

Supplementary Material

Captions

Figure S1 The lung score of Fructus Arctii in H1N1 infected mice.

Figure S2 The possible fragmentation pathway for Lappaol E (peak **81**).

Figure S3 The proposed fragmentation pathway for Lappaol F (peak **105**).

Figure S4 The proposed fragmentation pathway for Lappaol H (peak **40**).

Figure S5 The proposed fragmentation pathway for Neoarctin A (peak **116**).

Figure S6 The possible fragmentation pathway for Diarctigenin (peak **114**).

Table S1 Chemical constituents isolated from Fructus Arctii.

Table S2 Compounds identified or tentatively characterized in Fructus Arctii by UHPLC/Q-TOF MS.

Figure S1 The lung score of Fructus Arctii in H1N1 infected mice.

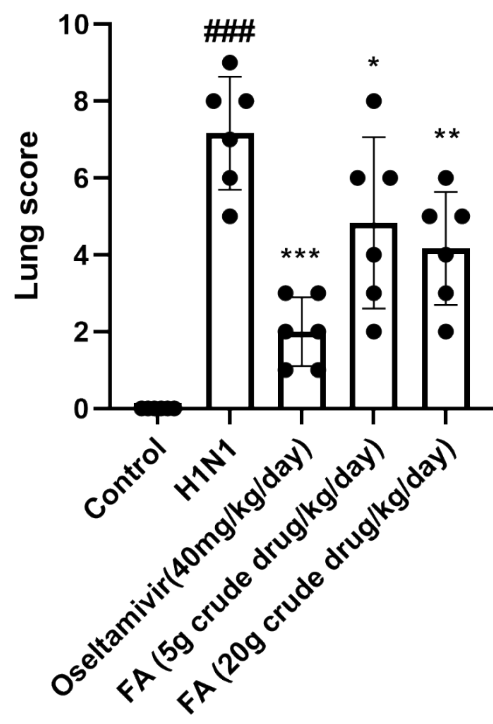


Figure S2 The possible fragmentation pathway for Lappaol E (peak **81**).

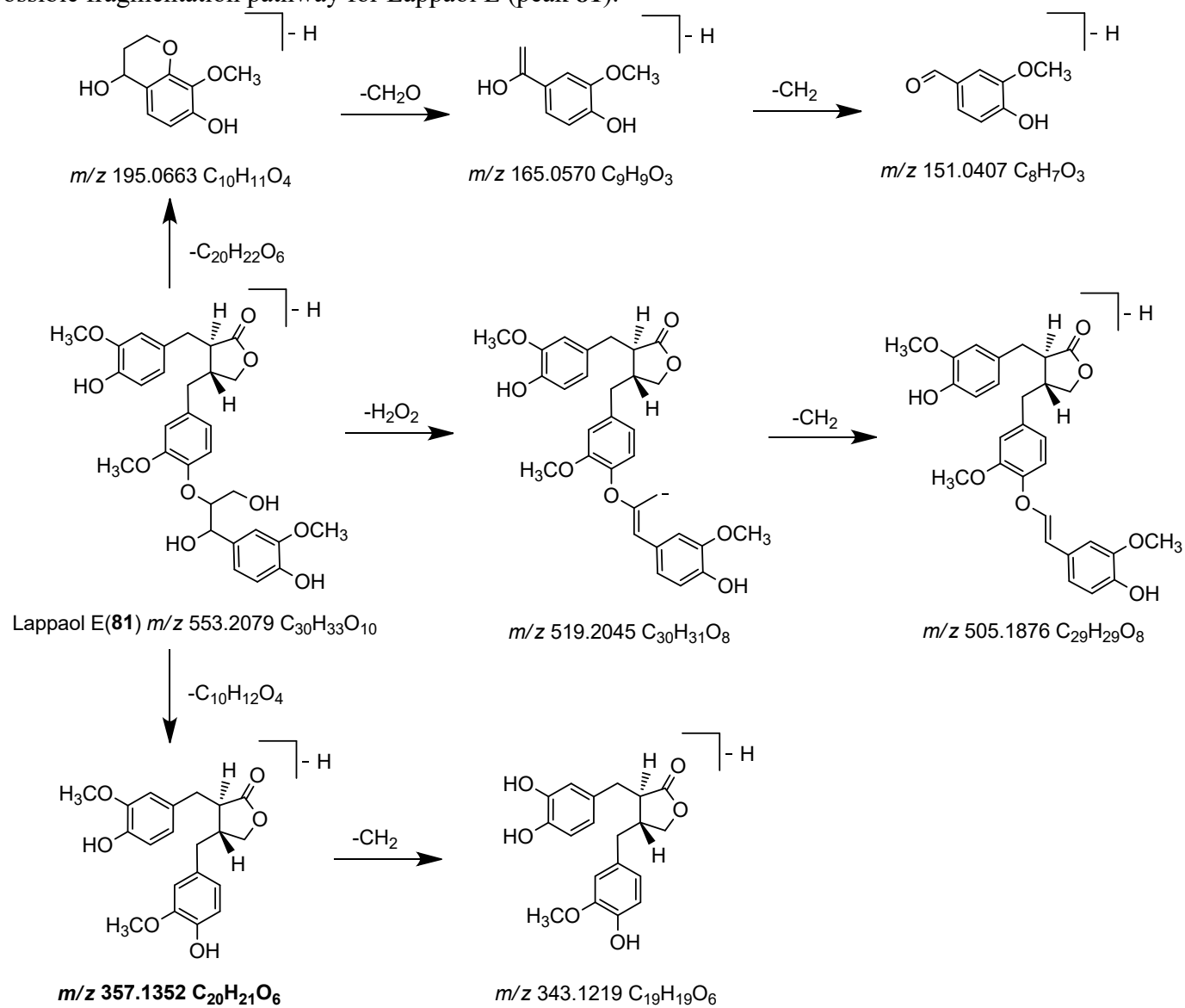


Figure S3 The proposed fragmentation pathway for Lappaol F (peak 105).

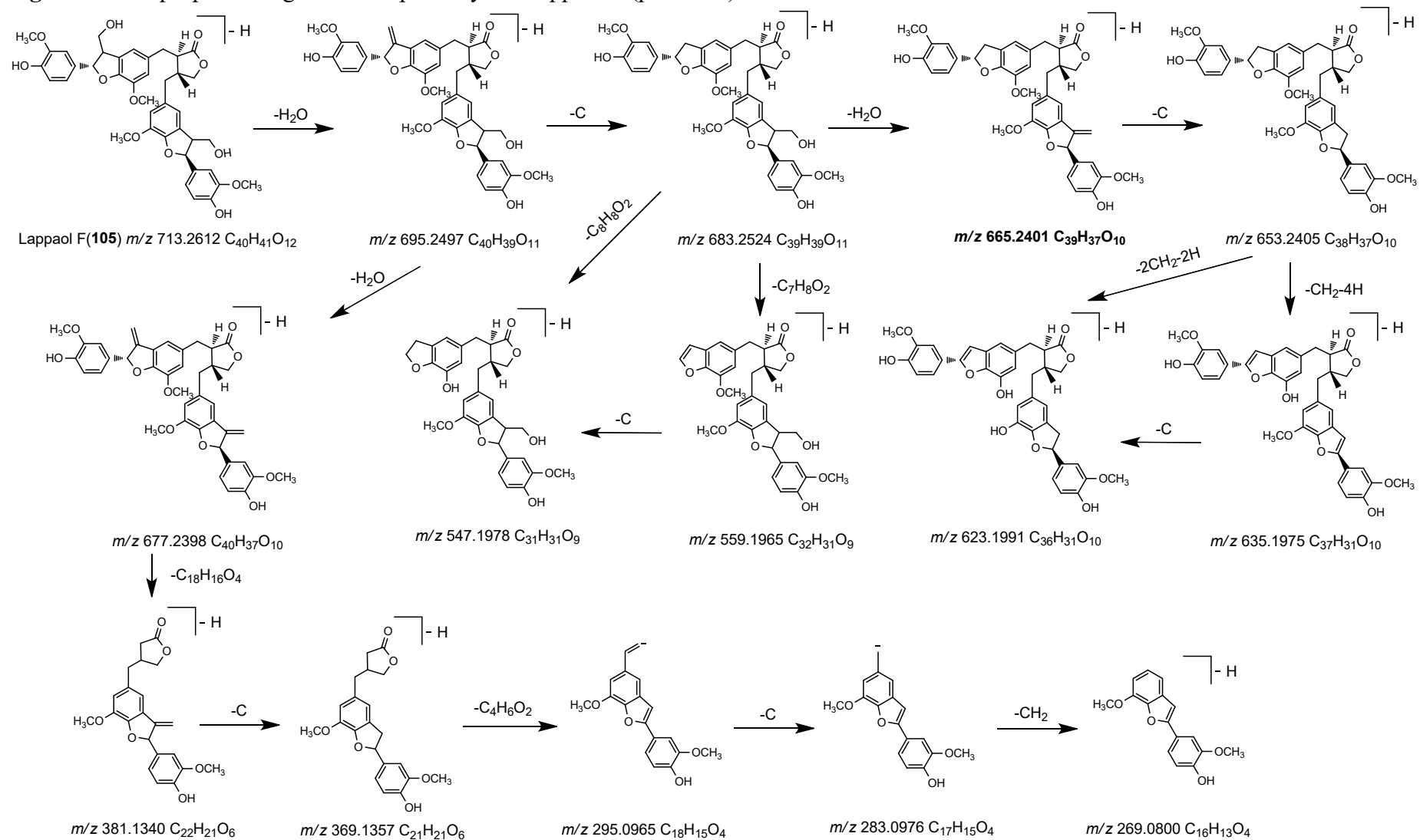


Figure S4 The proposed fragmentation pathway for Lappaol H (peak 40).

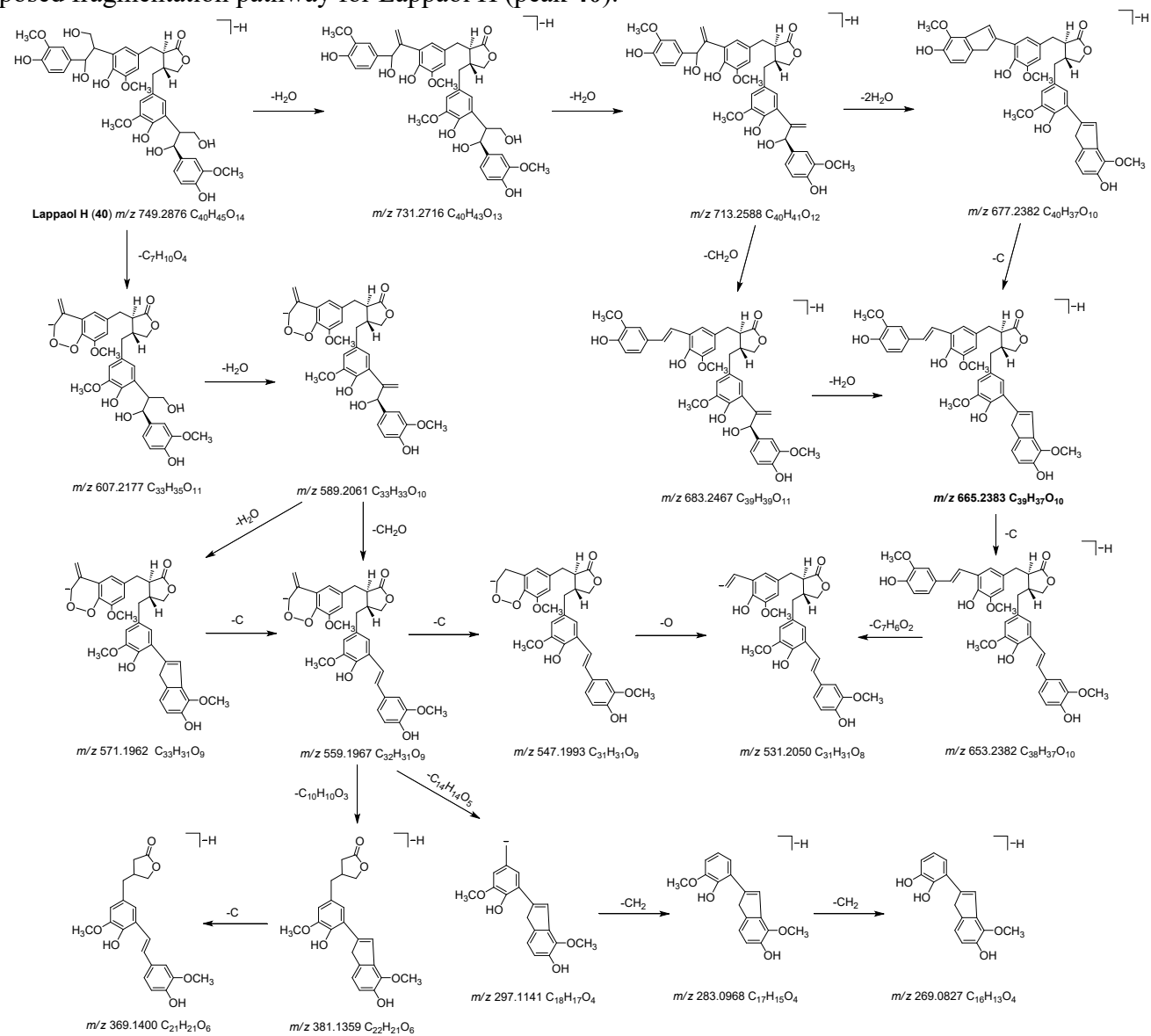


Figure S5 The proposed fragmentation pathway for Neoarctin A (peak 116).

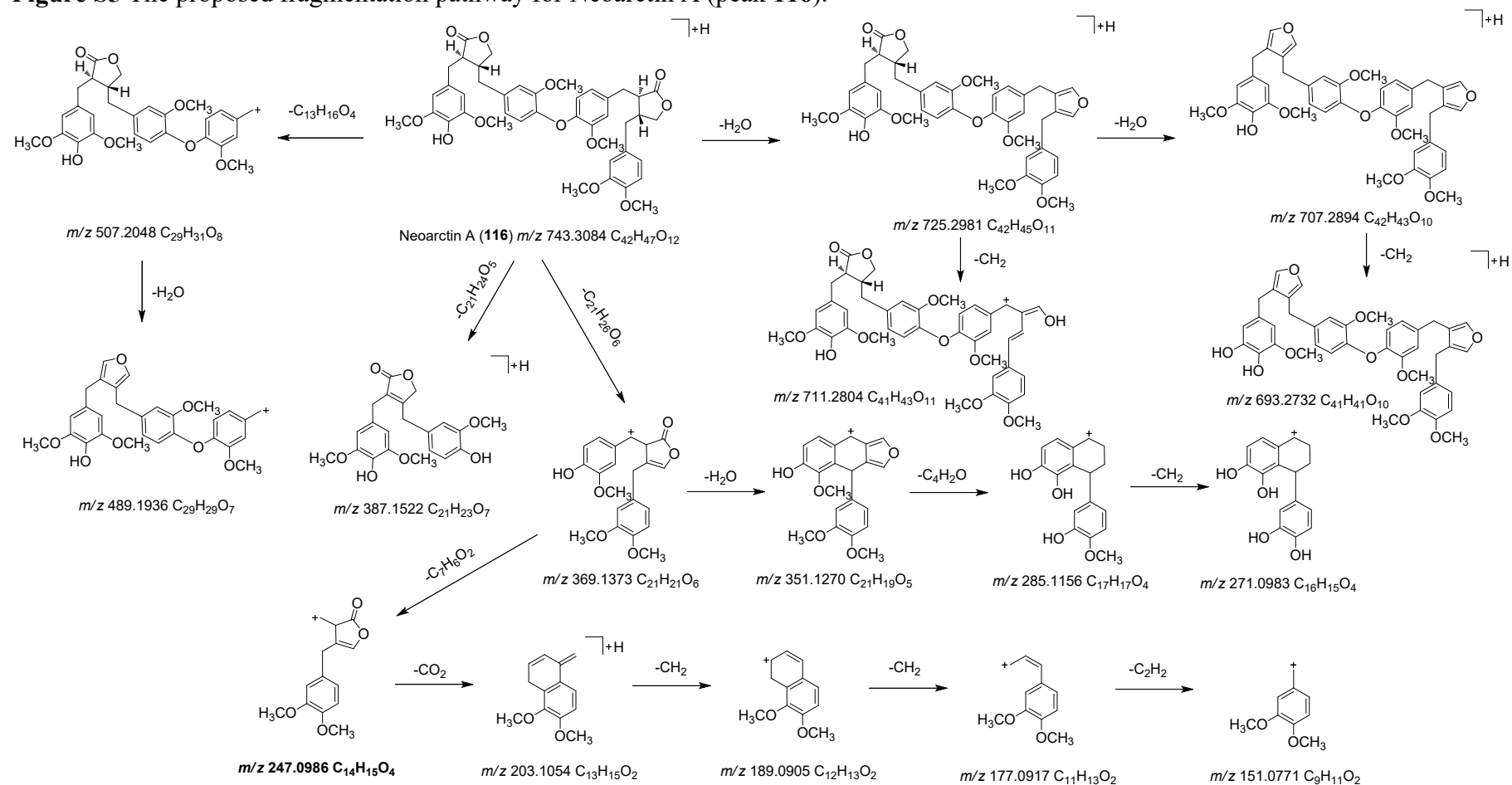


Figure S6 The possible fragmentation pathway for Diarctigenin (peak 114).

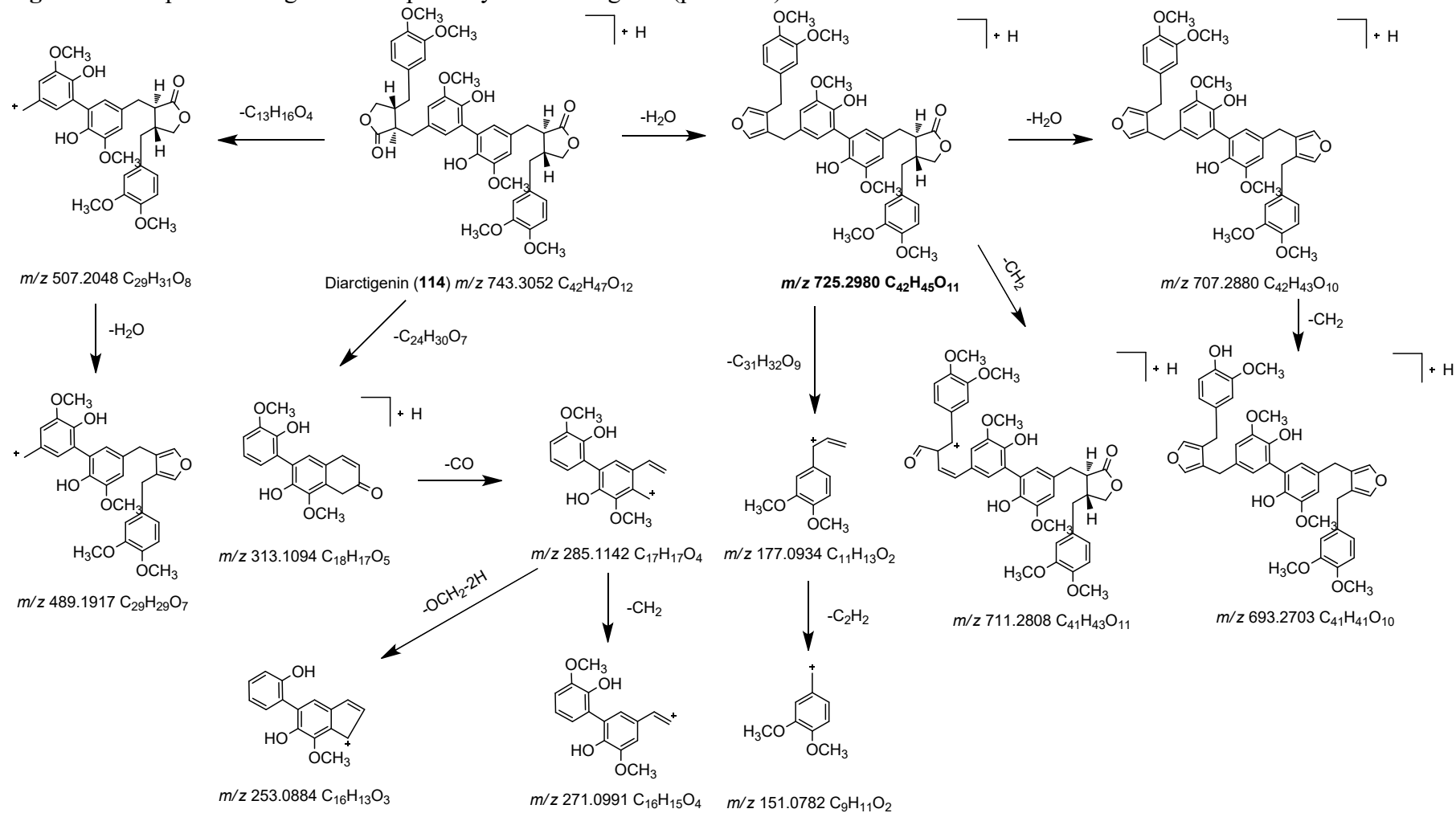


Table S1 Chemical constituents isolated from Fructus Arctii.

