

**Table S2.** Identification of the chemical constituents in Fufang Danshen Tablet (FDT)

N.	Identification	T <sub>R</sub> (min)	Formula	[M+H] <sup>+</sup> (error, ppm)	[M-H] <sup>-</sup> (error, ppm)	Fragment ions in positive (+) ion mode	Fragment ions in negative (-) ion mode	Source
1	Stachyose	2.11	C <sub>24</sub> H <sub>42</sub> O <sub>21</sub>	667.2295 (0.5)	665.2167 (3.2)	487.1631[M+H-Glc-H <sub>2</sub> O] <sup>+</sup> 325.1135[M+H-2Glc-H <sub>2</sub> O] <sup>+</sup>	485.1509[M-H-Glc-H <sub>2</sub> O] <sup>-</sup>	DS
2	Sucrose	2.18	C <sub>12</sub> H <sub>22</sub> O <sub>11</sub>	343.1234 (-0.3)	341.1088 (-0.5)	307.1228[M+H-2H <sub>2</sub> O] <sup>+</sup> 163.0587[M+H-Glc-H <sub>2</sub> O] <sup>+</sup> 145.0485[M+H-Glc-2H <sub>2</sub> O] <sup>+</sup> 127.0380[M+H-Glc-3H <sub>2</sub> O] <sup>+</sup>	179.0556[M-H-Glc] <sup>-</sup> 119.0343[M-H-Glc-COOH-CH <sub>3</sub> ] <sup>-</sup>	DS
3	Raffinose	2.24	C <sub>18</sub> H <sub>32</sub> O <sub>16</sub>	505.1758 (-0.9)	503.1616 (-0.2)	325.1137[M+H-Glc-H <sub>2</sub> O] <sup>+</sup> 163.0598[M+H-2Glc-H <sub>2</sub> O] <sup>+</sup>	ND	DS
4	Dencichin*	2.30	C <sub>5</sub> H <sub>8</sub> N <sub>2</sub> O <sub>5</sub>	177.0507 (0.8)	ND	160.0250[M+H-NH <sub>3</sub> ] <sup>+</sup> 116.0345[M+H-CO <sub>2</sub> -NH <sub>3</sub> ] <sup>+</sup> 88.0380[M+H-CO <sub>2</sub> -NH <sub>3</sub> -CO] <sup>+</sup>	ND	SQ
5	Adenosine	2.32	C <sub>10</sub> H <sub>13</sub> N <sub>5</sub> O <sub>4</sub>	268.1037 (-1.0)	ND	136.0615[M+H-C <sub>5</sub> H <sub>8</sub> O <sub>4</sub> ] <sup>+</sup>	ND	SQ
6	Pyroglutamate	2.83	C <sub>5</sub> H <sub>7</sub> NO <sub>3</sub>	130.0494 (-2.6)	128.0353 (-0.4)	84.0439[M+H-H <sub>2</sub> O-CO] <sup>+</sup>	82.0265[M-H-H <sub>2</sub> O-CO] <sup>-</sup>	DS
7	Succinic acid*	3.05	C <sub>4</sub> H <sub>6</sub> O <sub>4</sub>	ND	117.0193 (-0.4)	ND	99.0077[M-H-H <sub>2</sub> O] <sup>-</sup> 73.0290[M-H-CO <sub>2</sub> ] <sup>-</sup>	DS
8	Danshensu*	4.17	C <sub>9</sub> H <sub>10</sub> O <sub>5</sub>	ND	197.0464 (1.9)	ND	179.0348[M-H-H <sub>2</sub> O] <sup>-</sup> 135.0447[M-H-CO <sub>2</sub> -H <sub>2</sub> O] <sup>-</sup> 123.0446[M-H-2CO-H <sub>2</sub> O] <sup>-</sup>	DS
9	Protocatechuic acid*	4.84	C <sub>7</sub> H <sub>6</sub> O <sub>4</sub>	ND	153.0193 (-0.4)	ND	109.0281[M-H-CO <sub>2</sub> ] <sup>-</sup> 108.0195[M-H-COOH] <sup>-</sup>	DS
10	Pseudoginsenoside Rt <sub>5</sub> *	4.94	C <sub>36</sub> H <sub>62</sub> O <sub>10</sub>	655.4408 (-0.6)	ND	637.4310[M+H-H <sub>2</sub> O] <sup>+</sup> 457.3622[M+H-2H <sub>2</sub> O-Glc] <sup>+</sup> 439.3566[M+H-3H <sub>2</sub> O-Glc] <sup>+</sup> 143.1053[Glc-H <sub>2</sub> O] <sup>+</sup>	ND	SQ
