53	Caffeic acid	C <sub>9</sub> H <sub>8</sub> O <sub>4</sub>	180.0423	
54	Daphnetin	C <sub>9</sub> H <sub>6</sub> O <sub>4</sub>	178.0266	
55	Scopoletin	C <sub>10</sub> H <sub>8</sub> O <sub>4</sub>	192.0423	
56	Atractyloside A	C <sub>21</sub> H <sub>36</sub> O <sub>10</sub>	448.2308	
57	Atractylenolide I	C <sub>15</sub> H <sub>18</sub> O <sub>2</sub>	230.1307	
58	Atractylenolide II	C <sub>15</sub> H <sub>20</sub> O <sub>2</sub>	232.1463	
59	Atractylenolide III	C <sub>15</sub> H <sub>20</sub> O <sub>3</sub>	248.1412	
60	Uridine	C <sub>9</sub> H <sub>12</sub> N <sub>2</sub> O <sub>6</sub>	244.0695	
61	Rosavin	C <sub>20</sub> H <sub>28</sub> O <sub>10</sub>	428.1682	
62	Nystose	C <sub>24</sub> H <sub>42</sub> O <sub>21</sub>	666.2219	

**Table S2** The precursor ions list in the positive ESI mode.

<b>No.</b>	<b>Adduct</b>	<b><i>m/z</i></b>	<b>Integer mass (Da)</b>	<b>Mass defect (mDa)</b>
1	[M+H] <sup>+</sup>	116.0705	116	70.50
2	[M+H] <sup>+</sup>	124.0392	124	39.20
3	[M+H] <sup>+</sup>	126.0531	126	53.10
4	[M+H] <sup>+</sup>	127.0389	127	38.90
5	[M+H] <sup>+</sup>	136.0617	136	61.70
6	[M+Na] <sup>+</sup>	138.0531	138	53.10
7	[M+H] <sup>+</sup>	139.0389	139	38.90
8	[M+H] <sup>+</sup>	143.0338	143	33.80
9	[M+H] <sup>+</sup>	147.0440	147	44.00
10	[M+Na] <sup>+</sup>	149.0215	149	21.50
11	[M+H] <sup>+</sup>	163.0389	163	38.90
12	[M+H] <sup>+</sup>	175.1189	175	118.90
13	[M+Na] <sup>+</sup>	177.0528	177	52.80
14	[M+H] <sup>+</sup>	177.0981	177	98.10
15	[M+H] <sup>+</sup>	179.0702	179	70.20
16	[M+H] <sup>+</sup>	181.0706	181	70.60
17	[M+H] <sup>+</sup>	183.0862	183	86.20
18	[M+H] <sup>+</sup>	189.1121	189	112.10
19	[M+Na] <sup>+</sup>	191.0321	191	32.10
20	[M+H] <sup>+</sup>	193.0495	193	49.50
21	[M+H] <sup>+</sup>	195.0651	195	65.10
22	[M+H] <sup>+</sup>	195.0862	195	86.20
23	[M+H] <sup>+</sup>	197.0655	197	65.50
24	[M+Na] <sup>+</sup>	197.1015	197	101.50
25	[M+Na] <sup>+</sup>	199.0807	199	80.70
26	[M+H] <sup>+</sup>	210.0760	210	76.00
27	[M+H] <sup>+</sup>	219.1015	219	101.50
28	[M+H] <sup>+</sup>	219.1743	219	174.30
29	[M+H] <sup>+</sup>	231.1379	231	137.90
30	[M+Na] <sup>+</sup>	239.1412	239	141.20
31	[M+Na] <sup>+</sup>	240.1490	240	149.00
32	[M+Na] <sup>+</sup>	241.0841	241	84.10
33	[M+H] <sup>+</sup>	241.0858	241	85.80
34	[M+Na] <sup>+</sup>	241.1569	241	156.90
35	[M+H] <sup>+</sup>	245.0767	245	76.70
36	[M+H] <sup>+</sup>	249.1328	249	132.80
37	[M+Na] <sup>+</sup>	252.1365	252	136.50
38	[M+Na] <sup>+</sup>	253.1205	253	120.50

39	[M+H] <sup>+</sup>	255.0651	255	65.10
40	[M+Na] <sup>+</sup>	255.1361	255	136.10
41	[M+H] <sup>+</sup>	257.0808	257	80.80
42	[M+H] <sup>+</sup>	259.0964	259	96.40
43	[M+H] <sup>+</sup>	261.1121	261	112.10
44	[M+Na] <sup>+</sup>	261.1831	261	183.10
45	[M+Na] <sup>+</sup>	263.0684	263	68.40
46	[M+H] <sup>+</sup>	265.1434	265	143.40
47	[M+H] <sup>+</sup>	268.1040	268	104.00
48	[M+H] <sup>+</sup>	269.0808	269	80.80
49	[M+H] <sup>+</sup>	271.0600	271	60.00
50	[M+H] <sup>+</sup>	271.0964	271	96.40
51	[M+H] <sup>+</sup>	271.1288	271	128.80
52	[M+Na] <sup>+</sup>	271.1310	271	131.00
53	[M+H] <sup>+</sup>	273.0757	273	75.70
54	[M+Na] <sup>+</sup>	273.1831	273	183.10
55	[M+H] <sup>+</sup>	276.1719	276	171.90
56	[M+H] <sup>+</sup>	280.1331	280	133.10
57	[M+Na] <sup>+</sup>	281.0426	281	42.60
58	[M+Na] <sup>+</sup>	281.0790	281	79.00
59	[M+H] <sup>+</sup>	285.0757	285	75.70
60	[M+Na] <sup>+</sup>	285.1467	285	146.70
61	[M+Na] <sup>+</sup>	285.1831	285	183.10
62	[M+Na] <sup>+</sup>	286.0480	286	48.00
63	[M+H] <sup>+</sup>	286.1437	286	143.70
64	[M+H] <sup>+</sup>	287.0549	287	54.90
65	[M+H] <sup>+</sup>	287.0761	287	76.10
66	[M+H] <sup>+</sup>	287.0913	287	91.30
67	[M+Na] <sup>+</sup>	287.1260	287	126.00
68	[M+H] <sup>+</sup>	287.1277	287	127.70
69	[M+Na] <sup>+</sup>	291.0634	291	63.40
70	[M+Na] <sup>+</sup>	293.0790	293	79.00
71	[M+Na] <sup>+</sup>	293.1114	293	111.40
72	[M+H] <sup>+</sup>	294.1488	294	148.80
73	[M+Na] <sup>+</sup>	295.0583	295	58.30
74	[M+H] <sup>+</sup>	295.0964	295	96.40
75	[M+H] <sup>+</sup>	296.1644	296	164.40
76	[M+H] <sup>+</sup>	298.1437	298	143.70
77	[M+Na] <sup>+</sup>	298.1545	298	154.50
78	[M+H] <sup>+</sup>	299.0549	299	54.90
79	[M+H] <sup>+</sup>	299.0913	299	91.30
80	[M+H] <sup>+</sup>	299.1641	299	164.10

81	[M+H] <sup>+</sup>	300.1593	300	159.30
82	[M+H] <sup>+</sup>	301.0706	301	70.60
83	[M+H] <sup>+</sup>	301.1070	301	107.00
84	[M+H] <sup>+</sup>	301.1434	301	143.40
85	[M+H] <sup>+</sup>	303.0862	303	86.20
86	[M+H] <sup>+</sup>	303.1226	303	122.60
87	[M+Na] <sup>+</sup>	305.0790	305	79.00
88	[M+H] <sup>+</sup>	307.1719	307	171.90
89	[M+Na] <sup>+</sup>	309.0739	309	73.90
90	[M+Na] <sup>+</sup>	309.1103	309	110.30
91	[M+H] <sup>+</sup>	310.1437	310	143.70
92	[M+Na] <sup>+</sup>	311.0896	311	89.60
93	[M+H] <sup>+</sup>	313.1434	313	143.40
94	[M+H] <sup>+</sup>	315.0862	315	86.20
95	[M+Na] <sup>+</sup>	315.0957	315	95.70
96	[M+H] <sup>+</sup>	315.1226	315	122.60
97	[M+H] <sup>+</sup>	315.1590	315	159.00
98	[M+H] <sup>+</sup>	315.1823	315	182.30
99	[M+Na] <sup>+</sup>	315.1936	315	193.60
100	[M+H] <sup>+</sup>	317.1019	317	101.90
101	[M+Na] <sup>+</sup>	318.1470	318	147.00
102	[M+H] <sup>+</sup>	320.0553	320	55.30
103	[M+Na] <sup>+</sup>	320.1263	320	126.30
104	[M+H] <sup>+</sup>	320.1492	320	149.20
105	[M+Na] <sup>+</sup>	321.1467	321	146.70
106	[M+Na] <sup>+</sup>	322.1419	322	141.90
107	[M+Na] <sup>+</sup>	323.0532	323	53.20
108	[M+Na] <sup>+</sup>	323.1260	323	126.00
109	[M+H] <sup>+</sup>	323.1277	323	127.70
110	[M+H] <sup>+</sup>	324.1230	324	123.00
111	[M+Na] <sup>+</sup>	325.0325	325	32.50
112	[M+Na] <sup>+</sup>	325.0688	325	68.80
113	[M+Na] <sup>+</sup>	325.1052	325	105.20
114	[M+H] <sup>+</sup>	325.1302	325	130.20
115	[M+Na] <sup>+</sup>	325.1416	325	141.60
116	[M+H] <sup>+</sup>	325.1434	325	143.40
117	[M+H] <sup>+</sup>	326.1386	326	138.60
118	[M+Na] <sup>+</sup>	327.1573	327	157.30
119	[M+H] <sup>+</sup>	328.1543	328	154.30
120	[M+Na] <sup>+</sup>	329.1545	329	154.50
121	[M+H] <sup>+</sup>	329.1747	329	174.70
122	[M+H] <sup>+</sup>	331.1539	331	153.90



123	[M+Na] <sup>+</sup>	332.1627	332	162.70
124	[M+H] <sup>+</sup>	333.1928	333	192.80
125	[M+H] <sup>+</sup>	334.1648	334	164.80
126	[M+Na] <sup>+</sup>	337.0688	337	68.80
127	[M+Na] <sup>+</sup>	337.1052	337	105.20
128	[M+H] <sup>+</sup>	337.1070	337	107.00
129	[M+Na] <sup>+</sup>	337.1416	337	141.60
130	[M+Na] <sup>+</sup>	337.1649	337	164.90
131	[M+Na] <sup>+</sup>	339.1209	339	120.90
132	[M+H] <sup>+</sup>	339.1226	339	122.60
133	[M+H] <sup>+</sup>	339.1590	339	159.00
134	[M+H] <sup>+</sup>	340.1543	340	154.30
135	[M+H] <sup>+</sup>	341.1383	341	138.30
136	[M+H] <sup>+</sup>	341.1747	341	174.70
137	[M+Na] <sup>+</sup>	342.1318	342	131.80
138	[M+H] <sup>+</sup>	342.1699	342	169.90
139	[M+H] <sup>+</sup>	343.1539	343	153.90
140	[M+H] <sup>+</sup>	343.1772	343	177.20
141	[M+Na] <sup>+</sup>	345.1103	345	110.30
142	[M+H] <sup>+</sup>	345.1696	345	169.60
143	[M+Na] <sup>+</sup>	348.1212	348	121.20
144	[M+H] <sup>+</sup>	351.1226	351	122.60
145	[M+Na] <sup>+</sup>	351.1573	351	157.30
146	[M+Na] <sup>+</sup>	352.1525	352	152.50
147	[M+H] <sup>+</sup>	353.1019	353	101.90
148	[M+H] <sup>+</sup>	353.1046	353	104.60
149	[M+Na] <sup>+</sup>	353.1365	353	136.50
150	[M+H] <sup>+</sup>	353.1383	353	138.30
151	[M+Na] <sup>+</sup>	355.1158	355	115.80
152	[M+H] <sup>+</sup>	355.1539	355	153.90
153	[M+Na] <sup>+</sup>	355.1754	355	175.40
154	[M+Na] <sup>+</sup>	356.1474	356	147.40
155	[M+H] <sup>+</sup>	356.1856	356	185.60
156	[M+H] <sup>+</sup>	357.1332	357	133.20
157	[M+H] <sup>+</sup>	357.1928	357	192.80
158	[M+H] <sup>+</sup>	359.1852	359	185.20
159	[M+Na] <sup>+</sup>	362.1369	362	136.90
160	[M+Na] <sup>+</sup>	363.1209	363	120.90
161	[M+Na] <sup>+</sup>	363.1573	363	157.30
162	[M+Na] <sup>+</sup>	364.1525	364	152.50
163	[M+Na] <sup>+</sup>	365.1365	365	136.50
164	[M+H] <sup>+</sup>	367.1175	367	117.50