Types	Chemical name	Formula	Molecular weight	reference
Lignans				
1	diarctigenin	C ₄₂ H ₄₆ O ₁₂	742.2989	1
2	arctiin	C ₂₇ H ₃₄ O ₁₁	534.2101	1
3	arctigenin	C ₂₁ H ₂₄ O ₆	372.1573	1
4	4-acetylatearctiin	C ₂₉ H ₃₆ O ₁₂	576.2207	2
5	arctigenin-4- <i>O</i> - β -D-gentiobioside	C ₃₃ H ₄₄ O ₁₆	696.2629	1
6	arctigenin-4- <i>O</i> - α -D-galactopyranosyl-(1 \rightarrow 6)- <i>O</i> - β -D-glucopyranoside	C ₃₃ H ₄₄ O ₁₆	696.2629	1
7	arctigenin-4- <i>O</i> - β -D-apiofuranosyl-(1 \rightarrow 6)- <i>O</i> - β -D-glucopyranoside	C ₃₂ H ₄₂ O ₁₅	666.2524	1
8	3-benzyl-6-(1-hydroxyethyl)-2,5-piperazinedione	C ₁₃ H ₁₆ N ₂ O ₃	248.1161	1
9	3-benzyl-2,5- piperazinedione	C ₁₁ H ₁₂ N ₂ O ₂	204.0899	1
10	5'-propanediolmatairesinoid	C ₂₉ H ₃₈ O ₁₃	594.2312	1
11	(7 <i>R</i> ,8 <i>R</i> ,8' <i>R</i>)-rafanotrachelogenin-4- <i>O</i> - β -D-glucopyranoside	C ₂₇ H ₃₄ O ₁₂	550.2050	1
12	(7' <i>S</i> ,8 <i>R</i> ,8' <i>R</i>)-rafanotrachelogenin-4- <i>O</i> - β -D-glucopyranoside	C ₂₇ H ₃₄ O ₁₂	550.2050	1
13	(7 <i>S</i> ,8 <i>S</i> ,8' <i>R</i>)-4,7-dihydroxy-3,3',4'-trimethoxyl-9-oxo-dibenzylbutyrolactone lignan-4- <i>O</i> - β -D-glucopyranoside	C ₂₇ H ₃₄ O ₁₂	550.2050	1
14	(7 <i>S</i> ,8 <i>S</i> ,8' <i>R</i>)-4,7- dihydroxy-3,3',4'-trimethoxyl-9-oxo-dibenzylbutyrolactone lignan	C ₂₁ H ₂₄ O ₇	388.1522	1
15	(7 <i>R</i> ,8 <i>S</i> ,8' <i>R</i>)-4,7-dihydroxy-3,3',4'-trimethoxyl-9-oxo-dibenzylbutyrolactone lignan-4- <i>O</i> - β -D-glucopyranoside	C ₂₇ H ₃₄ O ₁₂	550.2050	1
16	(7 <i>R</i> ,8 <i>S</i> ,8' <i>R</i>)-4,7,4'-trihydroxy-3,3'- dimethoxyl-9-oxo-dibenzylbutyrolactone lignan-4- <i>O</i> - β -D-glucopyranoside	C ₂₆ H ₃₂ O ₁₂	536.1894	1
17	7,8-didehydroarctigenin	C ₂₁ H ₂₂ O ₆	370.1416	1
18	arctiidilactone	C ₂₀ H ₂₀ O ₈	388.1158	1
19	arctiapolignan A	C ₂₀ H ₂₈ O ₁₀	428.1682	1
20	arctiisesquineolignan A	C ₄₂ H ₅₂ O ₁₉	860.3103	1
21	arctiisesquineolignan B	C ₃₆ H ₄₆ O ₁₆	734.2786	1
22	arctiiphenolglycoside A	C ₁₉ H ₂₈ O ₁₃	464.1530	1
23	arctignan A	C ₃₀ H ₃₄ O ₁₀	554.2152	1
24	arctignan B	C ₃₀ H ₃₂ O ₁₀	552.1995	1
25	arctignan C	C ₃₀ H ₃₂ O ₁₀	552.1995	1
26	arctignan D	C ₄₀ H ₄₄ O ₁₃	732.2782	1
27	arctignan E	C ₄₀ H ₄₄ O ₁₃	732.2782	1

28	arctignan F	C ₄₀ H ₄₂ O ₁₃	730.2625	2
29	arctignan G	C ₄₀ H ₄₄ O ₁₃	732.2782	2
30	arctignan H	C ₄₀ H ₄₄ O ₁₃	732.2782	2
31	lappaol A	C ₃₀ H ₃₂ O ₉	536.2046	1
32	isolappaol A	C ₃₀ H ₃₂ O ₉	536.2046	3
33	lappaol B	C ₃₁ H ₃₄ O ₉	550.2203	1
34	isolappaol C	C ₃₀ H ₃₄ O ₁₀	554.2152	1
35	lappaol C	C ₃₀ H ₃₄ O ₁₀	554.2152	1
36	lappaol D	C ₃₁ H ₃₆ O ₁₀	568.2308	1
37	lappaol E	C ₃₀ H ₃₄ O ₁₀	554.2152	1
38	lappaol F	C ₄₀ H ₄₂ O ₁₂	714.2676	1
39	lappaol H	C ₄₀ H ₄₆ O ₁₄	750.2888	1
40	neoarctin A	C ₄₂ H ₄₆ O ₁₂	742.2989	1
41	neoarctin B	C ₄₂ H ₄₆ O ₁₂	742.2989	1
42	matairesinoside	C ₂₆ H ₃₂ O ₁₁	520.1945	1
43	matairesinol	C ₂₀ H ₂₂ O ₆	358.1416	1
44	matairesinol-4,4'-di- <i>O</i> - β -D-glucopyranoside	C ₃₂ H ₄₂ O ₁₆	682.2473	1
45	pinoresinol	C ₂₀ H ₂₂ O ₆	358.1416	1
46	phylligenin	C ₂₁ H ₂₄ O ₆	372.1573	1
47	styraxlignolide E	C ₂₆ H ₃₂ O ₁₁	520.1945	1
48	styraxlignolide D	C ₂₆ H ₃₂ O ₁₁	520.1945	1
49	syringaresinol	C ₂₂ H ₂₆ O ₈	418.1628	1
50	arctiinoside A	C ₂₆ H ₃₄ O ₁₃	554.1999	1
51	arctiinoside B	C ₃₂ H ₄₂ O ₁₇	698.2422	1
52	(7 <i>S</i> , 8 <i>R</i>)-4,7,9,9'-tetrahydroxy-3,3'-dimethoxy-8- <i>O</i> -4'-neolignan-9'- <i>O</i> - β -D-apiofuranosyl-(1 \rightarrow 6)- <i>O</i> - β -D-glucopyranoside	C ₃₁ H ₄₄ O ₁₆	672.2629	1
53	(8 <i>R</i>)-4,9,9'-trihydroxy-3,3'-dimethoxy-7-oxo-8- <i>O</i> -4'-neolignan-4- <i>O</i> - β -D-glucopyranoside	C ₂₆ H ₃₄ O ₁₂	538.2050	1
54	(7 <i>R</i> ,8 <i>S</i>)-dihydrodehydrodiconiferyl alcohol-7'-oxo-4- <i>O</i> - β -D-glucopyranoside	C ₂₆ H ₃₂ O ₁₂	536.1894	1
55	(7' <i>S</i> , 8' <i>R</i> ,8 <i>S</i>)-4,4',9'-trihydroxy-3,3'-dimethoxy-7',9'-epoxylignan-7-oxo-4- <i>O</i> - β -D-glucopyranoside	C ₂₆ H ₃₂ O ₁₂	536.1894	1
56	trachelogenin	C ₂₁ H ₂₄ O ₇	388.1522	1
57	(7 <i>S</i> ,8 <i>R</i> ,7' <i>S</i>)-Dihydrodehydrodiconiferyl Alcohol-7'-hydroxy-4- <i>O</i> - β -D-glucopyranoside	C ₂₆ H ₃₄ O ₁₂	538.2050	4
58	(7 <i>R</i> ,8 <i>S</i> ,7' <i>S</i>)-Dihydrodehydrodiconiferyl Alcohol-7'-hydroxy-4- <i>O</i> - β -D-glucopyranoside	C ₂₆ H ₃₄ O ₁₂	538.2050	4
59	(8 <i>R</i> ,7' <i>S</i>)-4,9,7',9'-Tetrahydroxy-3,3'-dimethoxy-7-oxo-8-4'-oxyneolignan-4- <i>O</i> - β -D-glucopyranoside	C ₂₆ H ₃₄ O ₁₃	554.1999	4

60	(8 <i>S</i> ,7' <i>S</i>)-4,9,7',9'-Tetrahydroxy-3,3'-dimethoxyl-7-oxo-8-4'-oxyneolignan-4- <i>O</i> - β -D-glucopyranoside	C ₂₆ H ₃₄ O ₁₃	554.1999	4
61	(8 <i>R</i> ,7' <i>R</i> ,8' <i>R</i>)-4,4',7'-Trihydroxy-3,3'-dimethoxyl-9-oxo Dibenzylybutyrolactone Lignan-4- <i>O</i> - β -D-glucopyranoside	C ₂₆ H ₃₂ O ₁₂	536.1894	4
62	(8 <i>R</i> ,7' <i>S</i> ,8' <i>R</i>)-4,4',7'-Trihydroxy-3,3'-dimethoxyl-9-oxo Dibenzylybutyrolactone Lignan-4- <i>O</i> - β -D-glucopyranoside	C ₂₆ H ₃₂ O ₁₂	536.1894	4
63	(7 <i>R</i> ,8 <i>S</i> ,7' <i>S</i> ,8' <i>R</i>)-4,9,4',7'-Tetrahydroxy-3,3'-dimethoxy-7,9'-epoxylignan-4'- <i>O</i> - β -D-glucopyranoside	C ₂₆ H ₃₄ O ₁₂	538.2050	4
64	(7 <i>S</i> ,8 <i>R</i> ,7' <i>R</i> ,8' <i>S</i>)-4,9,4',7'-Tetrahydroxy-3,3'-dimethoxy-7,9'-epoxylignan-4'- <i>O</i> - β -D-glucopyranoside	C ₂₆ H ₃₄ O ₁₂	538.2050	4
65	(7 <i>S</i> ,8 <i>R</i> ,7' <i>S</i> ,8' <i>S</i>)-4,9,4',7'-Tetrahydroxy-3,3'-dimethoxy-7,9'-epoxylignan-4'- <i>O</i> - β -D-glucopyranoside	C ₂₆ H ₃₄ O ₁₂	538.2050	4
66	(7 <i>S</i> ,8 <i>R</i> ,7' <i>R</i> ,8' <i>S</i>)-4,9,4',7'-Tetrahydroxy-3,3'-dimethoxy-7,9'-epoxylignan-4- <i>O</i> - β -D-glucopyranoside	C ₂₆ H ₃₄ O ₁₂	538.2050	4
67	(7 <i>R</i> ,8 <i>S</i>)-7,9,9'-trihydroxy-3,3'-dimethoxy-8- <i>O</i> -4'-neolignan-4- <i>O</i> - β -D-glucopyranoside	C ₂₆ H ₃₆ O ₁₂	540.2207	4
68	(7 <i>S</i> ,8 <i>R</i>)-7,9,9'-trihydroxy-3,3'-dimethoxy-8- <i>O</i> -4'-neolignan-4- <i>O</i> - β -D-glucopyranoside	C ₂₆ H ₃₆ O ₁₂	540.2207	4
69	(7 <i>R</i> ,8 <i>R</i>)-7,9,9'-trihydroxy-3,3'-dimethoxy-8- <i>O</i> -4'-neolignan-4- <i>O</i> - β -D-glucopyranoside	C ₂₆ H ₃₆ O ₁₂	540.2207	4
70	(7 <i>S</i> ,8 <i>S</i>)-7,9,9'-trihydroxy-3,3'-dimethoxy-8- <i>O</i> -4'-neolignan-4- <i>O</i> - β -D-glucopyranoside	C ₂₆ H ₃₆ O ₁₂	540.2207	4
71	(7 <i>R</i> ,7' <i>R</i> ,8 <i>S</i> ,8' <i>S</i>)-(+)-neo-olivil-4- <i>O</i> - β -D-glucopyranoside	C ₂₆ H ₃₄ O ₁₂	538.2050	4
72	Reported compound 1	C ₄₀ H ₄₆ O ₁₃	734.2938	5
73	Reported compound 2	C ₄₀ H ₄₂ O ₁₂	714.2676	5
74	Reported compound 3	C ₃₀ H ₃₄ O ₁₁	570.2101	5
75	(+)-Diasyringaresinol	C ₂₂ H ₂₆ O ₈	418.1628	6
76	Tanegool	C ₂₀ H ₂₄ O ₇	376.1522	6
77	Reported compound 4	C ₂₈ H ₃₀ O ₉	510.1890	5
78	Arctigenic acid	C ₂₁ H ₂₆ O ₇	390.1679	7
Carboxylic acids/Quinic acids and derivatives				
79	Caffeic acid	C ₉ H ₈ O ₄	180.0423	1
80	Caffeic acid 4- <i>O</i> -D-glucoside	C ₁₅ H ₁₈ O ₉	342.0951	1
81	Chlorogenic acid	C ₁₆ H ₁₈ O ₉	354.0951	1
82	<i>p</i> -coumaric acid	C ₉ H ₈ O ₃	164.0473	1
83	3-Coumaroylquinic acid	C ₁₆ H ₁₈ O ₈	338.1002	1
84	4-Coumaroylquinic acid	C ₁₆ H ₁₈ O ₈	338.1002	1
85	5-Coumaroylquinic acid	C ₁₆ H ₁₈ O ₈	338.1002	1
86	Benzoic Acid	C ₇ H ₆ O ₂	122.0368	1
87	Cynarin	C ₂₅ H ₂₄ O ₁₂	516.1268	1
88	Caffeoyl-hexose-hydroxyphenol	C ₂₁ H ₂₂ O ₁₀	434.1213	1

89	1- <i>O</i> -caffeoylquinic acid	C ₁₆ H ₁₈ O ₉	354.0951	1
90	4- <i>O</i> -caffeoylquinic acid	C ₁₆ H ₁₈ O ₉	354.0951	1
91	5- <i>O</i> -caffeoylquinic acid	C ₁₆ H ₁₈ O ₉	354.0951	1
92	1- <i>O</i> -, 5- <i>O</i> -dicaffeoyl-3- <i>O</i> -succinylquinic acid	C ₃₅ H ₄₀ O ₁₅	700.2367	1
93	1- <i>O</i> -, 5- <i>O</i> -dicaffeoyl-3- <i>O</i> -succinylquinic acid	C ₂₉ H ₂₈ O ₁₅	616.1428	1
94	1- <i>O</i> ,5- <i>O</i> -dicaffeoyl-4- <i>O</i> -succinylquinic acid	C ₂₉ H ₃₅ O ₁₅	623.1976	1
95	1- <i>O</i> ,5- <i>O</i> -dicaffeoyl-4- <i>O</i> -succinylquinic acid	C ₂₉ H ₂₈ O ₁₅	616.1428	1
96	1- <i>O</i> -,5- <i>O</i> -dicaffeoyl-3- <i>O</i> -4- <i>O</i> -disuccinylquaieniide	C ₃₃ H ₃₉ O ₁₈	723.2136	1
97	1- <i>O</i> -,5- <i>O</i> -dicaffeoyl-3- <i>O</i> -4- <i>O</i> -disuccinylquaieniide	C ₃₃ H ₃₂ O ₁₈	716.1589	1
98	1- <i>O</i> -,3,5- <i>O</i> -tricaffeoyl-4- <i>O</i> -succinylquinic acid	C ₃₈ H ₄₁ O ₁₈	785.2293	1
99	1- <i>O</i> -,3,5- <i>O</i> -tricaffeoyl-4- <i>O</i> -succinylquinic acid	C ₃₈ H ₃₄ O ₁₈	778.1745	1
100	1,3-di- <i>O</i> -caffeoylquinic acid	C ₂₅ H ₂₄ O ₁₂	516.1268	1
101	1,5-di- <i>O</i> -caffeoylquinic acid	C ₂₅ H ₂₄ O ₁₂	516.1268	1
102	1,5-di- <i>O</i> -caffeoyl-4- <i>O</i> -maloylquinic acid	C ₂₉ H ₂₈ O ₁₆	632.1377	1
103	1,5-di- <i>O</i> -caffeoyl-3- <i>O</i> -maloylquinic acid	C ₂₉ H ₂₈ O ₁₆	632.1377	1
104	1,3,5-tri- <i>O</i> -caffeoylquinic acid	C ₃₄ H ₃₀ O ₁₅	678.1585	1
105	1,5-di- <i>O</i> -caffeoyl-3- <i>O</i> -succinoyl-4- <i>O</i> -maloyquinic acid	C ₃₃ H ₃₂ O ₁₉	732.1538	1
106	5-sinapoylquinic acid	C ₁₈ H ₂₂ O ₁₀	398.1213	1
107	3-sinapoyl-5-caffeoylquinic acid	C ₂₇ H ₂₈ O ₁₃	560.1530	1
108	3-sinapoyl-5-caffeoyl-1-methoxyoxaloylquinic acid	C ₃₀ H ₃₀ O ₁₆	646.1534	1
109	4-sinapoyl-5-caffeoyl-1-methoxyoxaloylquinic acid	C ₃₀ H ₃₀ O ₁₆	646.1534	1
110	3,4- <i>O</i> -dicaffeoylquinic acid	C ₂₅ H ₂₄ O ₁₂	516.1268	1
111	1,4-di- <i>O</i> -caffeoylquinic acid	C ₂₅ H ₂₄ O ₁₂	516.1268	1
112	3,5-di- <i>O</i> -caffeoylquinic acid	C ₂₅ H ₂₄ O ₁₂	516.1268	1
113	4,5- <i>O</i> -dicaffeoylquinic acid	C ₂₅ H ₂₄ O ₁₂	516.1268	1
114	3,5- <i>O</i> -dicaffeoyl-1-methoxyoxaloylquinic acid	C ₂₈ H ₂₆ O ₁₅	602.1272	1
115	3-feruloyl-5-caffeoylquinic acid	C ₂₆ H ₂₆ O ₁₃	546.1373	1
116	4,5-dicaffeoyl-1-methoxyoxaloylquinic acid	C ₂₈ H ₂₆ O ₁₅	602.1272	1
117	3-sinapoyl-5-caffeoyl-4-methoxyoxaloylquinic acid	C ₃₀ H ₃₀ O ₁₆	646.1534	1
118	1,4,5-tricaffeoylquinic acid	C ₃₄ H ₃₀ O ₁₅	678.1585	1
119	3,4,5-tricaffeoylquinic acid	C ₃₄ H ₃₀ O ₁₅	678.1585	1
120	1,4,5-tricaffeoyl-3-methoxyoxaloylquinic acid	C ₃₇ H ₃₂ O ₁₈	764.1589	1
121	3-succinoyl-4,5-dicaffeoyl	C ₂₉ H ₂₈ O ₁₅	616.1428	1
122	1,5-dicaffeoyl-3-succinoylquinic acid	C ₂₉ H ₂₈ O ₁₅	616.1428	1

