

Table S1. The information table of 89 chromones was preliminarily identified from 24 batches of agarwood samples with different specifications.

Number	Compound	Formula	RT/time	Ion mode	Theoretical value	Measured value	Error/mDa	Fragment ion	Type
1	aquilarone a	C ₁₈ H ₂₀ O ₈	1.70	[M+H] ⁺	365.1236	365.1237	0.1	347.1116、329.1022、301.1053	THPECs
		C ₁₈ H ₂₀ O ₈	1.68	[M-H] ⁻	363.1080	363.1089	0.9	345.0964、327.0869	
2	aquilarone a(isomer1)	C ₁₈ H ₂₀ O ₈	1.93	[M+H] ⁺	365.1236	365.1237	0.1	347.1116、329.1022、301.1053	THPECs
		C ₁₈ H ₂₀ O ₈	1.93	[M-H] ⁻	363.1080	363.1089	0.9	345.0964、327.0869	
3	aquilarone a(isomer2)	C ₁₈ H ₂₀ O ₈	2.07	[M+H] ⁺	365.1236	365.1237	0.1	347.1116、329.1022、301.1089	THPECs
		C ₁₈ H ₂₀ O ₈	2.05	[M-H] ⁻	363.1080	363.1089	0.9	345.1003、327.0869	
4	aquilarone f	C ₁₇ H ₁₈ O ₇	2.41	[M+H] ⁺	335.1131	335.1144	1.3	317.1025、299.0963	THPECs
		C ₁₇ H ₁₈ O ₇	2.38	[M-H] ⁻	333.0974	333.0987	1.3	315.0858、297.0795	
5	5,6,7,8-tetrahydroxy-2-(4-methoxyphenethyl)-5,6,7,8-tetrahydrochromone	C ₁₈ H ₂₀ O ₇	2.97	[M+H] ⁺	349.1287	349.1304	1.7	331.1163、313.1667、279.0924	THPECs
		C ₁₈ H ₂₀ O ₇	2.96	[M-H] ⁻	347.1131	347.1142	1.1	329.1033、311.0956、275.0944	
6	agarotetrol	C ₁₇ H ₁₈ O ₆	3.57	[M+H] ⁺	319.1182	319.1199	1.7	301.1089、283.0977、255.1010、227.1076	THPECs
		C ₁₇ H ₁₈ O ₆	3.54	[M+COOH] ⁻	363.1080	363.1089	0.9	317.1013、299.0934、281.0798	
7	4'-methoxyagarotetrol	C ₁₈ H ₂₀ O ₇	3.79	[M+H] ⁺	349.1287	349.1304	1.7	331.1201、319.1199、313.1051、301.1089	THPECs
		C ₁₈ H ₂₀ O ₇	3.75	[M+COOH] ⁻	393.1186	393.1179	-0.7	347.1142、317.1050、311.0919、299.0898	
8	isoagarotetrol	C ₁₇ H ₁₈ O ₆	4.50	[M+H] ⁺	319.1182	319.1199	1.7	301.1053、283.0977	THPECs
		C ₁₇ H ₁₈ O ₆	4.46	[M+COOH] ⁻	363.1080	363.1089	0.9	317.1013、299.0934、281.0832	
9	4'-methoxyisoagarotetrol	C ₁₈ H ₂₀ O ₇	4.77	[M+H] ⁺	349.1287	349.1304	1.7	331.1201、319.1162、301.1089、	THPECs

