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Supporting Information

Skin-permeating components of *Lonicera japonica flos*: A comprehensive study from observations and model computations

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Table S1. Reported components of *LJF*, their ionization degrees and log K_p values calculated from Eq. (1) at pH 4.5 (Table 1 continued).

No.	Compounds[a]	Formula	pK_a[b]	F_n[c]	F_i[c]	log K_p (n)[d]	log K_p (i)[d]	log K_p (pred)[d]
Flavonoids								
13	3'-*O*-Methyl loniflavone	$C_{31}H_{20}O_{10}$	6.48	0.990	0.010	-7.24	—	-7.24
14	Hydnocarpin	$C_{25}H_{20}O_9$	6.49	0.990	0.010	-7.56	—	-7.56
15	Loniflavone	$C_{30}H_{18}O_{10}$	6.49	0.990	0.010	-7.64	—	-7.64
16	Luteolin 3'-*O*-*α*-L-rhamnopyranoside	$C_{21}H_{20}O_{10}$	6.49	0.990	0.010	-7.90	—	-7.90
17	Apigenin 7-*O*-rhamnoside	$C_{21}H_{20}O_9$	6.14	0.978	0.022	-8.08	—	-8.08
18	Luteolin 5-*O*-glucoside	$C_{21}H_{20}O_{11}$	6.42	0.988	0.012	-8.37	—	-8.37
19	Flavoyadorinin B	$C_{23}H_{24}O_{11}$	6.32	0.985	0.015	-8.56	—	-8.56
20	Apigenin 7-*O*-*β*-glucoside	$C_{21}H_{20}O_{10}$	6.12	0.977	0.023	-9.00	—	-9.00
21	Isorhamnetin 3-*O*-glucoside	$C_{22}H_{22}O_{12}$	6.17	0.979	0.021	-9.01	—	-9.01
22	Luteolin 7-*O*-glucoside	$C_{21}H_{20}O_{11}$	6.10	0.975	0.025	-9.09	—	-9.09
23	Luteolin 7-*O*-*β*-D-galactoside	$C_{21}H_{20}O_{11}$	6.10	0.975	0.025	-9.09	—	-9.09
24	Orientin	$C_{21}H_{20}O_{11}$	6.24	0.982	0.018	-9.15	—	-9.15
25	Chrysoeriol 7-*O*-neohesperidoside	$C_{28}H_{32}O_{15}$	6.08	0.974	0.026	-9.20	—	-9.20
26	Tricin 7-*O*-*β*-D-glucoside	$C_{23}H_{24}O_{12}$	6.08	0.974	0.026	-9.24	—	-9.24
27	Kaempferol 3-*O*-glucoside	$C_{21}H_{20}O_{11}$	6.20	0.980	0.020	-9.33	—	-9.33
28	Quercetin 3-*O*-*β*-D-glucoside	$C_{21}H_{20}O_{12}$	6.17	0.979	0.021	-9.42	—	-9.42
29	Hyperoside	$C_{21}H_{20}O_{12}$	6.17	0.979	0.021	-9.42	—	-9.42
30	Quercetin 7-*O*-*β*-D-glucoside	$C_{21}H_{20}O_{12}$	5.92	0.963	0.037	-9.42	—	-9.42
31	Rhoifolin	$C_{27}H_{30}O_{14}$	6.11	0.976	0.024	-9.52	—	-9.52
32	Lonicerin	$C_{27}H_{30}O_{15}$	6.08	0.974	0.026	-9.61	—	-9.61
33	Tricin 7-*O*-neohesperidoside	$C_{29}H_{34}O_{16}$	6.06	0.973	0.027	-9.76	—	-9.76
34	Kaempferol 3-*O*-*β*-rutinoside	$C_{27}H_{30}O_{15}$	6.20	0.980	0.020	-10.95	—	-10.95
35	Rutin	$C_{27}H_{30}O_{16}$	6.17	0.979	0.021	-11.03	—	-11.03
36	Madreselvin A	$C_{28}H_{32}O_{17}$	5.91	0.963	0.037	-11.44	—	-11.44
37	Implexaflavone	$C_{36}H_{36}O_{19}$	6.10	0.975	0.025	-11.65	—	-11.65
38	Madreselvin B	$C_{36}H_{36}O_{20}$	6.17	0.979	0.021	-12.08	—	-12.08
Iridoid glycosides								
39	Secoxyloganin 7-butyl ester	$C_{21}H_{32}O_{11}$	12.81	1.000	0.000	-8.83	—	-8.83
40	Sweroside	$C_{16}H_{22}O_9$	12.79	1.000	0.000	-9.18	—	-9.18
41	Adinoside A	$C_{20}H_{28}O_{11}$	12.81	1.000	0.000	-9.25	—	-9.25
42	Loniceracetalide A	$C_{21}H_{32}O_{11}$	12.81	1.000	0.000	-9.34	—	-9.34
43	Loniceracetalide B	$C_{21}H_{32}O_{11}$	12.81	1.000	0.000	-9.34	—	-9.34
44	Dimethylsecologanoside	$C_{18}H_{26}O_{11}$	12.81	1.000	0.000	-9.47	—	-9.47
45	7-*O*-Ethylsweroside	$C_{18}H_{26}O_{10}$	12.79	1.000	0.000	-9.54	—	-9.54
46	Dehydromorroniside	$C_{17}H_{24}O_{10}$	12.78	1.000	0.000	-9.57	—	-9.57
47	Secologanin dimethyl acetal	$C_{19}H_{30}O_{11}$	12.81	1.000	0.000	-9.60	—	-9.60
48	Ketologanin	$C_{17}H_{24}O_{10}$	12.79	1.000	0.000	-9.65	—	-9.65
49	Vogeloside	$C_{17}H_{24}O_{10}$	12.79	1.000	0.000	-9.69	—	-9.69
50	7-*epi*-Vogeloside	$C_{17}H_{24}O_{10}$	12.79	1.000	0.000	-9.69	—	-9.69
51	Kingiside	$C_{17}H_{24}O_{11}$	12.78	1.000	0.000	-9.83	—	-9.83
52	8-*epi*-Kingiside	$C_{17}H_{24}O_{11}$	12.78	1.000	0.000	-9.83	—	-9.83

53	L-Phenylalaninosecologanin C	$C_{26}H_{33}NO_{10}$	12.79	1.000	0.000	-9.90	—	-9.90
54	Stryspinoside	$C_{21}H_{28}O_{12}$	12.80	1.000	0.000	-10.03	—	-10.03
55	Secologanin	$C_{17}H_{24}O_{10}$	12.81	1.000	0.000	-10.09	—	-10.09
56	Ethyl secologanoside	$C_{18}H_{26}O_{11}$	4.62	0.569	0.431	-9.85	-12.57	-10.09
57	Loniphenyruviridoside A	$C_{24}H_{28}O_{10}$	4.51	0.506	0.494	-9.88	-12.77	-10.18
58	Secologanoside 7-methyl ester	$C_{17}H_{24}O_{11}$	4.53	0.517	0.483	-9.89	-12.55	-10.18
59	Loganin	$C_{17}H_{26}O_{10}$	12.80	1.000	0.000	-10.22	—	-10.22
60	7-*epi*-Loganin	$C_{17}H_{26}O_{10}$	12.80	1.000	0.000	-10.22	—	-10.22
61	8-*epi*-Loganin	$C_{17}H_{26}O_{10}$	12.80	1.000	0.000	-10.22	—	-10.22
62	Loniphenyruviridoside D	$C_{25}H_{28}O_{12}$	4.65	0.585	0.415	-10.00	-12.74	-10.23
63	Japonicaside C	$C_{31}H_{44}O_{13}$	4.67	0.597	0.403	-10.01	-13.41	-10.24
64	Secoxyloganin	$C_{17}H_{24}O_{11}$	4.40	0.443	0.557	-9.89	-12.53	-10.24
65	Secologanic acid	$C_{16}H_{22}O_{10}$	11.21	1.000	0.000	-10.32	—	-10.32
66	Loniphenyruviridoside B	$C_{25}H_{28}O_{12}$	4.15	0.309	0.691	-9.87	-12.62	-10.38
67	Loniphenyruviridoside C	$C_{25}H_{28}O_{12}$	4.15	0.309	0.691	-9.87	-12.62	-10.38
68	α-Morroniside	$C_{17}H_{26}O_{11}$	12.54	1.000	0.000	-10.60	—	-10.60
69	β-Morroniside	$C_{17}H_{26}O_{11}$	12.54	1.000	0.000	-10.60	—	-10.60
70	Secologanoside	$C_{16}H_{22}O_{11}$	4.40	0.443	0.557	-10.32	-12.81	-10.68
71	Loganic acid	$C_{16}H_{24}O_{10}$	4.55	0.529	0.471	-10.66	-13.22	-10.93
72	L-Phenylalaninosecologanin B	$C_{25}H_{31}NO_{10}$	3.65	0.124	0.876	-10.33	-13.38	-11.24
73	Secologanoside A	$C_{21}H_{32}O_{14}$	4.71	0.619	0.381	-12.23	-15.32	-12.44
74	(*Z*)-Aldosecologanin	$C_{34}H_{46}O_{19}$	12.81	1.000	0.000	-13.75	—	-13.75
75	(*E*)-Aldosecologanin	$C_{34}H_{46}O_{19}$	12.81	1.000	0.000	-13.75	—	-13.75
76	Lonijaposide A	$C_{27}H_{33}NO_{13}$	—	0.000	1.000	—	—	—
77	Lonijaposide B	$C_{25}H_{31}NO_{12}$	—	0.000	1.000	—	—	—
78	Lonijaposide C	$C_{24}H_{29}NO_{12}$	—	0.000	1.000	—	—	—
79	Lonijaposide D	$C_{26}H_{31}NO_{13}$	—	0.000	1.000	—	—	—
80	Lonijaposide E	$C_{25}H_{31}NO_{11}$	—	0.000	1.000	—	—	—
81	Lonijaposide F	$C_{24}H_{29}NO_{11}$	—	0.000	1.000	—	—	—
82	Lonijaposide G	$C_{24}H_{29}NO_{11}$	—	0.000	1.000	—	—	—
83	Lonijaposide H	$C_{27}H_{33}NO_{13}$	—	0.000	1.000	—	—	—
84	Lonijaposide I	$C_{23}H_{29}NO_{10}$	—	0.000	1.000	—	—	—
85	Lonijaposide J	$C_{24}H_{32}ClNO_{10}$	—	0.000	1.000	—	—	—
86	Lonijaposide K	$C_{23}H_{27}NO_{11}$	—	0.000	1.000	—	—	—
87	Lonijaposide L	$C_{24}H_{29}NO_{11}$	—	0.000	1.000	—	—	—
88	Lonijaposide M	$C_{25}H_{31}NO_{11}$	—	0.000	1.000	—	—	—
89	Lonijaposide N	$C_{26}H_{33}NO_{11}$	—	0.000	1.000	—	—	—
90	Lonijaposide O	$C_{24}H_{29}NO_{11}$	—	0.000	1.000	—	—	—
91	Lonijaposide P	$C_{25}H_{31}NO_{11}$	—	0.000	1.000	—	—	—
92	Lonijaposide Q	$C_{26}H_{32}N_2O_{12}$	—	0.000	1.000	—	—	—
93	Lonijaposide R	$C_{30}H_{33}NO_{11}$	—	0.000	1.000	—	—	—
94	Lonijaposide S	$C_{30}H_{33}NO_{11}$	—	0.000	1.000	—	—	—
95	Lonijaposide T	$C_{28}H_{35}NO_{13}$	—	0.000	1.000	—	—	—
96	Lonijaposide U	$C_{28}H_{35}NO_{13}$	—	0.000	1.000	—	—	—
97	Lonijaposide V	$C_{28}H_{35}NO_{13}$	—	0.000	1.000	—	—	—
98	Lonijaposide W	$C_{31}H_{33}NO_{13}$	—	0.000	1.000	—	—	—

Organic acids

111	3,5-*O*-Dicaffeoylquinic acid butyl ester	$C_{29}H_{32}O_{12}$	9.02	1.000	0.000	-7.28	—	-7.28
112	3-*O*-Caffeoylquinic acid butyl ester	$C_{20}H_{26}O_9$	9.32	1.000	0.000	-7.52	—	-7.52
113	5-*O*-Caffeoylquinic acid butyl ester	$C_{20}H_{26}O_9$	9.32	1.000	0.000	-7.52	—	-7.52
114	3,5-*O*-Dicaffeoylquinic acid ethyl ester	$C_{27}H_{28}O_{12}$	9.02	1.000	0.000	-7.89	—	-7.89
115	3,5-*O*-Dicaffeoylquinic acid methyl ester	$C_{26}H_{26}O_{12}$	9.02	1.000	0.000	-7.94	—	-7.94
116	Cinnamic acid, 3,4-dihydroxy-, ester with glycerol	$C_{12}H_{14}O_6$	8.45	1.000	0.000	-8.11	—	-8.11
117	3-*O*-Caffeoylquinic acid methyl ester	$C_{17}H_{20}O_9$	9.32	1.000	0.000	-8.15	—	-8.15
118	5-*O*-Caffeoylquinic acid methyl ester	$C_{17}H_{20}O_9$	8.44	1.000	0.000	-8.15	—	-8.15
119	3,4-*O*-Dicaffeoylquinic acid ethyl ester	$C_{27}H_{28}O_{12}$	9.32	1.000	0.000	-8.22	—	-8.22
120	4,5-*O*-Dicaffeoylquinic acid methyl ester	$C_{26}H_{26}O_{12}$	9.32	1.000	0.000	-8.25	—	-8.25
121	3,4-*O*-Dicaffeoylquinic acid methyl ester	$C_{26}H_{26}O_{12}$	8.43	1.000	0.000	-8.25	—	-8.25
122	4-*O*-Caffeoylquinic acid methyl ester	$C_{17}H_{20}O_9$	9.32	1.000	0.000	-8.28	—	-8.28
123	Vanillic acid 4-*O*-*β*-D-6-*O*-benzoylglucopyranoside	$C_{21}H_{22}O_{10}$	4.23	0.349	0.651	-7.83	-10.19	-8.29
124	5-*O*-*p*-Coumaroylquinic acid	$C_{16}H_{18}O_8$	3.91	0.204	0.796	-8.08	-9.95	-8.75
125	3-Feruloylquinic acid	$C_{17}H_{20}O_9$	3.91	0.204	0.796	-8.14	-10.20	-8.82
126	5-Feruloylquinic acid	$C_{17}H_{20}O_9$	3.91	0.204	0.796	-8.14	-10.20	-8.82
127	4-Feruloylquinic acid	$C_{17}H_{20}O_9$	4.07	0.271	0.729	-8.27	-10.44	-8.83
128	5-Caffeoylquinic acid	$C_{16}H_{18}O_9$	3.90	0.201	0.799	-8.56	-10.42	-9.24
129	4-Caffeoylquinic acid	$C_{16}H_{18}O_9$	4.07	0.271	0.729	-8.69	-10.66	-9.24
130	3,5-Dicaffeoylquinic acid	$C_{25}H_{24}O_{12}$	3.54	0.099	0.901	-8.33	-10.30	-9.29
131	3,4-Dicaffeoylquinic acid	$C_{25}H_{24}O_{12}$	3.70	0.137	0.863	-8.66	-10.69	-9.50
132	4,5-Dicaffeoylquinic acid	$C_{25}H_{24}O_{12}$	3.70	0.137	0.863	-8.66	-10.69	-9.50
133	Chlorogenic acid	$C_{16}H_{18}O_9$	3.91	0.204	0.796	-9.02	-11.23	-9.70[e]
134	3,4,5-*O*-Tricaffeoylquinic acid	$C_{34}H_{30}O_{15}$	3.31	0.061	0.939	-8.63	-10.73	-9.80
135	1-Caffeoylquinic acid	$C_{16}H_{18}O_9$	2.94	0.027	0.973	-9.26	-11.20	-10.68
136	(-)-3-*O*-(4-*O*-*β*-D-Glucopyranosylcaffeoyl) quinic acid	$C_{22}H_{28}O_{14}$	3.91	0.204	0.796	-11.19	-13.67	-11.88
137	(-)-5-*O*-(4-*O*-*β*-D-Glucopyranosylcaffeoyl) quinic acid	$C_{22}H_{28}O_{14}$	3.90	0.201	0.799	-11.19	-13.67	-11.89
138	(-)-4-*O*-(4-*O*-*β*-D-Glucopyranosylcaffeoyl) quinic acid	$C_{22}H_{28}O_{14}$	4.06	0.266	0.734	-11.33	-13.91	-11.90
Triterpenoids								
146	Hederagenin 3-*O*-*α*-L-rhamnopyranosyl-(1→2)-*β*-L-arabinopyranoside	$C_{41}H_{66}O_{12}$	4.63	0.574	0.426	-7.47	-10.45	-7.71
147	Hederagenin 3-*O*-*α*-L-rhamnopyranosyl-(1→2)-*α*-L-arabinopyranoside	$C_{41}H_{66}O_{12}$	4.63	0.574	0.426	-7.47	-10.45	-7.71
148	Hederagenin 28-*O*-*β*-D-glucopyranosyl-(1→6)-*β*-D-glucopyranoside	$C_{42}H_{68}O_{14}$	12.50	1.000	0.000	-8.80	—	-8.80
149	Loniceroside E	$C_{53}H_{86}O_{21}$	12.59	1.000	0.000	-10.32	—	-10.32
150	3-*O*-[*α*-L-Rhamnopyranosyl-(1→2)-*α*-L-arabinopyranosyl]-28-*O*-[*β*-D-glucopyranosyl (1→6)-*β*-D-glucopyranosyl]oleanolic acid	$C_{53}H_{86}O_{21}$	12.50	1.000	0.000	-10.32	—	-10.32
151	Loniceroside A	$C_{52}H_{84}O_{21}$	12.59	1.000	0.000	-10.43	—	-10.43
152	3-*O*-*α*-L-Rhamnopyranosyl-(1→2)-*α*-L-arabinopyranosyl-hederagenin-28-*O*-*β*-D-xylopyranosyl-(1→6)-*β*-D-glucopyranosyl ester	$C_{52}H_{84}O_{21}$	12.50	1.000	0.000	-10.43	—	-10.43
153	Macranthoside A	$C_{47}H_{76}O_{17}$	4.63	0.574	0.426	-10.62	-14.06	-10.86
154	Loniceroside C	$C_{53}H_{86}O_{22}$	12.59	1.000	0.000	-11.12	—	-11.12
155	Dipsacoside B	$C_{53}H_{86}O_{22}$	12.50	1.000	0.000	-11.12	—	-11.12
156	Macranthoside B	$C_{53}H_{86}O_{22}$	4.63	0.574	0.426	-11.38	-15.96	-11.62
157	Loniceroside D	$C_{53}H_{86}O_{23}$	12.59	1.000	0.000	-12.02	—	-12.02
158	Loniceroside B	$C_{58}H_{94}O_{25}$	12.59	1.000	0.000	-12.11	—	-12.11

159	Macranthoidin A	$C_{59}H_{96}O_{27}$	12.50	1.000	0.000	-13.96	—	-13.96
160	Macranthoidin B	$C_{65}H_{106}O_{32}$	12.50	1.000	0.000	-16.61	—	-16.61
Others								
231	Eugenyl-*β*-D-glucopyranoside	$C_{16}H_{22}O_7$	12.83	1.000	0.000	-7.68	—	-7.68
232	Benzyl-*O*-*β*-D-glucopyranoside	$C_{13}H_{18}O_6$	12.93	1.000	0.000	-7.78	—	-7.78
233	Syringin	$C_{17}H_{24}O_9$	12.75	1.000	0.000	-9.09	—	-9.09
234	(+)-Lyoniresinol 9-*O*-glucoside	$C_{28}H_{38}O_{13}$	10.05	1.000	0.000	-9.19	—	-9.19
235	Sasanquin	$C_{21}H_{30}O_{11}$	12.80	1.000	0.000	-9.67	—	-9.67
236	Sucrose	$C_{12}H_{22}O_{11}$	12.81	1.000	0.000	-11.11	—	-11.11[e]
237	Guanosine	$C_{10}H_{13}N_5O_5$	2.42	0.992	0.008	-11.18	—	-11.18
238	Shuangkangsu	$C_{20}H_{30}O_{14}$	12.51	1.000	0.000	-12.93	—	-12.93

[a] The references cited for these compounds are given in Supplementary Table S2; [b] Those are the most acidic pK_a for all compounds except guanosine, for which it is the most basic pK_a; Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994-2018 ACD/Labs) through the Scifinder database; [c] $F_n = 1/(1+10^{pH-pKa})$ for acids or $1/(1+10^{pKa-pH})$ for bases, and $F_i = 1 - F_n$; Compounds were viewed as neutral molecules when $F_n \geq 0.950$; [d] Units of cm/s; [e] Using experimental descriptors.

