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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.

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

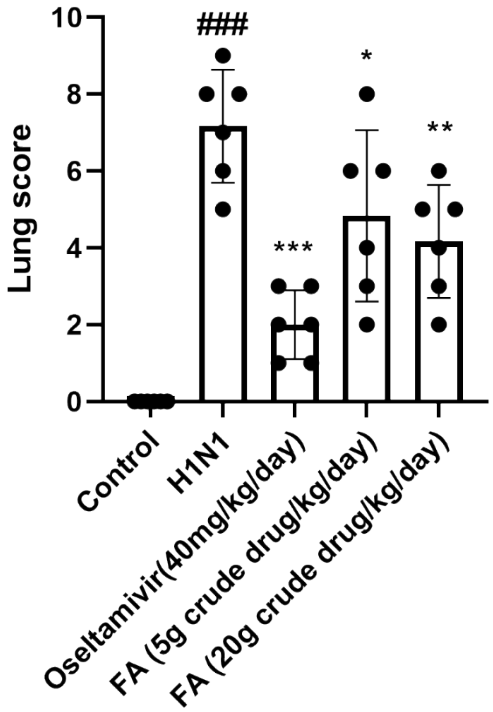

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Figure S2 The possible fragmentation pathway for Lappaol E (peak **81**).

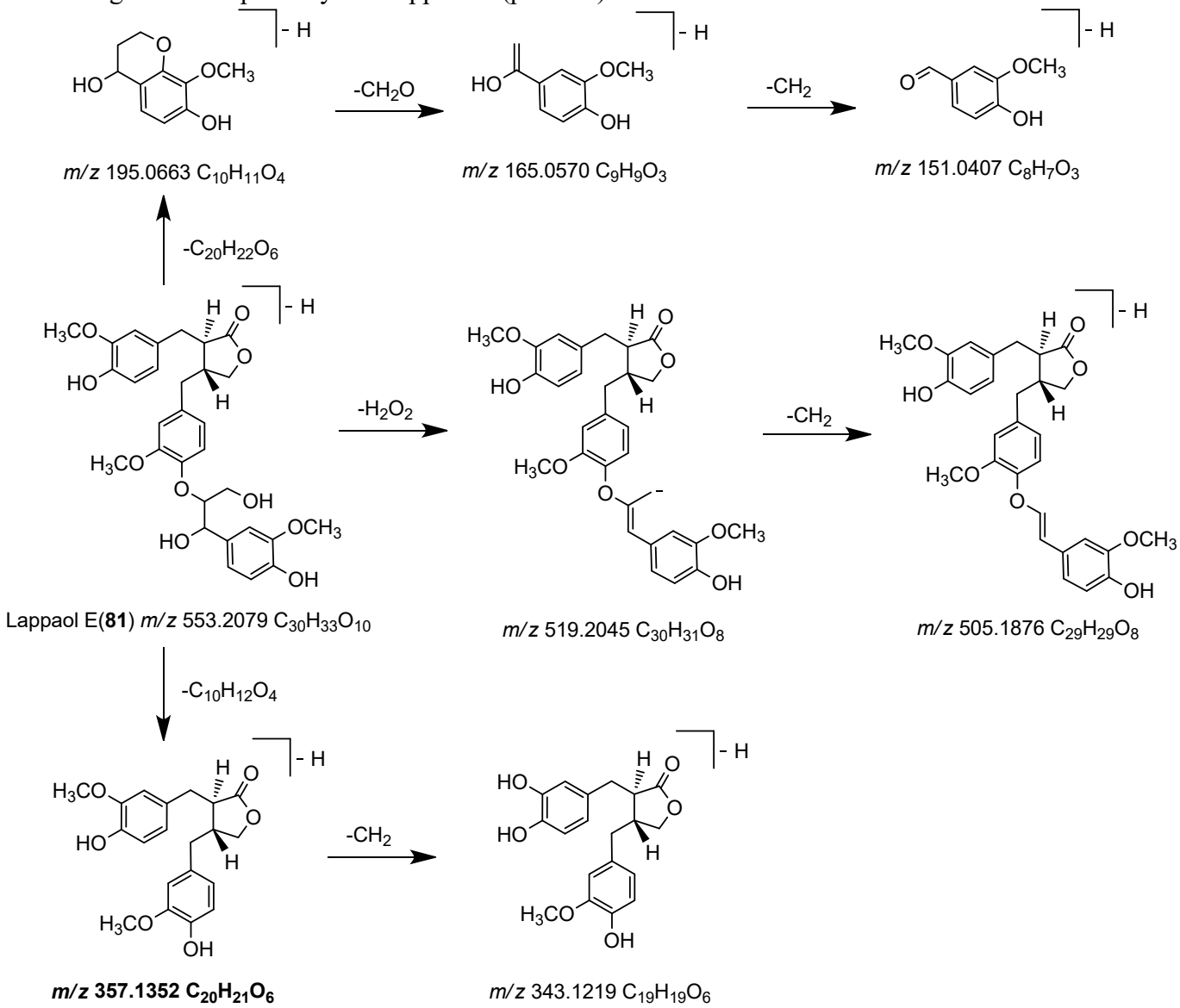

Figure S3 The proposed fragmentation pathway for Lappaol F (peak **105**).

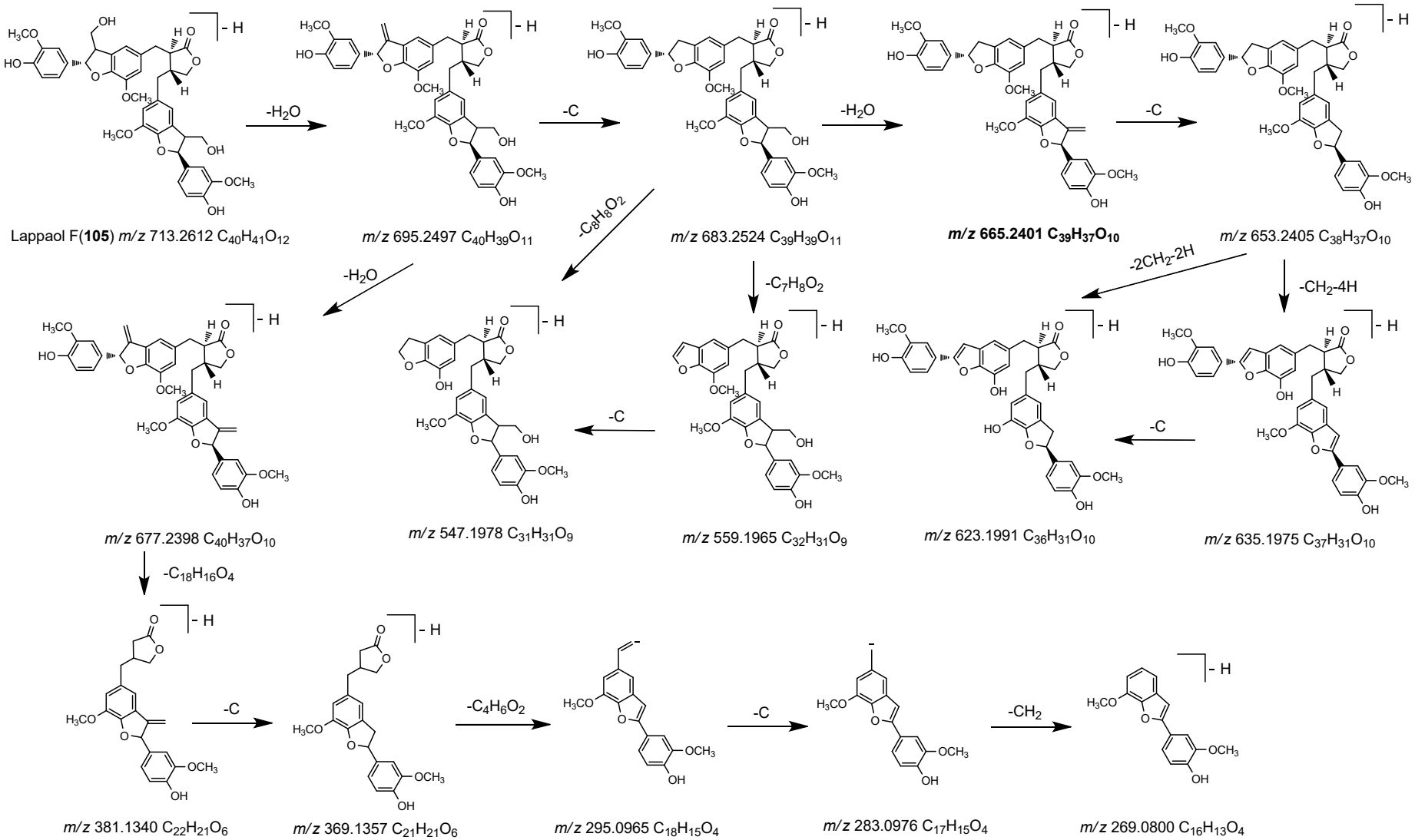

Figure S4 The proposed fragmentation pathway for Lappaol H (peak **40**).