								283.0977	
		C ₁₈ H ₂₀ O ₇	4.70	[M+COOH] ⁻	393.1186	393.1179	-0.7	347.1142、317.1013、299.0934、 281.0798	
10	aquilarone b	C ₁₇ H ₁₈ O ₆	4.91	[M+H] ⁺	319.1182	319.1199	1.7	301.1089、281.0977	THPECs
		C ₁₇ H ₁₈ O ₆	4.83	[M+COOH] ⁻	363.1080	363.1089	0.9	317.1013、299.0934、281.0832	
	5,6,7,8-tetrahydroxy-2-(4-methoxyphenethyl)-5,6,7,8-tetrahydrochromone	C ₁₈ H ₂₀ O ₇	5.24	[M+H] ⁺	349.1287	349.1265	-2.2	331.1201、313.1051、303.1211	
11		C ₁₈ H ₂₀ O ₇	5.16	[M+COOH] ⁻	393.1186	393.1179	-0.7	347.1142、329.1033、311.0919、 301.1069	THPECs
	5,6,7-trihydroxy-8-methoxy-5,6,7,8-tetrahydroxy-2-(2-phenylethyl)chromone	C ₁₈ H ₂₀ O ₆	5.46	[M+H] ⁺	333.1338	333.1329	-0.9	303.1211	THPECs
12		C ₁₈ H ₂₀ O ₆	5.41	[M+COOH] ⁻	377.1236	377.1235	-0.1	301.1069	
	8-chloro-5, 6, 7-trihydroxy-2-(3-hydroxy-4-methoxyphenethyl)-5, 6, 7, 8-tetrahydrochromen(or isomer)	C ₁₈ H ₁₉ Cl O ₇	6.73	[M+H] ⁺	383.0898	383.0909	1.1	365.0769、347.1116、331.1163、 137.9877	THPECs
13		C ₁₈ H ₁₉ Cl O ₇	6.65	[M-H] ⁻	381.0763	381.0760	-0.3	345.0964、329.1033	
	5;6-Epoxy-7β,8α-dihydroxy-2-[2-(3-hydroxy-4-methoxyphenyl)ethyl]-5,6,7,8-tetarhydrochromone	C ₁₈ H ₁₈ O ₇	6.89	[M+H] ⁺	347.1131	347.1116	-1.5	329.1022	EPECs
14		C ₁₈ H ₁₈ O ₇	6.80	[M-H] ⁻	345.0974	345.0964	-1.0	327.0869、265.1462、145.9309	
	5,6,7-trihydroxy-5,6,7,8-tetrahydroxy-2-(2-phenylethyl) chromone	C ₁₇ H ₁₈ O ₅	7.20	[M+H] ⁺	303.1232	303.1246	1.4	285.1110	THPECs
15		C ₁₈ H ₂₀ O ₆	7.47	[M+H] ⁺	333.1338	333.1329	-0.9	303.1211	THPECs
16	5,6,7-trihydroxy-2-(4-methoxyphenethyl)-5,6,7,8-tetrahydrochromone (isomer 2)	C ₁₈ H ₂₀ O ₆	7.47	[M+H] ⁺	333.1338	333.1329	-0.9	303.1211	THPECs
	7,8-epoxy-5,6-dihydroxy-2-[2-(4'-Methoxyphenyl)ethyl]-5,6,7,8-tetrahydrochrome(or isomer)	C ₁₈ H ₁₈ O ₆	7.60	[M+H] ⁺	331.1182	331.1163	-1.9	315.1243	EPECs
17		C ₁₈ H ₁₈ O ₆	7.60	[M+H] ⁺	331.1182	331.1163	-1.9	315.1243	EPECs
18	5,6;7,8-Diedroxy-2-[2-(2-hydroxy-4-	C ₁₈ H ₁₆ O ₆	8.80	[M+H] ⁺	329.1025	329.1022	-0.3	285.1145、137.9877	DEPECs

	methoxy)phenylethyl]-5,6,7,8-tetrahydrochromone	C ₁₈ H ₁₆ O ₆	8.75	[M-H] ⁻	327.0896	327.0896	0.0	283.0594	
19	5,6;7,8-diepoxy-2-(2-phenylethyl)-5,6,7,8-tetrahydrochromone(or isomer)	C ₁₇ H ₁₄ O ₄	9.11	[M+H] ⁺	283.0970	281.0977	0.7	255.1010、237.1705	DEPECs
20	7,8-epoxy-5,6-dihydroxy-2-[2-(4'-Methoxyphenyl)ethyl]-5,6,7,8-tetrahydrochrome(or isomer)	C ₁₈ H ₁₈ O ₆	9.16	[M+H] ⁺	331.1182	331.1163	-1.9	313.1088、301.1053、283.0977	EPECs
21	6,7-dihydroxy-5,6,7,8-tetrahydro-2-(2-phenylethyl) chromone	C ₁₇ H ₁₈ O ₄	9.33	[M+H] ⁺	287.1283	287.1280	-0.3	269.1168、251.1052	THPECs
22	5,6;7,8-Diedroxy-2-[2-(3-hydroxy-4-methoxy)phenylethyl]-5,6,7,8-tetrahydrochromone(or isomer)	C ₁₈ H ₁₆ O ₆	9.39	[M+H] ⁺	329.1025	329.1022	-0.3	313.1088、287.1280、279.0924	DEPECs
		C ₁₈ H ₁₆ O ₆	9.35	[M-H] ⁻	327.0896	327.0896	0.0	311.0919、285.1185、267.1627	
23*	2-[2-(3'-hydroxy-4'-methoxy phenyl)ethyl]-5,6,7-trihydroxy-5,6,7,8-tetrahydro-8-{5'',6''-epoxy-7''-hydroxy-2-[2-(3''-hydroxy-4''''-methoxyphenyl)ethyl]chromonyl-8-oxy} chromone(or isomer)	C ₃₆ H ₃₆ O ₁₄	9.73	[M+H] ⁺	693.2183	693.2157	-2.6	675.2077、347.1154、329.1022、299.0928	BI
		C ₃₆ H ₃₆ O ₁₄	9.69	[M-H] ⁻	691.2027	691.2029	0.2	673.1911、345.0964、327.0869、297.0760	
24*	2-[2-(3'-hydroxy-4'-methoxy phenyl)ethyl]-5,6,7-trihydroxy-5,6,7,8-tetrahydro-8-{5'',6''-epoxy-7''-hydroxy-2-[2-(3''-hydroxy-4''''-methoxyphenyl)ethyl]chromonyl-8-oxy} chromone(or isomer)	C ₃₆ H ₃₆ O ₁₄	10.18	[M+H] ⁺	693.2183	693.2157	-2.6	675.2077、347.1154、329.1022、299.0928	BI
		C ₃₆ H ₃₆ O ₁₄	10.15	[M-H] ⁻	691.2027	691.2029	0.2	673.1911、345.0964、327.0869、297.0760	
25*	2-[2-(3'-hydroxy-4'-methoxy phenyl)ethyl]-5,6,7-trihydroxy-5,6,7,8-tetrahydro-8-{6''-hydroxy-2-[2-(3''''-hydroxy-4''''-methoxy)phenylethyl]-5,6,7,8-tetrahydrochromone(or isomer)}	C ₃₆ H ₃₄ O ₁₃	10.39	[M+H] ⁺	675.2078	675.2077	-0.1	665.2213、645.1961、629.2065	
		C ₃₆ H ₃₄ O ₁₃	10.36	[M-H] ⁻	673.1921	673.1911	-1.0	663.2041、643.1790、627.1810	BI

