

## Supporting Information

### Chemical characterization and comparative for different parts of *Cocculus orbiculatus* through UHPLC-Q-TOF-MS

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**1** These authors made equal contributions to this work.

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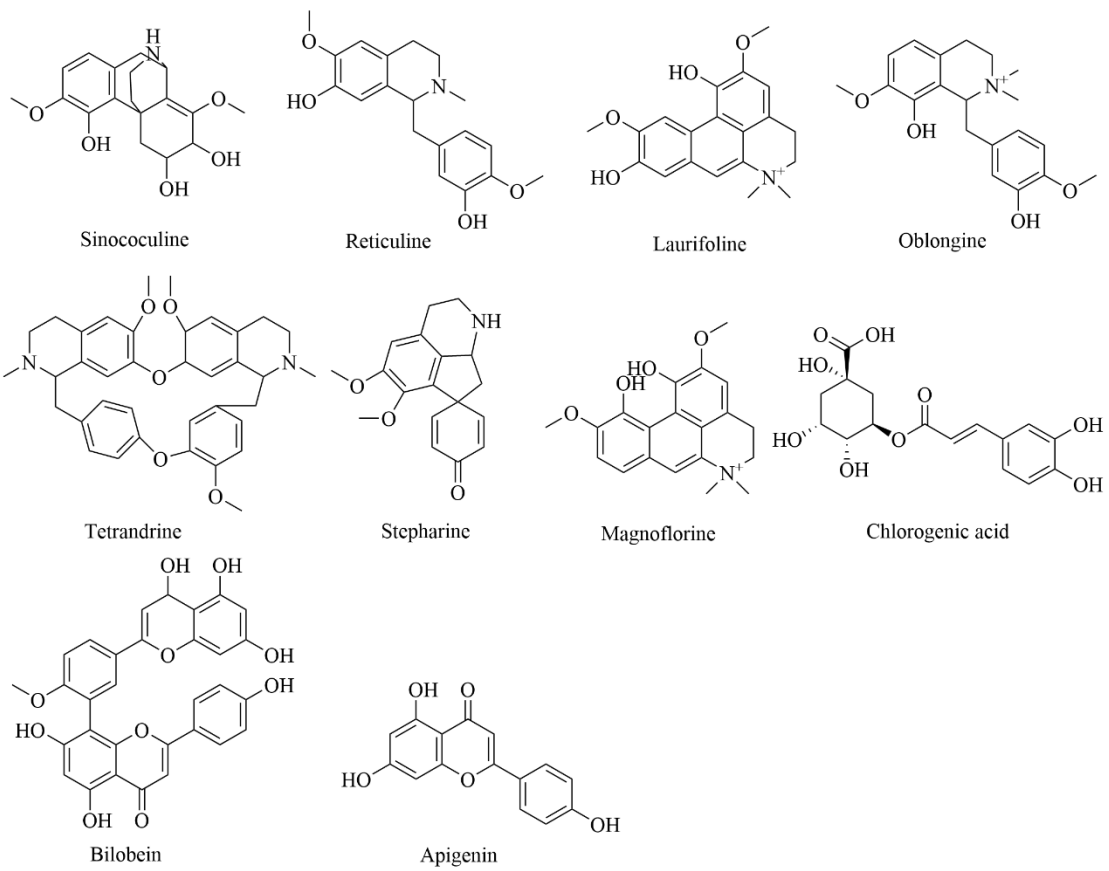
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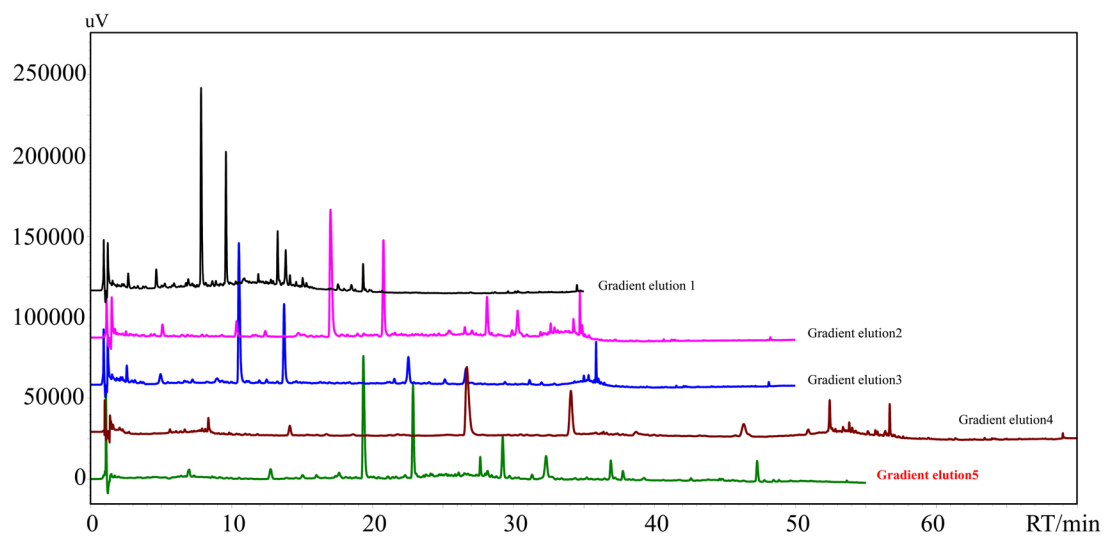


Figure S2

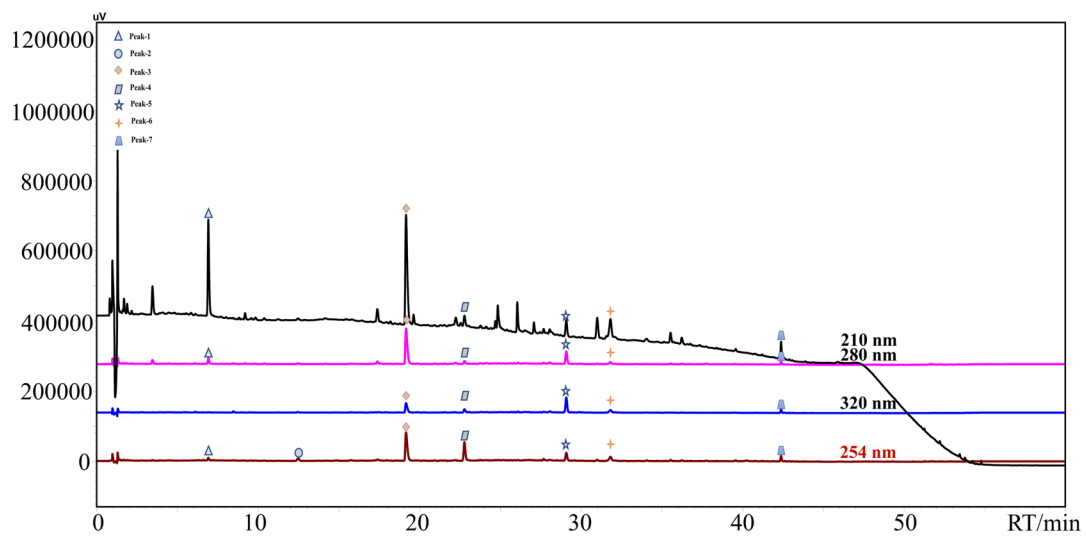
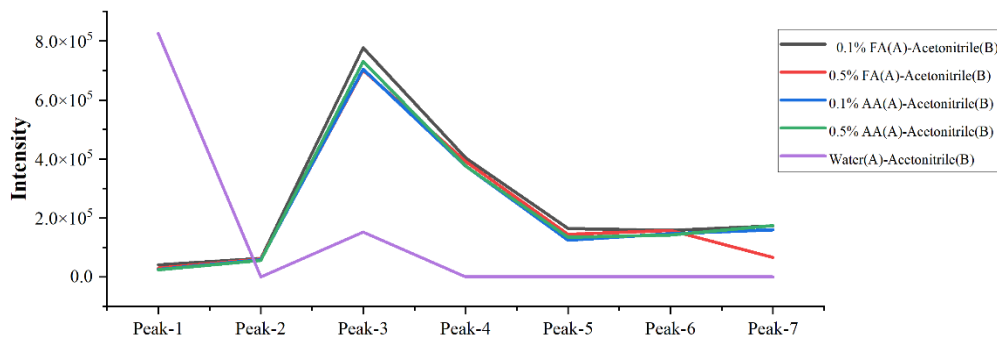
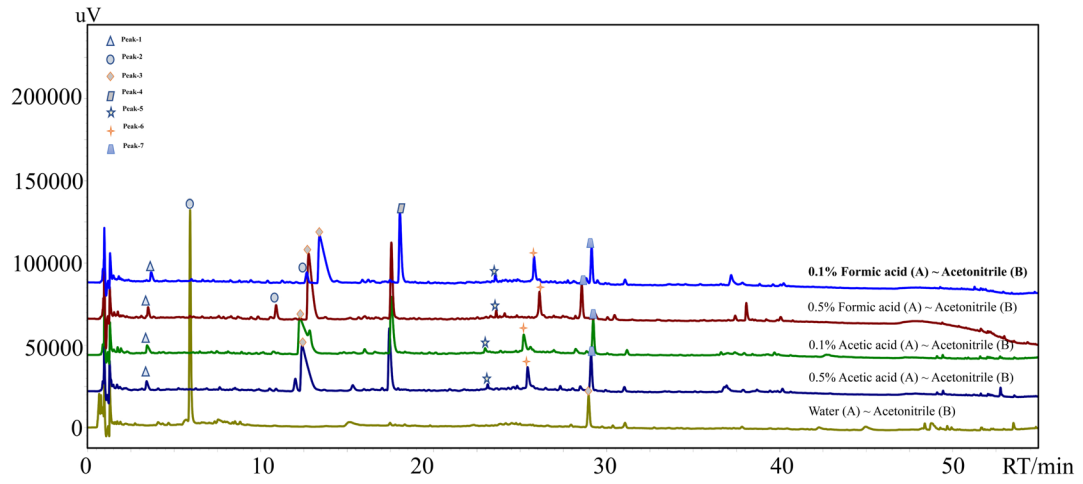


Figure S3



**Figure S4**



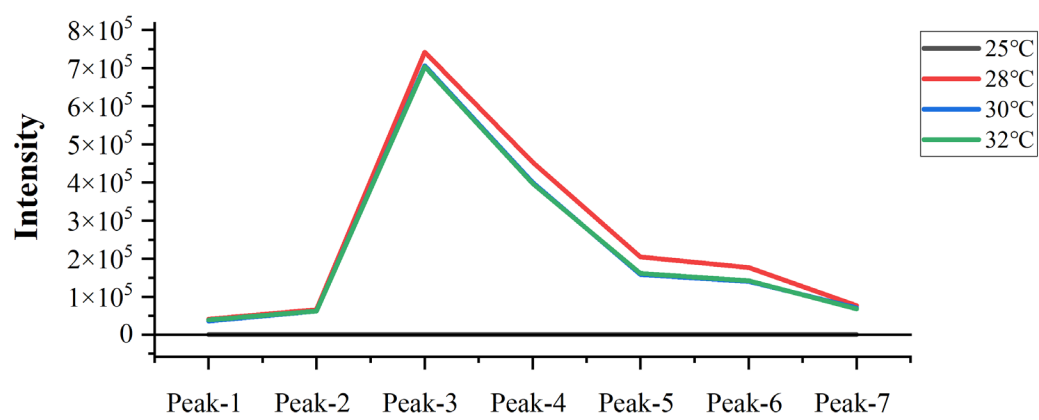
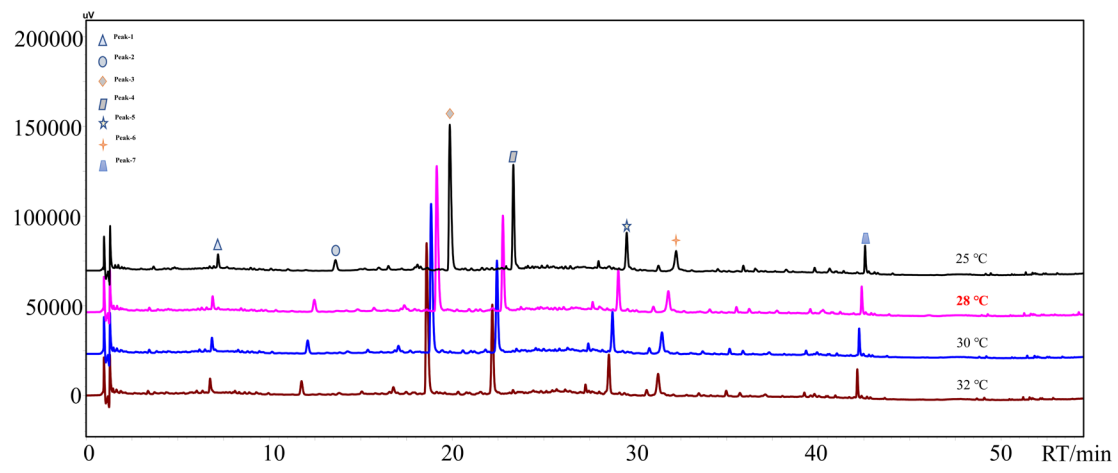