11	Ginsenoside F <sub>1</sub>	5.61	C <sub>36</sub> H <sub>62</sub> O <sub>9</sub>	639.4459 (-0.5)	ND	621.4290[M+H-H <sub>2</sub> O] <sup>+</sup> 603.4302[M+H-2H <sub>2</sub> O] <sup>+</sup> 441.3713[M+H-2H <sub>2</sub> O-Glc] <sup>+</sup> 423.3638[M+H-3H <sub>2</sub> O-Glc] <sup>+</sup>	ND	SQ
12	Unknow	5.63	C <sub>22</sub> H <sub>32</sub> O <sub>13</sub>	ND	503.1771 (0.1)	ND	341.1249[M-H-Glc] <sup>-</sup>	SQ
13	Protocatechualdehyde*	5.68	C <sub>7</sub> H <sub>6</sub> O <sub>3</sub>	139.0385 (-3.5)	137.0244 (0.1)	93.0325[M+H-H <sub>2</sub> O-CO] <sup>+</sup> 65.0386[M+H-CHO-COOH] <sup>+</sup>	136.0159[M-H-H] <sup>-</sup> 108.0204[M-H-CHO] <sup>-</sup> 92.0259[M-H-COOH] <sup>-</sup>	DS

14	Caffeic acid*	6.01	C <sub>9</sub> H <sub>8</sub> O <sub>4</sub>	ND	179.0351 (0.6)	ND	135.0445[M-H-CO <sub>2</sub> ] <sup>-</sup> 134.0358[M-H-COOH] <sup>-</sup>	DS
15	Quercetin	6.03	C <sub>15</sub> H <sub>10</sub> O <sub>7</sub>	303.0501 (0.4)	ND	257.0448[M+H-H <sub>2</sub> O-CO] <sup>+</sup> 229.0480[M+H-H <sub>2</sub> O-2CO] <sup>+</sup> 183.0456[M+H-C <sub>4</sub> H <sub>8</sub> O <sub>4</sub> ] <sup>+</sup>	ND	SQ
16	Quercetin 3-sambubioside	6.04	C <sub>26</sub> H <sub>28</sub> O <sub>16</sub>	597.1449 (-0.3)	595.1322 (2.9)	465.1012[M+H-Ara] <sup>+</sup> 303.0500[M+H-Ara-Glc] <sup>+</sup>	301.0361[M-H-Glc-Ara] <sup>-</sup>	SQ
17	Notoginsenoside C	6.19	C <sub>54</sub> H <sub>92</sub> O <sub>25</sub>	ND	1139.5919 (4.9)	ND	1093.5882[M-H-H <sub>2</sub> O-CO] <sup>-</sup>	SQ
18	Yunnaneic acid D	6.48	C <sub>27</sub> H <sub>24</sub> O <sub>12</sub>	ND	539.1206 (2.1)	ND	521.1001[M-H-H <sub>2</sub> O] <sup>-</sup> 359.0785[M-H-C <sub>9</sub> H <sub>8</sub> O <sub>4</sub> ] <sup>-</sup> 341.0680[M-H-DSS] <sup>-</sup> 197.0457[DSS-H] <sup>-</sup> 179.0329[C <sub>9</sub> H <sub>8</sub> O <sub>4</sub> -H] <sup>-</sup>	DS
19	Salviaflaside	6.53	C <sub>24</sub> H <sub>26</sub> O <sub>13</sub>	523.1436 (-2.0)	521.1312 (-0.3)	361.0946[M+H-Glc] <sup>+</sup> 325.0949[M+H-Glc-2H <sub>2</sub> O] <sup>+</sup> 163.0387[Glc+H] <sup>+</sup>	359.0775[M-H-Glc] <sup>-</sup> 323.0782[M-H-DSS] <sup>-</sup> 197.0437[DSS-H] <sup>-</sup> 179.0334[CA-H] <sup>-</sup>	DS
20	Yunnaneic acid F	6.55	C <sub>29</sub> H <sub>26</sub> O <sub>14</sub>	ND	597.1264 (1.7)	ND	553.1315[M-H-CO <sub>2</sub> ] <sup>-</sup> 417.0781[M-H-C <sub>9</sub> H <sub>8</sub> O <sub>4</sub> ] <sup>-</sup> 197.0431[DSS-H] <sup>-</sup> 179.0431[C <sub>9</sub> H <sub>8</sub> O <sub>4</sub> -H] <sup>-</sup>	DS
21	Notoginsenoside T <sub>5</sub>	6.94	C <sub>41</sub> H <sub>68</sub> O <sub>12</sub>	753.4778 (-0.7)	ND	441.3729[M+H-Xyl-Glc-H <sub>2</sub> O] <sup>+</sup> 423.3624[M+H-Xyl-Glc-2H <sub>2</sub> O] <sup>+</sup>	ND	SQ
