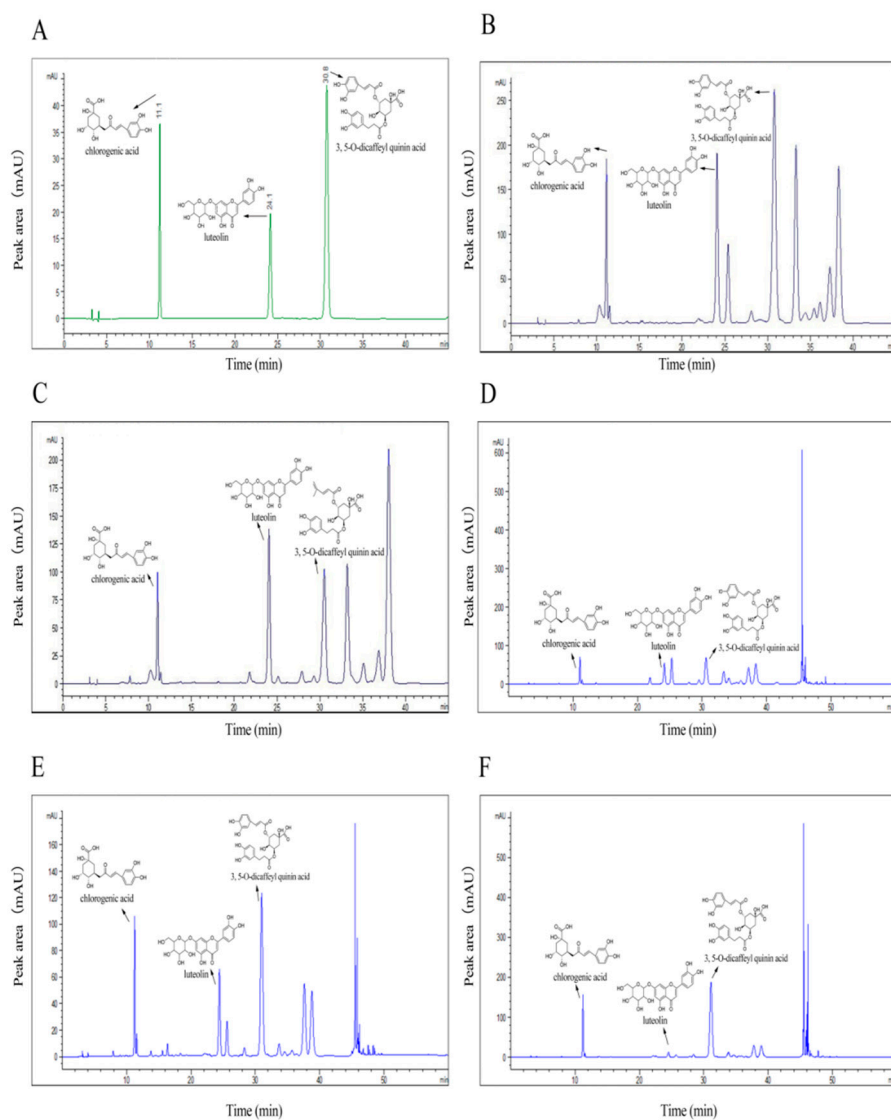


## Supplementary Material

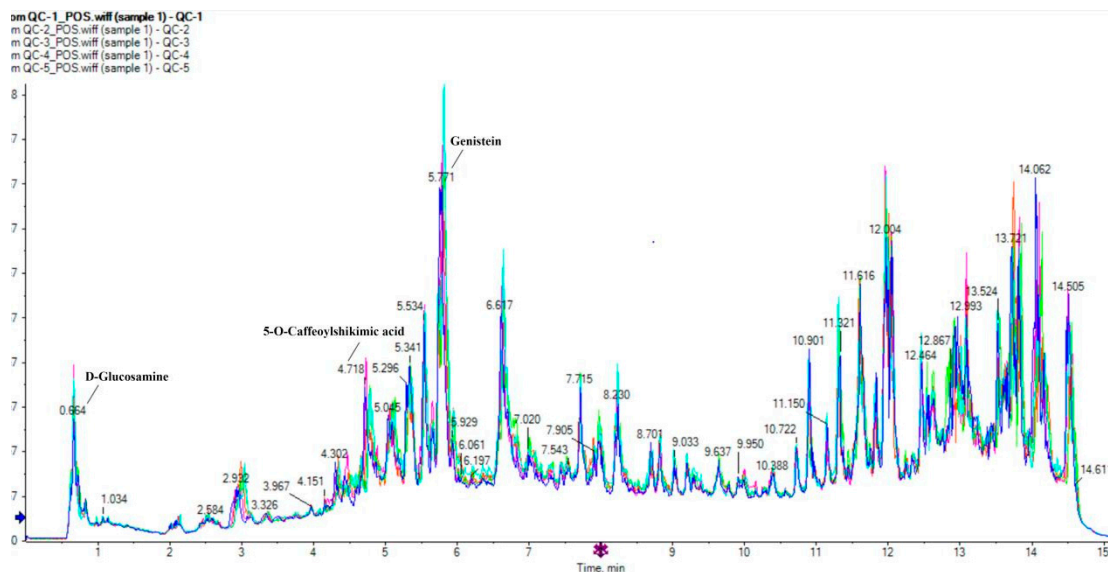
### Figure

Figure S1. The HPLC chromatogram of the five different varieties of *chrysanthemum* tea.