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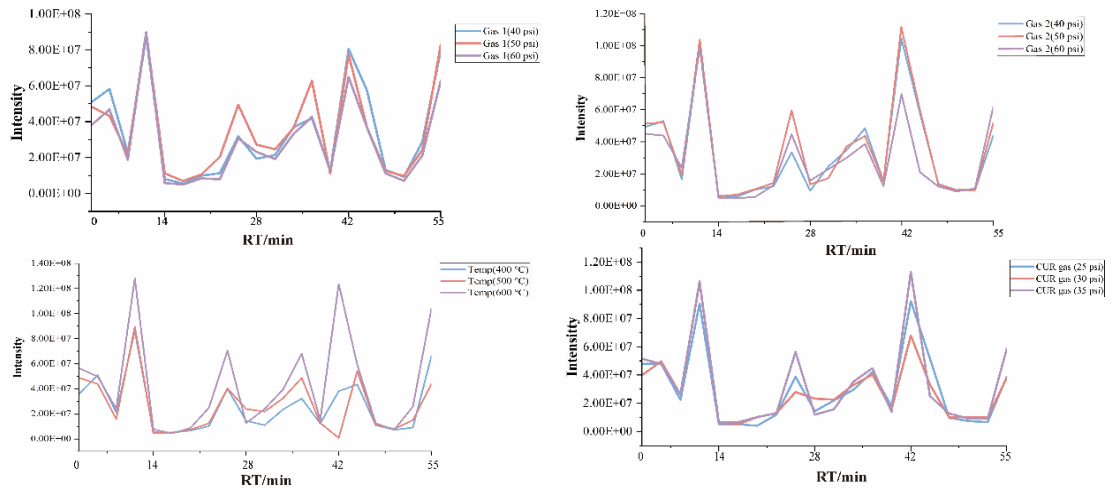
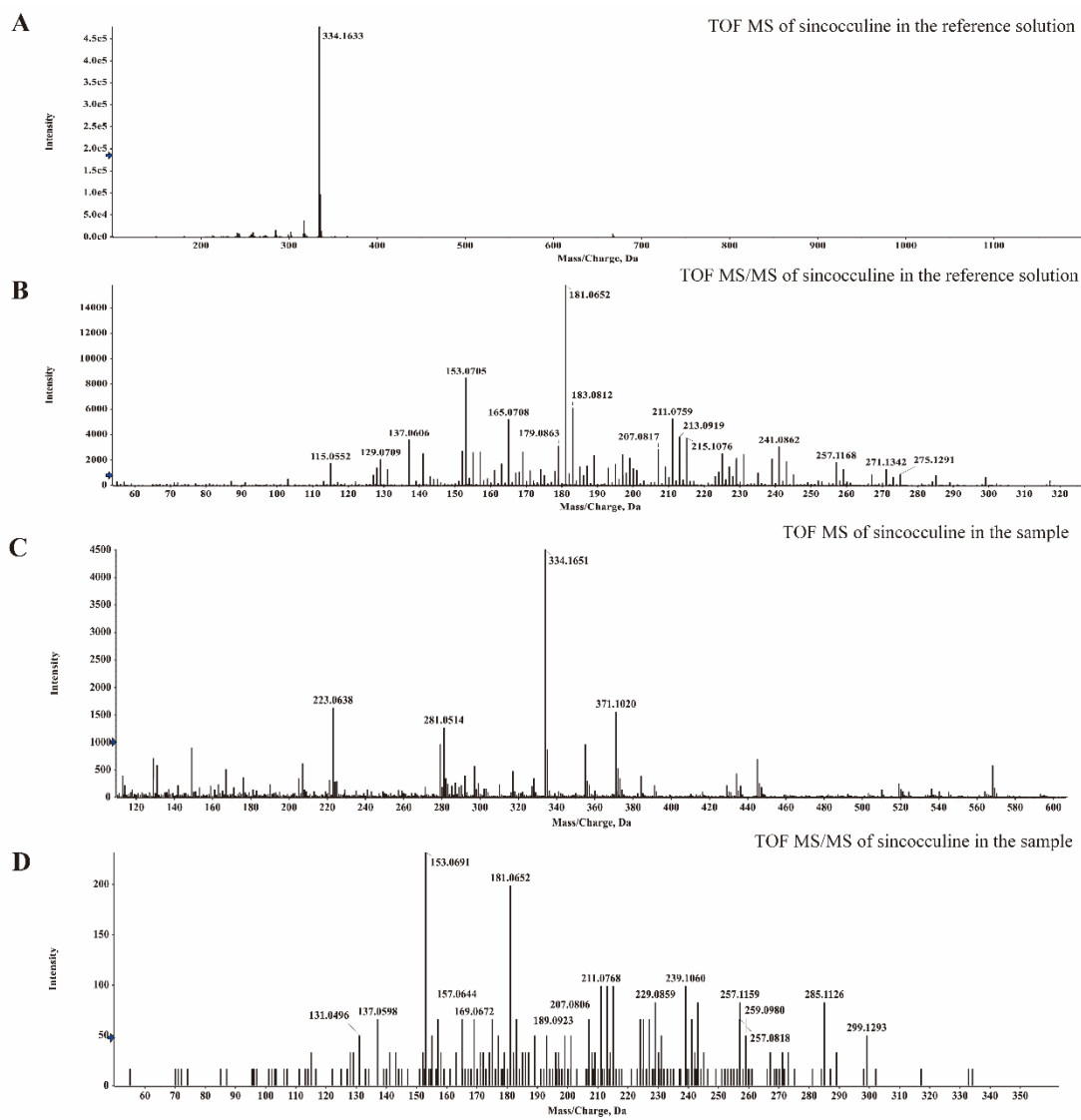
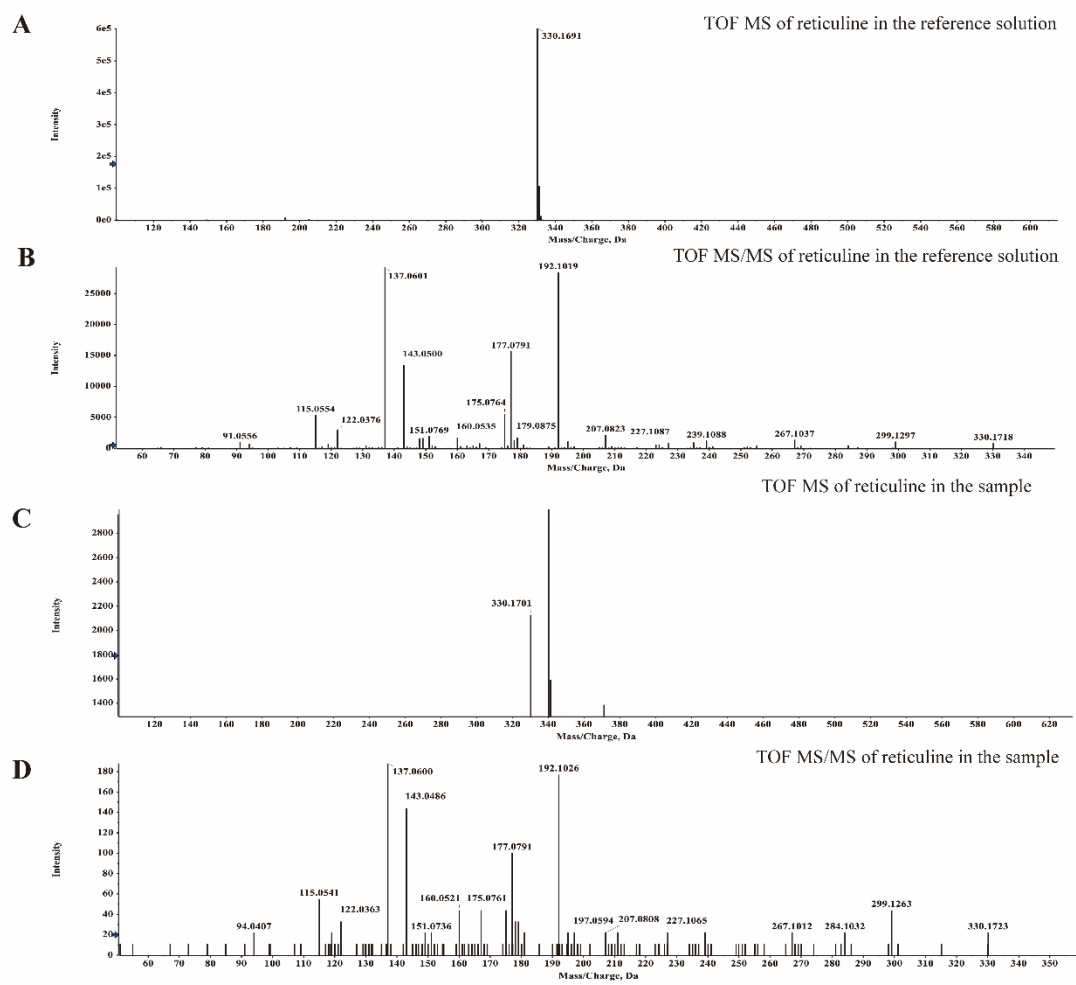