Table S2. Values of log K_p calculated through Eq. (1) and the compound descriptors used in this work.

Compounds	E	S	A	B	V	J^+	J^-	log K_p
Flavonoids								
Chrysin[a,b]	2.13	1.98	0.69	0.73	1.7871	0.0000	0.0000	-5.03[bm]
3',4',5',5,7-Pentamethoxyflavone[c]	2.11	2.12	0.12	1.55	2.6677	0.0000	0.0000	-5.33
5-Hydroxy-7,4'-dimethoxyflavone[d]	2.11	2.12	0.53	1.14	2.1276	0.0000	0.0000	-5.44
Luteolin 5,3'-dimethyl ether[b]	2.29	2.10	0.93	1.20	2.1863	0.0000	0.0000	-5.58
Flavoyadorigenin B[e]	2.29	2.10	0.93	1.20	2.1863	0.0000	0.0000	-5.58
5-Hydroxy-3',4',7-trimethoxyflavone[d]	2.17	2.19	0.53	1.34	2.3272	0.0000	0.0000	-5.60
5-Hydroxy-3',4',5',7-tetramethoxyflavone[d]	2.23	2.26	0.53	1.54	2.5268	0.0000	0.0000	-5.77
3'-Methoxyapigenin[b]	2.40	2.24	1.34	1.19	2.0454	0.0000	0.0000	-6.02
Luteolin[a,d]	2.50	2.28	1.57	1.13	1.9045	0.0000	0.0000	-6.21[bm]
Apigenin[b]	2.36	2.45	1.38	1.20	1.8458	0.0000	0.0000	-6.55[bm]
Tricin[f]	2.46	2.52	1.34	1.50	2.2450	0.0000	0.0000	-6.57
Quercetin[d]	2.68	2.20	1.92	1.40	1.9632	0.0000	0.0000	-6.81[bm]
3'-*O*-Methyl loniflavone[a]	4.31	5.13	1.87	2.25	3.7239	0.0000	0.0000	-7.24
Hydnocarpin[g]	3.55	3.72	1.36	2.33	3.1434	0.0000	0.0000	-7.56
Loniflavone[a]	4.42	5.26	2.27	2.23	3.5830	0.0000	0.0000	-7.64
Luteolin 3'-*O*-*α*-L-rhamnopyranoside[h]	3.34	2.97	1.98	2.36	2.8761	0.0000	0.0000	-7.90
Apigenin 7-*O*-rhamnoside[h]	3.06	2.92	1.75	2.42	2.8174	0.0000	0.0000	-8.08
Luteolin 5-*O*-glucoside[b]	3.59	3.76	2.31	2.37	2.9348	0.0000	0.0000	-8.37
Flavoyadorinin B[i]	3.30	3.26	1.49	2.88	3.2166	0.0000	0.0000	-8.56
Apigenin 7-*O*-*β*-glucoside[j]	3.31	3.61	2.07	2.64	2.8761	0.0000	0.0000	-9.00
Isorhamnetin 3-*O*-glucoside[k]	3.70	3.34	2.19	2.91	3.1344	0.0000	0.0000	-9.01
Luteolin 7-*O*-glucoside[l]	3.48	3.60	2.31	2.70	2.9348	0.0000	0.0000	-9.09
Luteolin 7-*O*-*β*-D-galactoside[m]	3.48	3.60	2.31	2.70	2.9348	0.0000	0.0000	-9.09
Orientin[g]	3.62	3.87	2.71	2.61	2.9348	0.0000	0.0000	-9.15
Chrysoeriol 7-*O*-neohesperidoside[f]	4.32	3.60	2.30	3.62	4.0473	0.0000	0.0000	-9.20
Tricin 7-*O*-*β*-D-glucoside[f]	3.43	3.75	1.90	3.03	3.2753	0.0000	0.0000	-9.24
Kaempferol 3-*O*-glucoside[c]	3.64	3.49	2.36	2.83	2.9348	0.0000	0.0000	-9.33
Quercetin 3-*O*-*β*-D-glucoside[d]	3.82	3.47	2.60	2.89	2.9935	0.0000	0.0000	-9.42
Hyperoside[m]	3.82	3.47	2.60	2.89	2.9935	0.0000	0.0000	-9.42
Quercetin 7-*O*-*β*-D-glucoside[n]	3.66	3.54	2.60	2.88	2.9935	0.0000	0.0000	-9.46
Rhoifolin[o]	4.26	3.74	2.48	3.54	3.8477	0.0000	0.0000	-9.52
Lonicerin[d]	4.44	3.73	2.71	3.60	3.9064	0.0000	0.0000	-9.61
Tricin 7-*O*-neohesperidoside[f]	4.38	3.88	2.30	3.93	4.2469	0.0000	0.0000	-9.76
Kaempferol 3-*O*-*β*-rutinoside[k]	4.23	4.19	2.74	4.02	3.9064	0.0000	0.0000	-10.95
Rutin[n]	4.41	4.18	2.97	4.08	3.9651	0.0000	0.0000	-11.03
Madreselvin A[p]	4.43	4.61	2.89	4.30	4.1647	0.0000	0.0000	-11.44
Implexaflavone[p]	5.51	5.60	3.73	4.76	5.0857	0.0000	0.0000	-11.63
Madreselvin B[p]	5.70	5.88	3.99	4.89	5.1444	0.0000	0.0000	-12.08
Iridoid glycosides								
Secoxyloganin 7-butyl ester[q]	2.00	2.98	0.97	3.14	3.3240	0.0000	0.0000	-8.83
Sweroside[r]	2.23	2.49	0.97	2.76	2.4365	0.0000	0.0000	-9.18

Adinoside A[h]	2.20	3.13	0.97	3.15	3.1401	0.0000	0.0000	-9.25
Loniceracetalide A[s]	2.21	2.50	0.97	3.43	3.2584	0.0000	0.0000	-9.34
Loniceracetalide B[s]	2.21	2.50	0.97	3.43	3.2584	0.0000	0.0000	-9.34
Dimethylsecologanoside[t]	2.04	3.02	0.97	3.08	2.9013	0.0000	0.0000	-9.47
7-*O*-Ethylsweroside[q]	2.23	2.54	0.97	3.15	2.7770	0.0000	0.0000	-9.54
Dehydromorroniside[s]	2.26	2.70	0.97	3.02	2.6361	0.0000	0.0000	-9.57
Secologanin dimethyl acetal[e]	2.00	2.70	0.97	3.35	3.0852	0.0000	0.0000	-9.60
Ketologanin[e]	2.19	2.85	0.97	3.01	2.6361	0.0000	0.0000	-9.65
Vogeloside[u]	2.23	2.53	0.97	3.11	2.6361	0.0000	0.0000	-9.69
7-*epi*-Vogeloside[r]	2.23	2.53	0.97	3.11	2.6361	0.0000	0.0000	-9.69
Kingiside[e]	2.15	3.04	0.97	3.08	2.6948	0.0000	0.0000	-9.83
8-*epi*-Kingiside[v]	2.15	3.04	0.97	3.08	2.6948	0.0000	0.0000	-9.83
L-Phenylalaninosecologanin C[w]	3.13	3.37	0.97	3.84	3.7234	0.0000	0.0000	-9.90
Stryspinoside[h]	2.45	3.07	0.97	3.52	3.1655	0.0000	0.0000	-10.03
Secologanin[u]	2.18	3.05	0.97	3.19	2.7017	0.0000	0.0000	-10.09
Ethyl secologanoside[v]	2.07	3.16	1.43	3.14	2.9013	0.0000	0.0000	-9.85
Ethyl secologanoside, anion[v]	2.22	7.03	0.34	6.24	2.8798	0.0000	2.7449	-12.57
Loniphenyruviridoside A[x]	2.92	3.16	1.43	3.48	3.2762	0.0000	0.0000	-9.88
Loniphenyruviridoside A, anion[x]	3.07	7.97	0.36	6.77	3.2547	0.0000	3.1031	-12.77
Secologanoside 7-methyl ester[u]	2.11	3.15	1.43	3.06	2.7604	0.0000	0.0000	-9.89
Secologanoside 7-methyl ester, anion[u]	2.26	7.00	0.33	6.10	2.7389	0.0000	2.7083	-12.55
Loganin[r]	2.26	3.17	1.20	3.17	2.6791	0.0000	0.0000	-10.22
7-*epi*-Loganin[r]	2.26	3.17	1.20	3.17	2.6791	0.0000	0.0000	-10.22
8-*epi*-Loganin[u]	2.26	3.17	1.20	3.17	2.6791	0.0000	0.0000	-10.22
Loniphenyruviridoside D[x]	3.15	3.99	1.73	3.50	3.5571	0.0000	0.0000	-10.00
Loniphenyruviridoside D, anion[x]	3.30	9.00	0.44	6.71	3.5356	0.0000	3.1010	-12.74
Japonicaside C[w]	3.60	3.45	1.73	4.35	4.4816	0.0000	0.0000	-10.01
Japonicaside C, anion[w]	3.75	9.38	0.54	8.15	4.4601	0.0000	3.6500	-13.41
Secoxyloganin[r]	2.16	3.15	1.43	3.06	2.7604	0.0000	0.0000	-9.89
Secoxyloganin, anion[r]	2.31	7.04	0.33	6.10	2.7389	0.0000	2.7216	-12.53
Secologanic acid[y]	2.42	2.67	1.27	3.20	2.4952	0.0000	0.0000	-10.32
Loniphenyruviridoside B[x]	3.32	3.82	1.73	3.50	3.5571	0.0000	0.0000	-9.87
Loniphenyruviridoside B, anion[x]	3.47	9.01	0.45	6.75	3.5356	0.0000	3.1795	-12.62
Loniphenyruviridoside C[x]	3.32	3.82	1.73	3.50	3.5571	0.0000	0.0000	-9.87
Loniphenyruviridoside C, anion[x]	3.47	9.01	0.45	6.75	3.5356	0.0000	3.1795	-12.62
α-Morroniside[e]	2.34	2.86	1.27	3.44	2.7378	0.0000	0.0000	-10.60
β-Morroniside[e]	2.34	2.86	1.27	3.44	2.7378	0.0000	0.0000	-10.60
Secologanoside[u]	2.22	3.29	1.89	3.04	2.6195	0.0000	0.0000	-10.32
Secologanoside, anion[u]	2.37	7.15	0.47	6.00	2.5980	0.0000	2.6610	-12.81
Loganic acid[u]	2.32	3.31	1.66	3.15	2.5382	0.0000	0.0000	-10.66
Loganic acid, anion[u]	2.47	7.22	0.38	6.11	2.5167	0.0000	2.6554	-13.22
L-Phenylalaninosecologanin B[w]	3.19	3.51	1.43	3.82	3.5825	0.0000	0.0000	-10.33
L-Phenylalaninosecologanin B, anion[w]	3.34	8.65	0.37	7.21	3.5610	0.0000	3.2142	-13.38
Secologanoside A[z]	2.98	3.81	2.20	4.30	3.4345	0.0000	0.0000	-12.23
Secologanoside A, anion[z]	3.13	8.64	0.61	7.68	3.4130	0.0000	3.0478	-15.32
(*Z*)-Aldosecologanin[aa]	4.35	5.51	1.93	5.95	5.2361	0.0000	0.0000	-13.75
(*E*)-Aldosecologanin[aa]	4.35	5.51	1.93	5.95	5.2361	0.0000	0.0000	-13.75
Lonijaposide A[x]	—	—	—	—	—	—	—	—

Lonijaposide B[x]	—	—	—	—	—	—	—	—
Lonijaposide C[x]	—	—	—	—	—	—	—	—
Lonijaposide D[x]	—	—	—	—	—	—	—	—
Lonijaposide E[x]	—	—	—	—	—	—	—	—
Lonijaposide F[x]	—	—	—	—	—	—	—	—
Lonijaposide G[x]	—	—	—	—	—	—	—	—
Lonijaposide H[x]	—	—	—	—	—	—	—	—
Lonijaposide I[x]	—	—	—	—	—	—	—	—
Lonijaposide J[x]	—	—	—	—	—	—	—	—
Lonijaposide K[x]	—	—	—	—	—	—	—	—
Lonijaposide L[x]	—	—	—	—	—	—	—	—
Lonijaposide M[x]	—	—	—	—	—	—	—	—
Lonijaposide N[x]	—	—	—	—	—	—	—	—
Lonijaposide O[ab]	—	—	—	—	—	—	—	—
Lonijaposide P[ab]	—	—	—	—	—	—	—	—
Lonijaposide Q[ab]	—	—	—	—	—	—	—	—
Lonijaposide R[ab]	—	—	—	—	—	—	—	—
Lonijaposide S[ab]	—	—	—	—	—	—	—	—
Lonijaposide T[ab]	—	—	—	—	—	—	—	—
Lonijaposide U[ab]	—	—	—	—	—	—	—	—
Lonijaposide V[ab]	—	—	—	—	—	—	—	—
Lonijaposide W[ab]	—	—	—	—	—	—	—	—
Organic acids								
Plamitic acid[ac]	0.04	0.65	0.62	0.45	2.4374	0.0000	0.0000	-2.64[bm]
Plamitic acid, anion[ac]	0.19	2.90	0.16	3.33	2.4159	0.0000	2.5300	-4.60
Myristic acid[ac]	0.06	0.65	0.62	0.45	2.1556	0.0000	0.0000	-3.14[bm]
Myristic acid, anion[ac]	0.21	2.79	0.14	3.24	2.1341	0.0000	2.4367	-5.05
4-Hydroxy cinnamic acid methyl ester[b]	1.18	1.44	0.53	0.73	1.3701	0.0000	0.0000	-5.53
trans-Cinnamic acid[h]	1.14	0.97	0.58	0.58	1.1705	0.0000	0.0000	-5.26[bm]
trans-Cinnamic acid, anion[h]	1.29	3.59	0.03	3.03	1.1490	0.0000	2.3179	-6.88
Methyl caffeate[b]	1.34	1.49	0.96	0.91	1.4288	0.0000	0.0000	-6.01
4-Hydroxy cinnamic acid[b]	1.33	1.41	0.99	0.70	1.2292	0.0000	0.0000	-5.82
4-Hydroxy cinnamic acid, anion[b]	1.48	4.15	0.15	3.10	1.2077	0.0000	2.3034	-7.35
1,4-Dihydroxybenzene[b]	1.06	1.27	1.06	0.57	0.8338	0.0000	0.0000	-6.19[bm]
Ferulic acid[ac]	1.25	1.53	0.80	0.91	1.4288	0.0000	0.0000	-5.99[bm]
Ferulic acid, anion[ac]	1.40	4.27	0.10	3.39	1.4073	0.0000	2.3285	-7.71
Protocatechuic acid[b]	1.14	1.29	1.22	0.70	1.0491	0.0000	0.0000	-6.18[bm]
Protocatechuic acid, anion[b]	1.29	3.80	0.23	3.07	1.0276	0.0000	2.2130	-7.66
1,2,4-Hydroxybenzene[b]	1.18	1.37	1.40	0.68	0.8925	0.0000	0.0000	-6.51[bm]
Caffeic acid[r]	1.50	1.55	1.36	0.90	1.2879	0.0000	0.0000	-6.39[bm]
Caffeic acid, anion[r]	1.65	4.45	0.28	3.33	1.2664	0.0000	2.3420	-7.92
3-(3,4-Dihydroxyphenyl)propionic acid[b]	1.12	1.68	1.38	0.95	1.3309	0.0000	0.0000	-6.57
3-(3,4-Dihydroxyphenyl)propionic acid, anion[b]	1.27	4.23	0.28	3.38	1.3094	0.0000	2.2303	-8.15
3,5-*O*-Dicaffeoylquinic acid butyl ester[ad]	3.29	3.80	2.52	2.73	4.1003	0.0000	0.0000	-7.28
3-*O*-Caffeoylquinic acid butyl ester[ae]	2.18	3.03	1.86	2.22	2.9797	0.0000	0.0000	-7.52
5-*O*-Caffeoylquinic acid butyl ester[ae]	2.18	3.03	1.86	2.22	2.9797	0.0000	0.0000	-7.52
3,5-*O*-Dicaffeoylquinic acid ethyl ester[af]	3.12	3.84	2.52	2.75	3.8185	0.0000	0.0000	-7.89