165	[M+Na] <sup>+</sup>	367.1522	367	152.20
166	[M+Na] <sup>+</sup>	367.1754	367	175.40
167	[M+H] <sup>+</sup>	367.2267	367	226.70
168	[M+H] <sup>+</sup>	369.1332	369	133.20
169	[M+H] <sup>+</sup>	369.1696	369	169.60
170	[M+H] <sup>+</sup>	371.1125	371	112.50
171	[M+H] <sup>+</sup>	371.1488	371	148.80
172	[M+H] <sup>+</sup>	371.1852	371	185.20
173	[M+Na] <sup>+</sup>	372.1343	372	134.30
174	[M+H] <sup>+</sup>	372.1805	372	180.50
175	[M+H] <sup>+</sup>	373.1645	373	164.50
176	[M+Na] <sup>+</sup>	377.1365	377	136.50
177	[M+H] <sup>+</sup>	377.1747	377	174.70
178	[M+Na] <sup>+</sup>	378.1318	378	131.80
179	[M+H] <sup>+</sup>	378.1466	378	146.60
180	[M+Na] <sup>+</sup>	378.1682	378	168.20
181	[M+Na] <sup>+</sup>	379.1158	379	115.80
182	[M+Na] <sup>+</sup>	379.1754	379	175.40
183	[M+Na] <sup>+</sup>	381.1314	381	131.40
184	[M+H] <sup>+</sup>	381.1332	381	133.20
185	[M+Na] <sup>+</sup>	381.1678	381	167.80
186	[M+H] <sup>+</sup>	382.2012	382	201.20
187	[M+H] <sup>+</sup>	383.1488	383	148.80
188	[M+H] <sup>+</sup>	384.1208	384	120.80
189	[M+H] <sup>+</sup>	385.1281	385	128.10
190	[M+Na] <sup>+</sup>	389.2093	389	209.30
191	[M+Na] <sup>+</sup>	391.1158	391	115.80
192	[M+Na] <sup>+</sup>	391.1886	391	188.60
193	[M+Na] <sup>+</sup>	394.1631	394	163.10
194	[M+H] <sup>+</sup>	399.1801	399	180.10
195	[M+Na] <sup>+</sup>	405.1314	405	131.40
196	[M+H] <sup>+</sup>	405.1696	405	169.60
197	[M+Na] <sup>+</sup>	407.1471	407	147.10
198	[M+Na] <sup>+</sup>	415.1886	415	188.60
199	[M+H] <sup>+</sup>	417.1179	417	117.90
200	[M+H] <sup>+</sup>	419.1336	419	133.60
201	[M+H] <sup>+</sup>	423.1801	423	180.10
202	[M+H] <sup>+</sup>	423.2165	423	216.50
203	[M+H] <sup>+</sup>	425.1958	425	195.80
204	[M+H] <sup>+</sup>	425.2322	425	232.20
205	[M+Na] <sup>+</sup>	427.1522	427	152.20
206	[M+H] <sup>+</sup>	431.1336	431	133.60

207	[M+Na] <sup>+</sup>	431.1835	431	183.50
208	[M+H] <sup>+</sup>	433.1340	433	134.00
209	[M+H] <sup>+</sup>	433.1492	433	149.20
210	[M+Na] <sup>+</sup>	433.1627	433	162.70
211	[M+H] <sup>+</sup>	434.1809	434	180.90
212	[M+H] <sup>+</sup>	437.1958	437	195.80
213	[M+Na] <sup>+</sup>	439.1005	439	100.50
214	[M+H] <sup>+</sup>	439.1751	439	175.10
215	[M+Na] <sup>+</sup>	441.1162	441	116.20
216	[M+H] <sup>+</sup>	445.1128	445	112.80
217	[M+H] <sup>+</sup>	447.1285	447	128.50
218	[M+Na] <sup>+</sup>	453.1162	453	116.20
219	[M+H] <sup>+</sup>	453.2271	453	227.10
220	[M+Na] <sup>+</sup>	454.1842	454	184.20
221	[M+Na] <sup>+</sup>	455.1166	455	116.60
222	[M+Na] <sup>+</sup>	455.1318	455	131.80
223	[M+H] <sup>+</sup>	455.3519	455	351.90
224	[M+Na] <sup>+</sup>	456.1635	456	163.50
225	[M+H] <sup>+</sup>	457.3675	457	367.50
226	[M+Na] <sup>+</sup>	459.2148	459	214.80
227	[M+H] <sup>+</sup>	461.1441	461	144.10
228	[M+Na] <sup>+</sup>	461.1940	461	194.00
229	[M+H] <sup>+</sup>	463.2842	463	284.20
230	[M+Na] <sup>+</sup>	469.1111	469	111.10
231	[M+H] <sup>+</sup>	469.3312	469	331.20
232	[M+Na] <sup>+</sup>	471.1864	471	186.40
233	[M+H] <sup>+</sup>	471.3468	471	346.80
234	[M+Na] <sup>+</sup>	473.1060	473	106.00
235	[M+H] <sup>+</sup>	473.1441	473	144.10
236	[M+Na] <sup>+</sup>	477.3345	477	334.50
237	[M+Na] <sup>+</sup>	479.3501	479	350.10
238	[M+Na] <sup>+</sup>	481.3658	481	365.80
239	[M+Na] <sup>+</sup>	483.1267	483	126.70
240	[M+Na] <sup>+</sup>	485.1424	485	142.40
241	[M+H] <sup>+</sup>	485.3261	485	326.10
242	[M+H] <sup>+</sup>	485.3625	485	362.50
243	[M+Na] <sup>+</sup>	487.1580	487	158.00
244	[M+H] <sup>+</sup>	487.3417	487	341.70
245	[M+H] <sup>+</sup>	489.1391	489	139.10
246	[M+H] <sup>+</sup>	489.3574	489	357.40
247	[M+Na] <sup>+</sup>	493.3294	493	329.40
248	[M+Na] <sup>+</sup>	495.1267	495	126.70

249	[M+Na] <sup>+</sup>	499.2195	499	219.50
250	[M+H] <sup>+</sup>	501.3574	501	357.40
251	[M+Na] <sup>+</sup>	503.1530	503	153.00
252	[M+H] <sup>+</sup>	503.1911	503	191.10
253	[M+Na] <sup>+</sup>	503.3138	503	313.80
254	[M+H] <sup>+</sup>	505.1704	505	170.40
255	[M+Na] <sup>+</sup>	509.3243	509	324.30
256	[M+Na] <sup>+</sup>	511.1217	511	121.70
257	[M+Na] <sup>+</sup>	511.3400	511	340.00
258	[M+H] <sup>+</sup>	513.3574	513	357.40
259	[M+H] <sup>+</sup>	525.1157	525	115.70
260	[M+Na] <sup>+</sup>	527.1530	527	153.00
261	[M+H] <sup>+</sup>	529.3523	529	352.30
262	[M+Na] <sup>+</sup>	531.0670	531	67.00
263	[M+H] <sup>+</sup>	535.1445	535	144.50
264	[M+Na] <sup>+</sup>	545.1635	545	163.50
265	[M+H] <sup>+</sup>	551.1758	551	175.80
266	[M+H] <sup>+</sup>	563.2540	563	254.00
267	[M+H] <sup>+</sup>	565.1551	565	155.10
268	[M+Na] <sup>+</sup>	573.1584	573	158.40
269	[M+H] <sup>+</sup>	579.1708	579	170.80
270	[M+H] <sup>+</sup>	581.1864	581	186.40
271	[M+Na] <sup>+</sup>	585.2002	585	200.20
272	[M+Na] <sup>+</sup>	587.1377	587	137.70
273	[M+H] <sup>+</sup>	593.1864	593	186.40
274	[M+H] <sup>+</sup>	595.1598	595	159.80
275	[M+H] <sup>+</sup>	595.1657	595	165.70
276	[M+Na] <sup>+</sup>	601.1534	601	153.40
277	[M+Na] <sup>+</sup>	603.1690	603	169.00
278	[M+H] <sup>+</sup>	613.1551	613	155.10
279	[M+Na] <sup>+</sup>	615.1690	615	169.00
280	[M+H] <sup>+</sup>	622.2595	622	259.50
281	[M+Na] <sup>+</sup>	631.2784	631	278.40
282	[M+Na] <sup>+</sup>	649.2109	649	210.90
283	[M+Na] <sup>+</sup>	673.3928	673	392.80
284	[M+Na] <sup>+</sup>	675.3399	675	339.90
285	[M+Na] <sup>+</sup>	675.4084	675	408.40
286	[M+Na] <sup>+</sup>	691.4034	691	403.40
287	[M+H] <sup>+</sup>	705.3844	705	384.40
288	[M+H] <sup>+</sup>	707.4000	707	400.00
289	[M+H] <sup>+</sup>	713.2287	713	228.70
290	[M+Na] <sup>+</sup>	727.3670	727	367.00

291	[M+Na] <sup>+</sup>	775.4245	775	424.50
292	[M+H] <sup>+</sup>	779.4575	779	457.50
293	[M+H] <sup>+</sup>	781.4732	781	473.20
294	[M+H] <sup>+</sup>	795.4525	795	452.50
295	[M+H] <sup>+</sup>	797.4681	797	468.10
296	[M+Na] <sup>+</sup>	801.4038	801	403.80
297	[M+H] <sup>+</sup>	821.3953	821	395.30
298	[M+H] <sup>+</sup>	823.4110	823	411.00
299	[M+H] <sup>+</sup>	825.4266	825	426.60
300	[M+H] <sup>+</sup>	839.4059	839	405.90
301	[M+Na] <sup>+</sup>	843.3779	843	377.90
302	[M+Na] <sup>+</sup>	845.3936	845	393.60
303	[M+Na] <sup>+</sup>	847.4092	847	409.20
304	[M+H] <sup>+</sup>	851.3695	851	369.50
305	[M+Na] <sup>+</sup>	861.3885	861	388.50
306	[M+H] <sup>+</sup>	869.4529	869	452.90
307	[M+Na] <sup>+</sup>	873.3521	873	352.10
308	[M+H] <sup>+</sup>	881.4165	881	416.50
309	[M+H] <sup>+</sup>	897.4114	897	411.40
310	[M+Na] <sup>+</sup>	903.3991	903	399.10
311	[M+Na] <sup>+</sup>	919.3940	919	394.00
312	[M+H] <sup>+</sup>	943.5260	943	526.00
313	[M+Na] <sup>+</sup>	957.5188	957	518.80
314	[M+Na] <sup>+</sup>	965.5086	965	508.60
315	[M+Na] <sup>+</sup>	977.5086	977	508.60
316	[M+H] <sup>+</sup>	985.4638	985	463.80

**Table S3** The precursor ions list in the negative ESI mode.

No.	Adduct	<i>m/z</i>	Integer mass (Da)	Mass defect (mDa)
1	[M-H] <sup>-</sup>	111.0088	111	8.80
2	[M-H] <sup>-</sup>	125.0245	125	24.50
3	[M-H] <sup>-</sup>	134.0473	134	47.30
4	[M-H] <sup>-</sup>	141.0194	141	19.40
5	[M-H] <sup>-</sup>	149.0456	149	45.60
6	[M-H] <sup>-</sup>	153.0194	153	19.40
7	[M-H] <sup>-</sup>	167.0351	167	35.10
8	[M-H] <sup>-</sup>	173.1045	173	104.50
9	[M-H] <sup>-</sup>	177.0194	177	19.40
10	[M-H] <sup>-</sup>	179.0351	179	35.10
11	[M-H] <sup>-</sup>	179.0562	179	56.20
12	[M-H] <sup>-</sup>	187.0977	187	97.70
13	[M-H] <sup>-</sup>	193.0355	193	35.50
14	[M-H] <sup>-</sup>	193.0507	193	50.70
15	[M-H] <sup>-</sup>	195.0511	195	51.10
16	[M-H] <sup>-</sup>	197.0456	197	45.60
17	[M-H] <sup>-</sup>	209.0456	209	45.60
18	[M-H+HCOOH] <sup>-</sup>	221.0892	221	89.20
19	[M-H+HCOOH] <sup>-</sup>	227.0773	227	77.30
20	[M-H+HCOOH] <sup>-</sup>	239.0562	239	56.20
21	[M-H] <sup>-</sup>	243.0623	243	62.30
22	[M-H] <sup>-</sup>	247.1184	247	118.40
23	[M-H] <sup>-</sup>	253.0507	253	50.70
24	[M-H+HCOOH] <sup>-</sup>	254.0671	254	67.10
25	[M-H] <sup>-</sup>	255.0664	255	66.40
26	[M-H] <sup>-</sup>	257.0820	257	82.00
27	[M-H] <sup>-</sup>	267.0664	267	66.40
28	[M-H] <sup>-</sup>	269.0456	269	45.60
29	[M-H] <sup>-</sup>	269.0820	269	82.00
30	[M-H] <sup>-</sup>	271.0613	271	61.30
31	[M-H] <sup>-</sup>	273.0405	273	40.50
32	[M-H] <sup>-</sup>	279.2330	279	233.00
33	[M-H] <sup>-</sup>	281.0820	281	82.00
34	[M-H] <sup>-</sup>	283.0613	283	61.30
35	[M-H] <sup>-</sup>	285.0405	285	40.50
36	[M-H] <sup>-</sup>	285.0617	285	61.70
37	[M-H] <sup>-</sup>	285.0769	285	76.90
38	[M-H] <sup>-</sup>	287.0926	287	92.60