22	Notoginsenoside R <sub>1</sub> *	6.96	C <sub>47</sub> H <sub>80</sub> O <sub>18</sub>	933.5420 (0.3)	931.5311 (4.2)	753.4961[M+H-Glc-H <sub>2</sub> O] <sup>+</sup> 621.4225[M+H-Glc-H <sub>2</sub> O-Xyl] <sup>+</sup> 441.3763[M+H-2Glc-Xyl-2H <sub>2</sub> O] <sup>+</sup> 423.3599[M+H-2Glc-Xyl-3H <sub>2</sub> O] <sup>+</sup>	799.4881[M-H-Xyl] <sup>-</sup>	SQ
23	Salvianolic acid D*	7.17	C <sub>20</sub> H <sub>18</sub> O <sub>10</sub>	ND	417.0831 (1.0)	ND	197.0451[DSS-H] <sup>-</sup> 179.0338[C <sub>9</sub> H <sub>8</sub> O <sub>4</sub> -H] <sup>-</sup> 174.0291[M-H-DSS-COOH] <sup>-</sup>	DS
24	Ginsenoside Re*	7.39	C <sub>48</sub> H <sub>82</sub> O <sub>18</sub>	947.5573 (-0.2)	ND	767.4891[M+H-Glc-H <sub>2</sub> O] <sup>+</sup> 441.3710[M+H-2Glc-Rha-2H <sub>2</sub> O] <sup>+</sup> 423.3576[M+H-2Glc-Rha-3H <sub>2</sub> O] <sup>+</sup> 405.3512[M+H-2Glc-Rha-4H <sub>2</sub> O] <sup>+</sup>	ND	SQ
25	Ginsenoside Rg <sub>1</sub> *	7.54	C <sub>42</sub> H <sub>72</sub> O <sub>14</sub>	801.4990 (-0.6)	ND	621.4339[M+H-Glc-H <sub>2</sub> O] <sup>+</sup> 441.3739[M+H-2Glc-2H <sub>2</sub> O] <sup>+</sup> 423.3614[M+H-2Glc-3H <sub>2</sub> O] <sup>+</sup>	ND	SQ
26	Rosmarinic acid*	8.13	C <sub>18</sub> H <sub>16</sub> O <sub>8</sub>	361.0916 (-0.4)	359.0781 (2.0)	163.0384[M+H-DSS] <sup>+</sup> 145.0275[M+H-DSS-H <sub>2</sub> O] <sup>+</sup>	197.0453[DSS-H] <sup>-</sup> 179.0344[CA-H] <sup>-</sup> 161.0239[M-H-DSS] <sup>-</sup>	DS

27	Salvianolic acid A*	8.66	C <sub>26</sub> H <sub>22</sub> O <sub>10</sub>	ND	493.1156 (2.0)	ND	313.0720[M-H-CA] <sup>-</sup> 295.0621[M-H-DSS] <sup>-</sup> 197.0446[DSS-H] <sup>-</sup>	DS
28	Lithospermic acid*	8.66	C <sub>27</sub> H <sub>22</sub> O <sub>12</sub>	539.1179 (-0.9)	537.1050 (2.2)	521.1080[M+H-H <sub>2</sub> O] <sup>+</sup> 323.0545[M+H-H <sub>2</sub> O-DSS] <sup>+</sup>	313.0728[M-H-CA-CO <sub>2</sub> ] <sup>-</sup> 295.0617[M-H-DSS-CO <sub>2</sub> ] <sup>-</sup> 197.0455[DSS-H] <sup>-</sup>	DS
29	Salvianolic acid B*	9.66	C <sub>36</sub> H <sub>30</sub> O <sub>16</sub>	719.1602 (-0.6)	717.1491 (4.2)	521.1070[M+H-DSS] <sup>+</sup> 493.1097[M+H-DSS-CO] <sup>+</sup> 323.0551[M+H-DSS-C <sub>9</sub> H <sub>8</sub> O <sub>4</sub> -H <sub>2</sub> O] <sup>+</sup>	519.0946[M-H-DSS] <sup>-</sup> 339.0516[M-H-DSS-C <sub>9</sub> H <sub>8</sub> O <sub>4</sub> ] <sup>-</sup> 321.0416[M-H-DSS-C <sub>9</sub> H <sub>8</sub> O <sub>4</sub> -H <sub>2</sub> O] <sup>-</sup>	DS
30	Salvianolic acid A isomer	11.38	C <sub>26</sub> H <sub>22</sub> O <sub>10</sub>	ND	493.1148 (1.7)	ND	313.0741[M-H-CA] <sup>-</sup> 295.0611[M-H-DSS] <sup>-</sup> 179.0345[CA-H] <sup>-</sup>	DS
