

# Combining Chemical Profiling and Network Analysis to Investigate the Pharmacology of Complex Prescriptions in Traditional Chinese Medicine

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**Supplementary information**

Supplementary Table S1. Chemical information of the ingredients identified from DJF formula.

T <sub>R</sub> (min)	Formula	ES <sup>-</sup> (m/z) [M-H] <sup>-</sup> (ppm)	MS <sup>2</sup>	ES(m/z) <sup>+</sup> [M+H] <sup>+</sup> (ppm)	MS <sup>2</sup>	Identification
1	C <sub>12</sub> H <sub>22</sub> O <sub>11</sub>	341.1095(3.2)	179.0560[M-H-Glc] <sup>-</sup> 161.0455[M-H-Glc-H <sub>2</sub> O] <sup>-</sup>	343.1240(0.0)	325.1138[M+H-H <sub>2</sub> O] <sup>+</sup>	Sucrose
2	C <sub>10</sub> H <sub>12</sub> N <sub>5</sub> O <sub>6</sub> P	328.0449(0.6)	134.0465[ADE] <sup>-</sup> 195.0653[DTFD] <sup>-</sup>	330.0596(-2.1)	136.0625[M+H-HDTDO] <sup>+</sup>	cAMP
3	C <sub>6</sub> H <sub>8</sub> O <sub>7</sub>	191.0195(1.6)	173.0086[M-H-H <sub>2</sub> O] <sup>-</sup> 111.0083[M-H-CO <sub>2</sub> -2 H <sub>2</sub> O] <sup>-</sup>	193.0347(-0.5)		Citric acid
4	C <sub>16</sub> H <sub>24</sub> O <sub>10</sub>	375.1293(0.5)	345.1188[M-H-CH <sub>2</sub> O] <sup>-</sup>	377.1438(-2.7)	215.0922[M+H-Glc] <sup>+</sup> 197.0816[M+H-Glc-H <sub>2</sub> O] <sup>+</sup>	8-Diebenzoylpaeoniflorin
5	C <sub>19</sub> H <sub>26</sub> O <sub>15</sub>	493.1193(0.0)	331.0663[M-H-Glc] <sup>-</sup> 313.0559[M-H-Glc-H <sub>2</sub> O] <sup>-</sup> 169.0136[GA-H] <sup>-</sup>	517.1171[M+Na] <sup>+</sup>	315.0743[M+H-Glc-H <sub>2</sub> O] <sup>+</sup> 153.0182[GA-H <sub>2</sub> O+H] <sup>+</sup>	6'-o-galloylsucroses or its isomer
6	C <sub>7</sub> H <sub>6</sub> O <sub>5</sub>	169.0135(-1.2)	125.0237[M-H-CO <sub>2</sub> ] <sup>-</sup>	171.0291(-1.2)		Gallic acid
7	C <sub>19</sub> H <sub>26</sub> O <sub>15</sub>	493.1200(1.4)	313.0572[M-H-Glc-H <sub>2</sub> O] <sup>-</sup> 169.0139[GA-H] <sup>-</sup>	517.1183[M+Na] <sup>+</sup>	315.0710[M+H-Glc-H <sub>2</sub> O] <sup>+</sup> 153.0185[GA-H <sub>2</sub> O+H] <sup>+</sup>	6'-o-galloylsucroses or its isomer
8	C <sub>19</sub> H <sub>26</sub> O <sub>15</sub>	493.1194(0.2)	331.0661[M-H-Glc] <sup>-</sup> 313.0560[M-H-Glc-H <sub>2</sub> O] <sup>-</sup>	517.1147[M+Na] <sup>+</sup>	315.0714[M+H-Glc-H <sub>2</sub> O] <sup>+</sup> 153.0185[GA-H <sub>2</sub> O+H] <sup>+</sup>	6'-o-galloylsucroses or its isomer
9	C <sub>16</sub> H <sub>24</sub> O <sub>9</sub>	359.1343(0.3)	197.0810[M-H-Glc] <sup>-</sup> 179.0704[M-H-Glc-H <sub>2</sub> O] <sup>-</sup>	361.1515(4.4)	199.0969[M+H-Glc] <sup>+</sup> 181.0863[M+H-Glc-H <sub>2</sub> O] <sup>+</sup> 163.0759[M+H-Glc-2H <sub>2</sub> O] <sup>+</sup>	1-o-β-D-glucopyranosyl-paeonisufrone
10	C <sub>23</sub> H <sub>28</sub> O <sub>14</sub> S	559.1129(1.3)	527.1439[M-H-CH <sub>2</sub> OH] <sup>-</sup> 483.0776[M-H-CH <sub>2</sub> OH-C			Oxypaeoniflorin sulfonate

				O <sub>2</sub> ] <sup>-</sup>			
11	1.806	C <sub>23</sub> H <sub>28</sub> O <sub>14</sub>	527.1393(-1.5)	397.1323[M-H-Glc] <sup>-</sup> 315.0714[M-H-GA-Glc] <sup>-</sup>			6'-o-galloyl desbenzoylpaeoniflorin isomer
12	2.104	C <sub>16</sub> H <sub>26</sub> O <sub>9</sub>	361.1482(-4.7)	169.0131[GA-H] <sup>-</sup>		201.0472[M+H-Glc] <sup>+</sup>	6-o-β-D-glucopyranosyl-lactinolid e
13	2.155	C <sub>23</sub> H <sub>28</sub> O <sub>14</sub>	527.1400(-0.2)	497.1293[M-H-HCHO] <sup>-</sup>		183.1027[M+H-Glc-H <sub>2</sub> O] <sup>+</sup>	8-o-galloyl desbenzoylpaeoniflorin
				479.1199[M-H-HCHO-H <sub>2</sub> O-H] <sup>-</sup>			
14	2.269	C <sub>21</sub> H <sub>24</sub> O <sub>11</sub>	451.1232(-1.8)	169.0138[GA-H] <sup>-</sup> 289.0709[M-H-Glc] <sup>-</sup>		291.0874[M+H-Glc] <sup>+</sup>	Catechin-5-o-glucoside
15	2.367	C <sub>29</sub> H <sub>38</sub> O <sub>18</sub> S	705.1693(-1.1)	583.1345[M-H-BZ] <sup>-</sup> 555.11733[M-H-BZ-CO] <sup>-</sup>		273.0793[M+H-Glc-H <sub>2</sub> O] <sup>+</sup> 501.1032[M+H-Glc-CO <sub>2</sub> ] <sup>+</sup>	Isomaltopaeoniflorin sulfonate
16	2.401	C <sub>23</sub> H <sub>28</sub> O <sub>14</sub>	527.1409(1.5)	543.1164[M-H-Glc] <sup>-</sup> 497.1272[M-H-HCHO] <sup>-</sup>		333.0446[GA+ Glc+H] <sup>+</sup>	6'-o-galloyl desbenzoylpaeoniflorin
				483.0770[M-H-CO <sub>2</sub> -H] <sup>-</sup>			
17	2.504	C <sub>23</sub> H <sub>28</sub> O <sub>12</sub>	495.1508(1.0)	313.0553[GA+ Glc-H] <sup>-</sup> 461.1665[M-H-2OH] <sup>-</sup> 345.1194[M-H-BZ-CO] <sup>-</sup> 333.0984[M-H-Glc] <sup>-</sup> 137.0240[4-OH-BZ-H] <sup>-</sup>	497.1665(1.2)	335.1119[M+H-Glc] <sup>+</sup>	Oxypaeoniflorin

18	2.549	C <sub>23</sub> H <sub>28</sub> O <sub>13</sub> S	543.1172(0.0)	421.0798[M-H-BZ] <sup>-</sup> 375.0751[M-H-BZ-HCOO H] <sup>-</sup> 121.0288[BZ-H] <sup>-</sup>		383.0782[M+H-Glc] <sup>+</sup> 261.0410[M+H-Glc-BZ] <sup>+</sup>	Paeoniflorin sulfonate
19	2.669	C <sub>23</sub> H <sub>28</sub> O <sub>12</sub>	495.1502(-0.2)	465.0675[M-H-HCHO] <sup>-</sup> 345.1180[M-H-BZ-CO] <sup>-</sup> 333.1013[M-H- Glc] <sup>-</sup> 313.0549[M-H-BZ-CH <sub>3</sub> OH -CO] <sup>-</sup> 137.0241[2-OH-BZ-H] <sup>-</sup>		317.1034[M+H-Glc-H <sub>2</sub> O] <sup>+</sup>	Palicylpaeoniflorin
20	2.915	C <sub>27</sub> H <sub>24</sub> O <sub>18</sub>	635.0890(0.9)	465.0662[M-H-GA] <sup>-</sup> 295.0473[M-H-2GA] <sup>-</sup> 169.0131[GA-H] <sup>-</sup>		467.0325[M+H-GA] <sup>+</sup> 449.0656[M+H-GA-H <sub>2</sub> O] <sup>+</sup>	Trigalloyglucose
21	2.967	C <sub>24</sub> H <sub>30</sub> O <sub>13</sub>	525.1608(0.0)	495.1511[M-H-HCHO] <sup>-</sup> 363.1055[M-H-Glc] <sup>-</sup> 167.0345[HB-H] <sup>-</sup>		347.1153[M+H-Glc-H <sub>2</sub> O] <sup>+</sup>	Mudanpioside E
22	3.001	C <sub>21</sub> H <sub>22</sub> O <sub>9</sub>	417.1177(-2.2)	255.0659[M-H-Glc] <sup>-</sup> 135.0083[M-H-VP] <sup>-</sup>	419.1339(-0.7)	257.0813[M+H-Glc] <sup>+</sup> 137.0233[M+H-VP] <sup>+</sup>	Liquiritin isomer
23	3.098	C <sub>32</sub> H <sub>40</sub> O <sub>18</sub>	711.2124(-1.7)	549.1597[M-H-Glc] <sup>-</sup>  417.1163[M-H-Glc-Api-H] - 255.0652[M-H-2Glc-Api] <sup>-</sup>		419.1306[M+H-Glc-Api] <sup>+</sup>  257.0802[M+H-2Glc-Api] <sup>+</sup>	Liquiritigenin-7-o-Glucoside-4'-o- Apiosyl-o-Glucoside
24	3.167	C <sub>20</sub> H <sub>16</sub> O <sub>13</sub>	463.0514(0.2)	300.9979 [M-H-Glc] <sup>-</sup>	465.0673(0.9)	303.0128[M+H-Glc] <sup>+</sup>	Ellagic acid-hexoside
25	3.247	C <sub>29</sub> H <sub>38</sub> O <sub>16</sub>	641.2088(0.9)	519.1747[M-H-BZ] <sup>-</sup> 489.1619[M-H-BZ-HCHO]		481.1619[M+H-Glc] <sup>+</sup> 319.1142[M+H-2Glc] <sup>+</sup>	6'-o-α-glucopyranosyl paeoniflorin