	methoxyphenyl)ethyl]chromonyl-7-oxy} chromone(or isomer)								
26	5,6;7,8-Diedroxy-2-[2-(4-hydroxy-3-methoxy)phenylethyl]-5,6,7,8-tetrahydrochromone (or isomer)	C ₁₈ H ₁₆ O ₆	10.50	[M+H] ⁺	329.1025	329.1022	-0.3	313.1160、269.1168、279.0924	DEPECs
		C ₁₈ H ₁₆ O ₆	10.43	[M-H] ⁻	327.0896	327.0896	0.0	311.0919、267.1593	
	2-[2-(3'-hydroxy-4'-methoxy phenyl)ethyl]-5,6,7-trihydroxy-5,6,7,8-tetrahydro-8-{6"-hydroxy-2-[2-(3'''-hydroxy-4'''-methoxyphenyl)ethyl]chromonyl-7-oxy} chromone(or isomer)	C ₃₆ H ₃₄ O ₁₃	10.73	[M+H] ⁺	675.2078	675.2078	0.0	615.2781、329.1022	
27*		C ₃₆ H ₃₄ O ₁₃	10.70	[M-H] ⁻	673.1921	673.1911	-1.0	613.2632、327.0869	BI
28	8-chloro-5,6,7-trihydroxy-2-(4-methoxyphenethyl)-5,6,7,8-tetrahydrochromene	C ₁₈ H ₁₉ Cl O ₆	10.89	[M+H] ⁺	367.0948	367.0962	1.4	337.0830、319.0724	THPECs
29	8-chloro-5,6,7-trihydroxy-2-(2-phenylethyl)-5,6,7,8-tetrahydrochromone	C ₁₇ H ₁₇ Cl O ₅	10.95	[M+H] ⁺	337.0843	337.0830	-1.3	319.0724、283.0942	THPECs
		C ₁₇ H ₁₇ Cl O ₅	10.93	[M-H] ⁻	335.0686	335.0698	1.2	317.0576、281.0798	
	2-[2-(3'-hydroxy-4'-methoxy phenyl)ethyl]-5,6,7-trihydroxy-5,6,7,8-tetrahydro-8-{6"-hydroxy-2-[2-(3'''-hydroxy-4'''-methoxyphenyl)ethyl]chromonyl-7-oxy} chromone(or isomer)	C ₃₆ H ₃₄ O ₁₃	11.11	[M+H] ⁺	675.2078	675.2078	0.0	329.1022、299.0928	
30*		C ₃₆ H ₃₄ O ₁₃	11.11	[M-H] ⁻	673.1921	673.1911	-1.0	327.0869、297.0760	BI
31	5,6-epoxy-7,8-dihydroxy-2-(2-phenylethyl)-5,6,7,8-tetrahydrochromone(or isomer)	C ₁₇ H ₁₆ O ₅	11.34	[M+H] ⁺	301.1076	301.1089	1.3	283.0977、255.1010	EPECs
32	5,6-epoxy-7,8-dihydroxy-2-[2-(4'-	C ₁₈ H ₁₈ O ₆	11.39	[M+H] ⁺	331.1182	331.1163	-1.9	301.1089、283.0977、255.1010	EPECs

