

Supplementary Materials: Qualitative Fingerprint Analysis and Multidirectional Assessment of Different Crude Extracts and Essential Oil from Wild *Artemisia santonicum* L.

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Abundance

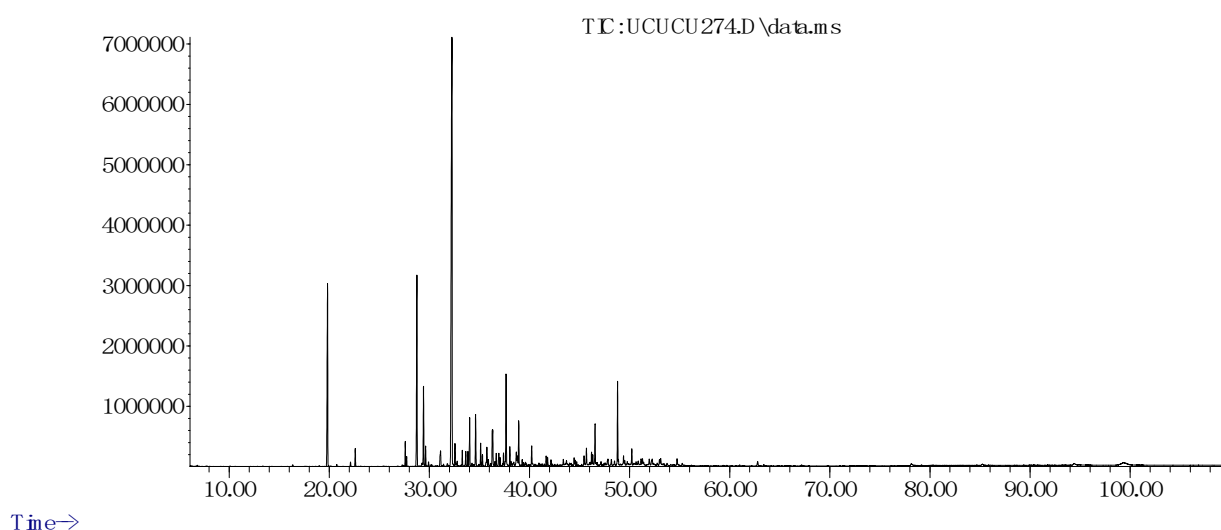
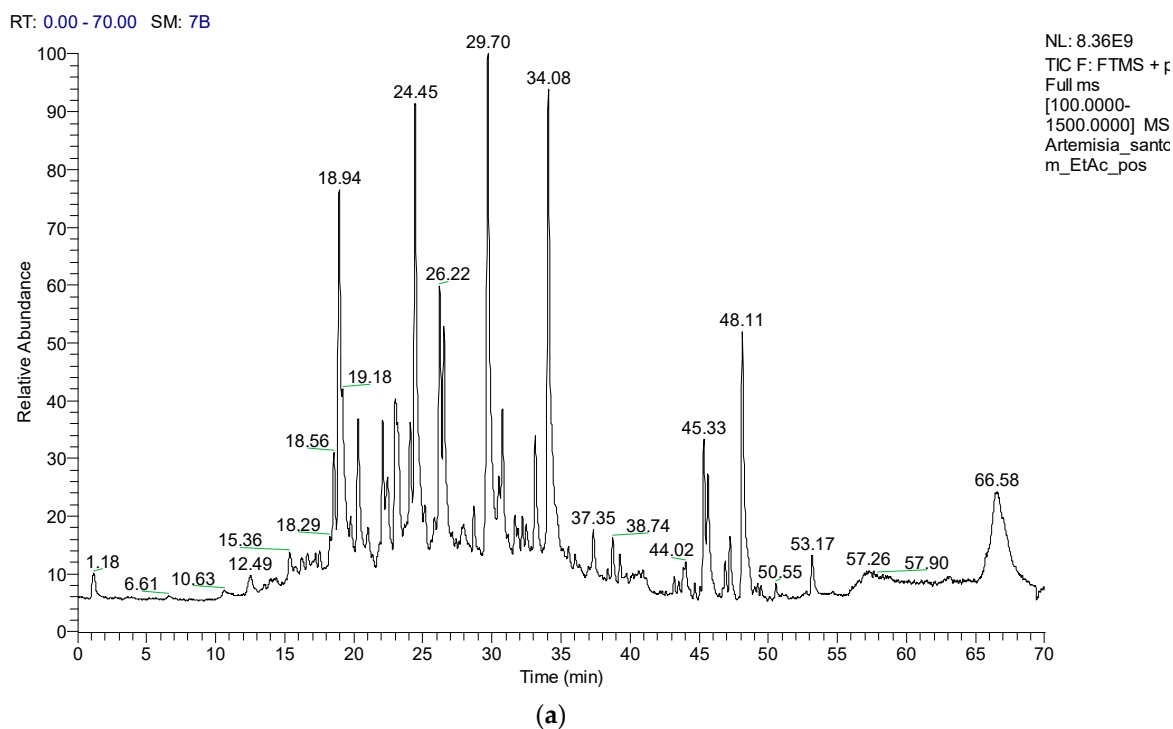