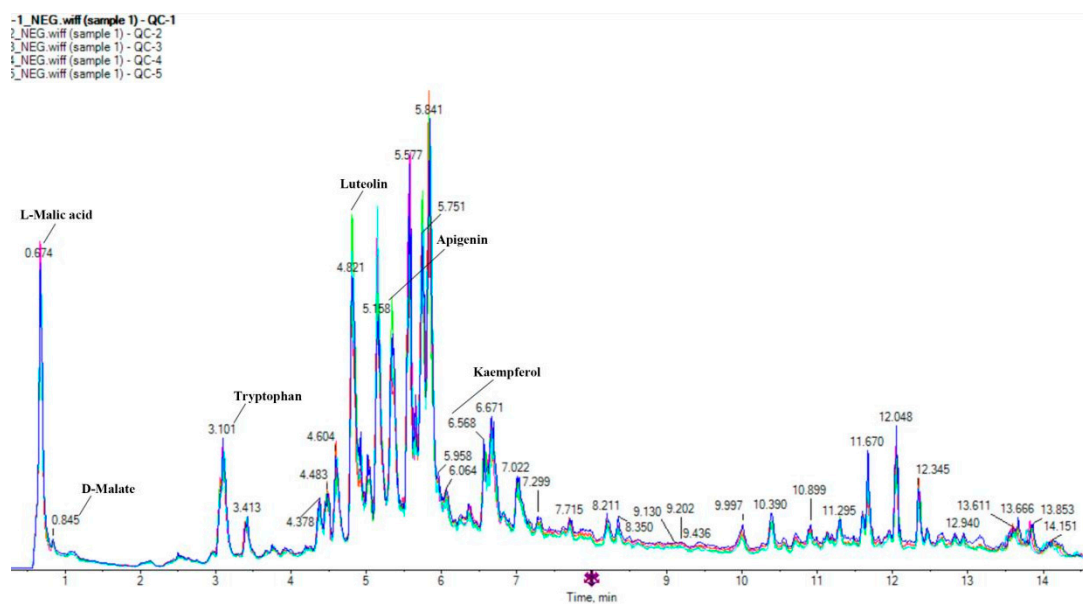


**Fig.S1 The HPLC chromatogram of the five different varieties of *chrysanthemum* tea.** (A) The HPLC chromatogram of the mixed sample standard ( chlorogenic acid, luteolin, and 3, 5-O-dicaffeoyl quinic acid ) ; (B)The HPLC chromatogram of 'Huangju' (X) O-dicaffeoyl quinic acid ) ; (C) The HPLC chromatogram of 'Jingsihuangju'(J) ;(D) The HPLC chromatogram of 'Boju'(B); (E) The HPLC chromatogram of 'Gongju'(G); (F) The HPLC chromatogram of 'Hangbaiju'(G);

**Figure S2 The TIC diagram in the ESI positive and negative modes for the five different varieties of *chrysanthemum* tea**



**Figure S2-a The TIC diagram in the ESI positive modes for the five different varieties of *chrysanthemum* tea**  
( Note: The abscissa represents the retention time of each chromatographic peak, and the ordinate represents the intensity value of the peak).



**Figure S2-b The TIC diagram in the ESI negative modes for the five different varieties of *chrysanthemum* tea**  
( Note: The abscissa represents the retention time of each chromatographic peak, and the ordinate represents the intensity value of the peak).

# Table

**Table S1 Contents of main bioactive substances of five different varieties of *chrysanthemum* tea**

<i>Chrysanthemum</i> varieties					
Dry matter content (%)	J	X	H	B	G
Chlorogenic acid	1.23 ± 0.03 <sup>c</sup>	2.11 ± 0.01 <sup>a</sup>	1.55 ± 0.02 <sup>b</sup>	0.66 ± 0.05 <sup>e</sup>	1.01 ± 0.01 <sup>d</sup>
Galuteolin	1.82 ± 0.01 <sup>b</sup>	2.62 ± 0.01 <sup>a</sup>	0.18 ± 0.01 <sup>e</sup>	0.67 ± 0.05 <sup>d</sup>	0.83 ± 0.02 <sup>c</sup>
Isochlorogenic acid	2.13 ± 0.04 <sup>d</sup>	5.93 ± 0.02 <sup>a</sup>	4.01 ± 0.10 <sup>b</sup>	1.26 ± 0.11 <sup>e</sup>	2.42 ± 0.03 <sup>c</sup>

Standard error of means (n = 3), <sup>a-d</sup> Means within the same row with different superscript differ significantly (*P* < 0.05)

**Table S2 Critical Compounds Metabolites Responsible for the Metabolomics Variation Caused between X and J Samples ((VIP>1, *P* < 0.01)**