3,5-*O*-Dicaffeoylquinic acid methyl ester[i]	3.33	3.84	2.52	2.68	3.6776	0.0000	0.0000	-7.94
Cinnamic acid, 3,4-dihydroxy-, ester with glycerol[j]	1.68	2.21	1.39	1.85	1.8280	0.0000	0.0000	-8.11
3-*O*-Caffeoylquinic acid methyl ester[ag]	2.22	3.06	1.86	2.16	2.5570	0.0000	0.0000	-8.15
5-*O*-Caffeoylquinic acid methyl ester[ae]	2.22	3.06	1.86	2.16	2.5570	0.0000	0.0000	-8.15
3,4-*O*-Dicaffeoylquinic acid ethyl ester[af]	3.23	3.86	2.51	2.89	3.8185	0.0000	0.0000	-8.22
4,5-*O*-Dicaffeoylquinic acid methyl ester[af]	3.44	3.86	2.51	2.81	3.6776	0.0000	0.0000	-8.25
3,4-*O*-Dicaffeoylquinic acid methyl ester[af]	3.44	3.86	2.51	2.81	3.6776	0.0000	0.0000	-8.25
4-*O*-Caffeoylquinic acid methyl ester[ah]	2.22	2.76	1.85	2.29	2.5570	0.0000	0.0000	-8.28
Vanillic acid 4-*O*-*β*-D-6-*O*-benzoylglucopyranoside[i]	2.41	3.05	1.35	2.43	2.9847	0.0000	0.0000	-7.83
Vanillic acid 4-*O*-*β*-D-6-*O*-benzoylglucopyranoside, anion[i]	2.56	7.29	0.32	5.42	2.9632	0.0000	2.8864	-10.19
5-*O*-*p*-Coumaroylquinic acid[j]	2.30	3.15	1.90	1.96	2.3574	0.0000	0.0000	-8.08
5-*O*-*p*-Coumaroylquinic acid, anion[j]	2.45	6.99	0.46	4.63	2.3359	0.0000	2.6179	-9.95
3-Feruloylquinic acid[j]	2.33	3.18	1.67	2.16	2.5570	0.0000	0.0000	-8.14
3-Feruloylquinic acid, anion[j]	2.48	7.13	0.39	4.93	2.5355	0.0000	2.6900	-10.20
5-Feruloylquinic acid[ai]	2.33	3.18	1.67	2.16	2.5570	0.0000	0.0000	-8.14
5-Feruloylquinic acid, anion[ai]	2.48	7.13	0.39	4.93	2.5355	0.0000	2.6900	-10.20
4-Feruloylquinic acid[ai]	2.33	2.87	1.66	2.29	2.5570	0.0000	0.0000	-8.27
4-Feruloylquinic acid, anion[ai]	2.48	6.87	0.41	5.15	2.5355	0.0000	2.7504	-10.44
5-Caffeoylquinic acid[ag]	2.45	3.20	2.32	2.14	2.4161	0.0000	0.0000	-8.56
5-Caffeoylquinic acid, anion[ag]	2.60	7.19	0.61	4.86	2.3946	0.0000	2.6688	-10.42
4-Caffeoylquinic acid[ag]	2.45	2.89	2.31	2.27	2.4161	0.0000	0.0000	-8.69
4-Caffeoylquinic acid, anion[ag]	2.60	6.93	0.63	5.08	2.3946	0.0000	2.7292	-10.66
3,5-Dicaffeoylquinic acid[i]	3.56	3.97	2.99	2.65	3.5367	0.0000	0.0000	-8.33
3,5-Dicaffeoylquinic acid, anion[i]	3.71	9.34	0.89	5.68	3.5152	0.0000	3.2072	-10.30
3,4-Dicaffeoylquinic acid[aj]	3.67	3.99	2.97	2.79	3.5367	0.0000	0.0000	-8.66
3,4-Dicaffeoylquinic acid, anion[aj]	3.82	9.46	0.88	5.84	3.5152	0.0000	3.2327	-10.69
4,5-Dicaffeoylquinic acid[i]	3.67	3.99	2.97	2.79	3.5367	0.0000	0.0000	-8.66
4,5-Dicaffeoylquinic acid, anion[i]	3.82	9.46	0.88	5.84	3.5152	0.0000	3.2327	-10.69
Chlorogenic acid[d]	2.13	2.61	2.08	2.49	2.4161	0.0000	0.0000	-9.02[bm]
Chlorogenic acid, anion[d]	2.28	6.41	0.56	5.41	2.3946	0.0000	2.6984	-11.23
3,4,5-*O*-Tricaffeoylquinic acid[ae]	4.88	5.09	3.64	3.31	4.6573	0.0000	0.0000	-8.63
3,4,5-O-Tricaffeoylquinic acid, anion[ae]	5.03	11.97	1.14	6.60	4.6358	0.0000	3.7335	-10.73
1-Caffeoylquinic acid[ak]	2.28	3.51	2.31	2.34	2.4161	0.0000	0.0000	-9.26
1-Caffeoylquinic acid, anion[ak]	2.43	7.29	0.59	5.04	2.3946	0.0000	2.5629	-11.20
(-)-3-*O*-(4-*O*-*β*-D-glucopyranosylcaffeoyl) quinic acid[al]	3.57	4.49	2.74	3.67	3.4464	0.0000	0.0000	-11.19
(-)-3-*O*-(4-*O*-*β*-D-glucopyranosylcaffeoyl) quinic acid, anion[al]	3.72	9.74	0.76	6.78	3.4249	0.0000	3.0769	-13.67
(-)-5-*O*-(4-*O*-*β*-D-glucopyranosylcaffeoyl) quinic acid[al]	3.57	4.49	2.74	3.67	3.4464	0.0000	0.0000	-11.19
(-)-5-*O*-(4-*O*-*β*-D-glucopyranosylcaffeoyl) quinic acid, anion[al]	3.72	9.74	0.76	6.78	3.4249	0.0000	3.0769	-13.67
(-)-4-*O*-(4-*O*-*β*-D-glucopyranosylcaffeoyl) quinic acid[al]	3.57	4.19	2.73	3.80	3.4464	0.0000	0.0000	-11.33
(-)-4-*O*-(4-*O*-*β*-D-glucopyranosylcaffeoyl) quinic acid, anion[al]	3.72	9.49	0.78	7.00	3.4249	0.0000	3.1354	-13.91
Triterpenoids								
Palmitic acid, ester with *β*-sitosterol glucoside[h]	2.24	2.59	0.70	2.11	7.0764	0.0000	0.0000	0.77
β-Sitosterol[r]	1.32	0.97	0.32	0.67	3.7760	0.0000	0.0000	-0.68[bm]
Ursolic acid[h]	1.66	1.94	0.77	1.27	3.8827	0.0000	0.0000	-2.64
Ursolic acid, anion[h]	1.81	6.09	0.25	4.52	3.8612	0.0000	3.2169	-4.93

Oleanic acid[h]	1.66	1.94	0.77	1.27	3.8827	0.0000	0.0000	-2.64
Oleanic acid, anion[h]	1.81	6.09	0.25	4.52	3.8612	0.0000	3.2169	-4.93
Daucosterol[d]	2.48	2.49	0.97	1.96	4.8063	0.0000	0.0000	-2.94
Limonin[am]	2.35	2.68	0.00	1.94	3.2664	0.0000	0.0000	-5.47
Hederagenin 3-*O*-*α*-L-arabinopyranoside[l]	2.88	4.02	1.64	2.84	4.7721	0.0000	0.0000	-6.24
Hederagenin 3-*O*-*α*-L-arabinopyranoside, anion[l]	3.03	9.33	0.50	6.28	4.7506	0.0000	3.4483	-8.92
Hederagenin 3-*O*-*α*-L-rhamnopyranosyl-(1→2)-*β*-L-arabinopyranoside[an]	3.74	5.38	1.99	3.73	5.7437	0.0000	0.0000	-7.47
Hederagenin 3-*O*-*α*-L-rhamnopyranosyl-(1→2)-*β*-L-arabinopyranoside, anion[an]	3.89	11.67	0.62	7.40	5.7222	0.0000	3.7528	-10.45
Hederagenin 3-*O*-*α*-L-rhamnopyranosyl-(1→2)-*α*-L-arabinopyranoside[ao]	3.74	5.38	1.99	3.73	5.7437	0.0000	0.0000	-7.47
Hederagenin 3-*O*-*α*-L-rhamnopyranosyl-(1→2)-*α*-L-arabinopyranoside, anion[ao]	3.89	11.67	0.62	7.40	5.7222	0.0000	3.7528	-10.45
Hederagenin 28-*O*-*β*-D-glucopyranosyl-(1→6)-*β*-D-glucopyranoside[an]	3.77	5.40	2.38	4.41	6.0020	0.0000	0.0000	-8.80
Loniceroside E[ap]	4.98	4.92	2.92	6.44	7.7456	0.0000	0.0000	-10.32
3-*O*-[*α*-L-Rhamnopyranosyl-(1→2)-*α*-L-arabinopyranosyl]-28-*O*-[*β*-D-glucopyranosyl (1→6)-*β*-D-glucopyranosyl]oleanolic acid[d]	4.98	4.92	2.92	6.44	7.7456	0.0000	0.0000	-10.32
Loniceroside A[aq]	4.95	4.96	2.97	6.36	7.6047	0.0000	0.0000	-10.43
3-*O*-*α*-L-Rhamnopyranosyl-(1→2)-*α*-L-arabinopyranosyl-hederagenin-28-*O*-*β*-D-xylopyranosyl-(1→6)-*β*-D-glucopyranosyl ester[aq]	4.95	4.96	2.97	6.36	7.6047	0.0000	0.0000	-10.43
Macranthoside A[an]	4.57	7.32	2.79	5.24	6.7740	0.0000	0.0000	-10.62
Macranthoside A, anion[an]	4.72	14.50	0.87	9.16	6.7525	0.0000	3.9567	-14.06
Loniceroside C[ap]	5.18	5.19	3.24	6.71	7.8043	0.0000	0.0000	-11.12
Dipsacoside B[ao]	5.18	5.19	3.24	6.71	7.8043	0.0000	0.0000	-11.12
Macranthoside B[an]	5.21	5.01	3.49	6.83	7.8043	0.0000	0.0000	-11.38
Macranthoside B, anion[an]	5.36	13.63	1.33	11.89	7.7828	0.0000	4.9386	-15.96
Loniceroside D[ap]	5.40	5.43	3.51	7.04	7.8630	0.0000	0.0000	-12.02
Loniceroside B[aq]	5.71	5.80	3.44	7.54	8.5763	0.0000	0.0000	-12.11
Macranthoidin A[ao]	6.22	6.18	3.94	8.36	8.8346	0.0000	0.0000	-13.96
Macranthoidin B[ao]	7.21	7.25	4.75	9.89	9.8649	0.0000	0.0000	-16.61
Essential oils								
Phytol[ar]	0.30	0.95	0.38	0.58	2.9423	0.0000	0.0000	-2.11[bm]
Longifolene[as]	0.77	0.20	0.00	0.15	1.8533	0.0000	0.0000	-2.38[bm]
β-Caryophyllene[at]	0.72	0.15	0.00	0.25	1.9189	0.0000	0.0000	-2.48[bm]
β-Elemene[au]	0.67	0.52	0.00	0.21	1.9845	0.0000	0.0000	-2.49
Caryophyllene oxide[av]	0.72	-0.24	0.00	0.36	1.9120	0.0000	0.0000	-2.52
β-Patchoulene[at]	0.72	0.18	0.00	0.24	1.8533	0.0000	0.0000	-2.59[bm]
β-Gurjunene[at]	0.78	0.23	0.00	0.26	1.8533	0.0000	0.0000	-2.66[bm]
Germacrene D[au]	0.40	0.34	0.00	0.31	1.9845	0.0000	0.0000	-2.67
α-Zingiberene[aw]	0.68	0.30	0.00	0.34	1.9845	0.0000	0.0000	-2.68[bm]
β-Sesquiphellandrene[ax]	0.70	0.36	0.00	0.33	1.9845	0.0000	0.0000	-2.68[bm]
γ-Elemene[as]	0.71	0.38	0.00	0.33	1.9845	0.0000	0.0000	-2.70[bm]
(-)-*β*-Elemene[au]	0.71	0.40	0.00	0.33	1.9845	0.0000	0.0000	-2.71[bm]
α-Cubebene[as]	0.62	0.17	0.00	0.29	1.8533	0.0000	0.0000	-2.72[bm]
(-)-Alloaromadendrene[ay]	0.72	0.23	0.00	0.29	1.8533	0.0000	0.0000	-2.74[bm]
Aromadendrene[at]	0.70	0.23	0.00	0.29	1.8533	0.0000	0.0000	-2.74[bm]
γ-Muurolene[az]	0.80	0.26	0.00	0.34	1.9189	0.0000	0.0000	-2.75[bm]
Copaene[as]	0.62	0.14	0.00	0.32	1.8533	0.0000	0.0000	-2.77[bm]
γ-Cadinene[au]	0.81	0.31	0.00	0.34	1.9189	0.0000	0.0000	-2.78[bm]

α-Ylangene[ba]	0.64	0.13	0.00	0.33	1.8533	0.0000	0.0000	-2.79[bm]
α-Muurolene[au]	0.80	0.25	0.00	0.36	1.9189	0.0000	0.0000	-2.80[bm]
δ-Cadinene[au]	0.82	0.29	0.00	0.36	1.9189	0.0000	0.0000	-2.82[bm]
α-Cadinene[au]	0.81	0.29	0.00	0.36	1.9189	0.0000	0.0000	-2.82[bm]
α-Farnesene[au]	0.71	0.38	0.00	0.45	2.0501	0.0000	0.0000	-2.87[bm]
Germacrene[bb]	0.49	0.34	0.00	0.41	1.9845	0.0000	0.0000	-2.90
Linoleic acid[bc]	0.41	0.73	0.57	0.74	2.6332	0.0000	0.0000	-2.97[bm]
Linoleic acid, anion[bc]	0.56	3.39	0.15	3.73	2.6117	0.0000	2.6817	-5.08
Carane[as]	0.27	0.35	0.00	0.00	1.3004	0.0000	0.0000	-3.17
2,3-Dihydrofarnesol[bd]	0.54	0.59	0.33	0.63	2.1948	0.0000	0.0000	-3.31
β-Eudesmol[at]	0.91	0.51	0.35	0.55	2.0206	0.0000	0.0000	-3.33[bm]
Farnesyl acetate[au]	0.59	0.81	0.00	0.83	2.4493	0.0000	0.0000	-3.35
Ledol[ba]	0.80	0.43	0.31	0.53	1.9550	0.0000	0.0000	-3.36[bm]
3-Carene[aw]	0.51	0.22	0.00	0.10	1.2574	0.0000	0.0000	-3.37[bm]
α-Pinene[at]	0.45	0.14	0.00	0.12	1.2574	0.0000	0.0000	-3.38[bm]
α-Terpinene[be]	0.53	0.25	0.00	0.15	1.3230	0.0000	0.0000	-3.39[bm]
α-Linolenic acid[bc]	0.55	0.84	0.57	0.83	2.5902	0.0000	0.0000	-3.31[bm]
α-Linolenic acid, anion[bc]	0.70	3.59	0.14	3.80	2.5687	0.0000	2.6826	-5.44
Guaiol[ba]	0.83	0.54	0.31	0.63	2.0206	0.0000	0.0000	-3.54
(±)-Nerolidol[au]	0.65	0.61	0.31	0.70	2.1518	0.0000	0.0000	-3.54
(+)-Nerolidol[au]	0.65	0.61	0.31	0.70	2.1518	0.0000	0.0000	-3.54
α-Elemol[au]	0.76	0.45	0.31	0.70	2.0862	0.0000	0.0000	-3.55
γ-Terpinene[bf]	0.50	0.32	0.00	0.20	1.3230	0.0000	0.0000	-3.56[bm]
Hinesol[ba]	0.76	0.32	0.31	0.70	2.0206	0.0000	0.0000	-3.59
β-Pinene[at]	0.53	0.24	0.00	0.19	1.2574	0.0000	0.0000	-3.60[bm]
Limonene[aw]	0.50	0.31	0.00	0.23	1.3230	0.0000	0.0000	-3.63[bm]
α-Cedrol[be]	0.80	0.50	0.32	0.64	1.9550	0.0000	0.0000	-3.67[bm]
Farnesal[au]	0.69	0.97	0.00	0.68	2.1088	0.0000	0.0000	-3.68
(2*E*,6*E*)-Farnesol[az]	0.71	0.70	0.33	0.74	2.1518	0.0000	0.0000	-3.70
Neryl acetate[bg]	0.35	0.70	0.00	0.65	1.7878	0.0000	0.0000	-4.07[bm]
Menthol[ba]	0.40	0.50	0.23	0.58	1.4677	0.0000	0.0000	-4.42[bm]
Citronellol[bh]	0.35	0.47	0.35	0.62	1.5333	0.0000	0.0000	-4.43[bm]
1-Octanol[ba]	0.20	0.42	0.37	0.48	1.2945	0.0000	0.0000	-4.52[bm]
Dihydrocarveol[bh]	0.60	0.55	0.31	0.58	1.4247	0.0000	0.0000	-4.53
(±)-Linalool[bi]	0.40	0.55	0.20	0.67	1.4903	0.0000	0.0000	-4.62[bm]
Nerol[az]	0.50	0.61	0.27	0.66	1.4903	0.0000	0.0000	-4.64[bm]
Geraniol[bi]	0.51	0.63	0.29	0.66	1.4903	0.0000	0.0000	-4.66[bm]
Linalool oxide[bb]	0.57	0.57	0.31	0.73	1.4834	0.0000	0.0000	-4.81
α-Terpineol[bi]	0.55	0.61	0.20	0.70	1.4247	0.0000	0.0000	-4.83[bm]
2-Caren-4-ol[ax]	0.61	0.74	0.31	0.59	1.3161	0.0000	0.0000	-4.86
1,8-Cineole[at]	0.38	0.33	0.00	0.76	1.3591	0.0000	0.0000	-4.88[bm]
Eugenol[ar]	0.95	0.98	0.26	0.65	1.3544	0.0000	0.0000	-5.02[bm]
Blaetteralkohol[bb]	0.34	0.56	0.29	0.57	0.9697	0.0000	0.0000	-5.36[bm]
Linalool oxide B[au]	0.55	0.73	0.31	0.92	1.4834	0.0000	0.0000	-5.37
Linalool oxide A[au]	0.55	0.73	0.31	0.92	1.4834	0.0000	0.0000	-5.37
Others								
Lonijaposide A_4[bj]	1.80	1.54	1.66	2.36	6.9560	0.0000	0.0000	0.20