Figure S1. Total ion chromatogram of essential oil from *Artemisia santonicum*.



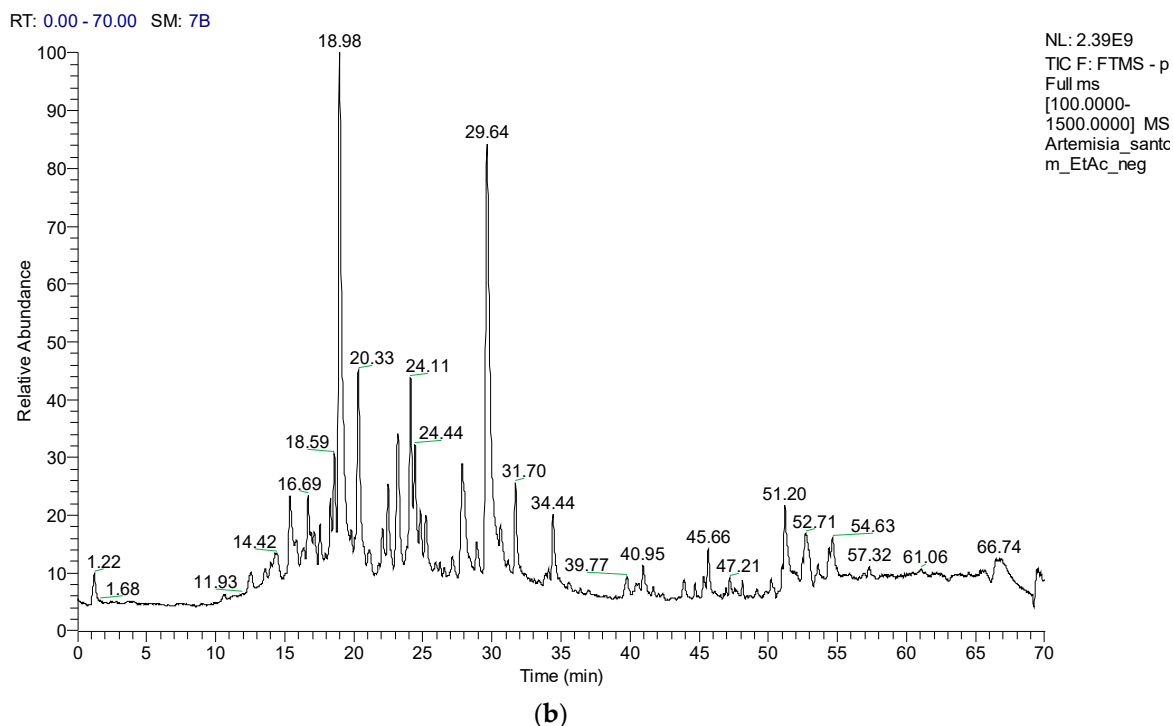
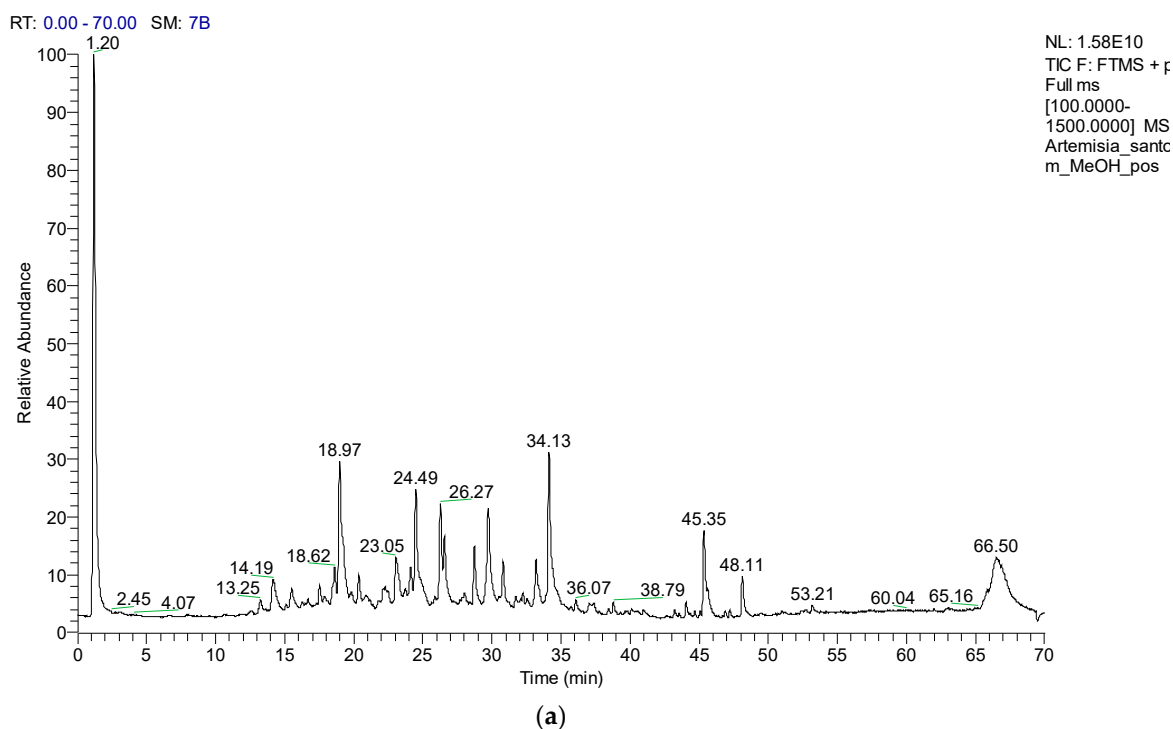