				121.0288[BZ-H] <sup>-</sup>				
26	3.333	C <sub>9</sub> H <sub>10</sub> O <sub>3</sub>	165.0549(-1.8)	150.0320[M-H-CH <sub>3</sub> ] <sup>-</sup>	167.0702(-3.6)	149.0600[M+H-H <sub>2</sub> O] <sup>+</sup>	Phloretic acid	
				137.0237[M-H-CO] <sup>-</sup>		121.0285[M+H-HCOOH] <sup>+</sup>		
27	3.378	C <sub>30</sub> H <sub>32</sub> O <sub>15</sub>	631.1653(-1.6)	495.1494[M-H-MB] <sup>-</sup>		315.0723[MG+H] <sup>+</sup>	Galloylpaconiflorin or its isomer	
				313.0561[MG-H] <sup>-</sup>		153.0184[GA+H-H <sub>2</sub> O] <sup>+</sup>		
				169.0133[GA-H] <sup>-</sup>				
28	3.430	C <sub>34</sub> H <sub>28</sub> O <sub>22</sub>	787.0996(0.3)	635.0877[M-H-GA+H <sub>2</sub> O] <sup>-</sup>		771.1032[M+H-H <sub>2</sub> O] <sup>+</sup>	1,2,3,6-tetra-o-galloyl-β-D-glucose	
				465.0655[M-H-2GA+H <sub>2</sub> O] <sup>-</sup>		619.0950[M+H-GA] <sup>+</sup>		
				-				
				449.1075[M-H-2GA] <sup>-</sup>		153.0184[GA+H-H <sub>2</sub> O] <sup>+</sup>		
				313.0581[M-H-3GA+2H <sub>2</sub> O] <sup>-</sup>				
				169.0139[GA-H] <sup>-</sup>				
29	3.527	C <sub>18</sub> H <sub>24</sub> O <sub>11</sub>	415.1237(-0.7)	327.1067[M-H-2CO <sub>2</sub> ] <sup>-</sup>		267.0866[M+H-Arab] <sup>+</sup>	2-o-[α-arabinopyranosyl-(1-6)-β-D-glucopyranoside]-Benzaldehyde	
				121.0287[BH-H] <sup>-</sup>				
30	3.578	C <sub>30</sub> H <sub>32</sub> O <sub>17</sub> S	695.1267(-2.2)	543.1160[M-H-GA+H <sub>2</sub> O] <sup>-</sup>		315.0689[GA+Glc-H <sub>2</sub> O+H] <sup>+</sup>	Galloylpaconiflorin sulfonate	
				313.0591[GA+Glc-H <sub>2</sub> O-H] <sup>-</sup>				
31	3.647	C <sub>23</sub> H <sub>28</sub> O <sub>11</sub>	479.1553(0.0)	435.1650[M-H-CO <sub>2</sub> ] <sup>-</sup>	481.1715(1.0)	463.1615[M+H-H <sub>2</sub> O] <sup>+</sup>	Albiflorin	
				357.1184[M-H-BZ] <sup>-</sup>		319.1186[M+H-Glc] <sup>+</sup>		
				327.1082[M-H-CH <sub>2</sub> O-BZ] <sup>-</sup>		301.1080[M+H-Glc-H <sub>2</sub> O] <sup>+</sup>		
				317.1027[M-H-Glc] <sup>-</sup>				

32	3.944	C <sub>23</sub> H <sub>28</sub> O <sub>11</sub>	479.1553(0.0)	121.0291[BZ-H] <sup>-</sup> 449.1448[M-H-HCHO] <sup>-</sup> 357.1186[M-H-BZ] <sup>-</sup> 327.1080[M-H-CH <sub>2</sub> O-BZ] <sup>-</sup>		463.1604[M+H-H <sub>2</sub> O] <sup>+</sup> 301.1075[M+H-Glc-H <sub>2</sub> O+H] <sup>+</sup>	Paeoniflorin
33	4.093	C <sub>34</sub> H <sub>28</sub> O <sub>22</sub>	787.0984(-1.3)	121.0292[BZ-H] <sup>-</sup> 617.0774[M-H-GA] <sup>-</sup>		619.0937[M+H-GA] <sup>+</sup>	1,3,4,6-tetra-o-galloyl-β-D-glucose
34	4.127	C <sub>21</sub> H <sub>22</sub> O <sub>10</sub>	433.1132(-0.7)	449.1446[M-H-2GA] <sup>-</sup> 169.0139[GA-H] <sup>-</sup> 271.0613[M-H-Glc] <sup>-</sup> 255.0657[M-H-Glc-OH] <sup>-</sup>		449.0680[M+H-2GA] <sup>+</sup> 153.0181[GA+H-H <sub>2</sub> O] <sup>+</sup> 273.0760[M+H-Glc] <sup>+</sup>	5-hydroxyliquiritin
35	4.131	C <sub>14</sub> H <sub>6</sub> O <sub>8</sub>	300.9989(1.7)	243.8993[M-H-CO-HCHO] ] <sup>-</sup> 225.9262[M-H-H <sub>2</sub> O-CO-H CHO] <sup>-</sup> 222.8290[M-H-CO <sub>2</sub> -2OH] <sup>-</sup>		287.8913[M+H-CH <sub>3</sub> ] <sup>+</sup> 241.8830[M+H-CO <sub>2</sub> -OH] <sup>+</sup>	Ellagic acid
36	4.207	C <sub>27</sub> H <sub>30</sub> O <sub>14</sub>	577.1565(1.4)	517.1263[M-H-C <sub>2</sub> H <sub>4</sub> O <sub>2</sub> ] <sup>-</sup> 487.1241[M-H-C <sub>3</sub> H <sub>6</sub> O <sub>3</sub> ] <sup>-</sup> 457.1148[M-H-C <sub>4</sub> H <sub>8</sub> O <sub>4</sub> ] <sup>-</sup>	579.1732(3.1)	561.1618[M+H-H <sub>2</sub> O] <sup>+</sup> 543.1476[M+H-2H <sub>2</sub> O] <sup>+</sup> 525.1397[M+H-3H <sub>2</sub> O] <sup>+</sup>	Isoviolanthin
37	4.327	C <sub>26</sub> H <sub>30</sub> O <sub>13</sub>	549.1614(1.1)	417.1184[M-H-Api] <sup>-</sup> 255.0661[M-H-Api-Glc] <sup>-</sup> 135.0083[M-H-Api-Glc-V P] <sup>-</sup>	551.1766(0.2)	257.0817[M+H-Api-Glc] <sup>+</sup> 419.1335[M+H-Api] <sup>+</sup> 137.0237[M+H-Api-Glc-VP] <sup>+</sup>	Liquiritin apioside
38	4.407	C <sub>21</sub> H <sub>22</sub> O <sub>9</sub>	417.1187(0.2)	255.0660[M-H-Glc] <sup>-</sup> 135.0083[M-H-VP] <sup>-</sup>	419.1335(-1.7)	257.0814[M+H-Glc] <sup>+</sup> 137.0235[M+H-VP] <sup>+</sup>	liquiritin
39	4.493	C <sub>41</sub> H <sub>32</sub> O <sub>26</sub>	939.1093(-1.2)	769.0878[M-H-GA] <sup>-</sup>		771.0992[M+H-GA] <sup>+</sup>	Pentagalloylglucose

				617.0768[M-H-2GA+H <sub>2</sub> O] -		431.0567[M+H-3GA] <sup>+</sup>	
40	4.573	C <sub>30</sub> H <sub>32</sub> O <sub>15</sub>	631.1666(0.5)	169.0136[GA-H] <sup>-</sup> 479.1559[M-H-GA+H <sub>2</sub> O] <sup>-</sup> 465.1393[M-H-BZ-CO <sub>2</sub> ] <sup>-</sup>	633.1809(-1.6)	153.0184[GA+H-H <sub>2</sub> O] <sup>+</sup> 503.1543[M+Na-GA+H <sub>2</sub> O] <sup>+</sup> 319.1180[M+H-GA+H <sub>2</sub> O-Glc] J <sup>+</sup>	Galloylpaconiflorin
41	4.642	C <sub>30</sub> H <sub>32</sub> O <sub>15</sub>	631.1666(0.5)	313.0557[GA+Glc-H <sub>2</sub> O-H] -		153.0185[GA+H-H <sub>2</sub> O] <sup>+</sup>	
41	4.642	C <sub>30</sub> H <sub>32</sub> O <sub>15</sub>	631.1666(0.5)	613.1561[M-H-H <sub>2</sub> O] <sup>-</sup> 491.1195[M-H-H <sub>2</sub> O-BZ] <sup>-</sup> 449.1448[M-H-GA-HCHO +H <sub>2</sub> O] <sup>-</sup> 313.0563[GA+Glc-H <sub>2</sub> O-H] -		615.1668[M+H-H <sub>2</sub> O] <sup>+</sup> 493.1360[M+H-H <sub>2</sub> O-BZ] <sup>+</sup> 315.0717[GA+Glc-H <sub>2</sub> O+H] <sup>+</sup>	4'-o-galloylpaconiflorin
42	4.773	C <sub>33</sub> H <sub>38</sub> O <sub>18</sub>	721.1987(1.0)	631.1658[M-H-C <sub>3</sub> H <sub>6</sub> O <sub>3</sub> ] <sup>-</sup>  463.2186[M-H-2C <sub>4</sub> H <sub>8</sub> O <sub>4</sub> -H <sub>2</sub> O] <sup>-</sup>	723.2150(1.9)	705.2054[M+H-H <sub>2</sub> O] <sup>+</sup>  687.2048[M+H-2H <sub>2</sub> O] <sup>+</sup>	Apigenin-6-C-α-L-rhamnopyranoside-8-C-[6'''-(3-hydroxy-3-methylglutaroyl)-β-D-glucopyranoside]
43	4.825	C <sub>30</sub> H <sub>32</sub> O <sub>15</sub>	631.1664(0.2)	479.1554[M-H-GA+H <sub>2</sub> O] <sup>-</sup> 449.1449[M-H-GA-HCHO +H <sub>2</sub> O] <sup>-</sup> 169.0139[GA-H] <sup>-</sup>	633.1827(1.3)	669.1925[M+H-3H <sub>2</sub> O] <sup>+</sup> 487.2126[M-HM-C <sub>3</sub> H <sub>6</sub> O <sub>3</sub> +H] <sup>+</sup> 503.1547[M+Na-GA+H <sub>2</sub> O] <sup>+</sup> 319.1184[M+H-GA+H <sub>2</sub> O-Glc] J <sup>+</sup>	6'-o-galloylbiflorin
44	5.019	C <sub>30</sub> H <sub>32</sub> O <sub>15</sub>	631.1668(0.8)	479.1561[M-H-GA+H <sub>2</sub> O] <sup>-</sup>	633.1823(0.6)	153.0189[GA-H <sub>2</sub> O+H] <sup>+</sup> 471.1298[M+H-Glc] <sup>+</sup>	4-o-galloylbiflorin