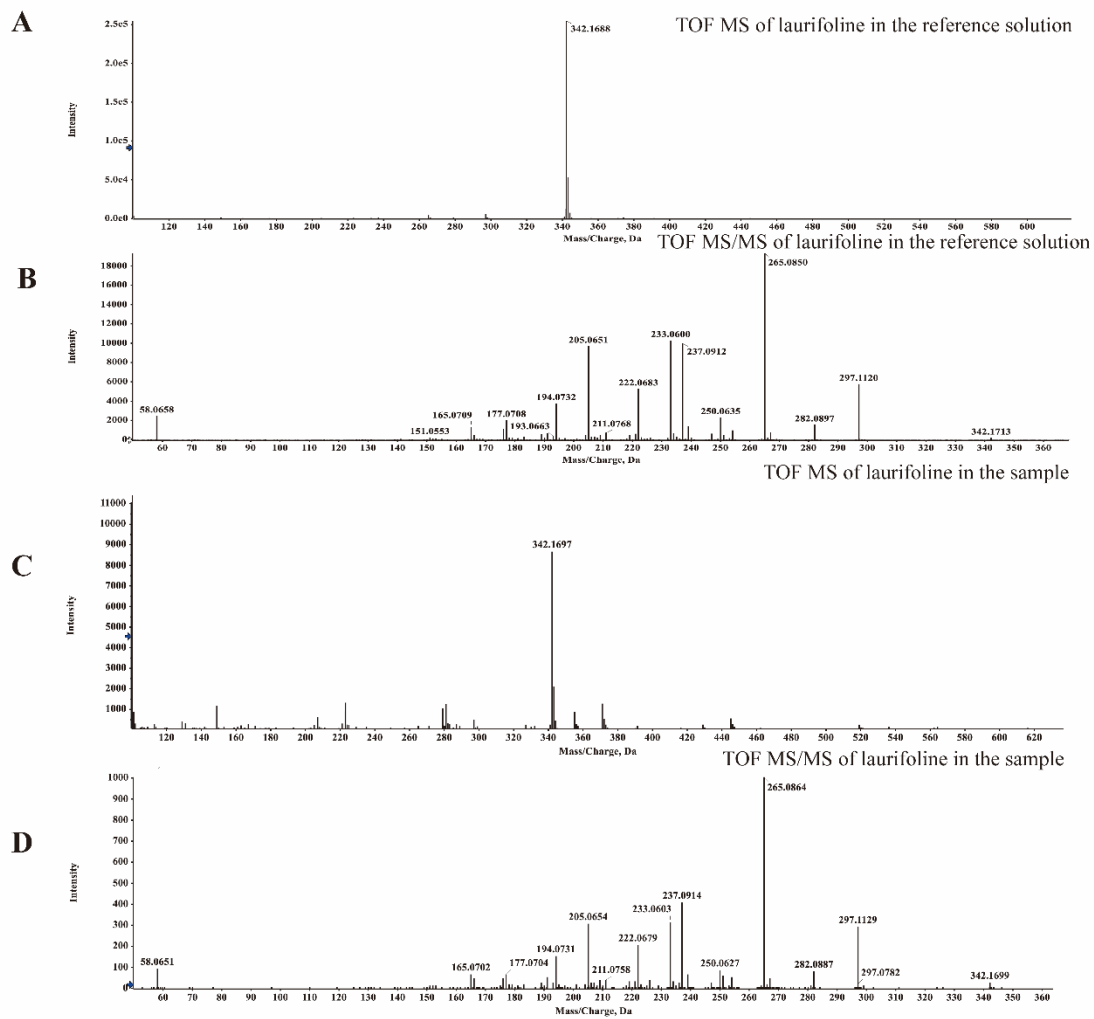
Figure S6



**Figure. S7**



**Figure. S8**



**Figure. S9**

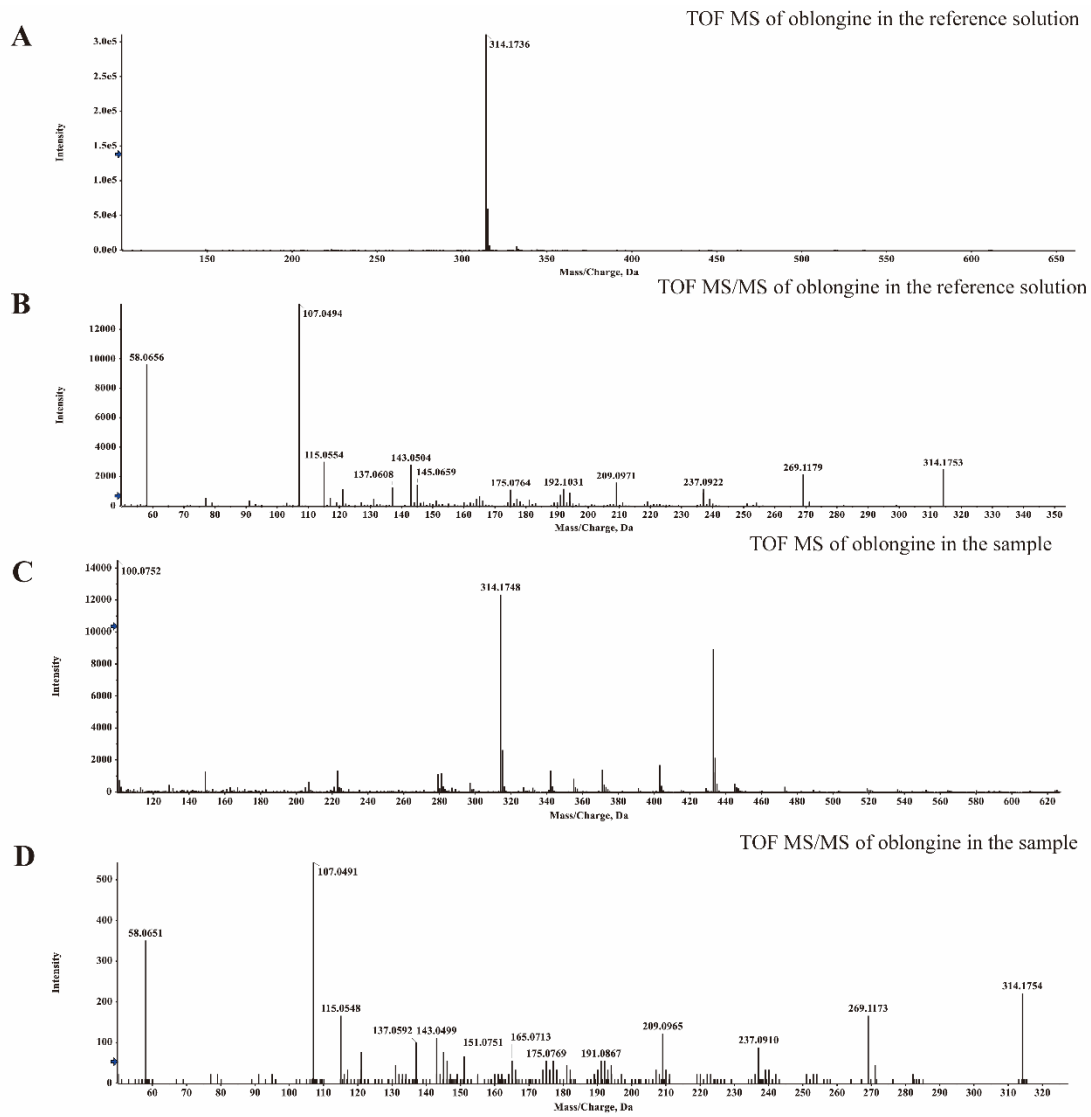


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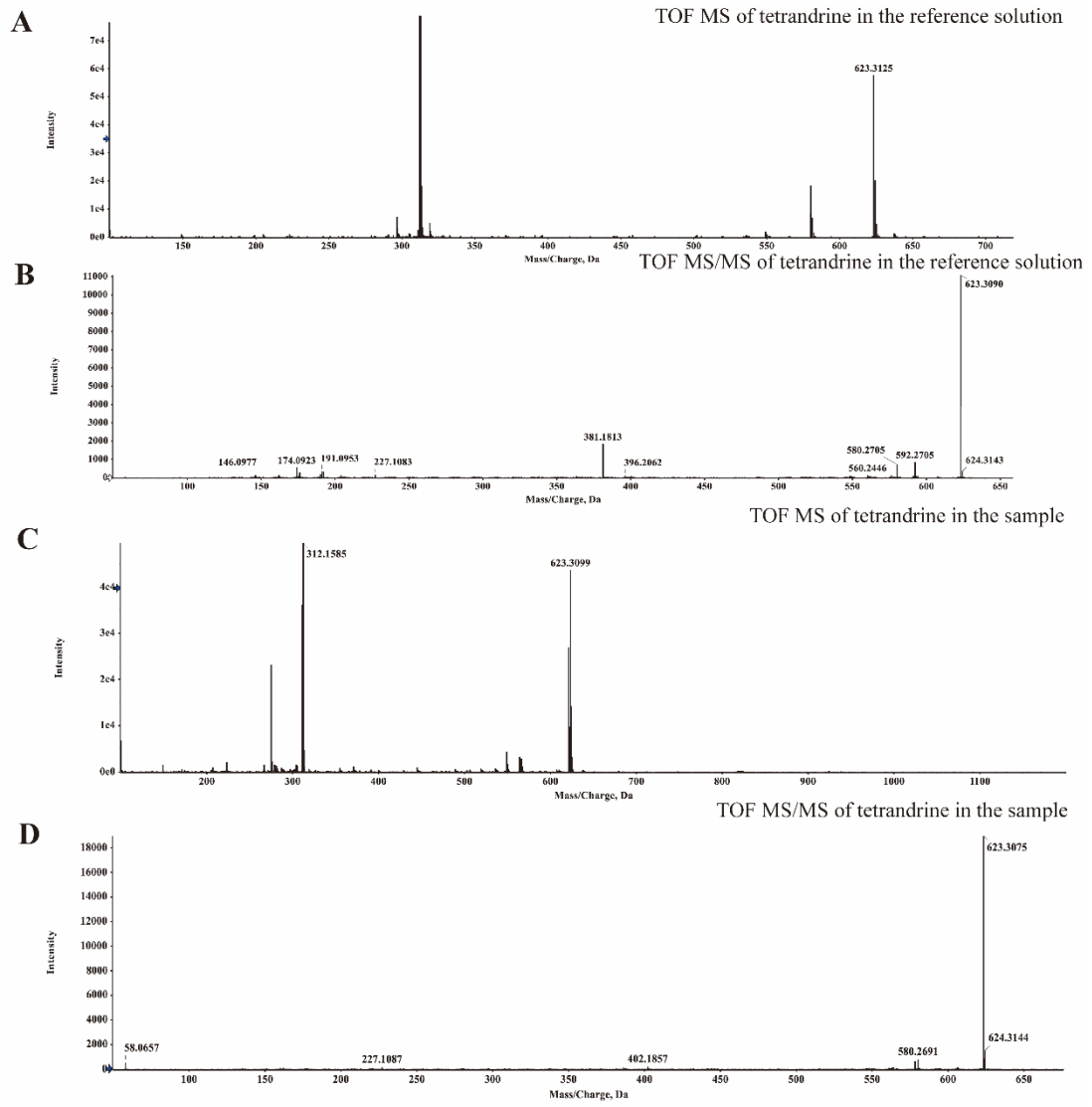


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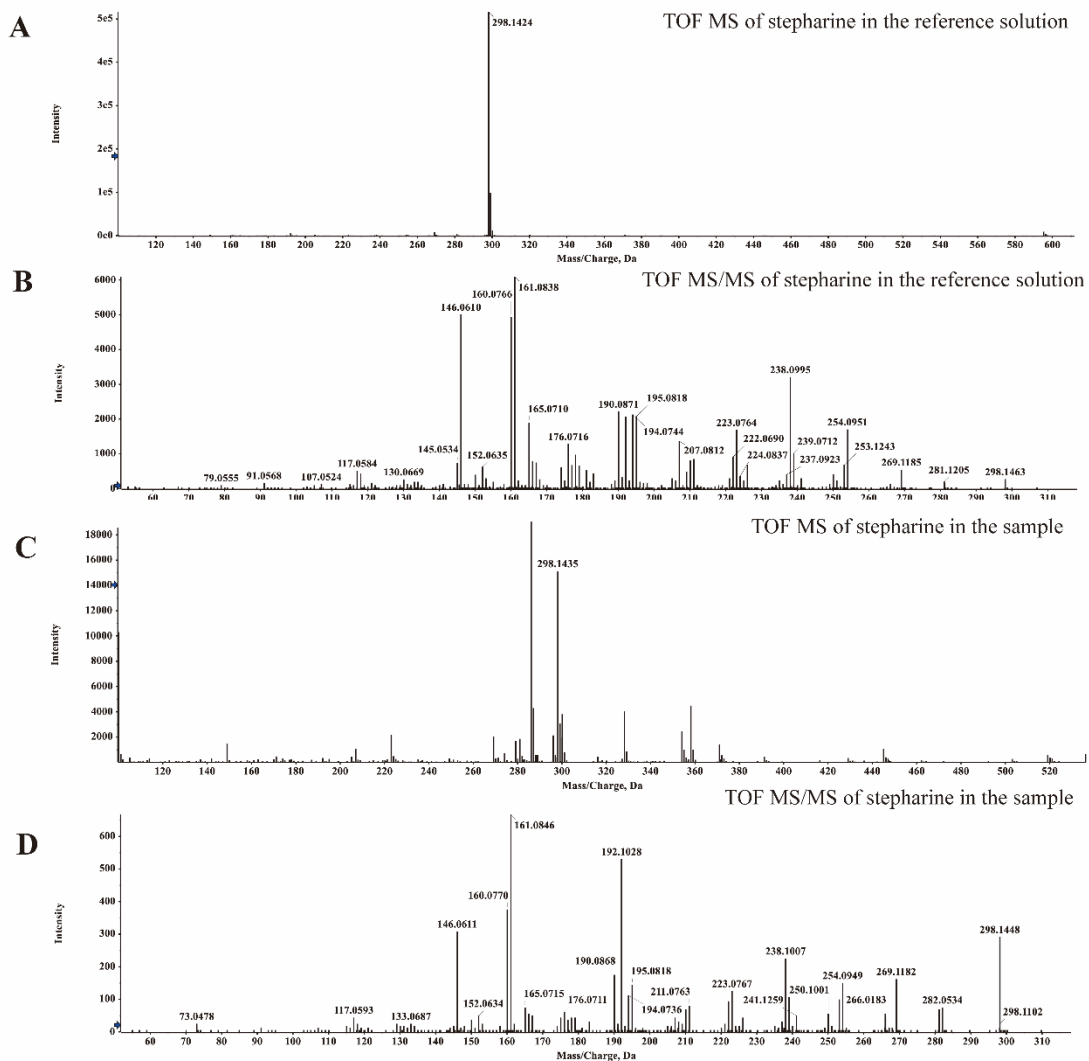