No.	ID	Compounds	Formula	m/z	RT (min)	Superclass	VIP
1	NEG_16900	3-(Hexopyranosyloxy)-2-hydroxypropyl ester, (9Z,12Z,15Z)-9,12,15-octadecatrienoic acid	C <sub>27</sub> H <sub>46</sub> O <sub>9</sub>	559.30	10.976	Lipids and lipid-like molecules	1.429
2	NEG_18146	Tiliroside	C <sub>30</sub> H <sub>26</sub> O <sub>13</sub>	593.12	6.595	Phenylpropanoids and polyketides	2.71
3	NEG_4360	Acacetin	C <sub>16</sub> H <sub>12</sub> O <sub>5</sub>	283.06	6.603	Phenylpropanoids and polyketides	4.879
4	NEG_17566	Apigenin-7-O-neohesperidoside	C <sub>27</sub> H <sub>30</sub> O <sub>14</sub>	577.15	5.678		3.371
5	NEG_653	Cinnamic acid	C <sub>9</sub> H <sub>8</sub> O <sub>2</sub>	147.04	3.614	Phenylpropanoids and polyketides	1.345
6	NEG_978	L-(-)-3-Phenyllactic acid	C <sub>9</sub> H <sub>10</sub> O <sub>3</sub>	165.05	3.614	Phenylpropanoids and polyketides	1.558
7	NEG_8089	Chrysosplenetin	C <sub>19</sub> H <sub>18</sub> O <sub>8</sub>	373.09	7.691	Phenylpropanoids and polyketides	3.689
8	NEG_19601	Acacetin-7-O-rutinoside	C <sub>28</sub> H <sub>32</sub> O <sub>14</sub>	637.17	6.595		1.795
9	NEG_7582	Jaceidin	C <sub>18</sub> H <sub>16</sub> O <sub>8</sub>	359.07	7.686	Phenylpropanoids and polyketides	2.292
10	NEG_11058	(Z)-2,6-Dimethyl-7-(4-methyl-5-oxooxolan-2-yl)-3-[[3,4,5-trihydroxy-6-	C <sub>21</sub> H <sub>34</sub> O <sub>10</sub>	445.20	6.76	Lipids and lipid-like molecules	1.144

		(hydroxymethyl)oxan-2-yl]oxymethyl]hept-5-enoic acid					
11	NEG_7051	5,7,3',4'-Tetrahydroxy-6,8-dimethoxyflavone	C <sub>17</sub> H <sub>14</sub> O <sub>8</sub>	345.05	6.73	Phenylpropanoids and polyketides	1.326
12	NEG_14917	Deacetoxy(7)-7-oxokhivorinic acid	C <sub>27</sub> H <sub>36</sub> O <sub>10</sub>	519.22	7.492	Organoheterocyclic compounds	2.419
13	NEG_14776	12-Acetoxyganoderic acid	C <sub>30</sub> H <sub>46</sub> O <sub>7</sub>	517.20	7.188	Lipids and lipid-like molecules	3.522
14	NEG_11153	Astragalin	C <sub>21</sub> H <sub>20</sub> O <sub>11</sub>	447.09	5.719	Phenylpropanoids and polyketides	1.868
15	NEG_6294	1-(4-Hydroxyphenyl)-3-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxypropan-1-one	C <sub>15</sub> H <sub>20</sub> O <sub>8</sub>	327.10	3.449	Lipids and lipid-like molecules	1.293
16	NEG_467	L-Malic acid	C <sub>4</sub> H <sub>6</sub> O <sub>5</sub>	133.01	0.667	Organic acids and derivatives	2.056
17	NEG_286	Hexanoic acid	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	115.00	0.667	Lipids and lipid-like molecules	1.195
18	NEG_4756	N-Fructosyl pyroglutamate	C <sub>11</sub> H <sub>17</sub> NO <sub>8</sub>	290.08	0.686		1.773
19	NEG_1722	Tryptophan	C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>	203.08	2.935	Organoheterocyclic compounds	1.784
20	NEG_10356	Vitexin	C <sub>21</sub> H <sub>20</sub> O <sub>10</sub>	431.09	5.144	Phenylpropanoids and polyketides	1.073
21	NEG_5261	Bracteatin	C <sub>15</sub> H <sub>10</sub> O <sub>7</sub>	301.03	6.559	Phenylpropanoids and polyketides	1.006
22	NEG_1272	2',6'-Dihydroxy-4'-methoxyacetophenone	C <sub>9</sub> H <sub>10</sub> O <sub>4</sub>	181.04	6.277	Organic oxygen compounds	2.581
23	NEG_22238	PG 34:3	C <sub>40</sub> H <sub>73</sub> O <sub>10</sub> P	743.48	13.79		1.185
24	NEG_280	Proline	C <sub>5</sub> H <sub>9</sub> NO <sub>2</sub>	114.05	0.681	Organic acids and derivatives	1.898
25	NEG_11166	Maritimein	C <sub>21</sub> H <sub>20</sub> O <sub>11</sub>	447.09	6.103	Phenylpropanoids and polyketides	1.221
26	NEG_4472	Luteolin	C <sub>15</sub> H <sub>10</sub> O <sub>6</sub>	285.03	4.796	Phenylpropanoids and polyketides	1.176
27	NEG_10472	Naringenin-7-O-glucoside	C <sub>21</sub> H <sub>22</sub> O <sub>10</sub>	433.11	5.482		1.334
28	NEG_10355	Apigenin-7-O-glucoside	C <sub>21</sub> H <sub>20</sub> O <sub>10</sub>	431.09	5.732		9.201
29	NEG_3694	Apigenin	C <sub>15</sub> H <sub>10</sub> O <sub>5</sub>	269.04	5.196	Phenylpropanoids and polyketides	1.199
30	NEG_4490	Kaempferol	C <sub>15</sub> H <sub>10</sub> O <sub>6</sub>	285.03	6.563	Phenylpropanoids and polyketides	6.100
31	NEG_11024	Apigenin 7-O-glucuronide	C <sub>21</sub> H <sub>18</sub> O <sub>11</sub>	445.07	5.195	Phenylpropanoids and polyketides	4.589
32	NEG_11964	Dalbinol	C <sub>23</sub> H <sub>22</sub> O <sub>8</sub>	463.08	4.437	Phenylpropanoids and	9.344