39	[M-H] <sup>-</sup>	291.0987	291	98.70
40	[M-H] <sup>-</sup>	293.0820	293	82.00
41	[M-H+HCOOH] <sup>-</sup>	293.1239	293	123.90
42	[M-H] <sup>-</sup>	295.0977	295	97.70
43	[M-H] <sup>-</sup>	297.0405	297	40.50
44	[M-H] <sup>-</sup>	297.0769	297	76.90
45	[M-H] <sup>-</sup>	297.1497	297	149.70
46	[M-H] <sup>-</sup>	299.0562	299	56.20
47	[M-H] <sup>-</sup>	299.1290	299	129.00
48	[M-H] <sup>-</sup>	301.0355	301	35.50
49	[M-H] <sup>-</sup>	301.0718	301	71.80
50	[M-H+HCOOH] <sup>-</sup>	307.1916	307	191.60
51	[M-H] <sup>-</sup>	308.1293	308	129.30
52	[M-H] <sup>-</sup>	311.1290	311	129.00
53	[M-H] <sup>-</sup>	313.0718	313	71.80
54	[M-H+HCOOH] <sup>-</sup>	313.0719	313	71.90
55	[M-H] <sup>-</sup>	313.1082	313	108.20
56	[M-H] <sup>-</sup>	315.0875	315	87.50
57	[M-H+HCOOH] <sup>-</sup>	315.0875	315	87.50
58	[M-H+HCOOH] <sup>-</sup>	317.0668	317	66.80
59	[M-H] <sup>-</sup>	318.0409	318	40.90
60	[M-H] <sup>-</sup>	321.1133	321	113.30
61	[M-H] <sup>-</sup>	323.1158	323	115.80
62	[M-H] <sup>-</sup>	323.1290	323	129.00
63	[M-H+HCOOH] <sup>-</sup>	324.1242	324	124.20
64	[M-H] <sup>-</sup>	324.1242	324	124.20
65	[M-H+HCOOH] <sup>-</sup>	327.0875	327	87.50
66	[M-H] <sup>-</sup>	329.1395	329	139.50
67	[M-H+HCOOH] <sup>-</sup>	331.0672	331	67.20
68	[M-H+HCOOH] <sup>-</sup>	331.1188	331	118.80
69	[M-H] <sup>-</sup>	331.1188	331	118.80
70	[M-H] <sup>-</sup>	335.0926	335	92.60
71	[M-H+HCOOH] <sup>-</sup>	337.1042	337	104.20
72	[M-H] <sup>-</sup>	337.1082	337	108.20
73	[M-H] <sup>-</sup>	337.1315	337	131.50
74	[M-H] <sup>-</sup>	337.1446	337	144.60
75	[M-H+HCOOH] <sup>-</sup>	337.2021	337	202.10
76	[M-H] <sup>-</sup>	338.1399	338	139.90
77	[M-H+HCOOH] <sup>-</sup>	338.1399	338	139.90
78	[M-H+HCOOH] <sup>-</sup>	339.0875	339	87.50
79	[M-H] <sup>-</sup>	339.1239	339	123.90
80	[M-H+HCOOH] <sup>-</sup>	341.1032	341	103.20

81	[M-H+HCOOH] <sup>-</sup>	343.1552	343	155.20
82	[M-H] <sup>-</sup>	343.1552	343	155.20
83	[M-H+HCOOH] <sup>-</sup>	344.1504	344	150.40
84	[M-H] <sup>-</sup>	349.1082	349	108.20
85	[M-H] <sup>-</sup>	351.0875	351	87.50
86	[M-H] <sup>-</sup>	351.0902	351	90.20
87	[M-H] <sup>-</sup>	351.1239	351	123.90
88	[M-H] <sup>-</sup>	353.0879	353	87.90
89	[M-H] <sup>-</sup>	353.1031	353	103.10
90	[M-H+HCOOH] <sup>-</sup>	353.1032	353	103.20
91	[M-H] <sup>-</sup>	353.1395	353	139.50
92	[M-H] <sup>-</sup>	355.1188	355	118.80
93	[M-H] <sup>-</sup>	357.1344	357	134.40
94	[M-H+HCOOH] <sup>-</sup>	357.1345	357	134.50
95	[M-H+HCOOH] <sup>-</sup>	361.0930	361	93.00
96	[M-H] <sup>-</sup>	365.1031	365	103.10
97	[M-H] <sup>-</sup>	367.1188	367	118.80
98	[M-H] <sup>-</sup>	367.1552	367	155.20
99	[M-H] <sup>-</sup>	369.0981	369	98.10
100	[M-H] <sup>-</sup>	369.1344	369	134.40
101	[M-H+HCOOH] <sup>-</sup>	369.1345	369	134.50
102	[M-H] <sup>-</sup>	369.1708	369	170.80
103	[M-H] <sup>-</sup>	371.1501	371	150.10
104	[M-H+HCOOH] <sup>-</sup>	373.1658	373	165.80
105	[M-H] <sup>-</sup>	375.1311	375	131.10
106	[M-H+HCOOH] <sup>-</sup>	381.0981	381	98.10
107	[M-H] <sup>-</sup>	381.1344	381	134.40
108	[M-H] <sup>-</sup>	382.1064	382	106.40
109	[M-H] <sup>-</sup>	383.1137	383	113.70
110	[M-H+HCOOH] <sup>-</sup>	383.1501	383	150.10
111	[M-H+HCOOH] <sup>-</sup>	385.1294	385	129.40
112	[M-H+HCOOH] <sup>-</sup>	387.1450	387	145.00
113	[M-H] <sup>-</sup>	387.1603	387	160.30
114	[M-H] <sup>-</sup>	391.1916	391	191.60
115	[M-H+HCOOH] <sup>-</sup>	395.1137	395	113.70
116	[M-H+HCOOH] <sup>-</sup>	397.0930	397	93.00
117	[M-H+HCOOH] <sup>-</sup>	397.1294	397	129.40
118	[M-H] <sup>-</sup>	397.1657	397	165.70
119	[M-H+HCOOH] <sup>-</sup>	399.0934	399	93.40
120	[M-H+HCOOH] <sup>-</sup>	399.1086	399	108.60
121	[M-H+HCOOH] <sup>-</sup>	399.1450	399	145.00
122	[M-H+HCOOH] <sup>-</sup>	401.1243	401	124.30



123	[M-H+HCOOH] <sup>-</sup>	403.1763	403	176.30
124	[M-H] <sup>-</sup>	405.1708	405	170.80
125	[M-H] <sup>-</sup>	415.1035	415	103.50
126	[M-H+HCOOH] <sup>-</sup>	415.1399	415	139.90
127	[M-H] <sup>-</sup>	417.1192	417	119.20
128	[M-H] <sup>-</sup>	417.1556	417	155.60
129	[M-H+HCOOH] <sup>-</sup>	417.1556	417	155.60
130	[M-H+HCOOH] <sup>-</sup>	421.1366	421	136.60
131	[M-H] <sup>-</sup>	421.1657	421	165.70
132	[M-H+HCOOH] <sup>-</sup>	421.1658	421	165.80
133	[M-H+HCOOH] <sup>-</sup>	422.1377	422	137.70
134	[M-H] <sup>-</sup>	423.2178	423	217.80
135	[M-H+HCOOH] <sup>-</sup>	426.1923	426	192.30
136	[M-H] <sup>-</sup>	429.1192	429	119.20
137	[M-H+HCOOH] <sup>-</sup>	429.1192	429	119.20
138	[M-H] <sup>-</sup>	431.1196	431	119.60
139	[M-H] <sup>-</sup>	431.1348	431	134.80
140	[M-H] <sup>-</sup>	431.2287	431	228.70
141	[M-H] <sup>-</sup>	433.2080	433	208.00
142	[M-H] <sup>-</sup>	435.2178	435	217.80
143	[M-H] <sup>-</sup>	437.1607	437	160.70
144	[M-H+HCOOH] <sup>-</sup>	439.2127	439	212.70
145	[M-H] <sup>-</sup>	443.0984	443	98.40
146	[M-H] <sup>-</sup>	443.1348	443	134.80
147	[M-H] <sup>-</sup>	445.1141	445	114.10
148	[M-H] <sup>-</sup>	447.0934	447	93.40
149	[M-H] <sup>-</sup>	447.1397	447	139.70
150	[M-H] <sup>-</sup>	447.1894	447	189.40
151	[M-H] <sup>-</sup>	449.1090	449	109.00
152	[M-H+HCOOH] <sup>-</sup>	451.1763	451	176.30
153	[M-H+HCOOH] <sup>-</sup>	455.2076	455	207.60
154	[M-H] <sup>-</sup>	459.1297	459	129.70
155	[M-H+HCOOH] <sup>-</sup>	459.3845	459	384.50
156	[M-H+HCOOH] <sup>-</sup>	461.1090	461	109.00
157	[M-H] <sup>-</sup>	461.1454	461	145.40
158	[M-H+HCOOH] <sup>-</sup>	463.1247	463	124.70
159	[M-H] <sup>-</sup>	465.1039	465	103.90
160	[M-H+HCOOH] <sup>-</sup>	467.1712	467	171.20
161	[M-H+HCOOH] <sup>-</sup>	467.2076	467	207.60
162	[M-H] <sup>-</sup>	467.3168	467	316.80
163	[M-H] <sup>-</sup>	469.3324	469	332.40
164	[M-H] <sup>-</sup>	471.1297	471	129.70

165	[M-H+HCOOH] <sup>-</sup>	475.1247	475	124.70
166	[M-H+HCOOH] <sup>-</sup>	477.1251	477	125.10
167	[M-H+HCOOH] <sup>-</sup>	477.1403	477	140.30
168	[M-H] <sup>-</sup>	477.2000	477	200.00
169	[M-H+HCOOH] <sup>-</sup>	477.2342	477	234.20
170	[M-H] <sup>-</sup>	479.1196	479	119.60
171	[M-H] <sup>-</sup>	484.1250	484	125.00
172	[M-H+HCOOH] <sup>-</sup>	484.1587	484	158.70
173	[M-H] <sup>-</sup>	485.3273	485	327.30
174	[M-H] <sup>-</sup>	487.1247	487	124.70
175	[M-H+HCOOH] <sup>-</sup>	489.1039	489	103.90
176	[M-H+HCOOH] <sup>-</sup>	489.1403	489	140.30
177	[M-H+HCOOH] <sup>-</sup>	491.1196	491	119.60
178	[M-H+HCOOH] <sup>-</sup>	491.1560	491	156.00
179	[M-H+HCOOH] <sup>-</sup>	493.1452	493	145.20
180	[M-H+HCOOH] <sup>-</sup>	495.1145	495	114.50
181	[M-H+HCOOH] <sup>-</sup>	497.2182	497	218.20
182	[M-H] <sup>-</sup>	503.1560	503	156.00
183	[M-H+HCOOH] <sup>-</sup>	503.3743	503	374.30
184	[M-H+HCOOH] <sup>-</sup>	505.1352	505	135.20
185	[M-H] <sup>-</sup>	506.1788	506	178.80
186	[M-H+HCOOH] <sup>-</sup>	517.1352	517	135.20
187	[M-H] <sup>-</sup>	521.1665	521	166.50
188	[M-H+HCOOH] <sup>-</sup>	525.1615	525	161.50
189	[M-H] <sup>-</sup>	527.3379	527	337.90
190	[M-H] <sup>-</sup>	533.1301	533	130.10
191	[M-H] <sup>-</sup>	549.1614	549	161.40
192	[M-H+HCOOH] <sup>-</sup>	549.1615	549	161.50
193	[M-H+HCOOH] <sup>-</sup>	552.1843	552	184.30
194	[M-H] <sup>-</sup>	561.2396	561	239.60
195	[M-H] <sup>-</sup>	563.1407	563	140.70
196	[M-H+HCOOH] <sup>-</sup>	567.1720	567	172.00
197	[M-H+HCOOH] <sup>-</sup>	569.1068	569	106.80
198	[M-H] <sup>-</sup>	577.1564	577	156.40
199	[M-H] <sup>-</sup>	579.1720	579	172.00
200	[M-H] <sup>-</sup>	591.1720	591	172.00
201	[M-H] <sup>-</sup>	593.1454	593	145.40
202	[M-H] <sup>-</sup>	593.1513	593	151.30
203	[M-H] <sup>-</sup>	593.1513	593	151.30
204	[M-H] <sup>-</sup>	593.2658	593	265.80
205	[M-H+HCOOH] <sup>-</sup>	595.1669	595	166.90
206	[M-H+HCOOH] <sup>-</sup>	607.2087	607	208.70

