

peak No.	t <sub>R</sub> /min	Ionisation mode	Mass(m/z)		Error (ppm)	Molecular formula	MS/MS fragments	Identification compound
			Theoretical Mass	Measured Mass				
1	0.91	[M-H] <sup>-</sup>	191.056 1	191.055 9	1.555	C <sub>7</sub> H <sub>12</sub> O <sub>6</sub>	191.056 1	Quinic acid
2	0.98	[M-H] <sup>-</sup>	173.045 5	173.045 3	1.512	C <sub>7</sub> H <sub>10</sub> O <sub>5</sub>	137.024 6, 111.045 4, 93.034 7	Shikimic acid
3	2.65	[M-H] <sup>-</sup>	391.124 6	391.124 5	1.134	C <sub>16</sub> H <sub>24</sub> O <sub>11</sub>	229.072 1, 167.071 3	Shanzhiside Isomers
4	2.81	[M-H] <sup>-</sup>	403.124 6	403.124 1	0.183	C <sub>17</sub> H <sub>24</sub> O <sub>11</sub>	241.072 3, 223.061 2, 127.040 2, 101.024 5	Deacetylasperulosidic acid methyl ester
5	2.84	[M-H] <sup>-</sup>	389.108 9	389.108 7	0.883	C <sub>16</sub> H <sub>22</sub> O <sub>11</sub>	389.109 2, 209.045 6, 183.066 2, 165.055 6, 147.045 2	Scandoside
6	2.98	[M-H] <sup>-</sup>	373.114 0	373.113 7	0.639	C <sub>16</sub> H <sub>22</sub> O <sub>10</sub>	373.110 4, 211.061 2, 193.050 5, 167.071 2, 149.060 7, 123.045 1	Gardoside*
7	3.13	[M-H] <sup>-</sup>	391.124 6	391.124 5	1.221	C <sub>16</sub> H <sub>24</sub> O <sub>11</sub>	229.071 7, 211.060 9, 185.081 3, 167.071 1	Shanziside*
8	3.32	[M-H] <sup>-</sup>	403.124 6	403.124 1	1.101	C <sub>17</sub> H <sub>24</sub> O <sub>11</sub>	241.072 2, 223.060 7, 193.050 1, 127.040 1, 101.024 6	Gardenosid
9	3.35	[M-H] <sup>-</sup>	373.114 0	373.113 6	0.478	C <sub>16</sub> H <sub>22</sub> O <sub>10</sub>	211.061 8, 193.050 3, 146.060 6, 123.045 0, 167.071 0, 121.056 7	Geniposidic acid*
10	3.38	[M-H] <sup>-</sup>	403.124 6	403.124 1	-0.561	C <sub>17</sub> H <sub>24</sub> O <sub>11</sub>	241.072 2, 223.061 4, 139.040 3	Feretoside
11	3.48	[M-H] <sup>-</sup>	405.140 2	405.139 9	0.503	C <sub>17</sub> H <sub>26</sub> O <sub>11</sub>	359.143 5, 197.082 4	Shanziside methyl ester*
12	3.57	[M-H] <sup>-</sup>	375.129 7	375.129 4	0.715	C <sub>16</sub> H <sub>24</sub> O <sub>10</sub>	213.077 4, 169.087 3, 151.076 7	Mussaenosidic acid
13	3.73	[M-H] <sup>-</sup>	345.155 5	345.155 2	0.775	C <sub>16</sub> H <sub>26</sub> O <sub>8</sub>	113.024 3, 101.024 2, 89.024 3	Jasminoside D
14	3.96	[M-H] <sup>-</sup>	327.144 9	327.144 7	0.832	C <sub>16</sub> H <sub>24</sub> O <sub>7</sub>	165.092 3	Zataroside B
15	4.04	[M-H] <sup>-</sup>	353.087 8	353.087 6	1.028	C <sub>16</sub> H <sub>18</sub> O <sub>9</sub>	191.056 4, 179.035 3, 135.045 3	5/3-O-Caffeoyl-quinic acid
16	4.20	[M-H] <sup>-</sup>	549.182 5	549.181 5	-0.883	C <sub>23</sub> H <sub>34</sub> O <sub>15</sub>	225. 077 4, 207. 066 7	Genipin 1-gentiobioside