				169.0138[GA-H] <sup>-</sup>		301.1074[M+H-Glc-GA] <sup>+</sup>	
45	5.236	C <sub>21</sub> H <sub>22</sub> O <sub>10</sub>	433.1133(-0.5)	271.0603[M-H-Glc] <sup>-</sup>		153.0187[GA-H <sub>2</sub> O+H] <sup>+</sup>	Naringenin-7-o-β-D-glucoside
				151.0029[M-H-Glc-VP] <sup>-</sup>		273.0754[M+H-Glc] <sup>+</sup>	
46	5.568	C <sub>26</sub> H <sub>30</sub> O <sub>13</sub>	549.1616(1.5)	417.1185[M-H-Api] <sup>-</sup>	551.1766(0.2)	153.0186[M+H-Glc-VP] <sup>+</sup>	Isoliquiritin apioside
				255.0665[M-H-Api-Glc] <sup>-</sup>		419.1333[M+H-Api] <sup>+</sup>	
				135.0087[M-H-Api-Glc-V P] <sup>-</sup>		257.0813[M+H-Api-Glc] <sup>+</sup>	
47	5.602	C <sub>23</sub> H <sub>28</sub> O <sub>11</sub>	479.1559(1.3)	357.1192[M-H-BZ] <sup>-</sup>	481.1703(-1.5)	137.0233[M+H-Api-Glc-VP] <sup>+</sup>	Isopaeoniflorin
				327.1069[M-H-CH <sub>2</sub> O-BZ] <sup>-</sup>		319.1190[M+H-Glc] <sup>+</sup>	
				121.0292[BZ-H] <sup>-</sup>		301.1094[M+H-Glc-H <sub>2</sub> O] <sup>+</sup>	
48	5.619	C <sub>37</sub> H <sub>36</sub> O <sub>19</sub>	783.1761(-1.5)	631.1647[M-H-GA+H <sub>2</sub> O] <sup>-</sup>	785.1942(1.7)	503.1532[M+Na-2GA+2H <sub>2</sub> O] <sup>+</sup>	3',6'-di-O-galloylpaeoniflorin
				479.1552[M-H-2GA+2H <sub>2</sub> O] ] <sup>-</sup>		481.1733[M+H-2GA+2H <sub>2</sub> O] <sup>+</sup>	
				313.0554[GA-H <sub>2</sub> O+Glc-H] - 169.0133[GA-H] <sup>-</sup>		319.1193[M+H-2GA+2H <sub>2</sub> O-G lc] <sup>+</sup>	
49	5.655	C <sub>48</sub> H <sub>74</sub> O <sub>21</sub>	985.4636(-0.8)	954.6343[M-H-OCH <sub>3</sub> ] <sup>-</sup> ;	987.4797(-0.4)	301.1072[M+H-2GA+H <sub>2</sub> O-Gl c] <sup>+</sup>	Yunganoside G1
				821.3953[M-H-Rha-H <sub>2</sub> O] <sup>-</sup>		841.4497[M+H-Rha] <sup>+</sup>	
50	5.682	C <sub>21</sub> H <sub>36</sub> O <sub>11</sub>	463.2187(1.7)	331.1761[M-H-Api] <sup>-</sup>	487.2132[M+Na] <sup>+</sup>	823.2448[M+H-Rha-H <sub>2</sub> O] <sup>+</sup>	Zansiumaloside A
51	5.734	C <sub>26</sub> H <sub>30</sub> O <sub>13</sub>	549.1608(0.0)	417.1183[M-H-Api] <sup>-</sup>		333.1894[M+H-Api] <sup>+</sup>	Licuraside
				255.0657[M-H-Api-Glc] <sup>-</sup>		257.0813[M+H-Api-Glc] <sup>+</sup>	
				135.0083[M-H-Api-Glc-V P] <sup>-</sup>		419.1342[M+H-Api] <sup>+</sup>	
						137.0237[M+H-Api-Glc-VP] <sup>+</sup>	



52	5.785	C <sub>21</sub> H <sub>22</sub> O <sub>9</sub>	417.1184(-0.5)	255.0658[M-H-Glc] <sup>-</sup> 135.0082[M-H-Glc-VP] <sup>-</sup>	419.1326(-3.8)	257.0817[M+H-Glc] <sup>+</sup> 137.0237[M+H-VP-Glc] <sup>+</sup>	Isoliquiritin
53	5.882	C <sub>16</sub> H <sub>12</sub> O <sub>4</sub>	267.0665(3.0)	252.0400[M-H-CH <sub>3</sub> ] <sup>-</sup>	269.0813(-0.4)	254.0460[M+H-CH <sub>3</sub> ] <sup>+</sup> 237.0555[M+H-CH <sub>3</sub> OH] <sup>+</sup> 201.0464[M+H-CH <sub>3</sub> OH-2H <sub>2</sub> O] <sup>+</sup>	Pallidiflorin
54	5.951	C <sub>21</sub> H <sub>22</sub> O <sub>9</sub>	417.1172(-3.4)	255.0655[M-H-Glc] <sup>-</sup> 135.0080[M-H-VP-Glc] <sup>-</sup>	419.1335(-1.7)	257.0816[M+H-Glc] <sup>+</sup> 137.0238[M+H-VP-Glc] <sup>+</sup>	Neoisoliquiritin
55	5.968	C <sub>35</sub> H <sub>36</sub> O <sub>15</sub>	695.1976(0.0)	549.1603[M-H-PC] <sup>-</sup> 531.1499[M-H-PC-H <sub>2</sub> O] <sup>-</sup> 417.1186[M-H-PC-Api] <sup>-</sup> 255.0657[M-H-PC-Api-Glc] <sup>-</sup>		419.1347[M+H-PC-Api] <sup>+</sup> 257.0817[M+H-PC-Api-Glc] <sup>+</sup>	Licorice-glycoside D2 or its isomer
56	6.014	C <sub>48</sub> H <sub>74</sub> O <sub>20</sub>	969.4691(-0.4)	793.4326[M-H-GlcA] <sup>-</sup> 497.1135[Rha+2GlcA-H] <sup>-</sup>		795.4532[M+H-GlcA] <sup>+</sup> 601.4107[M-2GlcA-H <sub>2</sub> O+H] <sup>+</sup>	3-o-[β-D-rhamnose]-24-hydroxyl-glycyrrhizic acid isomer
57	6.031	C <sub>22</sub> H <sub>22</sub> O <sub>9</sub>		267.0654[M-H-Glc] <sup>-</sup> 252.0420[M-H-Glc-CH <sub>3</sub> ] <sup>-</sup>	431.1331(-2.6)	269.0814[M+H-Glc] <sup>+</sup> 254.0569[M+H-Glc-CH <sub>3</sub> ] <sup>+</sup>	Ononin
58	6.065	C <sub>36</sub> H <sub>38</sub> O <sub>16</sub>	725.2077(-0.7)	549.1597[M-H-PM] <sup>-</sup> 531.1508[M-H-PM-H <sub>2</sub> O] <sup>-</sup> 255.0656[M-H-PM-Api-Glc] <sup>-</sup>			Licorice glycoside A
59	6.214	C <sub>15</sub> H <sub>12</sub> O <sub>4</sub>	255.0650(-2.7)	135.0080[M-H-VP]	257.0809(-1.9)	137.0238[M+H-VP] <sup>+</sup> 147.0455[M+H-RL] <sup>+</sup> 119.0504[M+H-RL-CO] <sup>+</sup>	Liquiritigenin

60	6.300	C <sub>42</sub> H <sub>62</sub> O <sub>18</sub>	853.3873(1.8)	351.0569[2GlcA-H] <sup>-</sup>	855.4020(0.7)	765.4501[M+H-HCOOH-CO <sub>2</sub> ] <sup>+</sup> 601.4045[M+H-GlcA-HCOOH-CH <sub>3</sub> OH] <sup>+</sup> 485.3323[M+H-2GlcA-H <sub>2</sub> O] <sup>+</sup>	22-Hydroxyl-licorice-saponin G2
61	6.380	C <sub>16</sub> H <sub>12</sub> O <sub>6</sub>	299.0568(4.0)	255.0673[M-H-CO <sub>2</sub> ] <sup>-</sup>	301.0716(1.3)	270.8882[M+H-OCH <sub>3</sub> ] <sup>+</sup> 257.0803[M+H-CO <sub>2</sub> ] <sup>+</sup>	Kaempferol 3-o-methyl ether
62	6.431	C <sub>35</sub> H <sub>36</sub> O <sub>15</sub>	695.1968(-1.2)	549.1606[M-H-PC] <sup>-</sup> 531.1500[M-H-PC-H <sub>2</sub> O] <sup>-</sup> 417.1193[M-H-PC-Api] <sup>-</sup> 255.0653[M-H-PC-Api-Glc] <sup>-</sup>		257.0812[M+H-PC-Api-Glc] <sup>+</sup> 147.0442[M+H-PC-Api-Glc-R] <sup>+</sup>	Licorice-glycoside D2 or its isomer
63	6.528	C <sub>21</sub> H <sub>34</sub> O <sub>10</sub>	445.2081(1.6)	313.1642[M-H-Api] <sup>-</sup> 293.0873[Api+Glc-H] <sup>-</sup>		429.1938[M+H-H <sub>2</sub> O] <sup>+</sup>	(1S,5R)-β-pinene-10-β-vicianoside
64	6.528	C <sub>30</sub> H <sub>32</sub> O <sub>13</sub>	599.1766(0.2)	477.1406[M-H-BZ] <sup>-</sup> 283.0605[BZ+Glc-H] <sup>-</sup> 137.0241[4-OH-BZ-H] <sup>-</sup>		285.0762[BZ+Glc+H] <sup>+</sup>	Benzoyloxypaeoniflorin
65	6.606	C <sub>42</sub> H <sub>64</sub> O <sub>16</sub>	823.4105(-1.3)	351.0581[2GlcA-H] <sup>-</sup>	825.4235(-4.6)	649.3922[M+H-GlcA] <sup>+</sup> 585.4132[M+H-HCOOH-H <sub>2</sub> O] <sup>+</sup>	Licorice-saponin J2
66	6.745	C <sub>35</sub> H <sub>36</sub> O <sub>15</sub>	695.1981(0.7)	549.1617[M-H-PC] <sup>-</sup> 531.1511[M-H-PC-H <sub>2</sub> O] <sup>-</sup> 255.0660[M-H-PC-Api-Glc] <sup>-</sup>		257.0822[M+H-PC-Api-Glc] <sup>+</sup>	Licorice glycoside B