Figure. S12



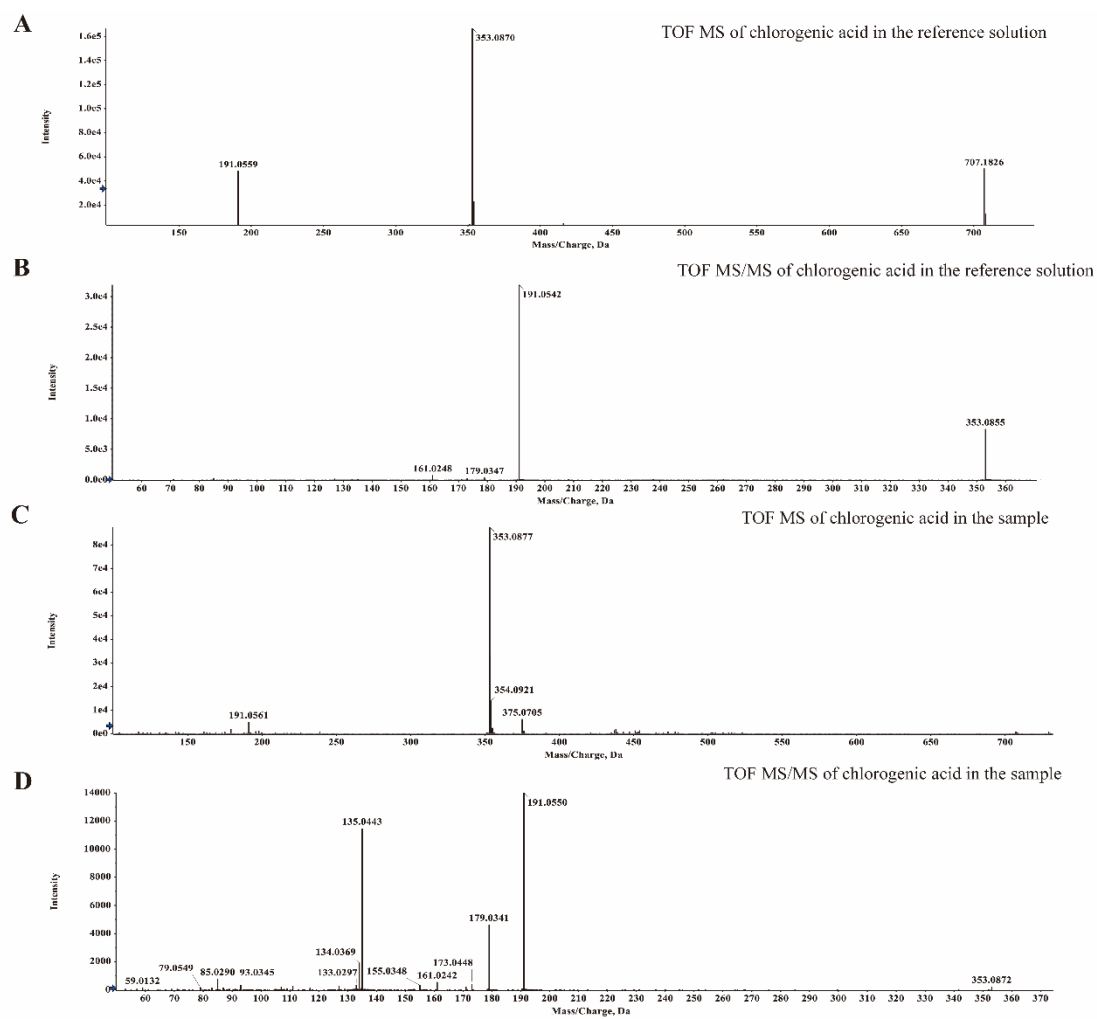
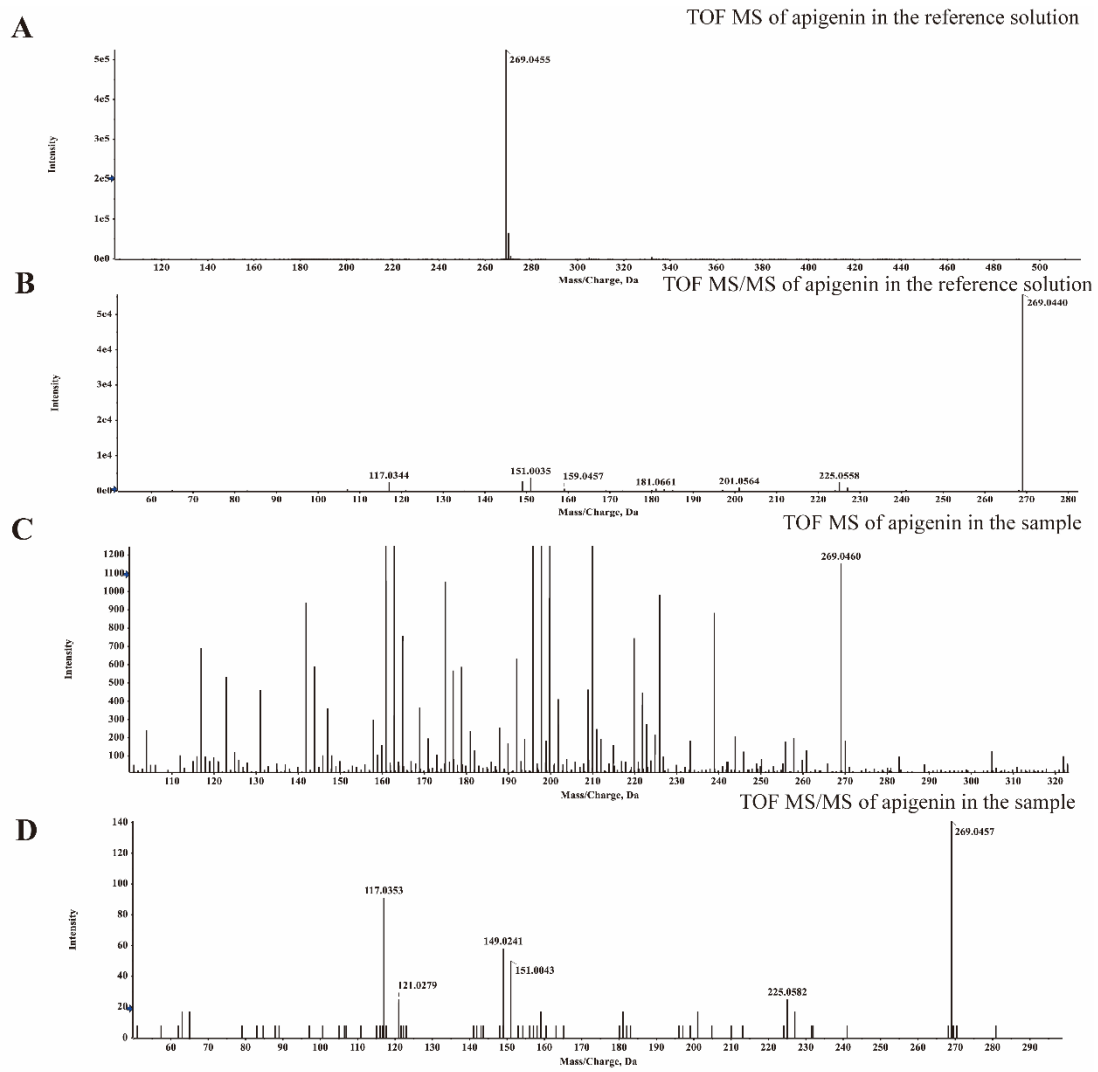
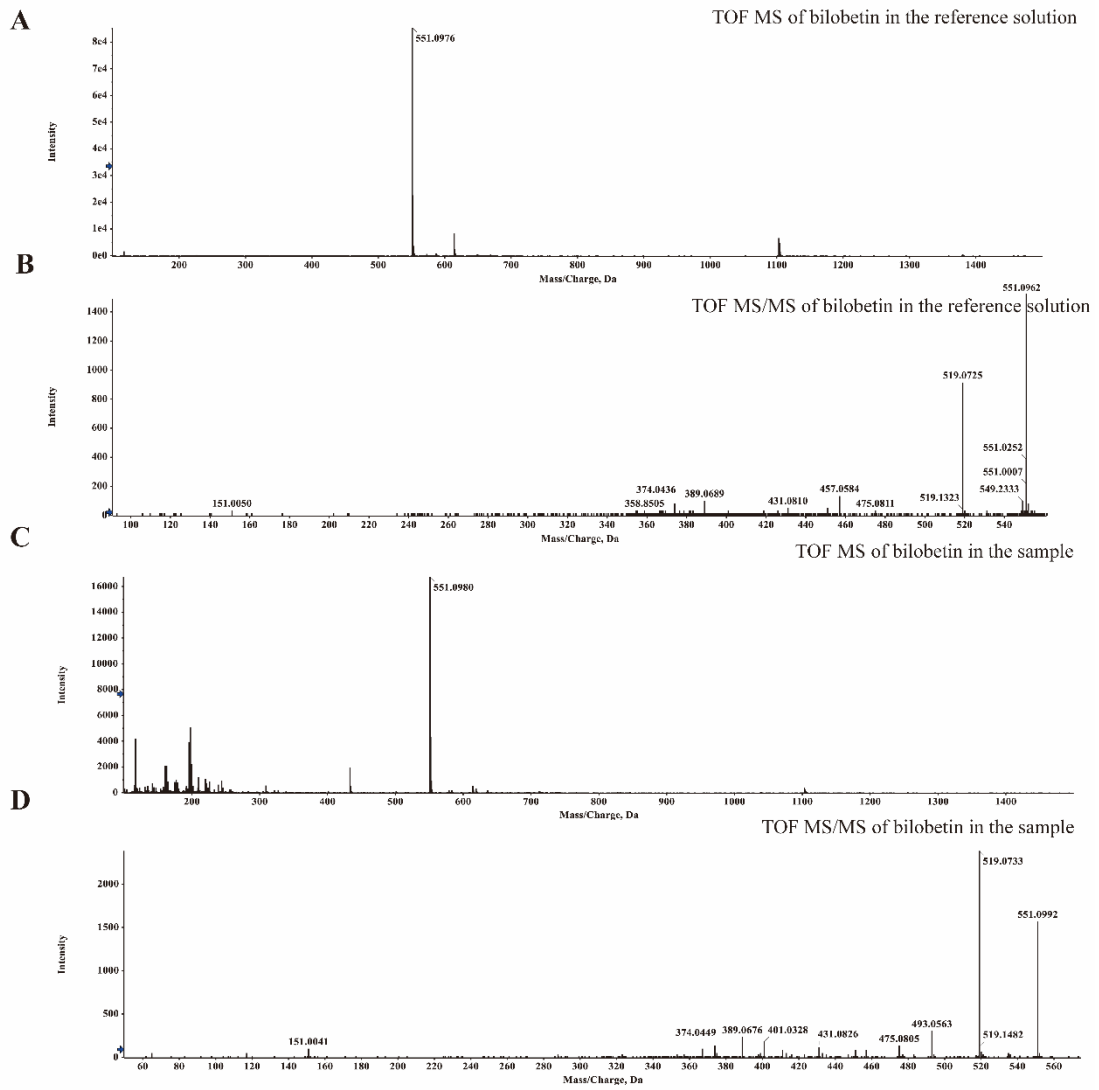