						polyketides	
33	NEG_8114	2-[2-[(Z)-pent-2-enyl]-3-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxycyclopentyl]acetic acid	C <sub>18</sub> H <sub>30</sub> O <sub>8</sub>	373.18	6.491	Lipids and lipid-like molecules	1.100
34	NEG_3828	Naringenin	C <sub>15</sub> H <sub>12</sub> O <sub>5</sub>	271.06	6.547	Phenylpropanoids and polyketides	1.707
35	NEG_6438	9,12,13-Trihydroxyoctadec-10-enoic acid	C <sub>18</sub> H <sub>34</sub> O <sub>5</sub>	329.23	7.565	Lipids and lipid-like molecules	1.281
36	NEG_11149	Orientin	C <sub>21</sub> H <sub>20</sub> O <sub>11</sub>	447.08	4.914	Phenylpropanoids and polyketides	1.511
37	NEG_6320	9,10-Dihydroxy-8-oxooctadec-12-enoic acid	C <sub>18</sub> H <sub>32</sub> O <sub>5</sub>	327.21	7.342	Lipids and lipid-like molecules	1.693
38	NEG_11171	Luteolin-7-O-glucoside	C <sub>21</sub> H <sub>20</sub> O <sub>11</sub>	447.09	5.353		6.826
39	NEG_466	D-Malate	C <sub>4</sub> H <sub>6</sub> O <sub>5</sub>	133.01	0.837	Organic acids and derivatives	1.045
40	NEG_24704	Baicalin	C <sub>21</sub> H <sub>18</sub> O <sub>11</sub>	891.16	5.196	Phenylpropanoids and polyketides	1.349
41	NEG_11289	Eriodictyol-7-O-glucoside	C <sub>21</sub> H <sub>22</sub> O <sub>11</sub>	449.10	5.031	Phenylpropanoids and polyketides	2.142
42	NEG_3562	5,9-Dihydroxy-5,7,7-trimethyl-4,5a,6,8,8a,9-hexahydro-1H-azuleno[5,6-c]furan-3-one	C <sub>15</sub> H <sub>22</sub> O <sub>4</sub>	265.15	6.751	Lipids and lipid-like molecules	1.459
43	NEG_19227	Quercetin 3-O-sophoroside	C <sub>15</sub> H <sub>10</sub> O <sub>7</sub>	625.14	3.99	Flavonoid glycosides	1.387
44	NEG_4873	Glutamylphenylalanine	C <sub>14</sub> H <sub>18</sub> N <sub>2</sub> O <sub>5</sub>	293.12	3.246	Organic acids and derivatives	1.010
45	NEG_5743	Cirsimaritin	C <sub>17</sub> H <sub>14</sub> O <sub>6</sub>	313.06	7.576	Phenylpropanoids and polyketides	1.205
46	NEG_11449	2-Azaniumylethyl (3-hexadecanoyloxy-2-hydroxypropyl) phosphate	C <sub>21</sub> H <sub>44</sub> NO <sub>7</sub> P	452.27	11.601	Lipids and lipid-like molecules	1.927
47	NEG_6974	Eupatilin	C <sub>18</sub> H <sub>16</sub> O <sub>7</sub>	343.08	7.627	Phenylpropanoids and polyketides	1.868
48	NEG_7382	Neochlorogenic acid	C <sub>16</sub> H <sub>18</sub> O <sub>9</sub>	353.08	2.215	Organic oxygen compounds	1.943
49	NEG_4998	9-Hydroxy-10E,12Z-octadecadienoic acid	C <sub>18</sub> H <sub>32</sub> O <sub>3</sub>	295.22	10.35	Lipids and lipid-like molecules	3.284
50	NEG_4305	trans-Vaccenic acid	C <sub>18</sub> H <sub>34</sub> O <sub>2</sub>	281.24	12.421	Lipids and lipid-like molecules	1.740
51	NEG_7372	3-[3-(3,4-Dihydroxyphenyl)prop-2-enoyloxy]-1,4,5-trihydroxycyclohexane-1-	C <sub>16</sub> H <sub>18</sub> O <sub>9</sub>	353.08	2.162	Organic oxygen compounds	2.032