	Methoxyphenyl)ethyl]-5,6,7,8-tetrahydrochrome(or isomer)								
33	6-hydroxy-7-methoxy-2-[2-(4-hydroxyphenyl)ethyl]chromone	C ₁₈ H ₁₆ O ₅	11.52	[M+H] ⁺	313.1076	313.1088	1.2	283.0977	FTPECs
		C ₁₈ H ₁₆ O ₅	11.44	[M-H] ⁻	311.0919	311.0919	0.0	281.0832	
34	6-hydroxy-7-methoxy-2-(4-hydroxy-3-methoxyphenethyl)chromone	C ₁₉ H ₁₈ O ₆	11.71	[M+H] ⁺	343.1182	343.1181	-0.1	313.1088	FTPECs
		C ₁₉ H ₁₈ O ₆	11.66	[M-H] ⁻	341.1025	341.1013	-1.2	311.0919	
35	6-hydroxy-7-methoxy-2-(3-hydroxy-4-methoxyphenethyl) chromone	C ₁₉ H ₁₈ O ₆	12.20	[M+H] ⁺	343.1182	343.1181	-0.1	283.0977	FTPECs
		C ₁₉ H ₁₈ O ₆	12.15	[M-H] ⁻	341.1025	341.1013	-1.2	281.0798	
36	6-Hydroxy-2-[2-(4-methoxyl-3-hydroxyphenyl)ethyl]chromone	C ₁₈ H ₁₆ O ₅	12.52	[M+H] ⁺	313.1076	313.1088	1.2	283.0942	FTPECs
		C ₁₈ H ₁₆ O ₅	12.48	[M-H] ⁻	311.0919	311.0919	0.0	281.0798	
	2-[2-(4'-methoxy phenyl)ethyl]-5,6,7-trihydroxy-5,6,7,8-tetrahydro-8-{5"-hydroxy-2-[2-(3'''-hydroxy-4'''-methoxyphenyl)ethyl]chromonyl-7-oxy} chromone	C ₃₆ H ₃₄ O ₁₂	12.74	[M+H] ⁺	659.2129	659.2104	-2.5	329.0985、313.1088、301.1089	
37		C ₃₆ H ₃₄ O ₁₂	12.74	[M-H] ⁻	657.1972	657.1995	2.3	327.0869、311.0919、299.0934	BI
	2-(2-phenylethyl)-5,6,7-trihydroxy-5,6,7,8-tetrahydro-8-{5",6"-epoxy-7"-hydroxy-2-[2-(3'''-hydroxy-4'''-methoxyphenyl)ethyl]chromonyl-8-0Xy} chromone	C ₃₅ H ₃₄ O ₁₂	12.78	[M+H] ⁺	647.2129	647.2135	0.6	629.2014、611.1907、283.0977	
38		C ₃₅ H ₃₄ O ₁₂	12.76	[M-H] ⁻	645.1972	645.1994	2.2	627.1862、609.1754、281.0832	DEPECs
	2-[2-(3',4'-hydroxy)-phenylethyl]-5,6,7-trihydroxy-5,6,7,8-tetrahydro-8- {6"-methoxy-2-[2-(4'''-methoxy)-phenylethyl]chromonyl-7-oxy} chromone	C ₃₅ H ₃₂ O ₁₁	12.90	[M+H] ⁺	629.2023	629.2014	-0.9	329.1022、283.0977	
39*		C ₃₅ H ₃₂ O ₁₁	12.84	[M-H] ⁻	627.1866	627.1862	-0.4	327.0869、281.0798	BI
40	6-Hydroxy-2-[2-(3-methoxyl-4-	C ₁₈ H ₁₆ O ₅	13.01	[M+H] ⁺	313.1076	313.1088	1.2	283.0977	FTPECs