207	[M-H] <sup>-</sup>	609.1462	609	146.20
208	[M-H+HCOOH] <sup>-</sup>	609.1462	609	146.20
209	[M-H] <sup>-</sup>	609.1826	609	182.60
210	[M-H] <sup>-</sup>	611.1407	611	140.70
211	[M-H] <sup>-</sup>	620.2451	620	245.10
212	[M-H] <sup>-</sup>	623.1618	623	161.80
213	[M-H+HCOOH] <sup>-</sup>	623.1619	623	161.90
214	[M-H] <sup>-</sup>	623.2764	623	276.40
215	[M-H+HCOOH] <sup>-</sup>	623.2863	623	286.30
216	[M-H+HCOOH] <sup>-</sup>	625.1352	625	135.20
217	[M-H+HCOOH] <sup>-</sup>	625.1775	625	177.50
218	[M-H+HCOOH] <sup>-</sup>	637.1775	637	177.50
219	[M-H] <sup>-</sup>	637.2920	637	292.00
220	[M-H+HCOOH] <sup>-</sup>	639.1509	639	150.90
221	[M-H] <sup>-</sup>	649.3958	649	395.80
222	[M-H+HCOOH] <sup>-</sup>	669.1673	669	167.30
223	[M-H] <sup>-</sup>	681.2401	681	240.10
224	[M-H+HCOOH] <sup>-</sup>	683.2611	683	261.10
225	[M-H+HCOOH] <sup>-</sup>	685.2323	685	232.30
226	[M-H+HCOOH] <sup>-</sup>	685.2350	685	235.00
227	[M-H+HCOOH] <sup>-</sup>	687.2143	687	214.30
228	[M-H] <sup>-</sup>	703.3700	703	370.00
229	[M-H] <sup>-</sup>	705.3856	705	385.60
230	[M-H] <sup>-</sup>	711.2143	711	214.30
231	[M-H+HCOOH] <sup>-</sup>	727.2456	727	245.60
232	[M-H] <sup>-</sup>	777.4068	777	406.80
233	[M-H] <sup>-</sup>	777.4431	777	443.10
234	[M-H] <sup>-</sup>	793.4381	793	438.10
235	[M-H] <sup>-</sup>	795.4537	795	453.70
236	[M-H] <sup>-</sup>	819.3809	819	380.90
237	[M-H] <sup>-</sup>	821.3966	821	396.60
238	[M-H] <sup>-</sup>	823.4122	823	412.20
239	[M-H+HCOOH] <sup>-</sup>	823.4123	823	412.30
240	[M-H] <sup>-</sup>	837.3915	837	391.50
241	[M-H] <sup>-</sup>	849.3551	849	355.10
242	[M-H+HCOOH] <sup>-</sup>	867.4021	867	402.10
243	[M-H] <sup>-</sup>	867.4385	867	438.50
244	[M-H+HCOOH] <sup>-</sup>	869.4177	869	417.70
245	[M-H] <sup>-</sup>	879.4021	879	402.10
246	[M-H+HCOOH] <sup>-</sup>	883.4334	883	433.40
247	[M-H] <sup>-</sup>	895.3970	895	397.00

248	[M-H+HCOOH] <sup>-</sup>	899.4283	899	428.30
249	[M-H] <sup>-</sup>	905.4905	905	490.50
250	[M-H] <sup>-</sup>	909.4854	909	485.40
251	[M-H+HCOOH] <sup>-</sup>	935.4283	935	428.30
252	[M-H+HCOOH] <sup>-</sup>	937.4803	937	480.30
253	[M-H] <sup>-</sup>	941.5116	941	511.60
254	[M-H+HCOOH] <sup>-</sup>	955.4909	955	490.90
255	[M-H] <sup>-</sup>	967.4909	967	490.90
256	[M-H] <sup>-</sup>	969.5065	969	506.50
257	[M-H] <sup>-</sup>	983.4494	983	449.40
258	[M-H+HCOOH] <sup>-</sup>	999.5171	999	517.10

**Table S4** Comparison of the ion response and signal-to-noise ratio (S/N) of the representative compounds acquired by the DDA and HDDDA approaches.

Compound type	Compound name	DDA						HDDDA					
		Peak Area			S/N			Peak Area			S/N		
		1	2	3	1	2	3	1	2	3	1	2	3
Alkaloid	fangchinoline ( <i>m/z</i> 609.2970)	6479117	6762308	5995285	12984	11862	10015	3703493	4357050	5393265	704	724	1317
		<b>6412237</b>			<b>11620</b>			<b>4484603</b>			<b>915</b>		
	tetrandrine ( <i>m/z</i> 623.3126)	11292354	10073175	11721253	22621	18393	19933	4919691	4968897	6344584	1038	868	1779
		<b>11028927</b>			<b>20315</b>			<b>5411057</b>			<b>1228</b>		
Lactone	atractylenolide I ( <i>m/z</i> 231.1384)	280242	285754	300823	115	70	79	220675	249091	265734	15	21	36
		<b>288940</b>			<b>88</b>			<b>245167</b>			<b>24</b>		
Flavonoid	liquiritin apioside ( <i>m/z</i> 549.1604)	19780311	18932268	17713457	2849	1747	1993	13746722	12624125	12120471	142	16	322
		<b>18808679</b>			<b>2196</b>			<b>12830439</b>			<b>160</b>		
	isomer of liquiritin ( <i>m/z</i> 417.1178)	6831742	6710850	6442924	946	606	648	3310640	3156184	2910020	13	2	40
		<b>6661839</b>			<b>733</b>			<b>3125615</b>			<b>19</b>		
Saponin	astragaloside A ( <i>m/z</i> 829.3808)	1149158	1098652	1018678	97	69	66	742203	678867	646220	6	1	17
		<b>1088829</b>			<b>77</b>			<b>689097</b>			<b>8</b>		
	glycyrrhizic acid ( <i>m/z</i> 821.3988)	43085677	41091714	38188627	4233	2947	2693	25891455	23989317	22795446	128	15	333
		<b>40788673</b>			<b>3291</b>			<b>24225406</b>			<b>159</b>		

Note: the numbers in bold refer to the average values (peak area and S/N).

**Table S5** The CCS values of some representative isomeric components characterized from FHD.

	<b>m/z</b>	<b>t<sub>R</sub> (min)</b>	<b>Name</b>	<b>CCS(Å<sup>2</sup>)</b>
<b>NEG</b>	283.0614	11.63	calycosin	168.42
		5.43	isomer of calycosin	226.81
	417.1189	5.65	isomer of Liquiritin	183.77
		9.87	Neoisoliquiritin	219.01
		3.42	isomer of Liquiritin	184.03
		7.26	isomer of Liquiritin	226.30
	549.1615	5.24	Liquirtin apioside	258.33
		10.80	isomer of Liquirtin apioside	222.16
	823.4114	27.84	isomer of Licorice-saponin J2	302.99
		14.23	isomer of Licorice-saponin J2	291.75
		22.41	isomer of Licorice-saponin J2	299.14
		29.60	isomer of Licorice-saponin J2	301.94
		25.16	isomer of Licorice-saponin J2	284.27
		16.78	isomer of Licorice-saponin J2	292.27
	821.3969	24.63	Glycyrrhizic acid	288.49
		22.74	isomer of Glycyrrhizic acid	290.63
		27.90	isomer of Glycyrrhizic acid	298.73
		27.62	isomer of Glycyrrhizic acid	293.00
		25.93	isomer of Glycyrrhizic acid	300.49
		23.57	isomer of Glycyrrhizic acid	306.48
14.72		isomer of Glycyrrhizic acid	288.99	
24.42		isomer of Glycyrrhizic acid	306.37	
<b>POS</b>	231.1369	35.84	Atractylenolide I	155.58
		23.56	isomer of Atractylenolide I	149.96
	269.0794	16.96	Formononetin	153.02
		9.48	isomer of Formononetin	206.02
	609.2957	7.61	Fangchinoline	229.56
		6.98	isomer of Fangchinoline	237.95
	623.3038	9.35	Tetrandrine	248.78
		7.09	isomer of Tetrandrine	241.84
		8.82	isomer of Tetrandrine	240.15

**Table S6** Detailed information of the 203 components characterized from the FHD.

No.	$t_R$	$m/z$	Adducts	Formula	Error (ppm)	CCS ( $\text{\AA}^2$ )	CID-MS <sup>2</sup>	Identification	Source
1	0.73	175.1187	[M+H] <sup>+</sup>	C <sub>16</sub> H <sub>14</sub> N <sub>4</sub> O <sub>2</sub>	-1.2	137.12	175.1174,158.0940,130.0978	Arginine	AR
2	1.12	136.0620	[M+H] <sup>+</sup>	C <sub>5</sub> H <sub>5</sub> N <sub>5</sub>	0.2	125.02	136.0620,119.0356	9H-purin-6-amine	STR
3	2.82	989.3203	[M+H] <sup>+</sup>	C <sub>45</sub> H <sub>64</sub> O <sub>24</sub>	1.3	284.56	989.3203,971.3097,827.2681,665.2151,503.1615,485.1498,341.1095,323.0989,179.0570,113.0240	C <sub>21</sub> H <sub>24</sub> O <sub>4</sub> -4Glc	GRR
4 <sup>a</sup>	3.20	449.1968	[M+H] <sup>+</sup>	C <sub>21</sub> H <sub>36</sub> O <sub>10</sub>	0.0	209.28	448.1954,286.1431,269.1168,237.0904,175.0755	Atractylenolide A	AMR
5	3.23	431.1190	[M-H] <sup>-</sup>	C <sub>18</sub> H <sub>24</sub> O <sub>12</sub>	-1.2	188.59	258.9946,215.0016,137.0247	Licoagroside B	GRR
6 <sup>a</sup>	3.28	447.1141	[M-H] <sup>-</sup>	C <sub>21</sub> H <sub>36</sub> O <sub>10</sub>	-2.4	193.12	152.0108,108.0209	Atractyloside A	AMR
7	3.32	300.1592	[M+H] <sup>+</sup>	C <sub>18</sub> H <sub>21</sub> NO <sub>3</sub>	-0.9	168.86	300.1602,255.1019,237.0921,107.0476	N-methylcoclaurine	STR
8	3.35	476.2279	[M+H] <sup>+</sup>	C <sub>24</sub> H <sub>29</sub> NO <sub>9</sub>	2.1	217.61	476.2269,314.1742,269.1164	C <sub>18</sub> H <sub>19</sub> NO <sub>4</sub> -Glc	STR
9	3.42	257.0804	[M+H] <sup>+</sup>	C <sub>15</sub> H <sub>12</sub> O <sub>4</sub>	-1.9	158.25	251.0813,242.0572,147.0432,137.0225	isomer of Liquiritigenin	GRR
10	3.47	461.1090	[M-H] <sup>-</sup>	C <sub>22</sub> H <sub>22</sub> O <sub>11</sub>	0.1	241.99	284.0317,255.0286	Kaempferol-4'-methoxy-3-O-β-D-glucopyranoside	AR
11	3.50	353.0882	[M-H] <sup>-</sup>	C <sub>16</sub> H <sub>18</sub> O <sub>9</sub>	1.1	173.69	191.0556,135.0448	Chlorogenic acid	AR
12	3.64	328.1543	[M+H] <sup>+</sup>	C <sub>19</sub> H <sub>21</sub> NO <sub>4</sub>	0.0	177.19	328.1536,285.1115,221.1049,192.1019,177.0774	Discretamine	STR
13	3.66	298.1437	[M+H] <sup>+</sup>	C <sub>18</sub> H <sub>19</sub> NO <sub>3</sub>	-0.2	168.03	298.1443,253.0848,191.0937,146.0358	Stepharine	STR
14	3.66	434.1806	[M+H] <sup>+</sup>	C <sub>22</sub> H <sub>27</sub> NO <sub>8</sub>	-0.7	198.62	434.1816,272.1278,255.1017	isomer of Fefangjine G	STR