Figure S2. Chromatogram of the ethyl acetate extract from *Artemisia santonicum* in positive (a) and negative (b) mode.



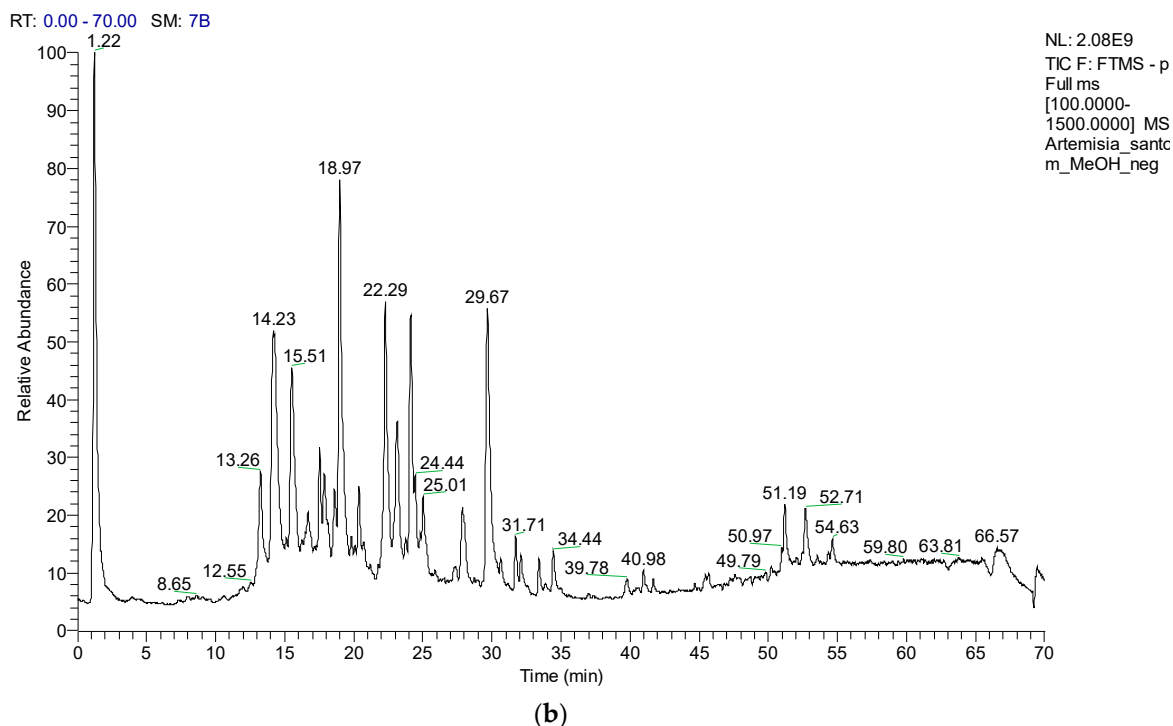