31	Dimethyl Lithospermate	13.98	C <sub>29</sub> H <sub>26</sub> O <sub>12</sub>	567.1495 (-0.4)	565.1370 (2.1)	369.0980[M+H-DSS] <sup>+</sup> 295.0604[M+H-DSS-2CO-H <sub>2</sub> O] <sup>+</sup>	519.0971[M-H-H <sub>2</sub> O-CO] <sup>-</sup> 367.0843[M-H-DSS] <sup>-</sup> 339.0514[M-H-DSS-CO] <sup>-</sup> 321.0406[M-H-DSS-CO-H <sub>2</sub> O] <sup>-</sup>	DS
32	Ethyl lithospermate	15.61	C <sub>29</sub> H <sub>26</sub> O <sub>12</sub>	567.1500 (0.5)	565.1370 (2.1)	521.1096[M+H-CO-H <sub>2</sub> O] <sup>+</sup> 493.1017[M+H-2CO-H <sub>2</sub> O] <sup>+</sup> 323.0580[M+H-CO-H <sub>2</sub> O-DSS] <sup>+</sup>	367.0820[M-H-DSS] <sup>-</sup> 321.0410[M-H-DSS-CO-H <sub>2</sub> O] <sup>-</sup>	DS
33	Notoginsenoside Fa*	18.67	C <sub>59</sub> H <sub>100</sub> O <sub>27</sub>	ND	1239.6455 (4.4)	ND	1239.6504 1107.6153[M-H-Xyl] <sup>-</sup>	SQ
34	Notoginsenoside R <sub>2</sub> /isomer	18.79	C <sub>41</sub> H <sub>70</sub> O <sub>13</sub>	ND	769.4778 (4.4)	ND	637.4372[M-H-Xyl] <sup>-</sup> 475.3788[M-H-Xyl-Glc] <sup>-</sup>	SQ
35	Ginsenoside Rb <sub>1</sub> *	18.88	C <sub>54</sub> H <sub>92</sub> O <sub>23</sub>	1109.6101 (-0.1)	1107.6025 (3.4)	767.4943[M+H-2Glc-H <sub>2</sub> O] <sup>+</sup> 605.4400[M+H-3Glc-H <sub>2</sub> O] <sup>+</sup> 425.3778[M+H-4Glc-2H <sub>2</sub> O] <sup>+</sup>	1107.6039	SQ
36	Ginsenoside Rh <sub>3</sub>	18.89	C <sub>36</sub> H <sub>60</sub> O <sub>7</sub>	605.4408 (-0.7)	ND	587.4431[M+H-H <sub>2</sub> O] <sup>+</sup> 425.3914[M+H-H <sub>2</sub> O-Glc] <sup>+</sup> 407.3692[M+H-2H <sub>2</sub> O-Glc] <sup>+</sup>	ND	SQ
37	Ginsenoside Rg <sub>2</sub> *	18.89	C <sub>42</sub> H <sub>72</sub> O <sub>13</sub>	785.5049 (0.5)	783.4927 (1.1)	605.4372[M+H-ORha-H <sub>2</sub> O] <sup>+</sup> 425.3756[M+H-ORha-Glc-2H <sub>2</sub> O] <sup>+</sup>	637.4336[M-H-Rha] <sup>-</sup>	SQ
38	Malonylginsenoside Rb <sub>1</sub>	18.99	C <sub>57</sub> H <sub>94</sub> O <sub>26</sub>	1195.6106 (0)	1193.6006 (3.6)	1015.4980[M+H-H <sub>2</sub> O-Glc] <sup>+</sup> 835.4798[M+H-2Glc-2H <sub>2</sub> O] <sup>+</sup> 673.4200[M+H-3Glc-2H <sub>2</sub> O] <sup>+</sup>	1149.6158[M-H-CO <sub>2</sub> ] <sup>-</sup> 1107.6050[M-H-C <sub>3</sub> H <sub>2</sub> O <sub>3</sub> ] <sup>-</sup>	SQ
39	Notoginsenoside A	19.07	C <sub>54</sub> H <sub>92</sub> O <sub>24</sub>	ND	1123.5947 (1.8)	ND	1077.5916[M-H-H <sub>2</sub> O-CO] <sup>-</sup>	SQ
40	Ginsenoside Rk <sub>3</sub> *	19.15	C <sub>36</sub> H <sub>60</sub> O <sub>8</sub>	621.4355 (-0.9)	ND	603.4289[M+H-H <sub>2</sub> O] <sup>+</sup> 441.3725[M+H-Glc-H <sub>2</sub> O] <sup>+</sup> 423.3631[M+H-Glc-2H <sub>2</sub> O] <sup>+</sup> 405.3492[M+H-Glc-3H <sub>2</sub> O] <sup>+</sup>	ND	SQ