Lonijaposide A_3[bj]	1.80	1.54	1.66	2.36	6.3924	0.0000	0.0000	-0.82
Lonijaposide A_1[bj]	1.80	1.54	1.66	2.36	6.2515	0.0000	0.0000	-1.07
Lonijaposide A_2[bj]	1.80	1.54	1.66	2.36	5.9697	0.0000	0.0000	-1.58
Lonijaposide B_1[bj]	2.79	2.74	2.36	3.77	7.4227	0.0000	0.0000	-3.21
p-Hydroxybenzaldehyde[h]	1.01	1.40	0.77	0.44	0.9317	0.0000	0.0000	-5.69[bm]
Lonijaposide B_2[bj]	3.40	4.41	2.92	5.57	9.0166	0.0000	0.0000	-5.83
5-Methoxyuracil[h]	0.91	1.06	0.43	0.85	0.9512	0.0000	0.0000	-6.34
Abscisic acid[h]	1.23	1.83	0.77	1.55	2.1333	0.0000	0.0000	-6.45
Abscisic acid, anion[h]	1.38	4.82	0.12	4.33	2.1118	0.0000	2.5112	-8.61
Eugenyl-*β*-D-glucopyranoside[h]	1.94	2.33	0.97	2.13	2.3847	0.0000	0.0000	-7.68
Benzyl-*O*-*β*-D-glucopyranoside[h]	1.86	2.05	0.97	1.91	1.9463	0.0000	0.0000	-7.78
Syringin[bk]	2.50	3.04	1.30	2.71	2.6430	0.0000	0.0000	-9.09
(+)-Lyoniresinol 9-*O*-glucoside[h]	3.66	4.07	2.05	3.55	4.1245	0.0000	0.0000	-9.19
Sasanquin[h]	2.55	3.20	1.47	3.31	3.2154	0.0000	0.0000	-9.67
Sucrose[d]	2.32	2.78	3.00	3.05	2.2279	0.0000	0.0000	-11.11[bm]
Guanosine[h]	2.75	3.35	1.53	2.86	1.8123	0.0000	0.0000	-11.18
Shuangkangsu[bl]	3.08	4.12	1.93	4.45	3.2936	0.0000	0.0000	-12.93

[a] Ref. 1; [b] Ref. 2; [c] Ref. 3; [d] Ref. 4; [e] Ref. 5; [f] Ref. 6; [g] Ref. 7; [h] Ref. 8; [i] Ref. 9; [j] Ref.10; [k] Ref.11; [l] Ref.12; [m] Ref.13; [n] Ref.14; [o] Ref.15; [p] Ref.16; [q] Ref.17; [r] Ref.18; [s] Ref.19; [t] Ref. 20; [u] Ref. 21; [v] Ref. 22; [w] Ref. 23; [x] Ref. 24; [y] Ref. 25; [z] Ref. 26; [aa] Ref. 27; [ab] Ref. 28; [ac] Ref. 29; [ad] Ref. 30; [ae] Ref. 31; [af] Ref. 32; [ag] Ref. 33; [ah] Ref. 34; [ai] Ref. 35; [aj] Ref. 36; [ak] Ref. 37; [al] Ref. 38; [am] Ref. 39; [an] Ref. 40; [ao] Ref. 41; [ap] Ref. 42; [aq] Ref. 43; [ar] Ref. 44; [as] Ref. 45; [at] Ref. 46; [au] Ref. 47; [av] Ref. 48; [aw] Ref. 49; [ax] Ref. 50; [ay] Ref. 51; [az] Ref. 52; [ba] Ref. 53; [bb] Ref. 54; [bc] Ref. 55; [bd] Ref. 56; [be] Ref. 57; [bf] Ref. 58; [bg] Ref. 59; [bh] Ref. 60; [bi] Ref. 61; [bj] Ref. 62; [bk] Ref. 63; [bl] Ref. 64; [bm] The experimental descriptors were directly taken from the UFZ-LSER database.

Table S3. Some compounds that structurally resemble some of the compounds in this work, and their calculated descriptors, predicted and observed log K_p values.

Compounds	E	S	A	B	V	J+	J-	log K_p (cal)	log K_p[a] (obs)
2-Naphthol	1.54	1.13	0.62	0.34	1.1441	0.0000	0.0000	-4.78	-4.65
2-Phenylethanol	0.82	0.85	0.33	0.56	1.0569	0.0000	0.0000	-5.30	-5.20
3,4-Xylenol	0.83	0.83	0.41	0.24	1.0569	0.0000	0.0000	-4.54	-4.52
3-Methylphenol	0.77	1.02	0.68	0.32	0.9160	0.0000	0.0000	-5.20	-4.89
4-Hydroxybenzyl alcohol	0.97	1.26	0.94	0.76	0.9747	0.0000	0.0000	-6.37	-6.26
4-Hydroxyphenylacetic acid	0.93	1.42	1.26	0.77	1.1313	0.0000	0.0000	-6.32	-6.16
5-Fluorouracil	0.74	0.92	0.43	0.63	0.7693	0.0000	0.0000	-6.07	-6.82
8-Methoxypsoralen	1.51	1.98	0.00	0.80	1.4504	0.0000	0.0000	-5.65	-5.12
Acetylsalicylic acid	0.81	1.51	0.69	0.74	1.2879	0.0000	0.0000	-5.84	-5.50
Amylobarbital	1.03	1.11	0.54	1.19	1.7966	0.0000	0.0000	-5.70	-6.00
Barbital	1.03	1.11	0.54	1.19	1.3739	0.0000	0.0000	-6.46	-7.31
Benzyl alcohol	0.82	0.85	0.33	0.50	0.9160	0.0000	0.0000	-5.41	-5.30
Betamethasone	2.15	3.31	1.00	2.02	2.9132	0.0000	0.0000	-7.04	-7.15
Betamethasone-17-valerate	1.97	3.50	0.70	2.12	3.6334	0.0000	0.0000	-6.03	-6.50
Butobarbital	1.03	1.11	0.50	1.19	1.6557	0.0000	0.0000	-5.94	-7.07
Butyl paraben	0.87	1.29	0.70	0.43	1.5540	0.0000	0.0000	-4.48	-4.34
3-Phenylpropanoic acid	0.78	1.22	0.57	0.61	1.2135	0.0000	0.0000	-5.45	-4.93
4-Phenylbutanoic acid	0.78	1.22	0.57	0.61	1.3544	0.0000	0.0000	-5.20	-4.85
5-Phenylpentanoic acid	0.78	1.22	0.57	0.61	1.4953	0.0000	0.0000	-4.94	-4.30
8-Phenyloctanoic acid	0.78	1.22	0.57	0.61	1.9180	0.0000	0.0000	-4.19	-3.86
Benzoic acid	0.78	1.11	0.46	0.43	0.9317	0.0000	0.0000	-5.42	-4.91
Caffeine	1.43	1.82	0.00	1.27	1.3632	0.0000	0.0000	-6.87	-6.85
Catechol	0.91	1.01	0.82	0.47	0.8338	0.0000	0.0000	-5.73	-5.87
Cortexolone	1.80	3.34	0.55	1.71	2.7389	0.0000	0.0000	-6.51	-7.20
Cortexone	1.68	2.59	0.33	1.38	2.6802	0.0000	0.0000	-5.31	-6.42
Corticosterone	1.87	2.30	0.63	2.09	2.7389	0.0000	0.0000	-6.83	-6.84
Cortisone	1.94	3.50	0.55	1.99	2.7546	0.0000	0.0000	-7.24	-7.38
Coumarin	1.08	1.37	0.00	0.65	1.0619	0.0000	0.0000	-5.68	-5.60
Cyclobarbitone	1.47	1.41	0.54	1.33	1.7859	0.0000	0.0000	-6.18	-6.65
Cytarabine	2.03	2.75	1.07	2.31	1.6234	0.0000	0.0000	-9.76	-8.66
Dexamethasone	2.15	3.31	1.00	2.02	2.9132	0.0000	0.0000	-7.04	-7.27
Digitoxin	3.65	4.04	1.23	5.07	5.6938	0.0000	0.0000	-9.76	-8.15
Estrone	1.81	2.36	0.52	1.11	2.1558	0.0000	0.0000	-5.50	-5.52
Flurbiprofen	1.40	1.57	0.57	0.74	1.8390	0.0000	0.0000	-4.77	-4.72
Flurbiprofen glucoside	2.37	2.75	0.94	2.16	2.8693	0.0000	0.0000	-7.07	-6.28
Flurbiprofen mannoside	2.37	2.75	0.94	2.16	2.8693	0.0000	0.0000	-7.07	-6.74
Griseofulvin	1.90	2.65	0.00	1.43	2.3947	0.0000	0.0000	-5.84	-6.44
Ibuprofen	0.77	1.04	0.57	0.67	1.7771	0.0000	0.0000	-4.48	-4.58
Ibuprofen glucoside	1.84	2.22	0.94	2.09	2.8074	0.0000	0.0000	-6.76	-6.94
Ibuprofen mannoside	1.84	2.22	0.94	2.09	2.8074	0.0000	0.0000	-6.76	-6.55
Ketoprofen	1.66	1.87	0.57	0.89	1.9779	0.0000	0.0000	-5.03	-5.22
Ketoprofen glucoside	2.68	3.05	0.94	2.31	3.0082	0.0000	0.0000	-7.32	-7.73
Ketoprofen mannoside	2.68	3.05	0.94	2.31	3.0082	0.0000	0.0000	-7.32	-7.59
Methyl 4-hydroxyphenylacetate	0.87	1.49	0.53	0.68	1.2722	0.0000	0.0000	-5.65	-5.26

Naproxen	1.53	2.06	0.57	0.85	1.7821	0.0000	0.0000	-5.42	-4.97
Naproxen glucoside	2.60	3.24	0.94	2.29	2.8124	0.0000	0.0000	-7.75	-7.89
Naproxen mannoside	2.60	3.24	0.94	2.29	2.8124	0.0000	0.0000	-7.75	-7.70
o-Cresol	0.76	0.82	0.41	0.34	0.9160	0.0000	0.0000	-5.04	-4.88
Ouabain	3.70	3.95	2.17	4.96	4.1615	0.0000	0.0000	-12.51	-9.66
p-Cresol	0.82	0.97	0.53	0.32	0.9160	0.0000	0.0000	-5.11	-4.83
Phenol	0.77	0.81	0.41	0.29	0.7751	0.0000	0.0000	-5.16	-5.27
Phloroglucinol	1.36	1.22	2.10	0.61	0.8925	0.0000	0.0000	-6.47	-5.87
Prednisolone	2.16	2.70	0.84	2.37	2.7546	0.0000	0.0000	-7.75	-7.91
Pregnenolone	1.41	2.04	0.31	1.18	2.6645	0.0000	0.0000	-4.55	-5.90
Progesterone	1.49	2.23	0.00	1.17	2.6215	0.0000	0.0000	-4.60	-4.90
Pyrogallol	1.11	1.22	1.11	0.65	0.8925	0.0000	0.0000	-6.26	-6.17
Resorcinol	0.92	1.41	1.36	0.45	0.8338	0.0000	0.0000	-6.11	-6.70
Testosterone	1.54	1.97	0.31	1.11	2.3827	0.0000	0.0000	-4.83	-5.54
Theophylline	1.42	1.84	0.62	1.29	1.2223	0.0000	0.0000	-7.39	-6.92

[a] Taken from the literature.[65]

Table S4. Experimentally observed skin-permeating components of *LJF* and the LC-MS/MS characteristics thereof (Table 2 continued).

No.	Compounds	Formula	$[M+H]^+$ Calc. *m/z*	$[M+H]^+$ Obs. *m/z*	Δ (ppm)	RT (min)	Targeted MS^2	Peak area[d]		
								S_{ME}[e]	S_{LJF}[e]	S_{ME}/S_{LJF}
Alkaloids										
14	Unidentified	$C_{15}H_{28}N_2O_6$	333.2026	333.2032	1.9	18.53	333.2032 (100)	1.29×10^5	6.93×10^5	0.19
15	Unidentified	$C_{15}H_{26}N_2O_6$	331.1869	331.1875	1.8	17.50	331.1876 (100)	4.07×10^4	1.57×10^5	0.26
16	Unidentified	$C_{18}H_{33}NO_4$	328.2488	328.2491	1.0	18.66	275.2011 (62), 213.1473 (13), 195.1384 (22), 181.1227 (19), 149.1329 (18), 145.1013 (17), 137.0962 (13), 135.1168 (26), 133.1015 (41), 123.117 (16), 119.0859 (25), 109.1016 (16), 107.0859 (44), 105.0705 (18), 97.0653 (16), 96.7663 (11), 95.0862 (41), 93.0704 (76), 91.0548 (52), 81.0705 (100), 79.055 (23), 74.9513 (10), 69.0707 (59), 67.3654 (11), 67.0552 (100), 57.8194 (10), 55.0551 (25)	1.71×10^4	6.96×10^4	0.25
17	Unidentified	$C_{19}H_{37}NO_4$	344.2801	344.2804	0.9	20.50	106.0502 (100), 88.0763 (51), 88.0398 (28), 71.0865 (24), 70.066 (13), 60.0452 (69), 57.0708 (27)	2.67×10^4	6.62×10^4	0.40
18	Unidentified	$C_{13}H_{17}NO_2$	220.1338	220.1337	-0.2	16.36	220.1323 (18), 138.055 (96), 109.0652 (48), 81.0706 (100), 70.0658 (18)	4.78×10^4	5.83×10^4	0.82
19	Unidentified	$C_{18}H_{33}NO_4$	328.2488	328.2491	1.0	18.38	269.9404 (29), 119.0863 (34), 116.5404 (26), 109.1018 (36), 107.0859 (33), 95.0858 (38), 95.0499 (24), 93.0704 (49), 91.0548 (50), 82.6714 (24), 81.0707 (40), 79.0549 (43), 67.0552 (100), 55.0551 (24), 54.3993 (23), 54.1577 (20), 50.6058 (22)	1.80×10^4	4.29×10^4	0.42
20	Unidentified	$C_{18}H_{37}NO_4$	332.2801	332.2803	0.7	17.09	332.1897 (100)	1.83×10^4	3.60×10^4	0.51
21	Unidentified	$C_{14}H_{25}NO_4$	272.1862	272.1864	0.8	14.80	248.0900 (43), 159.5778 (39), 158.0123 (51), 134.9967 (65), 130.0932 (56), 98.9759 (100), 98.3436 (42), 95.2277 (42), 71.0342 (38), 62.4919 (43), 62.0749 (38)	9.49×10^4	3.03×10^4	3.14
22	Unidentified	$C_{20}H_{33}NO_4$	352.2488	352.2496	2.3	18.05	352.255 (100), 348.7145 (91), 289.1785 (94), 250.0472 (98), 81.0704 (85), 78.3949 (85), 74.9987 (74), 53.6604 (74), 51.4678 (80)	2.22×10^4	2.21×10^4	1.00
Lipids										
23	Unidentified	$C_{18}H_{28}O_2$	277.2168	277.2171	1.2	19.45	277.2158 (60), 221.1173 (26), 165.0546 (35), 149.1326 (20), 147.044 (49), 137.0598 (54), 135.1168 (49), 133.1013 (13), 121.1014 (47), 119.0855 (12), 109.1017 (12), 107.086 (49), 105.0703 (15), 95.086 (25), 93.0704 (100), 91.0548 (17), 81.0706 (45), 79.0549 (60), 69.0707 (18), 67.0551 (25), 57.0708 (47), 55.0551 (20)	3.24×10^6	4.44×10^6	0.73
24	Unidentified	$C_{18}H_{28}O_2$	277.2168	277.2171	1.2	19.53	277.216 (64), 149.1326 (19), 135.1169 (49), 133.1013 (13), 121.1014 (43), 119.0858 (10), 109.1015 (12), 107.086 (48), 105.0703 (11), 95.0861 (20), 93.0705 (100), 91.0547 (19), 81.0705 (28), 79.0549 (58), 69.0706 (14), 67.0551 (27), 55.0551 (17)	2.09×10^6	3.15×10^6	0.67