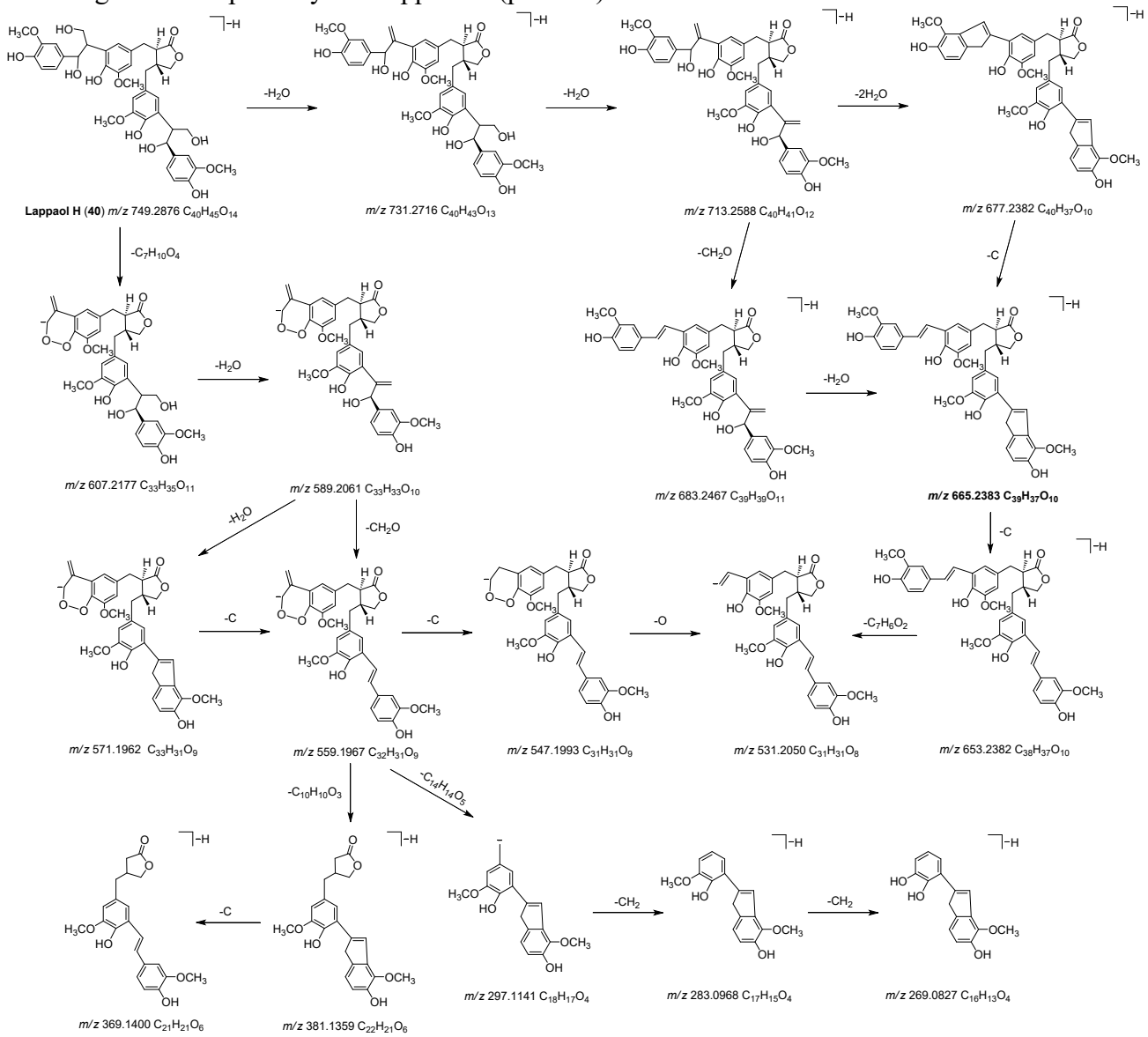

Figure S5 The proposed fragmentation pathway for Neoarctin A (peak **116**).

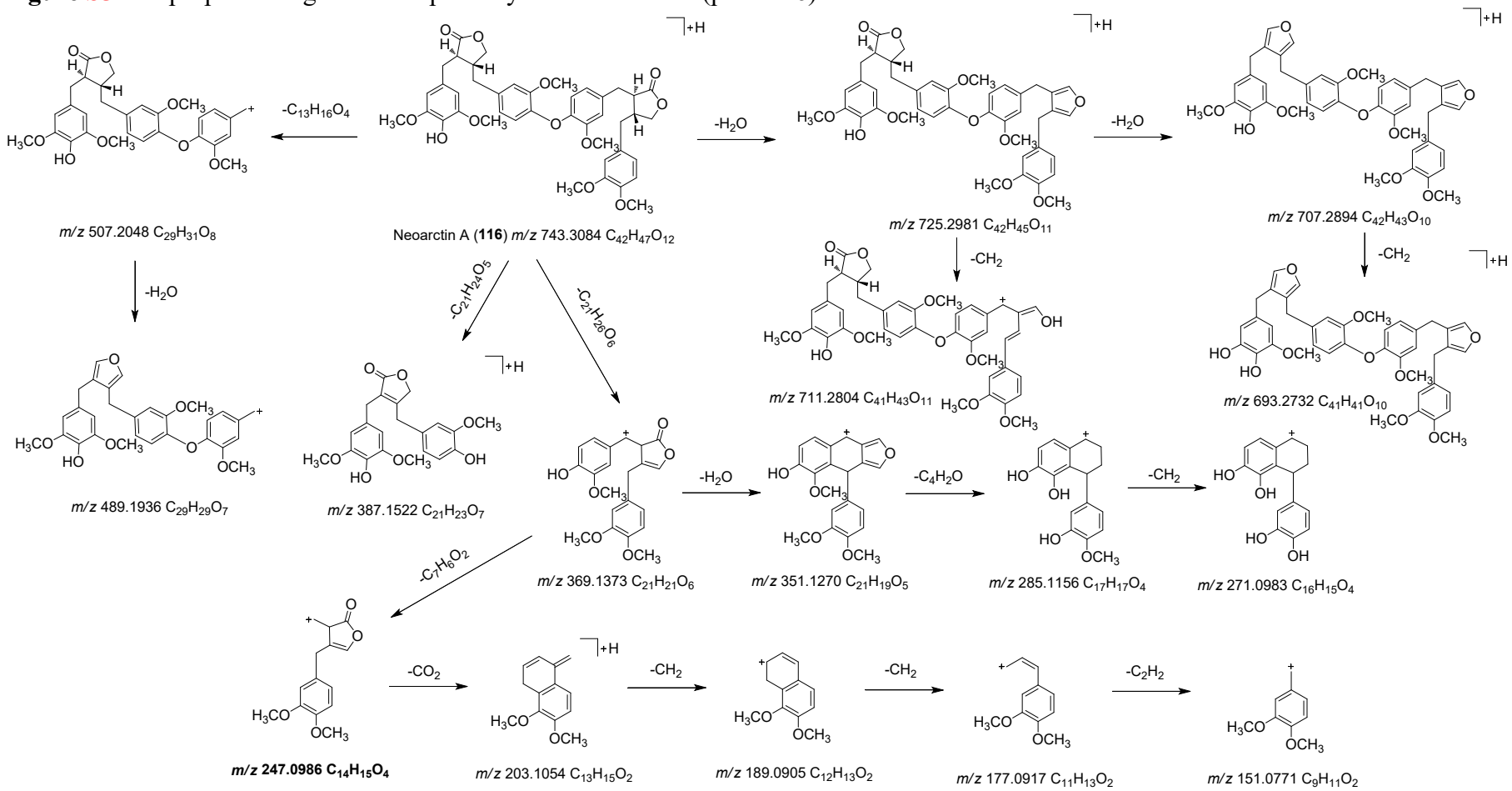

Figure S6 The possible fragmentation pathway for Diarctigenin (peak **114**).

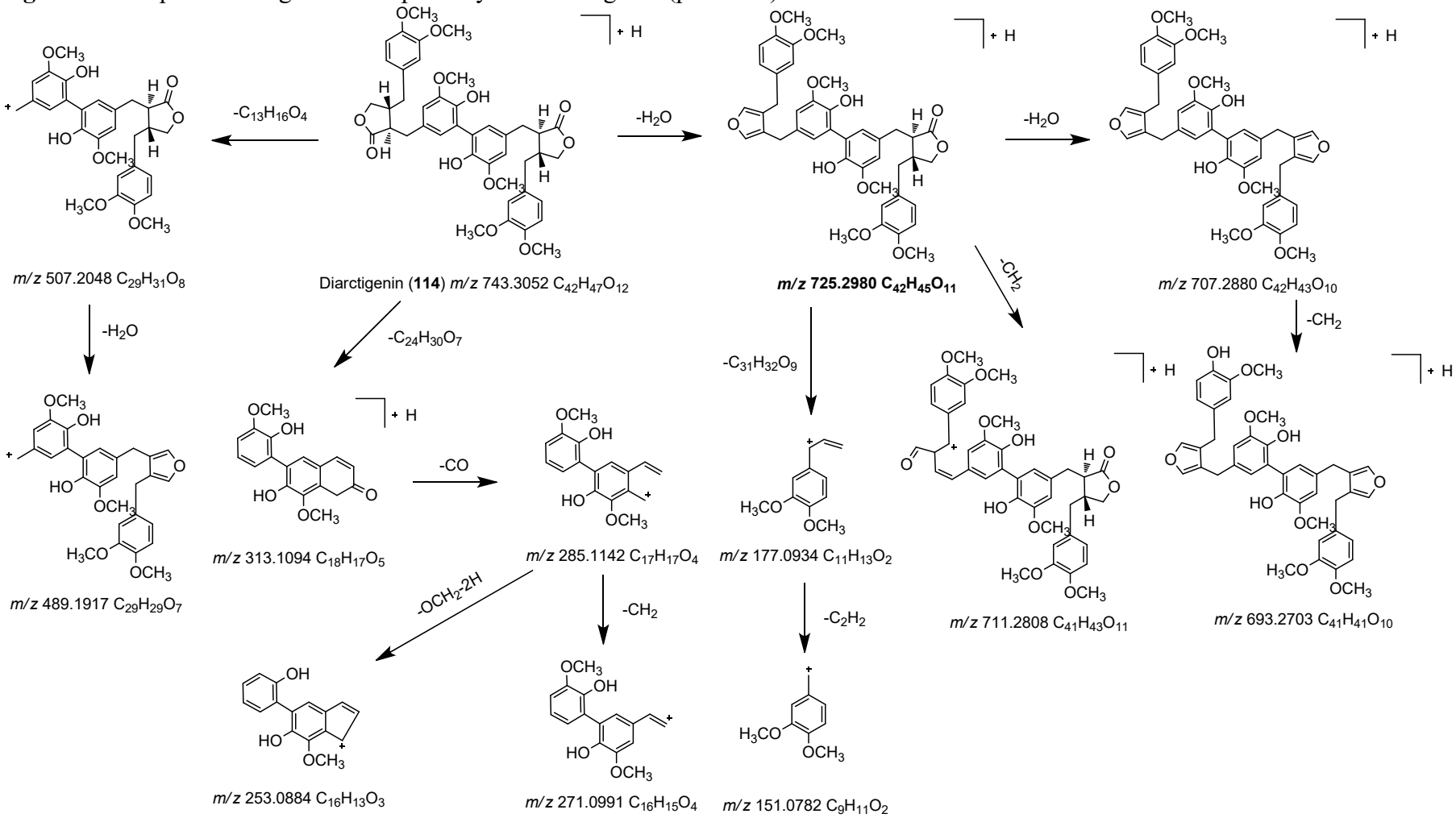

Table S1 Chemical constituents isolated from Fructus Arctii.