17	4.87	[M-H] <sup>-</sup>	387.129 7	387.129 4	0.693	C <sub>17</sub> H <sub>24</sub> O <sub>10</sub>	207.066 8, 225.077 4, 433.135 9, 123.045 4, 101.024 6	Geniposide*
18	5.34	[M-H] <sup>-</sup>	345.155 5	345.155 2	0.775	C <sub>16</sub> H <sub>26</sub> O <sub>8</sub>	301.042 5, 165.092 1, 183.102 8, 101.024 4, 89.024 5	Jasminoside B
19	5.49	[M-H] <sup>-</sup>	353.087 8	353.087 4	0.405	C <sub>16</sub> H <sub>18</sub> O <sub>9</sub>	191.056 6, 173.045 9, 179.065 8, 135.062 5	Chlorogenic acid
20	6.33	[M-H] <sup>-</sup>	179.035 0	179.034 8	1.832	C <sub>9</sub> H <sub>8</sub> O <sub>4</sub>	135.045 4	Caffeic acid
21	6.39	[M-H] <sup>-</sup>	183.102 7	183.102 3	1.206	C <sub>10</sub> H <sub>16</sub> O <sub>3</sub>	139.113 1, 111.009 0, 137.097 1, 109.065 7, 123.080 5	Jasminodiol
22	6.62	[M-H] <sup>-</sup>	503.177 0	503.176 9	0.883	C <sub>22</sub> H <sub>32</sub> O <sub>13</sub>	223.145 1, 205.087 9, 190.211 3	2-methyl-lerythritol-4-O-(6-O-transsinapoyl)- β -D-glu copyranoside
23	7.01	[M-H] <sup>-</sup>	359.134 8	359.134 7	1.372	C <sub>16</sub> H <sub>24</sub> O <sub>9</sub>	359.135 1, 197.081 9, 179.070 9	Ixoroside
24	7.44	[M-H] <sup>-</sup>	429.140 2	429.139 8	0.335	C <sub>19</sub> H <sub>26</sub> O <sub>11</sub>	383.133 2, 361.150 6, 239.090 1, 181.087 8	10-acetyl geniposide
25	7.57	[M-H] <sup>-</sup>	519.150 8	519.150 6	0.614	C <sub>25</sub> H <sub>28</sub> O <sub>12</sub>	163.040 1, 145.029 5, 123.045 2, 119.050 2, 149.060 8	6' -O-trans-coumaroyl Geniposidic acid
26	8.24	[M-H] <sup>-</sup>	551.177 0	551.176 8	0.643	C <sub>26</sub> H <sub>32</sub> O <sub>13</sub>	357.119 6, 213.077 5, 193.050 9, 175.040 3	6-O-trans-p-coumaroyl Gardenoside methyl ester
27	9.89	[M-H] <sup>-</sup>	491.213 4	491.213 3	0.954	C <sub>22</sub> H <sub>36</sub> O <sub>12</sub>	167.032 4, 323.101 5, 221.075 2, 161.058 0, 263.081 5	Jasminoside S/H/I
28	10.1 6	[M-H] <sup>-</sup>	579.171 9	579.172 1	1.174	C <sub>27</sub> H <sub>32</sub> O <sub>14</sub>	205.050 6, 325.093 1, 367.103 7, 385.114 4, 223.061 1, 123.045 1	6' -O-trans-sinapoyl gardoside
29	10.4 3	[M-H] <sup>-</sup>	565.192 7	565.192 4	0.574	C <sub>27</sub> H <sub>34</sub> O <sub>13</sub>	325.093 6, 295.082 8, 265.072 3, 223.061 8	11-(6-O-trans-sinapoyl)glucopyranosyl)gardendiol
30	10.7 9	[M-H] <sup>-</sup>	609.146 1	609.146 3	1.216	C <sub>27</sub> H <sub>30</sub> O <sub>16</sub>	301.035 9, 300.028 1, 271.025 5	Rutin
31	11.6 0	[M-H] <sup>-</sup>	465.102 8	465.101 8	0.938	C <sub>21</sub> H <sub>20</sub> O <sub>12</sub>	301.035 0, 271.024 5, 255.029 7	Isoquercitrin

32	11.8	[M-H] <sup>-</sup>	593.151 2	593.151 3	1.121	C <sub>27</sub> H <sub>30</sub> O <sub>15</sub>	325.092 5, 207.029 6, 93.034 4	Nicotiflorin