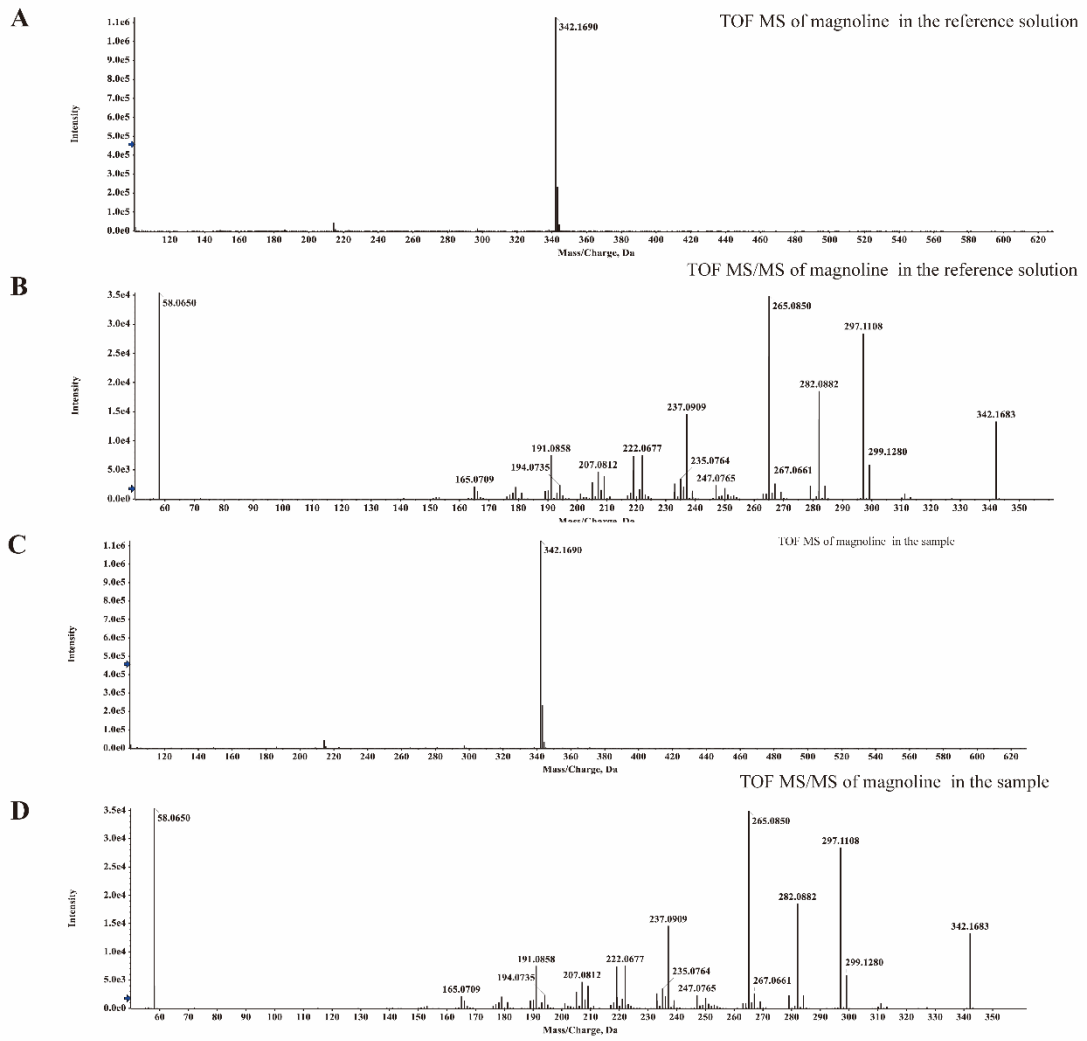
Figure. S13



**Figure. S14**



**Figure. S15**



**Figure. S16**

**Table S1**

No.	Sample batch	Sampling site	No.	Sample batch	Sampling site
S1	GZ-202212202	A	S47	GZ-20230623-7	B
S2	GZ-20230305-1	A	S48	GZ-20230906-1	C
S3	GZ-20230305-2	A	S49	GZ-20230906-2	C
S4	GZ-20230305-3	A	S50	GZ-20230906-3	C
S5	GZ-20230305-4	A	S51	GZ-20230906-4	C
S6	GZ-20230512-1	B	S52	GZ-20230906-5	D
S7	GZ-20230512-2	B	S53	GZ-20230906-6	D
S8	GZ-20230512-3	B	S54	GZ-20230906-7	D
S9	GZ-20230512-4	B	S55	GZ-20230906-8	C
S10	GZ-20230512-5	B	S56	GZ-20230906-9	C
S11	GZ-20230623-1	B	S57	GZ-20230909-1	E
S12	GZ-20230623-2	B	S58	GZ-20230909-2	E
S13	GZ-20230623-3	B	S59	GZ-20230909-3	E
S14	GZ-20230623-4	B	S60	GZ-20230909-4	E
S15	GZ-20230623-5	B	S61	GZ-20230909-5	E
S16	GZ-20230623-6	B	S62	GZ-20230512-1	B
S17	GZ-20230623-7	B	S63	GZ-20230512-2	B
S18	GZ-20230906-1	C	S64	GZ-20230512-3	B
S19	GZ-20230906-2	C	S65	GZ-20230512-4	B
S20	GZ-20230906-3	C	S66	GZ-20230512-5	B

S21	GZ-20230906-4	C	S67	GZ-20230623-1	B
S22	GZ-20230906-5	D	S68	GZ-20230623-2	B
S23	GZ-20230906-6	D	S69	GZ-20230623-3	B
S24	GZ-20230906-7	D	S70	GZ-20230623-4	B
S25	GZ-20230906-8	C	S71	GZ-20230623-5	B
S26	GZ-20230906-9	C	S72	GZ-20230623-6	B
S27	GZ-20230909-1	E	S73	GZ-20230623-7	B
S28	GZ-20230909-2	E	S74	GZ-20230906-1	C
S29	GZ-20230909-3	E	S75	GZ-20230906-2	C
S30	GZ-20230909-4	E	S76	GZ-20230906-3	C
S31	GZ-202212202	A	S77	GZ-20230906-4	C
S32	GZ-20230305-1	A	S78	GZ-20230906-5	D
S33	GZ-20230305-2	A	S79	GZ-20230906-6	D
S34	GZ-20230305-3	A	S80	GZ-20230906-7	D
S35	GZ-20230305-4	B	S81	GZ-20230906-8	C
S36	GZ-20230512-1	B	S82	GZ-20230906-9	C
S37	GZ-20230512-2	B	S83	GZ-20230909-1	E
S38	GZ-20230512-3	B	S84	GZ-20230909-2	E
S39	GZ-20230512-4	B	S85	GZ-20230909-3	E
S40	GZ-20230512-5	B	S86	GZ-20230909-3-1	E
S41	GZ-20230623-1	B	S87	GZ-20230909-3-2	E
S42	GZ-20230623-2	B	S88	GZ-20230909-3-3	E

S43	GZ-20230623-3	B	S89	GZ-20230909-3-1	E
S44	GZ-20230623-4	B	S90	GZ-20230909-3-2	E
S45	GZ-20230623-5	B	S91	GZ-20230909-3-3	E
S46	GZ-20230623-6	B			

Note: A: Guiyang Xintian Pharmaceutical Co., Ltd.; B: Qianxi City, Bijie City, Guizhou Province ; C: Honghuagang District, Zunyi City, Guizhou Province; D: Meitan County, Zunyi City, Guizhou Province; E: Huichuan District, Zunyi City, Guizhou Province.

**Table S2**

Standards	Formula	Lot No.	CAS No.	Purity	Manufacturer
Magnoflorine	$C_{20}H_{24}NO_4^+$	808F021	8841-09-5	HPLC>98%	A
Sinococuline	$C_{18}H_{23}NO_5$	BBP06007	109351-36-2	HPLC>98%	B
Tetrandrine	$C_{38}H_{42}N_2O_6$	BBP03852	518-34-3	HPLC>98%	B
Laurifoline	$C_{20}H_{24}NO_4$	BBP01501	7224-61-5	HPLC>98%	B
Stepharine	$C_{18}H_{19}NO_3$	BBP06021	2810-21-1	HPLC>98%	B
Reticuline	$C_{19}H_{23}NO_4$	BBP01159	485-19-8	HPLC>98%	B
Oblongine	$C_{19}H_{24}NO_3^+$	BBP01570	60008-01-7	HPLC>98%	B
Chlorogenic acid	$C_{16}H_{18}O_9$	BBP03169	327-97-9	HPLC>98%	B
Bilobetin	$C_{31}H_{20}O_{10}$	BBP02192	521-32-4	HPLC>98%	B
Apigenin	$C_{15}H_{10}O_5$	BBP00357	520-36-5	HPLC>98%	B

Note: A: Beijing Solarbio Science & Technology Co., Ltd.; B: BioBioPha Co., Ltd.



Table 3

No.	Compound	Formula	Molecular weight	No.	compound	formula	molecular weight
1	kohatine	C <sub>34</sub> H <sub>32</sub> N <sub>2</sub> O <sub>6</sub>	564.2252	130	jamtine- <i>N</i> -oxide	C <sub>20</sub> H <sub>25</sub> NO <sub>5</sub>	359.1726
2	2- <i>N</i> -methylkohatine	C <sub>35</sub> H <sub>32</sub> N <sub>2</sub> O <sub>6</sub>	576.2252	131	laurifinine	C <sub>20</sub> H <sub>25</sub> NO <sub>3</sub>	327.1828
3	5'-hydroxyapateline	C <sub>34</sub> H <sub>32</sub> N <sub>2</sub> O <sub>6</sub>	564.2252	132	hirsutine	C <sub>19</sub> H <sub>23</sub> NO <sub>4</sub>	329.1621
4	puertogaline B	C <sub>35</sub> H <sub>32</sub> N <sub>2</sub> O <sub>6</sub>	576.2252	133	cohirsitinine	C <sub>18</sub> H <sub>23</sub> NO <sub>3</sub>	301.1672
5	$\alpha,\alpha'$ -dioxo-7'- <i>O</i> -demethylstebisimine	C <sub>35</sub> H <sub>28</sub> N <sub>2</sub> O <sub>8</sub>	604.1838	134	coclafine	C <sub>16</sub> H <sub>19</sub> NO <sub>2</sub>	257.1411
6	tliafunimine	C <sub>36</sub> H <sub>36</sub> N <sub>2</sub> O <sub>6</sub>	592.2564	135	isocorydine	C <sub>21</sub> H <sub>26</sub> NO <sub>4</sub>	356.1855
7	demethylstebisimine	C <sub>36</sub> H <sub>36</sub> N <sub>2</sub> O <sub>6</sub>	592.2564	136	bavachinin	C <sub>21</sub> H <sub>22</sub> O <sub>4</sub>	339.1465
8	(+)-norberbamine	C <sub>36</sub> H <sub>38</sub> N <sub>2</sub> O <sub>6</sub>	594.272	137	Isoxanthohumol	C <sub>21</sub> H <sub>22</sub> O <sub>5</sub>	354.1461
9	coclobine	C <sub>37</sub> H <sub>38</sub> N <sub>2</sub> O <sub>6</sub>	606.272	138	leachianone G	C <sub>20</sub> H <sub>20</sub> O <sub>6</sub>	356.1254
10	cheratamine	C <sub>36</sub> H <sub>34</sub> N <sub>2</sub> O <sub>7</sub>	606.2357	139	pinnatifinoside I	C <sub>24</sub> H <sub>22</sub> O <sub>10</sub>	470.1206
11	cocsuline- <i>N</i> -2-oxide	C <sub>36</sub> H <sub>34</sub> N <sub>2</sub> O <sub>6</sub>	590.2408	140	isobavachin	C <sub>20</sub> H <sub>20</sub> O <sub>4</sub>	324.1356
12	isotrilobone- <i>N</i> -2-oxide	C <sub>36</sub> H <sub>36</sub> N <sub>2</sub> O <sub>6</sub>	592.2564	141	lupinifolin	C <sub>25</sub> H <sub>26</sub> O <sub>5</sub>	406.1773
13	<i>O</i> -methylthalmethine	C <sub>37</sub> H <sub>38</sub> N <sub>2</sub> O <sub>6</sub>	606.272	142	norkurainol	C <sub>25</sub> H <sub>28</sub> O <sub>7</sub>	440.1827
14	punjabine	C <sub>35</sub> H <sub>32</sub> N <sub>2</sub> O <sub>7</sub>	592.2201	143	sanggenon H	C <sub>20</sub> H <sub>18</sub> O <sub>6</sub>	354.1098
15	wattisine A	C <sub>36</sub> H <sub>38</sub> N <sub>2</sub> O <sub>6</sub>	594.272	144	kushenol B	C <sub>30</sub> H <sub>36</sub> O <sub>6</sub>	492.2502
16	stebisimine	C <sub>36</sub> H <sub>34</sub> N <sub>2</sub> O <sub>6</sub>	590.2408	145	5,7,8,2'-tetrahydroxy-flavone-7- <i>O</i> - $\beta$ - <i>D</i> -glucoside	C <sub>21</sub> H <sub>20</sub> O <sub>11</sub>	448.0999
17	siddiquamine	C <sub>35</sub> H <sub>30</sub> N <sub>2</sub> O <sub>6</sub>	608.2876	146	(2 <i>S</i> )-5,7-dihydroxy-6-methoxy-flavanone-7- <i>O</i> - $\beta$ - <i>D</i> -glucopyranoside	C <sub>22</sub> H <sub>24</sub> O <sub>10</sub>	448.1362
18	1,2-dehydrokohatine	C <sub>32</sub> H <sub>30</sub> N <sub>2</sub> O <sub>6</sub>	608.2876	147	liquiritigenin-4' - <i>O</i> - $\beta$ - <i>D</i> -glucopyranoside	C <sub>21</sub> H <sub>22</sub> O <sub>9</sub>	418.1257