		carboxylic acid					
52	NEG_23892	PI 34:2	C <sub>43</sub> H <sub>79</sub> O <sub>13</sub> P	833.51	14.046		3.259
53	NEG_15572	Flavone base + 4O, O-MalonylHex	C <sub>24</sub> H <sub>22</sub> O <sub>14</sub>	533.09	5.53	Phenylpropanoids and polyketides	5.904
54	NEG_1153	2-Isopropylmalic acid	C <sub>7</sub> H <sub>12</sub> O <sub>5</sub>	175.06	2.404	Lipids and lipid-like molecules	1.234
55	NEG_1446	Quinic acid	C <sub>7</sub> H <sub>12</sub> O <sub>6</sub>	191.05	0.631	Organic oxygen compounds	1.184
56	NEG_3875	FA 16:0;2O	C <sub>16</sub> H <sub>32</sub> O <sub>3</sub>	271.22	11.353	Lipids and lipid-like molecules	1.308
57	NEG_4907	9-HOTrE	C <sub>18</sub> H <sub>30</sub> O <sub>3</sub>	293.21	9.951	Lipids and lipid-like molecules	1.235
58	NEG_3698	Aloe-emodin	C <sub>15</sub> H <sub>10</sub> O <sub>5</sub>	269.04	5.646	Benzenoids	5.655
59	NEG_12660	[3-[2-Aminoethoxy(hydroxy)phosphoryl]oxy-2-hydroxypropyl]octadeca-9,12-dienoate	C <sub>23</sub> H <sub>44</sub> NO <sub>7</sub> P	476.27	11.298	Lipids and lipid-like molecules	1.001
60	POS_14378	4-Acetyl-3-hydroxy-5-methylphenyl beta-D-glucopyranoside	C <sub>15</sub> H <sub>20</sub> O <sub>8</sub>	351.10	3.534	Organic oxygen compounds	1.370
61	POS_10508	(5xi,9xi)-12-Hydroxyabieta-7,13-dien-18-oic acid	C <sub>20</sub> H <sub>30</sub> O <sub>3</sub>	301.21	8.211	Lipids and lipid-like molecules	1.609
62	POS_20040	Topotecan	C <sub>23</sub> H <sub>23</sub> N <sub>3</sub> O <sub>5</sub>	422.17	3.946	Alkaloids and derivatives	2.924
63	POS_17988	7-Hydroxy-5-methyl-2-(2-oxopropyl)-8-[3,4,5-trihydroxy-6-(hydroxymethyl)-2-oxanyl]-1-benzopyran-4-one	C <sub>19</sub> H <sub>22</sub> O <sub>9</sub>	395.13	3.567	Organic oxygen compounds	2.593
64	POS_19227	3-O-Methylfunicone	C <sub>20</sub> H <sub>20</sub> O <sub>8</sub>	411.10	8.237	Organic oxygen compounds	2.319
65	POS_15259	Fenofibrate	C <sub>20</sub> H <sub>21</sub> ClO <sub>4</sub>	361.125	4.068	Benzenoids	1.086
66	POS_6344	Thunalbene	C <sub>15</sub> H <sub>14</sub> O <sub>3</sub>	243.098	7.335	Phenylpropanoids and polyketides	1.238
67	POS_17448	Pyraclostrobin	C <sub>19</sub> H <sub>18</sub> ClN <sub>3</sub> O <sub>4</sub>	388.106	9.369	Organoheterocyclic compounds	3.075
68	POS_31781	Kaempferol-3,7-O-bis-alpha-L-rhamnoside	C <sub>27</sub> H <sub>30</sub> O <sub>14</sub>	579.170	5.681	Phenylpropanoids and polyketides	3.348
69	POS_15557	1,17,19-Trihydroxy-7-methyl-3-oxapentacyclo[9.8.0.02,4.05,10.013,18]nonadeca-5(10),13(18),14,16-tetraene-9,12-dione	C <sub>19</sub> H <sub>18</sub> O <sub>6</sub>	365.084	3.723	Benzenoids	1.380
70	POS_23706	Monotropitoside	C <sub>19</sub> H <sub>26</sub> O <sub>12</sub>	469.131	4.675	Organic oxygen compounds	3.107
71	POS_28038	3,5,5-Trimethyl-4-[3-[(6-O-beta-	C <sub>24</sub> H <sub>40</sub> O <sub>11</sub>	527.236	7.078	Lipids and lipid-like	2.002