	hydroxyphenyl)ethyl]chromone	C ₁₈ H ₁₆ O ₅	13.00	[M-H] ⁻	311.0919	311.0919	0.0	281.0798	
41	6,8-Dihydroxy-2-(2-phenylethyl) chromone	C ₁₇ H ₁₄ O ₄	13.40	[M+H] ⁺	283.097	283.0977	0.7	-	FTPECs
		C ₁₇ H ₁₄ O ₄	13.29	[M-H] ⁻	281.0814	281.0798	-1.6	-	
	2-[2-(4'-methoxy phenyl)ethyl]-5,6,7-trihydroxy-5,6,7,8-tetrahydro-8-{5"-	C ₃₆ H ₃₄ O ₁₂	13.75	[M+H] ⁺	659.2129	659.2104	-2.5	641.2019、313.1088、283.0977	
42	hydroxy-2-[2-(3'''-hydroxy-4'''-methoxyphenyl)ethyl]chromonyl-7-oxy}chromone	C ₃₆ H ₃₄ O ₁₂	13.69	[M-H] ⁻	657.1972	657.1942	-3.0	639.1839、311.0919、281.0798	BI
43*	6,7-Dimethoxy-2-[2-(4-hydroxyphenyl)ethyl]chromone	C ₁₉ H ₁₈ O ₅	14.09	[M+H] ⁺	327.1232	327.1237	0.5	313.1088、283.0977	FTPECs
44*	2-[2-(3-Hydroxyphenyl)ethyl]chromone	C ₁₇ H ₁₄ O ₃	14.26	[M+H] ⁺	267.1021	267.1006	-1.5	161.0601	FTPECs
45	6,7-dimethoxy-2-[2-(3-hydroxy-4-methoxyphenyl)ethyl]chromone	C ₂₀ H ₂₀ O ₆	14.36	[M+H] ⁺	357.1338	357.1364	2.6	327.1237、313.1088、283.0977	FTPECs
46	6,7-dihydroxy-2-[2-(4-methoxyphenyl)ethyl]chromone	C ₁₈ H ₁₆ O ₅	14.52	[M+H] ⁺	313.1076	313.1088	1.2	283.0942	FTPECs
		C ₁₈ H ₁₆ O ₅	14.50	[M-H] ⁻	311.0919	311.0919	0.0	281.0798	
47	6,7-Dimethoxy-2-[2-(4-hydroxyphenyl)ethyl]chromone(isomer)	C ₁₉ H ₁₈ O ₅	14.70	[M+H] ⁺	327.1232	327.1237	0.5	313.1088、283.0977	FTPECs
48	6,8-dihydroxy-2-(2-phenylethyl)chromone(or isomer)	C ₁₇ H ₁₄ O ₄	14.80	[M+H] ⁺	283.097	283.0977	0.7	235.1704	FTPECs
		C ₁₇ H ₁₄ O ₄	14.75	[M-H] ⁻	281.0814	281.0798	-1.6	116.9271	
49	6,8-dimethoxy-2-[2-(3-hydroxy-4-methoxyphenyl)ethyl]chromone	C ₂₀ H ₂₀ O ₆	15.05	[M+H] ⁺	357.1338	357.1325	-1.3	283.0977	FTPECs
50	2-[2-(4-Hydroxyphenyl)ethyl]chromone	C ₁₇ H ₁₄ O ₃	15.47	[M+H] ⁺	267.1021	267.1040	1.9	161.0601	FTPECs
51	2-[2-(3-Methoxy-4-hydroxyphenyl)ethyl]chromone	C ₁₈ H ₁₆ O ₄	15.81	[M+H] ⁺	297.1127	297.1117	-1.0	-	FTPECs
52*	2-[2-(3-Hydroxyphenyl)ethyl]chromone	C ₁₇ H ₁₄ O ₃	16.06	[M+H] ⁺	267.1021	267.1006	-1.5	-	FTPECs

53*	methoxy AH15(or isomer)	C ₃₅ H ₃₂ O ₁₀	16.18	[M+H] ⁺	613.2074	613.2099	2.5	595.2066、297.1152、267.1006	BI
54	6-methoxy-2-[2-(3-methoxy-4-hydroxyphenyl)ethyl]chromone (or isomer)	C ₁₉ H ₁₈ O ₅	16.30	[M+H] ⁺	327.1232	327.1237	0.5	203.1794	FTPECs
55	AH15 (or isomer)	C ₃₄ H ₃₀ O ₉	16.34	[M+H] ⁺	583.1968	583.1970	0.2	313.1015、297.1117	BI
56	6-hydroxy-2-[2-(4-methoxyphenyl)ethyl]chromone	C ₁₈ H ₁₆ O ₄	16.53	[M+H] ⁺	297.1127	297.1117	-1.0	-	FTPECs
57	4',4'''-dimethoxyaquisinenone K (or isomer)	C ₃₆ H ₃₄ O ₁₁	16.95	[M+H] ⁺	643.2179	643.2182	0.3	625.2009、313.1008	BI
58	6-Methoxy-7-hydroxy-2-[2-(4-methoxyphenyl)ethyl]chromone (or isomer)	C ₁₉ H ₁₈ O ₅	17.16	[M+H] ⁺	327.1232	327.1237	0.5	297.1117、167.1006	FTPECs
59	6-Methoxy-2-[2-(3-methoxy-4-hydroxyphenyl)ethyl]chromone (or isomer)	C ₁₉ H ₁₈ O ₅	17.53	[M+H] ⁺	327.1232	327.1237	0.5	297.1117	FTPECs
60	6-Hydroxy-7-methoxy-2-(2-phenylethyl)chromone (or isomer)	C ₁₈ H ₁₆ O ₄	17.73	[M+H] ⁺	297.1127	297.1117	-1.0	267.104	FTPECs
61	2-[2-(2-Hydroxyphenyl)ethyl]chromone (or isomer)	C ₁₇ H ₁₄ O ₃	17.90	[M+H] ⁺	267.1021	267.1040	1.9	161.0601	FTPECs
62	AH15 (or isomer)	C ₃₄ H ₃₀ O ₉	18.05	[M+H] ⁺	583.1968	583.1970	0.2	327.1237、297.1117	BI
63	6-Methoxy-2-[2-(3-hydroxy-4-methoxyphenyl)ethyl]chromone (or isomer)	C ₁₉ H ₁₈ O ₅	18.23	[M+H] ⁺	327.1232	327.1237	0.5	283.0904	FTPECs
64	6-Hydroxy-2-[2-(3-methoxyphenyl)ethyl]chromone(or isomer)	C ₁₈ H ₁₆ O ₄	18.63	[M+H] ⁺	297.1127	297.1117	-1.0	-	FTPECs
		C ₁₈ H ₁₆ O ₄	18.58	[M-H] ⁻	295.0907	295.0971	0.1	-	
65	6-Hydroxy-2-(2-phenylethyl) chromone	C ₁₇ H ₁₄ O ₃	19.01	[M+H] ⁺	267.1021	267.1040	1.9	-	FTPECs
		C ₁₇ H ₁₄ O ₃	18.89	[M-H] ⁻	265.0865	265.0863	-0.2	-	
66*	hydroxy aquisinenone D	C ₃₇ H ₃₄ O ₁₁	19.46	[M+H] ⁺	655.2179	655.2202	2.3	343.1181	BI
67*	4,4'-dimethoxy aquisinenone G (or isomer)	C ₃₆ H ₃₂ O ₁₀	20.67	[M+H] ⁺	625.2074	625.2060	-1.4	595.2016、313.1051、283.0977	BI
68	sesquiterpene-2-(2-phenylethyl)chromone	C ₃₃ H ₃₈ O ₁₀	20.82	[M+H] ⁺	595.2543	595.2565	2.2	577.2405、283.0977	BI