19	apateline	C <sub>34</sub> H <sub>32</sub> N <sub>2</sub> O <sub>5</sub>	548.2303	148	liquiritin	C <sub>21</sub> H <sub>22</sub> O <sub>9</sub>	418.1257
20	cocsoline	C <sub>34</sub> H <sub>32</sub> N <sub>2</sub> O <sub>5</sub>	548.2303	149	hispidulin7-(6- <i>E-p</i> -coumaroyl- $\beta$ - <i>D</i> -glucopyranoside)	C <sub>31</sub> H <sub>28</sub> O <sub>13</sub>	608.1521
21	hydroxyisotrilobine	C <sub>36</sub> H <sub>36</sub> N <sub>2</sub> O <sub>6</sub>	592.2564	150	7,4',7'',4'''-tetra- <i>O</i> -amentoflavone	C <sub>34</sub> H <sub>26</sub> O <sub>10</sub>	594.1518
22	kurramine	C <sub>33</sub> H <sub>28</sub> N <sub>2</sub> O <sub>5</sub>	532.1991	151	sanggenon G	C <sub>40</sub> H <sub>38</sub> O <sub>11</sub>	694.2403
23	(+)-cocsuline	C <sub>35</sub> H <sub>34</sub> N <sub>2</sub> O <sub>5</sub>	562.2459	152	gardenin C	C <sub>20</sub> H <sub>22</sub> O <sub>9</sub>	406.1257
24	N-methylapateline	C <sub>35</sub> H <sub>34</sub> N <sub>2</sub> O <sub>5</sub>	562.2459	153	flavone	C <sub>15</sub> H <sub>10</sub> O <sub>2</sub>	222.0678
25	(+)-kohatamine	C <sub>35</sub> H <sub>34</sub> N <sub>2</sub> O <sub>6</sub>	578.2408	154	isosakuranetin	C <sub>16</sub> H <sub>14</sub> O <sub>5</sub>	286.0837
26	kurramine-2'- $\alpha$ - <i>N</i> -oxide	C <sub>33</sub> H <sub>28</sub> N <sub>2</sub> O <sub>6</sub>	548.194	155	5,7,8,3',4'-pentamethoxyflavone	C <sub>20</sub> H <sub>20</sub> O <sub>7</sub>	372.1203
27	kurramine-2'- $\beta$ - <i>N</i> -oxide	C <sub>33</sub> H <sub>28</sub> N <sub>2</sub> O <sub>6</sub>	548.194	156	flavonol	C <sub>15</sub> H <sub>10</sub> O <sub>3</sub>	238.0627
28	(+)-coccuorbiculatine A	C <sub>38</sub> H <sub>42</sub> N <sub>2</sub> O <sub>6</sub>	622.3032	157	quercetin	C <sub>15</sub> H <sub>10</sub> O <sub>7</sub>	302.0423
29	(+)- <i>O</i> -methylcocsoline	C <sub>35</sub> H <sub>34</sub> N <sub>2</sub> O <sub>5</sub>	562.2459	158	kushenol G	C <sub>25</sub> H <sub>28</sub> O <sub>8</sub>	456.1776
30	oxyacanthine	C <sub>37</sub> H <sub>40</sub> N <sub>2</sub> O <sub>6</sub>	608.2876	159	patuletin-7- <i>O</i> -[6'- <i>O</i> -(2-methylbutyryl)]-glucoside	C <sub>27</sub> H <sub>30</sub> O <sub>14</sub>	578.1626
31	trilobamine	C <sub>35</sub> H <sub>36</sub> N <sub>2</sub> O <sub>6</sub>	580.2564	160	kaempferol-3- <i>O</i> -neohesperidoside	C <sub>27</sub> H <sub>30</sub> O <sub>15</sub>	594.1575
32	(+)-siddiquine	C <sub>34</sub> H <sub>28</sub> N <sub>2</sub> O <sub>6</sub>	560.194	161	quercetin-7- <i>O</i> -rutinoside	C <sub>27</sub> H <sub>30</sub> O <sub>16</sub>	610.1524
33	cocsupendine	C <sub>36</sub> H <sub>34</sub> N <sub>2</sub> O <sub>6</sub>	590.2408	162	sagittatoside B	C <sub>32</sub> H <sub>38</sub> O <sub>14</sub>	646.225
34	normenisarine	C <sub>34</sub> H <sub>32</sub> N <sub>2</sub> O <sub>5</sub>	548.2303	163	kaempferol-3- <i>O</i> -lathyroside(Nikotoflorin)	C <sub>26</sub> H <sub>28</sub> O <sub>15</sub>	580.1419
35	menisarine	C <sub>36</sub> H <sub>34</sub> N <sub>2</sub> O <sub>6</sub>	590.2408	164	rutin	C <sub>27</sub> H <sub>30</sub> O <sub>16</sub>	610.1524
36	tetrandrine	C <sub>38</sub> H <sub>42</sub> N <sub>2</sub> O <sub>5</sub>	606.3083	165	baohuoside I	C <sub>27</sub> H <sub>30</sub> O <sub>10</sub>	514.183
37	norpenduline	C <sub>36</sub> H <sub>38</sub> N <sub>2</sub> O <sub>6</sub>	594.272	166	ermanin	C <sub>17</sub> H <sub>14</sub> O <sub>6</sub>	314.0786
38	hernandezine	C <sub>39</sub> H <sub>44</sub> N <sub>2</sub> O <sub>7</sub>	652.3137	167	kaempferol	C <sub>15</sub> H <sub>10</sub> O <sub>6</sub>	286.0474

39	penduline	C <sub>37</sub> H <sub>40</sub> N <sub>2</sub> O <sub>6</sub>	608.2876	168	ombuin-3- <i>O</i> -β- <i>D</i> -glucoside	C <sub>23</sub> H <sub>24</sub> O <sub>12</sub>	492.126
40	(+)-1,2-dehydro-2'-nortelobine	C <sub>34</sub> H <sub>30</sub> N <sub>2</sub> O <sub>5</sub>	546.2147	169	kaempferide-4' -methylether-3-glucoside	C <sub>22</sub> H <sub>22</sub> O <sub>11</sub>	462.1155
41	<i>O,O</i> -dimethy-1',2'-dehydronorkohatine	C <sub>35</sub> H <sub>32</sub> N <sub>2</sub> O <sub>6</sub>	576.2252	170	isorhamnetin-3- <i>O</i> -β- <i>D</i> -galactoside	C <sub>22</sub> H <sub>22</sub> O <sub>12</sub>	478.1104
42	1,2-dehydroapateline	C <sub>34</sub> H <sub>30</sub> N <sub>2</sub> O <sub>5</sub>	546.2147	171	kaempferol-3-glucuronide	C <sub>21</sub> H <sub>18</sub> O <sub>12</sub>	462.0792
43	orbiculatinine	C <sub>34</sub> H <sub>30</sub> N <sub>2</sub> O <sub>6</sub>	562.2096	172	trifolin	C <sub>21</sub> H <sub>20</sub> O <sub>11</sub>	448.0999
44	1,2-dehydrokohatamine	C <sub>35</sub> H <sub>32</sub> N <sub>2</sub> O <sub>6</sub>	576.2252	173	2,5-dimethyl-7-hydroxychromone	C <sub>11</sub> H <sub>10</sub> O <sub>3</sub>	190.0627
45	dehydrokohatine	C <sub>34</sub> H <sub>30</sub> N <sub>2</sub> O <sub>6</sub>	562.2096	174	5- <i>O</i> -methylvisamminol	C <sub>16</sub> H <sub>18</sub> O <sub>5</sub>	290.1149
46	1,2-dehydro-2'-nortelobine	C <sub>34</sub> H <sub>30</sub> N <sub>2</sub> O <sub>5</sub>	546.2147	175	ledebouriellol	C <sub>20</sub> H <sub>22</sub> O <sub>7</sub>	374.1359
47	<i>N</i> -norcocsulinin	C <sub>34</sub> H <sub>32</sub> N <sub>2</sub> O <sub>6</sub>	564.2252	176	1,5-dihydrxy-2,3,4,7-tetramethoxyxanthone	C <sub>17</sub> H <sub>16</sub> O <sub>8</sub>	348.084
48	cocsilinine	C <sub>33</sub> H <sub>30</sub> N <sub>2</sub> O <sub>6</sub>	550.2096	177	2''- <i>O</i> -feruloylaloetin	C <sub>29</sub> H <sub>30</sub> O <sub>12</sub>	570.1728
49	<i>O</i> -methylcocsulinine	C <sub>36</sub> H <sub>36</sub> N <sub>2</sub> O <sub>6</sub>	592.2564	178	aloeresin	C <sub>19</sub> H <sub>22</sub> O <sub>9</sub>	394.1257
50	cocsiline	C <sub>35</sub> H <sub>34</sub> N <sub>2</sub> O <sub>6</sub>	578.2408	179	prim- <i>O</i> -glucosylcimifugin	C <sub>22</sub> H <sub>28</sub> O <sub>11</sub>	468.1623
51	cocsulinine	C <sub>35</sub> H <sub>34</sub> N <sub>2</sub> O <sub>6</sub>	578.2408	180	sec- <i>O</i> -glucosylhamaudol	C <sub>21</sub> H <sub>26</sub> O <sub>10</sub>	438.1518
52	pendulinine	C <sub>35</sub> H <sub>34</sub> N <sub>2</sub> O <sub>6</sub>	578.2408	181	aloeresin G	C <sub>29</sub> H <sub>30</sub> O <sub>10</sub>	538.183
53	pendilinine	C <sub>36</sub> H <sub>36</sub> N <sub>2</sub> O <sub>6</sub>	592.2564	182	6-methoxy-2-[2-(3'-methoxyphenyl)ethyl]chromone	C <sub>19</sub> H <sub>18</sub> O <sub>4</sub>	310.12
54	pendine	C <sub>35</sub> H <sub>34</sub> N <sub>2</sub> O <sub>6</sub>	578.2408	183	6,7-dimethoxy-2-(2- <i>p</i> -methoxyphenylethyl)chromone	C <sub>20</sub> H <sub>20</sub> O <sub>5</sub>	340.1305