25	Unidentified	$C_{18}H_{28}O_3$	293.2117	293.2118	0.4	19.75	275.2005 (100), 257.1892 (20), 189.1126 (21), 149.0963 (83), 147.117 (14), 145.1015 (11), 135.0805 (13), 133.1011 (22), 131.0857 (13), 125.0961 (28), 121.1015 (27), 119.0859 (29), 117.0702 (13), 109.1016 (26), 107.0859 (68), 107.0495 (35), 105.0703 (30), 97.1017 (30), 97.0653 (10), 95.0862 (20), 93.0704 (44), 91.0548 (25), 83.0863 (13), 83.0499 (29), 81.0706 (35), 79.055 (62), 69.0708 (16), 67.0551 (41), 55.0552 (54), 55.0187 (15)	1.11×10^6	2.13×10^6	0.52
26	Unidentified	$C_{18}H_{26}O_3$	291.1960	291.1962	0.6	17.50	291.1954 (100), 273.1849 (46), 161.0961 (12), 147.0805 (24), 145.1012 (24), 143.0855 (11), 135.0806 (35), 131.0857 (24), 121.1016 (12), 121.0649 (17), 119.0858 (27), 117.07 (22), 109.0653 (16), 107.0858 (21), 105.0705 (22), 95.0861 (14), 95.0498 (11), 93.0705 (18), 91.0549 (25), 81.0706 (39), 79.055 (21), 67.0551 (23), 57.0344 (20), 55.0551 (21), 55.0187 (14)	3.98×10^5	1.23×10^6	0.32
27	Unidentified	$C_{16}H_{30}O_4$	287.2222	287.2223	0.2	17.09	269.2115 (46), 251.2008 (100), 233.1907 (15), 215.1793 (12), 175.0154 (38), 147.1167 (11), 125.097 (10), 123.1169 (11), 121.1013 (41), 109.1014 (48), 107.0857 (12), 97.1015 (17), 95.086 (92), 93.0705 (45), 91.055 (11), 83.0861 (18), 81.0707 (84), 79.0549 (33), 69.0706 (33), 67.055 (54), 57.0708 (29), 56.9657 (13), 55.0552 (30)	4.31×10^4	8.23×10^5	0.05
28	Unidentified	$C_{14}H_{22}O_3$	239.1647	239.1648	0.3	17.65	239.1645 (19), 109.1017 (20), 95.0865 (14), 89.0605 (12), 69.0707 (13), 57.0708 (100)	1.69×10^5	7.65×10^5	0.22
29	Unidentified	$C_{18}H_{26}O_4$	307.1909	307.1911	0.5	18.05	289.1795 (100), 271.1685 (23), 188.6333 (24), 165.0667 (19), 159.08 (32), 135.0807 (30), 135.0653 (19), 117.7874 (21), 107.0859 (19), 107.0502 (23), 101.4446 (20), 97.1022 (22), 93.0703 (27), 91.2829 (17), 91.0542 (21), 81.0706 (36), 80.1921 (18), 79.0547 (19), 76.006 (18), 68.2027 (15), 67.0551 (38), 64.1044 (15), 57.0344 (89), 55.0552 (28), 50.5106 (16)	2.49×10^5	4.67×10^5	0.53
30	Unidentified	$C_{16}H_{32}O_4$	289.2379	289.2379	0.1	16.84	246.1632 (22), 226.1812 (34), 225.2562 (22), 177.9113 (23), 132.3614 (20), 110.2516 (22), 100.5394 (19), 93.8926 (19), 93.0704 (20), 71.4196 (22), 67.055 (19), 51.9726 (18)	5.21×10^5	4.60×10^5	1.13
31	Unidentified	$C_{18}H_{28}O_3$	293.2117	293.2118	0.4	18.68	277.2163 (58), 221.1167 (45), 193.1222 (21), 175.1117 (24), 151.1117 (14), 149.1327 (15), 147.1169 (22), 139.1116 (24), 135.1166 (33), 133.1012 (36), 125.0962 (19), 123.1172 (19), 121.1013 (47), 119.0858 (28), 111.0809 (18), 109.1016 (50), 107.086 (43), 105.0703 (22), 101.0236 (36), 99.0812 (18), 97.1016 (29), 95.086 (78), 93.0704 (63), 91.0549 (29), 85.029 (47), 83.0863 (52), 81.0706 (100), 79.055 (31), 73.0291 (14), 71.0862 (19), 69.0707 (39), 67.0551 (96), 57.0708 (64), 55.0552 (51), 55.0187 (15)	1.83×10^5	4.36×10^5	0.42
32	Unidentified	$C_{17}H_{26}O_4$	295.1909	295.1910	0.2	19.42	277.2161 (56), 277.1818 (18), 231.1739 (11), 203.0153 (12), 162.9179 (11), 151.1127 (12), 137.0597 (100), 135.1174 (16), 130.8849 (11), 121.1013 (52), 111.0442 (11), 109.1014 (19), 107.0864 (24), 95.0858 (51), 93.0705 (22), 91.055 (12), 83.0861 (17), 81.0705 (76), 79.7425 (11), 79.0551 (22), 71.0864 (18), 71.0501 (17), 69.333 (10), 69.0707 (19), 67.0549 (46), 57.0707 (23), 55.055 (21), 55.0187 (16)	1.87×10^5	4.18×10^5	0.45

33	Unidentified	$C_{17}H_{26}O_4$	295.1909	295.1910	0.2	19.24	277.2161 (100), 259.2055 (10), 189.1125 (13), 165.1276 (13), 161.1323 (17), 151.1122 (18), 149.1325 (21), 147.1168 (24), 139.1115 (15), 135.117 (22), 133.1013 (25), 125.0963 (18), 121.1016 (26), 119.0858 (23), 111.0808 (32), 109.1018 (28), 107.0861 (44), 105.0703 (28), 99.0809 (18), 97.1017 (29), 95.0861 (57), 95.0498 (14), 93.0705 (68), 91.0548 (36), 83.0862 (41), 83.0499 (20), 81.0707 (85), 79.055 (42), 71.0863 (27), 69.0707 (36), 67.0551 (90), 57.0709 (16), 55.0552 (63), 55.0187 (28)	2.30×10^5	3.44×10^5	0.67
34	Unidentified	$C_{11}H_{16}O_3$	197.1178	197.1178	0.2	9.24	197.1172 (85), 179.1067 (100), 161.0962 (29), 135.1169 (59), 133.1013 (55), 107.086 (52), 105.0704 (13), 93.0705 (19)	1.36×10^6	2.43×10^5	5.58
35	Unidentified	$C_{13}H_{20}O_2$	209.1542	209.1542	0.2	13.74	209.1537 (47), 165.1275 (100), 123.0806 (11), 121.1015 (11)	3.00×10^5	1.78×10^5	1.68
36	Unidentified	$C_{17}H_{26}O_4$	295.1909	295.1911	0.6	17.81	137.0596 (100), 111.0441 (12), 109.1015 (11), 109.0651 (11), 95.0859 (15), 93.0703 (12), 81.0705 (30), 67.0549 (13)	2.26×10^5	1.62×10^5	1.40
37	Unidentified	$C_{11}H_{18}O_3$	199.1334	199.1332	-1.1	16.57	181.1224 (33), 163.112 (21), 158.1542 (83), 145.1013 (16), 135.117 (19), 135.0806 (16), 125.0601 (29), 111.0445 (100), 107.086 (16), 102.0919 (16), 95.0862 (10), 83.0499 (10), 74.0973 (10), 57.0708 (20), 55.0552 (15)	5.80×10^4	1.16×10^5	0.50
38	Unidentified	$C_{20}H_{38}O_3$	327.2899	327.2892	-2.2	20.38	267.2679 (32), 249.2578 (16), 137.1321 (12), 123.1167 (22), 111.117 (16), 109.1012 (45), 97.1013 (40), 95.0858 (100), 83.0859 (44), 81.0703 (48), 69.0704 (45), 67.0549 (49), 57.0705 (24), 55.055 (27)	1.95×10^4	8.66×10^4	0.23
39	Unidentified	$C_{21}H_{38}O_4$	355.2848	355.2848	-0.1	20.06	355.2907 (12), 337.2736 (22), 331.9138 (19), 308.9 (19), 280.6996 (11), 263.2369 (65), 245.2272 (41), 218.8675 (15), 204.0113 (10), 163.8128 (11), 163.1476 (12), 163.039 (18), 133.101 (12), 123.1175 (13), 121.1014 (23), 109.1018 (42), 107.086 (16), 105.0706 (10), 97.1013 (12), 95.0861 (78), 93.0701 (21), 83.0864 (12), 81.0705 (100), 79.0549 (21), 69.0708 (22), 67.0551 (63), 57.0707 (17), 55.0552 (21)	5.13×10^4	6.89×10^4	0.75
40	Unidentified	$C_{17}H_{32}O_4$	301.2379	301.2379	0.0	18.78	301.141 (100), 269.2102 (39), 256.2269 (54), 251.2001 (60), 240.2318 (12), 221.1895 (12), 139.1122 (11), 123.117 (12), 121.1015 (32), 109.1015 (36), 107.0865 (12), 97.1018 (28), 95.0861 (73), 93.0706 (37), 83.0864 (23), 81.0706 (58), 69.0707 (29), 67.0551 (40), 55.055 (15)	1.03×10^4	5.00×10^4	0.21
41	Unidentified	$C_{18}H_{32}O_4$	313.2379	313.2379	0.0	18.29	295.2253 (17), 277.216 (60), 187.1481 (17), 173.1328 (24), 149.1328 (15), 133.1012 (13), 131.0858 (19), 121.1016 (50), 119.0859 (16), 118.8901 (14), 109.1018 (27), 108.0104 (11), 107.1227 (11), 107.0857 (56), 105.0703 (17), 97.0659 (14), 95.086 (88), 93.0703 (46), 91.2225 (12), 84.9606 (12), 83.0861 (21), 81.0706 (100), 79.0549 (19), 77.6297 (11), 77.6248 (13), 71.1473 (11), 71.0498 (21), 69.0706 (22), 67.055 (66), 64.0821 (11), 57.0341 (18), 55.0551 (42), 51.1001 (10)	9.43×10^4	4.89×10^4	1.93
42	Unidentified	$C_{22}H_{42}O_3$	355.3212	355.3205	-2.0	20.90	295.2986 (59), 277.2881 (21), 142.1586 (15), 137.1321 (11), 125.1322 (13), 123.1167 (21), 111.1169 (28), 109.1013 (49), 97.1014 (56), 95.0858 (100), 93.0704 (11), 83.086 (55), 81.0704	2.82×10^5	4.24×10^4	6.64

							(77), 71.0861 (12), 69.0705 (60), 67.0548 (44), 57.0706 (33), 55.055 (39)			
43	Unidentified	$C_{24}H_{38}O_3$	375.2899	375.2893	-1.7	17.49	375.2893 (74), 235.1693 (100), 189.1638 (28), 147.1169 (20), 133.1013 (24), 119.0858 (14), 105.0703 (11)	1.80×10^5	4.06×10^4	4.42

[d] Specific to the chromatographic peak areas of the quasi-molecular ions ($[M+H]^+$); [e] S_{ME}, the methanol solution of *LJF* extract (10 mg/mL); S_{LJF}, the skin-permeating sample of *LJF* extract.

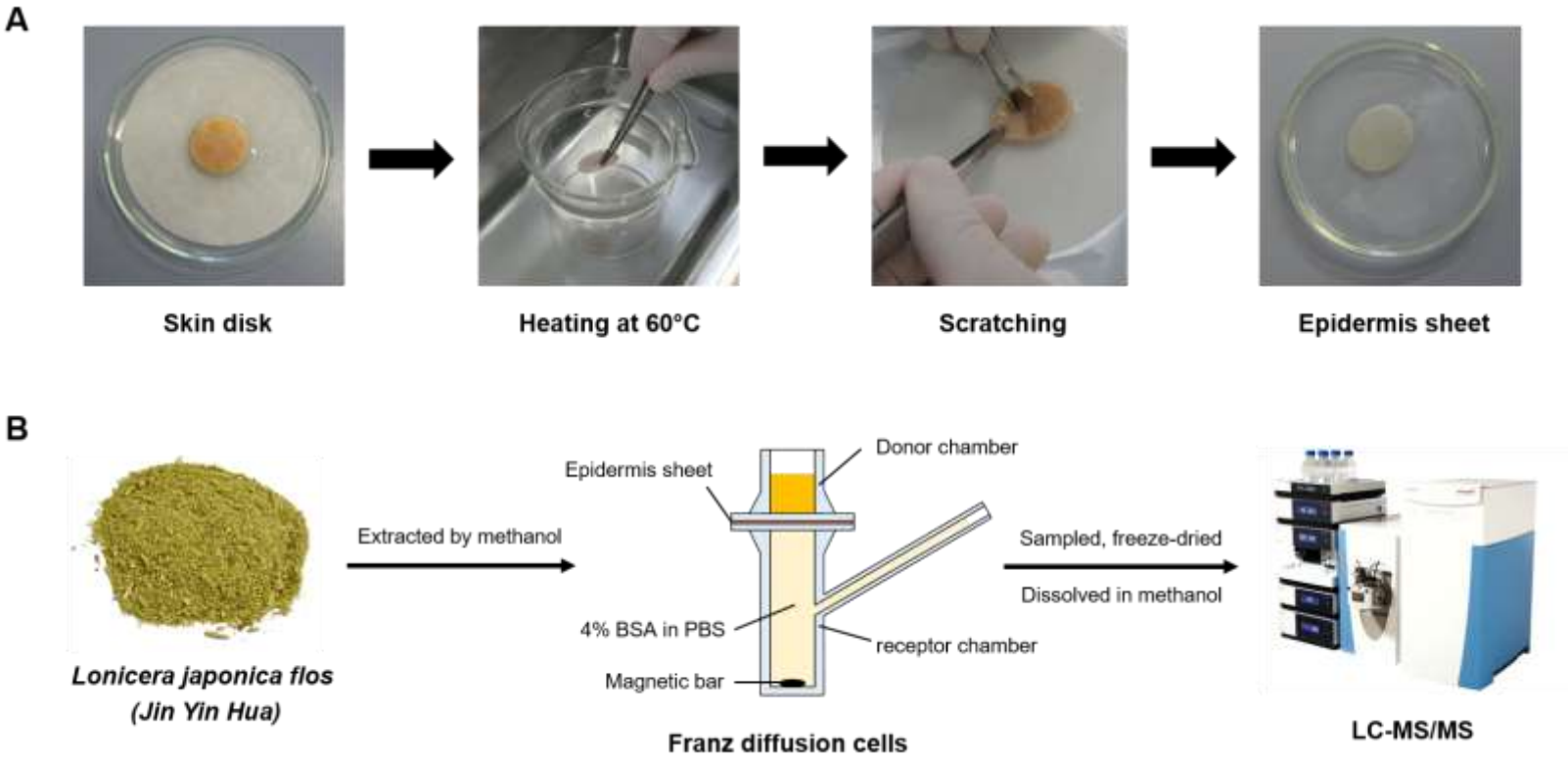

Figure S1. Experimental procedures of *in vitro* skin permeation study. (**A**) Preparation of human skin epidermis; (**B**) Skin permeation experiments, preparation of test samples and LC-MS/MS measurements.

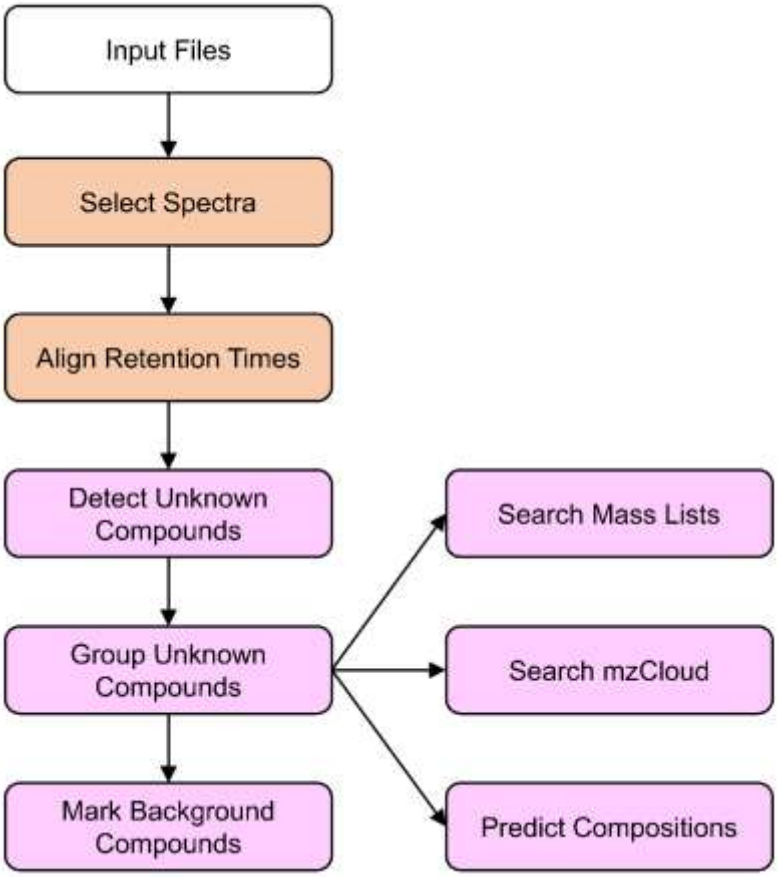

Figure S2. An untargeted screening workflow applied for finding and identifying skin-permeating components of *LJF* in Compound Discoverer^{TM} software

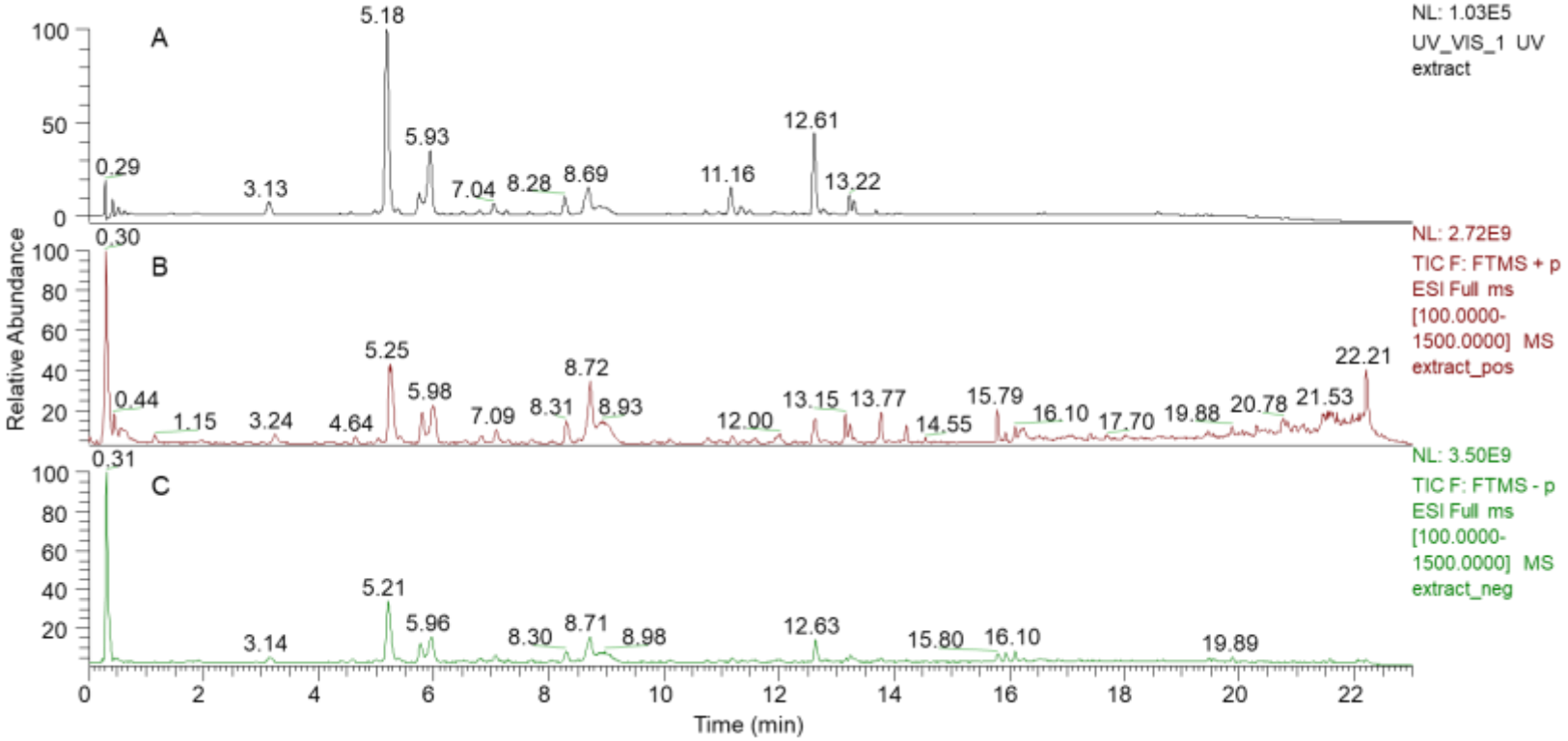

Figure S3. Representative UV and total ion chromatographs of the methanol extract of *LJF* at 254 nm (A), in positive ion mode (B) and negative ion mode (C)