123	1,5-di- <i>O</i> -caffeoyl-4- <i>O</i> -succinoylquinic acid	C ₂₉ H ₂₈ O ₁₅	616.1428	1
124	3,4-dicaffeoyl-5-succinoylquinic acid	C ₂₉ H ₂₈ O ₁₅	616.1428	1
125	1,3-dicaffeoyl-5-fumaroylquinic acid	C ₂₉ H ₂₆ O ₁₅	614.1272	1
126	1,5-dicaffeoyl-4-fumaroylquinic acid	C ₂₉ H ₂₆ O ₁₅	614.1272	1
127	1,5-dicaffeoyl-3-maloylquinic acid	C ₂₉ H ₂₈ O ₁₆	632.1377	1
128	1,4-di- <i>O</i> -caffeoyl-3- <i>O</i> -maloylquinic acid	C ₂₉ H ₂₈ O ₁₆	632.1377	1
129	1,3-di- <i>O</i> -caffeoyl-4,5-di- <i>O</i> -maloylquinic acid	C ₃₃ H ₃₂ O ₂₀	748.1487	1
130	1,5-dicaffeoyl-4-maloylquinic acid	C ₂₉ H ₂₈ O ₁₆	632.1377	1
131	1,4-di- <i>O</i> -maloyl-3,5-di- <i>O</i> -caffeoylquinic acid	C ₃₃ H ₃₂ O ₂₀	748.1487	1
132	1,3,5-tricaffeoyl-4-succinoylquinic acid	C ₃₈ H ₃₄ O ₁₈	778.1745	1
133	1,5-dicaffeoyl-3,4-disuccinoylquinic acid	C ₃₃ H ₃₂ O ₁₈	716.1589	1
134	1,5-dicaffeoyl-3-fumaroyl-4-succinoylquinic acid	C ₃₃ H ₃₀ O ₁₈	714.1432	1
135	1-fumaroyl-3,5-dicaffeoyl-4-succinoylquinic acid	C ₃₃ H ₃₀ O ₁₈	714.1432	1
136	1,5-di- <i>O</i> -caffeoyl-3- <i>O</i> -succinoyl-4- <i>O</i> -maloylquinic acid	C ₃₃ H ₃₂ O ₁₉	732.1538	1
137	Dimaloyl-dicaffeoylquinic acid isomer 1	C ₃₃ H ₃₂ O ₂₀	748.1487	1
138	Succinoyl-tricaffeoylquinic acid isomer	C ₃₈ H ₃₄ O ₁₈	778.1745	1
139	Maloyl-dicaffeoylquinic acid isomer	C ₂₉ H ₂₈ O ₁₅	616.1428	1
140	Dicaffeoyl-succinoylmalonylquinic acid isomer 1	C ₃₃ H ₃₂ O ₁₉	732.1538	1
141	Dicaffeoyl-succinoylmalonylquinic acid isomer 2	C ₃₃ H ₃₂ O ₂₀	748.1487	1
142	Dimaloyl-dicaffeoylquinic acid isomer 2	C ₃₃ H ₃₂ O ₂₀	748.1487	1
143	Dimaloyl-dicaffeoylquinic acid isomer 3	C ₃₃ H ₃₂ O ₂₀	748.1487	1
144	Maloyl-tricaffeoylquinic isomer	C ₂₈ H ₃₂ O ₁₉	672.1538	1
145	1,3,5-tri- <i>O</i> -caffeoyl-4- <i>O</i> -maloylquinic Acid	C ₃₈ H ₃₄ O ₁₉	794.1694	1
146	5-hydroxymaltol	C ₆ H ₆ O ₄	142.0266	1
147	Succinic acid	C ₄ H ₆ O ₄	118.0266	1
Flavonoids				
148	Baicalin	C ₂₁ H ₁₈ O ₁₁	446.0849	1
149	Luteolin	C ₁₅ H ₁₀ O ₆	286.0477	1
150	Rutin	C ₂₇ H ₃₀ O ₁₆	610.1534	1
151	Quercitrin	C ₂₁ H ₂₀ O ₁₁	448.1006	1
152	Quercetin	C ₁₅ H ₁₀ O ₇	302.0427	1
153	Quercetin-3- <i>O</i> -glucuronide	C ₂₁ H ₁₈ O ₁₃	478.0747	1
154	Quercetin-3-vicianoside	C ₂₆ H ₂₈ O ₁₆	596.1377	1
155	Quercetin rhamnoside (Quercitrin)	C ₂₁ H ₂₀ O ₁₁	448.1006	1

156	Quercimeritrin	$C_{21}H_{20}O_{12}$	464.0955	1
157	Isoquercetin	$C_{21}H_{20}O_{12}$	464.0955	1
158	Astragalin	$C_{21}H_{20}O_{11}$	448.1006	1
159	Kaempferol 3- <i>O</i> - β -rutinoside	$C_{27}H_{30}O_{15}$	594.1585	1
160	Biachanin A	$C_{16}H_{12}O_5$	284.0685	1
161	Genestein	$C_{15}H_{10}O_5$	270.0528	1
162	Nobiletin	$C_{21}H_{22}O_8$	402.1315	1
163	Tangeretin	$C_{20}H_{20}O_7$	372.1209	1
164	8,4'-dimethoxy-6-(2-oxopropyl)-flavone	$C_{20}H_{18}O_5$	338.1154	1
165	8,4'-dimethoxy-6-(3-hydroxypropyl)-flavone	$C_{20}H_{20}O_5$	340.1311	1
Terpenes/Terpenoids				
166	β -eudesmol	$C_{15}H_{26}O$	222.1984	1
167	Ursolic acid	$C_{30}H_{48}O_3$	456.3603	1
168	Oleanolic acid	$C_{30}H_{48}O_3$	456.3603	1
169	Arctiopicrin	$C_{19}H_{26}O_6$	350.1729	1
170	Onopordopicrin	$C_{19}H_{24}O_6$	348.1573	1
171	Dehydrovomifoliol	$C_{13}H_{18}O_3$	222.1256	1
172	Loliolide	$C_{11}H_{16}O_3$	196.1099	1
173	Dehydromelitensin-8-(4'-hydroxymethacrylate)	$C_{15}H_{24}O_6$	300.1573	1
174	Dehydromelitensin	$C_{15}H_{20}O_4$	264.1362	1
175	Melitensin	$C_{15}H_{22}O_4$	266.1518	1
176	3 α -acetoxypop-22(29)-ene	$C_{30}H_{49}O_2$	441.3733	1
177	3 α -hydroxylanosta-5,15-diene	$C_{30}H_{50}O$	426.3862	1
Saccharides/Polysaccharides				
178	Rhamnogalacturonan	$C_{117}H_{178}O_{101}$	3198.8792	1
179	Arabinan	$C_9H_{13}N_3O_5$	243.0855	1
180	Arabinogalactan	$C_{20}H_{36}O_{14}$	500.2105	1
181	Galactan	$C_{18}H_{32}O_{16}$	504.1690	1
182	Cellulose	$C_{64}H_{124}O_{30}$	1372.8177	1
183	Xyloglucan	$C_{51}H_{86}O_{42}$	1370.4594	1
184	Galacturonic acid	$C_6H_{10}O_7$	194.0427	1
185	Galacturonic acid	$C_6H_{10}O_7$	194.0427	1
186	Galactose	$C_6H_{12}O_6$	180.0634	1
187	Glucose	$C_6H_{12}O_6$	180.0634	1

188	Mannose	$C_6H_{12}O_6$	180.0634	1
189	Sucrose	$C_{12}H_{22}O_{11}$	342.1162	1
190	Raffinose	$C_{18}H_{32}O_{16}$	504.1690	1
191	Rhamnose	$C_6H_{12}O_5$	164.0685	1
192	Arabinose	$C_5H_{10}O_5$	150.0528	1
193	Fructose	$C_6H_{12}O_6$	180.0634	1
194	Sorbitol	$C_6H_{14}O_6$	182.0790	1
195	Mannitol	$C_6H_{14}O_6$	182.0790	1
Sterols				
196	β -sitosterol	$C_{29}H_{50}O$	414.3862	1
197	daucosterol	$C_{35}H_{60}O_6$	576.4390	1
198	Daucosterol	$C_{35}H_{60}O_6$	576.4390	1
Fatty acids				
199	Docosanoic acid	$C_{22}H_{44}O_2$	340.3341	1
200	Eicosanoic acid	$C_{20}H_{40}O_2$	312.3028	1
201	cis-13-eicosenoic acid	$C_{20}H_{38}O_2$	310.2872	1
202	Methyl palmitate	$C_{17}H_{34}O_2$	270.2559	1
203	Methyl linoleate	$C_{19}H_{34}O_2$	294.2559	1
204	Methyl linolenate	$C_{19}H_{32}O_2$	292.2402	1
205	Methyl stearate	$C_{19}H_{38}O_2$	298.2872	1
206	Methyl oleate	$C_{19}H_{36}O_2$	296.2715	1
207	Hexadecanoic acid	$C_{16}H_{32}O_2$	256.2402	1
208	9-hexadecenoic acid	$C_{16}H_{30}O_2$	254.2246	1
209	Linoleic acid	$C_{18}H_{32}O_2$	280.2402	1
210	Linolenic acid	$C_{18}H_{30}O_2$	278.2246	1
211	Stearic acid	$C_{18}H_{36}O_2$	284.2715	1
212	9,12-octadecadienoic acid	$C_{18}H_{32}O_2$	280.2402	1
213	Oleic acid	$C_{18}H_{34}O_2$	282.2559	1
214	Oxiraneoctanoic acid	$C_{19}H_{36}O_3$	312.2664	1
215	Tetracosanoic acid	$C_{24}H_{48}O_2$	368.3654	1
Others				
216	Crocin	$C_{44}H_{64}O_{24}$	976.3788	1
217	β -asparagine	$C_4H_8N_2O_3$	132.0535	1

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Table S2 Compounds identified or tentatively characterized in Fructus Arctii by UHPLC/Q-TOF MS.

NO.	t _R (min)	Molecular Formula	Selected ion	Measured ion	Error (mDa)	(ESI-/ESI+) MS fragmentaions	Identification or characterization	Types
1 ⁿ	2.38	C ₁₆ H ₁₉ NO ₉	[M-H] ⁻	368.0975	-0.7	352.1042 [M+H-H ₂ O] ⁺ , 208.0620 [M+H-Glc] ⁺ , 188.0717 [0.2X+H-COOH-OH] ⁺ , 146.0631 [0.2X+H-C ₃ H ₄ O ₄] ⁺	N-glc-3-hydroxy-indoleacetic acid	alkaloid
2*	3.65	C ₁₆ H ₁₈ O ₉	[M-H] ⁻	353.0866	-0.7	191.0571 [M-H-caffeoyl] ⁻ , 179.0347 [M-H-QA] ⁻ , 135.0455 [M-H-QA-CO ₂] ⁻	5-O-caffeoylquinic acid	CA
3	4.83	C ₁₅ H ₁₈ O ₉	[M-H] ⁻	341.0884	1.1	179.0312 [M-H-Glc] ⁻ , 135.0296 [M-H-Glc-CO ₂] ⁻	Caffeic acid 4-O-glucoside	CA
4*	4.97	C ₁₆ H ₁₈ O ₉	[M-H] ⁻	353.0874	0.1	191.0557 [M-H-caffeoyl] ⁻ , 179.0339[M-H-QA] ⁻ , 161.0245 [M-H-QA-H ₂ O] ⁻ , 135.0447 [M-H-QA-CO ₂] ⁻	Chlorogenic acid	CA
5	5.17	C ₂₆ H ₃₄ O ₁₂	[M-H] ⁻	537.1983	1.1	375.1392 [M-H-Glc] ⁻ , 327.1234 [M-H-Glc-2H ₂ O-C] ⁻ , 297.1145 [M-H-Glc-3H ₂ O-2C] ⁻ , 282.0943	Neo-olivil-4-O-β-D-glucopyranoside1	Lignans
6*	5.25	C ₁₆ H ₁₈ O ₉	[M-H] ⁻	353.0872	-0.1	191.0563 [M-H-caffeoyl] ⁻ , 179.0357[M-H-QA] ⁻ , 173.0455, 161.0248 [M-H-QA-H ₂ O] ⁻ , 135.0442 [M-H-QA-CO ₂] ⁻	4-O-caffeoylquinic acid	CA
7	5.28	C ₂₆ H ₃₄ O ₁₂	[M-H] ⁻	537.2000	2.8	375.1207 [M-H-Glc] ⁻ , 327.1264 [M-H-Glc-2H ₂ O-C] ⁻ , 297.1139 [M-H-Glc-3H ₂ O-2C] ⁻ , 282.0923	Neo-olivil-4-O-β-D-glucopyranoside2	Lignans
8	5.45	C ₉ H ₈ O ₄	[M-H] ⁻	179.0352	0.8	135.0454 [M-H-CO ₂] ⁻	caffèic acid	CA
9	5.95	C ₁₆ H ₁₈ O ₈	[M-H] ⁻	337.0916	-0.7	191.0569 [M-H-coumaroyl] ⁻ , 163.0339[M-H-QA] ⁻	3-coumaroylquinic acid	CA
10	5.95	C ₂₆ H ₃₄ O ₁₂	[M-H] ⁻	537.1971	-0.1	375.1424 [M-H-Glc] ⁻ , 357.1353 [M-H-Glc-H ₂ O] ⁻ , 345.1342 [M-H-Glc-H ₂ O-C] ⁻ , 327.1248 [M-H-Glc-C-2H ₂ O] ⁻ , 312.1039,297.1121 [M-H-Glc-3H ₂ O-2C] ⁻ , 191.0624 C ₁₁ H ₁₁ O ₃ , 151.0337 C ₈ H ₇ O ₃	4,9,4',7'-Tetrahydroxy-3,3'-dimethoxy-7,9'-epoxylignan-4-O-β-D-glucopyranoside	Lignans
11	6.11	C ₂₆ H ₃₄ O ₁₂	[M-H] ⁻	537.1971	-0.1	375.1346 [M-H-Glc] ⁻ , 357.1292 [M-H-Glc-H ₂ O] ⁻ , 345.1124 [M-H-Glc-H ₂ O-C] ⁻ , 327.1235 [M-H-Glc-2H ₂ O-C] ⁻ , 312.0995, 297.1056 [M-H-Glc-3H ₂ O-2C] ⁻ , 191.0648 C ₁₁ H ₁₁ O ₃ , 151.0318 C ₈ H ₇ O ₃	4,9,4',7'-Tetrahydroxy-3,3'-dimethoxy-7,9'-epoxylignan-4'-O-β-D-glucopyranoside	Lignans
12	6.64	C ₂₆ H ₃₄ O ₁₂	[M-H] ⁻	537.1964	-0.8	327.1214 [M-H-Glc-2H ₂ O-C] ⁻ , 297.1453 [M-H-Glc-3H ₂ O-2C] ⁻ , 165.0536 C ₉ H ₉ O ₃ , 150.0296 C ₈ H ₆ O ₃	(8R)-4,9,9'-trihydroxy-3,3'-dimethoxy-7-oxo-8-O-4'-neolignan-4-O-β-D-glucopyranoside	Lignans
13	6.72	C ₂₆ H ₃₂ O ₁₂	[M-H] ⁻	535.1814	-0.2	373.1283 [M-H-Glc] ⁻ , 355.1190 [M-H-Glc-H ₂ O] ⁻ , 311.1202 [M-H-Glc-H ₂ O-CO ₂] ⁻ , 173.0650 C ₁₁ H ₉ O ₂	4,7,4'-trihydroxy-3,3'- dimethoxyl-9-oxo-dibenzylbutyrolactonelignan-4-O-β-D-glucopyranoside1	Lignans
14	6.91	C ₃₁ H ₄₄ O ₁₆	[M-H] ⁻	671.2592	4.1	623.2292 [M-H-2H ₂ O-C] ⁻ , 491.1847 [M-H-2H ₂ O-C-Dapi] ⁻ , 343.1339 [M-H-Dapi-C ₁₀ H ₁₂ O ₄] ⁻ , 297.1088 [M-H-Dapi-Glc-C ₂ H ₈ O ₃] ⁻ , 217.0552 C ₁₂ H ₉ O ₄ , 173.0612 C ₁₁ H ₉ O ₂	(7S,8R)-4,7,9,9'-tetrahydroxy-3,3'-dimethoxy-8-O-4'-neolignan-9'-O-β-Dapiofuranosyl-(1+6)-O-β-D-glucopyranoside	Lignans
15	6.92	C ₂₆ H ₃₂ O ₁₂	[M-H] ⁻	535.1808	-0.8	373.1288 [M-H-Glc] ⁻ , 355.1178 [M-H-Glc-H ₂ O] ⁻ , 311.1270 [M-H-Glc-H ₂ O-CO ₂] ⁻ , 173.0567 C ₁₁ H ₉ O ₂	4,7,4'-trihydroxy-3,3'- dimethoxyl-9-oxo-dibenzylbutyrolactonelignan-4-O-β-D-glucopyranoside2	Lignans
16	6.97	C ₂₆ H ₃₆ O ₁₂	[M-H] ⁻	539.2131	0.2	491.1918 [M-H-2HO ₂ -C] ⁻ , 195.0679 C ₁₀ H ₁₁ O ₄ , 165.0475 C ₉ H ₉ O ₃	(7S,8R)-7,9,9'-trihydroxy-3,3'-dimethoxy-8-O-4'-neolignan-4-O-β-D-glucopyranoside	Lignans
17	7.02	C ₂₆ H ₃₂ O ₁₂	[M-H] ⁻	535.1826	1.0	373.1277 [M-H-Glc] ⁻ , 313.1082 [M-H-Glc-CH ₂ O-CO] ⁻ , 298.0839 , 136.0152	7,8-dihydrodehydrodiconiferylalcohol-	Lignans