<b>55</b>	12'- <i>O</i> - methyldehydrokohatine	C <sub>35</sub> H <sub>34</sub> N <sub>2</sub> O <sub>6</sub>	578.2408	<b>184</b>	6-hydroxy-2-(2-phenylethyl) chromone	C <sub>17</sub> H <sub>14</sub> O <sub>3</sub>	266.0939
<b>56</b>	5'-hydroxytelobine	C <sub>35</sub> H <sub>34</sub> N <sub>2</sub> O <sub>6</sub>	578.2408	<b>185</b>	6,7-dihydroxy-2-(2-phenylethyl) chromone	C <sub>19</sub> H <sub>18</sub> O <sub>4</sub>	310.12
<b>57</b>	1,2-dihydrokurramine	C <sub>33</sub> H <sub>30</sub> N <sub>2</sub> O <sub>5</sub>	534.2147	<b>186</b>	6-methoxy-2-(2-phenylethyl) chromone	C <sub>18</sub> H <sub>16</sub> O <sub>3</sub>	280.1095
<b>58</b>	trilobine	C <sub>35</sub> H <sub>34</sub> N <sub>2</sub> O <sub>5</sub>	562.2459	<b>187</b>	6-hydroxy-2-[2-(4'-methoxyphenyl)ethyl] chromone	C <sub>18</sub> H <sub>16</sub> O <sub>4</sub>	296.1044
<b>59</b>	nortrilobine	C <sub>34</sub> H <sub>32</sub> N <sub>2</sub> O <sub>5</sub>	548.2303	<b>188</b>	chrysin	C <sub>15</sub> H <sub>10</sub> O <sub>4</sub>	254.0576
<b>60</b>	tricordatine	C <sub>34</sub> H <sub>32</sub> N <sub>2</sub> O <sub>5</sub>	548.2303	<b>189</b>	tangeritin	C <sub>20</sub> H <sub>20</sub> O <sub>7</sub>	372.1203
<b>61</b>	isotrilobine	C <sub>35</sub> H <sub>36</sub> N <sub>2</sub> O <sub>6</sub>	580.2564	<b>190</b>	5,6,4'-trihydroxy-7,8-dimethoxyflavone	C <sub>17</sub> H <sub>14</sub> O <sub>7</sub>	330.0735
<b>62</b>	laurifoline	C <sub>20</sub> H <sub>24</sub> NO <sub>4</sub>	342.1699	<b>191</b>	4',5,7,8-tetramethoxy-flavone	C <sub>19</sub> H <sub>18</sub> O <sub>6</sub>	342.1098
<b>63</b>	<i>N,O</i> - dimethylisocorydine	C <sub>22</sub> H <sub>28</sub> NO <sub>4</sub> +	370.2011	<b>192</b>	5,7,4'-trihydroxy-8,3'-diprenylflavone	C <sub>25</sub> H <sub>26</sub> O <sub>5</sub>	406.1773
<b>64</b>	<i>N</i> -methylboldine	C <sub>20</sub> H <sub>24</sub> NO <sub>4</sub> +	342.1699	<b>193</b>	genkwanin-4'- <i>O</i> - $\beta$ - <i>D</i> -rutinoside	C <sub>28</sub> H <sub>32</sub> O <sub>14</sub>	592.1782
<b>65</b>	norisoboldine	C <sub>18</sub> H <sub>19</sub> NO <sub>4</sub>	313.1309	<b>194</b>	licoflavone A	C <sub>20</sub> H <sub>18</sub> O <sub>4</sub>	322.12
<b>66</b>	magnoflorine	C <sub>20</sub> H <sub>24</sub> NO <sub>4</sub>	342.1699	<b>195</b>	bilobetin	C <sub>31</sub> H <sub>20</sub> O <sub>10</sub>	552.105
<b>67</b>	stepharine	C <sub>18</sub> H <sub>19</sub> NO <sub>3</sub>	297.136	<b>196</b>	sotetsuflavone	C <sub>31</sub> H <sub>20</sub> O <sub>10</sub>	552.105
<b>68</b>	cocsarmine	C <sub>23</sub> H <sub>30</sub> NO <sub>4</sub> +	384.2167	<b>197</b>	5'-methoxy-bilobetin	C <sub>32</sub> H <sub>22</sub> O <sub>11</sub>	582.1155
<b>69</b>	( <i>S</i> )-dicentrine	C <sub>20</sub> H <sub>21</sub> NO <sub>4</sub>	339.1465	<b>198</b>	hinokiflavone	C <sub>30</sub> H <sub>18</sub> O <sub>10</sub>	538.0894
<b>70</b>	isoboldine	C <sub>19</sub> H <sub>21</sub> NO <sub>4</sub>	327.1465	<b>199</b>	flavanonol	C <sub>15</sub> H <sub>12</sub> O <sub>3</sub>	240.0783
<b>71</b>	norboldine	C <sub>18</sub> H <sub>19</sub> NO <sub>4</sub>	313.1309	<b>200</b>	(2 <i>R</i> ,3 <i>R</i> )-3,7-dihydroxy-6-methoxyflavanone	C <sub>16</sub> H <sub>14</sub> O <sub>5</sub>	286.0837

<b>72</b>	(±)- laurelliptinhexadecan- 1-one	C <sub>34</sub> H <sub>49</sub> NO <sub>5</sub>	551.3598	<b>201</b>	3,4',5-trihydroxy-7-methoxy-8- isopentenylflavone	C <sub>21</sub> H <sub>20</sub> O <sub>6</sub>	368.1254
<b>73</b>	(±)- laurelliptinoctadecan-1- one	C <sub>36</sub> H <sub>53</sub> NO <sub>5</sub>	579.391	<b>202</b>	kushenol M	C <sub>30</sub> H <sub>36</sub> O <sub>7</sub>	508.2451
<b>74</b>	menisperine	C <sub>21</sub> H <sub>26</sub> NO <sub>4</sub> +	356.1855	<b>203</b>	kushenol J	C <sub>27</sub> H <sub>32</sub> O <sub>14</sub>	580.1782
<b>75</b>	trilobinine	C <sub>20</sub> H <sub>24</sub> NO <sub>4</sub> +	342.1699	<b>204</b>	isosilybin	C <sub>26</sub> H <sub>24</sub> O <sub>10</sub>	496.1362
<b>76</b>	<i>N</i> -methylboldine	C <sub>20</sub> H <sub>23</sub> NO <sub>4</sub>	327.1465	<b>205</b>	kushenol H	C <sub>26</sub> H <sub>32</sub> O <sub>8</sub>	472.2088
<b>77</b>	peruvianine	C <sub>18</sub> H <sub>13</sub> NO <sub>4</sub>	307.0841	<b>206</b>	isoanhydroicaritin	C <sub>22</sub> H <sub>24</sub> O <sub>6</sub>	384.1566
<b>78</b>	haiderine	C <sub>18</sub> H <sub>21</sub> NO <sub>4</sub>	315.1465	<b>207</b>	corylin	C <sub>20</sub> H <sub>16</sub> O <sub>4</sub>	320.1044
<b>79</b>	palmatine	C <sub>21</sub> H <sub>22</sub> NO <sub>4</sub> +	352.1543	<b>208</b>	licoricone	C <sub>22</sub> H <sub>22</sub> O <sub>6</sub>	382.141
<b>80</b>	oxypalmatine	C <sub>21</sub> H <sub>21</sub> NO <sub>5</sub>	367.1414	<b>209</b>	genistin	C <sub>21</sub> H <sub>20</sub> O <sub>10</sub>	432.105
<b>81</b>	<i>N</i> -methylcoclaurine	C <sub>18</sub> H <sub>21</sub> NO <sub>3</sub>	299.1516	<b>210</b>	sophoraisoflavone A	C <sub>20</sub> H <sub>16</sub> O <sub>6</sub>	352.0942
<b>82</b>	coclaurine	C <sub>17</sub> H <sub>19</sub> NO <sub>3</sub>	285.136	<b>211</b>	odoratin-7- <i>O</i> -β- <i>D</i> -glucoside	C <sub>23</sub> H <sub>24</sub> O <sub>11</sub>	476.1311
<b>83</b>	( <i>S</i> )-reticuline	C <sub>19</sub> H <sub>23</sub> NO <sub>4</sub>	329.1621	<b>212</b>	2',6'-dihydroxy-4,4'-dimethoxydihydrochalcone	C <sub>17</sub> H <sub>18</sub> O <sub>5</sub>	302.1149

<b>84</b>	laudanine	C <sub>20</sub> H <sub>25</sub> NO <sub>4</sub>	343.1777	<b>213</b>	2',6'-dihydroxy-4'-methoxy-dihydrochalcone	C <sub>16</sub> H <sub>16</sub> O <sub>4</sub>	272.1044
<b>85</b>	oblongine	C <sub>19</sub> H <sub>24</sub> NO <sub>3</sub> +	314.175	<b>214</b>	3',5',β-Trihydroxy-3,4,4',α-tetramethoxychalcone	C <sub>15</sub> H <sub>12</sub> O <sub>2</sub>	224.0834
<b>86</b>	isococclaurine	C <sub>17</sub> H <sub>20</sub> NO <sub>3</sub>	286.1438	<b>215</b>	7-hydroxy-3',4'dimethoxy-isoflavan-5',2'-di- <i>O</i> -β- <i>D</i> -glucoside	C <sub>29</sub> H <sub>38</sub> O <sub>16</sub>	642.2148
<b>87</b>	cohirsine	C <sub>20</sub> H <sub>25</sub> NO <sub>4</sub>	343.1777	<b>216</b>	3'- <i>O</i> -Methylviolanone	C <sub>18</sub> H <sub>18</sub> O <sub>6</sub>	330.1098
<b>88</b>	cohirsinine	C <sub>19</sub> H <sub>23</sub> NO <sub>4</sub>	329.1621	<b>217</b>	methyl ophiopogonanone A	C <sub>19</sub> H <sub>18</sub> O <sub>6</sub>	342.1098
<b>89</b>	shaheenine	C <sub>18</sub> H <sub>21</sub> NO <sub>4</sub>	315.1465	<b>218</b>	methyl ophiopogonone A	C <sub>19</sub> H <sub>16</sub> O <sub>6</sub>	340.0942
<b>90</b>	cohrisitine	C <sub>24</sub> H <sub>29</sub> NO <sub>7</sub>	443.1936	<b>219</b>	6-hydroxy-2-[2-3'-methoxy-4'-hydroxy-phenyl)ethyl]chromone	C <sub>18</sub> H <sub>16</sub> O <sub>5</sub>	312.0993
<b>91</b>	jamtinine	C <sub>20</sub> H <sub>23</sub> NO <sub>5</sub>	357.157	<b>220</b>	cyclomorusin	C <sub>25</sub> H <sub>22</sub> O <sub>6</sub>	418.141
<b>92</b>	( <i>R</i> )-ophiocarpinone	C <sub>20</sub> H <sub>19</sub> NO <sub>5</sub>	353.1258	<b>221</b>	morusin hydroperoxide	C <sub>25</sub> H <sub>24</sub> O <sub>8</sub>	452.1464

<b>93</b>	stepholidine	C <sub>19</sub> H <sub>21</sub> NO <sub>4</sub>	339.1465	<b>222</b>	sanggenon A	C <sub>25</sub> H <sub>24</sub> O <sub>7</sub>	436.1515
<b>94</b>	4-methoxy-13,14-dihydrooxypalmatine	C <sub>22</sub> H <sub>25</sub> NO <sub>6</sub>	399.1675	<b>223</b>	(-)-epicatechin-pentaacetate	C <sub>25</sub> H <sub>24</sub> O <sub>11</sub>	500.1311
<b>95</b>	4-methoxypalmatine	C <sub>22</sub> H <sub>24</sub> NO <sub>5</sub> +	382.1648	<b>224</b>	(3R,4S)-3,4-dihydroxy-3-(3',4'-dimethoxybenzyl)-7-methoxy-chroman	C <sub>19</sub> H <sub>22</sub> O <sub>6</sub>	346.141
<b>96</b>	coclanoline	C <sub>20</sub> H <sub>24</sub> NO <sub>4</sub> +	342.1699	<b>225</b>	bavachromanol	C <sub>20</sub> H <sub>20</sub> O <sub>5</sub>	340.1305
<b>97</b>	coccoline	C <sub>17</sub> H <sub>17</sub> NO <sub>3</sub>	283.1204	<b>226</b>	3'-O-angeloylhamaudol	C <sub>20</sub> H <sub>22</sub> O <sub>6</sub>	358.141
<b>98</b>	coccolinine	C <sub>18</sub> H <sub>19</sub> NO <sub>3</sub>	297.136	<b>227</b>	psorachalcone A	C <sub>20</sub> H <sub>20</sub> O <sub>5</sub>	340.1305
<b>99</b>	coccudienone	C <sub>18</sub> H <sub>19</sub> NO <sub>3</sub>	297.136	<b>228</b>	nordracorhodin	C <sub>16</sub> H <sub>12</sub> O <sub>3</sub>	252.0783
<b>100</b>	cocculidinone	C <sub>18</sub> H <sub>21</sub> NO <sub>3</sub>	299.1516	<b>229</b>	3'-deoxysappanol	C <sub>16</sub> H <sub>16</sub> O <sub>5</sub>	288.0993
<b>101</b>	cocconvine	C <sub>17</sub> H <sub>19</sub> NO <sub>2</sub>	269.1411	<b>230</b>	(3R,4S)-4',7-dimethoxy-3'-deoxysappanol	C <sub>18</sub> H <sub>20</sub> O <sub>5</sub>	316.1305
<b>102</b>	cocconvinine	C <sub>18</sub> H <sub>21</sub> NO <sub>2</sub>	283.1567	<b>231</b>	methylophiopogonanone B	C <sub>19</sub> H <sub>20</sub> O <sub>5</sub>	328.1305
<b>103</b>	cocculolidine	C <sub>15</sub> H <sub>19</sub> NO <sub>3</sub>	261.136	<b>232</b>	5,7-dihydroxy-6-methyl-3-(4'-hydroxybenzyl)chroman-4-one	C <sub>17</sub> H <sub>16</sub> O <sub>5</sub>	300.0993
<b>104</b>	isococculidine	C <sub>18</sub> H <sub>23</sub> NO <sub>2</sub>	285.1723	<b>233</b>	3'-deoxysappanone B	C <sub>18</sub> H <sub>18</sub> O <sub>5</sub>	314.1149
<b>105</b>	cocculimine	C <sub>18</sub> H <sub>23</sub> NO <sub>3</sub>	301.1672	<b>234</b>	methylophiopogonone B	C <sub>19</sub> H <sub>18</sub> O <sub>5</sub>	326.1149
<b>106</b>	isococculine	C <sub>17</sub> H <sub>21</sub> NO <sub>2</sub>	271.1567	<b>235</b>	5,7-dihydroxy-3-(4'-hydroxybenzyl) chromone	C <sub>16</sub> H <sub>12</sub> O <sub>5</sub>	284.0681