67	6.713	C <sub>42</sub> H <sub>64</sub> O <sub>16</sub>	823.4116(0.0)	c] 351.0570[2GlcA-H] <sup>-</sup>		649.3967[M+H-GlcA] <sup>+</sup> 455.3535[M+H-2GlcA-H <sub>2</sub> O] <sup>+</sup>	Uralsaponin C
68	6.789	C <sub>42</sub> H <sub>62</sub> O <sub>17</sub>	837.3875(-4.1)	351.0562 [2GlcA-H] <sup>-</sup> , 289.0730 [2GlcA-H <sub>2</sub> O-CO <sub>2</sub> -H] <sup>-</sup>	839.4051(-1.7)	663.3754[M+H-GlcA] <sup>+</sup> 487.3426[M+H-2GlcA] <sup>+</sup>  469.3330[M+H-2GlcA-H <sub>2</sub> O] <sup>+</sup>	24-Hydroxyl-glycyrrhizin
69	6.843	C <sub>48</sub> H <sub>72</sub> O <sub>22</sub>	999.4428(-0.9)	837.3889[M-H-Glc] <sup>-</sup> 351.0555[2GlcA-H] <sup>-</sup>	1001.4576(-1.7)	825.4209[M+H-GlcA] <sup>+</sup> 649.3965[M+H-2GlcA] <sup>+</sup> 631.3855[M+H-2GlcA-H <sub>2</sub> O] <sup>+</sup> 487.3429[M+H-2GlcA-Glc] <sup>+</sup> 469.3321[M+H-2GlcA-Glc-H 2O] <sup>+</sup>	24-Hydroxyl-licoricesaponinA3
70	7.060	C <sub>44</sub> H <sub>64</sub> O <sub>19</sub>	895.3948(-1.8)	351.0562[2GlcA-H] <sup>-</sup>		545.3487[M+H-2GlcA] <sup>+</sup> 527.3367[M+H-2GlcA-H <sub>2</sub> O] <sup>+</sup>	Uralsaponin F
71	7.226	C <sub>42</sub> H <sub>62</sub> O <sub>18</sub>	853.3848(-1.2)	351.0561[2GlcA-H] <sup>-</sup>	855.4004(-1.2)	503.3370[M+H-2GlcA] <sup>+</sup> 485.3263[M+H-2GlcA-H <sub>2</sub> O] <sup>+</sup> 467.3147[M+H-2GlcA-2H <sub>2</sub> O] +	22-Hydroxyl-licorice-saponin G2
72	7.340	C <sub>48</sub> H <sub>72</sub> O <sub>21</sub>	983.4476(-1.2)	821.3977[M-H-Glc] <sup>-</sup> 351.0550[2GlcA-H] <sup>-</sup>	985.4650(0.6)	809.4406[M+H-GlcA] <sup>+</sup> 615.3862[M+H-GlcA-H <sub>2</sub> O] <sup>+</sup> 453.3372[M+H-2GlcA-Glc-H <sub>2</sub> O] <sup>+</sup>	Licorice saponin A3
73	7.391	C <sub>30</sub> H <sub>32</sub> O <sub>12</sub>	583.1817(0.2)	461.1450[M-H-BZ] <sup>-</sup> 121.0291[BZ-H] <sup>-</sup>		445.1501[M+H-BZ-H <sub>2</sub> O] <sup>+</sup> 427.1391[M+H-BZ-2H <sub>2</sub> O] <sup>+</sup> 301.1074[M+H-BZ-Glc] <sup>+</sup>	Benzoylpaconiflorin

74	7.540	C <sub>30</sub> H <sub>32</sub> O <sub>12</sub>	583.1812(-0.7)	121.0289[BZ-H] <sup>-</sup>	585.1970(-0.3)	267.0871[BZ+ Glc-H <sub>2</sub> O+H] <sup>+</sup> 319.1181[M+NA-BZ-Glc-CO <sub>2</sub> ] <sup>+</sup> 301.1076[M+H-BZ-Glc] <sup>+</sup> 267.0871[BZ+ Glc-H <sub>2</sub> O+H] <sup>+</sup> 249.0764[BZ+Glc-2H <sub>2</sub> O+H] <sup>+</sup>	Isobenzoylpaconiflorin
75	7.626	C <sub>44</sub> H <sub>64</sub> O <sub>18</sub>	879.4022(0.9)	351.0559[2GlcA-H] <sup>-</sup>		705.3859[M+H-GlcA] <sup>+</sup> 511.3423[M+H-2GlcA-H <sub>2</sub> O] <sup>+</sup> 451.3203[M+H-2GlcA-H <sub>2</sub> O-AceOH] <sup>+</sup>	22-Acetoxyglycyrrhizin
76	7.854	C <sub>42</sub> H <sub>62</sub> O <sub>17</sub>	837.3898(-1.3)	661.3580[M-H-GlcA] <sup>-</sup> 351.0556[2GlcA-H] <sup>-</sup>	839.4050(-1.8)	663.3726[M+H-GlcA] <sup>+</sup> 469.3322[M +H-2GlcA-H <sub>2</sub> O] <sup>+</sup>	Isolicorice saponin G2
77	7.969	C <sub>42</sub> H <sub>62</sub> O <sub>17</sub>	837.3915(0.7)	351.0585[M-H-2GlcA] <sup>-</sup>	839.4075(1.2)	663.3738[M+H-GlcA] <sup>+</sup> , 487.3447[M+H-2GlcA] <sup>+</sup> , 469.3324[M+H-2GlcA-H <sub>2</sub> O] <sup>+</sup>	Yunganoside K2
78	8.003	C <sub>48</sub> H <sub>74</sub> O <sub>20</sub>	969.4692(-0.3)	823.4121[M-H-Rha] <sup>-</sup>  497.1143[2GlcA+Rha-H] <sup>-</sup>		825.4094[M+H-Rha] <sup>+</sup>  795.4512[M+H-GlcA] <sup>+</sup>	3-o-[β-D-rhamnose]-24-hydroxyl-glycyrrhizic acid
79	8.224	C <sub>15</sub> H <sub>12</sub> O <sub>4</sub>	255.0673(1.6)	135.0092[M-H-VP] <sup>-</sup> 119.0509[VP-H] <sup>-</sup>		147.0465[M+H-RL] <sup>+</sup> 137.0249[M+H-VP] <sup>+</sup>	Isoliquiritigenin
80	8.500	C <sub>42</sub> H <sub>62</sub> O <sub>17</sub>	837.3906(-0.4)	819.3802[M-H-H <sub>2</sub> O] <sup>-</sup> 775.3896[M-H-H <sub>2</sub> O-CO <sub>2</sub> ] <sup>-</sup> 351.0566[2GlcA-H] <sup>-</sup>	839.4058(-0.8)	663.3759[M+H-GlcA] <sup>+</sup> 487.3425[M+H-2GlcA] <sup>+</sup> 469.3321[M+H-2GlcA-H <sub>2</sub> O] <sup>+</sup> 451.3215[M+H-2GlcA-2H <sub>2</sub> O] <sup>+</sup>	Licorice saponin G2
81	8.586	C <sub>16</sub> H <sub>12</sub> O <sub>4</sub>	266.0667(2.7)	252.0426[M-H-CH <sub>3</sub> ] <sup>-</sup>	269.0826(4.5)	237.0558[M+H-CH <sub>3</sub> OH] <sup>+</sup>	Formononetin