15	3.70	286.1435	[M+H] <sup>+</sup>	C <sub>17</sub> H <sub>19</sub> NO <sub>3</sub>	-1.1	169.99	286.1430,269.1176,254.0936,237.0899,209.0959,191.0864,175.0752,165.0520,137.0598,107.0493	Coclaurine	STR
16 <sup>a</sup>	3.77	328.1541	[M+H] <sup>+</sup>	C <sub>19</sub> H <sub>21</sub> NO <sub>4</sub>	-0.6	177.42	328.1538,283.0957,268.0727	Isoboldine	STR
17	3.78	595.1660	[M+H] <sup>+</sup>	C <sub>27</sub> H <sub>30</sub> O <sub>15</sub>	0.4	261.64	541.1395,523.1240,457.1125,379.0822,3256.0705	Vicenin-II	GRR
18	3.83	377.1458	[M+H] <sup>+</sup>	C <sub>17</sub> H <sub>20</sub> N <sub>4</sub> O <sub>6</sub>	0.6	187.20	377.1446,243.0880,172.0861	Riboflavin	AR
19	4.00	328.1546	[M+H] <sup>+</sup>	C <sub>19</sub> H <sub>21</sub> NO <sub>4</sub>	0.7	176.13	328.1528,178.0863,176.0707	Stepholidine/isoscoulerine/corytuberine	STR
20 <sup>a</sup>	4.06	342.1703	[M+H] <sup>+</sup>	C <sub>20</sub> H <sub>23</sub> NO <sub>4</sub>	0.8	180.86	342.1699,297.1119,265.0856,237.0902,217.0798	Magnoflorine	STR
21	4.07	356.1492	[M+H] <sup>+</sup>	C <sub>20</sub> H <sub>21</sub> NO <sub>5</sub>	-0.1	183.40	356.1482,192.1007	(+)-Norphoebine	STR
22	4.17	326.1385	[M+H] <sup>+</sup>	C <sub>19</sub> H <sub>19</sub> NO <sub>4</sub>	-0.4	176.61	326.1397,311.1151,265.1106	(S)-Fenfangjine T/Cassythicine	STR
23	4.19	163.0389	[M+H] <sup>+</sup>	C <sub>9</sub> H <sub>6</sub> O <sub>3</sub>	-0.2	128.34	163.0399	7-Hydroxycoumarin	AMR
24	4.25	340.1537	[M+H] <sup>+</sup>	C <sub>20</sub> H <sub>21</sub> NO <sub>4</sub>	-1.8	176.95	342.1696,297.1121,190.0866	Dicentrine/Nantenine/Crebanine	STR
25	4.27	301.0704	[M+H] <sup>+</sup>	C <sub>16</sub> H <sub>12</sub> O <sub>6</sub>	-0.7	165.16	301.0706,241.0499,213.0549,197.0598	Rhamnocitin	AR
26	4.41	593.1515	[M-H] <sup>-</sup>	C <sub>27</sub> H <sub>30</sub> O <sub>15</sub>	0.5	242.63	473.1078,383.0773,353.0665,297.0765,282.0535,175.0413	Nicotiflorin	GRR
27	4.42	328.1538	[M+H] <sup>+</sup>	C <sub>19</sub> H <sub>21</sub> NO <sub>4</sub>	-1.5	177.99	283.0963,255.1024,237.0906,137.0256	Stepholidine/Isoscoulerine/Corytuberine	STR
28	4.45	565.1551	[M+H] <sup>+</sup>	C <sub>26</sub> H <sub>28</sub> O <sub>14</sub>	-0.2	234.00	511.1239,481.1112,427.1014,409.0920,391.0819,379.0798,325.0706,295.0598	Schaftoside	GRR
29 <sup>a</sup>	4.76	314.1753	[M+H] <sup>+</sup>	C <sub>18</sub> H <sub>19</sub> NO <sub>4</sub>	1.1	173.33	314.1748,269.1173,237.0906,209.0963,175.0753,143.0487	(+)-Norisoboldine	STR



30	4.83	340.1561	[M+H] <sup>+</sup>	C <sub>20</sub> H <sub>21</sub> NO <sub>4</sub>	3.2	190.66	310.1093,282.1137,252.0435,224.0477,196.0538	isomer of Tetrahydroberberine	STR
31 <sup>a</sup>	4.85	255.0647	[M+H] <sup>+</sup>	C <sub>15</sub> H <sub>10</sub> O <sub>4</sub>	-2.0	202.08	255.0654	Daidzein	GRR
32	4.93	449.1092	[M-H] <sup>-</sup>	C <sub>21</sub> H <sub>22</sub> O <sub>11</sub>	0.6	199.49	269.0459,259.0617,125.0249	Scutellarein 6- <i>o</i> -glucoside	AMR
33	5.00	434.1810	[M+H] <sup>+</sup>	C <sub>22</sub> H <sub>27</sub> NO <sub>8</sub>	0.1	201.92	356.1519,314.1380,271.0961,225.0543,211.0752,197.0594,181.0653	Fenfangjine G	STR
34	5.01	271.0964	[M+H] <sup>+</sup>	C <sub>16</sub> H <sub>12</sub> O <sub>4</sub>	-0.4	201.34	271.0991,256.0742,239.0703,211.0748,196.0523,183.0811	Medicarpin	GRR
35	5.07	356.1492	[M+H] <sup>+</sup>	C <sub>20</sub> H <sub>21</sub> NO <sub>5</sub>	-0.2	182.29	356.1486,285.1115,253.0861,206.0810,191.0576,151.0758	(+)-N-formylnorisocorydine	STR
36	5.11	461.1087	[M-H] <sup>-</sup>	C <sub>22</sub> H <sub>22</sub> O <sub>11</sub>	-0.5	213.14	299.0565,284.0322,,255.0299,240.0415,227.0340	Rhamnocitin-3- <i>o</i> -β-D-glucopyranoside	AR
37	5.18	419.1336	[M+H] <sup>+</sup>	C <sub>21</sub> H <sub>22</sub> O <sub>9</sub>	-0.2	262.19	257.0792	Liquiritin	GRR
38 <sup>a</sup>	5.24	549.1980	[M-H] <sup>-</sup>	C <sub>26</sub> H <sub>30</sub> O <sub>13</sub>	0.6	258.33	549.1595,399.1066,255.0662,135.0089	Liquirtin apioside	GRR
39	5.26	563.1409	[M-H] <sup>-</sup>	C <sub>26</sub> H <sub>28</sub> O <sub>14</sub>	0.5	231.24	384.0801,383.0774,353.0662,297.0765,296.0670,283.0603	Isoschaftoside	GRR
40	5.36	711.2143	[M-H] <sup>-</sup>	C <sub>32</sub> H <sub>40</sub> O <sub>18</sub>	0.2	236.95	255.0668,135.0087	Glucoliquiritin apioside	GRR
41 <sup>a</sup>	5.37	342.1706	[M+H] <sup>+</sup>	C <sub>20</sub> H <sub>23</sub> NO <sub>4</sub>	1.7	180.56	342.1700,192.1018,177.0782	Aristolochic acid I	STR
42 <sup>a</sup>	5.37	192.1013	[M-e] <sup>+</sup>	C <sub>10</sub> H <sub>8</sub> O <sub>4</sub>	3.0	180.57	192.1020,177.0779,149.0841	Scopoletin	AMR
43	5.43	285.0758	[M+H] <sup>+</sup>	C <sub>16</sub> H <sub>12</sub> O <sub>5</sub>	0.3	210.96	285.0754,270.0517,253.0493,225.0542	Genkwanin	GRR
44	5.59	579.1709	[M+H] <sup>+</sup>	C <sub>27</sub> H <sub>30</sub> O <sub>14</sub>	0.1	240.02	525.1423,507.1314,465.1202,447.1087,423.1072,405.0962,379.0813,325.0707	Isoviolanthin/Violanthin	GRR
45	5.60	579.1725	[M-H] <sup>-</sup>	C <sub>27</sub> H <sub>32</sub> O <sub>14</sub>	1.0	230.91	255.0654,135.0089	Liquiritigenin-7,4-di-glucoside/Naringin	GRR

46 <sup>a</sup>	5.62	257.0810	[M+H] <sup>+</sup>	C <sub>15</sub> H <sub>12</sub> O <sub>4</sub>	0.8	159.18	257.0805,239.0702,211.0753,165.0708,147.0439,137.0234,119.0488,107.0495	Liquiritigenin	GRR
47	5.65	342.1703	[M+H] <sup>+</sup>	C <sub>20</sub> H <sub>23</sub> NO <sub>4</sub>	2.5	180.15	342.1702,192.1020,177.0792	isomer of Aristolochic acid I	STR
48	5.76	315.0860	[M+H] <sup>+</sup>	C <sub>17</sub> H <sub>14</sub> O <sub>6</sub>	-1.0	171.00	315.0860, 300.0619, 283.0596, 167.0323	Kumatakenin	GRR
49	5.84	447.1292	[M-H] <sup>-</sup>	C <sub>22</sub> H <sub>24</sub> O <sub>10</sub>	-1.0	236.42	270.0538	6β-D-glucopyranosyloxy-5-hydroxy-7-methoxy-flavonone	AMR
50	6.03	415.1038	[M-H] <sup>-</sup>	C <sub>21</sub> H <sub>20</sub> O <sub>9</sub>	0.9	210.71	252.0437,223.0405	Genistein/Soybean glycoside	GRR
51	6.25	711.2146	[M-H] <sup>-</sup>	C <sub>32</sub> H <sub>40</sub> O <sub>18</sub>	0.6	248.42	255.0656,135.0087	isomer of Glucoliquiritin apioside	GRR
52	6.33	324.1247	[M-H] <sup>-</sup>	C <sub>19</sub> H <sub>19</sub> NO <sub>4</sub>	1.7	176.95	294.0776,265.0501,237.0532,209.0598	Cassythicine/(S)-Fenfangjine T	STR
53	6.52	303.0867	[M+H] <sup>+</sup>	C <sub>16</sub> H <sub>14</sub> O <sub>6</sub>	1.3	168.68	303.0874,193.0498,165.0550	Tetrahydroxymethoxychalcone	GRR
54	6.52	283.0613	[M-H] <sup>-</sup>	C <sub>16</sub> H <sub>12</sub> O <sub>5</sub>	0.4	228.60	267.0295,239.0360,211.0401,195.0457,183.0451,148.0171	isomer of Prunetin	GRR
55	6.53	491.1198	[M+H] <sup>+</sup>	C <sub>30</sub> H <sub>46</sub> O <sub>4</sub>	1.5	232.75	283.0610,268.0377,239.0340,211.0413	isomer of Cycloastragenol	AR
56	6.59	577.1568	[M-H] <sup>-</sup>	C <sub>27</sub> H <sub>30</sub> O <sub>14</sub>	0.9	238.42	413.0878,395.0785,383.0775,353.0673,297.0765,296.0692,255.0667	Isoviolanthin/Violanthin	GRR
57	6.77	549.1619	[M-H] <sup>-</sup>	C <sub>26</sub> H <sub>30</sub> O <sub>13</sub>	1.0	212.21	549.1595,399.1066,255.0662,135.0089	isomer of Liquirtin apioside	GRR
58	6.89	255.0661	[M-H] <sup>-</sup>	C <sub>15</sub> H <sub>12</sub> O <sub>4</sub>	-0.6	184.59	119.0503	isomer of Pinocembrin	GRR
59	6.94	417.1186	[M-H] <sup>-</sup>	C <sub>21</sub> H <sub>22</sub> O <sub>9</sub>	-1.1	183.32	255.0656,213.0579,135.0088,119.0503	Isoliquiritin/Neoisoliquiritin/Liquiritin/Neoliquiritin	GRR
60	7.50	301.0706	[M+H] <sup>+</sup>	C <sub>16</sub> H <sub>12</sub> O <sub>6</sub>	-0.3	166.71	301.0704, 286.0455	Chrysoeriol	GRR
61	7.53	356.1859	[M+H] <sup>+</sup>	C <sub>21</sub> H <sub>25</sub> NO <sub>4</sub>	0.7	186.91	356.1857,206.1175,190.0862	Tetrahydropalmatine	STR
62 <sup>a</sup>	7.61	609.2986	[M+H] <sup>+</sup>	C <sub>37</sub> H <sub>40</sub> N <sub>2</sub> O <sub>6</sub>	-0.5	229.56	609.2962,578.2543,566.2447,383.1906,367.1640,351.1790,192.1011,146.0931	Fangchinoline	STR