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-*O*-*β*-D-gentiobioside	$C_{33}H_{44}O_{16}$	696.2629	[1]
6	arctigenin-4-*O*-*α*-D-galactopyranosyl-(1→6)-*O*-*β*-D-glucopyranoside	$C_{33}H_{44}O_{16}$	696.2629	[1]
7	arctigenin-4-*O*-*β*-D-apiofuranosyl-(1→6)-*O*-*β*-D-glucopyranoside	$C_{32}H_{42}O_{15}$	666.2524	[1]
8	3-benzyl-6-(1-hydroxyethyl)-2,5-piperazinedione	$C_{13}H_{16}N_2O_3$	248.1161	[1]
9	3-benzyl-2,5- piperazinedione	$C_{11}H_{12}N_2O_2$	204.0899	[1]
10	5'-propanediolmatairesinoside	$C_{29}H_{38}O_{13}$	594.2312	[1]
11	(7'*R*,8*R*,8'*R*)-rafanotrachelogenin-4-*O*-*β*-D-glucopyranoside	$C_{27}H_{34}O_{12}$	550.2050	[1]
12	(7'*S*,8*R*,8'*R*)-rafanotrachelogenin-4-*O*-*β*-D-glucopyranoside	$C_{27}H_{34}O_{12}$	550.2050	[1]
13	(7*S*,8*S*,8'*R*)-4,7-dihydroxy-3,3',4'-trimethoxyl-9-oxo-dibenzylbutyrolactone lignan-4-*O*-*β*-D-glucopyranoside	$C_{27}H_{34}O_{12}$	550.2050	[1]
14	(7*S*,8*S*,8'*R*)-4,7- dihydroxy-3,3',4'-trimethoxyl-9-oxo-dibenzylbutyrolactone lignan	$C_{21}H_{24}O_7$	388.1522	[1]
15	(7*R*,8*S*,8′*R*)-4,7-dihydroxy-3,3′,4′-trimethoxyl-9-oxo-dibenzylbutyrolactone lignan-4-*O*-*β*-D-glucopyranoside	$C_{27}H_{34}O_{12}$	550.2050	[1]
16	(7*R*,8*S*,8'*R*)-4,7,4′-trihydroxy-3,3′- dimethoxyl-9-oxo-dibenzylbutyrolactone lignan-4-*O*-*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	arctiiapolignan 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-*O*-*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*S*, 8*R*)-4,7,9,9'-tetrahydroxy-3,3'-dimethoxy-8-*O*-4'-neolignan-9'-*O*-*β*-D-apiofuranosyl-(1→6)-*O*-*β*-D-glucopyranoside	$C_{31}H_{44}O_{16}$	672.2629	1
53	(8*R*)-4,9,9'-trihydroxy-3,3'-dimethoxy-7-oxo-8-*O*-4'-neolignan-4-*O*-*β*-D-glucopyranoside	$C_{26}H_{34}O_{12}$	538.2050	1
54	(7*R*,8*S*)-dihydrodehydrodiconiferyl alcohol-7'-oxo-4-*O*-*β*-D-glucopyranoside	$C_{26}H_{32}O_{12}$	536.1894	1
55	(7'*S*, 8'*R*,8*S*)-4,4',9'-trihydroxy-3,3'-dimethoxy-7',9-epoxylignan-7-oxo-4-*O*-*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*S*,8*R*,7′*S*)-Dihydrodehydrodiconiferyl Alcohol-7′-hydroxy-4-*O*-*β*-D-glucopyranoside	$C_{26}H_{34}O_{12}$	538.2050	4

58	(7*R*,8*S*,7′*S*)-Dihydrodehydrodiconiferyl Alcohol-7′-hydroxy-4-*O*-*β*-D-glucopyranoside	$C_{26}H_{34}O_{12}$	538.2050	4
59	(8*R*,7′*S*)-4,9,7′,9′-Tetrahydroxy-3,3′-dimethoxyl-7-oxo-8-4′-oxyneolignan-4-*O*-*β*-D-glucopyranoside	$C_{26}H_{34}O_{13}$	554.1999	4
60	(8*S*,7′*S*)-4,9,7′,9′-Tetrahydroxy-3,3′-dimethoxyl-7-oxo-8-4′-oxyneolignan-4-*O*-*β*-D-glucopyranoside	$C_{26}H_{34}O_{13}$	554.1999	4
61	(8*R*,7′*R*,8′*R*)-4,4′,7′-Trihydroxy-3,3′-dimethoxyl-9-oxo Dibenzylbutyrolactone Lignan-4-*O*-*β*-D-glucopyranoside	$C_{26}H_{32}O_{12}$	536.1894	4
62	(8*R*,7′*S*,8′*R*)-4,4′,7′-Trihydroxy-3,3′-dimethoxyl-9-oxo Dibenzylbutyrolactone Lignan-4-*O*-*β*-D-glucopyranoside	$C_{26}H_{32}O_{12}$	536.1894	4
63	(7*R*,8*S*,7′*S*,8′*R*)-4,9,4′,7′-Tetrahydroy-3,3′-dimethoxy-7,9′-epoxylignan-4′-*O*-*β*-D-glucopyranoside	$C_{26}H_{34}O_{12}$	538.2050	4
64	(7*S*,8*R*,7′*R*,8′*S*)-4,9,4′,7′-Tetrahydroy-3,3′-dimethoxy-7,9′-epoxylignan-4′-*O*-*β*-D-glucopyranoside	$C_{26}H_{34}O_{12}$	538.2050	4
65	(7*S*,8*R*,7′*S*,8′*S*)-4,9,4′,7′-Tetrahydroy-3,3′-dimethoxy-7,9′-epoxylignan-4′-*O*-*β*-D-glucopyranoside	$C_{26}H_{34}O_{12}$	538.2050	4
66	(7*S*,8*R*,7′*R*,8′*S*)-4,9,4′,7′-Tetrahydroy-3,3′-dimethoxy-7,9′-epoxylignan-4-*O*-*β*-D-glucopyranoside	$C_{26}H_{34}O_{12}$	538.2050	4
67	(7*R*,8*S*)-7,9,9′-trihydroxy-3,3′-dimethoxy-8-*O*-4′-neolignan-4-*O*-*β*-D-glucopyranoside	$C_{26}H_{36}O_{12}$	540.2207	4
68	(7*S*,8*R*)-7,9,9′-trihydroxy-3,3′-dimethoxy-8-*O*-4′-neolignan-4-*O*-*β*-D-glucopyranoside	$C_{26}H_{36}O_{12}$	540.2207	4
69	(7*R*,8*R*)-7,9,9′-trihydroxy-3,3′-dimethoxy-8-*O*-4′-neolignan-4-*O*-*β*-D-glucopyranoside	$C_{26}H_{36}O_{12}$	540.2207	4
70	(7*S*,8*S*)-7,9,9′-trihydroxy-3,3′-dimethoxy-8-*O*-4′-neolignan-4-*O*-*β*-D-glucopyranoside	$C_{26}H_{36}O_{12}$	540.2207	4
71	(7*R*,7′*R*,8*S*,8′*S*)-(+)-neo-olivil-4-*O*-*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	$C_9H_8O_4$	180.0423	1
80	Caffeic acid 4-*O*-D-glucoside	$C_{15}H_{18}O_9$	342.0951	1
81	Chlorogenic acid	$C_{16}H_{18}O_9$	354.0951	1
82	*p*-coumaric acid	$C_9H_8O_3$	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	$C_7H_6O_2$	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-*O*-caffeoylquinic acid	$C_{16}H_{18}O_9$	354.0951	[1]
90	4-*O*-caffeoylquinic acid	$C_{16}H_{18}O_9$	354.0951	[1]
91	5-*O*-caffeoylquinic acid	$C_{16}H_{18}O_9$	354.0951	[1]
92	1-*O*-, 5-*O*-dicaffeoyl-3-*O*-succinylquinic acid	$C_{35}H_{40}O_{15}$	700.2367	[1]
93	1-*O*-, 5-*O*-dicaffeoyl-3-*O*-succinylquinic acid	$C_{29}H_{28}O_{15}$	616.1428	[1]
94	1-*O*,5-*O*-dicaffeoyl-4-*O*-succinylquinic acid	$C_{29}H_{35}O_{15}$	623.1976	[1]
95	1-*O*,5-*O*-dicaffeoyl-4-*O*-succinylquinic acid	$C_{29}H_{28}O_{15}$	616.1428	[1]
96	1-*O*-,5-*O*-dicaffeoyl-3-*O*-4-*O*-disuccinylquaicniidc	$C_{33}H_{39}O_{18}$	723.2136	[1]
97	1-*O*-,5-*O*-dicaffeoyl-3-*O*-4-*O*-disuccinylquaicniidc	$C_{33}H_{32}O_{18}$	716.1589	[1]
98	1-*O*-,3,5-O-tricaffeoyl-4-*O*-succinylquinic acid	$C_{38}H_{41}O_{18}$	785.2293	[1]
99	1-*O*-,3,5-*O*-tricaffeoyl-4-*O*-succinylquinic acid	$C_{38}H_{34}O_{18}$	778.1745	[1]
100	1,3-di-*O*-caffeoylquinic acid	$C_{25}H_{24}O_{12}$	516.1268	[1]
101	1,5-di-*O*-caffeoylquinic acid	$C_{25}H_{24}O_{12}$	516.1268	[1]
102	1,5-di-*O*-caffeoyl-4-*O*-maloylquinic acid	$C_{29}H_{28}O_{16}$	632.1377	[1]
103	1,5-di-*O*-caffeoyl-3-*O*-maloylquinic acid	$C_{29}H_{28}O_{16}$	632.1377	[1]
104	1,3,5-tri-*O*-caffeoylquinic acid	$C_{34}H_{30}O_{15}$	678.1585	[1]
105	1,5-di-*O*-caffeoyl-3-*O*-succinoyl-4-*O*-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-*O*-dicaffeoylquinic acid	$C_{25}H_{24}O_{12}$	516.1268	[1]
111	1,4-di-*O*-caffeoylquinic acid	$C_{25}H_{24}O_{12}$	516.1268	[1]
112	3,5-di-*O*-caffeoylquinic acid	$C_{25}H_{24}O_{12}$	516.1268	[1]
113	4,5-*O*-dicaffeoylquinic acid	$C_{25}H_{24}O_{12}$	516.1268	[1]
114	3,5-*O*-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-*O*-caffeoyl-4-*O*-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-*O*-caffeoyl-3-*O*-maloylquinic acid	$C_{29}H_{28}O_{16}$	632.1377	[1]
129	1,3-di-*O*-caffeoyl-4,5-di-*O*-maloylquinicacid	$C_{33}H_{32}O_{20}$	748.1487	[1]
130	1,5-dicaffeoyl-4-maloylquinic acid	$C_{29}H_{28}O_{16}$	632.1377	[1]
131	1,4-di-*O*-maloyl-3,5-di-*O*-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-*O*-caffeoyl-3-*O*-succinoyl-4-*O*-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-*O*-caffeoyl-4-*O*-maloylquinic Acid	$C_{38}H_{34}O_{19}$	794.1694	[1]
146	5-hydroxymaltol	$C_6H_6O_4$	142.0266	[1]
147	Succinic acid	$C_4H_6O_4$	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-*O*-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-*O*-*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	3α-acetoxyhop-22(29)-ene	$C_{30}H_{49}O_2$	441.3733	[1]
177	3α-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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89 **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 $[M+H-H_2O]^+$, 208.0620 $[M+H-Glc]^+$, 188.0717 $[^{0,2}X+H-COOH-OH]^+$, **146.0631 $[^{0,2}X+H-C_3H_4O_4]^+$**	*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 $[M-H-QA-H_2O]^-$, 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 $[M-H-Glc-2H_2O-C]^-$, **297.1145 $[M-H-Glc-3H_2O-2C]^-$**, 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 $[M-H-QA-H_2O]^-$, 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 $[M-H-Glc-2H_2O-C]^-$, **297.1139 $[M-H-Glc-3H_2O-2C]^-$**, 282.0923	Neo-olivil-4-*O*-*β*-D-glucopyranoside2	Lignans
8	5.45	$C_9H_8O_4$	$[M-H]^-$	179.0352	0.8	135.0454 $[M-H-CO_2]^-$	caffeic 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 $[M-H-Glc-H_2O]^-$, 345.1342 $[M-H-Glc-H_2O-C]^-$, **327.1248 $[M-H-Glc-C-2H_2O]^-$**, 312.1039,297.1121 $[M-H-Glc-3H_2O-2C]^-$, 191.0624 $C_{11}H_{11}O_3$, 151.0337 $C_8H_7O_3$	4,9,4′,7′-Tetrahydroy-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 $[M-H-Glc-H_2O]^-$, 345.1124 $[M-H-Glc-H_2O-C]^-$, **327.1235 $[M-H-Glc-2H_2O-C]^-$**, 312.0995, 297.1056 $[M-H-Glc-3H_2O-2C]^-$, 191.0648 $C_{11}H_{11}O_3$, 151.0318 $C_8H_7O_3$	4,9,4′,7′-Tetrahydroy-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 $[M-H-Glc-2H_2O-C]^-$, 297.1453 $[M-H-Glc-3H_2O-2C]^-$, **165.0536 $C_9H_9O_3$**, 150.0296 $C_8H_6O_3$	(8*R*)-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 $[M-H-Glc-H_2O]^-$,311.1202 $[M-H-Glc-H_2O-CO_2]^-$**,173.0650$C_{11}H_9O_2$	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 $[M-H-2H_2O-C]^-$, 491.1847 $[M-H-2H_2O-C-Dapi]^-$, 343.1339 $[M-H-Dapi-C_{10}H_{12}O_4]^-$, 297.1088 $[M-H-Dapi-Glc-C_2H_8O_3]^-$, **217.0552 $C_{12}H_9O_4$**, 173.0612 $C_{11}H_9O_2$	(7*S*,8*R*)-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 $[M-H-Glc-H_2O]^-$**, **311.1270 $[M-H-Glc-H_2O-CO_2]^-$**, 173.0567 $C_{11}H_9O_2$	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 $C_9H_9O_3$	(7*S*,8*R*)-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 $[M-H-Glc-CH_2O-CO]^-$**, **298.0839**, 136.0152	7,8-dihydrodehydrodiconiferylalcohol-7′-oxo-4-*O*-*β*-D-glucopyranoside 1	Lignans
18	7.14	$C_{26}H_{32}O_{12}$	$[M-H]^-$	535.1856	4.0	**373.1277 $[M-H-Glc]^-$**, **355.1158 $[M-H-Glc-H_2O]^-$**, **311.1235 $[M-H-Glc-H_2O-CO_2]^-$**, 173.0597 $C_{11}H_9O_2$	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 $[M-H-Glc-CH_2O-CO]^-$**, 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 $[M-H-H_2O-C]^-$, **193.0476 $C_{10}H_9O_4$**	Tanegool	Lignans
21	7.56	$C_{26}H_{32}O_{12}$	$[M-H]^-$	535.1825	0.9	**373.1334 $[M-H-Glc]^-$**, **151.0410 $C_8H_7O_3$**,136.0178	(7'*S*,8'*R*,8*S*)-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$[M-H-Glc-C_2H_2O]^-$, **357.1339 $[M-H-2Glc]^-$**, 313.1310 $[M-H-2Glc-CO_2]^-$, 161.0608$C_{10}H_9O_2$	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 $[M-H-Glc-H_2O]^-$, 401.1588 $[M-H-Glc-H_2O-C]^-$, 383.1470 $[M-H-Glc-2H_2O-C]^-$	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 $[M+H-Glc-H_2O]^+$**, 233.0812 $[M+H-Glc-H_2O-CH_4]^+$, 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 $[M-H-caffeoyl-H_2O]^-$, 191.0568 $[M-H-2caffeoyl]^-$, **179.0347 $[M-H-caffeoyl-QA]^-$**, 161.0244 $[M-H-caffeoyl-QA-H_2O]^-$, 135.0461 $[M-H-caffeoyl-QA-2H_2O]^-$	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 $[M-H-H_2O]^-$, 715.2670 $[M-H-2H_2O]^-$, 685.2666 $[M-H-3H_2O-C]^-$, 679.2513 $[M-H-4H_2O]^-$, **667.2418 $[M-H-4H_2O-C]^-$**, 637.2427 $[M-H-4H_2O-2C]^-$, 625.2454 $[M-H-4H_2O-3C]^-$, 573.2029 $[M-H-C_7H_{10}O_4-2H_2O]^-$, 561.2121 $[M-H-C_7H_{10}O_4-2H_2O-C]^-$, 531.2042 $[M-H-C_7H_{10}O_4-3H_2O-2C]^-$, 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 $[M-H-caffeoyl-QA-H_2O]^-$, 135.0451 $[M-H-caffeoyl-QA-2H_2O]^-$	3,5-*O*-dicaffeoylquinic acid	CA
29	8.83	$C_{30}H_{34}O_{11}$	$[M-H]^-$	569.2009	-1.4	**533.1802 $[M-H-2H_2O]^-$**, **521.1802 $[M-H-2H_2O-C]^-$**, 503.1741 $[M-H-3H_2O-C]^-$, 459.1791 $[M-H-3H_2O-2C]^-$, **427.1400 $[M-H-C_7H_{10}O_3]^-$**, 415.1392 $[M-H-C_8H_{10}O_3]^-$, 397.1281 $[M-H-C_8H_{10}O_3-H_2O]^-$, 367.1194 $[M-H-C_8H_{10}O_3-2H_2O-C]^-$	Reported compound 1	Lignans
30[n,a]	8.90	$C_{40}H_{48}O_{14}$	$[M-H]^-$	751.2966	0.1	733.2831 $[M-H-H_2O]^-$, 715.2712 $[M-H-2H_2O]^-$, 679.2539 $[M-H-4H_2O]^-$, **667.2507 $[M-H-4H_2O-C]^-$**, 655.2531 $[M-H-4H_2O-2C]^-$,609.2316 $[M-H-C_7H_{10}O_4]^-$, 591.2097 $[M-H-C_7H_{10}O_4-H_2O]^-$, 573.2109 $[M-H-C_7H_{10}O_4-2H_2O]^-$, 561.2130 $[M-H-C_7H_{10}O_4-2H_2O-C]^-$, 549.2144 $[M-H-C_7H_{10}O_4-2H_2O-2C]^-$,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 $[M-H-2H_2O]^-$**, **521.1889 $[M-H-2H_2O-C]^-$**,503.1702 $[M-H-3H_2O-C]^-$, 459.1726 $[M-H-3H_2O-2C]^-$, **427.1318 $[M-H-C_7H_{10}O_3]^-$**, 415.1403 $[M-H-C_8H_{10}O_3]^-$, 397.1143 [M-H-	Isomer of reported compound 1	Lignans