18	7.14	C ₂₆ H ₃₂ O ₁₂	[M-H] ⁻	535.1856	4.0	373.1277 [M-H-Glc] ⁻ , 355.1158 [M-H-Glc-H ₂ O] ⁻ , 311.1235 [M-H-Glc-H ₂ O-CO ₂] ⁻ , 173.0597 C ₁₁ H ₉ O ₂	7'-oxo-4-O-β-D-glucopyranoside 1 4,7,4'-trihydroxy-3,3'-dimethoxyl-9-oxo-dibenzylbutyrolactonelignan-4-O-β-D-glucopyranoside3	Lignans
19	7.32	C ₂₆ H ₃₂ O ₁₂	[M-H] ⁻	535.1841	2.5	373.1285 [M-H-Glc] ⁻ , 343.1227, 313.1086 [M-H-Glc-CH ₂ O-CO] ⁻ , 298.0806	7,8-dihydrodehydrodiconiferylalcohol-7'-oxo-4-O-β-D-glucopyranoside 2	Lignans
20	7.50	C ₂₀ H ₂₄ O ₇	[M-H] ⁻	375.1476	3.2	345.1269 [M-H-H ₂ O-C] ⁻ , 193.0476 C ₁₀ H ₉ O ₄	Tanegool	Lignans
21	7.56	C ₂₆ H ₃₂ O ₁₂	[M-H] ⁻	535.1825	0.9	373.1334 [M-H-Glc] ⁻ , 151.0410 C ₈ H ₇ O ₃ , 136.0178	(7'S,8'R,8S)-4,4',9'-trihydroxy-3,3'-dimethoxy-7',9-epoxylignan-7-oxo-4-O-β-D-glucopyranoside	Lignans
22	7.71	C ₃₂ H ₄₂ O ₁₆	[M-H] ⁻	681.2393	-0.2	519.1833 [M-H-Glc] ⁻ , 477.1788[M-H-Glc-C ₂ H ₂ O] ⁻ , 357.1339 [M-H-2Glc] ⁻ , 313.1310 [M-H-2Glc-CO ₂] ⁻ , 161.0608C ₁₀ H ₉ O ₂	Matairesinol-4,4'-di-O-β-D-glucopyranoside	Lignans
23	7.89	C ₂₉ H ₃₈ O ₁₃	[M-H] ⁻	593.2267	3.3	431.1768 [M-H-Glc] ⁻ , 413.1558 [M-H-Glc-H ₂ O] ⁻ , 401.1588 [M-H-Glc-H ₂ O-C] ⁻ , 383.1470 [M-H-Glc-2H ₂ O-C] ⁻	5'-propanediolmatairesinoside	Lignans
24 ^{n.a}	7.90	C ₂₈ H ₃₈ O ₁₅	[M-H] ⁻	613.2163	3.1	451.1562 [M-H-Glc] ⁻ , 179.0375 [caffeic acid-H] ⁻ , 161.0246, 135.0453 [caffeic acid-H-CO ₂] ⁻	Unknown	Others
25	7.94	C ₂₀ H ₂₈ O ₁₀	[M-H+HCOOH] ⁻	473.1672	1.3	249.1073 [M+H-Glc-H ₂ O] ⁺ , 233.0812 [M+H-Glc-H ₂ O-CH ₄] ⁺ , 189.0884 C ₁₂ H ₁₃ O ₂	Arctiiapolignan A	Lignans
26*	8.47	C ₂₅ H ₂₄ O ₁₂	[M-H] ⁻	515.1189	-0.1	353.0875 [M-H-caffeoyl] ⁻ , 335.0766 [M-H-caffeoyl-H ₂ O] ⁻ , 191.0568 [M-H-2caffeoyl] ⁻ , 179.0347 [M-H-caffeoyl-QA] ⁻ , 161.0244 [M-H-caffeoyl-QA-H ₂ O] ⁻ , 135.0461 [M-H-caffeoyl-QA-2H ₂ O] ⁻	3,4-O-dicaffeoylquinic acid	CA
27 ^{n.a}	8.50	C ₄₀ H ₄₈ O ₁₄	[M-H] ⁻	751.3006	4.0	733.2917 [M-H-H ₂ O] ⁻ , 715.2670 [M-H-2H ₂ O] ⁻ , 685.2666 [M-H-3H ₂ O-C] ⁻ , 679.2513 [M-H-4H ₂ O] ⁻ , 667.2418 [M-H-4H ₂ O-C] ⁻ , 637.2427 [M-H-4H ₂ O-2C] ⁻ , 625.2454 [M-H-4H ₂ O-3C] ⁻ , 573.2029 [M-H-C ₇ H ₁₀ O ₄ -2H ₂ O] ⁻ , 561.2121 [M-H-C ₇ H ₁₀ O ₄ -2H ₂ O-C] ⁻ , 531.2042 [M-H-C ₇ H ₁₀ O ₄ -3H ₂ O-2C] ⁻ , 283.0987 C ₁₇ H ₁₅ O ₄	Lappaol H+2H 1	Lignans
28*	8.69	C ₂₅ H ₂₄ O ₁₂	[M-H] ⁻	515.1192	0.2	353.0879 [M-H-caffeoyl] ⁻ , 191.0558 [M-H-2caffeoyl] ⁻ , 179.0353 [M-H-caffeoyl-QA] ⁻ , 161.0239 [M-H-caffeoyl-QA-H ₂ O] ⁻ , 135.0451 [M-H-caffeoyl-QA-2H ₂ O] ⁻	3,5-O-dicaffeoylquinic acid	CA
29	8.83	C ₃₀ H ₃₄ O ₁₁	[M-H] ⁻	569.2009	-1.4	533.1802 [M-H-2H ₂ O] ⁻ , 521.1802 [M-H-2H ₂ O-C] ⁻ , 503.1741 [M-H-3H ₂ O-C] ⁻ , 459.1791 [M-H-3H ₂ O-2C] ⁻ , 427.1400 [M-H-C ₇ H ₁₀ O ₃] ⁻ , 415.1392 [M-H-C ₈ H ₁₀ O ₃] ⁻ , 397.1281 [M-H-C ₈ H ₁₀ O ₃ -H ₂ O] ⁻ , 367.1194 [M-H-C ₈ H ₁₀ O ₃ -2H ₂ O-C] ⁻	Reported compound 1	Lignans
30 ^{n.a}	8.90	C ₄₀ H ₄₈ O ₁₄	[M-H] ⁻	751.2966	0.1	733.2831 [M-H-H ₂ O] ⁻ , 715.2712 [M-H-2H ₂ O] ⁻ , 679.2539 [M-H-4H ₂ O] ⁻ , 667.2507 [M-H-4H ₂ O-C] ⁻ , 655.2531 [M-H-4H ₂ O-2C] ⁻ , 609.2316 [M-H-C ₇ H ₁₀ O ₄] ⁻ , 591.2097 [M-H-C ₇ H ₁₀ O ₄ -H ₂ O] ⁻ , 573.2109 [M-H-C ₇ H ₁₀ O ₄ -2H ₂ O] ⁻ , 561.2130 [M-H-C ₇ H ₁₀ O ₄ -2H ₂ O-C] ⁻ , 549.2144 [M-H-C ₇ H ₁₀ O ₄ -2H ₂ O-2C] ⁻ , 383.1477 C ₂₂ H ₂₃ O ₆ , 371.1492 C ₂₁ H ₂₃ O ₆ , 283.0945 C ₁₇ H ₁₅ O ₄	Lappaol H+2H 2	Lignans
31 ^{n.a}	8.95	C ₃₀ H ₃₄ O ₁₁	[M-H] ⁻	569.2004	-1.9	533.1821 [M-H-2H ₂ O] ⁻ , 521.1889 [M-H-2H ₂ O-C] ⁻ , 503.1702 [M-H-3H ₂ O-C] ⁻ , 459.1726 [M-H-3H ₂ O-2C] ⁻ , 427.1318 [M-H-C ₇ H ₁₀ O ₃] ⁻ , 415.1403 [M-H-C ₈ H ₁₀ O ₃] ⁻ , 397.1143 [M-H-C ₈ H ₁₀ O ₃ -H ₂ O] ⁻ , 367.1235 [M-H-C ₈ H ₁₀ O ₃ -2H ₂ O-C] ⁻	Isomer of reported compound 1	Lignans

32*	8.97	C ₂₅ H ₂₄ O ₁₂	[M-H] ⁻	515.1187	-0.3	353.0867 [M-H-caffeoyl] ⁻ , 191.0557 [M-H-2caffeoyl] ⁻ , 179.0346 [M-H-caffeoyl-QA] ⁻ , 161.0256 [M-H-caffeoyl-QA-H ₂ O] ⁻ , 135.0450 [M-H-caffeoyl-QA-2H ₂ O] ⁻	4,5- <i>O</i> -dicaffeoylquinic acid	CA
33	9.22	C ₂₇ H ₃₄ O ₁₂	[M-H+HCOOH] ⁻	595.2048	2.1	371.1485 [M+H-Glc-H ₂ O] ⁺ , 247.0966 [M+H-Glc-H ₂ O-C ₇ H ₈ O ₂] ⁺ , 203.1089 C ₁₃ H ₁₅ O ₂ , 151.0738 C ₉ H ₁₁ O ₂	(7 <i>S</i> ,8 <i>S</i> ,8' <i>R</i>)-4,7-dihydroxy-3,3',4'-trimethoxyl-9-oxo-dibenzylbutyrolactonelignan-4- <i>O</i> -β-D-glucopyranoside	Lignans
34	9.35	C ₂₅ H ₂₄ O ₁₂	[M-H] ⁻	515.1198	0.8	353.0872 [M-H-caffeoyl] ⁻ , 191.0560 [M-H-2caffeoyl] ⁻ , 179.0350 [M-H-caffeoyl-QA] ⁻ , 161.0234 [M-H-caffeoyl-QA-H ₂ O] ⁻ , 135.0452 [M-H-caffeoyl-QA-2H ₂ O] ⁻	1,5- <i>O</i> -dicaffeoylquinic acid	CA
35	9.84	C ₄₂ H ₅₂ O ₁₉	[M-H] ⁻	859.3033	0.8	697.2508 [M-H-Glc] ⁻ , 535.1967 [M-H-2Glc] ⁻ , 517.1878 [M-H-2Glc-H ₂ O] ⁻ , 505.1885 [M-H-2Glc-H ₂ O-C] ⁻	Arctiisquineolignan A	Lignans
36	9.87	C ₂₆ H ₃₂ O ₁₁	[M-H] ⁻	519.1865	-0.1	357.1334 [M-H-Glc] ⁻ , 342.1086 [M-H-Glc-CH ₃] ⁻ , 313.1322 [M-H-Glc-CO ₂] ⁻	Styraxlignolide E	Lignans
37 ^{n.a}	9.95	C ₅₀ H ₅₈ O ₁₈	[M-H] ⁻	945.3549	0.4	927.3462 [M-H-H ₂ O] ⁻ , 909.3406 [M-H-2H ₂ O] ⁻ , 897.3348 [M-H-2H ₂ O-C] ⁻ , 891.3221 [M-H-3H ₂ O] ⁻ , 879.3265 [M-H-3H ₂ O-C] ⁻ , 873.3196 [M-H-4H ₂ O] ⁻ , 861.3143 [M-H-4H ₂ O-C] ⁻ , 843.2952 [M-H-5H ₂ O-C] ⁻ , 837.2925 [M-H-6H ₂ O] ⁻ , 731.2539 [M-H-5H ₂ O-C ₇ H ₈ O ₂] ⁻ , 719.2501 [M-H-5H ₂ O-C ₇ H ₈ O ₂ -C] ⁻ , 707.2517 [M-H-5H ₂ O-C ₇ H ₈ O ₂ -2C] ⁻ , 607.2224 [M-H-C ₁₇ H ₂₂ O ₇] ⁻ , 595.2129 [M-H-C ₁₇ H ₂₂ O ₇ -C] ⁻ , 589.2062 [M-H-C ₁₇ H ₂₂ O ₇ -H ₂ O] ⁻ , 571.1993 [M-H-C ₁₇ H ₂₂ O ₇ -2H ₂ O] ⁻ , 559.1963 [M-H-C ₁₇ H ₂₂ O ₇ -2H ₂ O-C] ⁻ , 547.2011 [M-H-C ₁₇ H ₂₂ O ₇ -2H ₂ O-2C] ⁻	Unknown	Lignans
38*	10.04	C ₂₆ H ₃₂ O ₁₁	[M-H] ⁻	519.1865	-0.1	357.1344 [M-H-Glc] ⁻ , 342.1103 [M-H-Glc-CH ₃] ⁻ , 313.1451 [M-H-Glc-CO ₂] ⁻ , 221.0825 C ₁₂ H ₁₃ O ₄ , 209.0807 C ₁₁ H ₁₃ O ₄	Matairesinoside	Lignans
39 ^{n.a}	10.08	C ₅₀ H ₅₈ O ₁₈	[M-H] ⁻	945.3546	0.1	927.3482 [M-H-H ₂ O] ⁻ , 909.3420 [M-H-2H ₂ O] ⁻ , 897.3309 [M-H-2H ₂ O-C] ⁻ , 879.3152 [M-H-3H ₂ O-C] ⁻ , 861.3094 [M-H-4H ₂ O-C] ⁻ , 785.2729 [M-H-C ₇ H ₁₂ O ₄] ⁻ , 719.2399 [M-H-C ₈ H ₁₈ O ₇] ⁻ , 707.2440 [M-H-C ₈ H ₁₈ O ₇ -C] ⁻ , 695.2475 [M-H-C ₈ H ₁₈ O ₇ -2C] ⁻ , 607.2203 [M-H-C ₁₇ H ₂₂ O ₇] ⁻ , 589.2079 [M-H-C ₁₇ H ₂₂ O ₇ -H ₂ O] ⁻ , 571.1993 [M-H-C ₁₇ H ₂₂ O ₇ -2H ₂ O] ⁻ , 559.1992 [M-H-C ₁₇ H ₂₂ O ₇ -2H ₂ O-C] ⁻ , 547.1976 [M-H-C ₁₇ H ₂₂ O ₇ -2H ₂ O-2C] ⁻	Unknown	Lignans
40	10.12	C ₄₀ H ₄₆ O ₁₄	[M-H] ⁻	749.2876	-3.3	731.2716 [M-H-H ₂ O] ⁻ , 713.2588 [M-H-2H ₂ O] ⁻ , 683.2467 [M-H-2H ₂ O-CH ₂ O] ⁻ , 677.2382 [M-H-4H ₂ O] ⁻ , 665.2383 [M-H-4H ₂ O-C] ⁻ , 653.2382 [M-H-4H ₂ O-2C] ⁻ , 607.2177 [M-H-C ₇ H ₁₀ O ₄] ⁻ , 589.2061 [M-H-C ₇ H ₁₀ O ₄ -H ₂ O] ⁻ , 571.1962 [M-H-C ₇ H ₁₀ O ₄ -2H ₂ O] ⁻ , 559.1967 [M-H-C ₇ H ₁₀ O ₄ -2H ₂ O-C] ⁻ , 547.1993 [M-H-C ₇ H ₁₀ O ₄ -2H ₂ O-2C] ⁻ , 531.2050 [M-H-C ₇ H ₁₀ O ₄ -2H ₂ O-2C-O] ⁻ , 381.1359 C ₂₂ H ₂₁ O ₆ , 369.1400 C ₂₁ H ₂₁ O ₆ , 297.1141 C ₁₈ H ₁₇ O ₄ , 283.0968 C ₁₇ H ₁₅ O ₄ , 269.0827 C ₁₆ H ₁₃ O ₄	Lappaol H	Lignans
41	10.21	C ₃₃ H ₄₄ O ₁₆	[M-H+HCOOH] ⁻	741.2603	-0.3	371.1504 [M-H-Gal-Glc] ⁻ , 357.1302 [M-H-Gal-Glc-CH ₂] ⁻	Arctigenin-4- <i>O</i> -α-D-galactopyranosyl-(1→6)- <i>O</i> -β-D-glucopyranoside	Lignans