41	Salvianolic acid F	19.15	C <sub>17</sub> H <sub>14</sub> O <sub>6</sub>	ND	313.0717 (-0.1)	ND	161.0226[CA-H-H <sub>2</sub> O] <sup>-</sup> 151.0417[CA-H-CO] <sup>-</sup> 133.0289[M-H-CA] <sup>-</sup>	DS
42	Ginsenoside Rd*	19.25	C <sub>48</sub> H <sub>82</sub> O <sub>18</sub>	947.5569 (-0.6)	945.5462 (3.5)	767.4859 [M+H-Glc-H <sub>2</sub> O] <sup>+</sup> 605.4373 [M+H-2Glc-H <sub>2</sub> O] <sup>+</sup> 425.3763 [M+H-3Glc-2H <sub>2</sub> O] <sup>+</sup>	945.5477	SQ
43	Ginsenoside Rk <sub>2</sub> *	19.27	C <sub>36</sub> H <sub>60</sub> O <sub>7</sub>	605.4411 (-0.2)	ND	587.4269[M+H-H <sub>2</sub> O] <sup>+</sup> 551.4097[M+H-3H <sub>2</sub> O] <sup>+</sup> 425.3812[M+H-H <sub>2</sub> O-Glc] <sup>+</sup> 407.3680[M+H-2H <sub>2</sub> O-Glc] <sup>+</sup>	ND	SQ
44	Acetyl-ginsenoside F <sub>1</sub>	19.35	C <sub>38</sub> H <sub>64</sub> O <sub>10</sub>	ND	679.4454 (4.0)	ND	619.4284[M-H-HOAc] <sup>-</sup>	SQ
45	Hydroxycryptotanshinone/ isomer	19.40	C <sub>19</sub> H <sub>20</sub> O <sub>4</sub>	313.1435 (0.2)	ND	295.1332[M+H-H <sub>2</sub> O] <sup>+</sup> 277.1239[M+H-2H <sub>2</sub> O] <sup>+</sup> 267.1372[M+H-H <sub>2</sub> O-CO] <sup>+</sup> 255.0994[M+H-2CH <sub>3</sub> -CO] <sup>+</sup>	ND	DS
46	Salvianolic acid C*	19.42	C <sub>26</sub> H <sub>20</sub> O <sub>10</sub>	ND	491.0988 (0.9)	ND	447.1073[M-H-CO <sub>2</sub> ] <sup>-</sup> 293.0480[M-H-DSS] <sup>-</sup> 197.0433[DSS-H] <sup>-</sup> 179.0342[C <sub>9</sub> H <sub>8</sub> O <sub>4</sub> -H] <sup>-</sup>	DS
47	20(S)-sanchirrhinosides A <sub>2</sub>	20.09	C <sub>43</sub> H <sub>72</sub> O <sub>14</sub>	ND	811.4894 (3.8)	ND	765.4835[M-H-CO-H <sub>2</sub> O] <sup>-</sup> 619.4240[M-H-2CH <sub>3</sub> -Glc] <sup>-</sup>	SQ
48	Tanshinol B	20.22	C <sub>18</sub> H <sub>16</sub> O <sub>4</sub>	297.1122 (0.1)	ND	279.1010[M+H-H <sub>2</sub> O] <sup>+</sup> 261.0905[M+H-2H <sub>2</sub> O] <sup>+</sup> 233.0959[M+H-2H <sub>2</sub> O-CO] <sup>+</sup>	ND	DS
49	Ginsenoside Rg <sub>3</sub>	20.45	C <sub>42</sub> H <sub>72</sub> O <sub>13</sub>	785.5048 (0.3)	783.4929 (2.2)	749.5063[M+H-2H <sub>2</sub> O] <sup>+</sup> 443.3958[M+H-2Glc-H <sub>2</sub> O] <sup>+</sup> 425.3758[M+H-2Glc-2H <sub>2</sub> O] <sup>+</sup>	621.4244[M-H-Glc] <sup>-</sup>	SQ
50	3β-Hydroxymethylenetanshinquinone	20.48	C <sub>18</sub> H <sub>14</sub> O <sub>4</sub>	295.0965 (0.1)	293.0817 (-1)	249.0914[M+H-CO-H <sub>2</sub> O] <sup>+</sup> 221.0956[M+H-H <sub>2</sub> O-2CO] <sup>+</sup>	265.0877[M-H-CO] <sup>-</sup> 250.0647[M-H-CO-CH <sub>3</sub> ] <sup>-</sup>	DS