<b>107</b>	cocclafine	C <sub>16</sub> H <sub>19</sub> NO <sub>2</sub>	257.1411	<b>236</b>	6-hydroxy-7-methoxy-2-(2-phenylethyl) chromone	C <sub>18</sub> H <sub>16</sub> O <sub>4</sub>	296.1044
<b>108</b>	cocculidine	C <sub>18</sub> H <sub>23</sub> NO <sub>2</sub>	285.1723	<b>237</b>	20-hydroxyecdysone	C <sub>27</sub> H <sub>44</sub> O <sub>7</sub>	480.3075
<b>109</b>	cocculine	C <sub>17</sub> H <sub>21</sub> NO <sub>2</sub>	271.1567	<b>238</b>	makisterone A	C <sub>28</sub> H <sub>46</sub> O <sub>7</sub>	494.3231
<b>110</b>	cocculitine	C <sub>18</sub> H <sub>23</sub> NO <sub>3</sub>	301.1672	<b>239</b>	β-sitosterol	C <sub>29</sub> H <sub>50</sub> O	414.3849
<b>111</b>	coccutrine	C <sub>18</sub> H <sub>23</sub> NO <sub>3</sub>	301.1672	<b>240</b>	daucosterol	C <sub>35</sub> H <sub>60</sub> O <sub>6</sub>	576.4374
<b>112</b>	dihydroerysodine	C <sub>18</sub> H <sub>23</sub> NO <sub>3</sub>	301.1672	<b>241</b>	cholesta-8,24-Dien-3-ol,4-methyl-, (3.β.,4.α.)-	C <sub>28</sub> H <sub>46</sub> O	398.3537
<b>113</b>	dihydroerysotrine	C <sub>19</sub> H <sub>25</sub> NO <sub>3</sub>	315.1828	<b>242</b>	stigmasteryl tosylate	C <sub>36</sub> H <sub>54</sub> O <sub>3</sub> S	566.378
<b>114</b>	dihydroerysovine	C <sub>18</sub> H <sub>23</sub> NO <sub>3</sub>	301.1672	<b>243</b>	4,22-stigmastadiene-3-one	C <sub>29</sub> H <sub>46</sub> O	410.3537
<b>115</b>	cocculitinine	C <sub>17</sub> H <sub>21</sub> NO <sub>3</sub>	287.1516	<b>244</b>	ethyl iso-allocholate	C <sub>27</sub> H <sub>48</sub> O <sub>5</sub>	452.3489
<b>116</b>	erythramide	C <sub>19</sub> H <sub>24</sub> N <sub>2</sub> O <sub>3</sub>	328.1781	<b>245</b>	stigmasterol	C <sub>29</sub> H <sub>48</sub> O	412.3693
<b>117</b>	erythroculine	C <sub>20</sub> H <sub>25</sub> NO <sub>4</sub>	343.1777	<b>246</b>	syringaresinol	C <sub>22</sub> H <sub>26</sub> O <sub>8</sub>	432.1651
<b>118</b>	<i>O</i> -methylcoccutrine	C <sub>19</sub> H <sub>25</sub> NO <sub>3</sub>	315.1828	<b>247</b>	<i>N</i> -trans-feruloyltyramine	C <sub>18</sub> H <sub>19</sub> NO <sub>4</sub>	313.1309
<b>119</b>	erythlaurine	C <sub>20</sub> H <sub>25</sub> NO <sub>5</sub>	359.1726	<b>248</b>	phytol	C <sub>20</sub> H <sub>40</sub> O	296.3069
<b>120</b>	carococculine	C <sub>19</sub> H <sub>23</sub> NO <sub>5</sub>	345.157	<b>249</b>	octadecanoic acid, ethyl ester	C <sub>20</sub> H <sub>40</sub> O <sub>2</sub>	312.3018
<b>121</b>	sinococculine	C <sub>18</sub> H <sub>23</sub> NO <sub>5</sub>	333.157	<b>250</b>	oleic acid	C <sub>18</sub> H <sub>34</sub> O <sub>2</sub>	282.255
<b>122</b>	isosinococculine	C <sub>18</sub> H <sub>23</sub> NO <sub>5</sub>	333.157	<b>251</b>	sulfurous acid, pentadecyl 2-propyl ester	C <sub>18</sub> H <sub>38</sub> O <sub>3</sub> S	334.2532
<b>123</b>	corsutine	C <sub>21</sub> H <sub>27</sub> NO <sub>7</sub>	405.178	<b>252</b>	4,4,6A,6B,8A,11,11,14B-Octamethyl-1,4,4A,5,6,6A,6B,7,8,8A,9,10,11,12,12A,14,14A,12,12A,14,14A,14B-octadecahydro-2	C <sub>30</sub> H <sub>48</sub> O	424.3693



<b>124</b>	14- hydroxyisostephodoline	C <sub>21</sub> H <sub>27</sub> NO <sub>6</sub>	389.1831	<b>253</b>	9,19-cyclolanost-24-en-3-ol, acetate,(3β)-	C <sub>32</sub> H <sub>52</sub> O <sub>2</sub>	468.3954
<b>125</b>	sinoacutine	C <sub>19</sub> H <sub>21</sub> NO <sub>4</sub>	327.1465	<b>254</b>	1-hexyl-2-nitrocyclohexane	C <sub>12</sub> H <sub>23</sub> NO <sub>2</sub>	213.1723
<b>126</b>	sebiferine	C <sub>20</sub> H <sub>23</sub> NO <sub>4</sub>	341.1621	<b>255</b>	cis-Z-.α-bisabolene epoxide	C <sub>15</sub> H <sub>24</sub> O	220.1821
<b>127</b>	N-methylstepharine	C <sub>19</sub> H <sub>21</sub> NO <sub>3</sub>	311.1516	<b>256</b>	(+)-quercitol	C <sub>6</sub> H <sub>12</sub> O <sub>5</sub>	164.0681
<b>128</b>	laurifine	C <sub>19</sub> H <sub>23</sub> NO <sub>3</sub>	313.1672	<b>257</b>	(-)-viburnitol	C <sub>6</sub> H <sub>12</sub> O <sub>5</sub>	164.0681
<b>129</b>	laurifonine	C <sub>20</sub> H <sub>25</sub> NO <sub>3</sub>	327.1828	<b>258</b>	coclauril	C <sub>8</sub> H <sub>9</sub> NO <sub>2</sub>	151.0631

**Table S4**

RT/min	<i>m/z</i>	FC	<i>P</i>	VIP	[M+Na] <sup>+</sup>	Formule	Error(ppm)	RDB	Fragment ions	Compound
6.17	147.0441	127.84	4.12E-35	1.9485	169.0325	C <sub>9</sub> H <sub>6</sub> O <sub>2</sub>	0.3	7	119.0496, 101.0410, 91.0539, 77.0373, 75.0533	Unkown
23.85	304.1428	24.513	1.65E-13	2.2099	326.1255	C <sub>16</sub> H <sub>19</sub> N <sub>2</sub> O <sub>4</sub>	3.4	8.5	304.1429, 281.1115, 266.1182, 188.0842, 176.0723, 128.0628, 115.0550	Unkown
2.59	336.1436	165.43	3.01E-39	1.8692	358.1284	C <sub>17</sub> H <sub>21</sub> NO <sub>6</sub>	-1.7	8	336.1442, 276.1237, 248.1279, 200.1084, 110.0607, 105.0703	Unkown
17.13	342.1335	84.761	7.57E-29	2.1733	364.1182	C <sub>19</sub> H <sub>19</sub> NO <sub>5</sub>	-0.3	11	342.1347, 326.1033, 311.0796, 265.0881, 164.0715	Unkown
4.46	377.0839	53.787	1.63E-22	2.225	399.1638	C <sub>13</sub> H <sub>16</sub> N <sub>2</sub> O <sub>11</sub>	3.2	7	215.0515, 163.0390, 89.0351	Unkown

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53.34	384.1434	99.686	2.89E-31	1.6286	406.1269	C <sub>21</sub> H <sub>21</sub> NO <sub>6</sub>	-2	12	384.1446, 354.0979, 308.09321, 293.0693	Unkown
20.38	432.1451	143.1	6.65E-37	2.158	454.1255	C <sub>25</sub> H <sub>21</sub> NO <sub>6</sub>	-2.1	3	432.1459, 414.1355, 402.1364, 268.0987, 174.0567	Unkown
22.97	520.2129	193.52	7.92E-42	2.3302	542.1939	C <sub>33</sub> H <sub>29</sub> NO <sub>5</sub>	2	20	520.2124, 489.1715, 458.1529, 277.0848, 147.0674	Unkown
21.49	563.2188	199.07	2.68E-42	2.3505	585.2057	C <sub>34</sub> H <sub>30</sub> N <sub>2</sub> O <sub>6</sub>	2	21	563.2190, 545.2074, 437.1439, 364.1417	Unkown
24.79	598.2654	138.7	2.10E-36	2.3402	620.2535	C <sub>32</sub> H <sub>39</sub> NO <sub>10</sub>	1.2	14	598.2648, 436.2141, 3287.1556, 275.1076	Coumarin

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Note: "RDB" means that is the unsaturation of the compound.

**Table S5**

RT/min	<i>m/z</i>	FC	<i>P</i>	VIP	[M+Na] <sup>+</sup>	Formule	Error(ppm)	RDB	Fragment ions	Compound
54.36	261.2221	12.833	2.13E-32	1.516563	283.2263	C <sub>18</sub> H <sub>28</sub> O	3.1	5	243.2122, 159.1183, 147.1193, 119.0881, 107.0879	Unkown
54.37	279.2312	18.335	5.55E-33	1.509106	301.1422	C <sub>18</sub> H <sub>30</sub> O <sub>2</sub>	-2.4	4	201.0477, 173.1330, 149.0238, 109.1023, 95.0859	Unkown
54.7	295.2271	10.194	3.03E-25	1.481581	317.2087	C <sub>18</sub> H <sub>30</sub> O <sub>3</sub>	1.1	4	277.2176, 231.2112, 165.1127, 151.1127, 147.1184	Unkown
23.06	679.5108	218430	4.75E-50	1.538095	701.493	C <sub>35</sub> H <sub>70</sub> N <sub>2</sub> O <sub>10</sub>	0.7	2	679.5113m 548.4171, 322.2499, 209.1642	Unkown
25.52	453.3428	57070	7.02E-47	1.537757	[2M+H] <sup>+</sup> : 905.6794	C <sub>23</sub> H <sub>48</sub> O <sub>8</sub>	1.3	0	435.3375, 387.3066, 114.0921, 96.0799	Unkown

Note: "RDB" means that is the unsaturation of the compound.