63	7.78	301.0711	[M+H] <sup>+</sup>	C <sub>16</sub> H <sub>12</sub> O <sub>6</sub>	1.3	164.91	301.0705,283.0594,231.0643,167.0333	isomer of Chrysoeriol	GRR
64	7.87	271.0604	[M+H] <sup>+</sup>	C <sub>15</sub> H <sub>10</sub> O <sub>5</sub>	1.1	159.61	271.0599,153.0183	Apigenin/Galangin	GRR/AR
65	8.44	287.0911	[M+H] <sup>+</sup>	C <sub>16</sub> H <sub>14</sub> O <sub>5</sub>	-1.1	163.44	167.0334	(+)-Vesticarpan	AR
66	8.48	309.1111	[M+H] <sup>+</sup>	C <sub>19</sub> H <sub>16</sub> O <sub>4</sub>	-3.2	181.28	309.1124,279.1004,251.1052	Glabrocoumarone A kanzonol U/Glabrocoumarone B	GRR
67	8.49	340.1530	[M+H] <sup>+</sup>	C <sub>20</sub> H <sub>21</sub> NO <sub>4</sub>	-3.8	183.94	309.1118,279.1016,192.1025	Dicentrine/Nantenine/Crebanine	STR
68	8.55	417.1552	[M-H] <sup>-</sup>	C <sub>22</sub> H <sub>26</sub> O <sub>8</sub>	-0.7	219.07	166.0278,151.0039	Syringaresinol	STR
69	8.65	447.1275	[M+H] <sup>+</sup>	C <sub>22</sub> H <sub>22</sub> O <sub>10</sub>	-2.5	205.01	285.0757	Sissotrin/Calycosin-7- <i>o</i> -β-D- glucopyranoside	AR
70	8.71	355.1180	[M+H] <sup>+</sup>	C <sub>20</sub> H <sub>18</sub> O <sub>6</sub>	1.2	182.33	355.1182,267.0297	isomer of Licoisoflavanone	GRR
71	8.71	625.2136	[M-H] <sup>-</sup>	C <sub>29</sub> H <sub>38</sub> O <sub>15</sub>	-0.3	251.07	301.1081,286.0837,271.0610	isomer of Isomucronulatol 7,2'-di- <i>o</i> - glucoside	AR
72	8.73	463.1612	[M-H] <sup>-</sup>	C <sub>23</sub> H <sub>28</sub> O <sub>10</sub>	0.4	247.30	271.0604	2'-hydroxy-3',4'-dimethoxy- isoflavone-7- <i>o</i> -β- glycoside/isomucronulatol 7- <i>o</i> - glucoside/3S(-)-mucronulatol-7- <i>o</i> - β-D-glucopyranoside	AR
73	8.80	445.1139	[M-H] <sup>-</sup>	C <sub>22</sub> H <sub>22</sub> O <sub>10</sub>	-0.3	205.74	281.0464,268.0394,239.0347	Sissotrin/Calycosin-7- <i>o</i> -β-D- glucopyranoside	AR
74	9.20	299.0565	[M-H] <sup>-</sup>	C <sub>16</sub> H <sub>12</sub> O <sub>6</sub>	1.4	170.71	255.0295,227.0355,211.0394	isomer of Rhamnocitin	AR
75	9.29	447.1291	[M-H] <sup>-</sup>	C <sub>22</sub> H <sub>24</sub> O <sub>10</sub>	-1.2	203.28	270.0530	isomer of 6β-D-glucopyranosyloxy- 5-hydroxy-7-methoxy-flavonone	AMR
76 <sup>a</sup>	9.35	623.3116	[M+H] <sup>+</sup>	C <sub>38</sub> H <sub>42</sub> N <sub>2</sub> O <sub>6</sub>	0.1	248.78	623.3118,592.2706,580.2684,381.1800,1 92.1023	Tetrandrine	STR

77	9.44	461.1093	[M-H] <sup>-</sup>	C <sub>22</sub> H <sub>22</sub> O <sub>11</sub>	0.7	217.87	297.0401,255.0309	Kaempferol-4'-methoxy-3- <i>o</i> -β-D-glucopyranoside/Rhamnocitin-3- <i>o</i> -β-D-glucopyranoside	AR
78	9.48	269.0810	[M+H] <sup>+</sup>	C <sub>16</sub> H <sub>12</sub> O <sub>4</sub>	0.8	206.02	269.0814,254.0572,237.0548,226.0619,213.0917	7-dihydroxy-3'-methoxyisoflavanone/3'-dihydroxy-5'-methoxyisoflavanone	AR
79	9.56	257.0809	[M+H] <sup>+</sup>	C <sub>15</sub> H <sub>12</sub> O <sub>4</sub>	3.1	160.35	257.0800,211.0770,137.0229	isomer of Liquiritigenin	GRR
80	9.82	459.1305	[M-H] <sup>-</sup>	C <sub>23</sub> H <sub>24</sub> O <sub>10</sub>	1.9	198.28	255.0675	isomer of 6''- <i>o</i> -Acetyllicuritin	GRR
81 <sup>a</sup>	9.87	419.1340	[M+H] <sup>+</sup>	C <sub>21</sub> H <sub>22</sub> O <sub>9</sub>	0.7	213.92	257.0810,137.0225	Neoisoliquiritin	GRR
82	10.29	255.0650	[M+H] <sup>+</sup>	C <sub>15</sub> H <sub>10</sub> O <sub>4</sub>	-0.7	155.00	255.0651,199.0756	7,4'-Dihydroxyflavone	GRR
83	10.42	287.0911	[M+H] <sup>+</sup>	C <sub>16</sub> H <sub>14</sub> O <sub>5</sub>	-1.0	167.42	121.0288	Licochicone B	GRR
84	10.54	257.0810	[M+H] <sup>+</sup>	C <sub>15</sub> H <sub>12</sub> O <sub>4</sub>	0.8	160.08	257.0804,211.0754,147.0436,137.0233	Pinocembrin/2',4',4'-trihydroxy-chalcone	GRR/AR
85	10.67	795.4507	[M+H] <sup>+</sup>	C <sub>42</sub> H <sub>66</sub> O <sub>14</sub>	-2.3	304.76	601.4106	Huangqiyeinins E	AR
86	10.76	301.1068	[M+H] <sup>+</sup>	C <sub>17</sub> H <sub>16</sub> O <sub>5</sub>	-1.0	169.96	303.0867,301.1062,285.0754,269.0806,241.0857,169.0502,167.0706,163.0388	(6αR, 11αR) 3, 9-dimethoxy-10-hydroxy pterocarpan	AR
87	10.80	549.1621	[M-H] <sup>-</sup>	C <sub>26</sub> H <sub>30</sub> O <sub>13</sub>	1.3	222.16	255.0671,151.0404,135.0087	isomer of Liquirtin apioside	GRR
88	10.81	625.2146	[M-H] <sup>-</sup>	C <sub>29</sub> H <sub>38</sub> O <sub>15</sub>	1.3	235.52	301.1077,286.0868	Isomucronulatol 7,2'- <i>di</i> - <i>o</i> -glucoside	AR
89	10.87	591.1723	[M-H] <sup>-</sup>	C <sub>28</sub> H <sub>32</sub> O <sub>14</sub>	0.7	228.11	549.1637,255.0667,135.0087	Scolymoside	AR
90	11.01	267.0663	[M-H] <sup>-</sup>	C <sub>16</sub> H <sub>12</sub> O <sub>4</sub>	0.0	165.04	251.0345,223.0399,195.0452	7-Dihydroxy-3'-methoxyisoflavanone/3'-dihydroxy-5'-methoxyisoflavanone	AR
91	11.05	459.1297	[M-H] <sup>-</sup>	C <sub>23</sub> H <sub>24</sub> O <sub>10</sub>	0.0	194.49	255.0663,135.0091,119.0505	isomer of 6''- <i>o</i> -Acetyllicuritin	GRR
92	11.13	385.1290	[M+H] <sup>+</sup>	C <sub>21</sub> H <sub>20</sub> O <sub>7</sub>	2.1	193.16	367.1192	isomer of Isolicopyranocoumarin	GRR

93	11.15	296.1646	[M+H] <sup>+</sup>	C <sub>19</sub> H <sub>21</sub> NO <sub>2</sub>	0.3	171.00	251.1079,219.0822,191.0853	(-)-Nuciferine/Argentinine/Noratherosperminine	STR
94	11.33	417.1192	[M-H] <sup>-</sup>	C <sub>21</sub> H <sub>22</sub> O <sub>9</sub>	0.2	221.05	255.0662,253.0513,213.0546,148.0166,119.0505	Isoliquiritin/Neoisoliquiritin/Liquiritin/Neoliquiritin	GRR
95 <sup>a</sup>	11.63	285.0759	[M+H] <sup>+</sup>	C <sub>16</sub> H <sub>12</sub> O <sub>5</sub>	0.6	162.50	285.0756,270.0519,253.0490,225.0544	Calycosin	GRR/AR
96	12.00	285.0770	[M-H] <sup>-</sup>	C <sub>16</sub> H <sub>14</sub> O <sub>5</sub>	0.4	171.43	150.0328	isomer of (+)-Vesticarpan	AR
97	12.32	255.0664	[M-H] <sup>-</sup>	C <sub>15</sub> H <sub>12</sub> O <sub>4</sub>	0.4	160.39	119.0503	Pinocembrin	GRR
98	12.35	315.0862	[M+H] <sup>+</sup>	C <sub>17</sub> H <sub>14</sub> O <sub>6</sub>	-0.3	171.17	315.0858,300.0621,283.0593,255.0656,244.0719	2',3'-dihydroxy-7,4'-dimethoxyisoflavone	AR
99	12.39	299.0927	[M-H] <sup>-</sup>	C <sub>17</sub> H <sub>16</sub> O <sub>5</sub>	0.5	234.87	241.0506	(6 $\alpha$ R, 11 $\alpha$ R) 3, 9-dimethoxy-10-hydroxy pterocarpan/( -)-Methylnissolin(6 $\alpha$ R, 11 $\alpha$ R) 9, 10-dimethoxy-3-hydroxypterocarpan/Astrapterocarpan	AR
100	13.12	825.4275	[M+H] <sup>+</sup>	C <sub>42</sub> H <sub>64</sub> O <sub>16</sub>	1.0	301.16	455.3513,437.3406	Astraisoolesaponins E2/Uralsaponin C/Licorice-saponin J2	AR
101	13.13	301.1082	[M-H] <sup>-</sup>	C <sub>17</sub> H <sub>18</sub> O <sub>5</sub>	0.0	204.18	149.0247,121.0298	7,2'-dihydroxy-3',4'-dimethoxyisoflavane	AR
102 <sup>a</sup>	13.14	463.1607	[M-H] <sup>-</sup>	C <sub>23</sub> H <sub>28</sub> O <sub>10</sub>	-0.6	207.16	301.1081,271.0604,256.0378,253.0510,149.0244	Astraisoflavan-7- <i>o</i> - $\beta$ -D-glucoside	AR
103	13.15	455.3525	[M+H] <sup>+</sup>	C <sub>30</sub> H <sub>46</sub> O <sub>3</sub>	1.2	216.83	455.3519,437.3419,419.3314,189.1649	Isomacedonic acid/9,11-Dehydro-11-deoxo-18 $\beta$ -glycyrrhetic acid	GRR