33	12.1	[M-H] <sup>-</sup>	755.240 4	755.240 8	1.306	C <sub>34</sub> H <sub>44</sub> O <sub>19</sub>	123.076 5, 223.077 4, 205.425 5, 101.218 2, 427.066 5	6' '-O-trans-sinapoylgenipin Gentiobioside
34	12.6	[M-H] <sup>-</sup>	725.229 8	725.230 2	1.201	C <sub>33</sub> H <sub>42</sub> O <sub>18</sub>	225.077 3, 193.051 2, 123.045 4	6' '-O-trans-feruloylgenipin Gentiobioside
35	12.6	[M-H] <sup>-</sup>	695.219 3	695.219 2	0.742	C <sub>32</sub> H <sub>40</sub> O <sub>17</sub>	663.196 5, 469.136 3, 225.077 3, 145.029 8, 207.066 9	6' '-O-trans-p-coumaroylgenipin gentiobioside
36	13.0	[M-H] <sup>-</sup>	551.213 4	551.213 3	0.742	C <sub>27</sub> H <sub>36</sub> O <sub>12</sub>	521.204 1, 367.014 2, 165.092 3	6' '-O-trans-sinapoyl Jasminoside L
37	13.3	[M-H] <sup>-</sup>	975.371 5	975.371 0	0.044	C <sub>44</sub> H <sub>64</sub> O <sub>24</sub>	651.267 4, 327.160 9, 283.1700, 239.1800	trans-crocin I /cis-crocin I
38	14.0	[M-H] <sup>-</sup>	593.187 6	593.187 7	1.095	C <sub>28</sub> H <sub>34</sub> O <sub>14</sub>	367.105 5, 225.077 2, 223.061 0, 207.065 8, 205.051 2, 123.046 5, 353.088 8, 191.056 5, 173.045 8	6' '-O-sinapoylgeniposide
39	14.6	[M-H] <sup>-</sup>	515.119 5	515.119 1	0.251	C <sub>25</sub> H <sub>24</sub> O <sub>12</sub>		3,5-Dicaffeoylquinic acid
40	15.5	[M-H] <sup>-</sup>	533.166 4	533.166 3	0.786	C <sub>26</sub> H <sub>30</sub> O <sub>12</sub>	145.132 3, 123.130 5, 307.114 8, 225.087 9	6' '-O-p-coumaroylgeniposide
41	15.6	[M-H] <sup>-</sup>	659.161 8	659.162 1	1.366	C <sub>31</sub> H <sub>32</sub> O <sub>16</sub>	497.131 3, 191.056 4, 161.045 7	3,4-dicaffeoyl-5-(3-hydroxy-3-methyl glutaroyl)quinic acid
42	16.4	[M-H] <sup>-</sup>	559.145 7	559.145 5	0.616	C <sub>27</sub> H <sub>28</sub> O <sub>13</sub>	397.114 9, 173.045 9	3-caffeoyl-4-sinapoylquinatone
43	17.4	[M-H] <sup>-</sup>	535.218 5	535.218 3	0.716	C <sub>27</sub> H <sub>36</sub> O <sub>11</sub>	325.092 6, 265.071 5, 223.060 9, 205.050 4	6' '-O-trans-sinapoyl Jasminoside A
44	18.5	[M-H] <sup>-</sup>	533.202 8	533.202 5	0.419	C <sub>27</sub> H <sub>34</sub> O <sub>11</sub>	205.051 1, 367.104 1, 223.061 3, 165.055 3, 190.027 5	6' '-O-trans-sinapoyl Jasminoside C
45	19.5	[M-H] <sup>-</sup>	345.061 6	345.061 4	0.950	C <sub>17</sub> H <sub>14</sub> O <sub>8</sub>	315.014 9, 330.038 3, 287.019 9	5,7,3',4' -tetrahydroxy-6,8-dimethoxy flavone
46	21.7	[M-H] <sup>-</sup>	813.318 7	813.319 2	1.286	C <sub>38</sub> H <sub>54</sub> O <sub>19</sub>	651.267 6, 489.213 7, 369.170 9, 327.161 1, 283.170 9, 179.056 4	Crocin II

\* represented components compared with reference standards;