42	10.36	C ₃₃ H ₄₄ O ₁₆	[M-H+HCOOH] ⁻	741.2603	-0.3	371.1467 [M-H-Gen] ⁻ , 357.1354 [M-H-Gen-CH ₂] ⁻ 927.3464 [M-H-H ₂ O] ⁻ , 909.3374 [M-H-2H ₂ O] ⁻ , 897.3365 [M-H-2H ₂ O-C] ⁻ , 803.2944 [M-H-C ₇ H ₁₀ O ₃] ⁻ , 791.2944 [M-H-C ₇ H ₁₀ O ₃ -C] ⁻ , 779.2865 [M-H-C ₇ H ₁₀ O ₃ -2C] ⁻ , 747.2700 [M-H-C ₁₀ H ₁₄ O ₄] ⁻ , 729.2593 [M-H-C ₁₀ H ₁₄ O ₄ -H ₂ O] ⁻ , 561.2154 [M-H-C ₁₈ H ₂₄ O ₉] ⁻ , 549.2164 [M-H-C ₁₈ H ₂₄ O ₉ -C] ⁻ , 543.2064 [M-H-C ₁₈ H ₂₄ O ₉ -H ₂ O] ⁻ , 531.2056 [M-H-C ₁₈ H ₂₄ O ₉ -H ₂ O-C] ⁻ , 517.1867 [M-H-C ₁₈ H ₂₄ O ₉ -H ₂ O-C-CH ₂] ⁻ , 505.1927 [M-H-C ₁₈ H ₂₄ O ₉ -H ₂ O-2C-CH ₂] ⁻ , 455.1721 [M-H-C ₂₅ H ₃₀ O ₁₀] ⁻ , 443.1726 [M-H-C ₂₅ H ₃₀ O ₁₀ -C] ⁻ , 437.1549 [M-H-C ₂₅ H ₃₀ O ₁₀ -H ₂ O] ⁻ , 425.1621 [M-H-C ₂₅ H ₃₀ O ₁₀ -C-H ₂ O] ⁻ , 409.1605 [M-H-C ₂₅ H ₃₀ O ₁₀ -CO-H ₂ O] ⁻ 517.1909 [M-H-2H ₂ O] ⁻ , 505.1886 [M-H-2H ₂ O-C] ⁻ , 475.1722 [M-H-2H ₂ O-C-CH ₂ O] ⁻ , 411.1457 [M-H-C ₇ H ₁₀ O ₃] ⁻ , 399.1420 [M-H-C ₇ H ₁₀ O ₃ -C] ⁻	Arctigenin-4- <i>O</i> -β-D-gentiobioside	Lignans
43 ^{n,a}	10.53	C ₅₀ H ₅₈ O ₁₈	[M-H] ⁻	945.3549	0.4	C ₁₈ H ₂₄ O ₉ -H ₂ O] ⁻ , 531.2056 [M-H-C ₁₈ H ₂₄ O ₉ -H ₂ O-C] ⁻ , 517.1867 [M-H-C ₁₈ H ₂₄ O ₉ -H ₂ O-C-CH ₂] ⁻ , 505.1927 [M-H-C ₁₈ H ₂₄ O ₉ -H ₂ O-2C-CH ₂] ⁻ , 455.1721 [M-H-C ₂₅ H ₃₀ O ₁₀] ⁻ , 443.1726 [M-H-C ₂₅ H ₃₀ O ₁₀ -C] ⁻ , 437.1549 [M-H-C ₂₅ H ₃₀ O ₁₀ -H ₂ O] ⁻ , 425.1621 [M-H-C ₂₅ H ₃₀ O ₁₀ -C-H ₂ O] ⁻ , 409.1605 [M-H-C ₂₅ H ₃₀ O ₁₀ -CO-H ₂ O] ⁻ 517.1909 [M-H-2H ₂ O] ⁻ , 505.1886 [M-H-2H ₂ O-C] ⁻ , 475.1722 [M-H-2H ₂ O-C-CH ₂ O] ⁻ , 411.1457 [M-H-C ₇ H ₁₀ O ₃] ⁻ , 399.1420 [M-H-C ₇ H ₁₀ O ₃ -C] ⁻	Unknown	Lignans
44	10.57	C ₃₀ H ₃₄ O ₁₀	[M-H] ⁻	553.2079	0.5	[M-H-2H ₂ O-C-CH ₂ O] ⁻ , 411.1457 [M-H-C ₇ H ₁₀ O ₃] ⁻ , 399.1420 [M-H-C ₇ H ₁₀ O ₃ -C] ⁻	Arctignan A	Lignans
45	10.88	C ₃₂ H ₄₂ O ₁₅	[M-H+HCOOH] ⁻	711.2520	2.0	373.1568 [M+H-Api-Glc] ⁺ , 355.1512 [M+H-Api-Glc-H ₂ O] ⁺ 927.3433 [M-H-H ₂ O] ⁻ , 909.3214 [M-H-2H ₂ O] ⁻ , 879.3303 [M-H-3H ₂ O-C] ⁻ , 861.3129 [M-H-4H ₂ O-C] ⁻ , 747.2651 [M-H-C ₁₀ H ₁₄ O ₄] ⁻ , 729.2482 [M-H-C ₁₀ H ₁₄ O ₄ -H ₂ O] ⁻ , 663.2224 [M-H-C ₁₀ H ₁₄ O ₄ -4H ₂ O-C] ⁻ , 651.2294 [M-H-C ₁₀ H ₁₄ O ₄ -4H ₂ O-2C] ⁻ , 557.1829 [M-H-C ₁₈ H ₂₈ O ₉] ⁻ , 531.1929 [M-H-C ₁₈ H ₂₈ O ₉ -H ₂ O-C] ⁻ , 517.1909 [M-H-C ₁₈ H ₂₈ O ₉ -H ₂ O-2C-2H] ⁻ , 505.1860 [M-H-C ₁₈ H ₂₈ O ₉ -O-3C] ⁻	Arctigenin-4- <i>O</i> -β-D-apiofuranosyl-(1→6)- <i>O</i> -β-D-glucopyranoside1	Lignans
46 ^{n,a}	11.05	C ₅₀ H ₅₈ O ₁₈	[M-H] ⁻	945.3549	0.4	C ₁₀ H ₁₄ O ₄ -4H ₂ O-C] ⁻ , 651.2294 [M-H-C ₁₀ H ₁₄ O ₄ -4H ₂ O-2C] ⁻ , 557.1829 [M-H-C ₁₈ H ₂₈ O ₉] ⁻ , 531.1929 [M-H-C ₁₈ H ₂₈ O ₉ -H ₂ O-C] ⁻ , 517.1909 [M-H-C ₁₈ H ₂₈ O ₉ -H ₂ O-2C-2H] ⁻ , 505.1860 [M-H-C ₁₈ H ₂₈ O ₉ -O-3C] ⁻	Unknown	Lignans
47	11.07	C ₃₂ H ₄₂ O ₁₅	[M-H+HCOOH] ⁻	711.2532	3.2	373.1621 [M+H-Api-Glc] ⁺ , 355.1624 [M+H-Api-Glc-H ₂ O] ⁺	Arctigenin-4- <i>O</i> -β-D-apiofuranosyl-(1→6)- <i>O</i> -β-D-glucopyranoside2	Lignans
48 ⁿ	11.22	C ₂₇ H ₃₂ O ₁₁	[M-H+HCOOH] ⁻	577.1937	1.6	369.1364 [M-H-Glc] ⁻ , 354.1084 [M-H-Glc-CH ₃] ⁻ , 203.0352 C ₁₁ H ₇ O ₄ , 174.0683 C ₁₁ H ₁₀ O ₂ , 159.0374 C ₁₀ H ₇ O ₂ 927.3427 [M-H-H ₂ O] ⁻ , 909.3539 [M-H-2H ₂ O] ⁻ , 897.3338 [M-H-2H ₂ O-C] ⁻ , 879.3211 [M-H-3H ₂ O-C] ⁻ , 861.3249 [M-H-4H ₂ O-C] ⁻ , 849.3149 [M-H-4H ₂ O-2C] ⁻ , 803.2888 [M-H-C ₇ H ₁₀ O ₃] ⁻ , 665.2405 [M-H-C ₁₁ H ₂₀ O ₈] ⁻ , 561.2144 [M-H-C ₁₈ H ₂₄ O ₉] ⁻ , 549.2159 [M-H-C ₁₈ H ₂₄ O ₉ -C] ⁻ , 543.2045 [M-H-C ₁₈ H ₂₄ O ₉ -H ₂ O] ⁻ , 531.2003 [M-H-C ₁₈ H ₂₄ O ₉ -H ₂ O-C] ⁻ , 517.1884 [M-H-C ₁₈ H ₂₄ O ₉ -H ₂ O-C-CH ₂] ⁻ , 505.1880 [M-H-C ₁₈ H ₂₄ O ₉ -H ₂ O-2C-CH ₂] ⁻ , 455.1650 [M-H-C ₂₅ H ₃₀ O ₁₀] ⁻ 927.3459 [M-H-H ₂ O] ⁻ , 909.3396 [M-H-2H ₂ O] ⁻ , 897.3337 [M-H-2H ₂ O-C] ⁻ , 879.3193 [M-H-3H ₂ O-C] ⁻ , 861.3155 [M-H-4H ₂ O-C] ⁻ , 849.3155 [M-H-4H ₂ O-2C] ⁻ , 803.2881 [M-H-C ₇ H ₁₀ O ₃] ⁻ , 665.2411 [M-H-C ₁₁ H ₂₀ O ₈] ⁻ , 653.2399 [M-H-C ₁₁ H ₂₀ O ₈ -C] ⁻ , 561.2106 [M-H-C ₁₈ H ₂₄ O ₉] ⁻ , 549.2118 [M-H-C ₁₈ H ₂₄ O ₉ -C] ⁻ , 531.1990 [M-H-C ₁₈ H ₂₄ O ₉ -H ₂ O-C] ⁻ , 517.1878 [M-H-C ₁₈ H ₂₄ O ₉ -H ₂ O-C-CH ₂] ⁻ , 505.1909 [M-H-C ₁₈ H ₂₄ O ₉ -H ₂ O-2C-CH ₂] ⁻ , 455.1564 [M-H-C ₂₅ H ₃₀ O ₁₀] ⁻ , 443.1540 [M-H-C ₂₅ H ₃₀ O ₁₀ -C] ⁻	Hemislienoside	Lignans
49 ^{n,a}	11.29	C ₅₀ H ₅₈ O ₁₈	[M-H] ⁻	945.3549	0.4	C ₁₈ H ₂₄ O ₉ -H ₂ O] ⁻ , 531.2003 [M-H-C ₁₈ H ₂₄ O ₉ -H ₂ O-C] ⁻ , 517.1884 [M-H-C ₁₈ H ₂₄ O ₉ -H ₂ O-C-CH ₂] ⁻ , 505.1880 [M-H-C ₁₈ H ₂₄ O ₉ -H ₂ O-2C-CH ₂] ⁻ , 455.1650 [M-H-C ₂₅ H ₃₀ O ₁₀] ⁻ 927.3459 [M-H-H ₂ O] ⁻ , 909.3396 [M-H-2H ₂ O] ⁻ , 897.3337 [M-H-2H ₂ O-C] ⁻ , 879.3193 [M-H-3H ₂ O-C] ⁻ , 861.3155 [M-H-4H ₂ O-C] ⁻ , 849.3155 [M-H-4H ₂ O-2C] ⁻ , 803.2881 [M-H-C ₇ H ₁₀ O ₃] ⁻ , 665.2411 [M-H-C ₁₁ H ₂₀ O ₈] ⁻ , 653.2399 [M-H-C ₁₁ H ₂₀ O ₈ -C] ⁻ , 561.2106 [M-H-C ₁₈ H ₂₄ O ₉] ⁻ , 549.2118 [M-H-C ₁₈ H ₂₄ O ₉ -C] ⁻ , 531.1990 [M-H-C ₁₈ H ₂₄ O ₉ -H ₂ O-C] ⁻ , 517.1878 [M-H-C ₁₈ H ₂₄ O ₉ -H ₂ O-C-CH ₂] ⁻ , 505.1909 [M-H-C ₁₈ H ₂₄ O ₉ -H ₂ O-2C-CH ₂] ⁻ , 455.1564 [M-H-C ₂₅ H ₃₀ O ₁₀] ⁻ , 443.1540 [M-H-C ₂₅ H ₃₀ O ₁₀ -C] ⁻	Unknown	Lignans
50 ^{n,a}	11.39	C ₅₀ H ₅₈ O ₁₈	[M-H] ⁻	945.3549	0.4	C ₁₁ H ₂₀ O ₈ -C] ⁻ , 561.2106 [M-H-C ₁₈ H ₂₄ O ₉] ⁻ , 549.2118 [M-H-C ₁₈ H ₂₄ O ₉ -C] ⁻ , 531.1990 [M-H-C ₁₈ H ₂₄ O ₉ -H ₂ O-C] ⁻ , 517.1878 [M-H-C ₁₈ H ₂₄ O ₉ -H ₂ O-C-CH ₂] ⁻ , 505.1909 [M-H-C ₁₈ H ₂₄ O ₉ -H ₂ O-2C-CH ₂] ⁻ , 455.1564 [M-H-C ₂₅ H ₃₀ O ₁₀] ⁻ , 443.1540 [M-H-C ₂₅ H ₃₀ O ₁₀ -C] ⁻	Unknown	Lignans
51 ^{n,a}	11.41	C ₄₀ H ₄₆ O ₁₄	[M-H] ⁻	749.2803	-0.6	731.2734 [M-H-H ₂ O] ⁻ , 713.2621 [M-H-2H ₂ O] ⁻ , 701.2598 [M-	Unknown	Lignans

52	11.46	C ₃₀ H ₃₄ O ₁₀	[M-H] ⁻	553.2084	1.0	H-2H ₂ O-C ⁻], 695.2499 [M-H-3H ₂ O] ⁻ , 677.2419 [M-H-4H ₂ O] ⁻ , 665.2399 [M-H-4H₂O-C]⁻ , 653.2397 [M-H-4H ₂ O-2C] ⁻ , 607.2142 [M-H-C ₇ H ₁₀ O ₃] ⁻ , 571.2095 [M-H-C ₇ H ₁₀ O ₃ -2H ₂ O] ⁻ , 559.1992 [M-H-C ₇ H ₁₀ O ₃ -2H ₂ O-C] ⁻ , 547.1972 [M-H-C ₇ H ₁₀ O ₃ -2H ₂ O-2C] ⁻ , 283.1004 C ₁₇ H ₁₅ O ₄ , 269.0808 C ₁₆ H ₁₃ O ₄ , 517.1888 [M-H-2H ₂ O] ⁻ , 505.1888 [M-H-2H₂O-C]⁻ , 475.1426 [M-H-2H ₂ O-C-CH ₂ O] ⁻ , 411.1464 [M-H-C ₇ H ₁₀ O ₃] ⁻ , 399.1460 [M-H-C ₇ H ₁₀ O ₃ -C] ⁻ , 731.2726 [M-H-H ₂ O] ⁻ , 713.2621 [M-H-2H ₂ O] ⁻ , 701.2627[M-H-2H₂O-C]⁻ , 683.2510[M-H-2H ₂ O-CH ₂ O] ⁻ , 665.2396 [M-H-4H ₂ O-C] ⁻ , 653.2400 [M-H-4H ₂ O-2C] ⁻ , 607.2191 [M-H-C ₇ H ₁₀ O ₃] ⁻ , 589.2055 [M-H-C ₇ H ₁₀ O ₃ -H ₂ O] ⁻ , 571.2007 [M-H-C ₇ H ₁₀ O ₃ -2H ₂ O] ⁻ , 559.2000 [M-H-C ₇ H ₁₀ O ₃ -2H ₂ O-C] ⁻ , 283.0990 C ₁₇ H ₁₅ O ₄ , 269.0835 C ₁₆ H ₁₃ O ₄ , 371.1519 [M-H-Glc]⁻ , 357.1269 [M-H-Glc-H ₂ O] ⁻ , 235.0983 C ₁₃ H ₁₅ O ₄ , 121.0359 C ₇ H ₅ O ₂	Isolappaol C	Lignans
53 ^{n.a}	11.49	C ₄₀ H ₄₆ O ₁₄	[M-H] ⁻	749.2817	0.8	517.1885 [M-H-2H ₂ O] ⁻ , 505.1881 [M-H-2H₂O-C]⁻ , 411.1461 [M-H-C ₇ H ₁₀ O ₃] ⁻ , 399.1470 [M-H-C ₇ H ₁₀ O ₃ -C] ⁻ , 731.2709 [M-H-H ₂ O] ⁻ , 713.2628 [M-H-2H ₂ O] ⁻ , 701.2604 [M-H-2H₂O-C]⁻ , 695.2542 [M-H-3H ₂ O] ⁻ , 683.2504 [M-H-2H ₂ O-CH ₂ O] ⁻ , 665.2426[M-H-4H ₂ O-C] ⁻ , 653.2403 [M-H-4H ₂ O-2C] ⁻ , 607.2191 [M-H-C ₇ H ₁₀ O ₃] ⁻ , 589.2085 [M-H-C ₇ H ₁₀ O ₃ -H ₂ O] ⁻ , 571.1968 [M-H-C ₇ H ₁₀ O ₃ -2H ₂ O] ⁻ , 381.1357 C ₂₂ H ₂₁ O ₆ , 297.1127 C ₁₈ H ₁₇ O ₄	Unknown	Lignans
54*	11.56	C ₂₇ H ₃₄ O ₁₁	[M-H+HCOOH] ⁻	579.2119	4.1	371.1519 [M-H-Glc]⁻ , 357.1269 [M-H-Glc-H ₂ O] ⁻ , 235.0983 C ₁₃ H ₁₅ O ₄ , 121.0359 C ₇ H ₅ O ₂	Arctiin	Lignans
55	11.69	C ₃₀ H ₃₄ O ₁₀	[M-H] ⁻	553.2084	1.0	517.1885 [M-H-2H ₂ O] ⁻ , 505.1881 [M-H-2H₂O-C]⁻ , 411.1461 [M-H-C ₇ H ₁₀ O ₃] ⁻ , 399.1470 [M-H-C ₇ H ₁₀ O ₃ -C] ⁻ , 731.2709 [M-H-H ₂ O] ⁻ , 713.2628 [M-H-2H ₂ O] ⁻ , 701.2604 [M-H-2H₂O-C]⁻ , 695.2542 [M-H-3H ₂ O] ⁻ , 683.2504 [M-H-2H ₂ O-CH ₂ O] ⁻ , 665.2426[M-H-4H ₂ O-C] ⁻ , 653.2403 [M-H-4H ₂ O-2C] ⁻ , 607.2191 [M-H-C ₇ H ₁₀ O ₃] ⁻ , 589.2085 [M-H-C ₇ H ₁₀ O ₃ -H ₂ O] ⁻ , 571.1968 [M-H-C ₇ H ₁₀ O ₃ -2H ₂ O] ⁻ , 381.1357 C ₂₂ H ₂₁ O ₆ , 297.1127 C ₁₈ H ₁₇ O ₄	Lappaol C	Lignans
56 ⁿ	11.75	C ₄₀ H ₄₆ O ₁₄	[M-H] ⁻	749.2809	0.0	371.1504 [M-H-H ₂ O] ⁻ , 330.1502 [M-H-COOH-CH₂]⁻ , 909.3343 [M-H-H ₂ O] ⁻ , 879.3279 [M-H-2H ₂ O-C] ⁻ , 861.3060 [M-H-3H ₂ O-C] ⁻ , 843.3069 [M-H-4H ₂ O-C] ⁻ , 837.3087[M-H-5H ₂ O] ⁻ , 825.2944 [M-H-5H ₂ O-C] ⁻ , 813.2916 [M-H-5H₂O-2C]⁻ , 801.2926 [M-H-5H ₂ O-3C] ⁻ , 785.2798 [M-H-C ₇ H ₁₀ O ₃] ⁻ , 737.2724 [M-H-C ₇ H ₁₀ O ₃ -4C] ⁻ , 719.2517 [M-H-C ₈ H ₁₆ O ₆] ⁻ , 707.2501 [M-H-C ₈ H ₁₆ O ₆ -C] ⁻ , 567.2302 [M-H-Glc] ⁻ , 553.2021 [M-H-Glc-CH ₂] ⁻ , 549.2149[M-H-Glc-H ₂ O] ⁻ , 531.1986 [M-H-Glc-2H ₂ O] ⁻ , 519.2030[M-H-Glc-2H ₂ O-C] ⁻ , 517.1917 [M-H-Glc-2H ₂ O-CH ₂] ⁻ , 505.1887 [M-H-Glc-2H ₂ O-CH ₂ -C] ⁻ , 411.1429 [M-H-C ₁₄ H ₂₂ O ₈] ⁻ , 401.1627 [M-H-C₁₅H₂₀O₈]⁻ , 383.1520 [M-H-C ₁₅ H ₂₀ O ₈ -H ₂ O] ⁻ , 371.1513 [M-H-C ₁₅ H ₂₀ O ₈ -H ₂ O-C] ⁻ , 165.0569 C ₉ H ₉ O ₃ , 731.2668 [M-H-H ₂ O] ⁻ , 683.2380 [M-H-2H ₂ O-CH ₂ O] ⁻ , 607.2179 [M-H-C ₇ H ₁₀ O ₃] ⁻ , 589.1982 [M-H-C ₇ H ₁₀ O ₃ -H ₂ O] ⁻ , 571.1968 [M-H-C ₇ H ₁₀ O ₃ -2H ₂ O] ⁻ , 559.1964 [M-H-C ₇ H ₁₀ O ₃ -2H ₂ O-C] ⁻ , 401.1620 [M-H-C₁₈H₂₀O₇]⁻ , 383.1521 [M-H-C ₁₈ H ₂₀ O ₇ -H ₂ O] ⁻ , 909.3367 [M-H-H ₂ O] ⁻ , 879.3209 [M-H-2H ₂ O-C] ⁻ , 861.3148 [M-H-3H ₂ O-C] ⁻ , 843.3069 [M-H-4H ₂ O-C] ⁻ , 837.2950 [M-H-5H ₂ O] ⁻ , 825.2936 [M-H-5H ₂ O-C] ⁻ , 813.2916 [M-H-5H₂O-2C]⁻ , 801.2901 [M-H-5H ₂ O-3C] ⁻ , 785.2778 [M-H-C ₇ H ₁₀ O ₃] ⁻ ,	Cerberalignan A	Lignans
57	11.85	C ₂₁ H ₂₆ O ₇	[M-H] ⁻	389.1626	2.6	371.1504 [M-H-H ₂ O] ⁻ , 330.1502 [M-H-COOH-CH₂]⁻ , 909.3343 [M-H-H ₂ O] ⁻ , 879.3279 [M-H-2H ₂ O-C] ⁻ , 861.3060 [M-H-3H ₂ O-C] ⁻ , 843.3069 [M-H-4H ₂ O-C] ⁻ , 837.3087[M-H-5H ₂ O] ⁻ , 825.2944 [M-H-5H ₂ O-C] ⁻ , 813.2916 [M-H-5H₂O-2C]⁻ , 801.2926 [M-H-5H ₂ O-3C] ⁻ , 785.2798 [M-H-C ₇ H ₁₀ O ₃] ⁻ , 737.2724 [M-H-C ₇ H ₁₀ O ₃ -4C] ⁻ , 719.2517 [M-H-C ₈ H ₁₆ O ₆] ⁻ , 707.2501 [M-H-C ₈ H ₁₆ O ₆ -C] ⁻ , 567.2302 [M-H-Glc] ⁻ , 553.2021 [M-H-Glc-CH ₂] ⁻ , 549.2149[M-H-Glc-H ₂ O] ⁻ , 531.1986 [M-H-Glc-2H ₂ O] ⁻ , 519.2030[M-H-Glc-2H ₂ O-C] ⁻ , 517.1917 [M-H-Glc-2H ₂ O-CH ₂] ⁻ , 505.1887 [M-H-Glc-2H ₂ O-CH ₂ -C] ⁻ , 411.1429 [M-H-C ₁₄ H ₂₂ O ₈] ⁻ , 401.1627 [M-H-C₁₅H₂₀O₈]⁻ , 383.1520 [M-H-C ₁₅ H ₂₀ O ₈ -H ₂ O] ⁻ , 371.1513 [M-H-C ₁₅ H ₂₀ O ₈ -H ₂ O-C] ⁻ , 165.0569 C ₉ H ₉ O ₃ , 731.2668 [M-H-H ₂ O] ⁻ , 683.2380 [M-H-2H ₂ O-CH ₂ O] ⁻ , 607.2179 [M-H-C ₇ H ₁₀ O ₃] ⁻ , 589.1982 [M-H-C ₇ H ₁₀ O ₃ -H ₂ O] ⁻ , 571.1968 [M-H-C ₇ H ₁₀ O ₃ -2H ₂ O] ⁻ , 559.1964 [M-H-C ₇ H ₁₀ O ₃ -2H ₂ O-C] ⁻ , 401.1620 [M-H-C₁₈H₂₀O₇]⁻ , 383.1521 [M-H-C ₁₈ H ₂₀ O ₇ -H ₂ O] ⁻ , 909.3367 [M-H-H ₂ O] ⁻ , 879.3209 [M-H-2H ₂ O-C] ⁻ , 861.3148 [M-H-3H ₂ O-C] ⁻ , 843.3069 [M-H-4H ₂ O-C] ⁻ , 837.2950 [M-H-5H ₂ O] ⁻ , 825.2936 [M-H-5H ₂ O-C] ⁻ , 813.2916 [M-H-5H₂O-2C]⁻ , 801.2901 [M-H-5H ₂ O-3C] ⁻ , 785.2778 [M-H-C ₇ H ₁₀ O ₃] ⁻ ,	Arctigenic acid	Lignans
58 ^{n.a}	11.88	C ₅₀ H ₅₆ O ₁₇	[M-H] ⁻	927.3446	0.7	567.2302 [M-H-Glc] ⁻ , 553.2021 [M-H-Glc-CH ₂] ⁻ , 549.2149[M-H-Glc-H ₂ O] ⁻ , 531.1986 [M-H-Glc-2H ₂ O] ⁻ , 519.2030[M-H-Glc-2H ₂ O-C] ⁻ , 517.1917 [M-H-Glc-2H ₂ O-CH ₂] ⁻ , 505.1887 [M-H-Glc-2H ₂ O-CH ₂ -C] ⁻ , 411.1429 [M-H-C ₁₄ H ₂₂ O ₈] ⁻ , 401.1627 [M-H-C₁₅H₂₀O₈]⁻ , 383.1520 [M-H-C ₁₅ H ₂₀ O ₈ -H ₂ O] ⁻ , 371.1513 [M-H-C ₁₅ H ₂₀ O ₈ -H ₂ O-C] ⁻ , 165.0569 C ₉ H ₉ O ₃ , 731.2668 [M-H-H ₂ O] ⁻ , 683.2380 [M-H-2H ₂ O-CH ₂ O] ⁻ , 607.2179 [M-H-C ₇ H ₁₀ O ₃] ⁻ , 589.1982 [M-H-C ₇ H ₁₀ O ₃ -H ₂ O] ⁻ , 571.1968 [M-H-C ₇ H ₁₀ O ₃ -2H ₂ O] ⁻ , 559.1964 [M-H-C ₇ H ₁₀ O ₃ -2H ₂ O-C] ⁻ , 401.1620 [M-H-C₁₈H₂₀O₇]⁻ , 383.1521 [M-H-C ₁₈ H ₂₀ O ₇ -H ₂ O] ⁻ , 909.3367 [M-H-H ₂ O] ⁻ , 879.3209 [M-H-2H ₂ O-C] ⁻ , 861.3148 [M-H-3H ₂ O-C] ⁻ , 843.3069 [M-H-4H ₂ O-C] ⁻ , 837.2950 [M-H-5H ₂ O] ⁻ , 825.2936 [M-H-5H ₂ O-C] ⁻ , 813.2916 [M-H-5H₂O-2C]⁻ , 801.2901 [M-H-5H ₂ O-3C] ⁻ , 785.2778 [M-H-C ₇ H ₁₀ O ₃] ⁻ ,	Unknown	Lignans
59 ^{n.a}	11.92	C ₃₇ H ₄₆ O ₁₅	[M-H+HCOOH] ⁻	775.2833	2.0	567.2302 [M-H-Glc] ⁻ , 553.2021 [M-H-Glc-CH ₂] ⁻ , 549.2149[M-H-Glc-H ₂ O] ⁻ , 531.1986 [M-H-Glc-2H ₂ O] ⁻ , 519.2030[M-H-Glc-2H ₂ O-C] ⁻ , 517.1917 [M-H-Glc-2H ₂ O-CH ₂] ⁻ , 505.1887 [M-H-Glc-2H ₂ O-CH ₂ -C] ⁻ , 411.1429 [M-H-C ₁₄ H ₂₂ O ₈] ⁻ , 401.1627 [M-H-C₁₅H₂₀O₈]⁻ , 383.1520 [M-H-C ₁₅ H ₂₀ O ₈ -H ₂ O] ⁻ , 371.1513 [M-H-C ₁₅ H ₂₀ O ₈ -H ₂ O-C] ⁻ , 165.0569 C ₉ H ₉ O ₃ , 731.2668 [M-H-H ₂ O] ⁻ , 683.2380 [M-H-2H ₂ O-CH ₂ O] ⁻ , 607.2179 [M-H-C ₇ H ₁₀ O ₃] ⁻ , 589.1982 [M-H-C ₇ H ₁₀ O ₃ -H ₂ O] ⁻ , 571.1968 [M-H-C ₇ H ₁₀ O ₃ -2H ₂ O] ⁻ , 559.1964 [M-H-C ₇ H ₁₀ O ₃ -2H ₂ O-C] ⁻ , 401.1620 [M-H-C₁₈H₂₀O₇]⁻ , 383.1521 [M-H-C ₁₈ H ₂₀ O ₇ -H ₂ O] ⁻ , 909.3367 [M-H-H ₂ O] ⁻ , 879.3209 [M-H-2H ₂ O-C] ⁻ , 861.3148 [M-H-3H ₂ O-C] ⁻ , 843.3069 [M-H-4H ₂ O-C] ⁻ , 837.2950 [M-H-5H ₂ O] ⁻ , 825.2936 [M-H-5H ₂ O-C] ⁻ , 813.2916 [M-H-5H₂O-2C]⁻ , 801.2901 [M-H-5H ₂ O-3C] ⁻ , 785.2778 [M-H-C ₇ H ₁₀ O ₃] ⁻ ,	Lappaol D isomer 2+Glc	Lignans
60 ^{n.a}	11.94	C ₄₀ H ₄₆ O ₁₄	[M-H] ⁻	749.2806	-0.3	909.3367 [M-H-H ₂ O] ⁻ , 879.3209 [M-H-2H ₂ O-C] ⁻ , 861.3148 [M-H-3H ₂ O-C] ⁻ , 843.3069 [M-H-4H ₂ O-C] ⁻ , 837.2950 [M-H-5H ₂ O] ⁻ , 825.2936 [M-H-5H ₂ O-C] ⁻ , 813.2916 [M-H-5H₂O-2C]⁻ , 801.2901 [M-H-5H ₂ O-3C] ⁻ , 785.2778 [M-H-C ₇ H ₁₀ O ₃] ⁻ ,	Unknown	Lignans
61 ^{n.a}	11.98	C ₅₀ H ₅₆ O ₁₇	[M-H] ⁻	927.3468	2.9	909.3367 [M-H-H ₂ O] ⁻ , 879.3209 [M-H-2H ₂ O-C] ⁻ , 861.3148 [M-H-3H ₂ O-C] ⁻ , 843.3069 [M-H-4H ₂ O-C] ⁻ , 837.2950 [M-H-5H ₂ O] ⁻ , 825.2936 [M-H-5H ₂ O-C] ⁻ , 813.2916 [M-H-5H₂O-2C]⁻ , 801.2901 [M-H-5H ₂ O-3C] ⁻ , 785.2778 [M-H-C ₇ H ₁₀ O ₃] ⁻ ,	Unknown	Lignans