		D-xylopyranosyl-beta-D-glucopyranosyl)oxy]butyl]-2-cyclohexen-1-one				molecules	
72	POS_21718	11,12,13-Trihydroxy-4,5,8-trimethyl-3-(2-methylpropyl)-1H,2H,3H,4H,6aH,9H,10H,11H,12H,13H,14H,15H,15bH-cycloundeca[e]isoindole-1,15-dione	C <sub>24</sub> H <sub>37</sub> NO <sub>5</sub>	442.270	4.116	Organoheterocyclic compounds	8.167
73	POS_8718	(3S,3aR,4S,9aS,9bR)-4-Hydroxy-9-(hydroxymethyl)-3,6-dimethyl-3,3a,4,5,9a,9b-hexahydroazuleno[4,5-b]furan-2,7-dione	C <sub>15</sub> H <sub>18</sub> O <sub>5</sub>	279.121	4.679	Organoheterocyclic compounds	1.401
74	POS_21421	Sayaendoside	C <sub>19</sub> H <sub>28</sub> O <sub>10</sub>	439.151	5.727	Organic oxygen compounds	1.306
75	POS_27104	Tauromuricholic acid	C <sub>26</sub> H <sub>45</sub> NO <sub>7</sub> S	516.306	9.139	Lipids and lipid-like molecules	1.326
76	POS_33486	(S)-7-(((2-O-6-Deoxy-alpha-L-mannopyranosyl)-beta-D-glucopyranosyl)oxy)-2,3-dihydro-5-hydroxy-2-(3-hydroxy-4-methoxyphenyl)-4H-1-benzopyran-4-one	C <sub>28</sub> H <sub>34</sub> O <sub>15</sub>	611.463	12.653	Phenylpropanoids and polyketides	4.196
77	POS_21638	Simvastatin	C <sub>25</sub> H <sub>38</sub> O <sub>5</sub>	441.257	9.904	Organoheterocyclic compounds	1.564
78	POS_18121	3',5-Dihydroxy-3,4',5',7-tetramethoxyflavone	C <sub>19</sub> H <sub>18</sub> O <sub>8</sub>	397.086	7.894	Phenylpropanoids and polyketides	1.978
79	POS_22389	(3R,3aR,4S,6S,7aR)-6-ethenyl-4-hydroxy-3,6-dimethyl-7-[(E)-1-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyprop-1-en-2-yl]-3,3a,4,5,7,7a-hexahydro-1-benzofuran-2-one	C <sub>21</sub> H <sub>32</sub> O <sub>9</sub>	451.194	5.515	Lipids and lipid-like molecules	1.002
80	POS_29937	Lutein		551.414	13.622	Lipids and lipid-like molecules	1.294
81	POS_21553	3-Hydroxy-2-[[3-(3-hydroxy-6-methylheptanoyl)oxy-8-methylnonanoyl]amino]propanoic acid	C <sub>21</sub> H <sub>39</sub> NO <sub>7</sub>	440.252	4.864	Organic acids and derivatives	15.676
82	POS_6080	[(6S,9aS)-6,9a-Dimethyl-1,3,4,5,5a,7,8,9-	C <sub>15</sub> H <sub>24</sub> O <sub>2</sub>	237.185	8.258	Organoheterocyclic compounds	1.298

83	POS_6921	octahydrobenzo[e][2]benzofuran-6-yl]methanol 3a-Hydroxy-3,5a,9-trimethyl-3a,4,5,5a,6,7,8,9b-octahydronaphtho[1,2-b]furan-2(3H)-one 3,3a,4,5,9a,9b-Hexahydro-9a-hydroxy-6,9-dimethyl-3-methylene-, (9aR,9bS)-azuleno[4,5-b]furan-2,7-dione	C <sub>15</sub> H <sub>22</sub> O <sub>3</sub>	251.166	6.813	Lipids and lipid-like molecules	3.660
84	POS_7479	Sempervirine	C <sub>15</sub> H <sub>16</sub> O <sub>4</sub>	261.109	4.674	Organoheterocyclic compounds	1.976
85	POS_8297	5,5,9,13-tetramethyl-7-(phenylmethylidene)tetracyclo[11.2.1.01,10.04,9]hexadec-14-en-6-one (2R,3S,4S,5R,6R)-2-(hydroxymethyl)-6-(2-hydroxy-2-methylbut-3-enoxy)oxane-3,4,5-triol [(3Ar,4R,5R,6E,9Z,11aR)-4-hydroxy-6,10-dimethyl-3-methylidene-2,8-dioxo-4,5,11,11a-tetrahydro-3aH-cyclodeca[b]furan-5-yl] (Z)-2-methylbut-2-enoate	C <sub>19</sub> H <sub>16</sub> N <sub>2</sub>	273.145	8.467	Organoheterocyclic compounds	1.243
86	POS_16518	Biochanin A 7-(6-malonylglucoside)	C <sub>27</sub> H <sub>34</sub> O	375.266	11.26		1.032
87	POS_9463	Sinapaldehyde glucoside	C <sub>11</sub> H <sub>20</sub> O <sub>7</sub>	287.108	2.119	Lipids and lipid-like molecules	1.676
88	POS_16713	Cafestol	C <sub>20</sub> H <sub>24</sub> O <sub>6</sub>	378.183	7.47	Lipids and lipid-like molecules	1.158
89	POS_28471	Isoschaftoside	C <sub>25</sub> H <sub>24</sub> O <sub>13</sub>	533.133	6.642	Phenylpropanoids and polyketides	4.801
90	POS_17813	22-Hydroxy-2-hopen-1-one	C <sub>17</sub> H <sub>22</sub> O <sub>9</sub>	393.111	5.05	Organic oxygen compounds	2.966
91	POS_11705	2-[[[3,4-Dihydroxy-4-(hydroxymethyl)oxolan-2-yl]oxymethyl]-6-[(6,6-dimethyl-4-bicyclo[3.1.1]hept-3-enyl)methoxy]oxane-3,4,5-triol	C <sub>20</sub> H <sub>28</sub> O <sub>3</sub>	317.206	10.259	Organoheterocyclic compounds	1.086
92	POS_30933	2-Phenylethyl beta-D-glucopyranoside	C <sub>26</sub> H <sub>28</sub> O <sub>14</sub>	565.151	4.809	Phenylpropanoids and polyketides	1.237
93	POS_21669	(4Ar,5R,6R)-6-hydroxy-3-	C <sub>30</sub> H <sub>48</sub> O <sub>2</sub>	441.363	11.845	Lipids and lipid-like molecules	1.619
94	POS_23382		C <sub>21</sub> H <sub>34</sub> O <sub>10</sub>	464.246	6.769	Lipids and lipid-like molecules	1.131
95	POS_10541		C <sub>14</sub> H <sub>20</sub> O <sub>6</sub>	302.159	5.092	Organic oxygen compounds	1.231
96	POS_4759		C <sub>15</sub> H <sub>20</sub> O <sub>2</sub>	215.139	6.796	Lipids and lipid-like molecules	1.528