						$C_8H_{10}O_3$-H_2O]$^-$, 367.1235 [M-H-$C_8H_{10}O_3$-2H_2O-C]$^-$		
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_2O]$^-$, 135.0450 [M-H-caffeoyl-QA-2H_2O]$^-$	4,5-*O*-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_2O]$^+$, **247.0966** [M+H-Glc-H_2O-$C_7H_8O_2$]$^+$, 203.1089 $C_{13}H_{15}O_2$, 151.0738 $C_9H_{11}O_2$	(7*S*,8*S*,8'*R*)-4,7-dihydroxy-3,3',4'-trimethoxyl-9-oxo-dibenzylbutyrolactonelignan-4-*O*-*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_2O]$^-$, 135.0452 [M-H-caffeoyl-QA-2H_2O]$^-$	1,5-*O*-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_2O]**$^-$, **505.1885 [M-H-2Glc-H_2O-C]**$^-$	Arctiisesquineolignan 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_2O]**$^-$, 909.3406 [M-H-2H_2O]$^-$, 897.3348 [M-H-2H_2O-C]$^-$, 891.3221 [M-H-3H_2O]$^-$, 879.3265 [M-H-3H_2O-C]$^-$, 873.3196 [M-H-4H_2O]$^-$, 861.3143 [M-H-4H_2O-C]$^-$, 843.2952 [M-H-5H_2O-C]$^-$, 837.2925 [M-H-6H_2O]$^-$, 731.2539 [M-H-5H_2O-$C_7H_8O_2$]$^-$, 719.2501 [M-H-5H_2O-$C_7H_8O_2$-C]$^-$, 707.2517 [M-H-5H_2O-$C_7H_8O_2$-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_2O]$^-$, 571.1993 [M-H-$C_{17}H_{22}O_7$-2H_2O]$^-$,559.1963 [M-H-$C_{17}H_{22}O_7$-2H_2O-C]$^-$,547.2011 [M-H-$C_{17}H_{22}O_7$-2H_2O-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_2O]$^-$, 909.3420 [M-H-2H_2O]$^-$, 897.3309 [M-H-2H_2O-C]$^-$, 879.3152 [M-H-3H_2O-C]$^-$, 861.3094 [M-H-4H_2O-C]$^-$, 785.2729 [M-H-$C_7H_{12}O_4$]$^-$, 719.2399 [M-H-$C_8H_{18}O_7$]$^-$, 707.2440 [M-H-$C_8H_{18}O_7$-C]$^-$, 695.2475 [M-H-$C_8H_{18}O_7$-2C]$^-$, 607.2203 [M-H-$C_{17}H_{22}O_7$]$^-$, 589.2079 [M-H-$C_{17}H_{22}O_7$-H_2O]$^-$, 571.1993 [M-H-$C_{17}H_{22}O_7$-2H_2O]$^-$, **559.1992 [M-H-$C_{17}H_{22}O_7$-2H_2O-C]**$^-$, 547.1976 [M-H-$C_{17}H_{22}O_7$-2H_2O-2C]$^-$	Unknown	Lignans
40	10.12	$C_{40}H_{46}O_{14}$	[M-H]$^-$	749.2876	-3.3	731.2716 [M-H-H_2O]$^-$, 713.2588 [M-H-2H_2O]$^-$, 683.2467 [M-H-2H_2O-CH_2O]$^-$, 677.2382 [M-H-4H_2O]$^-$, **665.2383 [M-H-4H_2O-C]**$^-$, 653.2382 [M-H-4H_2O-2C]$^-$, 607.2177 [M-H-$C_7H_{10}O_4$]$^-$, 589.2061 [M-H-$C_7H_{10}O_4$-H_2O]$^-$, 571.1962 [M-H-$C_7H_{10}O_4$-2H_2O]$^-$, 559.1967 [M-H-$C_7H_{10}O_4$-2H_2O-C]$^-$, 547.1993 [M-H-$C_7H_{10}O_4$-2H_2O-2C]$^-$, 531.2050 [M-H-$C_7H_{10}O_4$-2H_2O-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-*O*-*α*-D-galactopyranosyl-(1→6)-*O*-*β*-D-	Lignans