51	Tanshinone II <sub>B</sub>	20.59	C <sub>19</sub> H <sub>18</sub> O <sub>4</sub>	311.1279 (0.4)	ND	267.1382[M+H-CO <sub>2</sub> ] <sup>+</sup> 252.1153[M+H-CO <sub>2</sub> -CH <sub>3</sub> ] <sup>+</sup>	ND	DS
52	Salvianonol	20.62	C <sub>18</sub> H <sub>20</sub> O <sub>4</sub>	301.1433 (-0.4)	ND	283.1334[M+H-H <sub>2</sub> O] <sup>+</sup> 265.1238[M+H-2H <sub>2</sub> O] <sup>+</sup> 241.1232[M+H-COOH-CH <sub>3</sub> ] <sup>+</sup>	ND	DS
53	Hydroxytanshinone	20.80	C <sub>19</sub> H <sub>18</sub> O <sub>4</sub>	311.1281 (0.9)	ND	293.1183[M+H-H <sub>2</sub> O] <sup>+</sup> 275.1074[M+H-2H <sub>2</sub> O] <sup>+</sup>	ND	DS
54	Nortanshinone	20.81	C <sub>17</sub> H <sub>12</sub> O <sub>4</sub>	281.0807 (-0.3)	ND	235.0757[M+H-H <sub>2</sub> O-CO] <sup>+</sup> 207.0808[M+H-H <sub>2</sub> O-2CO] <sup>+</sup>	ND	DS
55	Didehydrotanshinone II <sub>A</sub>	20.82	C <sub>19</sub> H <sub>16</sub> O <sub>3</sub>	293.1172 (-0.1)	ND	247.0749[M+H-H <sub>2</sub> O-CO] <sup>+</sup> 219.0803[M+H-H <sub>2</sub> O-2CO] <sup>+</sup>	ND	DS

56	Panaxydol	21.17	C <sub>17</sub> H <sub>24</sub> O <sub>2</sub>	261.1847 (-0.8)	ND	168.9769[M+H-C <sub>6</sub> H <sub>4</sub> O] <sup>+</sup> 141.1260[M+H-C <sub>6</sub> H <sub>4</sub> O-CO] <sup>+</sup>	ND	SQ
57	Danshenxinkun A	21.30	C <sub>18</sub> H <sub>16</sub> O <sub>4</sub>	297.1123 (0.4)	295.0981 (1.5)	261.0911[M+H-2H <sub>2</sub> O] <sup>+</sup> 233.0967[M+H-2H <sub>2</sub> O-CO] <sup>+</sup>	265.0856[M-H-2CH <sub>3</sub> ] <sup>-</sup> 237.0923[M-H-2CH <sub>3</sub> -CO] <sup>-</sup>	
58	Isocryptotanshinone	21.52	C <sub>19</sub> H <sub>20</sub> O <sub>3</sub>	297.1486 (0.3)	ND	253.1585[M+H-CH <sub>3</sub> -CHO] <sup>+</sup> 238.1347[M+H-CHO-2CH <sub>3</sub> ] <sup>+</sup>	ND	DS
59	Neocryptotanshinone isomer	21.53	C <sub>19</sub> H <sub>22</sub> O <sub>4</sub>	315.1591 (-0.1)	313.1450 (1.4)	297.1493[M+H-H <sub>2</sub> O] <sup>+</sup> 253.1592[M+H-H <sub>2</sub> O-CHO-CH <sub>3</sub> ] <sup>+</sup> 238.1350[M+H-H <sub>2</sub> O-CHO-2CH <sub>3</sub> ] <sup>+</sup>	269.1549[M-H-CHO-CH <sub>3</sub> ] <sup>-</sup> 213.1280[M-H-CHO-CH <sub>3</sub> -2CO] <sup>-</sup>	DS
60	Przewaquinone B	21.57	C <sub>18</sub> H <sub>18</sub> O <sub>4</sub>	299.1279 (0.3)	297.1135 (0.9)	281.1193[M+H-H <sub>2</sub> O] <sup>+</sup> 263.1066[M+H-2H <sub>2</sub> O] <sup>+</sup> 235.1086[M+H-2H <sub>2</sub> O-CO] <sup>+</sup>	253.1228[M-H-CHO-CH <sub>3</sub> ] <sup>-</sup> 209.1338[M-H-2CHO-2CH <sub>3</sub> ] <sup>-</sup>	DS
61	Dehydromiltirone/ Sibiriquinone A	21.90	C <sub>19</sub> H <sub>20</sub> O <sub>2</sub>	281.1536 (0.2)	ND	263.1409[M+H-H <sub>2</sub> O] <sup>+</sup> 252.1154[M+H-CHO] <sup>+</sup> 238.0980[M+H-CH <sub>3</sub> -CO] <sup>+</sup>	ND	DS