		isopropenyl-4a,5-dimethyl-5,6,7,8-tetrahydronaphthalen-2-one				molecules	
97	POS_10100	9-Oxo-octadeca-10,12-dienoic acid	C <sub>18</sub> H <sub>30</sub> O <sub>3</sub>	295.224	9.473	Lipids and lipid-like molecules	1.101
98	POS_21629	N-Methyl-N-[(2E,4E,6E)-2,4,6-octatrienoyl]valylalanylprolinamide	C <sub>22</sub> H <sub>34</sub> N <sub>4</sub> O <sub>4</sub>	441.236	6.894	Organic acids and derivatives	1.712
99	POS_31058	4-Oxogazaniaxanthin	C <sub>40</sub> H <sub>54</sub> O <sub>2</sub>	567.416	12.568	Lipids and lipid-like molecules	2.327
100	POS_23401	Delphinidin 3-glucoside	[C <sub>21</sub> H <sub>21</sub> O <sub>12</sub> ] +	465.101	5.151	Phenylpropanoids and polyketides	1.018
101	POS_33626	5-Hydroxy-3-(4-methoxyphenyl)-7-[3,4,5-trihydroxy-6-[(3,4,5-trihydroxy-6-methyloxan-2-yl)oxymethyl]oxan-2-yl]oxychromen-4-one	C <sub>28</sub> H <sub>32</sub> O <sub>14</sub>	615.165	6.606	Phenylpropanoids and polyketides	1.236
102	POS_36352	Rutaresin	C <sub>31</sub> H <sub>30</sub> O <sub>16</sub>	681.1422	6.593	Phenylpropanoids and polyketides	4.461
103	POS_4919	Pymetrozine	C <sub>10</sub> H <sub>11</sub> N <sub>5</sub> O	218.101	3.993	Benzenoids	1.033
104	POS_20872	beta-D-Glucopyranoside, 4-hydroxy-5-methyl-2-(1-methylethyl)phenyl, 6-(2-carboxyacetate)	C <sub>19</sub> H <sub>26</sub> O <sub>10</sub>	432.179	5.064	Lipids and lipid-like molecules	1.376
105	POS_18049	Fucosterol	C <sub>29</sub> H <sub>48</sub> O	395.365	12.632	Lipids and lipid-like molecules	1.075
106	POS_10105	(9E,11Z)-13-Oxo-9,11-octadecadienoic acid	C <sub>18</sub> H <sub>30</sub> O <sub>3</sub>	295.226	10.261	Lipids and lipid-like molecules	1.530
107	POS_30165	(-)-Maackiain-3-O-glucosyl-6"-O-malonate	C <sub>25</sub> H <sub>24</sub> O <sub>13</sub>	555.108	6.642	Phenylpropanoids and polyketides	1.165
108	POS_15590	7,8-Dihydroxycalonectrin	C <sub>19</sub> H <sub>26</sub> O <sub>8</sub>	365.153	5.159	Lipids and lipid-like molecules	1.372
109	POS_21418	Phenethyl 2-O-(beta-D-xylopyranosyl)-beta-D-glucopyranoside	C <sub>19</sub> H <sub>28</sub> O <sub>10</sub>	439.149	5.406	Organic oxygen compounds	1.413
110	POS_22368	(2R,2S)-Eriodictyol 7-O-beta-D-glucoside	C <sub>21</sub> H <sub>22</sub> O <sub>11</sub>	451.122	5.035	Phenylpropanoids and polyketides	2.060
111	POS_29451	Triferric doxorubicin	C <sub>27</sub> H <sub>29</sub> NO <sub>11</sub>	544.179	5.763	Phenylpropanoids and polyketides	3.502
112	POS_4391	Sinapoyl malate	C <sub>15</sub> H <sub>16</sub> O <sub>9</sub>	207.137	4.628	Phenylpropanoids and polyketides	1.236
113	POS_1293	Trigonelline HCl	C <sub>7</sub> H <sub>7</sub> NO <sub>2</sub> .H Cl	138.055	0.666		1.221
114	POS_32891	Violanthin	C <sub>27</sub> H <sub>30</sub> O <sub>14</sub>	601.152	5.693	Phenylpropanoids and	2.430