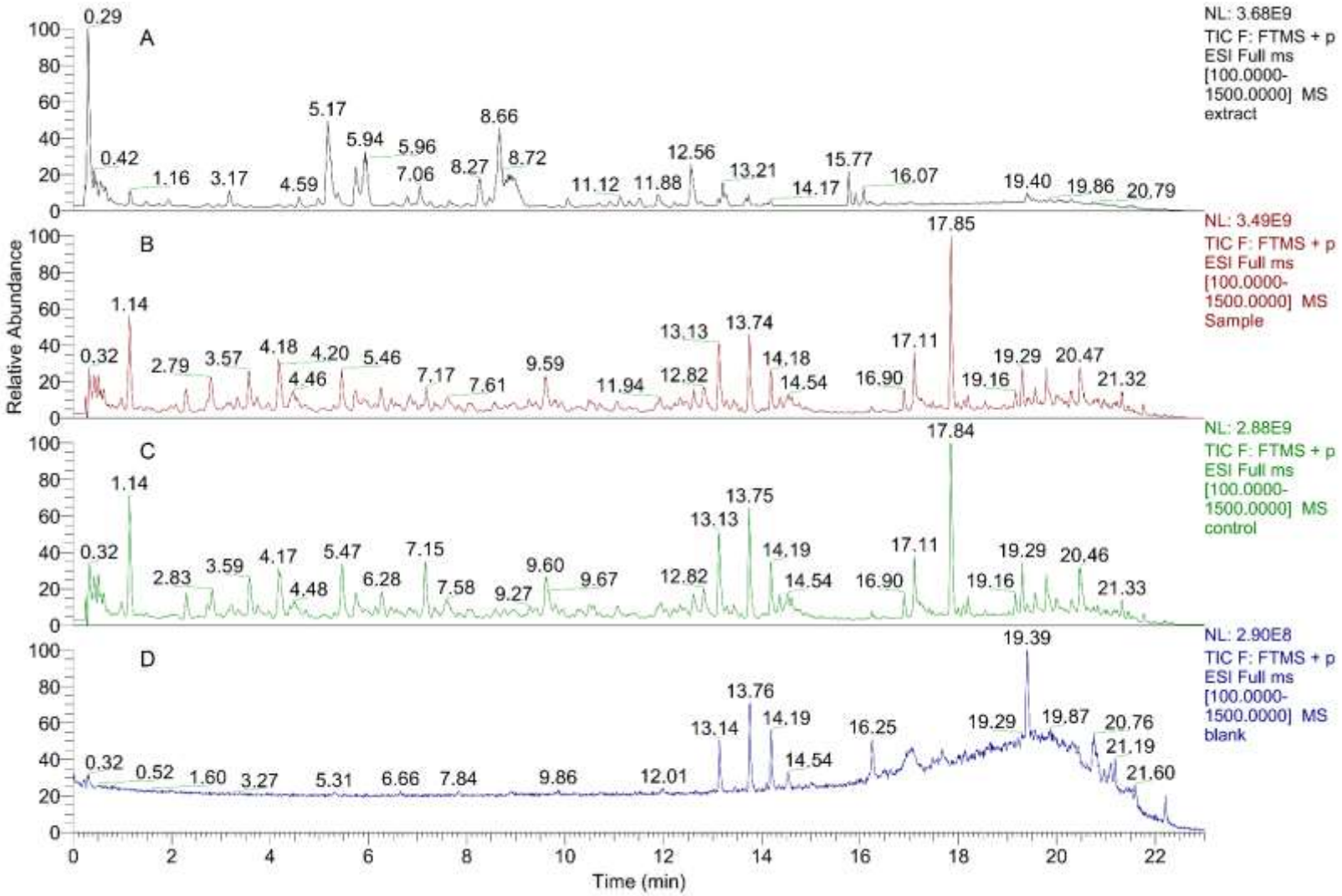

Figure S4. Representative total ion chromatographs of the methanol extract of *LJF* (A), the skin-permeating sample of *LJF* extract (B), the control (C) and the blank, methanol (D) in positive ion mode

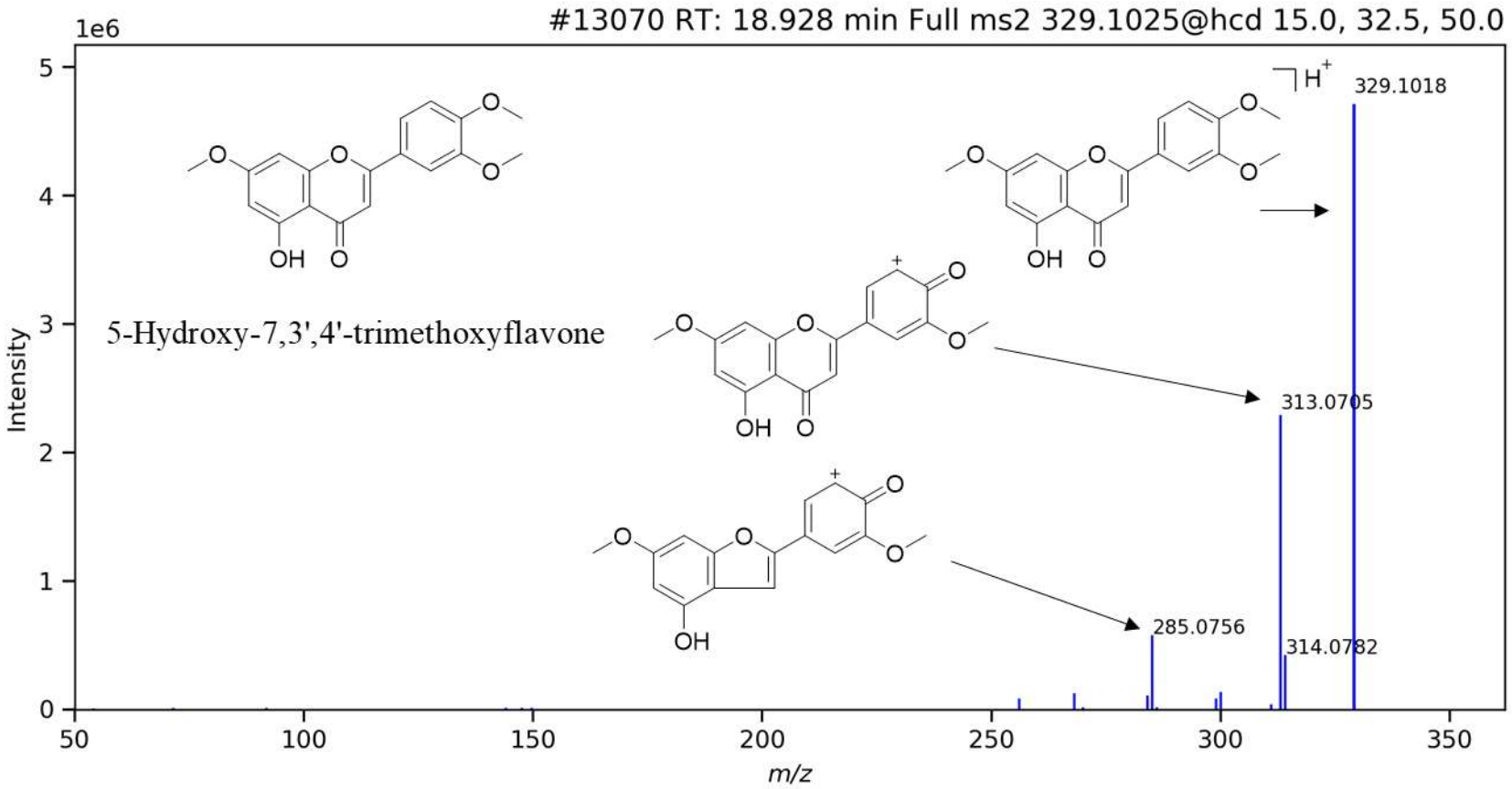

Figure S5. The MS/MS spectrum of 5-hydroxy-7,3',4'-trimethoxyflavone with fragment annotations in positive ion mode

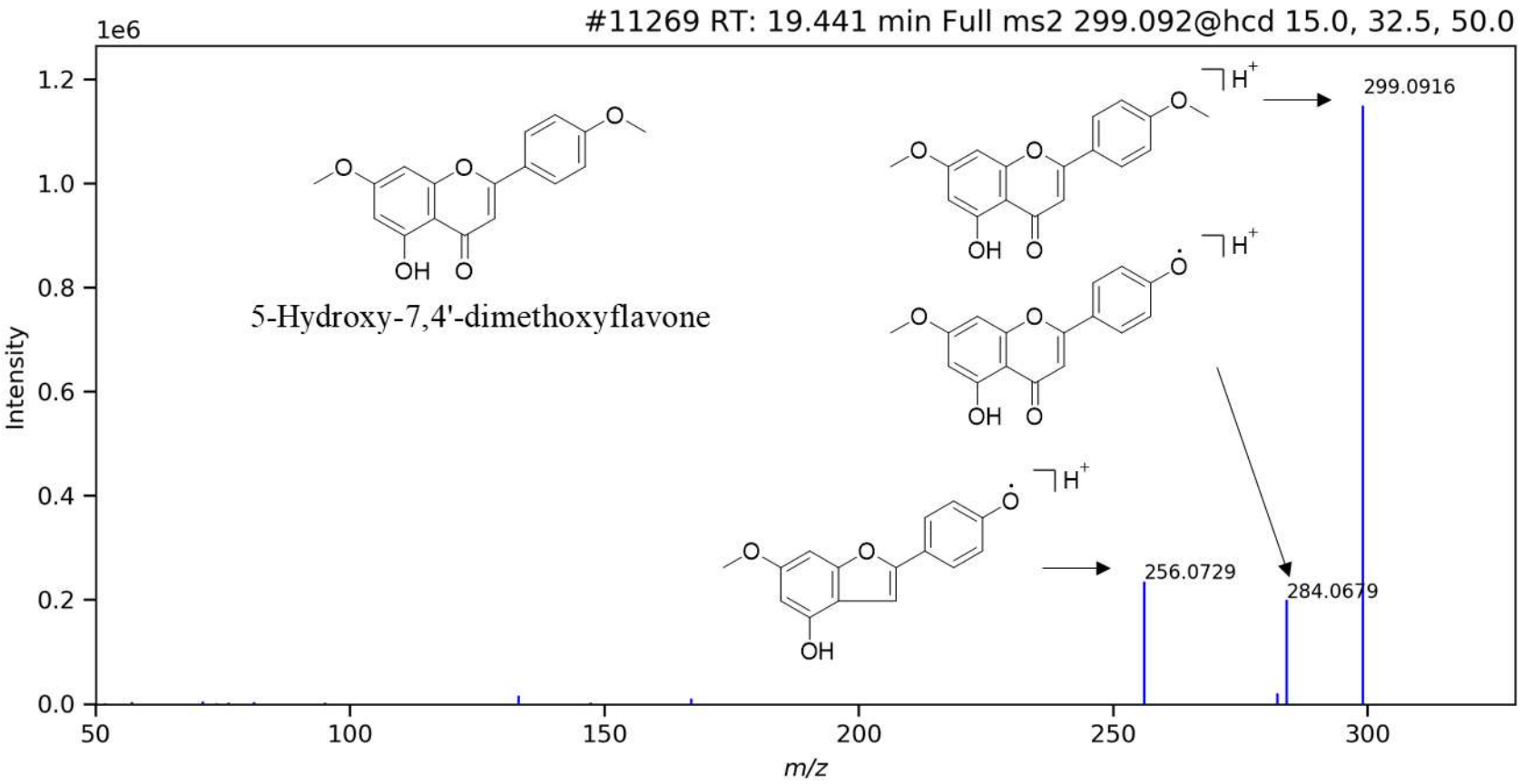

Figure S6. The MS/MS spectrum of 5-hydroxy-7,4'-dimethoxyflavone with fragment annotations in positive ion mode

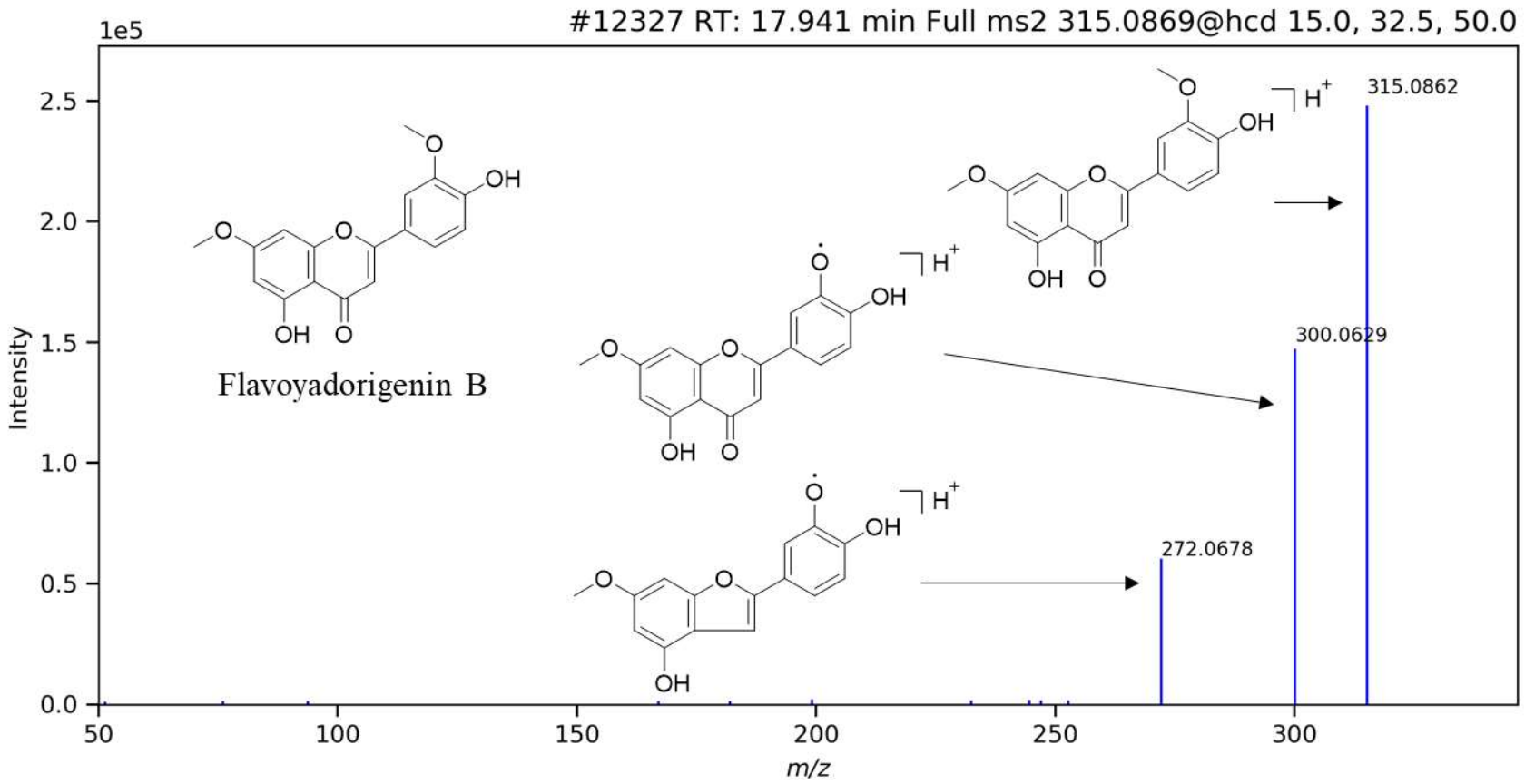

Figure S7. The MS/MS spectrum of flavoyadorigenin B with fragment annotations in positive ion mode

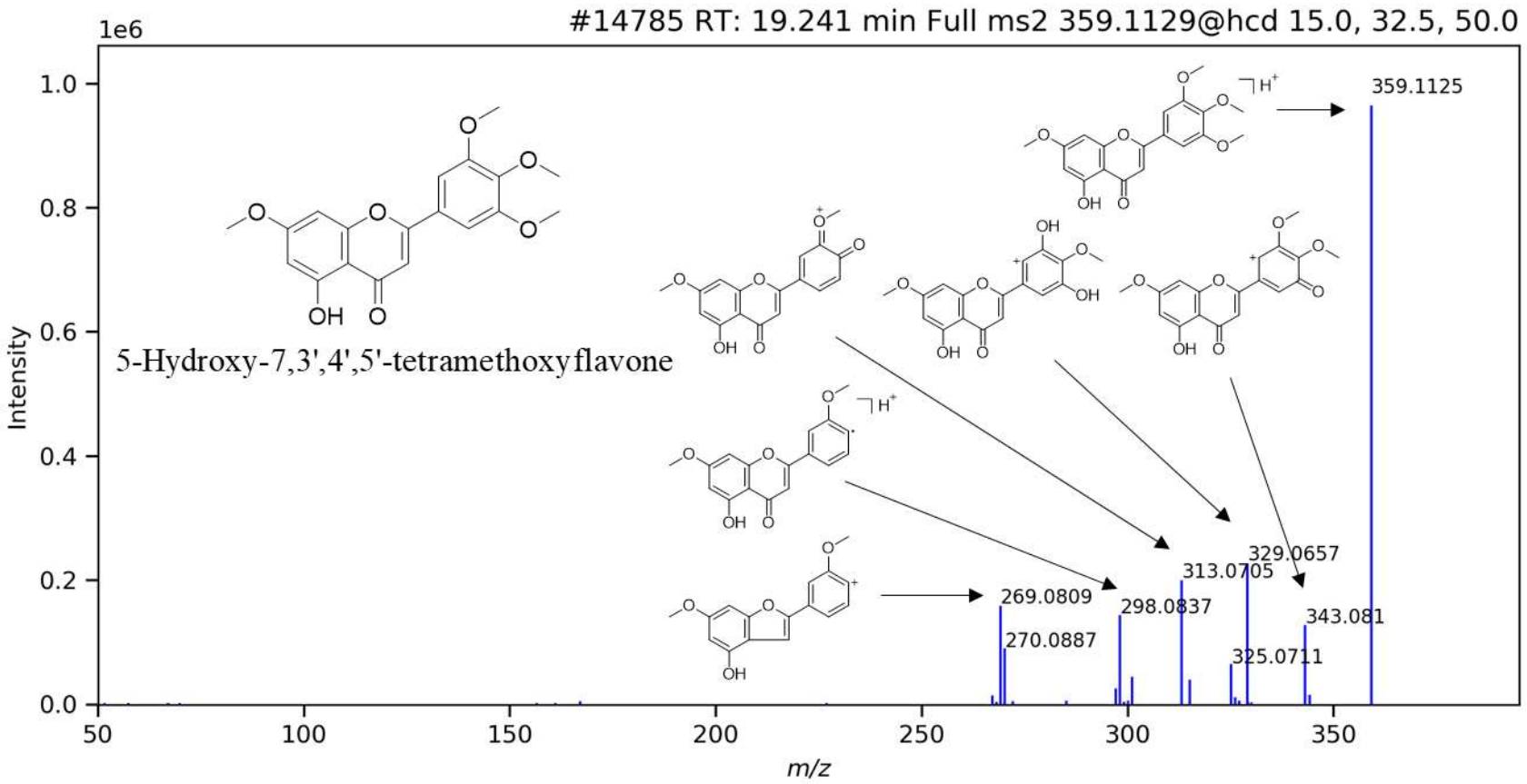

Figure S8. The MS/MS spectrum of 5-hydroxy-7,3',4',5'-tetramethoxyflavone with fragment annotations in positive ion mode