62	Hydroxycryptotanshinone/ isomer	22.00	C <sub>19</sub> H <sub>20</sub> O <sub>4</sub>	313.1433 (-0.5)	ND	295.1345[M+H-H <sub>2</sub> O] <sup>+</sup> 277.1248[M+H-2H <sub>2</sub> O] <sup>+</sup> 269.1536[M+H-CHO-CH <sub>3</sub> ] <sup>+</sup> 251.1433[M+H-H <sub>2</sub> O-CHO-CH <sub>3</sub> ] <sup>+</sup>	ND	DS
63	Ginsenoside Rg <sub>5</sub> <sup>*</sup>	22.21	C <sub>42</sub> H <sub>70</sub> O <sub>12</sub>	767.4934 (-0.7)	765.4825 (4.0)	605.4399[M+H-Glc] <sup>+</sup> 425.3786[M+H-2Glc-H <sub>2</sub> O] <sup>+</sup> 407.3653[M+H-2Glc-2H <sub>2</sub> O] <sup>+</sup>	719.2866[M-H-CO-H <sub>2</sub> O] <sup>-</sup> 603.4265[M-H-Glc] <sup>-</sup>	SQ
64	Dihydrotanshinone I <sup>*</sup>	22.46	C <sub>18</sub> H <sub>14</sub> O <sub>3</sub>	279.1013 (-0.9)	ND	233.0967[M+H-CO-H <sub>2</sub> O] <sup>+</sup> 205.1011[M+H-2CO-H <sub>2</sub> O] <sup>+</sup> 190.0780[M+H-2CO-H <sub>2</sub> O-CH <sub>3</sub> ] <sup>+</sup>	ND	DS
65	Horminone	22.66	C <sub>20</sub> H <sub>28</sub> O <sub>4</sub>	333.2064 (1.0)	331.1918 (1.0)	315.1917[M+H-H <sub>2</sub> O] <sup>+</sup> 297.1904[M+H-2H <sub>2</sub> O] <sup>+</sup>	301.1810[M-H-2CH <sub>3</sub> ] <sup>-</sup>	DS
66	Norsalvioxide	22.66	C <sub>18</sub> H <sub>24</sub> O <sub>2</sub>	273.1847 (-0.7)	271.1707 (1.1)	255.1746[M+H-H <sub>2</sub> O] <sup>+</sup> 243.1738[M+H-2CH <sub>3</sub> ] <sup>+</sup> 199.1101[M+H-3CH <sub>3</sub> -CHO] <sup>+</sup>	241.1595[M-H-2CH <sub>3</sub> ] <sup>-</sup> 199.0769[M-H-CO-CHO-CH <sub>3</sub> ] <sup>-</sup>	DS
67	Neocryptotanshinone	22.75	C <sub>19</sub> H <sub>22</sub> O <sub>4</sub>	315.1590 (-0.2)	313.1449 (1.2)	297.1479[M+H-H <sub>2</sub> O] <sup>+</sup> 279.1374[M+H-2H <sub>2</sub> O] <sup>+</sup> 254.0931[M+H-H <sub>2</sub> O-CO-CH <sub>3</sub> ] <sup>+</sup>	283.1351[M-H-2CH <sub>3</sub> ] <sup>-</sup> 267.1396[M-H-CO-H <sub>2</sub> O] <sup>-</sup> 255.1398[M-H-2CH <sub>3</sub> -CO] <sup>-</sup>	DS
68	Microstegiol	22.78	C <sub>20</sub> H <sub>26</sub> O <sub>2</sub>	299.2003 (-0.8)	297.1861 (0.5)	257.1543[M+H-C <sub>3</sub> H <sub>6</sub> ] <sup>+</sup> 229.1227[M+H-CO-C <sub>3</sub> H <sub>6</sub> ] <sup>+</sup>	282.1627[M-H-CH <sub>3</sub> ] <sup>-</sup> 254.1321[M-H-CO-CH <sub>3</sub> ] <sup>-</sup>	DS
69	Isotanshinone II <sub>A</sub>	23.34	C <sub>19</sub> H <sub>18</sub> O <sub>3</sub>	295.1329 (0)	ND	277.1215[M+H-H <sub>2</sub> O] <sup>+</sup> 225.1268[M+H-3CH <sub>2</sub> -CO] <sup>+</sup>	ND	DS
70	Epidanshenspiroketallactone	23.51	C <sub>17</sub> H <sub>16</sub> O <sub>3</sub>	269.1171 (-0.4)	ND	251.1061[M+H-H <sub>2</sub> O] <sup>+</sup> 223.1118[M+H-H <sub>2</sub> O-CO] <sup>+</sup> 195.1153[M+H-H <sub>2</sub> O-2CO] <sup>+</sup>	ND	DS