							glucopyranoside	
42	10.36	$C_{33}H_{44}O_{16}$	$[M-H+HCOOH]^-$	741.2603	-0.3	371.1467 $[M-H-Gen]^-$, **357.1354** $[M-H-Gen-CH_2]^-$	Arctigenin-4-*O*-*β*-D-gentiobioside	Lignans
43[n,a]	10.53	$C_{50}H_{58}O_{18}$	$[M-H]^-$	945.3549	0.4	927.3464 $[M-H-H_2O]^-$, 909.3374 $[M-H-2H_2O]^-$, 897.3365 $[M-H-2H_2O-C]^-$, 803.2944 $[M-H-C_7H_{10}O_3]^-$, 791.2944 $[M-H-C_7H_{10}O_3-C]^-$, 779.2865 $[M-H-C_7H_{10}O_3-2C]^-$, 747.2700 $[M-H-C_{10}H_{14}O_4]^-$, 729.2593 $[M-H-C_{10}H_{14}O_4-H_2O]^-$, 561.2154 $[M-H-C_{18}H_{24}O_9]^-$, **549.2164 $[M-H-C_{18}H_{24}O_9-C]^-$**, 543.2064 $[M-H-C_{18}H_{24}O_9-H_2O]^-$, 531.2056 $[M-H-C_{18}H_{24}O_9-H_2O-C]^-$, 517.1867 $[M-H-C_{18}H_{24}O_9-H_2O-C-CH_2]^-$, 505.1927 $[M-H-C_{18}H_{24}O_9-H_2O-2C-CH_2]^-$, 455.1721 $[M-H-C_{25}H_{30}O_{10}]^-$, 443.1726 $[M-H-C_{25}H_{30}O_{10}-C]^-$, 437.1549 $[M-H-C_{25}H_{30}O_{10}-H_2O]^-$, 425.1621 $[M-H-C_{25}H_{30}O_{10}-C-H_2O]^-$, 409.1605 $[M-H-C_{25}H_{30}O_{10}-CO-H_2O]^-$	Unknown	Lignans
44	10.57	$C_{30}H_{34}O_{10}$	$[M-H]^-$	553.2079	0.5	**517.1909 $[M-H-2H_2O]^-$**, 505.1886 $[M-H-2H_2O-C]^-$, 475.1722 $[M-H-2H_2O-C-CH_2O]^-$, 411.1457 $[M-H-C_7H_{10}O_3]^-$, 399.1420 $[M-H-C_7H_{10}O_3-C]^-$	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 $[M+H-Api-Glc-H_2O]^+$	Arctigenin-4-*O*-*β*-D-apiofuranosyl-(1→6)-*O*-*β*-D-glucopyranoside1	Lignans
46[n,a]	11.05	$C_{50}H_{58}O_{18}$	$[M-H]^-$	945.3549	0.4	927.3433 $[M-H-H_2O]^-$, 909.3214 $[M-H-2H_2O]^-$, 879.3303 $[M-H-3H_2O-C]^-$, 861.3129 $[M-H-4H_2O-C]^-$, **747.2651 $[M-H-C_{10}H_{14}O_4]^-$**, 729.2482 $[M-H-C_{10}H_{14}O_4-H_2O]^-$, 663.2224 $[M-H-C_{10}H_{14}O_4-4H_2O-C]^-$, 651.2294 $[M-H-C_{10}H_{14}O_4-4H_2O-2C]^-$, 557.1829$[M-H-C_{18}H_{28}O_9]^-$, 531.1929 $[M-H-C_{18}H_{28}O_9-H_2O-C]^-$, 517.1909 $[M-H-C_{18}H_{28}O_9-H_2O-2C-2H]^-$, **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 $[M+H-Api-Glc-H_2O]^+$	Arctigenin-4-*O*-*β*-D-apiofuranosyl-(1→6)-*O*-*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 $C_{11}H_7O_4$, 174.0683 $C_{11}H_{10}O_2$, 159.0374 $C_{10}H_7O_2$	Hemislienoside	Lignans
49[n,a]	11.29	$C_{50}H_{58}O_{18}$	$[M-H]^-$	945.3549	0.4	927.3427 $[M-H-H_2O]^-$, 909.3539 $[M-H-2H_2O]^-$, 897.3338 $[M-H-2H_2O-C]^-$, 879.3211 $[M-H-3H_2O-C]^-$, 861.3249 $[M-H-4H_2O-C]^-$, 849.3149 $[M-H-4H_2O-2C]^-$, 803.2888 $[M-H-C_7H_{10}O_3]^-$, 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 $[M-H-C_{18}H_{24}O_9-H_2O]^-$, 531.2003 $[M-H-C_{18}H_{24}O_9-H_2O-C]^-$, 517.1884 $[M-H-C_{18}H_{24}O_9-H_2O-C-CH_2]^-$, 505.1880 $[M-H-C_{18}H_{24}O_9-H_2O-2C-CH_2]^-$, 455.1650 $[M-H-C_{25}H_{30}O_{10}]^-$	Unknown	Lignans
50[n,a]	11.39	$C_{50}H_{58}O_{18}$	$[M-H]^-$	945.3549	0.4	927.3459 $[M-H-H_2O]^-$, 909.3396 $[M-H-2H_2O]^-$, 897.3337 $[M-H-2H_2O-C]^-$, 879.3193 $[M-H-3H_2O-C]^-$, 861.3155 $[M-H-4H_2O-C]^-$, 849.3155 $[M-H-4H_2O-2C]^-$, 803.2881 $[M-H-C_7H_{10}O_3]^-$, **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 $[M-H-C_{18}H_{24}O_9-H_2O-C]^-$, 517.1878 $[M-H-C_{18}H_{24}O_9-H_2O-C-CH_2]^-$, 505.1909 $[M-H-C_{18}H_{24}O_9-H_2O-2C-CH_2]^-$, 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 $[M-H-H_2O]^-$, 713.2621 $[M-H-2H_2O]^-$, 701.2598 $[M-H-2H_2O-C]^-$, 695.2499 $[M-H-3H_2O]^-$, 677.2419 $[M-H-4H_2O]^-$, **665.2399 $[M-H-4H_2O-C]^-$**, 653.2397 $[M-H-4H_2O-2C]^-$, 607.2142 $[M-H-C_7H_{10}O_3]^-$, 571.2095 $[M-H-C_7H_{10}O_3-2H_2O]^-$, 559.1992 $[M-H-C_7H_{10}O_3-2H_2O-C]^-$, 547.1972 $[M-H-C_7H_{10}O_3-2H_2O-2C]^-$, 283.1004 $C_{17}H_{15}O_4$, 269.0808 $C_{16}H_{13}O_4$	Unknown	Lignans
52	11.46	$C_{30}H_{34}O_{10}$	$[M-H]^-$	553.2084	1.0	517.1888 $[M-H-2H_2O]^-$, **505.1888 $[M-H-2H_2O-C]^-$**, 475.1426 $[M-H-2H_2O-C-CH_2O]^-$, 411.1464 $[M-H-C_7H_{10}O_3]^-$, 399.1460 $[M-H-C_7H_{10}O_3-C]^-$	Isolappaol C	Lignans
53[n,a]	11.49	$C_{40}H_{46}O_{14}$	$[M-H]^-$	749.2817	0.8	731.2726 $[M-H-H_2O]^-$, 713.2621 $[M-H-2H_2O]^-$, **701.2627$[M-H-2H_2O-C]^-$**, 683.2510$[M-H-2H_2O-CH_2O]^-$, 665.2396 $[M-H-4H_2O-C]^-$, 653.2400 $[M-H-4H_2O-2C]^-$, 607.2191 $[M-H-C_7H_{10}O_3]^-$, 589.2055 $[M-H-C_7H_{10}O_3-H_2O]^-$, 571.2007 $[M-H-C_7H_{10}O_3-2H_2O]^-$, 559.2000 $[M-H-C_7H_{10}O_3-2H_2O-C]^-$, 283.0990 $C_{17}H_{15}O_4$, 269.0835 $C_{16}H_{13}O_4$	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 $[M-H-Glc-H_2O]^-$, 235.0983 $C_{13}H_{15}O_4$, 121.0359 $C_7H_5O_2$	Arctiin	Lignans
55	11.69	$C_{30}H_{34}O_{10}$	$[M-H]^-$	553.2084	1.0	517.1885 $[M-H-2H_2O]^-$, **505.1881 $[M-H-2H_2O-C]^-$**, 411.1461 $[M-H-C_7H_{10}O_3]^-$, 399.1470 $[M-H-C_7H_{10}O_3-C]^-$	Lappaol C	Lignans
56[n]	11.75	$C_{40}H_{46}O_{14}$	$[M-H]^-$	749.2809	0.0	731.2709 $[M-H-H_2O]^-$, 713.2628 $[M-H-2H_2O]^-$, **701.2604 $[M-H-2H_2O-C]^-$**, 695.2542 $[M-H-3H_2O]^-$, 683.2504 $[M-H-2H_2O-CH_2O]^-$, 665.2426$[M-H-4H_2O-C]^-$, 653.2403 $[M-H-4H_2O-2C]^-$, 607.2191 $[M-H-C_7H_{10}O_3]^-$, 589.2085 $[M-H-C_7H_{10}O_3-H_2O]^-$, 571.1968 $[M-H-C_7H_{10}O_3-2H_2O]^-$, 381.1357 $C_{22}H_{21}O_6$, 297.1127 $C_{18}H_{17}O_4$	Cerberalignan A	Lignans
57	11.85	$C_{21}H_{26}O_7$	$[M-H]^-$	389.1626	2.6	371.1504 $[M-H-H_2O]^-$, **330.1502 $[M-H-COOH-CH_2]^-$**	Arctigenic acid	Lignans
58[n,a]	11.88	$C_{50}H_{56}O_{17}$	$[M-H]^-$	927.3446	0.7	909.3343 $[M-H-H_2O]^-$, 879.3279 $[M-H-2H_2O-C]^-$, 861.3060 $[M-H-3H_2O-C]^-$, 843.3069 $[M-H-4H_2O-C]^-$, 837.3087$[M-H-5H_2O]^-$, 825.2944 $[M-H-5H_2O-C]^-$, **813.2916 $[M-H-5H_2O-2C]^-$**, 801.2926 $[M-H-5H_2O-3C]^-$, 785.2798 $[M-H-C_7H_{10}O_3]^-$, 737.2724 $[M-H-C_7H_{10}O_3-4C]^-$, 719.2517 $[M-H-C_8H_{16}O_6]^-$, 707.2501 $[M-H-C_8H_{16}O_6-C]^-$	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$[M-H-Glc-H_2O]^-$, 531.1986 $[M-H-Glc-2H_2O]^-$,519.2030$[M-H-Glc-2H_2O-C]^-$, 517.1917 $[M-H-Glc-2H_2O-CH_2]^-$, 505.1887 $[M-H-Glc-2H_2O-CH_2-C]^-$, 411.1429 $[M-H-C_{14}H_{22}O_8]^-$, **401.1627 $[M-H-C_{15}H_{20}O_8]^-$**, 383.1520 $[M-H-C_{15}H_{20}O_8-H_2O]^-$,371.1513 $[M-H-C_{15}H_{20}O_8-H_2O-C]^-$, 165.0569 $C_9H_9O_3$	Lappaol D isomer 2+Glc	Lignans
60[n,a]	11.94	$C_{40}H_{46}O_{14}$	$[M-H]^-$	749.2806	-0.3	731.2668 $[M-H-H_2O]^-$, 683.2380 $[M-H-2H_2O-CH_2O]^-$, 607.2179 $[M-H-C_7H_{10}O_3]^-$, 589.1982 $[M-H-C_7H_{10}O_3-H_2O]^-$, 571.1968 $[M-H-C_7H_{10}O_3-2H_2O]^-$, 559.1964 $[M-H-C_7H_{10}O_3-2H_2O-C]^-$, **401.1620 $[M-H-C_{18}H_{20}O_7]^-$**, 383.1521 $[M-H-C_{18}H_{20}O_7-H_2O]^-$	Unknown	Lignans
61[n,a]	11.98	$C_{50}H_{56}O_{17}$	$[M-H]^-$	927.3468	2.9	909.3367 $[M-H-H_2O]^-$, 879.3209 $[M-H-2H_2O-C]^-$, 861.3148 $[M-H-3H_2O-C]^-$, 843.3069 $[M-H-4H_2O-C]^-$, 837.2950 $[M-H-5H_2O]^-$, 825.2936 $[M-H-5H_2O-C]^-$, **813.2916 $[M-H-5H_2O-2C]^-$**	Unknown	Lignans