69*	derivative (or isomer) 6,7-Dimethoxy-2-[2-(4-methoxyphenyl)ethyl]chromone	C ₂₀ H ₂₀ O ₅	21.16	[M+H] ⁺	341.1389	341.1395	0.6	-	FTPECs
70	6-methoxy-2-[2-(3-methoxyphenyl)ethyl]chromone	C ₁₉ H ₁₈ O ₄	21.60	[M+H] ⁺	311.1342	311.1358	1.6	-	FTPECs
71*	4,4'-dimethoxy aquisinenone G (or isomer)	C ₃₆ H ₃₂ O ₁₀	22.15	[M+H] ⁺	625.2074	625.2060	-1.4	579.2029、283.0977	BI
		C ₃₆ H ₃₂ O ₁₀	22.15	[M-H] ⁻	623.1917	623.1901	-1.6	575、1722、281.0798	
72	4,4'-dimethoxyaquisinenone A (or isomer)	C ₃₆ H ₃₂ O ₉	22.30	[M+H] ⁺	609.2125	609.2101	-2.4	595.1967、583.2859、283.0977	BI
		C ₃₆ H ₃₂ O ₉	22.29	[M+COOH] ⁻	653.2023	653.2028	0.5	593.1801、581.1802、281.0832	
73	sesquiterpene-2-(2-phenylethyl)chromone derivative (or isomer)	C ₃₅ H ₃₀ O ₉	22.45	[M+H] ⁺	595.1968	595.1967	-0.1	577.1865、283.0977	BI
74	AH21	C ₃₄ H ₂₈ O ₈	22.80	[M+H] ⁺	565.1862	565.1860	-0.2	547.1751、267.1006	BI
75	2-(2-phenylethyl)-5,6,7-trihydroxy-5,6,7,8-tetrahydro-8-[2-(2-phenylethyl)chromonyl-6-oxy]chromone	C ₃₄ H ₃₀ O ₈	23.25	[M+H] ⁺	567.2019	567.2009	-1.0	549.1412、531.1846	BI
76*	2-[2-(4-methoxyphenyl)ethyl]chromone	C ₁₈ H ₁₆ O ₃	23.63	[M+H] ⁺	281.1178	281.1189	1.1	121.0666	FTPECs
77*	2-(2-phenylethyl)chromone	C ₁₇ H ₁₄ O ₂	24.09	[M+H] ⁺	251.1072	251.1084	1.2	160.052	FTPECs
78*	4,4'-dimethoxy aquisinenone G (or isomer)	C ₃₆ H ₃₃ O ₁₀	24.94	[M+H] ⁺	625.2074	625.2060	-1.4	595.1967、579.2023、301.0627、283.0942	BI
79	6,7-Dimethoxy-2-(2-phenylethyl)chromone	C ₁₉ H ₁₈ O ₄	25.47	[M+H] ⁺	311.1283	311.1286	0.3	-	FTPECs
80*	6-methoxy-2-(2-phenylethyl)chromone	C ₁₈ H ₁₆ O ₃	25.93	[M+H] ⁺	281.1178	281.1189	1.1	-	FTPECs
81	methoxy AH21 (or isomer)	C ₃₃ H ₃₈ O ₉	26.64	[M+H] ⁺	579.2594	579.2571	-2.3	313.1088	BI
82	4,4'-dimethoxyaquisinenone A (or isomer)	C ₃₆ H ₃₂ O ₉	27.24	[M+H] ⁺	609.2125	609.2101	-2.4	595.1967、327.1237	BI
83	7-hydroxy-6-methoxy-2-(4-methoxyphenethyl)chromone (or isomer)	C ₁₉ H ₁₈ O ₅	27.53	[M+H] ⁺	327.1232	327.1237	0.5	283.0977、267.1006	FTPECs