71	Horminon isomer	24.07	C <sub>20</sub> H <sub>28</sub> O <sub>4</sub>	333.2066	331.1923	315.1944[M+H-H <sub>2</sub> O] <sup>+</sup>	313.1817[M-H-H <sub>2</sub> O] <sup>-</sup>	DS

			(1.6)	(2.4)	287.2042[M+H-H <sub>2</sub> O-CO] <sup>+</sup>	298.1568[M-H-CH <sub>3</sub> -H <sub>2</sub> O] <sup>-</sup> 270.1630[M-H-CH <sub>3</sub> -H <sub>2</sub> O-CO] <sup>-</sup> 227.1084[M-H-C <sub>3</sub> H <sub>6</sub> -2CH <sub>3</sub> ] <sup>-</sup>	DS
72	Sugiol	24.35	C <sub>20</sub> H <sub>28</sub> O <sub>2</sub> 301.2160 (-0.6)	299.2023 (2.3)	259.1689[M+H-C <sub>3</sub> H <sub>6</sub> ] <sup>+</sup> 213.1277[M+H-H <sub>2</sub> O-CO-C <sub>3</sub> H <sub>6</sub> ] <sup>+</sup>		
73	Cryptotanshinone*	24.43	C <sub>19</sub> H <sub>20</sub> O <sub>3</sub> 297.1487 (0.5)	ND	254.0942[M+H-CO-CH <sub>3</sub> ] <sup>+</sup> 251.1428[M+H-CO-H <sub>2</sub> O] <sup>+</sup>	ND	DS
74	Tanshinone I*	24.59	C <sub>18</sub> H <sub>12</sub> O <sub>3</sub> 277.0858 (-0.5)	ND	249.0906[M+H-CO] <sup>+</sup> 178.0776[M+H-3CO-CH <sub>3</sub> ] <sup>+</sup>	ND	DS
75	Miltirone I	25.06	C <sub>18</sub> H <sub>16</sub> O <sub>2</sub> 265.1221 (-0.8)	ND	223.0756[M+H-C <sub>3</sub> H <sub>6</sub> ] <sup>+</sup> 204.0929[M+H-CO-H <sub>2</sub> O-CH <sub>3</sub> ] <sup>+</sup> 195.0800[M+H-C <sub>3</sub> H <sub>6</sub> -CO] <sup>+</sup>	ND	DS
76	Dihydrotanshinone I isomer	25.59	C <sub>18</sub> H <sub>14</sub> O <sub>3</sub> 279.1015 (-0.4)	ND	261.0905[M+H-H <sub>2</sub> O] <sup>+</sup> 205.1012[M+H-2CO-H <sub>2</sub> O] <sup>+</sup>	ND	DS
77	Dehydromiltirone/ Sibiriquinone A	26.62	C <sub>19</sub> H <sub>20</sub> O <sub>2</sub> 281.1535 (-0.2)	ND	221.0963[M+H-4CH <sub>3</sub> ] <sup>+</sup> 193.1014[M+H-4CH <sub>3</sub> -CO] <sup>+</sup>	ND	DS
78	Tanshinone II <sub>A</sub> *	27.24	C <sub>19</sub> H <sub>18</sub> O <sub>3</sub> 295.1328 (-0.3)	ND	277.1220[M+H-H <sub>2</sub> O] <sup>+</sup> 252.0790[M+H-CO-CH <sub>3</sub> ] <sup>+</sup> 249.1265[M+H-H <sub>2</sub> O-CO] <sup>+</sup>	ND	DS
79	Miltirone	28.17	C <sub>19</sub> H <sub>22</sub> O <sub>2</sub> 283.1694 (0.4)	ND	223.1121[M+H-HOAc] <sup>+</sup> 208.0889[M+H-CH <sub>3</sub> -HOAc] <sup>+</sup>	ND	DS
80	Salviolone	28.45	C <sub>18</sub> H <sub>20</sub> O <sub>2</sub> 269.1535 (-0.4)	ND	254.1302[M+H-CH <sub>3</sub> ] <sup>+</sup> 239.1059[M+H-2CH <sub>3</sub> ] <sup>+</sup>	ND	DS
81	Oleanolic acid	31.92	C <sub>30</sub> H <sub>48</sub> O <sub>3</sub> 457.3677 (0.2)	455.3534 (0.8)	439.3573[M+H-H <sub>2</sub> O] <sup>+</sup> 411.3653[M+H-H <sub>2</sub> O-CO] <sup>+</sup>	455.3528	DS