						, 801.2901 [M-H-5H_2O-3C]$^-$, 785.2778 [M-H-$C_7H_{10}O_3$]$^-$, 737.2511 [M-H-$C_7H_{10}O_3$-4C]$^-$, 719.2506 [M-H-$C_8H_{16}O_6$]$^-$, 707.2485 [M-H-$C_8H_{16}O_6$-C]$^-$		
62	12.04	$C_{40}H_{46}O_{13}$	[M-H]$^-$	733.2875	1.5	715.2650 [M-H-H_2O]$^-$, 679.2506 [M-H-3H_2O]$^-$, **667.2499[M-H-3H_2O-C]$^-$**, 655.2571 [M-H-3H_2O-2C]$^-$, 561.2104 [M-H-$C_8H_{12}O_4$]$^-$, 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_2O]$^-$, 703.2774 [M-H-H_2O-C]$^-$, 685.2607 [M-H-2H_2O]$^-$, 679.2534 [M-H-3H_2O]$^-$, **667.2510 [M-H-3H_2O-C]$^-$**, 655.2532 [M-H-3H_2O-2C]$^-$, 607.2153 [M-H-$C_7H_{10}O_2$]$^-$, 561.2122 [M-H-$C_8H_{12}O_4$]$^-$	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_2O]$^-$, 533.1823 [M-H-Glc-CH_4-H_2O]$^-$, 519.2036 [M-H-Glc-2H_2O-C]$^-$,517.1891 [M-H-Glc-2H_2O-CH_2]$^-$, **505.1881 [M-H-Glc-2H_2O-CH_2-C]$^-$**, 411.1393 [M-H-$C_{14}H_{22}O_8$]$^-$, 195.0673 $C_{10}H_{11}O_4$, 165.0571 $C_9H_9O_3$	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_2O]$^-$, 835.2906 [M-H-2H_2O]$^-$, 823.3036 [M-H-2H_2O-C]$^-$, 805.2818 [M-H-3H_2O-C]$^-$, 787.2744 [M-H-4H_2O-C]$^-$, 775.2717 [M-H-4H_2O-2C]$^-$, 731.2573 [M-H-5H_2O-4C]$^-$, 687.3163 [M-H-$C_7H_4O_6$]$^-$, 683.2485 [M-H-$C_8H_{12}O_5$]$^-$, 681.2343 [M-H-$C_8H_{12}O_5$-2H]$^-$, 671.2440 [M-H-$C_8H_{12}O_5$-C]$^-$, 665.2408 [M-H-$C_8H_{12}O_5$-H_2O]$^-$, 653.2430 [M-H-$C_8H_{12}O_5$-H_2O-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_2O]$^-$, 897.3375 [M-H-H_2O-C]$^-$, 879.3265 [M-H-2H_2O-C]$^-$, 861.3177 [M-H-3H_2O-C]$^-$, 843.2952 [M-H-4H_2O-C]$^-$, 837.3044 [M-H-5H_2O]$^-$, 825.2925 [M-H-5H_2O-C]$^-$, **813.2953 [M-H-5H_2O-2C]$^-$**,801.2835[M-H-5H_2O-3C]$^-$, 785.2709 [M-H-$C_7H_{10}O_3$]$^-$, 737.2626 [M-H-$C_7H_{10}O_3$-4C]$^-$, 719.2507 [M-H-$C_8H_{16}O_6$]$^-$	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 $C_{11}H_7O_4$, **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_2O]$^-$, 897.3338 [M-H-H_2O-C]$^-$, 879.3309 [M-H-2H_2O-C]$^-$, 861.3174 [M-H-3H_2O-C]$^-$, 843.3010 [M-H-4H_2O-C]$^-$, 825.2930 [M-H-5H_2O-C]$^-$, **813.2962 [M-H-5H_2O-2C]$^-$**, 801.2856 [M-H-5H_2O-3C]$^-$, 785.2724 [M-H-$C_7H_{10}O_3$]$^-$, 719.2539 [M-H-$C_8H_{16}O_6$]$^-$, 707.2502 [M-H-$C_8H_{16}O_6$-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_2O]$^-$, 909.3270 [M-H-2H_2O]$^-$, 897.3295 [M-H-2H_2O-C]$^-$, 879.3223 [M-H-3H_2O-C]$^-$, 683.2411 [M-H-$C_{11}H_{18}O_7$]$^-$, 665.2435 [M-H-$C_{11}H_{18}O_7$-H_2O]$^-$, 653.2437 [M-H-$C_{11}H_{18}O_7$-H_2O-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_2O]$^-$, 559.1985 [M-H-$C_{17}H_{22}O_7$-2H_2O-C]$^-$, 547.1966 [M-H-$C_{17}H_{22}O_7$-2H_2O-2C]$^-$, 531.2022 [M-H-$C_{17}H_{22}O_7$-2H_2O-2C-O]$^-$, 517.1854 [M-H-$C_{17}H_{22}O_7$-2H_2O-2C-O-CH_2]$^-$, 505.1920 [M-H-$C_{17}H_{22}O_7$-2H_2O-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-acetyGlc]$^-$**, 357.1390 [M-H-acetyGlc-H_2O]$^-$,	4-acetylate arctiin	Lignans

						121.0315 $C_7H_5O_2$		
71[n,a]	12.57	$C_{50}H_{56}O_{17}$	$[M-H]^-$	927.3446	0.7	897.3338 $[M-H-H_2O-C]^-$, 879.3191 $[M-H-2H_2O-C]^-$, 861.3163 $[M-H-3H_2O-C]^-$, 849.3130 $[M-H-3H_2O-2C]^-$, 717.2673 $[M-H-C_7H_{14}O_7]^-$, **665.2462 $[M-H-C_{11}H_{18}O_7]^-$**, 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 $[M-H-H_2O]^-$, 717.2548 $[M-H-H_2O-CH_2]^-$,701.2609 $[M-H-2H_2O-C]^-$, 683.2492 $[M-H-2H_2O-CH_2O]^-$, 665.2360 $[M-H-4H_2O-C]^-$, 653.2383 $[M-H-4H_2O-2C]^-$, 607.2093 $[M-H-C_7H_{10}O_3]^-$, **597.2381 $[M-H-C_8H_8O_3]^-$**, 579.2252 $[M-H-C_8H_8O_3-H_2O]^-$, 553.2095 $[M-H-C_8H_8O_3-H_2O-C_2H_2]^-$, 549.2150 $[M-H-C_8H_8O_3-2H_2O-C]^-$, 531.2081$[M-H-C_8H_8O_3-3H_2O-C]^-$, 371.1486 $C_{21}H_{23}O_6$, 165.0563 $C_9H_9O_3$, 151.0418 $C_8H_7O_3$	Unknown	Lignans
73[n,a]	12.70	$C_{50}H_{56}O_{17}$	$[M-H]^-$	927.3468	2.9	897.3341 $[M-H-H_2O-C]^-$, 879.3291 $[M-H-2H_2O-C]^-$, 861.3128 $[M-H-3H_2O-C]^-$, 849.3044 $[M-H-3H_2O-2C]^-$, 717.2560 $[M-H-C_7H_{14}O_7]^-$, **665.2368 $[M-H-C_{11}H_{18}O_7]^-$**, 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 $[M-H-H_2O]^-$, **505.1876 $[M-H-H_2O-CO]^-$**, 411.1492 $[M-H-C_7H_8O_3]^-$, 409.1315 $[M-H-C_7H_{10}O_3]^-$, 151.0434 $C_8H_7O_3$	Arctignan B	Lignans
75[n,a]	12.75	$C_{50}H_{58}O_{18}$	$[M-H]^-$	945.3549	0.4	927.3477 $[M-H-H_2O]^-$, 909.3370 $[M-H-2H_2O]^-$, 895.3121 $[M-H-2H_2O-CH_2]^-$, 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 $[M-H-C_{28}H_{32}O_{11}]^-$**	Unknown	Lignans
76[n,a]	12.79	$C_{40}H_{46}O_{14}$	$[M-H]^-$	749.2825	1.6	731.2772 $[M-H-H_2O]^-$, 701.2621 $[M-H-2H_2O-C]^-$, 683.2510 $[M-H-2H_2O-CH_2O]^-$, 665.2330 $[M-H-4H_2O-C]^-$, 653.2362 $[M-H-4H_2O-2C]^-$, 607.2049 $[M-H-C_7H_{10}O_3]^-$, 597.2292 $[M-H-C_8H_8O_3]^-$, 553.2123 $[M-H-C_8H_8O_3-H_2O-C_2H_2]^-$, **521.1825 $[M-H-C_8H_8O_3-2H_2O-C_2H_2-2C]^-$**, 165.0565 $C_9H_9O_3$, 151.0416 $C_8H_7O_3$	Unknown	Lignans
77	12.80	$C_{30}H_{32}O_{10}$	$[M-H]^-$	551.1938	2.1	533.1797 $[M-H-H_2O]^-$, **505.1893 $[M-H-H_2O-CO]^-$**, 409.1314 $[M-H-C_7H_{10}O_3]^-$, 397.1305 $[M-H-C_7H_{10}O_3-C]^-$, 151.0404 $C_8H_7O_3$	Arctignan C	Lignans
78[n,a]	12.94	$C_{50}H_{56}O_{17}$	$[M-H]^-$	927.3455	1.6	**909.3322 $[M-H-H_2O]^-$**, 897.3328 $[M-H-H_2O-C]^-$, 891.3290 $[M-H-2H_2O]^-$, 879.3211 $[M-H-2H_2O-C]^-$, 861.3118 $[M-H-3H_2O-C]^-$, 843.3008 $[M-H-4H_2O-C]^-$, 837.3062 $[M-H-5H_2O]^-$, 825.2917 $[M-H-5H_2O-C]^-$, **813.2915 $[M-H-5H_2O-2C]^-$**, 719.2421 $[M-H-C_8H_{16}O_6]^-$, 707.2502 $[M-H-C_8H_{16}O_6-C]^-$, 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 $[M-H-H_2O]^-$**, 891.3240 $[M-H-2H_2O]^-$, 879.3223$[M-H-2H_2O-C]^-$, 861.3185 $[M-H-3H_2O-C]^-$, 843.3040 $[M-H-4H_2O-C]^-$, 837.2908 $[M-H-5H_2O]^-$, 825.2959 $[M-H-5H_2O-C]^-$, 813.2939 $[M-H-5H_2O-2C]^-$, 801.2922 $[M-H-5H_2O-3C]^-$, 719.2479 $[M-H-C_8H_{16}O_6]^-$, 707.2469 $[M-H-C_8H_{16}O_6-C]^-$, 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 $[M-H-H_2O]^-$, 695.2530 $[M-H-2H_2O]^-$, 683.2480 $[M-H-2H_2O-C]^-$, 677.2429 $[M-H-3H_2O]^-$, **665.2401 $[M-H-3H_2O-C]^-$**, 653.2403 $[M-H-3H_2O-2C]^-$, 589.2047 $[M-H-C_7H_{10}O_3]^-$,	Unknown	Lignans