104	13.25	283.0612	[M-H] <sup>-</sup>	C <sub>16</sub> H <sub>12</sub> O <sub>5</sub>	0.0	168.77	267.0289,251.0362,239.0349,240.0391,239.0349,211.0400,195.0451,183.0448,156.0579,148.0165,135.0087,119.0135	Prunetin	GRR
105	13.39	779.4567	[M+H] <sup>+</sup>	C <sub>42</sub> H <sub>66</sub> O <sub>13</sub>	-1.2	302.37	585.4149	Licorice-saponin C2	GRR
106 <sup>a</sup>	13.64	273.0747	[M+H] <sup>+</sup>	C <sub>15</sub> H <sub>12</sub> O <sub>5</sub>	-3.9	161.45	273.0749,153.0181,147.0444	Naringenine	GRR
107	13.84	487.3410	[M+H] <sup>+</sup>	C <sub>30</sub> H <sub>46</sub> O <sub>5</sub>	-1.6	218.41	487.3403	18 $\alpha$ -hydroxyglycyrrhetic acid	GRR
108 <sup>a</sup>	14.11	271.0958	[M+H] <sup>+</sup>	C <sub>16</sub> H <sub>14</sub> O <sub>4</sub>	-2.4	165.27	271.0592	echinatin	GRR
109	14.23	823.4117	[M-H] <sup>-</sup>	C <sub>42</sub> H <sub>64</sub> O <sub>16</sub>	-0.5	291.75	823.4116,761.4087,647.3806,585.3790,471.3475,351.0567,289.0559,193.0357,113.0243	Astraisoolesaponins E2/Uralsaponin C/Licorice-saponin J2	AR
110	14.28	473.1446	[M+H] <sup>+</sup>	C <sub>24</sub> H <sub>24</sub> O <sub>10</sub>	0.7	220.72	269.0807	6''-o-acetyl-ononin	AR
111	14.31	897.4126	[M+H] <sup>+</sup>	C <sub>42</sub> H <sub>64</sub> O <sub>19</sub>	1.3	325.83	703.3702,685.3584,545.3474,527.3368,509.3259,403.2987	Uralsaponin F	GRR
112	14.42	385.1286	[M+H] <sup>+</sup>	C <sub>21</sub> H <sub>20</sub> O <sub>7</sub>	1.0	194.15	385.1281	isomer of Gancaonin D	GRR
113	14.43	299.0930	[M-H] <sup>-</sup>	C <sub>17</sub> H <sub>16</sub> O <sub>5</sub>	1.7	237.59	241.0497	(6 $\alpha$ R, 11 $\alpha$ R) 3,9-dimethoxy-10-hydroxy pterocarpan/( - )-methylnissolin(6 $\alpha$ R,11 $\alpha$ R) 9,10-dimethoxy-3-hydroxypterocarpan/Astrapterocarpan	AR
114	14.66	779.4577	[M+H] <sup>+</sup>	C <sub>42</sub> H <sub>66</sub> O <sub>13</sub>	0.1	301.10	585.4154	isomer of Licorice-saponin C2	GRR
115	14.78	294.1491	[M+H] <sup>+</sup>	C <sub>19</sub> H <sub>19</sub> NO <sub>2</sub>	0.8	170.66	249.0911	Stephenanthrine/Tephenanthrine	STR
116	15.10	317.1014	[M+H] <sup>+</sup>	C <sub>17</sub> H <sub>16</sub> O <sub>6</sub>	-1.9	172.78	317.1020,285.0755,253.0448,183.0649,163.0370	2',4'-dihydro-xy-5,6-dimethylisoflawaone	AR

117	15.43	985.4664	[M+H] <sup>+</sup>	C <sub>48</sub> H <sub>72</sub> O <sub>21</sub>	2.6	326.64	809.4347,615.3904,597.3816,471.3475,453.3371,357.2425	isomer of Licorice-saponin A3	GRR
118	15.48	895.3966	[M-H] <sup>-</sup>	C <sub>44</sub> H <sub>64</sub> O <sub>19</sub>	-0.4	302.65	895.3963,833.3987,719.3622,659.3445,597.3447,553.3543,439.3222,351.0570,289.0562,193.0352,113.0247	isomer of Uralsaponin F	GRR
119	15.71	459.1297	[M-H] <sup>-</sup>	C <sub>23</sub> H <sub>24</sub> O <sub>10</sub>	0.2	231.36	253.0510,148.0168,119.0509	isomer of 6''-o-Acetyllicquiritin	GRR
120	15.71	301.0711	[M+H] <sup>+</sup>	C <sub>16</sub> H <sub>12</sub> O <sub>6</sub>	1.3	163.75	301.0704,286.0474,258.0517	isomer of Chrysoeriol	GRR
121	15.77	383.1144	[M-H] <sup>-</sup>	C <sub>21</sub> H <sub>20</sub> O <sub>7</sub>	2.0	197.70	268.0381	Isolicopyranocoumarin	GRR
122	15.97	485.3262	[M+H] <sup>+</sup>	C <sub>30</sub> H <sub>44</sub> O <sub>5</sub>	0.1	303.15	485.3258,315.1954	21-Hydroxyisoglabrolide/liquoric acid	GRR
123	16.21	895.3962	[M-H] <sup>-</sup>	C <sub>44</sub> H <sub>64</sub> O <sub>19</sub>	-0.8	299.91	895.3957,773.3784,659.3424,439.3218,351.0565,289.0551,193.0352,175.0250	isomer of Uralsaponin F	GRR
124	16.32	511.3429	[M+H] <sup>+</sup>	C <sub>32</sub> H <sub>46</sub> O <sub>5</sub>	2.2	228.10	511.3420,451.3199,405.3156,297.1829,227.1797,187.1477,145.1002	3β-Acetyoxyglabrolide	GRR
125	16.46	369.1332	[M+H] <sup>+</sup>	C <sub>21</sub> H <sub>20</sub> O <sub>6</sub>	-0.1	192.34	369.1331,299.0910,193.0494,165.0544	isomer of Isoglycycoumarin	GRR
126	16.52	983.4485	[M-H] <sup>-</sup>	C <sub>48</sub> H <sub>72</sub> O <sub>21</sub>	-0.8	311.03	941.0418,821.3961,759.3948,645.3650,627.3536,583.3635,469.3316,351.0568,289.0569,193.0352,113.0249	Licorice-saponin A3	GRR
127	16.62	849.3545	[M-H] <sup>-</sup>	C <sub>42</sub> H <sub>58</sub> O <sub>18</sub>	-0.7	284.87	849.3548,743.3657,629.3311,409.3100,351.0566,289.0562,193.0351,113.0240	Uralsaponin D	GRR
128	16.64	983.4482	[M-H] <sup>-</sup>	C <sub>39</sub> H <sub>64</sub> O <sub>29</sub>	1.2	312.38	983.4499,821.3953,645.3640,351.0564,289.0549,193.0348	C <sub>16</sub> H <sub>20</sub> O <sub>9</sub> -2Glc-Xyl-GluA	AR
129 <sup>a</sup>	16.78	257.0807	[M+H] <sup>+</sup>	C <sub>15</sub> H <sub>12</sub> O <sub>4</sub>	-0.3	159.95	257.0800,147.0442,137.0234	Isoliquiritigenin	GRR
130 <sup>a</sup>	16.96	267.0663	[M-H] <sup>-</sup>	C <sub>16</sub> H <sub>12</sub> O <sub>4</sub>	0.2	165.14	251.0340,223.0400,195.0451,167.0499,132.0213	Formononetin	GRR/AR

131	17.16	705.3845	[M+H] <sup>+</sup>	C <sub>38</sub> H <sub>56</sub> O <sub>12</sub>	0.1	274.60	511.3410,493.3332,451.3199	Huangqiyeinins H	AR
132	17.55	301.1072	[M+H] <sup>+</sup>	C <sub>17</sub> H <sub>16</sub> O <sub>5</sub>	0.6	168.46	301.1083,269.0810,241.0861,167.0703,147.0443	isomer of (6 $\alpha$ R, 11 $\alpha$ R) 3, 9-dimethoxy-10-hydroxy pterocarpan	AR
133	17.70	299.0916	[M+H] <sup>+</sup>	C <sub>17</sub> H <sub>14</sub> O <sub>5</sub>	0.7	167.44	299.0913,284.0683,241.0852,167.0710	Afromosin	GRR
134	17.72	879.4024	[M-H] <sup>-</sup>	C <sub>44</sub> H <sub>64</sub> O <sub>18</sub>	0.4	300.41	879.4009,817.4009,757.3788,643.3490,581.3483,537.3568,423.3259,351.0566,289.0570,193.0354,113.0242	22 $\beta$ -Acetoxylglycyrrhizin	GRR
135	17.76	371.1487	[M+H] <sup>+</sup>	C <sub>21</sub> H <sub>22</sub> O <sub>6</sub>	-0.4	194.51	193.0498,165.0537	12-Seneciolyloxytetradeca-2E,8E,10E-trien-4,6-diyne-1,14-diacetate	AMR
136	17.90	881.4174	[M+H] <sup>+</sup>	C <sub>44</sub> H <sub>64</sub> O <sub>18</sub>	1.0	324.49	511.3452,451.3202,433.3100,405.3151,393.2800	Isomer of 22 $\beta$ -Acetoxylglycyrrhizin	GRR
137	18.00	367.1178	[M+H] <sup>+</sup>	C <sub>21</sub> H <sub>18</sub> O <sub>6</sub>	0.6	192.30	367.1169,167.0342	Glycyrol/Isoglycyrol/Neoglycyrol	GRR
138	18.72	415.1393	[M+H] <sup>+</sup>	C <sub>22</sub> H <sub>22</sub> O <sub>8</sub>	1.4	191.69	415.1389,383.1137,350.0821	Formononetin-7- <i>o</i> - $\beta$ -D-glycoside	AR
139	19.21	469.3315	[M+H] <sup>+</sup>	C <sub>30</sub> H <sub>44</sub> O <sub>4</sub>	0.6	305.62	469.3317, 451.3205, 423.3237, 315.1964,217.1591,189.1635	Uralenolide	GRR
140	19.22	839.4074	[M+H] <sup>+</sup>	C <sub>42</sub> H <sub>62</sub> O <sub>17</sub>	1.7	311.81	645.3666,627.3561,488.3450,487.3420,469.3316,451.3214,439.3211,141.0177	Licorice-saponin G2	GRR
141	19.37	267.0663	[M-H] <sup>-</sup>	C <sub>16</sub> H <sub>12</sub> O <sub>4</sub>	0.2	165.14	251.0350,223.0395,195.0450	isomer of Formononetin	GRR/AR
142	19.63	879.4002	[M-H] <sup>-</sup>	C <sub>34</sub> H <sub>42</sub> O <sub>27</sub>	1.5	314.11	879.3995,703.3681,351.1561,193.0356	C <sub>16</sub> H <sub>18</sub> O <sub>9</sub> -3GluA	AR
143	19.83	881.4174	[M+H] <sup>+</sup>	C <sub>44</sub> H <sub>64</sub> O <sub>18</sub>	1.0	329.09	511.3431,451.3205,433.3105,405.3153,393.2806	isomer of 22 $\beta$ -Acetoxylglycyrrhizin	GRR
144	19.93	355.1533	[M+H] <sup>+</sup>	C <sub>21</sub> H <sub>22</sub> O <sub>5</sub>	-2.0	188.10	355.1539,299.0920,287.0892,193.0499,165.0546	isomer of Licochalcone D	GRR
145	20.04	705.3849	[M+H] <sup>+</sup>	C <sub>38</sub> H <sub>56</sub> O <sub>12</sub>	0.7	271.55	511.3415	isomer of Huangqiyeinins H	AR



146	20.25	983.4851	[M-H] <sup>-</sup>	C <sub>39</sub> H <sub>62</sub> O <sub>29</sub>	2.3	344.11	983.4838,879.4732,733.4146,645.3632	C <sub>16</sub> H <sub>18</sub> O <sub>9</sub> -2Glc-Xyl-GluA	AR
147	20.41	839.4074	[M+H] <sup>+</sup>	C <sub>42</sub> H <sub>62</sub> O <sub>17</sub>	1.7	311.14	487.3415,469.3308,451.3206,439.3204	isomer of Licorice-saponin G2	GRR
148	20.55	819.3805	[M-H] <sup>-</sup>	C <sub>34</sub> H <sub>46</sub> O <sub>23</sub>	1.8	289.98	819.3802,757.3799,643.3494,351.0570	C <sub>16</sub> H <sub>18</sub> O <sub>9</sub> -2Rha-GluA	AR
149 <sup>a</sup>	20.70	819.3803	[M+Cl] <sup>-</sup>	C <sub>42</sub> H <sub>60</sub> O <sub>16</sub>	-0.7	278.95	819.3793,757.3790,685.3590,643.3466,535.3470,465.2974,353.0602,351.0563,289.0573,193.0351,113.0241	Astragaloside III	AR
150	20.78	369.1334	[M+H] <sup>+</sup>	C <sub>21</sub> H <sub>20</sub> O <sub>6</sub>	0.4	190.53	313.0706,271.0598	Gancaonin N	GRR
151	20.82	821.3964	[M-H] <sup>-</sup>	C <sub>34</sub> H <sub>48</sub> O <sub>23</sub>	1.7	300.91	821.3955,645.3648,469.3292,351.0570,193.0353	C <sub>20</sub> H <sub>26</sub> O <sub>14</sub> -2GluA	AR
152	21.07	837.3913	[M-H] <sup>-</sup>	C <sub>42</sub> H <sub>62</sub> O <sub>17</sub>	-0.2	298.04	837.3913,775.3900,661.3586,643.3495,527.3374,485.3263,353.0614,351.0569,289.0562,193.0355,113.0246	isomer of Licorice-saponin G2	GRR
153	22.35	471.3471	[M+H] <sup>+</sup>	C <sub>30</sub> H <sub>46</sub> O <sub>4</sub>	0.4	217.57	471.3466,425.3419,317.2110,189.1635	Oleana-11,13(18)-dien-30-oic acid,3.beta.-hydroxy,methyl ester	GRR
154	22.41	823.4118	[M+H] <sup>+</sup>	C <sub>42</sub> H <sub>62</sub> O <sub>16</sub>	0.8	299.14	647.3794,471.3465,453.3362,435.3254,357.2423,189.1635	isomer of Glycyrrhizic acid	GRR
155	23.13	353.1381	[M+H] <sup>+</sup>	C <sub>21</sub> H <sub>20</sub> O <sub>5</sub>	-0.8	188.07	353.1383	isomer of Gancaonin A	GRR
156	23.56	367.1189	[M-H] <sup>-</sup>	C <sub>21</sub> H <sub>20</sub> O <sub>6</sub>	0.5	195.47	265.0497,255.0294,211.0398	isomer of Gancaonin N	GRR
157	23.57	821.3961	[M+H] <sup>+</sup>	C <sub>42</sub> H <sub>60</sub> O <sub>16</sub>	0.9	306.48	451.3205,433.3088	Licorice-saponin E2	GRR
158	23.92	353.1378	[M+H] <sup>+</sup>	C <sub>21</sub> H <sub>20</sub> O <sub>5</sub>	-1.5	188.91	353.1388,298.0838	isomer of Gancaonin A	GRR
159	24.06	487.3412	[M+H] <sup>+</sup>	C <sub>30</sub> H <sub>46</sub> O <sub>5</sub>	-1.2	221.55	487.3418	24-Hydroxy-glycyrrhetate	GRR
160	24.15	353.1386	[M+H] <sup>+</sup>	C <sub>21</sub> H <sub>20</sub> O <sub>5</sub>	0.6	188.32	298.0828	isomer of Gancaonin A	GRR
161	24.35	457.3675	[M+H] <sup>+</sup>	C <sub>30</sub> H <sub>48</sub> O <sub>3</sub>	-0.2	213.78	457.3689	Ursolic acid/Betulic acid	GRR