				224.0464[M-H-CH <sub>3</sub> -CO] <sup>-</sup>		226.0627[M+H-CH <sub>3</sub> -CO] <sup>+</sup>	
				223.0409[M-H-CH <sub>3</sub> -CHO] <sup>-</sup>			
				-			
82	8.683	C <sub>48</sub> H <sub>72</sub> O <sub>20</sub>	967.4517(-2.3)	351.0561[2GlcA-H] <sup>-</sup>		823.4158[M+H-Rha] <sup>+</sup>	Rhaoglycyrrhizin
						647.3723[M+H-Rha-GlcA] <sup>+</sup>	
						471.3460[M+H-Rha-2GlcA] <sup>+</sup>	
						453.3364[M+H-Rha-2GlcA-H <sub>2</sub> O] <sup>+</sup>	
83	8.718	C <sub>42</sub> H <sub>62</sub> O <sub>17</sub>	837.3906(-0.4)	661.3574[M-H]-GlcA] <sup>-</sup>		663.3690[M+H- GlcA] <sup>+</sup>	Macedonoside B
				351.0569[2GlcA-H] <sup>-</sup>		487.3421[M+H-2GlcA] <sup>+</sup>	
						469.3312[M+H-2GlcA-H <sub>2</sub> O] <sup>+</sup>	
84	8.751	C <sub>42</sub> H <sub>62</sub> O <sub>16</sub>		351.0578[2GlcA-H] <sup>-</sup>	823.4081(-4.3)	647.3756[M+H-GlcA] <sup>+</sup>	Licorice saponin H2
						471.3464[M+H-2GlcA] <sup>+</sup>	
						453.3356[M+H-2GlcA-H <sub>2</sub> O] <sup>+</sup>	
85	8.786	C <sub>44</sub> H <sub>64</sub> O <sub>17</sub>	863.4056(-1.0)	583.1813[M-H-GlcA-Ace OH-CO <sub>2</sub> ] <sup>-</sup>	865.4239(2.0)	689.3988[M+H-GlcA] <sup>+</sup>	22-Acetoxy glycyrrhaldehyde
				351.0557[2GlcA-H] <sup>-</sup>		495.3459[M+H-2GlcA-H <sub>2</sub> O] <sup>+</sup>	
86	9.015	C <sub>42</sub> H <sub>62</sub> O <sub>16</sub>	821.3946(-1.7)	645.3725[M-H-GlcA] <sup>-</sup>	823.4142(3.2)	647.3801[M+H-GlcA] <sup>+</sup>	Glycyrrhizin
				351.0559[2GlcA-H] <sup>-</sup>		453.3367[M+H-2GlcA-H <sub>2</sub> O] <sup>+</sup>	
						471.3483[M+H-2GlcA] <sup>+</sup>	
87	9.215	C <sub>25</sub> H <sub>32</sub> O <sub>9</sub>	475.1971(0.6)	415.1762[M-H-AceOH] <sup>-</sup>	499.1912[M+Na] <sup>+</sup>	417.1903[M+H-AceOH] <sup>+</sup>	3,5-Diacetoxy-1-(4-hydroxy-3-met hoxyphenyl)-7-(3,4-dihydroxy-5- methoxyphenyl)heptane
				355.1543[M-H-2AceOH] <sup>-</sup>		357.1695[M+H-2AceOH] <sup>+</sup>	
				295.1696[M-H-PE] <sup>-</sup>			
88	9.629	C <sub>42</sub> H <sub>64</sub> O <sub>15</sub>	807.4144(-2.8)	631.3853[M-H-GlcA] <sup>-</sup>	809.4285(-4.6)	633.3987[M+H-GlcA] <sup>+</sup> ,	22-dehydroxyl uralsaponinC

						457.3666[M+H-2GlcA] <sup>+</sup> 439.3572[M+H-2GlcA-H <sub>2</sub> O] <sup>+</sup> 421.3664[M+H-2GlcA-2H <sub>2</sub> O] +	
89	9.661	C <sub>42</sub> H <sub>62</sub> O <sub>16</sub>	821.3950(-1.2)	351.0552[2GlcA-H] <sup>-</sup>	823.4147(3.7)	647.3833[M+H-GlcA] <sup>+</sup> 471.3437[M+H-2GlcA] <sup>+</sup> 453.3353[M+H-2GlcA-H <sub>2</sub> O] <sup>+</sup>	18α-glycyrrhizin
90	9.895	C <sub>21</sub> H <sub>22</sub> O <sub>5</sub>	353.1382(-2.0)	338.1149[M-CH <sub>3</sub> -H] <sup>-</sup> 295.0597[M-H-2CH <sub>3</sub> -CO] <sup>-</sup>	355.1537(-2.3)	299.0947[M+H-BT] <sup>+</sup> 189.0934[M-H-MVD] <sup>+</sup>	Licoagrochalcone D
91	9.924	C <sub>42</sub> H <sub>62</sub> O <sub>16</sub>	821.3934(-3.2)	351.0574[2GlcA-H] <sup>-</sup>	823.4133(2.1)	647.3770[M+H-GlcA] <sup>+</sup> 471.3464[M+H-2GlcA] <sup>+</sup> 453.3368[M+H-2GlcA-H <sub>2</sub> O] <sup>+</sup>	UralsaponinB
92	9.930	C <sub>41</sub> H <sub>62</sub> O <sub>14</sub>	777.4058(-0.4)	627.3535[M-H-Arab-H <sub>2</sub> O] <sup>-</sup> 449.1499[M-H-Arab-GlcA-H <sub>2</sub> O] <sup>-</sup>		647.3787[M+H-Arab] <sup>+</sup> 453.3366[M+H-Arab-GlcA-H <sub>2</sub> O] <sup>+</sup>	Araboglycyrrhizin
93	10.021	C <sub>20</sub> H <sub>16</sub> O <sub>6</sub>	351.0879(2.8)	283.0987[M-H-PA] <sup>-</sup>	353.1031(1.7)	335.0930[M+H-H <sub>2</sub> O] <sup>+</sup> 311.0569[M+H-PP] <sup>+</sup>	LicoisoflavoneB/SemilicoisoflavoneB/allolicoisoflavone B
94	10.247	C <sub>20</sub> H <sub>18</sub> O <sub>6</sub>	353.1024(-0.3)	297.0398[M-H-BT] <sup>-</sup>	355.1187(1.4)	299.0583[M+H-BT] <sup>+</sup>	Licoflavonol or its isomer
95	10.324	C <sub>20</sub> H <sub>20</sub> O <sub>6</sub>	355.1185(0.8)	337.1077[M-H-H <sub>2</sub> O] <sup>-</sup> 293.0453[M-H-CO-2OH] <sup>-</sup> 281.0457[M-H-H <sub>2</sub> O-BT] <sup>-</sup> 229.0868[M-H-BE] <sup>-</sup> 125.0241[BE-H] <sup>-</sup>		339.1212[M+H-H <sub>2</sub> O] <sup>+</sup> 283.0604[M+H-H <sub>2</sub> O-BT] <sup>+</sup> 301.0708[M+H-BT] <sup>+</sup>	Uralenin
96	10.410	C <sub>21</sub> H <sub>20</sub> O <sub>6</sub>	367.1173(-2.5)	339.1223[M-H-CO] <sup>-</sup> 333.0754[M-H-2OH] <sup>-</sup>	369.1342(1.1)	335.0929[M+H-2OH] <sup>+</sup> 313.0712[M+H-BT] <sup>+</sup>	Glycyrrhisoflavanone

				309.0397[M-H-CO-2CH <sub>3</sub> ] <sup>-</sup>				
				297.0398[M-H-PI] <sup>-</sup>				
97	10.483	C <sub>21</sub> H <sub>20</sub> O <sub>6</sub>	367.1192(2.7)	337.1081[M-H-CH <sub>2</sub> O] <sup>-</sup> , 309.0408[M-H-CH <sub>2</sub> O-CO] <sup>-</sup>	369.1342(1.1)	313.0718[M+H-IB] <sup>+</sup> , 285.0764[M+H-BT-CO] <sup>+</sup> , 269.0478[M+H-BT-CO-CH <sub>4</sub> ] <sup>+</sup>	Glycycomarin	
98	10.623	C <sub>21</sub> H <sub>24</sub> O <sub>5</sub>	355.1549(1.1)	321.1107[M-H-2OH] <sup>-</sup> 323.1283[M-H-CH <sub>4</sub> O] <sup>-</sup> 337.1086[M-H-H <sub>2</sub> O] <sup>-</sup>	357.1712(2.8)	301.1091[M+H-BT] <sup>+</sup> ; 321.1140[M+H-2H <sub>2</sub> O] <sup>+</sup> 313.1096[M+H-CO <sub>2</sub> ] <sup>+</sup>	Glyasperins C	
99	10.777	C <sub>20</sub> H <sub>18</sub> O <sub>6</sub>	353.1022(-0.8)	297.0396[M-H-BT] <sup>-</sup> 269.0458[M-H-BT-CO] <sup>-</sup>	355.1190(2.3)	299.0564[M+H-BT] <sup>+</sup> , 287.0574[M+H-IP] <sup>+</sup>	Licoflavonol or its isomer	
100	11.022	C <sub>20</sub> H <sub>18</sub> O <sub>6</sub>	353.1020(-1.4)	309.1120[M-H-CO <sub>2</sub> ] <sup>-</sup> 285.1125[M-H-IP] <sup>-</sup>	355.1194(3.4)	340.0794[M+H-CH <sub>3</sub> ] <sup>+</sup> 299.0556[M+H-BT] <sup>+</sup>	Licoflavonol or its isomer	
101	11.090	C <sub>20</sub> H <sub>18</sub> O <sub>6</sub>	353.1025(0.0)	307.0964[M-H-CO-H <sub>2</sub> O] <sup>-</sup> 227.0707[M-H-BE] <sup>-</sup> 125.0239[BE-H] <sup>-</sup>	355.1183(0.3)	337.1064[M+H-H <sub>2</sub> O] <sup>+</sup> 179.0342[M+H-DCO] <sup>+</sup>	Licoisoflavanone	
102	11.165	C <sub>20</sub> H <sub>18</sub> O <sub>6</sub>	353.1027(0.6)	325.1858[M-H-CO] <sup>-</sup>	355.1190(2.3)	299.0558[M+H-BT] <sup>+</sup> 327.1252[M+H-CO] <sup>+</sup>	Licoflavonol or its isomer	
103	11.248	C <sub>21</sub> H <sub>22</sub> O <sub>4</sub>	337.1447(2.1)	281.0833[M-H-2CH <sub>3</sub> -C <sub>2</sub> H <sub>2</sub> ] <sup>-</sup> 187.0768[M-H-2CH <sub>3</sub> -OCD] <sup>-</sup>	339.1600(1.2)	271.0978[M+H-IP] <sup>+</sup> 245.1198[M+H-PH] <sup>+</sup>	Licochalcone A	
104	11.353	C <sub>21</sub> H <sub>18</sub> O <sub>6</sub>	365.1023(-0.5)	337.1076[M-H-CO] <sup>-</sup> 307.0236[M-H-CO-2CH <sub>3</sub> ] <sup>-</sup>	367.1172(-2.7)	121.0299[M+H-MMEV] <sup>+</sup> 339.1227[M+H-CO] <sup>+</sup> 323.0545[M+H-CO <sub>2</sub> ] <sup>+</sup> 311.0550[M+H-2CO] <sup>+</sup> 283.0602[M+H-3CO] <sup>+</sup>	Isoglycyrol	