81	13.10	$C_{30}H_{34}O_{10}$	$[M-H]^-$	553.2079	0.5	571.1968[M-H-$C_7H_{10}O_3$-H_2O]$^-$, 559.1990 [M-H-$C_7H_{10}O_3$-H_2O-C]$^-$, 369.1319$C_{21}H_{21}O_6$ 519.2045 [M-H-H_2O-O]$^-$, 505.1876 [M-H-H_2O-O-CH_2]$^-$, **357.1352 [M-H-$C_{10}H_{12}O_4$]$^-$**, 343.1219 [M-H-$C_{10}H_{12}O_4$-CH_2]$^-$, 195.0663 $C_{10}H_{11}O_4$,165.0570 $C_9H_9O_3$, 151.0407 $C_8H_7O_3$	Lappaol E	Lignans
82	13.12	$C_{31}H_{36}O_{10}$	$[M-H]^-$	567.2251	2.1	535.1983 [M-H-H_2O-CH_2]$^-$, 531.2048 [M-H-2H_2O]$^-$, 519.2055 [M-H-2H_2O-C]$^-$, **505.1878 [M-H-2H_2O-C-CH_2]$^-$**, 411.1467 [M-H-$C_8H_{12}O_3$]$^-$, 397.1608 [M-H-$C_8H_{10}O_4$]$^-$, 195.0684 $C_{10}H_{11}O_4$, 165.0574 $C_9H_9O_3$	Lappaol D	Lignans
83	13.24	$C_{40}H_{44}O_{13}$	$[M-H]^-$	731.2704	0.0	713.2620 [M-H-H_2O]$^-$, 683.2524 [M-H-2H_2O-C]$^-$, 677.2406 [M-H-3H_2O]$^-$, **665.2405 [M-H-3H_2O-C]$^-$**, 653.2401 [M-H-3H_2O-2C]$^-$, 589.2093 [M-H-$C_7H_{10}O_3$]$^-$, 571.1992 [M-H-$C_7H_{10}O_3$-H_2O]$^-$, 559.1985 [M-H-$C_7H_{10}O_3$-H_2O-C]$^-$, 547.1989 [M-H-$C_7H_{10}O_3$-H_2O-2C]$^-$, 531.2033 [M-H-$C_7H_{10}O_3$-H_2O-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_2O]$^-$, 683.2505 [M-H-2H_2O-C]$^-$, 677.2407 [M-H-3H_2O]$^-$, **665.2402 [M-H-3H_2O-C]$^-$**, 653.2402 [M-H-3H_2O-2C]$^-$, 589.2103 [M-H-$C_7H_{10}O_3$]$^-$, 571.1998 [M-H-$C_7H_{10}O_3$-H_2O]$^-$, 559.1996 [M-H-$C_7H_{10}O_3$-H_2O-C]$^-$, 547.1982 [M-H-$C_7H_{10}O_3$-H_2O-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-$C_{16}H_{22}O_7$]$^-$**	lappaolB+Glc	Lignans
86*	13.40	$C_{20}H_{22}O_6$	$[M-H]^-$	357.1339	0.1	**342.1113 [M-H-CH_3]$^-$**, 313.1397 [M-H-CO_2]$^-$, 221.0824 [M-H-$C_8H_8O_2$]$^-$, 209.0840 [M-H-$C_8H_8O_2$-C]$^-$, 161.0561 $C_{10}H_9O_2$, 147.0455 $C_9H_7O_2$, 137.0598 $C_8H_9O_2$	Matairesinol	Lignans
87[n]	13.64	$C_{40}H_{44}O_{13}$	$[M-H]^-$	731.2705	0.1	713.2582 [M-H-H_2O]$^-$, 701.2607 [M-H-H_2O-C]$^-$, 683.2511 [M-H-2H_2O-C]$^-$, 677.2402 [M-H-3H_2O]$^-$, **665.2399 [M-H-3H_2O-C]$^-$**, 653.2388 [M-H-3H_2O-2C]$^-$, 589.2103 [M-H-$C_7H_{10}O_3$]$^-$, 571.1971 [M-H-$C_7H_{10}O_3$-H_2O]$^-$, 559.1985 [M-H-$C_7H_{10}O_3$-H_2O-C]$^-$, 547.1985 [M-H-$C_7H_{10}O_3$-H_2O-2C]$^-$, 505.1901[M-H-$C_7H_{10}O_3$-2H_2O-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_2O]$^-$, 699.2462 [M-H-H_2O-C]$^-$, 681.2343 [M-H-2H_2O-C]$^-$, 669.2336 [M-H-2H_2O-2C]$^-$, 663.2287 [M-H-3H_2O-C]$^-$, 651.2331 [M-H-3H_2O-2C]$^-$, 557.1816 [M-H-$C_8H_{12}O_4$]$^-$, 545.1883 [M-H-$C_8H_8O_5$]$^-$, 517.1910 [M-H-$C_{10}H_{12}O_5$]$^-$, **505.1897 [M-H-$C_{10}H_{12}O_5$-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_2O]$^-$, 423.1431 [M-H-$C_7H_{10}O_3$]$^-$, **411.1470 [M-H-$C_7H_{10}O_3$-C]$^-$**	Unknown	Lignans
90[n]	14.15	$C_{40}H_{42}O_{13}$	$[M-H]^-$	729.2573	2.6	711.2453 [M-H-H_2O]$^-$, 701.2621 [M-H-CO]$^-$, 681.2374 [M-H-2H_2O-C]$^-$, 669.2408 [M-H-2H_2O-2C]$^-$, 557.1811 [M-H-$C_8H_{12}O_4$]$^-$, 545.1851 [M-H-$C_8H_8O_5$]$^-$, **517.1887 [M-H-$C_{10}H_{12}O_5$]$^-$**, 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_2O]$^-$, **701.2632[M-H-H_2O-C]$^-$**, 683.2512[M-	Arctignan G	Lignans

						H-2H_2O-C]$^-$, 665.2419 [M-H-3H_2O-C]$^-$, 653.2443 [M-H-3H_2O-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 $C_9H_9O_3$		
92[n,a]	14.25	$C_{31}H_{34}O_{10}$	[M-H]$^-$	565.2089	1.5	**533.1855** [M-H-H_2O-CH_2]$^-$, 195.0680 $C_{10}H_{11}O_4$, 165.0573 $C_9H_9O_3$	Unknown	Lignans
93[n,a]	14.28	$C_{41}H_{46}O_{13}$	[M-H]$^-$	745.2889	2.9	715.2682 [M-H-CH_2O]$^-$, 697.2602 [M-H-CH_2O-H_2O]$^-$, 679.2489 [M-H-CH_2O-2H_2O]$^-$, **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_2O]$^-$, 299.0938 [M-H-$C_{21}H_{24}O_7$-2CH_2-CH_2O]$^-$	Unknown	Lignans
94[n,a]	14.41	$C_{31}H_{36}O_{10}$	[M-H]$^-$	567.2259	2.9	519.2019 [M-H-2H_2O-C]$^-$, 517.1876 [M-H-2H_2O-CH_2]$^-$, **505.1916 [M-H-2H_2O-CH_2-C]$^-$**, 195.0666 $C_{10}H_{11}O_4$, 165.0569 $C_9H_9O_3$	Lappaol D isomer 1	Lignans
95	14.51	$C_{40}H_{44}O_{13}$	[M-H]$^-$	731.2709	0.5	713.2590 [M-H-H_2O]$^-$, **701.2591 [M-H-H_2O-C]$^-$**, 683.2518 [M-H-2H_2O-C]$^-$, 653.2387 [M-H-3H_2O-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 $C_9H_9O_3$	Arctignan H	Lignans
96[n,a]	14.52	$C_{31}H_{36}O_{10}$	[M-H]$^-$	567.2258	2.8	553.2089 [M-H-CH_2]$^-$, 549.2127 [M-H-H_2O]$^-$, 531.2034 [M-H-2H_2O]$^-$, 519.2059 [M-H-2H_2O-C]$^-$, 505.1860 [M-H-2H_2O-C-CH_2]$^-$, 411.1432 [M-H-$C_8H_{12}O_3$]$^-$, 401.1594 [M-H-$C_9H_{10}O_3$]$^-$, **383.1515 [M-H-$C_9H_{10}O_3$-H_2O]$^-$**, 371.1532 [M-H-$C_9H_{10}O_3$-H_2O-C]$^-$, 165.0559 $C_9H_9O_3$	Lappaol D isomer 2	Lignans
97	14.74	$C_{30}H_{32}O_9$	[M-H]$^-$	535.1975	0.7	517.1887 [M-H-H_2O]$^-$, **505.1882 [M-H-H_2O-C]$^-$**, 475.1490 [M-H-H_2O-3CH_2]$^-$, 283.0989 $C_{17}H_{15}O_4$, 269.0843 $C_{16}H_{13}O_4$	Isolappaol A	Lignans
98	14.83	$C_{30}H_{32}O_9$	[M-H]$^-$	535.1979	1.1	517.1884 [M-H-H_2O]$^-$, **505.1893 [M-H-H_2O-C]$^-$**, 475.1647 [M-H-H_2O-3CH_2]$^-$, 381.1360 [M-H-$C_8H_{10}O_3$]$^-$, 282.0918 $C_{17}H_{14}O_4$, 270.0905 $C_{16}H_{14}O_4$	Lappaol A	Lignans
99[n]	15.03	$C_{30}H_{32}O_9$	[M-H]$^-$	535.1995	2.7	517.1885 [M-H-H_2O]$^-$, **505.1914 [M-H-H_2O-C]$^-$**, 475.1573 [M-H-H_2O-3CH_2]$^-$, 283.0939 $C_{17}H_{15}O_4$, 269.0769 $C_{16}H_{13}O_4$	Hedyotol A	Lignans
100[n,a]	15.12	$C_{30}H_{32}O_9$	[M-H]$^-$	535.1992	2.4	517.1925 [M-H-H_2O]$^-$, **505.1894 [M-H-H_2O-C]$^-$**, 475.1506 [M-H-H_2O-3CH_2]$^-$, 381.1313 [M-H-$C_8H_{10}O_3$]$^-$, 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 $C_{11}H_7O_4$, **174.0708 $C_{11}H_{10}O_2$**	7,8-didehydroarctigenin	Lignans
102*	15.15	$C_{21}H_{24}O_6$	[M-H]$^-$	371.1503	0.8	357.1280 [M-H-H_2O]$^-$, 255.0606 $C_{15}H_{11}O_4$, 235.0959 $C_{13}H_{15}O_4$, 203.0382 $C_{11}H_7O_4$, 174.0697 $C_{11}H_{10}O_2$, **121.0314 $C_7H_5O_2$**	Arctigenin	Lignans
103[n,a]	15.49	$C_{41}H_{46}O_{13}$	[M-H]$^-$	745.2889	1.7	727.2732 [M-H-H_2O]$^-$, 715.2813 [M-H-CH_2O]$^-$, 697.2618 [M-H-CH_2O-H_2O]$^-$, 677.2297 [M-H-CH_2O-2H_2O-2H]$^-$, 667.2585 [M-H-3H_2O-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 $C_9H_9O_3$	Arctignan G+CH_2	Lignans
104[n]	15.53	$C_{31}H_{34}O_{10}$	[M-H]$^-$	565.2094	2.0	**531.2008 [M-H-H_2O_2]$^-$**, 519.2096 [M-H-H_2O_2-C]$^-$, 397.1608 [M-H-$C_8H_8O_4$]$^-$	2-Hydroxylappaol B	Lignans
105	15.62	$C_{40}H_{42}O_{12}$	[M-H]$^-$	713.2612	1.4	695.2497 [M-H-H_2O]$^-$, 683.2524 [M-H-H_2O-C]$^-$, 677.2398 [M-H-2H_2O]$^-$, **665.2401 [M-H-2H_2O-C]$^-$**, 653.2405 [M-H-2H_2O-2C]$^-$, 635.1975 [M-H-2H_2O-3CH_2]$^-$, 623.1991 [M-H-2H_2O-3CH_2-C]$^-$, 559.1965 [M-H-$C_8H_{10}O_3$]$^-$, 547.1978 [M-H-	Lappaol F	Lignans