84	methoxy AH21 (or isomer)	C ₃₅ H ₃₀ O ₈	27.71	[M+H] ⁺	579.2019	579.2029	1.0	327.1237	BI
85*	5-hydroxy-6-methoxy-2-(2-phenylethyl)chromone	C ₁₈ H ₁₆ O ₄	27.95	[M+H] ⁺	297.1127	297.1117	-1.0	-	FTPECs
86	4,4'-dimethoxyaquisinone A (or isomer)	C ₃₆ H ₃₂ O ₉	29.97	[M+H] ⁺	609.2125	609.2101	-2.4	313.1088、283.0977	BI
87	methoxy AH21	C ₃₅ H ₃₀ O ₈	30.33	[M+H] ⁺	579.2019	579.2029	1.0	545.3525、283.0977	BI
88	dehydroxy AH21	C ₃₄ H ₂₈ O ₇	30.59	[M+H] ⁺	549.1913	549.1912	-0.1	515.2454、283.0977	BI
89	hydroxy AH11 (or isomer)	C ₃₃ H ₃₈ O ₇	31.15	[M+H] ⁺	547.2696	547.2708	1.2	529.2535、313.1051、283.0942	BI

The green line indicates the negative ion mode. * Represents 19 different components.

Table S2. 19 different components between Group A and Group (B+C).

Number	RT/min	<i>m/z</i>	VIP	<i>P</i>	Fold change	Type	Low-Density	High-Density	Variation Tendency	Compound
							($\rho < 0.7$) Average relative abundances/%	($\rho \geq 0.7$) Average relative abundance/%		
23*	9.72	693.2258	8.3172	0.0006	2.8863	BI	5.02	10.16	↑	2-[2-(3'-hydroxy-4'-methoxyphenyl)ethyl]-5,6,7-trihydroxy-5,6,7,8-tetrahydro-8-{5'',6''-epoxy-7''-hydroxy-2-[2-(3''-hydroxy-4''''-methoxyphenyl)ethyl]chromonyl-8-oxy} chromone(or isomer)
24*	10.16	693.2246	6.3714	0.0004	2.6200	BI	3.93	6.99	↑	2-[2-(3'-hydroxy-4'-methoxyphenyl)ethyl]-5,6,7-trihydroxy-5,6,7,8-tetrahydro-8-{5'',6''-epoxy-7''-hydroxy-2-[2-(3''-hydroxy-4''''-methoxyphenyl)ethyl]chromonyl-8-oxy} chromone(or isomer)
25*	10.4	675.2136	6.6314	0.0007	2.7369	BI	3.89	7.07	↑	2-[2-(3'-hydroxy-4'-methoxy phenyl)ethyl]-5,6,7-trihydroxy-5,6,7,8-tetrahydro-8-{6''-hydroxy-2-[2-(3''''-hydroxy-4''''-methoxyphenyl)ethyl]chromonyl-7-oxy} chromone(or isomer)
27*	10.84	675.2153	6.7404	0.0009	2.7580	BI	3.90	7.29	↑	2-[2-(3'-hydroxy-4'-methoxy phenyl)ethyl]-5,6,7-trihydroxy-5,6,7,8-tetrahydro-8-{6''-hydroxy-2-[2-(3''''-hydroxy-4''''-methoxyphenyl)ethyl]chromonyl-7-oxy} chromone(or isomer)
30*	11.13	675.2147	5.3909	0.0012	2.7417	BI	2.66	4.96	↑	2-[2-(3'-hydroxy-4'-methoxy phenyl)ethyl]-5,6,7-trihydroxy-5,6,7,8-tetrahydro-8-{6''-hydroxy-2-[2-(3''''-hydroxy-4''''-methoxyphenyl)ethyl]chromonyl-7-