62	12.04	C ₄₀ H ₄₆ O ₁₃	[M-H] ⁻	733.2875	1.5	737.2511 [M-H-C ₇ H ₁₀ O ₃ -4C] ⁻ , 719.2506 [M-H-C ₈ H ₁₆ O ₆] ⁻ , 707.2485 [M-H-C ₈ H ₁₆ O ₆ -C] ⁻ , 715.2650 [M-H-H ₂ O] ⁻ , 679.2506 [M-H-3H ₂ O] ⁻ , 667.2499 [M-H-3H ₂ O-C] ⁻ , 655.2571 [M-H-3H ₂ O-2C] ⁻ , 561.2104 [M-H-C ₈ H ₁₂ O ₄] ⁻ , 283.1009 C ₁₇ H ₁₅ O ₄	Reported compound 2	Lignans
63 ^{n.a}	12.13	C ₄₀ H ₄₆ O ₁₃	[M-H] ⁻	733.2857	-0.3	715.2682 [M-H-H ₂ O] ⁻ , 703.2774 [M-H-H ₂ O-C] ⁻ , 685.2607 [M-H-2H ₂ O] ⁻ , 679.2534 [M-H-3H ₂ O] ⁻ , 667.2510 [M-H-3H ₂ O-C] ⁻ , 655.2532 [M-H-3H ₂ O-2C] ⁻ , 607.2153 [M-H-C ₇ H ₁₀ O ₂] ⁻ , 561.2122 [M-H-C ₈ H ₁₂ O ₄] ⁻	Isomer of reported compound 2	Lignans
64 ^{n.a}	12.17	C ₃₇ H ₄₆ O ₁₅	[M-H+HCOOH] ⁻	775.2836	2.3	567.2255 [M-H-Glc] ⁻ , 551.1943 [M-H-Glc-CH ₄] ⁻ , 535.2009 [M-H-Glc-CH ₂ -H ₂ O] ⁻ , 533.1823 [M-H-Glc-CH ₄ -H ₂ O] ⁻ , 519.2036 [M-H-Glc-2H ₂ O-C] ⁻ , 517.1891 [M-H-Glc-2H ₂ O-CH ₂] ⁻ , 505.1881 [M-H-Glc-2H ₂ O-CH ₂ -C] ⁻ , 411.1393 [M-H-C ₁₄ H ₂₂ O ₈] ⁻ , 195.0673 C ₁₀ H ₁₁ O ₄ , 165.0571 C ₉ H ₉ O ₃	LappaolD+Glc	Lignans
65 ^{n.a}	12.25	C ₄₇ H ₅₂ O ₁₆	[M-H] ⁻	871.3205	2.8	853.3063 [M-H-H ₂ O] ⁻ , 835.2906 [M-H-2H ₂ O] ⁻ , 823.3036 [M-H-2H ₂ O-C] ⁻ , 805.2818 [M-H-3H ₂ O-C] ⁻ , 787.2744 [M-H-4H ₂ O-C] ⁻ , 775.2717 [M-H-4H ₂ O-2C] ⁻ , 731.2573 [M-H-5H ₂ O-4C] ⁻ , 687.3163 [M-H-C ₇ H ₄ O ₆] ⁻ , 683.2485 [M-H-C ₈ H ₁₂ O ₅] ⁻ , 681.2343 [M-H-C ₈ H ₁₂ O ₅ -2H] ⁻ , 671.2440 [M-H-C ₈ H ₁₂ O ₅ -C] ⁻ , 665.2408 [M-H-C ₈ H ₁₂ O ₅ -H ₂ O] ⁻ , 653.2430 [M-H-C ₈ H ₁₂ O ₅ -H ₂ O-C] ⁻ , 479.2620 C ₂₆ H ₃₉ O ₈	Unknown	Lignans
66 ^{n.a}	12.25	C ₅₀ H ₅₆ O ₁₇	[M-H] ⁻	927.3452	1.3	909.3383 [M-H-H ₂ O] ⁻ , 897.3375 [M-H-H ₂ O-C] ⁻ , 879.3265 [M-H-2H ₂ O-C] ⁻ , 861.3177 [M-H-3H ₂ O-C] ⁻ , 843.2952 [M-H-4H ₂ O-C] ⁻ , 837.3044 [M-H-5H ₂ O] ⁻ , 825.2925 [M-H-5H ₂ O-C] ⁻ , 813.2953 [M-H-5H ₂ O-2C] ⁻ , 801.2835 [M-H-5H ₂ O-3C] ⁻ , 785.2709 [M-H-C ₇ H ₁₀ O ₃] ⁻ , 737.2626 [M-H-C ₇ H ₁₀ O ₃ -4C] ⁻ , 719.2507 [M-H-C ₈ H ₁₆ O ₆] ⁻	Unknown	Lignans
67 ^{n.a}	12.31	C ₂₁ H ₂₂ O ₆	[M-H] ⁻	369.1373	3.5	354.1124 [M-H-CH ₃] ⁻ , 203.0363 C ₁₁ H ₇ O ₄ , 174.0703 C ₁₁ H ₁₀ O ₂	7,8-didehydroarctigenin isomer	Lignans
68 ^{n.a}	12.35	C ₅₀ H ₅₆ O ₁₇	[M-H] ⁻	927.3463	2.4	909.3338 [M-H-H ₂ O] ⁻ , 897.3338 [M-H-H ₂ O-C] ⁻ , 879.3309 [M-H-2H ₂ O-C] ⁻ , 861.3174 [M-H-3H ₂ O-C] ⁻ , 843.3010 [M-H-4H ₂ O-C] ⁻ , 825.2930 [M-H-5H ₂ O-C] ⁻ , 813.2962 [M-H-5H ₂ O-2C] ⁻ , 801.2856 [M-H-5H ₂ O-3C] ⁻ , 785.2724 [M-H-C ₇ H ₁₀ O ₃] ⁻ , 719.2539 [M-H-C ₈ H ₁₆ O ₆] ⁻ , 707.2502 [M-H-C ₈ H ₁₆ O ₆ -C] ⁻	Unknown	Lignans
69 ^{n.a}	12.43	C ₅₀ H ₅₈ O ₁₈	[M-H] ⁻	945.3549	0.4	927.3447 [M-H-H ₂ O] ⁻ , 909.3270 [M-H-2H ₂ O] ⁻ , 897.3295 [M-H-2H ₂ O-C] ⁻ , 879.3223 [M-H-3H ₂ O-C] ⁻ , 683.2411 [M-H-C ₁₁ H ₁₈ O ₇] ⁻ , 665.2435 [M-H-C ₁₁ H ₁₈ O ₇ -H ₂ O] ⁻ , 653.2437 [M-H-C ₁₁ H ₁₈ O ₇ -H ₂ O-C] ⁻ , 607.2193 [M-H-C ₁₇ H ₂₂ O ₇] ⁻ , 597.2333 [M-H-C ₁₈ H ₂₀ O ₇] ⁻ , 583.2204 [M-H-C ₁₇ H ₂₂ O ₇ -2C] ⁻ , 579.2265 [M-H-C ₁₇ H ₂₂ O ₇ -2C-CO] ⁻ , 571.2001 [M-H-C ₁₇ H ₂₂ O ₇ -2H ₂ O] ⁻ , 559.1985 [M-H-C ₁₇ H ₂₂ O ₇ -2H ₂ O-C] ⁻ , 547.1966 [M-H-C ₁₇ H ₂₂ O ₇ -2H ₂ O-2C] ⁻ , 531.2022 [M-H-C ₁₇ H ₂₂ O ₇ -2H ₂ O-2C-O] ⁻ , 517.1854 [M-H-C ₁₇ H ₂₂ O ₇ -2H ₂ O-2C-O-CH ₂] ⁻ , 505.1920 [M-H-C ₁₇ H ₂₂ O ₇ -2H ₂ O-3C-O-CH ₂] ⁻ , 411.1458 [M-H-C ₂₇ H ₃₄ O ₁₁] ⁻ , 401.1599 [M-H-C ₂₈ H ₃₂ O ₁₁] ⁻	Unknown	Lignans
70	12.45	C ₂₉ H ₃₆ O ₁₂	[M-H] ⁻	575.2137	0.8	371.118 [M-H-acetylGlc] ⁻ , 357.1390 [M-H-acetylGlc-H ₂ O] ⁻ , 121.0315 C ₇ H ₅ O ₂	4-acetylate arctiin	Lignans

71 ^{n.a}	12.57	C ₅₀ H ₅₆ O ₁₇	[M-H] ⁻	927.3446	0.7	897.3338 [M-H-H ₂ O-C] ⁻ , 879.3191 [M-H-2H ₂ O-C] ⁻ , 861.3163 [M-H-3H ₂ O-C] ⁻ , 849.3130 [M-H-3H ₂ O-2C] ⁻ , 717.2673 [M-H-C ₇ H ₁₄ O ₇] ⁻ , 665.2462 [M-H-C₁₁H₁₈O₇]⁻ , 653.2407 [M-H-C ₁₁ H ₁₈ O ₇ -C] ⁻	Unknown	Lignans
72 ^{n.a}	12.66	C ₄₀ H ₄₆ O ₁₄	[M-H] ⁻	749.2832	2.3	731.2729 [M-H-H ₂ O] ⁻ , 717.2548 [M-H-H ₂ O-CH ₂] ⁻ , 701.2609 [M-H-2H ₂ O-C] ⁻ , 683.2492 [M-H-2H ₂ O-CH ₂ O] ⁻ , 665.2360 [M-H-4H ₂ O-C] ⁻ , 653.2383 [M-H-4H ₂ O-2C] ⁻ , 607.2093 [M-H-C ₇ H ₁₀ O ₃] ⁻ , 597.2381 [M-H-C₈H₈O₃]⁻ , 579.2252 [M-H-C ₈ H ₈ O ₃ -H ₂ O] ⁻ , 553.2095 [M-H-C ₈ H ₈ O ₃ -H ₂ O-C ₂ H ₂] ⁻ , 549.2150 [M-H-C ₈ H ₈ O ₃ -2H ₂ O-C] ⁻ , 531.2081 [M-H-C ₈ H ₈ O ₃ -3H ₂ O-C] ⁻ , 371.1486 C ₂₁ H ₂₃ O ₆ , 165.0563 C ₉ H ₉ O ₃ , 151.0418 C ₈ H ₇ O ₃	Unknown	Lignans
73 ^{n.a}	12.70	C ₅₀ H ₅₆ O ₁₇	[M-H] ⁻	927.3468	2.9	897.3341 [M-H-H ₂ O-C] ⁻ , 879.3291 [M-H-2H ₂ O-C] ⁻ , 861.3128 [M-H-3H ₂ O-C] ⁻ , 849.3044 [M-H-3H ₂ O-2C] ⁻ , 717.2560 [M-H-C ₇ H ₁₄ O ₇] ⁻ , 665.2368 [M-H-C₁₁H₁₈O₇]⁻ , 653.2411 [M-H-C ₁₁ H ₁₈ O ₇ -C] ⁻	Unknown	Lignans
74	12.70	C ₃₀ H ₃₂ O ₁₀	[M-H] ⁻	551.1948	3.1	535.1965 [M-H-O] ⁻ , 533.1805 [M-H-H ₂ O] ⁻ , 505.1876 [M-H-H₂O-CO]⁻ , 411.1492 [M-H-C ₇ H ₈ O ₃] ⁻ , 409.1315 [M-H-C ₇ H ₁₀ O ₃] ⁻ , 151.0434 C ₈ H ₇ O ₃	Arctignan B	Lignans
75 ^{n.a}	12.75	C ₅₀ H ₅₈ O ₁₈	[M-H] ⁻	945.3549	0.4	927.3477 [M-H-H ₂ O] ⁻ , 909.3370 [M-H-2H ₂ O] ⁻ , 895.3121 [M-H-2H ₂ O-CH ₂] ⁻ , 701.2589 [M-H-C ₁₁ H ₁₆ O ₆] ⁻ , 597.2343 [M-H-C ₁₈ H ₂₀ O ₇] ⁻ , 505.1879 [M-H-C ₂₁ H ₂₈ O ₁₀] ⁻ , 401.1604 [M-H-C₂₈H₃₂O₁₁]⁻	Unknown	Lignans
76 ^{n.a}	12.79	C ₄₀ H ₄₆ O ₁₄	[M-H] ⁻	749.2825	1.6	731.2772 [M-H-H ₂ O] ⁻ , 701.2621 [M-H-2H ₂ O-C] ⁻ , 683.2510 [M-H-2H ₂ O-CH ₂ O] ⁻ , 665.2330 [M-H-4H ₂ O-C] ⁻ , 653.2362 [M-H-4H ₂ O-2C] ⁻ , 607.2049 [M-H-C ₇ H ₁₀ O ₃] ⁻ , 597.2292 [M-H-C ₈ H ₈ O ₃] ⁻ , 553.2123 [M-H-C ₈ H ₈ O ₃ -H ₂ O-C ₂ H ₂] ⁻ , 521.1825 [M-H-C₈H₈O₃-2H₂O-C₂H₂-2C]⁻ , 165.0565 C ₉ H ₉ O ₃ , 151.0416 C ₈ H ₇ O ₃	Unknown	Lignans
77	12.80	C ₃₀ H ₃₂ O ₁₀	[M-H] ⁻	551.1938	2.1	533.1797 [M-H-H ₂ O] ⁻ , 505.1893 [M-H-H₂O-CO]⁻ , 409.1314 [M-H-C ₇ H ₁₀ O ₃] ⁻ , 397.1305 [M-H-C ₇ H ₁₀ O ₃ -C] ⁻ , 151.0404 C ₈ H ₇ O ₃	Arctignan C	Lignans
78 ^{n.a}	12.94	C ₅₀ H ₅₆ O ₁₇	[M-H] ⁻	927.3455	1.6	909.3322 [M-H-H₂O]⁻ , 897.3328 [M-H-H ₂ O-C] ⁻ , 891.3290 [M-H-2H ₂ O] ⁻ , 879.3211 [M-H-2H ₂ O-C] ⁻ , 861.3118 [M-H-3H ₂ O-C] ⁻ , 843.3008 [M-H-4H ₂ O-C] ⁻ , 837.3062 [M-H-5H ₂ O] ⁻ , 825.2917 [M-H-5H ₂ O-C] ⁻ , 813.2915 [M-H-5H₂O-2C]⁻ , 719.2421 [M-H-C ₈ H ₁₆ O ₆] ⁻ , 707.2502 [M-H-C ₈ H ₁₆ O ₆ -C] ⁻ , 589.2107 [M-H-C ₁₇ H ₂₂ O ₇] ⁻	Unknown	Lignans
79 ^{n.a}	13.05	C ₅₀ H ₅₆ O ₁₇	[M-H] ⁻	927.3468	2.9	909.3373 [M-H-H₂O]⁻ , 891.3240 [M-H-2H ₂ O] ⁻ , 879.3223 [M-H-2H ₂ O-C] ⁻ , 861.3185 [M-H-3H ₂ O-C] ⁻ , 843.3040 [M-H-4H ₂ O-C] ⁻ , 837.2908 [M-H-5H ₂ O] ⁻ , 825.2959 [M-H-5H ₂ O-C] ⁻ , 813.2939 [M-H-5H ₂ O-2C] ⁻ , 801.2922 [M-H-5H ₂ O-3C] ⁻ , 719.2479 [M-H-C ₈ H ₁₆ O ₆] ⁻ , 707.2469 [M-H-C ₈ H ₁₆ O ₆ -C] ⁻ , 589.2076 [M-H-C ₁₇ H ₂₂ O ₇] ⁻	Unknown	Lignans
80 ^{n.a}	13.06	C ₄₀ H ₄₄ O ₁₃	[M-H] ⁻	731.2736	3.2	713.2542 [M-H-H ₂ O] ⁻ , 695.2530 [M-H-2H ₂ O] ⁻ , 683.2480 [M-H-2H ₂ O-C] ⁻ , 677.2429 [M-H-3H ₂ O] ⁻ , 665.2401 [M-H-3H₂O-C]⁻ , 653.2403 [M-H-3H ₂ O-2C] ⁻ , 589.2047 [M-H-C ₇ H ₁₀ O ₃] ⁻ , 571.1968 [M-H-C ₇ H ₁₀ O ₃ -H ₂ O] ⁻ , 559.1990 [M-H-C ₇ H ₁₀ O ₃ -H ₂ O-	Unknown	Lignans