162	24.36	819.3808	[M-H] <sup>-</sup>	C <sub>42</sub> H <sub>60</sub> O <sub>16</sub>	0.0	284.77	821.3968,759.3939,697.3955,645.3646,6 27.3547,469.3316,351.0571,289.0563,19 3.0354,113.0245	isomer of Licorice-saponin E2	GRR
163	24.46	353.1025	[M+H] <sup>+</sup>	C <sub>20</sub> H <sub>16</sub> O <sub>6</sub>	1.6	178.33	353.1004,311.0560	isomer of Sophoraisoflavone	GRR
164 <sup>a</sup>	24.63	821.3963	[M-H] <sup>-</sup>	C <sub>42</sub> H <sub>62</sub> O <sub>16</sub>	-0.3	288.49	821.3961,759.3956,697.3952,645.3650,6 27.3536,583.3635,469.3316,353.0612,35 1.0568,289.0569,193.0352,113.0244	Glycyrrhizic acid	GRR
165	25.25	797.4682	[M+H] <sup>+</sup>	C <sub>42</sub> H <sub>68</sub> O <sub>14</sub>	0.0	307.48		Astramembranosides A	AR
166	25.32	943.5283	[M+H] <sup>+</sup>	C <sub>48</sub> H <sub>78</sub> O <sub>18</sub>	2.3	339.19	599.3948,441.3729,423.3624,405.3511,2 03.1804	Soyasaponin I	AR
167	25.42	705.3849	[M+H] <sup>+</sup>	C <sub>38</sub> H <sub>56</sub> O <sub>12</sub>	0.6	270.69	511.3414,451.3202	isomer of Huangqiyenins H	AR
168	25.93	821.3958	[M+H] <sup>+</sup>	C <sub>42</sub> H <sub>60</sub> O <sub>16</sub>	0.4	300.49	453.3348,435.3249,407.3314	isomer of Licorice-saponin E2	GRR
169	26.00	315.0861	[M+H] <sup>+</sup>	C <sub>17</sub> H <sub>14</sub> O <sub>6</sub>	-0.7	169.30	315.0862,300.0624,299.0553	Odoratin	GRR
170	26.06	967.4903	[M-H] <sup>-</sup>	C <sub>49</sub> H <sub>76</sub> O <sub>19</sub>	-0.5	342.33	967.4920,629.3705	Astraisoolesaponins D	AR
171	26.58	705.3874	[M-H] <sup>-</sup>	C <sub>38</sub> H <sub>58</sub> O <sub>12</sub>	2.6	282.62	705.3892,487.3447	Huangqiyenins G	AR
172	26.99	369.1330	[M+H] <sup>+</sup>	C <sub>21</sub> H <sub>20</sub> O <sub>6</sub>	-0.6	194.02	369.1332,313.0701,285.0753,270.0520,2 43.0651	7-O-Methyluteone	GRR
173 <sup>a</sup>	27.01	353.1014	[M+H] <sup>+</sup>	C <sub>20</sub> H <sub>16</sub> O <sub>6</sub>	-1.6	186.37	353.1020,335.0911,153.0179	Semilicoisoflavone B	GRR
174	27.13	367.1175	[M+H] <sup>+</sup>	C <sub>21</sub> H <sub>18</sub> O <sub>6</sub>	-0.2	186.91	369.1315,313.0707,285.0753	Glycyrol/Isoglycyrol/Neoglycyrol	GRR
175	27.41	941.5111	[M-H] <sup>-</sup>	C <sub>48</sub> H <sub>78</sub> O <sub>18</sub>	-0.4	333.06	941.5111,923.5006,795.4527,733.4534,6 15.3906,457.3692,205.0718	isomer of Soyasaponin I	AR
176	27.51	825.4270	[M+H] <sup>+</sup>	C <sub>42</sub> H <sub>64</sub> O <sub>16</sub>	0.3	308.86	455.3501,437.3409,409.3457,189.1630	Astraisoolesaponins E2/Uralsaponin C/Licorice-saponin J2	AR
177	27.72	703.3697	[M-H] <sup>-</sup>	C <sub>38</sub> H <sub>56</sub> O <sub>12</sub>	-0.3	286.72	643.3488,599.3580,537.3578,477.3391,4 23.3285,408.3014	isomer of Huangqiyenins H	AR

178	27.76	355.1537	[M+H] <sup>+</sup>	C <sub>21</sub> H <sub>22</sub> O <sub>5</sub>	-1.0	186.23	301.1070,221.1180,165.0544	1-Methoxyphaseollidin/Licobenzofurane	GRR
179	28.95	967.4890	[M-H] <sup>-</sup>	C <sub>49</sub> H <sub>76</sub> O <sub>19</sub>	-1.9	347.27	967.4940	isomer of Astraisoolesaponins D	AR
180 <sup>a</sup>	28.96	355.1176	[M+H] <sup>+</sup>	C <sub>20</sub> H <sub>18</sub> O <sub>6</sub>	-0.1	190.28	299.0539,287.0544	Glycyrrhisoflavone	GRR
181	29.34	313.0726	[M-H] <sup>-</sup>	C <sub>17</sub> H <sub>14</sub> O <sub>6</sub>	2.8	173.61	255.0294	isomer of Odoratin	GRR
182	29.60	823.4120	[M-H] <sup>-</sup>	C <sub>42</sub> H <sub>64</sub> O <sub>16</sub>	-0.2	301.94	823.4116,761.4123,647.3813,629.3707,471.3463,351.0569,289.0574,193.0350,113.0249	Astraisoolesaponins E2/Uralsaponin C/Licorice-saponin J2	AR
183	29.60	777.4066	[M-H] <sup>-</sup>	C <sub>41</sub> H <sub>62</sub> O <sub>14</sub>	-0.1	298.32	777.4060,715.4060,627.3533,583.3638,537.3587,469.3322	Apioglycyrrhizin/Araboglycyrrhizin	GRR
184	29.82	367.1192	[M-H] <sup>-</sup>	C <sub>21</sub> H <sub>20</sub> O <sub>6</sub>	1.2	195.25	309.0398,201.0198	isomer of Gancaonin N	GRR
185	30.37	383.1486	[M+H] <sup>+</sup>	C <sub>22</sub> H <sub>22</sub> O <sub>6</sub>	-0.9	195.40	327.0869,299.0914	Glycyrin/Kanzonol O/Licoricone	GRR
186	31.40	355.1520	[M+H] <sup>+</sup>	C <sub>21</sub> H <sub>22</sub> O <sub>5</sub>	-5.6	191.30	299.0905	isomer of 1-Methoxyphaseollidin/licobenzofurane	GRR
187	31.50	353.1377	[M+H] <sup>+</sup>	C <sub>21</sub> H <sub>20</sub> O <sub>5</sub>	-2.0	185.53	299.0909	isomer of Gancaonin A	GRR
188	31.51	793.4369	[M-H] <sup>-</sup>	C <sub>42</sub> H <sub>66</sub> O <sub>14</sub>	-1.4	290.11	793.4361,351.0573	isomer of Huangqiyenins E	AR
189	31.7	805.4012	[M-H] <sup>-</sup>	C <sub>33</sub> H <sub>44</sub> O <sub>23</sub>	2.3	289.3	805.4013,629.3662,351.0559,193.0357	C <sub>16</sub> H <sub>18</sub> O <sub>9</sub> -Rha-Xyl-GluA	AMR
190 <sup>a</sup>	32.18	233.1537	[M+H] <sup>+</sup>	C <sub>15</sub> H <sub>20</sub> O <sub>2</sub>	0.3	154.04	233.1534	Atractylenolide II	AMR
191	32.79	381.1342	[M-H] <sup>-</sup>	C <sub>22</sub> H <sub>22</sub> O <sub>6</sub>	-0.5	200.44	351.0861,323.0929,308.0318,279.0298,201.0194,199.0404	Glycyrin/kanzonol O/Licoricone	GRR
192	32.88	309.1117	[M+H] <sup>+</sup>	C <sub>19</sub> H <sub>16</sub> O <sub>4</sub>	-1.3	171.05	173.0589	Glabrocoumarone A kanzonol U/Glabrocoumarone B	GRR

193	33.8	645.3632	[M-H] <sup>-</sup>	C <sub>27</sub> H <sub>34</sub> O <sub>18</sub>	2.5	273.58	645.3643,569.3491,523.3433,469.3317,425.3414	C <sub>20</sub> H <sub>26</sub> O <sub>10</sub> -2GluA	AMR
194	34.59	485.3268	[M-H] <sup>-</sup>	C <sub>30</sub> H <sub>46</sub> O <sub>5</sub>	-0.9	235.54	485.3283,441.3362	isomer of Glabric acid	GRR
195	35.15	529.3527	[M+H] <sup>+</sup>	C <sub>32</sub> H <sub>48</sub> O <sub>6</sub>	0.6	229.16	529.3538	22β-Acethylglbric acid	GRR
196 <sup>a</sup>	35.84	231.1378	[M+H] <sup>+</sup>	C <sub>15</sub> H <sub>18</sub> O <sub>2</sub>	-0.6	155.58	235.1698,231.1384,185.1332,179.1074,157.1021	Atractylenolide I	AMR
197 <sup>a</sup>	35.92	249.1849	[M+H] <sup>+</sup>	C <sub>15</sub> H <sub>20</sub> O <sub>3</sub>	1.5	169.50		Atractylenolide III	AMR
198	36.43	276.1710	[M+H] <sup>+</sup>	C <sub>17</sub> H <sub>23</sub> O <sub>3</sub>	-3.7	172.46	261.1473	8β-Ethoxyasterolid	AMR
199	37.06	341.1746	[M+H] <sup>+</sup>	C <sub>21</sub> H <sub>24</sub> O <sub>4</sub>	-0.3	188.25	341.1753,285.1122	α,α'-Dihydroxy-4'-acetoxy-5'isopentenylstilbene	GRR
200 <sup>a</sup>	38.53	471.3468	[M+H] <sup>+</sup>	C <sub>30</sub> H <sub>46</sub> O <sub>4</sub>	0.0	218.38	471.3459	Glycyrrhethic acid	GRR
201	40.41	339.2001	[M+H] <sup>+</sup>	C <sub>21</sub> H <sub>22</sub> O <sub>4</sub>	1.1	203.24	339.1979,183.0121	isomer of Licochalcone A	AMR
202	40.93	381.2042	[M+H] <sup>+</sup>	C <sub>24</sub> H <sub>28</sub> O <sub>4</sub>	-4.7	208.89	381.2086	Gancaonin U	GRR
203	41.16	367.2643	[M+H] <sup>+</sup>	C <sub>21</sub> H <sub>18</sub> O <sub>6</sub>	3.3	209.93	205.1596,149.0974	Glycyrol/Isoglycyrol/Neoglycyrol	AMR

<sup>a</sup>: The components confirmed by comparison with the reference standards.