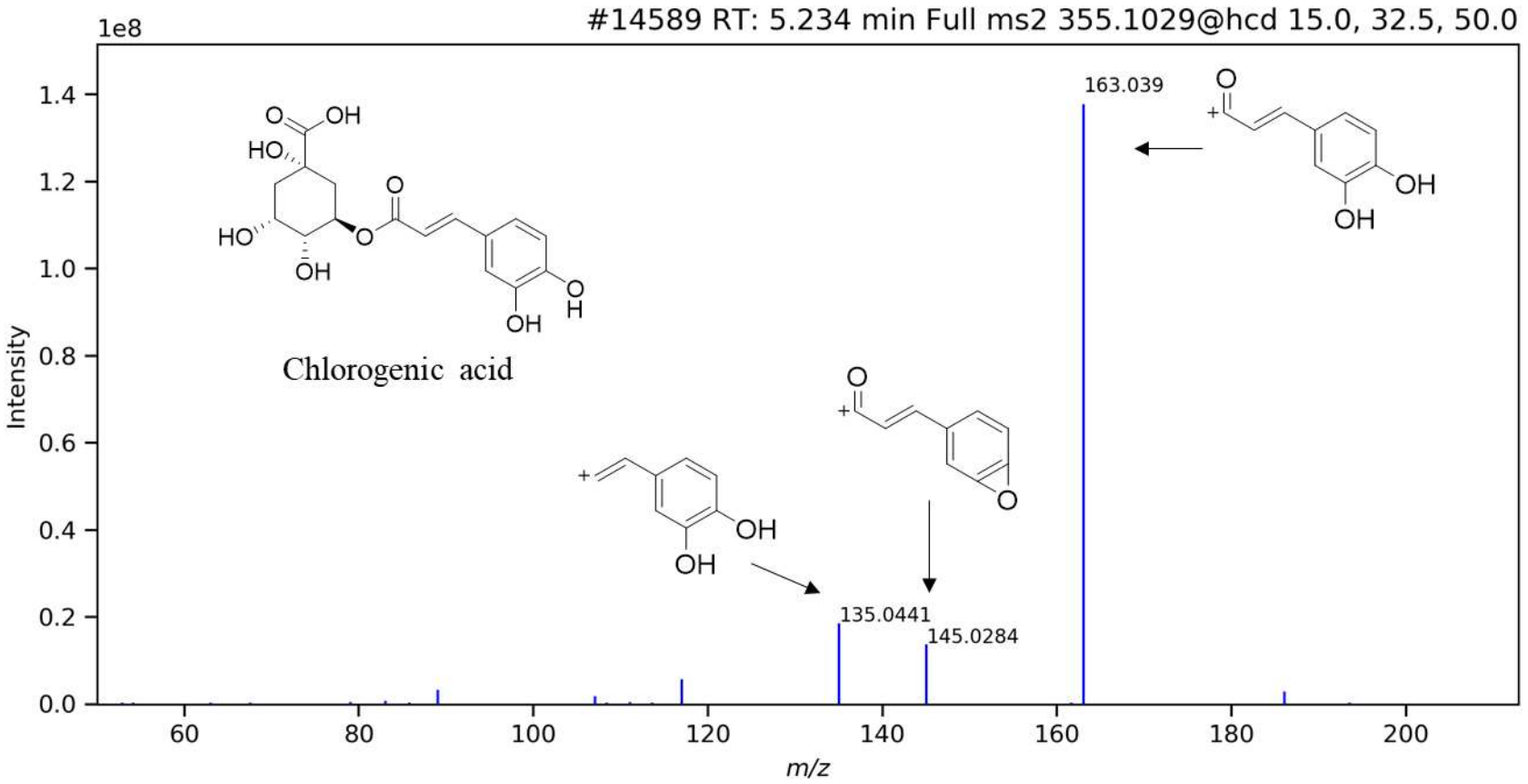

Figure S9. The MS/MS spectrum of chlorogenic acid with fragment annotations in positive ion mode

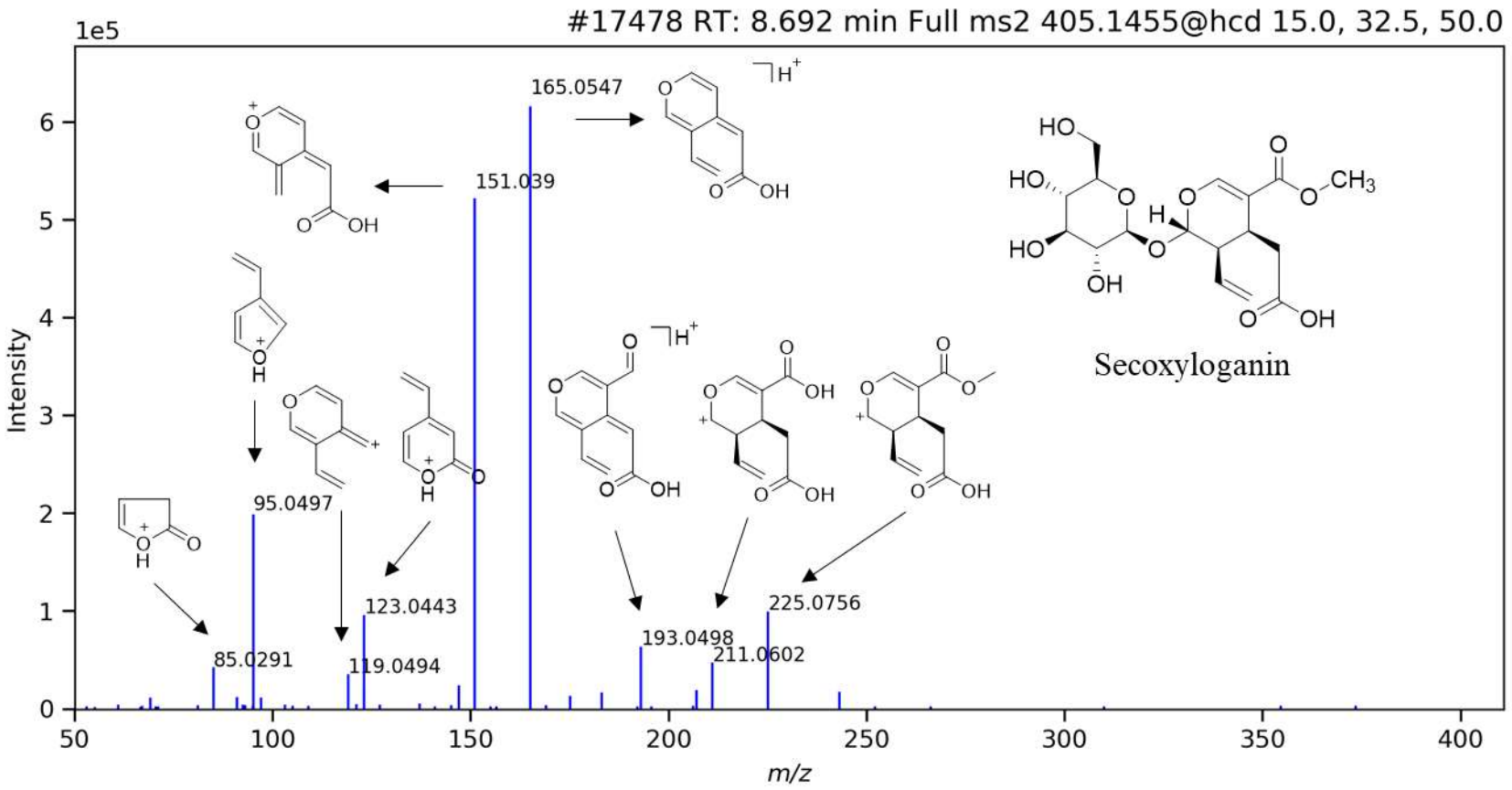

Figure S10. The MS/MS spectrum of secoxyloganin with fragment annotations in positive ion mode

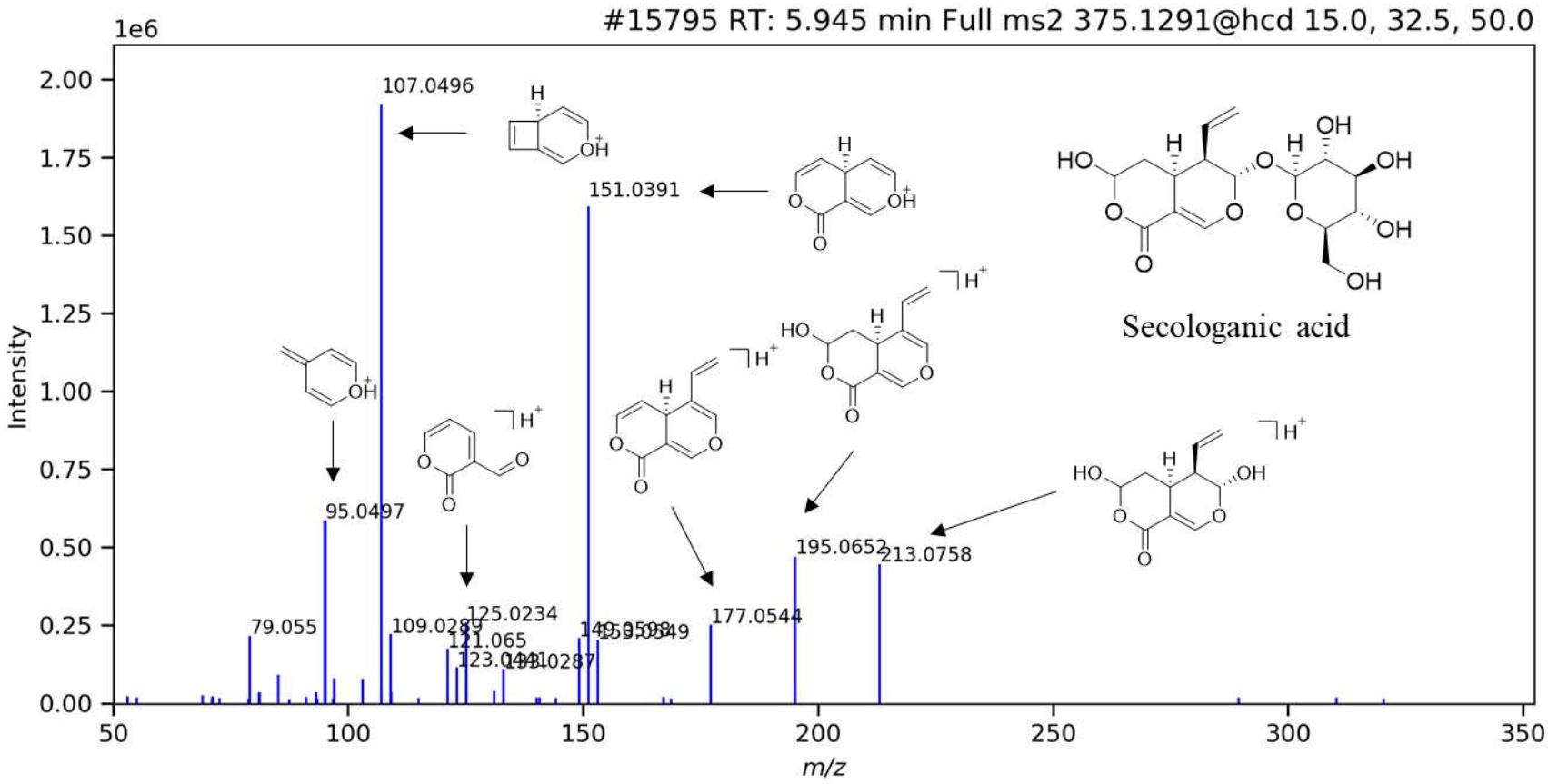

Figure S11. The MS/MS spectrum of secologanic acid with fragment annotations in positive ion mode

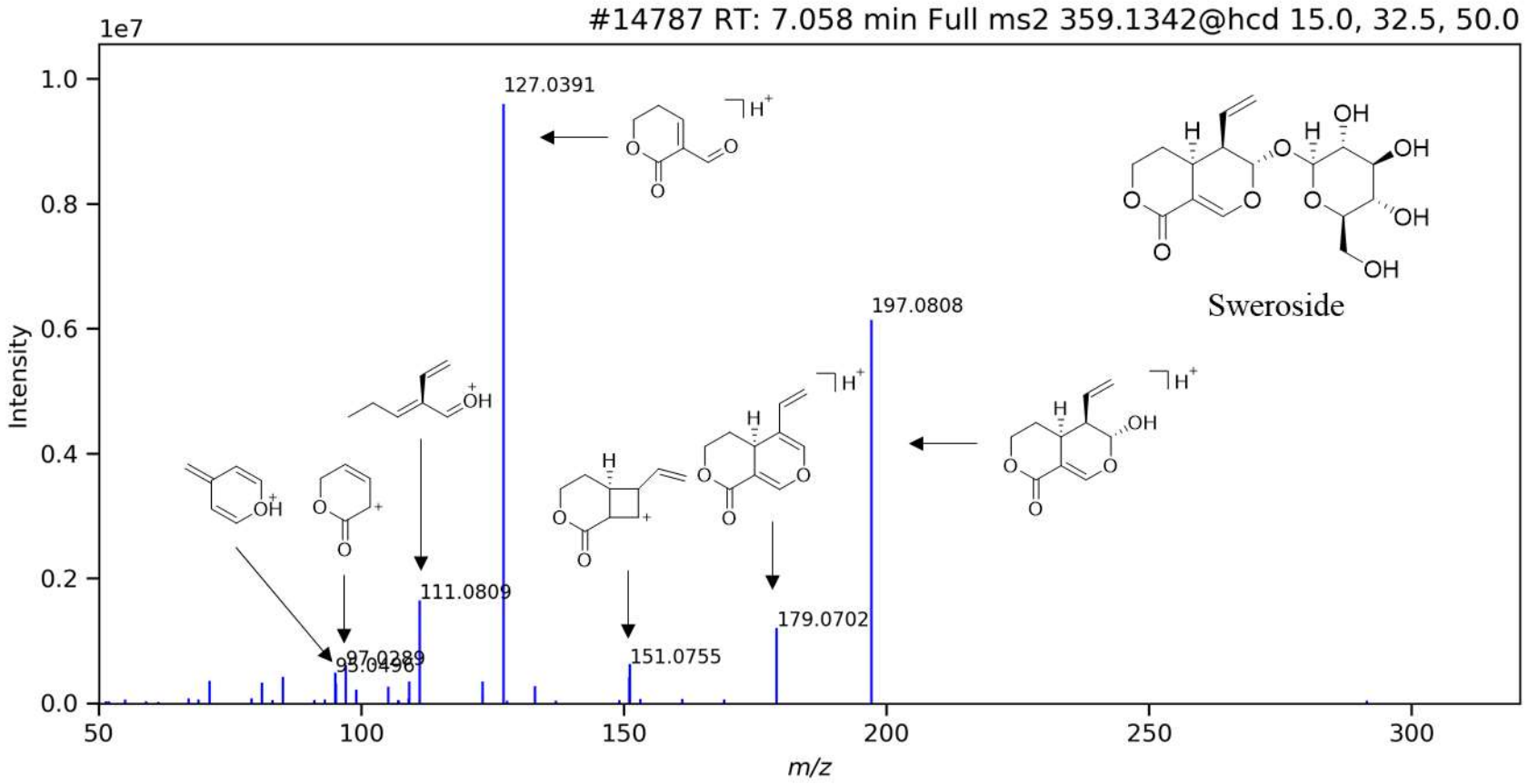

Figure S12. The MS/MS spectrum of sweroside with fragment annotations in positive ion mode