						C ⁻], 369.1319C ₂₁ H ₂₁ O ₆			
81	13.10	C ₃₀ H ₃₄ O ₁₀	[M-H] ⁻	553.2079	0.5	519.2045 [M-H-H ₂ O-O] ⁻ , 505.1876 [M-H-H ₂ O-O-CH ₂] ⁻ , 357.1352 [M-H-C₁₀H₁₂O₄]⁻ , 343.1219 [M-H-C ₁₀ H ₁₂ O ₄ -CH ₂] ⁻ , 195.0663 C ₁₀ H ₁₁ O ₄ , 165.0570 C ₉ H ₉ O ₃ , 151.0407 C ₈ H ₇ O ₃	Lappaol E	Lignans	
82	13.12	C ₃₁ H ₃₆ O ₁₀	[M-H] ⁻	567.2251	2.1	535.1983 [M-H-H ₂ O-CH ₂] ⁻ , 531.2048 [M-H-2H ₂ O] ⁻ , 519.2055 [M-H-2H ₂ O-C] ⁻ , 505.1878 [M-H-2H₂O-C-CH₂]⁻ , 411.1467 [M-H-C ₈ H ₁₂ O ₃] ⁻ , 397.1608 [M-H-C ₈ H ₁₀ O ₄] ⁻ , 195.0684 C ₁₀ H ₁₁ O ₄ , 165.0574 C ₉ H ₉ O ₃	Lappaol D	Lignans	
83	13.24	C ₄₀ H ₄₄ O ₁₃	[M-H] ⁻	731.2704	0.0	713.2620 [M-H-H ₂ O] ⁻ , 683.2524 [M-H-2H ₂ O-C] ⁻ , 677.2406 [M-H-3H ₂ O] ⁻ , 665.2405 [M-H-3H₂O-C]⁻ , 653.2401 [M-H- 3H ₂ O-2C] ⁻ , 589.2093 [M-H-C ₇ H ₁₀ O ₃] ⁻ , 571.1992 [M-H- C ₇ H ₁₀ O ₃ -H ₂ O] ⁻ , 559.1985 [M-H-C ₇ H ₁₀ O ₃ -H ₂ O-C] ⁻ , 547.1989 [M-H-C ₇ H ₁₀ O ₃ -H ₂ O-2C] ⁻ , 531.2033 [M-H-C ₇ H ₁₀ O ₃ -H ₂ O-2C- O] ⁻ , 381.1353 C ₂₂ H ₂₁ O ₆ , 369.1357 C ₂₁ H ₂₁ O ₆ , 297.1125 C ₁₈ H ₁₇ O ₄ , 283.0972 C ₁₇ H ₁₅ O ₄ , 269.0817 C ₁₆ H ₁₃ O ₄	Arctignan D	Lignans	
84	13.29	C ₄₀ H ₄₄ O ₁₃	[M-H] ⁻	731.2722	1.8	713.2620 [M-H-H ₂ O] ⁻ , 683.2505 [M-H-2H ₂ O-C] ⁻ , 677.2407 [M-H-3H ₂ O] ⁻ , 665.2402 [M-H-3H₂O-C]⁻ , 653.2402 [M-H- 3H ₂ O-2C] ⁻ , 589.2103 [M-H-C ₇ H ₁₀ O ₃] ⁻ , 571.1998 [M-H- C ₇ H ₁₀ O ₃ -H ₂ O] ⁻ , 559.1996 [M-H-C ₇ H ₁₀ O ₃ -H ₂ O-C] ⁻ , 547.1982 [M-H-C ₇ H ₁₀ O ₃ -H ₂ O-2C] ⁻ , 381.1362 C ₂₂ H ₂₁ O ₆ , 283.0973 C ₁₇ H ₁₅ O ₄ , 269.0849 C ₁₆ H ₁₃ O ₄	Arctignan E	Lignans	
85 ^{n,a}	13.36	C ₃₇ H ₄₄ O ₁₄	[M-H+HCOOH] ⁻	757.2730	2.2	549.2117 [M-H-Glc]⁻ , 519.2048 [M-H-Glc-CO] ⁻ , 385.1299 [M-H-C₁₆H₂₂O₇]⁻	lappaolB+Glc	Lignans	
86*	13.40	C ₂₀ H ₂₂ O ₆	[M-H] ⁻	357.1339	0.1	342.1113 [M-H-CH₃]⁻ , 313.1397 [M-H-CO ₂] ⁻ , 221.0824 [M- H-C ₈ H ₈ O ₂] ⁻ , 209.0840 [M-H-C ₈ H ₈ O ₂ -C] ⁻ , 161.0561 C ₁₀ H ₉ O ₂ , 147.0455 C ₉ H ₇ O ₂ , 137.0598 C ₈ H ₉ O ₂	Matairesinol	Lignans	
87 ⁿ	13.64	C ₄₀ H ₄₄ O ₁₃	[M-H] ⁻	731.2705	0.1	713.2582 [M-H-H ₂ O] ⁻ , 701.2607 [M-H-H ₂ O-C] ⁻ , 683.2511 [M- H-2H ₂ O-C] ⁻ , 677.2402 [M-H-3H ₂ O] ⁻ , 665.2399 [M-H-3H₂O- C]⁻ , 653.2388 [M-H-3H ₂ O-2C] ⁻ , 589.2103 [M-H-C ₇ H ₁₀ O ₃] ⁻ , 571.1971 [M-H-C ₇ H ₁₀ O ₃ -H ₂ O] ⁻ , 559.1985 [M-H-C ₇ H ₁₀ O ₃ - H ₂ O-C] ⁻ , 547.1985 [M-H-C ₇ H ₁₀ O ₃ -H ₂ O-2C] ⁻ , 505.1901[M-H- C ₇ H ₁₀ O ₃ -2H ₂ O-4C] ⁻ , 283.0889 C ₁₇ H ₁₅ O ₄	Arctignan H isomer	Lignans	
88	14.02	C ₄₀ H ₄₂ O ₁₃	[M-H] ⁻	729.2568	2.1	711.2444 [M-H-H ₂ O] ⁻ , 699.2462 [M-H-H ₂ O-C] ⁻ , 681.2343 [M- H-2H ₂ O-C] ⁻ , 669.2336 [M-H-2H ₂ O-2C] ⁻ , 663.2287 [M-H- 3H ₂ O-C] ⁻ , 651.2331 [M-H-3H ₂ O-2C] ⁻ , 557.1816 [M-H- C ₈ H ₁₂ O ₄] ⁻ , 545.1883 [M-H-C ₈ H ₈ O ₅] ⁻ , 517.1910 [M-H- C ₁₀ H ₁₂ O ₅] ⁻ , 505.1897 [M-H-C₁₀H₁₂O₅-C]⁻ , 415.1454 [M-H- C ₁₄ H ₁₈ O ₈] ⁻ , 283.0960 C ₁₇ H ₁₅ O ₄ , 269.0805 C ₁₆ H ₁₃ O ₄	Arctignan F	Lignans	
89 ^{n,a}	14.08	C ₃₁ H ₃₄ O ₁₀	[M-H] ⁻	565.2117	4.3	441.1544 [M-H-CH ₂ O] ⁻ , 423.1431 [M-H-C ₇ H ₁₀ O ₃] ⁻ , 411.1470 [M-H-C₇H₁₀O₃-C]⁻	Unknown	Lignans	
90 ⁿ	14.15	C ₄₀ H ₄₂ O ₁₃	[M-H] ⁻	729.2573	2.6	711.2453 [M-H-H ₂ O] ⁻ , 701.2621 [M-H-CO] ⁻ , 681.2374 [M-H- 2H ₂ O-C] ⁻ , 669.2408 [M-H-2H ₂ O-2C] ⁻ , 557.1811 [M-H- C ₈ H ₁₂ O ₄] ⁻ , 545.1851 [M-H-C ₈ H ₈ O ₅] ⁻ , 517.1887 [M-H- C₁₀H₁₂O₅]⁻ , 505.1899[M-H-C ₁₀ H ₁₂ O ₅ -C] ⁻ , 415.1427 [M-H- C ₁₄ H ₁₈ O ₈] ⁻ , 283.0966 C ₁₇ H ₁₅ O ₄	Herpetetrone	Lignans	
91	14.21	C ₄₀ H ₄₄ O ₁₃	[M-H] ⁻	731.2698	-0.6	713.2633 [M-H-H ₂ O] ⁻ , 701.2632[M-H-H₂O-C]⁻ , 683.2512[M- H-2H ₂ O-C] ⁻ , 665.2419 [M-H-3H ₂ O-C] ⁻ , 653.2443 [M-H-	Arctignan G	Lignans	

92 ^{n,a}	14.25	C ₃₁ H ₃₄ O ₁₀	[M-H] ⁻	565.2089	1.5	3H ₂ O-2C], 517.1887 [M-H-C ₁₀ H ₁₄ O ₅] ⁻ , 505.1878 [M-H-C ₁₀ H ₁₄ O ₅ -C] ⁻ , 283.0968 C ₁₇ H ₁₅ O ₄ , 269.0761 C ₁₆ H ₁₃ O ₄ , 195.0677 C ₁₀ H ₁₁ O ₄ , 165.0569 C ₉ H ₉ O ₃	Unknown	Lignans
93 ^{n,a}	14.28	C ₄₁ H ₄₆ O ₁₃	[M-H] ⁻	745.2889	2.9	533.1855 [M-H-H ₂ O-CH ₂] ⁻ , 195.0680 C ₁₀ H ₁₁ O ₄ , 165.0573 C ₉ H ₉ O ₃ 715.2682 [M-H-CH ₂ O] ⁻ , 697.2602 [M-H-CH ₂ O-H ₂ O] ⁻ , 679.2489 [M-H-CH ₂ O-2H ₂ O] ⁻ , 357.1341 [M-H-C ₂₁ H ₂₄ O ₇] ⁻ , 343.117 5[M-H-C ₂₁ H ₂₄ O ₇ -CH ₂] ⁻ , 313.1090 [M-H-C ₂₁ H ₂₄ O ₇ -CH ₂ -CH ₂ O] ⁻ , 299.0938 [M-H-C ₂₁ H ₂₄ O ₇ -2CH ₂ -CH ₂ O] ⁻ 519.2019 [M-H-2H ₂ O-C] ⁻ , 517.1876 [M-H-2H ₂ O-CH ₂] ⁻ , 505.1916 [M-H-2H ₂ O-CH ₂ -C] ⁻ , 195.0666 C ₁₀ H ₁₁ O ₄ , 165.0569 C ₉ H ₉ O ₃	Unknown	Lignans
94 ^{n,a}	14.41	C ₃₁ H ₃₆ O ₁₀	[M-H] ⁻	567.2259	2.9	505.1916 [M-H-2H ₂ O-CH ₂ -C] ⁻ , 195.0666 C ₁₀ H ₁₁ O ₄ , 165.0569 C ₉ H ₉ O ₃ 713.2590 [M-H-H ₂ O] ⁻ , 701.2591 [M-H-H ₂ O-C] ⁻ , 683.2518 [M-H-2H ₂ O-C] ⁻ , 653.2387 [M-H-3H ₂ O-2C] ⁻ , 517.1902 [M-H-C ₁₀ H ₁₄ O ₅] ⁻ , 505.1855 [M-H-C ₁₀ H ₁₄ O ₅ -C] ⁻ , 283.1042 C ₁₇ H ₁₅ O ₄ , 195.0679 C ₁₀ H ₁₁ O ₄ , 165.0565 C ₉ H ₉ O ₃	Lappaol D isomer 1	Lignans
95	14.51	C ₄₀ H ₄₄ O ₁₃	[M-H] ⁻	731.2709	0.5	553.2089 [M-H-CH ₂] ⁻ , 549.2127 [M-H-H ₂ O] ⁻ , 531.2034 [M-H-2H ₂ O] ⁻ , 519.2059 [M-H-2H ₂ O-C] ⁻ , 505.1860 [M-H-2H ₂ O-C-CH ₂] ⁻ , 411.1432 [M-H-C ₈ H ₁₂ O ₃] ⁻ , 401.1594 [M-H-C ₉ H ₁₀ O ₃] ⁻ , 383.1515 [M-H-C ₉ H ₁₀ O ₃ -H ₂ O] ⁻ , 371.1532 [M-H-C ₉ H ₁₀ O ₃ -H ₂ O-C] ⁻ , 165.0559 C ₉ H ₉ O ₃	Arctignan H	Lignans
96 ^{n,a}	14.52	C ₃₁ H ₃₆ O ₁₀	[M-H] ⁻	567.2258	2.8	517.1887 [M-H-H ₂ O] ⁻ , 505.1882 [M-H-H ₂ O-C] ⁻ , 475.1490 [M-H-H ₂ O-3CH ₂] ⁻ , 283.0989 C ₁₇ H ₁₅ O ₄ , 269.0843 C ₁₆ H ₁₃ O ₄ 517.1884 [M-H-H ₂ O] ⁻ , 505.1893 [M-H-H ₂ O-C] ⁻ , 475.1647 [M-H-H ₂ O-3CH ₂] ⁻ , 381.1360 [M-H-C ₈ H ₁₀ O ₃] ⁻ , 282.0918 C ₁₇ H ₁₄ O ₄ , 270.0905 C ₁₆ H ₁₄ O ₄	Lappaol D isomer 2	Lignans
97	14.74	C ₃₀ H ₃₂ O ₉	[M-H] ⁻	535.1975	0.7	517.1885 [M-H-H ₂ O] ⁻ , 505.1914 [M-H-H ₂ O-C] ⁻ , 475.1573 [M-H-H ₂ O-3CH ₂] ⁻ , 283.0939 C ₁₇ H ₁₅ O ₄ , 269.0769 C ₁₆ H ₁₃ O ₄ 517.1925 [M-H-H ₂ O] ⁻ , 505.1894 [M-H-H ₂ O-C] ⁻ , 475.1506 [M-H-H ₂ O-3CH ₂] ⁻ , 381.1313 [M-H-C ₈ H ₁₀ O ₃] ⁻ , 282.0913 C ₁₇ H ₁₄ O ₄	Isolappaol A	Lignans
98	14.83	C ₃₀ H ₃₂ O ₉	[M-H] ⁻	535.1979	1.1	517.1885 [M-H-H ₂ O] ⁻ , 505.1914 [M-H-H ₂ O-C] ⁻ , 475.1573 [M-H-H ₂ O-3CH ₂] ⁻ , 283.0939 C ₁₇ H ₁₅ O ₄ , 269.0769 C ₁₆ H ₁₃ O ₄ 517.1925 [M-H-H ₂ O] ⁻ , 505.1894 [M-H-H ₂ O-C] ⁻ , 475.1506 [M-H-H ₂ O-3CH ₂] ⁻ , 381.1313 [M-H-C ₈ H ₁₀ O ₃] ⁻ , 282.0913 C ₁₇ H ₁₄ O ₄	Lappaol A	Lignans
99 ⁿ	15.03	C ₃₀ H ₃₂ O ₉	[M-H] ⁻	535.1995	2.7	517.1885 [M-H-H ₂ O] ⁻ , 505.1914 [M-H-H ₂ O-C] ⁻ , 475.1573 [M-H-H ₂ O-3CH ₂] ⁻ , 283.0939 C ₁₇ H ₁₅ O ₄ , 269.0769 C ₁₆ H ₁₃ O ₄ 517.1925 [M-H-H ₂ O] ⁻ , 505.1894 [M-H-H ₂ O-C] ⁻ , 475.1506 [M-H-H ₂ O-3CH ₂] ⁻ , 381.1313 [M-H-C ₈ H ₁₀ O ₃] ⁻ , 282.0913 C ₁₇ H ₁₄ O ₄	Hedyotol A	Lignans
100 ^{n,a}	15.12	C ₃₀ H ₃₂ O ₉	[M-H] ⁻	535.1992	2.4	517.1885 [M-H-H ₂ O] ⁻ , 505.1914 [M-H-H ₂ O-C] ⁻ , 475.1573 [M-H-H ₂ O-3CH ₂] ⁻ , 283.0939 C ₁₇ H ₁₅ O ₄ , 269.0769 C ₁₆ H ₁₃ O ₄ 517.1925 [M-H-H ₂ O] ⁻ , 505.1894 [M-H-H ₂ O-C] ⁻ , 475.1506 [M-H-H ₂ O-3CH ₂] ⁻ , 381.1313 [M-H-C ₈ H ₁₀ O ₃] ⁻ , 282.0913 C ₁₇ H ₁₄ O ₄	LappaolA isomer	Lignans
101	15.13	C ₂₁ H ₂₂ O ₆	[M-H] ⁻	369.1352	1.4	354.1135 [M-H-CH ₃] ⁻ , 203.0376 C ₁₁ H ₇ O ₄ , 174.0708 C ₁₁ H ₁₀ O ₂ 357.1280 [M-H-H ₂ O] ⁻ , 255.0606 C ₁₅ H ₁₁ O ₄ , 235.0959 C ₁₃ H ₁₅ O ₄ , 203.0382 C ₁₁ H ₇ O ₄ , 174.0697 C ₁₁ H ₁₀ O ₂ , 121.0314 C ₇ H ₅ O ₂	7,8-didehydroarctigenin	Lignans
102*	15.15	C ₂₁ H ₂₄ O ₆	[M-H] ⁻	371.1503	0.8	727.2732 [M-H-H ₂ O] ⁻ , 715.2813 [M-H-CH ₂ O] ⁻ , 697.2618 [M-H-CH ₂ O-H ₂ O] ⁻ , 677.2297 [M-H-CH ₂ O-2H ₂ O-2H] ⁻ , 667.2585 [M-H-3H ₂ O-2CH ₂] ⁻ , 531.1987 [M-H-C ₁₀ H ₁₄ O ₅] ⁻ , 519.2054 [M-H-C ₁₀ H ₁₄ O ₅ -C] ⁻ , 325.1098 [M-H-C ₂₂ H ₂₈ O ₈] ⁻ , 313.1075 [M-H-C ₂₂ H ₂₈ O ₈ -C] ⁻ , 195.0658 C ₁₀ H ₁₁ O ₄ , 165.0538 C ₉ H ₉ O ₃	Arctigenin	Lignans
103 ^{n,a}	15.49	C ₄₁ H ₄₆ O ₁₃	[M-H] ⁻	745.2889	1.7	531.2008 [M-H-H ₂ O ₂] ⁻ , 519.2096 [M-H-H ₂ O ₂ -C] ⁻ , 397.1608 [M-H-C ₈ H ₈ O ₄] ⁻ 695.2497 [M-H-H ₂ O] ⁻ , 683.2524 [M-H-H ₂ O-C] ⁻ , 677.2398 [M-H-2H ₂ O] ⁻ , 665.2401 [M-H-2H ₂ O-C] ⁻ , 653.2405 [M-H-2H ₂ O-2C] ⁻ , 635.1975 [M-H-2H ₂ O-3CH ₂] ⁻ , 623.1991 [M-H-2H ₂ O-3CH ₂ -C] ⁻ , 559.1965 [M-H-C ₈ H ₁₀ O ₃] ⁻ , 547.1978 [M-H-C ₈ H ₁₀ O ₃ -C] ⁻ , 381.1340 [M-H-C ₁₈ H ₂₀ O ₆] ⁻ , 369.1329 [M-H-	Arctignan G+CH ₂	Lignans
104 ⁿ	15.53	C ₃₁ H ₃₄ O ₁₀	[M-H] ⁻	565.2094	2.0	695.2497 [M-H-H ₂ O] ⁻ , 683.2524 [M-H-H ₂ O-C] ⁻ , 677.2398 [M-H-2H ₂ O] ⁻ , 665.2401 [M-H-2H ₂ O-C] ⁻ , 653.2405 [M-H-2H ₂ O-2C] ⁻ , 635.1975 [M-H-2H ₂ O-3CH ₂] ⁻ , 623.1991 [M-H-2H ₂ O-3CH ₂ -C] ⁻ , 559.1965 [M-H-C ₈ H ₁₀ O ₃] ⁻ , 547.1978 [M-H-C ₈ H ₁₀ O ₃ -C] ⁻ , 381.1340 [M-H-C ₁₈ H ₂₀ O ₆] ⁻ , 369.1329 [M-H-	2-Hydroxylappaol B	Lignans
105	15.62	C ₄₀ H ₄₂ O ₁₂	[M-H] ⁻	713.2612	1.4	695.2497 [M-H-H ₂ O] ⁻ , 683.2524 [M-H-H ₂ O-C] ⁻ , 677.2398 [M-H-2H ₂ O] ⁻ , 665.2401 [M-H-2H ₂ O-C] ⁻ , 653.2405 [M-H-2H ₂ O-2C] ⁻ , 635.1975 [M-H-2H ₂ O-3CH ₂] ⁻ , 623.1991 [M-H-2H ₂ O-3CH ₂ -C] ⁻ , 559.1965 [M-H-C ₈ H ₁₀ O ₃] ⁻ , 547.1978 [M-H-C ₈ H ₁₀ O ₃ -C] ⁻ , 381.1340 [M-H-C ₁₈ H ₂₀ O ₆] ⁻ , 369.1329 [M-H-	Lappaol F	Lignans