						polyketides	
115	POS_33707	Kaempferol 3-O-beta-D-glucopyranosyl-7-O-alpha-L-rhamnopyranoside	C <sub>27</sub> H <sub>30</sub> O <sub>15</sub>	617.146	5.341	Phenylpropanoids and polyketides	1.911
116	POS_29757	Flavone base + 3O, 1MeO, O-MalonylHex	C <sub>25</sub> H <sub>24</sub> O <sub>14</sub>	549.116	5.943	Phenylpropanoids and polyketides	1.695
117	POS_21371	Lunarine	C <sub>25</sub> H <sub>31</sub> N <sub>3</sub> O <sub>4</sub>	438.231	4.844	Phenylpropanoids and polyketides	2.2391
118	POS_31471	3-{7-[5-(1-hydroxyhenicosa-4,8-dien-1-yl)oxolan-2-yl]heptyl}-5-methyl-5H-furan-2-one	C <sub>37</sub> H <sub>64</sub> O <sub>4</sub>	573.484	13.921		2.663
119	POS_5800	Isoalantolactone	C <sub>15</sub> H <sub>20</sub> O <sub>2</sub>	233.151	8.014	Lipids and lipid-like molecules	1.559
120	POS_5743	alpha-Pyrrolidinovalerophenone	C <sub>15</sub> H <sub>21</sub> NO	232.1679	8.268	Organic oxygen compounds	1.575
121	POS_39499	N1,N5,N10,N14-Tetra-trans-p-coumaroylspermine	C <sub>46</sub> H <sub>50</sub> N <sub>4</sub> O <sub>8</sub>	787.372	7.006	Phenylpropanoids and polyketides	1.5905 0
122	POS_13176	5-O-Caffeoylshikimic acid	C <sub>16</sub> H <sub>16</sub> O <sub>8</sub>	337.084	4.758	Phenylpropanoids and polyketides	1.328
123	POS_6063	3,7-Epoxycaryophyllan-6-One	C <sub>15</sub> H <sub>24</sub> O <sub>2</sub>	237.1826	7.572	Organoheterocyclic compounds	1.2343 67
124	POS_9312	Retinal	C <sub>20</sub> H <sub>28</sub> O	285.2187	9.92	Lipids and lipid-like molecules	1.0188 04
125	POS_6911	2-[(2R,4aS,7R)-7-Hydroxy-4a-methyl-8-methylenedecahydro-2-naphthalenyl]acrylic acid	C <sub>15</sub> H <sub>22</sub> O <sub>3</sub>	251.1643	7.821	Lipids and lipid-like molecules	1.5261 48
126	POS_29643	3-(4-{[1,3-Dihydroxy-1-(4-hydroxy-3-methoxyphenyl)-2-propanyl]oxy}-3-methoxyphenyl)propyl 6-deoxy-alpha-L-mannopyranoside	C <sub>26</sub> H <sub>36</sub> O <sub>11</sub>	547.210	4.969	Lignans, neolignans and related compounds	1.164
127	POS_29936	Echinone	C <sub>40</sub> H <sub>54</sub> O	551.414	12.861	Lipids and lipid-like molecules	1.367
128	POS_8156	Genistein	C <sub>15</sub> H <sub>10</sub> O <sub>5</sub>	271.059	5.753	Phenylpropanoids and polyketides	4.520
129	POS_27732	cyclo[DL-Ala-DL-Trp-DL-Ala-DL-Val-Gly]	C <sub>24</sub> H <sub>32</sub> N <sub>6</sub> O <sub>5</sub>	523.202	5.667	Organic acids and derivatives	1.131
130	POS_31987	Diadinoxchrome A	C <sub>40</sub> H <sub>54</sub> O <sub>3</sub>	583.408	12.538	Lipids and lipid-like molecules	1.681
131	POS_27525	Anthocyanidin base+3O, O-MalonylHex	C <sub>24</sub> H <sub>24</sub> O <sub>13</sub>	521.129	5.512	Phenylpropanoids and polyketides	1.595
132	POS_33324	Diosmin	C <sub>28</sub> H <sub>32</sub> O <sub>15</sub>	609.180	5.784	Phenylpropanoids and polyketides	1.323
133	POS_2246	Rosmarinic acid	C <sub>18</sub> H <sub>16</sub> O <sub>8</sub>	163.029	2.934	Phenylpropanoids and	2.958

						polyketides	
134	POS_15079	5-Hydroxy-2',4',7,8-tetramethoxyflavone	C <sub>19</sub> H <sub>18</sub> O <sub>7</sub>	359.110	7.988	Phenylpropanoids and polyketides	2.939
135	POS_25818	Primeverin	C <sub>20</sub> H <sub>28</sub> O <sub>13</sub>	499.136	3.646	Organic oxygen compounds	1.712
136	POS_27320	6"-O-Malonylgenistin	C <sub>24</sub> H <sub>22</sub> O <sub>13</sub>	519.112	5.657	Phenylpropanoids and polyketides	3.044
137	POS_6214	Triacetin	C <sub>9</sub> H <sub>14</sub> O <sub>6</sub>	241.065	3.398	Lipids and lipid-like molecules	1.012
138	POS_32588	Luteolin 7-O-rutinoside	C <sub>27</sub> H <sub>30</sub> O <sub>15</sub>	595.165	5.321	Phenylpropanoids and polyketides	2.245
139	POS_4891	Zizanoic acid	C <sub>15</sub> H <sub>22</sub> O <sub>2</sub>	217.158	9.424	Lipids and lipid-like molecules	1.038
140	POS_32507	Deoxykhivorin	C <sub>32</sub> H <sub>42</sub> O <sub>9</sub>	593.277	12.467	Organoheterocyclic compounds	1.508
141	POS_3007	D-Glucosamine	C <sub>6</sub> H <sub>13</sub> NO <sub>5</sub>	180.086	0.659	Organic oxygen compounds	1.007
142	POS_15169	Palatinose	C <sub>12</sub> H <sub>22</sub> O <sub>11</sub>	360.150	0.677	Organic oxygen compounds	2.068
143	POS_7201	Palmitic amide	C <sub>16</sub> H <sub>33</sub> NO	256.263	11.829	Others	2.805

---