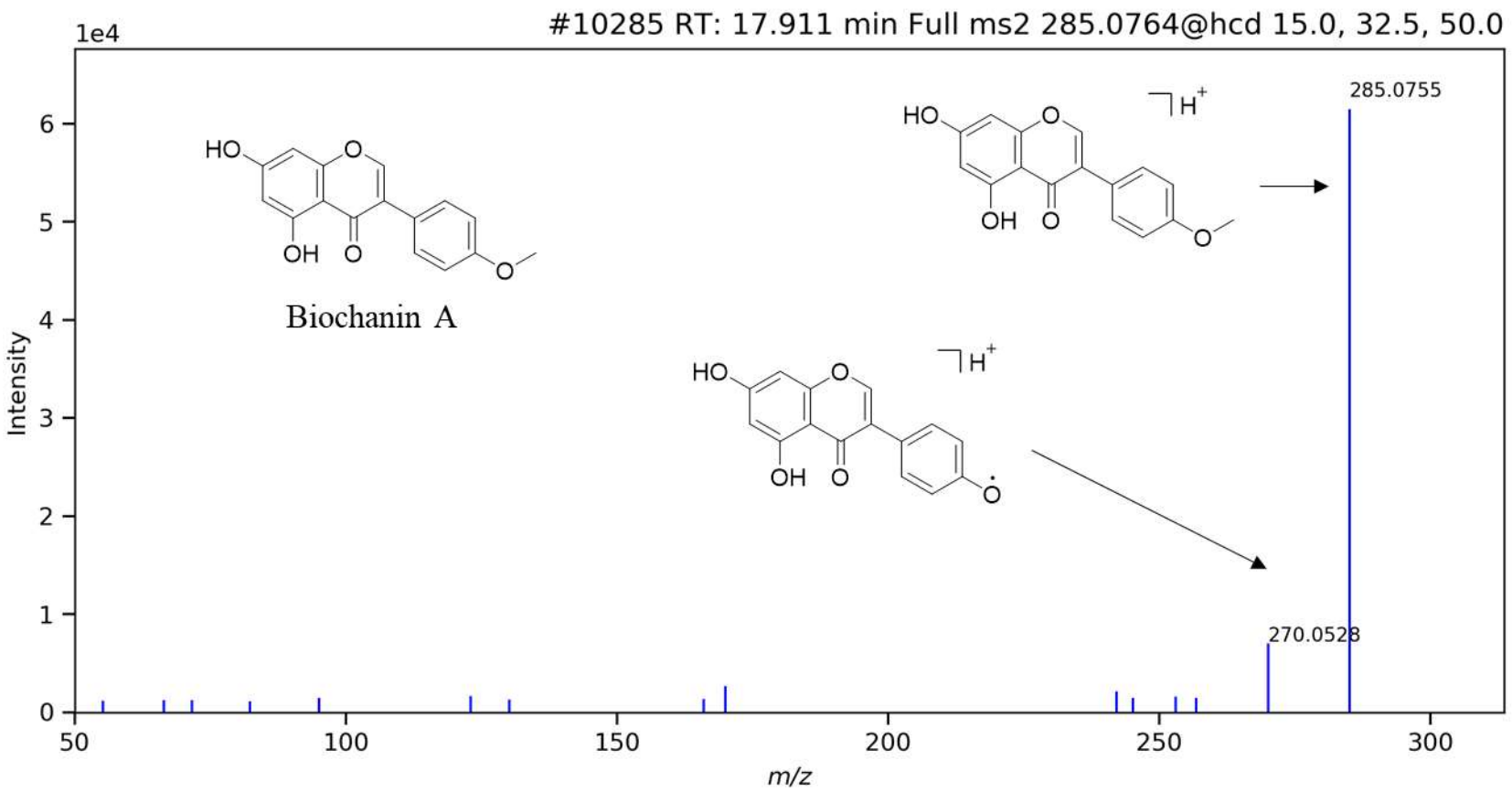

Figure S13. The MS/MS spectrum of biochanin A with fragment annotations in positive ion mode

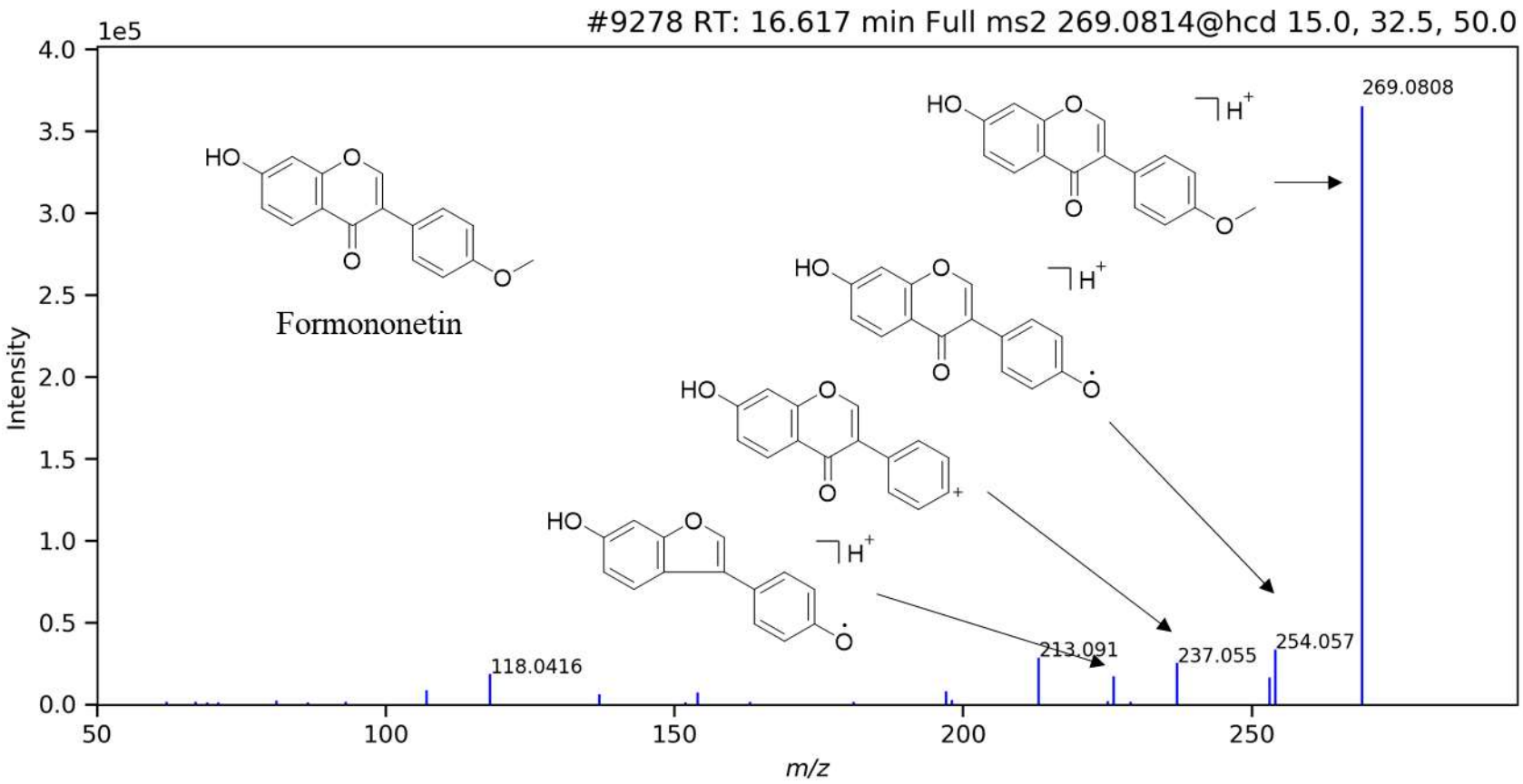

Figure S14. The MS/MS spectrum of formononetin with fragment annotations in positive ion mode

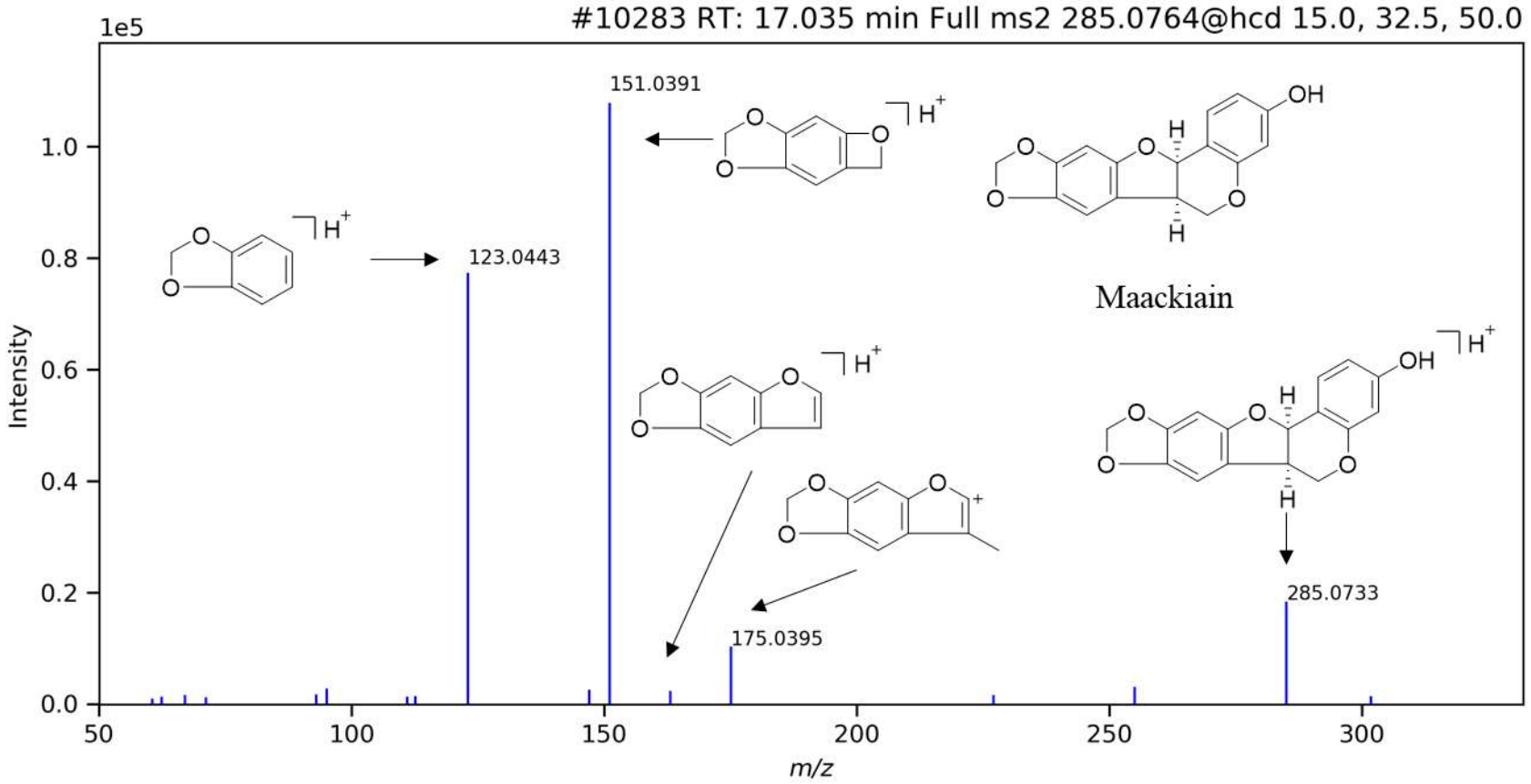

Figure S15. The MS/MS spectrum of maackiain with fragment annotations in positive ion mode

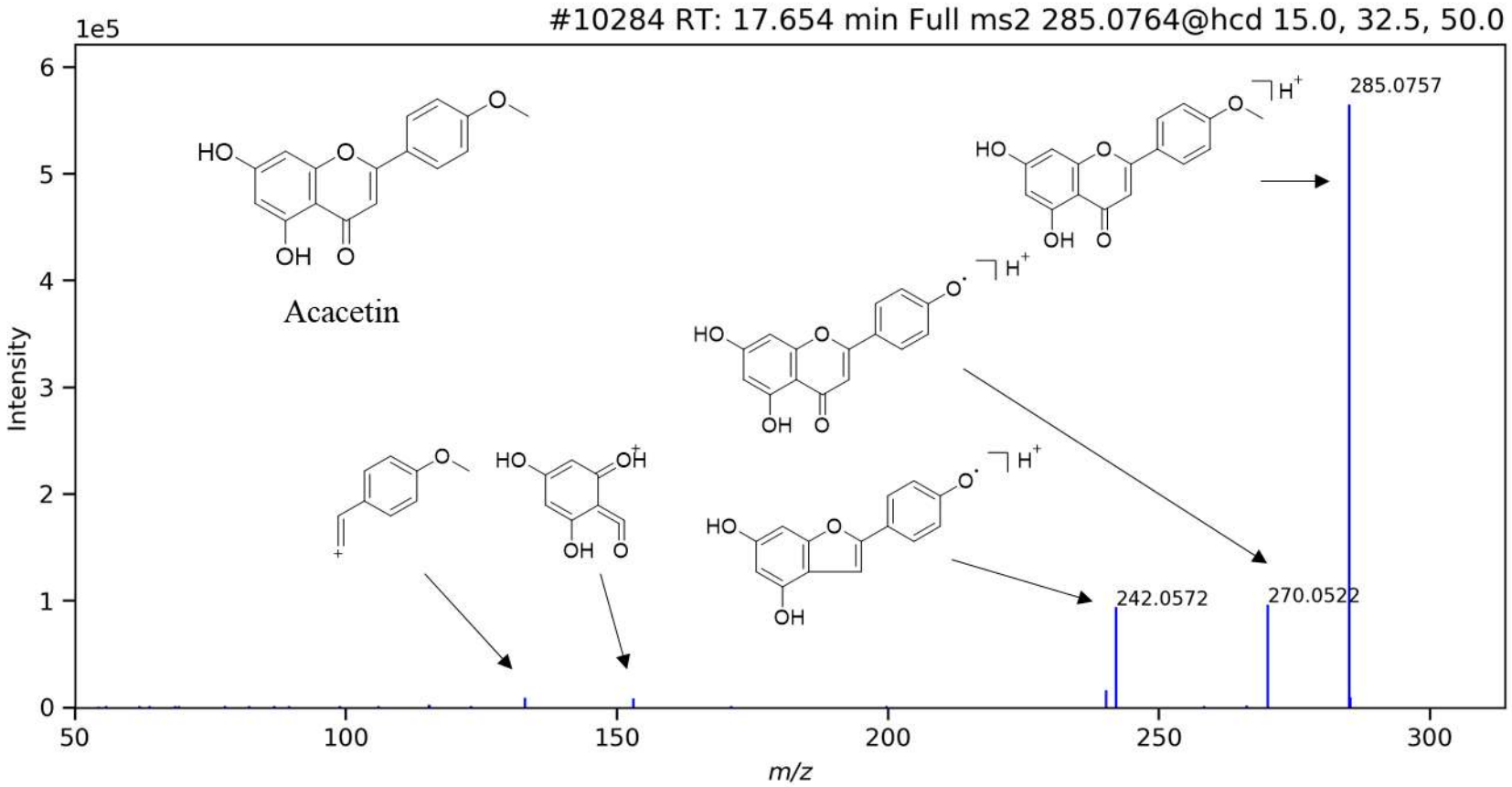

Figure S16. The MS/MS spectrum of acacetin with fragment annotations in positive ion mode

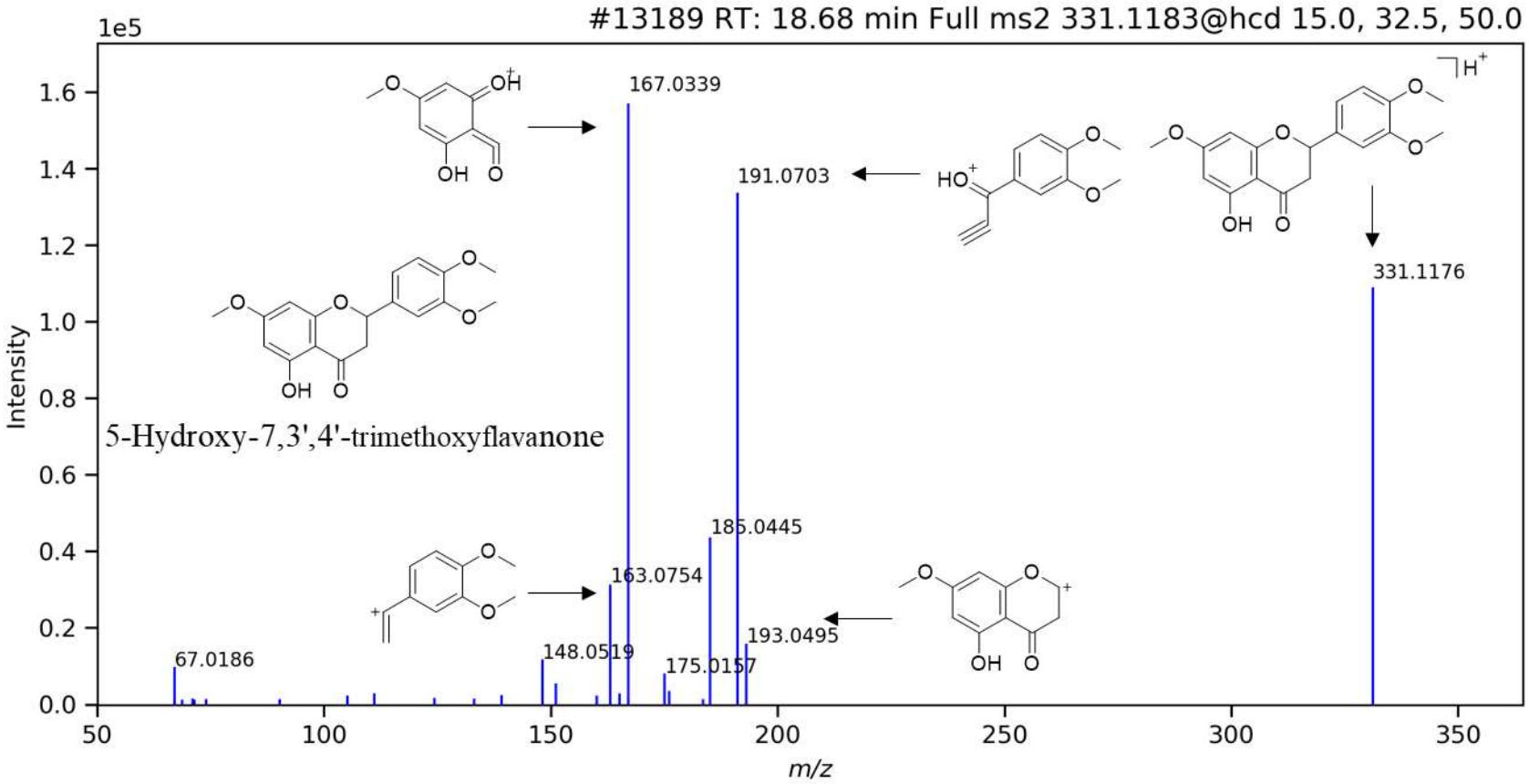

Figure S17. The MS/MS spectrum of 5-hydroxy-7,3',4'-trimethoxyflavanone with fragment annotations in positive ion mode

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