105	11.370	C <sub>25</sub> H <sub>26</sub> O <sub>7</sub>	437.1595(-1.1)	381.1332[M-H-BT] <sup>-</sup> 337.1071[M-H-MPEO] <sup>-</sup> 307.0240[M-H-MPEO-2C H <sub>3</sub> ] <sup>-</sup>	439.1745(-2.7)	383.1125[M+H-BT] <sup>+</sup>	Kanzonol T
106	11.816	C <sub>20</sub> H <sub>16</sub> O <sub>5</sub>	335.0922(0.9)	320.0675[M-H-CH <sub>3</sub> ] <sup>-</sup> 305.0450[M-H-2CH <sub>3</sub> ] <sup>-</sup> 291.1021[M-H-CHO-CH <sub>3</sub> ] <sup>-</sup>	337.1076(0.0)	319.0964[M+H-H <sub>2</sub> O] <sup>+</sup> 295.0607[M+H-PP] <sup>+</sup>	Glabrone
107	11.850	C <sub>12</sub> H <sub>14</sub> O <sub>2</sub>			191.1074(1.0)	173.0964[M+H-H <sub>2</sub> O] <sup>+</sup> 145.1011[M+H-HCOOH] <sup>+</sup> 117.0699[M+H-HCOOH-C <sub>2</sub> H 4] <sup>+</sup>	Z-/E-ligustilide
108	12.016	C <sub>20</sub> H <sub>18</sub> O <sub>6</sub>	353.1023(-0.6)	323.1281[M-H-2CH <sub>3</sub> ] <sup>-</sup> 269.0445[M-H-2DO] <sup>-</sup> 241.0493[M-H-2DO-CO] <sup>-</sup>	355.1195(3.7)	299.0556[M+H-BT] <sup>+</sup>	Glyasperin F
109	12.314	C <sub>20</sub> H <sub>16</sub> O <sub>6</sub>	351.0872(0.9)	336.0628[M-H-CH <sub>3</sub> ] <sup>-</sup> 307.0968[M-H-CO <sub>2</sub> ] <sup>-</sup> 283.0972[M-H-PA] <sup>-</sup> 241.0862[M-H-RL] <sup>-</sup>	353.1026(0.3)	335.0917[M+H-H <sub>2</sub> O] <sup>+</sup> 311.0558[M+H-PP] <sup>+</sup> 299.0558[M+H-3H <sub>2</sub> O] <sup>+</sup> 283.0614[M+H-PI] <sup>+</sup>	Demethylglycyrol
110	12.765	C <sub>20</sub> H <sub>16</sub> O <sub>5</sub>	335.0915(-1.2)	317.0812[M-H-H <sub>2</sub> O] <sup>-</sup> 305.0452[M-H-2CH <sub>3</sub> ] <sup>-</sup> 291.0655[M-H-CO <sub>2</sub> ] <sup>-</sup>	337.1074(-0.6)	295.0581[M+H-PP] <sup>+</sup>	Isoglabrone
111	12.879	C <sub>25</sub> H <sub>28</sub> O <sub>4</sub>	391.1915(1.5)	203.0716[M-H-MBV] <sup>-</sup> 187.1129[MBV-H] <sup>-</sup> 132.0577[MBV-BT-H] <sup>-</sup>	393.2063(-0.8)	337.1436[M+H-BT] <sup>+</sup>	Glabrol
112	13.280	C <sub>22</sub> H <sub>26</sub> O <sub>5</sub>	369.1704(0.5)	339.1235[M-H-CH <sub>2</sub> O] <sup>-</sup> 311.0923[M-H-CH <sub>2</sub> O-CO] <sup>-</sup>	371.1841(-4.6)	315.1224[M+H-BT] <sup>+</sup> 235.1329[M+H-MLT] <sup>+</sup>	Glyasperins D



				279.0654[M-H-CH <sub>2</sub> O-CO-CH <sub>3</sub> OH] <sup>-</sup>			
				135.0449[M-H-DOT] <sup>-</sup>			
113	13.394	C <sub>25</sub> H <sub>28</sub> O <sub>6</sub>	423.1821(3.1)	367.1166[M-H-BT] <sup>-</sup>		369.1359[M+H-BT] <sup>+</sup>	Glyinflanin F
				229.0867[M-H-BF] <sup>-</sup>		365.1031[M+H-ISP] <sup>+</sup>	
				193.0867[BF-H] <sup>-</sup>		351.1235[M+H-ISD] <sup>+</sup>	
						221.1181[M+H-APP] <sup>+</sup>	
						191.1073[M+H-APP-2CH <sub>3</sub> ] <sup>+</sup>	
114	13.577	C <sub>25</sub> H <sub>28</sub> O <sub>5</sub>	407.1862(1.0)	337.1442[M-H-PI] <sup>-</sup>	409.2012(-0.7)	353.1389[M+H-BT] <sup>+</sup>	Glycyrdione A
				219.0658[M-H-HMDB] <sup>-</sup>		191.1072[HMBB+H] <sup>+</sup>	
				187.1122[HMDB-H] <sup>-</sup>			
115	13.708	C <sub>25</sub> H <sub>26</sub> O <sub>6</sub>	421.1647(-0.9)	352.0945[M-H-C <sub>3</sub> H <sub>9</sub> ] <sup>-</sup>	423.1805(-0.7)	367.1177[M+H-BT] <sup>+</sup>	6,8-diprenylorobol
				309.0397[M-H-4CO] <sup>-</sup>		311.0555[M+H-2BT] <sup>+</sup>	
						261.1852[M+H-DCE] <sup>+</sup>	
						163.0756[DCE+H] <sup>+</sup>	
116	13.743	C <sub>24</sub> H <sub>28</sub> O <sub>4</sub>			381.2065(-0.3)	335.2004[M+H-H <sub>2</sub> O-CO] <sup>+</sup>	Senkyunolide O or its isomer
						191.1071[M+H]-ZBD] <sup>+</sup>	
						173.0963[M+H-ZBD-H <sub>2</sub> O] <sup>+</sup>	
						145.1013[M+H-ZBD-HCOO H] <sup>+</sup>	
117	13.908	C <sub>25</sub> H <sub>28</sub> O <sub>6</sub>	423.1799(-2.1)	299.0861[M-H-MBT] <sup>-</sup>	425.1959(-1.2)	369.1337[M+H-BT] <sup>+</sup>	GancaoninE/ 3'-(γ,γ-dimethylallyl)-kievitone
				193.0862[MBT-H] <sup>-</sup>		191.1073[M+H-DMP] <sup>+</sup>	
						135.0443[M+H-DMP-BT] <sup>+</sup>	
118	14.040	C <sub>25</sub> H <sub>26</sub> O <sub>6</sub>	421.1646(-1.2)	309.0398[M-H-2BT] <sup>-</sup>	423.1812(0.9)	367.1180[M+H-BT] <sup>+</sup>	Glyurallin B/Isoangustone A /Angustone A

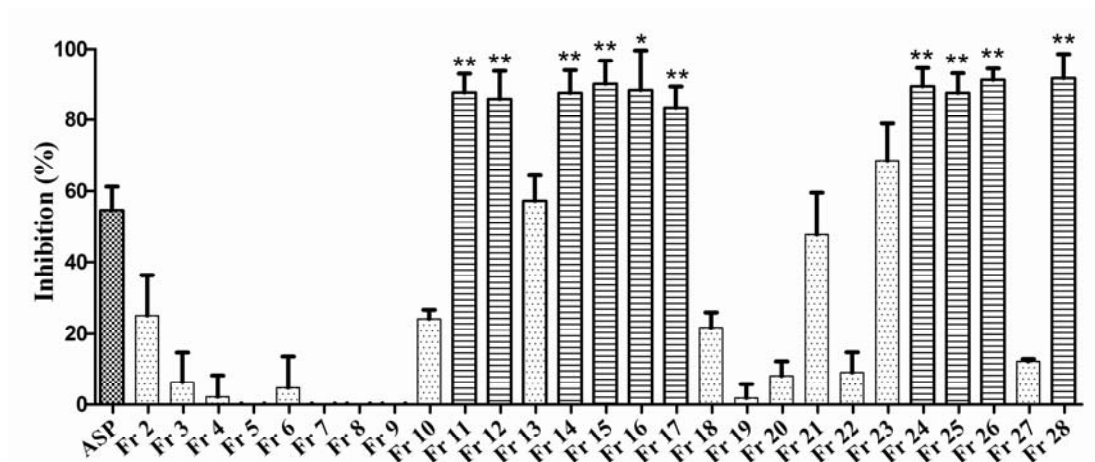
						311.0553[M+H-2BT] <sup>+</sup>	
						283.0581[M+H-2BT-CO] <sup>+</sup>	
						255.0659[M+H-2BT-2CO] <sup>+</sup>	
119	14.537	C <sub>30</sub> H <sub>46</sub> O <sub>4</sub>	469.3306(-2.6)	425.3416[M-H-CO <sub>2</sub> ] <sup>-</sup>	471.3479(1.1)	453.3398[M+H-H <sub>2</sub> O] <sup>+</sup>	Glycyrrhetic acid
				355.2609[M-H-CO <sub>2</sub> -ME] <sup>-</sup>		425.2890[M+H-HCOOH] <sup>+</sup>	
						407.2775[M+H-HCOOH-H <sub>2</sub> O] <sup>+</sup>	
120	14.606	C <sub>25</sub> H <sub>26</sub> O <sub>6</sub>	421.1646(-1.2)	193.0862[MBT-H] <sup>-</sup>			Glyurallin B/Isoangustone A /Angustone A
121	14.634	C <sub>24</sub> H <sub>28</sub> O <sub>4</sub>			381.2062(-1.0)	363.1953[M+H-H <sub>2</sub> O] <sup>+</sup>	Tokinolide B or its isomer
						335.2003[M+H-H <sub>2</sub> O-CO] <sup>+</sup>	
						191.1071[M+H-ZBD] <sup>+</sup>	
						173.0966[M+H-ZBD-H <sub>2</sub> O] <sup>+</sup>	
122	14.852	C <sub>24</sub> H <sub>28</sub> O <sub>4</sub>			381.2070(1.0)	363.1960[M+H-H <sub>2</sub> O] <sup>+</sup>	Levistolide A
						335.2015[M+H-H <sub>2</sub> O-CO] <sup>+</sup>	
						191.1076[M+H-ZBD] <sup>+</sup>	
						173.0966[M+H-ZBD-H <sub>2</sub> O] <sup>+</sup>	
123	14.966	C <sub>24</sub> H <sub>28</sub> O <sub>4</sub>			381.2063(-0.8)	363.1958[M+H-H <sub>2</sub> O] <sup>+</sup>	Angelicide or its isomer
						335.2008[M+H-H <sub>2</sub> O-CO] <sup>+</sup>	
						191.1082[M+H-ZBD] <sup>+</sup>	
						173.0966[M+H-ZBD-H <sub>2</sub> O] <sup>+</sup>	
124	15.052	C <sub>24</sub> H <sub>28</sub> O <sub>4</sub>			381.2068(0.5)	363.1956[M+H-H <sub>2</sub> O] <sup>+</sup>	Z,Z'-6.8',7.3'-Diligustilide or its isomer
						191.1077[M+H-ZBD] <sup>+</sup>	
						173.0965[M+H-ZBD-H <sub>2</sub> O] <sup>+</sup>	
125	15.481	C <sub>24</sub> H <sub>28</sub> O <sub>4</sub>			381.2057(-2.4)	191.1071[M+H-ZBD] <sup>+</sup>	Z-Ligustilide dimer E-232 or its