						C ₁₈ H ₂₀ O ₆ -C] ⁻ , 295.0965 C ₁₈ H ₁₅ O ₄ , 283.0976 C ₁₇ H ₁₅ O ₄ , 269.0800 C ₁₆ H ₁₃ O ₄			
106 ^{n.a}	15.92	C ₄₀ H ₄₂ O ₁₂	[M-H] ⁻	713.2585	-1.0	695.2422 [M-H-H ₂ O] ⁻ , 683.2530 [M-H-H ₂ O-C] ⁻ , 677.2423 [M-H-2H ₂ O] ⁻ , 665.2425 [M-H-2H ₂ O-C] ⁻ , 653.2393 [M-H-2H ₂ O-2C] ⁻ , 635.1962 [M-H-2H ₂ O-3CH ₂] ⁻ , 623.1805 [M-H-2H ₂ O-3CH ₂ -C] ⁻ , 561.2067 [M-H-C ₈ H ₈ O ₃] ⁻ , 559.1877 [M-H-C ₈ H ₁₀ O ₃] ⁻ , 547.1923 [M-H-C ₈ H ₁₀ O ₃ -C] ⁻ , 295.0545 C ₁₈ H ₁₅ O ₄	Lappaol F isomer	Lignans	
107	16.09	C ₃₁ H ₃₄ O ₉	[M-H] ⁻	549.2154	2.9	531.2045 [M-H-H ₂ O] ⁻ , 519.2037 [M-H-H ₂ O-C] ⁻ , 489.1574 [M-H-H ₂ O-3CH ₂] ⁻ , 283.0963 C ₁₇ H ₁₅ O ₄ , 269.0837 C ₁₆ H ₁₃ O ₄	Lappaol B	Lignans	
108 ^{n.a}	16.35	C ₄₈ H ₅₆ O ₁₇	[M-H] ⁻	903.3448	0.9	743.3075 [M+H-Glc] ⁺ , 725.2974 [M+H-Glc-H ₂ O] ⁺ , 531.2089[M+H-Glc-C ₁₁ H ₁₆ O ₄] ⁺ , 507.2070 [M+H-Glc-C ₁₃ H ₁₆ O ₄] ⁺ , 489.1970 [M+H-Glc-C ₁₃ H ₁₆ O ₄ -H ₂ O] ⁺ , 371.1369 [M+H-Glc-C ₂₁ H ₂₄ O ₆] ⁺ , 335.1316 [M+H-Glc-C ₂₁ H ₂₄ O ₆ -2H ₂ O] ⁺ , 285.1158 C ₁₇ H ₁₇ O ₄ , 176.0862 C ₁₁ H ₁₂ O ₂ , 151.0781 C ₉ H ₁₁ O ₂	NeoarctinA+Glc	Lignans	
109 ^{n.a}	16.46	C ₄₈ H ₅₄ O ₁₇	[M+NH ₄] ⁺	920.3708	0.3	741.2930 [M+H-Glc] ⁺ , 723.2812 [M+H-Glc-H ₂ O] ⁺ , 505.1924 [M+H-Glc-C ₁₃ H ₁₆ O ₄] ⁺ , 247.0989 C ₁₄ H ₁₅ O ₄ , 203.0999 C ₁₃ H ₁₅ O ₂ , 151.0753 C ₉ H ₁₁ O ₂	Neoarctin A-2H+Glc	Lignans	
110 ^{n.a}	16.62	C ₄₈ H ₅₆ O ₁₇	[M+Na] ⁺	927.3460	4.5	743.3107 [M+H-Glc] ⁺ , 725.2971 [M+H-Glc-H ₂ O] ⁺ , 711.2950 [M+H-Glc-H ₂ O-CH ₂] ⁺ , 507.2085 [M+H-Glc-C ₁₃ H ₁₆ O ₄] ⁺ , 489.1880 [M+H-Glc-C ₁₃ H ₁₆ O ₄ -H ₂ O] ⁺ , 285.1181 C ₁₇ H ₁₇ O ₄ , 247.0996 C ₁₄ H ₁₅ O ₄ , 177.0902 C ₁₁ H ₁₃ O ₂ , 151.0727 C ₉ H ₁₁ O ₂	Diarctigenin+Glc	Lignans	
111 ^{n.a}	17.03	C ₄₀ H ₄₂ O ₁₂	[M-H] ⁻	713.2594	-0.4	697.2672 [M+H-H ₂ O] ⁺ , 679.2571 [M+H-2H ₂ O] ⁺ , 665.2425 [M+H-2H ₂ O-CH ₂] ⁺ , 561.2168 [M+H-C ₈ H ₁₀ O ₃] ⁺ , 543.2048 [M+H-C ₈ H ₁₀ O ₃ -H ₂ O] ⁺ , 531.1977 [M+H-C ₈ H ₁₀ O ₃ -H ₂ O-C] ⁺	Unknown	Lignans	
112 ^{n.a}	17.14	C ₄₀ H ₄₂ O ₁₂	[M-H] ⁻	713.2596	-0.2	697.2721 [M+H-H ₂ O] ⁺ , 679.2600[M+H-2H ₂ O] ⁺ , 665.2600 [M+H-2H ₂ O-CH ₂] ⁺ , 561.2126 [M+H-C ₈ H ₁₀ O ₃] ⁺ , 543.1943 [M+H-C ₈ H ₁₀ O ₃ -H ₂ O] ⁺ , 531.2034 [M+H-C ₈ H ₁₀ O ₃ -H ₂ O-C] ⁺	Unknown	Lignans	
113 ⁿ	18.98	C ₄₂ H ₄₄ O ₁₂	[M-H] ⁻	739.2763	0.8	723.2827 [M+H-H ₂ O] ⁺ , 705.2745[M+H-2H ₂ O] ⁺ , 505.1902 [M+H-C ₁₃ H ₁₆ O ₄] ⁺ , 487.1755 [M+H-C ₁₃ H ₁₆ O ₄ -H ₂ O] ⁺ , 477.1955 [M+H-C ₁₃ H ₁₆ O ₄ -CO] ⁺ , 469.1721 [M+H-C ₁₃ H ₁₆ O ₄ -2H ₂ O] ⁺ , 455.1549 [M+H-C ₁₃ H ₁₆ O ₄ -2H ₂ O-CH ₂] ⁺ , 283.1037 C ₁₇ H ₁₅ O ₄ , 271.0990 C ₁₆ H ₁₅ O ₄ , 259.1006 C ₁₅ H ₁₅ O ₄ , 247.0996 C ₁₄ H ₁₅ O ₄ , 229.0877 C ₁₄ H ₁₃ O ₃ , 219.1035 C ₁₃ H ₁₅ O ₃ , 203.1056 C ₁₃ H ₁₅ O ₂ , 189.0903 C ₁₂ H ₁₃ O ₂ , 151.0771 C ₉ H ₁₁ O ₂	Viridissimaol E	Lignans	
114	19.18	C ₄₂ H ₄₆ O ₁₂	[M-H] ⁻	741.2931	2.0	725.2980 [M+H-H ₂ O] ⁺ , 711.2808 [M+H-H ₂ O-CH ₂] ⁺ , 707.2880 [M+H-2H ₂ O] ⁺ , 693.2703 [M+H-2H ₂ O-CH ₂] ⁺ , 507.2048 [M+H-C ₁₃ H ₁₆ O ₄] ⁺ , 489.1917 [M+H-C ₁₃ H ₁₆ O ₄ -H ₂ O] ⁺ , 313.1094 C ₁₈ H ₁₇ O ₅ , 285.1142 C ₁₇ H ₁₇ O ₄ , 271.0991 C ₁₆ H ₁₅ O ₄ , 253.0884 C ₁₆ H ₁₃ O ₃ , 177.0934 C ₁₁ H ₁₃ O ₂ , 151.0782 C ₉ H ₁₁ O ₂	Diarctigenin	Lignans	
115 ^{n.a}	19.79	C ₄₂ H ₄₄ O ₁₂	[M-H] ⁻	739.2771	1.6	723.2832 [M+H-H ₂ O] ⁺ , 705.2687 [M+H-2H ₂ O] ⁺ , 589.2172 [M+H-C ₉ H ₁₂ O ₂] ⁺ , 571.2095 [M+H-C ₉ H ₁₂ O ₂ -H ₂ O] ⁺ , 559.2019 [M+H-C ₉ H ₁₂ O ₂ -H ₂ O-C] ⁺ , 505.1884[M+H-C ₁₃ H ₁₆ O ₄] ⁺ , 487.1982 [M+H-C ₁₃ H ₁₆ O ₄ -H ₂ O] ⁺ , 367.1272 [M+H-C ₂₁ H ₂₆ O ₆] ⁺ , 247.0988 C ₁₄ H ₁₅ O ₄ , 203.1028 C ₁₃ H ₁₅ O ₂ , 151.0764 C ₉ H ₁₁ O ₂	Diarctigenin/Neoarctin A-2H 1	Lignans	

116	19.86	C ₄₂ H ₄₆ O ₁₂	[M-H] ⁻	741.2911	0.0	725.2981 [M+H-H ₂ O] ⁺ , 711.2804 [M+H-H ₂ O-CH ₂] ⁺ , 707.2894 [M+H-2H ₂ O] ⁺ , 693.2732 [M+H-2H ₂ O-CH ₂] ⁺ , 507.2048 [M+H-C ₁₃ H ₁₆ O ₄] ⁺ , 489.1936 [M+H-C ₁₃ H ₁₆ O ₄ -H ₂ O] ⁺ , 387.1522 [M+H-C ₂₁ H ₂₄ O ₅] ⁺ , 369.1373 [M+H-C ₂₁ H ₂₆ O ₆] ⁺ , 351.1270 [M+H-C ₂₁ H ₂₆ O ₆ -H ₂ O] ⁺ , 285.1156 C ₁₇ H ₁₇ O ₄ , 271.0983 C ₁₆ H ₁₅ O ₄ , 247.0986 C ₁₄ H ₁₅ O ₄ , 203.1054 C ₁₃ H ₁₅ O ₂ , 189.0905 C ₁₂ H ₁₃ O ₂ , 177.0917 C ₁₁ H ₁₃ O ₂ , 151.0771 C ₉ H ₁₁ O ₂	Neoarctin A	Lignans
117 ^{n,a}	19.99	C ₄₂ H ₄₄ O ₁₂	[M-H] ⁻	739.2772	1.7	723.2817 [M+H-H ₂ O] ⁺ , 705.2703 [M+H-2H ₂ O] ⁺ , 505.1875 [M+H-C ₁₃ H ₁₆ O ₄] ⁺ , 495.1952[M+H-C ₁₄ H ₁₄ O ₄] ⁺ , 487.1716 [M+H-C ₁₃ H ₁₆ O ₄ -H ₂ O] ⁺ , 477.1905 [M+H-C ₁₃ H ₁₆ O ₄ -CO] ⁺ , 336.1324[M+H-C ₂₁ H ₂₅ O ₈] ⁺ , 247.0978 C ₁₄ H ₁₅ O ₄ , 203.1091 C ₁₃ H ₁₅ O ₂ , 151.0745 C ₉ H ₁₁ O ₂	Diarctigenin/Neoarctin A-2H 2	Lignans
118 ^{n,a}	20.07	C ₄₂ H ₄₄ O ₁₂	[M-H] ⁻	739.2775	2.0	723.2791 [M+H-H ₂ O] ⁺ , 705.2693 [M+H-2H ₂ O] ⁺ , 505.1943 [M+H-C ₁₃ H ₁₆ O ₄] ⁺ , 495.2081 [M+H-C ₁₄ H ₁₄ O ₄] ⁺ , 487.1748 [M+H-C ₁₃ H ₁₆ O ₄ -H ₂ O] ⁺ , 477.1933 [M+H-C ₁₃ H ₁₆ O ₄ -CO] ⁺ , 469.1742 [M+H-C ₁₃ H ₁₆ O ₄ -2H ₂ O] ⁺ , 283.0984 C ₁₇ H ₁₅ O ₄ , 271.1070 C ₁₆ H ₁₅ O ₄ , 247.0989 C ₁₄ H ₁₅ O ₄ , 203.1091 C ₁₃ H ₁₅ O ₂ , 151.0745 C ₉ H ₁₁ O ₂	Diarctigenin/Neoarctin A-2H 3	Lignans
119 ^{n,a}	20.60	C ₄₂ H ₄₄ O ₁₂	[M-H] ⁻	739.2784	2.9	723.2852 [M+H-H ₂ O] ⁺ , 705.2712 [M+H-2H ₂ O] ⁺ , 559.1881 [M+H-C ₁₀ H ₁₄ O ₃] ⁺ , 505.1881 [M+H-C ₁₃ H ₁₆ O ₄] ⁺ , 351.1277 [M+H-C ₂₁ H ₂₆ O ₇] ⁺ , 247.1002 C ₁₄ H ₁₅ O ₄ , 203.1028 C ₁₃ H ₁₅ O ₂ , 151.0808 C ₉ H ₁₁ O ₂	Diarctigenin/Neoarctin A-2H 4	Lignans
120 ^{n,a}	20.79	C ₆₃ H ₆₆ O ₁₈	[M-H] ⁻	1109.4159	-1.2	893.3486 [M+H-C ₉ H ₁₄ O ₆] ⁺ , 865.3491 [M+H-C ₉ H ₁₄ O ₆ -CO] ⁺ , 741.2865 [M+H-C ₂₁ H ₂₂ O ₆] ⁺ , 727.3124 [M+H-C ₂₁ H ₂₀ O ₇] ⁺ , 709.2972 [M+H-C ₂₁ H ₂₀ O ₇ -H ₂ O] ⁺ , 247.1004 C ₁₄ H ₁₅ O ₄ , 203.1090 C ₁₃ H ₁₅ O ₂ , 151.0717 C ₉ H ₁₁ O ₂	Neoarctin A+7,8-didehydroarctigenin	Lignans
121 ^{n,a}	20.83	C ₄₂ H ₄₄ O ₁₂	[M-H] ⁻	739.2723	-3.2	723.2852 [M+H-H ₂ O] ⁺ , 247.0995 C ₁₄ H ₁₅ O ₄ , 203.1043 C ₁₃ H ₁₅ O ₂ , 151.0728 C ₉ H ₁₁ O ₂	Diarctigenin/Neoarctin A-2H 5	Lignans
122 ^{n,a}	21.02	C ₆₃ H ₆₈ O ₁₈	[M+H] ⁺	1113.4509	2.5	1095.4423 [M+H-H ₂ O] ⁺ , 1081.4221 [M+H-H ₂ O-CH ₂] ⁺ , 727.3146 [M+H-C ₂₁ H ₂₂ O ₆ -O] ⁺ , 709.3037 [M+H-C ₂₁ H ₂₂ O ₇ -H ₂ O] ⁺ , 691.2857 [M+H-C ₂₁ H ₂₂ O ₇ -2H ₂ O] ⁺ , 491.2132 [M+H-C ₃₄ H ₃₈ O ₁₁] ⁺ , 473.1907 [M+H-C ₃₄ H ₃₈ O ₁₁ -H ₂ O] ⁺ , 247.0997 C ₁₄ H ₁₅ O ₄ , 151.0720 C ₉ H ₁₁ O ₂	Diarctigenin+arctigenin	Lignans
123 ^{n,a}	21.81	C ₆₃ H ₆₈ O ₁₈	[M+H] ⁺	1113.4509	2.5	1095.4404 [M+H-H ₂ O] ⁺ , 1081.4243 [M+H-H ₂ O-CH ₂] ⁺ , 727.3138 [M+H-C ₂₁ H ₂₂ O ₆ -O] ⁺ , 709.3027 [M+H-C ₂₁ H ₂₂ O ₇ -H ₂ O] ⁺ , 691.2892 [M+H-C ₂₁ H ₂₂ O ₇ -2H ₂ O] ⁺ , 491.2039 [M+H-C ₃₄ H ₃₈ O ₁₁] ⁺ , 247.0991 C ₁₄ H ₁₅ O ₄ , 203.1071 C ₁₃ H ₁₅ O ₂ , 151.0746 C ₉ H ₁₁ O ₂	NeoarctinA+arctigenin	Lignans

Notes: CA, caffeoylquinic acids;quinicacid:QA;Glucopyranosyl, Glc; Dapiofuranosyl, Dapi; galactopyranosyl, Gal; gentiobiosyl, Gen; apiofuranosyl, Api;ⁿ-Nontarget compounds; ^a-potential novel compounds; *-unambitiously identified by comparison with reference standards.