						$C_8H_{10}O_3$-C]$^-$, 381.1340 [M-H-$C_{18}H_{20}O_6$]$^-$, 369.1329 [M-H-$C_{18}H_{20}O_6$-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_2O]$^-$, 683.2530 [M-H-H_2O-C]$^-$, 677.2423 [M-H-2H_2O]$^-$, **665.2425 [M-H-2H_2O-C]$^-$**, 653.2393 [M-H-2H_2O-2C]$^-$, 635.1962 [M-H-2H_2O-3CH_2]$^-$, 623.1805 [M-H-2H_2O-3CH_2-C]$^-$, 561.2067 [M-$C_8H_8O_3$]$^-$, 559.1877 [M-$C_8H_{10}O_3$]$^-$, 547.1923 [M-$C_8H_{10}O_3$-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_2O]$^-$, **519.2037 [M-H-H_2O-C]$^-$**, 489.1574 [M-H-H_2O-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_2O]$^+$, 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_2O]$^+$, 371.1369 [M+H-Glc-$C_{21}H_{24}O_6$]$^+$, 335.1316 [M+H-Glc-$C_{21}H_{24}O_6$-2H_2O]$^+$, 285.1158 $C_{17}H_{17}O_4$, 176.0862 $C_{11}H_{12}O_2$, **151.0781 $C_9H_{11}O_2$**	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_2O]$^+$, 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 $C_9H_{11}O_2$**	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_2O]$^+$, 711.2950 [M+H-Glc-H_2O-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_2O]$^+$, 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 $C_9H_{11}O_2$	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_2O]$^+$**, 679.2571 [M+H-2H_2O]$^+$, 665.2425 [M+H-2H_2O-CH_2]$^+$, 561.2168 [M+H-$C_8H_{10}O_3$]$^+$, 543.2048 [M+H-$C_8H_{10}O_3$-H_2O]$^+$, 531.1977 [M+H-$C_8H_{10}O_3$-H_2O-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_2O]$^+$**, 679.2600[M+H-2H_2O]$^+$, 665.2600 [M+H-2H_2O-CH_2]$^+$, 561.2126 [M+H-$C_8H_{10}O_3$]$^+$, 543.1943 [M+H-$C_8H_{10}O_3$-H_2O]$^+$, 531.2034 [M+H-$C_8H_{10}O_3$-H_2O-C]$^+$	Unknown	Lignans
113[n]	18.98	$C_{42}H_{44}O_{12}$	[M-H]$^-$	739.2763	0.8	723.2827 [M+H-H_2O]$^+$, 705.2745[M+H-2H_2O]$^+$, 505.1902 [M+H-$C_{13}H_{16}O_4$]$^+$, 487.1755 [M+H-$C_{13}H_{16}O_4$-H_2O]$^+$, 477.1955 [M+H-$C_{13}H_{16}O_4$-CO]$^+$, 469.1721 [M+H-$C_{13}H_{16}O_4$-2H_2O]$^+$, 455.1549 [M+H-$C_{13}H_{16}O_4$-2H_2O-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 $C_9H_{11}O_2$	Viridissimaol E	Lignans
114	19.18	$C_{42}H_{46}O_{12}$	[M-H]$^-$	741.2931	2.0	**725.2980 [M+H-H_2O]$^+$**, 711.2808 [M+H-H_2O-CH_2]$^+$, 707.2880 [M+H-2H_2O]$^+$, 693.2703 [M+H-2H_2O-CH_2]$^+$, 507.2048 [M+H-$C_{13}H_{16}O_4$]$^+$, 489.1917 [M+H-$C_{13}H_{16}O_4$-H_2O]$^+$, 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 $C_9H_{11}O_2$	Diarctigenin	Lignans
115[n,a]	19.79	$C_{42}H_{44}O_{12}$	[M-H]$^-$	739.2771	1.6	**723.2832 [M+H-H_2O]$^+$**, 705.2687 [M+H-2H_2O]$^+$, 589.2172 [M+H-$C_9H_{12}O_2$]$^+$, 571.2095 [M+H-$C_9H_{12}O_2$-H_2O]$^+$, 559.2019 [M+H-$C_9H_{12}O_2$-H_2O-C]$^+$, 505.1884[M+H-$C_{13}H_{16}O_4$]$^+$, 487.1982 [M+H-$C_{13}H_{16}O_4$-H_2O]$^+$, 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	Diarctigenin/Neoarctin A-2H 1	Lignans

						$C_9H_{11}O_2$		
116	19.86	$C_{42}H_{46}O_{12}$	$[M-H]^-$	741.2911	0.0	725.2981 $[M+H-H_2O]^+$, 711.2804 $[M+H-H_2O-CH_2]^+$, 707.2894 $[M+H-2H_2O]^+$, 693.2732 $[M+H-2H_2O-CH_2]^+$, 507.2048 $[M+H-C_{13}H_{16}O_4]^+$, 489.1936 $[M+H-C_{13}H_{16}O_4-H_2O]^+$, 387.1522 $[M+H-C_{21}H_{24}O_5]^+$, 369.1373 $[M+H-C_{21}H_{26}O_6]^+$, 351.1270 $[M+H-C_{21}H_{26}O_6-H_2O]^+$, 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 $C_9H_{11}O_2$	Neoarctin A	Lignans
117[n,a]	19.99	$C_{42}H_{44}O_{12}$	$[M-H]^-$	739.2772	1.7	723.2817 $[M+H-H_2O]^+$, 705.2703 $[M+H-2H_2O]^+$, 505.1875 $[M+H-C_{13}H_{16}O_4]^+$, 495.1952$[M+H-C_{14}H_{14}O_4]^+$, 487.1716 $[M+H-C_{13}H_{16}O_4-H_2O]^+$, 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 $C_9H_{11}O_2$	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 $[M+H-H_2O]^+$, 705.2693 $[M+H-2H_2O]^+$, 505.1943 $[M+H-C_{13}H_{16}O_4]^+$, 495.2081 $[M+H-C_{14}H_{14}O_4]^+$, 487.1748 $[M+H-C_{13}H_{16}O_4-H_2O]^+$, 477.1933 $[M+H-C_{13}H_{16}O_4-CO]^+$, 469.1742 $[M+H-C_{13}H_{16}O_4-2H_2O]^+$, 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 $C_9H_{11}O_2$	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 $[M+H-H_2O]^+$, 705.2712 $[M+H-2H_2O]^+$, 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 $C_9H_{11}O_2$	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 $[M+H-C_9H_{14}O_6]^+$, 865.3491 $[M+H-C_9H_{14}O_6-CO]^+$, 741.2865 $[M+H-C_{21}H_{22}O_6]^+$, 727.3124 $[M+H-C_{21}H_{20}O_7]^+$, 709.2972 $[M+H-C_{21}H_{20}O_7-H_2O]^+$, **247.1004 $C_{14}H_{15}O_4$**, 203.1090 $C_{13}H_{15}O_2$, 151.0717 $C_9H_{11}O_2$	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 $[M+H-H_2O]^+$, **247.0995 $C_{14}H_{15}O_4$**, 203.1043 $C_{13}H_{15}O_2$, 151.0728 $C_9H_{11}O_2$	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 $[M+H-H_2O]^+$, 1081.4221 $[M+H-H_2O-CH_2]^+$, **727.3146 $[M+H-C_{21}H_{22}O_6-O]^+$**, 709.3037 $[M+H-C_{21}H_{22}O_7-H_2O]^+$, 691.2857 $[M+H-C_{21}H_{22}O_7-2H_2O]^+$, 491.2132 $[M+H-C_{34}H_{38}O_{11}]^+$, 473.1907 $[M+H-C_{34}H_{38}O_{11}-H_2O]^+$, 247.0997 $C_{14}H_{15}O_4$,151.0720 $C_9H_{11}O_2$	Diarctigenin+arctigenin	Lignans
123[n,a]	21.81	$C_{63}H_{68}O_{18}$	$[M+H]^+$	1113.4509	2.5	1095.4404 $[M+H-H_2O]^+$, 1081.4243 $[M+H-H_2O-CH_2]^+$, **727.3138 $[M+H-C_{21}H_{22}O_6-O]^+$**, 709.3027 $[M+H-C_{21}H_{22}O_7-H_2O]^+$, 691.2892 $[M+H-C_{21}H_{22}O_7-2H_2O]^+$, 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 $C_9H_{11}O_2$	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.