							isomer
126	15.601	C <sub>39</sub> H <sub>54</sub> O <sub>6</sub>	617.3837(-0.8)	573.3922[M-H-CO <sub>2</sub> ] <sup>-</sup> 453.3256[M-H-HDPA] <sup>-</sup>	619.3985(-2.3)	173.0959[M+H-ZBD-H <sub>2</sub> O] <sup>+</sup> 601.3856[M+H-H <sub>2</sub> O] <sup>+</sup> 455.3493[M+H-HDPA] <sup>+</sup> 437.3414[M+H-HDPA-H <sub>2</sub> O] <sup>+</sup>	p-Coumaroyl maslinic acid
127	15.681	C <sub>24</sub> H <sub>28</sub> O <sub>4</sub>			381.2047(-5.0)	363.1944[M+H-H <sub>2</sub> O] <sup>+</sup> 191.1069[M+H-ZBD] <sup>+</sup> 173.0961[M+H-ZBD-H <sub>2</sub> O] <sup>+</sup> 145.1018[M+H-ZBD-HCOO H] <sup>+</sup>	Neodiligustilide or its isomer
128	15.932	C <sub>25</sub> H <sub>24</sub> O <sub>6</sub>	419.1495(0.0)	404.1255[M-H-CH <sub>3</sub> ] <sup>-</sup> 375.1601[M-H-CO <sub>2</sub> ] <sup>-</sup> 219.0655[M-H-EDC] <sup>-</sup> 199.0754[EDC-H] <sup>-</sup>		403.1885[M+H-H <sub>2</sub> O] <sup>+</sup> 365.1022[M+H-BT] <sup>+</sup> 347.0907[M+H-BT-H <sub>2</sub> O] <sup>+</sup>	gancaonin H
129	16.098	C <sub>24</sub> H <sub>28</sub> O <sub>4</sub>			381.2064(-0.5)	363.1938[M+H-H <sub>2</sub> O] <sup>+</sup>  335.2002[M+H-H <sub>2</sub> O-CO] <sup>+</sup> 191.1073[M+H-ZBD] <sup>+</sup> 173.0967[M+H-ZBD-H <sub>2</sub> O] <sup>+</sup>	Z,Z'-3.3',8.8'-Diligustilide or its isomer
130	16.195	C <sub>24</sub> H <sub>28</sub> O <sub>4</sub>			381.2068(0.5)	191.1067[M+H-ZBD] <sup>+</sup>  173.0962[M+H-ZBD-H <sub>2</sub> O] <sup>+</sup> 145.1012[M+H-ZBD-HCOO H] <sup>+</sup>	E,E'-3.3', 8.8'-Diligustilide or its isomer
131	16.292	C <sub>24</sub> H <sub>28</sub> O <sub>4</sub>			381.2062(-1.0)	363.1955[M+H-H <sub>2</sub> O] <sup>+</sup>	E,E'-3.8', 8.3'-Isodiligustilide or its isomer

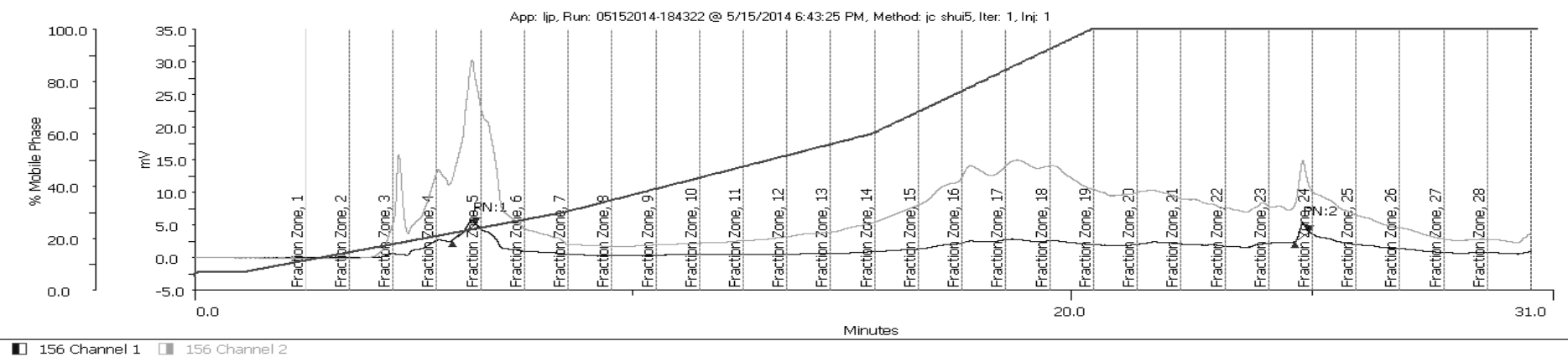
132	17.390	C <sub>24</sub> H <sub>28</sub> O <sub>4</sub>	381.2059(-1.8)	335.2032[M+H-H <sub>2</sub> O-CO] <sup>+</sup> 191.1073[M+H-ZBD] <sup>+</sup> 173.0963[M+H-ZBD-H <sub>2</sub> O] <sup>+</sup> 363.1923[M+H-H <sub>2</sub> O] <sup>+</sup>	3,3'Z-6.7',7.6'-Diligustilide or its isomer
133	17.521	C <sub>24</sub> H <sub>28</sub> O <sub>4</sub>	381.2062(-1.0)	335.2007[M+H-H <sub>2</sub> O-CO] <sup>+</sup> 191.1071[M+H-ZBD] <sup>+</sup> 173.0965[M+H-ZBD-H <sub>2</sub> O] <sup>+</sup> 363.1971[M+H-H <sub>2</sub> O] <sup>+</sup>	3α.7'α,7α.3'α-Diligustilide or its isomer
134	17.784	C <sub>24</sub> H <sub>28</sub> O <sub>4</sub>	381.2063(-0.8)	335.1998[M+H-H <sub>2</sub> O-CO] <sup>+</sup> 191.1070[M+H-ZBD] <sup>+</sup> 173.0964[M+H-ZBD-H <sub>2</sub> O] <sup>+</sup> 363.1975[M+H-H <sub>2</sub> O] <sup>+</sup>  335.2022[M+H-H <sub>2</sub> O-CO] <sup>+</sup> 191.1069[M+H-ZBD] <sup>+</sup> 173.0958[M+H-ZBD-H <sub>2</sub> O] <sup>+</sup>	(3')-(3R, 8S, 3'aR, 6'S)-3.3a', 8.6'-Biligustilide or its isomer

Glc: Glucose, ADE: Adenine, HDTDO: (1aS,1bS,3S,5aR,6aS)-3-hydroxytetrahydro-5H-oxireno[2',3':4,5]furo[3,2-d][1,3,2]dioxaphosphinine 3-oxide, DTFD: (4aR,7S,7aS)-2,7-dihydroxytetrahydro-4H-furo[3,2-d][1,3,2]dioxaphosphinin-6-ide 2-oxide, GA: Gallic acid, BZ: Benzoic Acid, 4-OH-BZ: 4-hydroxyl-benzoic acid, 2-OH-BZ: 2-hydroxyl-benzoic acid, HB: 4-hydroxy-3-methoxybenzoic acid, VP: 4-vinylphenol, Api:apiose, MB: methyl benzoate, MG: ((2R,3S,4R,5S)-3,4,5-trihydroxytetrahydro-6H-pyran-2-yl)methyl 3,4,5-trihydroxybenzoate, Arab: Arabinose, BH:2-o-Benzaldehyde, RL:resorcinol, HM: 3-hydroxy-3-methylglutaroyl, Rha: rhamnose, PC: P-coumaroyl, GlcA: glucuronic acid, PM:2-methoxy-coumaroyl, PE: 3-methoxy-5-(3H-propyl)benzene-1,2-diol, BT: isobutylene, MVD: 3-methoxy-4-vinylbenzene-1,2-diol, PP: propylene, PA: 3-methylbuta-1,2-diene, BE: benzene-1,3,5-triol, PI: pentanol-iosprene, IP: isoprene, DCO: 2,2-dimethyl-2H-chromen-5-ol, OCD: 4-oxomethylidenecyclohexa-2,5-dienone, PH: phenol, MMEV: 5-methoxy-2-(2-methylbut-3-en-2-yl)-4-vinylphenol, MPEO:

2-methylpent-4-en-2-ol, PP: propylene, 2DO:2,2-dimethyl-2H-oxete, MBV: 2-(3-methylbut-2-en-1-yl)-4-vinylphenol, DOT: 2,4-dimethoxy-3-(3-methylbut-2-en-1-yl)-7-oxabicyclo[4.2.0]octa-1,3,5-triene, MLT: 4-vinylbenzene-1,3-diol, BF: 2-(2-hydroxypropan-2-yl)-2,3-dihydrobenzofuran-6-ol, APP: 1-(4-hydroxy-3-(3-methylbut-2-en-1-yl)phenyl)ethan-1-one, ISD: 2-methylpropan-2-ol, ISP: propan-2-ol, HMDB:4-hydroxy-3-(3-methylbuta-1,2-dien-1-yl)benzaldehyde, HMBB:4-hydroxy-3-(3-methylbut-2-en-1-yl)benzaldehyde, DCE: 2-(3,4-dihydroxyphenyl)cycloprop-2-en-1-one, ZBD: (Z)-3-butylidene-4,5-dihydroisobenzofuran-1(3H)-one, DMP: 2-(2,4-dihydroxy-3-(3-methylbut-2-en-1-yl)phenyl)propanal, MBT: 2-(3-methylbut-2-en-1-yl)benzene-1,3,5-triol, ME:3-methylbut-1-ene, HDPA: (E)-3-(4-hydroxyphenyl)acrylic acid, EDC: 6-ethynyl-2,2-dimethyl-2H-chromen-8-ol



Supplementary Figure S1. The anti-platelet effects of the fractions from DJF. Significant difference with respect to aspirin (ASP): \*,  $p < 0.05$ ; \*\*,  $p < 0.01$ .