										oxy}chromone(or isomer)
39*	12.83	629.2097	5.6907	0.0122	2.0280	BI	4.40	6.14	↑	2-[2-(3',4'-hydroxy)-phenylethyl]-5,6,7-trihydroxy-5,6,7,8-tetrahydro-8- {6"-methoxy-2-[2-(4"-methoxy)-phenylethyl]chromonyl-7-oxy}chromone(or isomer)
43*	14.1	327.1288	5.1350	0.0040	0.2708	FTPECs	3.79	1.12	↓	6,7-Dimethoxy-2-[2-(4-hydroxyphenyl)ethyl]chromone
44*	14.19	267.0960	1.5242	0.0200	0.2733	FTPECs	0.31	0.09	↓	2-[2-(3-Hydroxyphenyl)ethyl]chromone(or isomer)
52*	16.05	267.1034	3.1213	0.0290	0.4412	FTPECs	2.03	0.79	↓	2-[2-(3-Hydroxyphenyl)ethyl]chromone(or isomer)
53*	16.14	613.2149	5.3554	0.0204	2.0615	BI	3.56	5.12	↑	methoxy AH15(or isomer)
66*	19.45	655.2243	5.4989	0.0083	2.7323	BI	3.39	6.07	↑	hydroxy aquisitionone D(or isomer)
67*	20.51	625.2137	8.1653	0.0007	2.3602	BI	7.60	11.93	↑	4,4'-dimethoxy aquisitionone G (or isomer)
69*	21.15	341.3304	2.7187	0.0238	0.4724	FTPECs	1.74	0.76	↓	6,7-Dimethoxy-2-[2-(4-methoxyphenyl)ethyl]chromone
71*	22.14	625.2144	8.4384	0.0007	2.1523	BI	9.97	14.58	↑	4,4'-dimethoxy aquisitionone G (or isomer)
76*	23.84	281.1193	5.1979	0.0120	0.4596	FTPECs	5.71	2.26	↓	2-[2-(4-methoxyphenyl)ethyl]chromone
77*	23.88	251.1084	6.9471	0.0454	0.1847	FTPECs	6.03	1.08	↓	2-(2-phenylethyl)chromone
78*	24.95	625.2143	6.0259	0.0017	2.4723	BI	4.65	7.77	↑	4,4'-dimethoxy aquisitionone G (or isomer)
80*	25.94	281.1142	13.7038	0.0325	0.2429	FTPECs	24.34	5.03	↓	6-methoxy-2-(2-phenylethyl)chromone
85*	27.99	297.1174	4.8094	0.0194	0.2730	FTPECs	3.08	0.82	↓	5-hydroxy-6-methoxy-2-(2-phenylethyl)chromone(or isomer)

Table S3. Method validation results

1. Linearity Results								
Compound	Regression Equation	Linear Range (µg/ml)			Correlation Coefficient (r)	n		
2-(2-phenylethyl) chromone	Y= 2875840x + 2028	0.0012-0.6313			0.9999	7		
2-[(4-methoxyphenyl) ethyl] chromone	Y= 6610520x + 6252	0.0005-1.9656			0.9999	7		
6-methoxy-2-(2-phenylethyl) chromone	Y= 4434900x + 580	0.0006-4, 5250			0.9997	7		
6,7-dimethoxy-2-[2-(4-hydroxyphenyl) ethyl] chromone	Y= 722733x + 123	0.0008-3.2625			0.9999	7		
2. Precision Results								
Compound	Peak area 1	Peak area 2	Peak area 3	Peak area 4	Peak area 5	Peak area 6	RSD/%	
2-(2-phenylethyl) chromone	3496000	3478000	3552000	3551000	3607000	3533000	1.3	
2-[(4-methoxyphenyl) ethyl] chromone	12900000	12610000	13070000	12680000	12900000	12830000	1.3	
6-methoxy-2-(2-phenylethyl) chromone	2597000	2446000	2551000	2603000	2538000	2660000	2.84	
6,7-dimethoxy-2-[2-(4-hydroxyphenyl) ethyl] chromone	565600	593900	597300	582200	616800	628900	3.83	
3. Stability Results								
Compound	0h	2h	4h	8h	12h	24h	RSD/%	
2-(2-phenylethyl) chromone	25400000	24960000	25210000	25070000	26140000	25530000	1.67	
2-[(4-methoxyphenyl) ethyl] chromone	40840000	39700000	39790000	39710000	39790000	40190000	1.12	
6-methoxy-2-(2-phenylethyl) chromone	3309000	3321000	3288000	3313000	3238000	3309000	0.93	
6,7-dimethoxy-2-[2-(4-hydroxyphenyl) ethyl] chromone	39610	37360	38140	41020	37340	38210	3.73	
4. Repeatability Results								
Compound	1	2	3	4	5	6	RSD/%	

2-(2-phenylethyl) chromone	0.000715	0.000645	0.000674	0.000681	0.000663	0.000688	3.51
2-[(4-methoxyphenyl) ethyl] chromone	0.000153	0.000146	0.000148	0.000152	0.000165	0.000155	4.45
6-methoxy-2-(2-phenylethyl) chromone	0.005581	0.005392	0.005258	0.005758	0.00519	0.005502	3.87
6,7-dimethoxy-2-[2-(4-hydroxyphenyl) ethyl] chromone	0.000187	0.000178	0.000165	0.00019	0.000164	0.000181	6.04

5. Recovery Test Results

Compound	1	2	3	4	5	6	Average recovery	RSD
2-(2-phenylethyl) chromone	104.70%	100.50%	97.11%	99.23%	104.42%	103.36%	101.55%	3.04%
2-[(4-methoxyphenyl) ethyl] chromone	100.62%	102.06%	98.26%	102.95%	99.32%	97.94%	100.19%	2.04%
6-methoxy-2-(2-phenylethyl) chromone	100.53%	96.87%	103.76%	97.80%	105.16%	100.49%	100.77%	3.21%
6,7-dimethoxy-2-[2-(4-hydroxyphenyl) ethyl] chromone	103.95%	91.70%	100.63%	102.64%	105.40%	98.47%	100.47%	4.92%