Supplementary Figure S2. The preparative chromatogram of DJF extractions.

Supplementary Table S2. The potential target proteins in the DT network.

Protein name	Uniprot ID
Thrombin	P00734
Thromboxane A2 receptor	P21731
Proteinase-activated receptor 1	P25116
Proteinase-activated receptor 4	Q96RI0
P2Y purinoceptor 1	P47900
P2Y purinoceptor 12	Q9H244
Prostacyclin receptor	P43119
Cytosolic phospholipase A2	P47712
Guanine nucleotide-binding protein G(q) subunit a	P50148
Guanine nucleotide-binding protein G(s) subunit a	P63092
Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit a	P42336
Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit b	P42338
Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit g	P48736
Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit d	O00329
Phosphatidylinositol 3-kinase regulatory subunit a	P27986
Phosphatidylinositol 3-kinase regulatory subunit b	O00459
Phosphatidylinositol 3-kinase regulatory subunit g	Q92569
Phosphatidylinositol 3-kinase regulatory subunit 5	Q8WYR1
1-phosphatidylinositol 4,5-bisphosphate phosphodiesterase b-1	Q9NQ66
1-phosphatidylinositol 4,5-bisphosphate phosphodiesterase b-2	Q00722
1-phosphatidylinositol 4,5-bisphosphate phosphodiesterase b-3	Q01970
1-phosphatidylinositol 4,5-bisphosphate phosphodiesterase b-4	Q15147
Adenylate cyclase type 1	Q08828
Adenylate cyclase type 2	Q08462
Adenylate cyclase type 3	O60266
Adenylate cyclase type 4	Q8NFM4
Adenylate cyclase type 5	O95622
Adenylate cyclase type 6	O43306
Adenylate cyclase type 7	P51828
Adenylate cyclase type 8	P40145
Adenylate cyclase type 9	O60503
Lymphocyte cytosolic protein 2	Q13094
1-phosphatidylinositol 4,5-bisphosphate phosphodiesterase g-2	P16885
Tyrosine-protein kinase BTK	Q06187
Prostaglandin G/H synthase 1 (COX-1)	P23219
Protein kinase C	P41743
RAS guanyl-releasing protein 1	O95267
RAS guanyl-releasing protein 2	Q7LDG7
cAMP-dependent protein kinase catalytic subunit a	P17612
Thromboxane-A synthase	P24557
Ras-related protein Rap-1A	P62834
Ras-related protein Rap-1b	P61224
Vasodilator-stimulated phosphoprotein	P50552
Amyloid b A4 precursor protein-binding family B member 1-interacting protein	Q7Z5R6
Actin, cytoplasmic 1	P60709
Fermitin family homolog 3	Q86UX7
Talin-1	Q9Y490
Talin-2	Q9Y4G6
Integrin a-IIb	P08514
Integrin b-3	P05106
Fibrinogen a chain	P02671
Fibrinogen b chain	P02675

Fibrinogen g chain	P02679
Guanine nucleotide-binding protein G(i) subunit a-1	P63096
Synaptosomal-associated protein 23	O00161
Vesicle-associated membrane protein 8	Q9BV40

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Supplementary Table S3. The elution condition for DJF fractionating

Time (min)	A%	B%
0	95	5
8	70	30
15	40	60
20	0	100
30	0	100

Supplementary Table S4. The elution condition for ingredient identification

Time(min)	A%	B%
0	95	5
20	5	95
22	5	95

Supplementary Table S5. The elution condition for the plasma concentration testing

Time (min)	A%	B%
0	95	5
3	85	15
8	75	25
36	5	95
37	0	100
40	0	100



Supplementary Table S6. The composition of the Tris buffer solution.

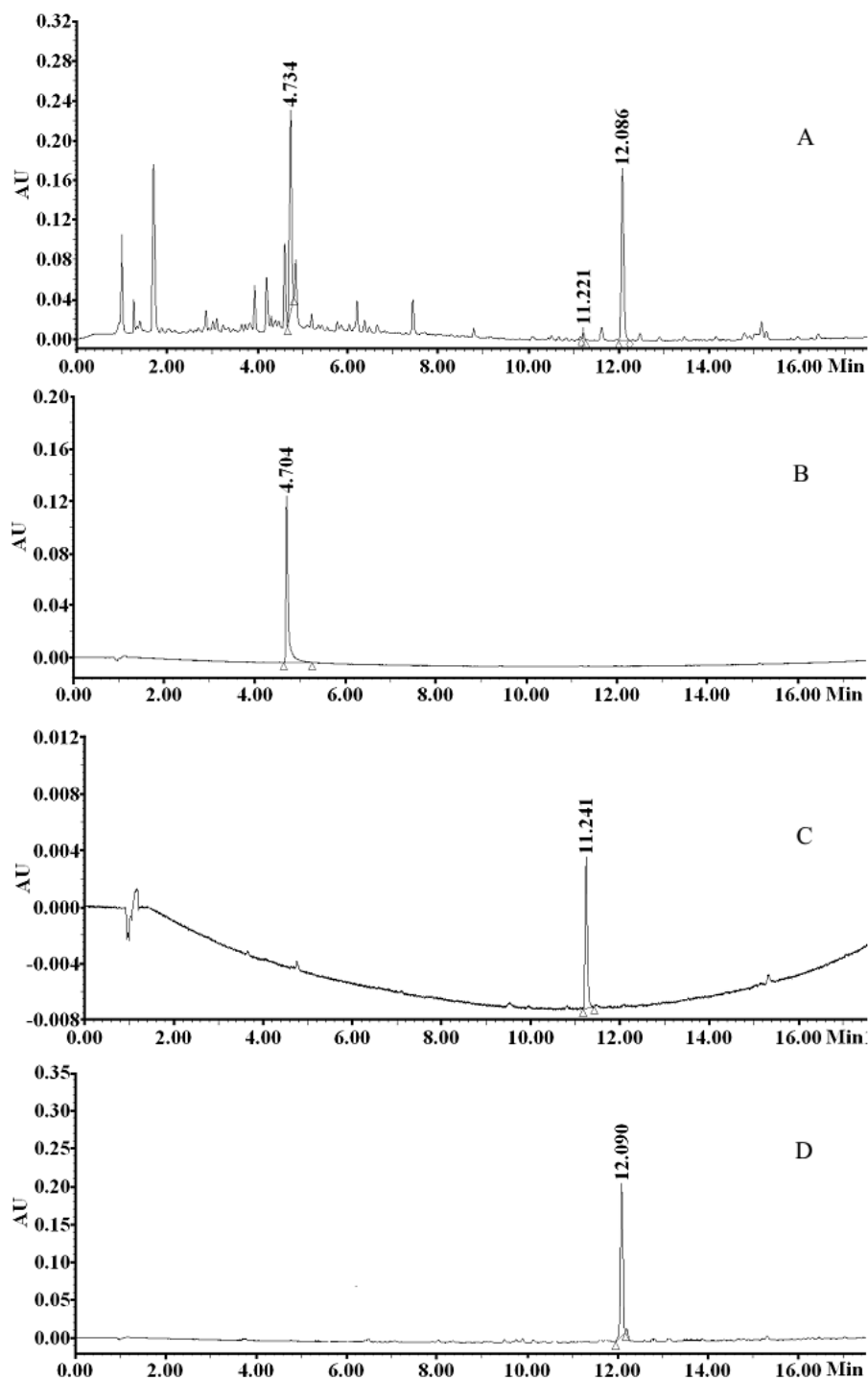
Chemicals	Concentration (mM)	Weight (g)
NaCl	130	3.042
Sodium citrate	10	1.1764
NaHCO <sub>3</sub>	9	0.3024
Glucose	6	0.432
MgCl <sub>2</sub>	0.9	0.0342
KH <sub>2</sub> PO <sub>4</sub>	0.81	0.04406
Tris-base	10	0.4844

Supplementary Table S7. The composition of the ACD solution.

Chemicals	Concentration (mM)	Weight (g)
Sodium citrate	75	0.882
Glucose	124	0.893
Citrate acid	38	0.292

Supplementary Table S8. The grouping of the platelet aggregation experiments.

Group	Constituent
Negative	100mL platelets + 50mL buffer solution + 50mL (agonist and CaCl <sub>2</sub> )
Positive	100mL platelets + 50mL reagent solution + 50mL (agonist and CaCl <sub>2</sub> )
Investigating	100mL platelets + 50mL compound solution + 50mL (agonist and CaCl <sub>2</sub> )
Control	150mL buffer solution + 50mL compound solution



Supplementary Figure S3. The UPLC-DAD chromatograms of DJF, showing the full formula (A, 40.88mg/mL ), along with the data of the standard solutions of Pentagalloylglucose (B, 28.9 $\mu$ g/mL ), Licochalcone A (C, 0.96 $\mu$ g/mL) and (Z)-ligustilide (D, 128.0 $\mu$ g/mL).

Supplementary Table S9. The composition of the 3-compound formulae

Composition Groups	Pentagalloylglucose	Licochalcone A	(Z)-Ligustilide
RF <sub>1</sub> -C <sub>1</sub>	46.25µg/mL	46.25µg/mL	47.50µg/mL
RF <sub>1</sub> -C <sub>2</sub>	23.13µg/mL	23.13µg/mL	23.75µg/mL
RF <sub>1</sub> -C <sub>3</sub>	11.57µg/mL	11.57µg/mL	11.88µg/mL
RF <sub>2</sub> -C <sub>1</sub>	45.00µg/mL	1.25µg/mL	155.00µg/mL
RF <sub>2</sub> -C <sub>2</sub>	22.50µg/mL	0.63µg/mL	77.50µg/mL
RF <sub>2</sub> -C <sub>3</sub>	11.25µg/mL	0.32µg/mL	38.75µg/mL