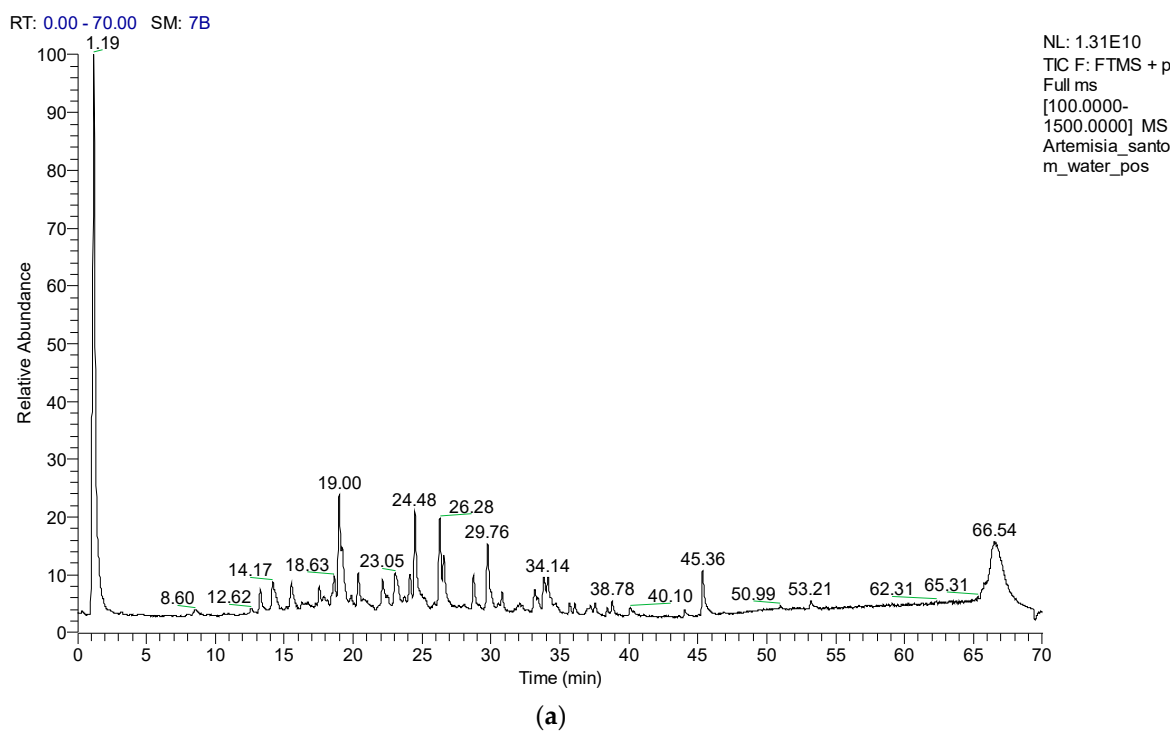


Figure S3. Chromatogram of the methanol extract from *Artemisia santonicum* in positive (a) and negative (b) mode.



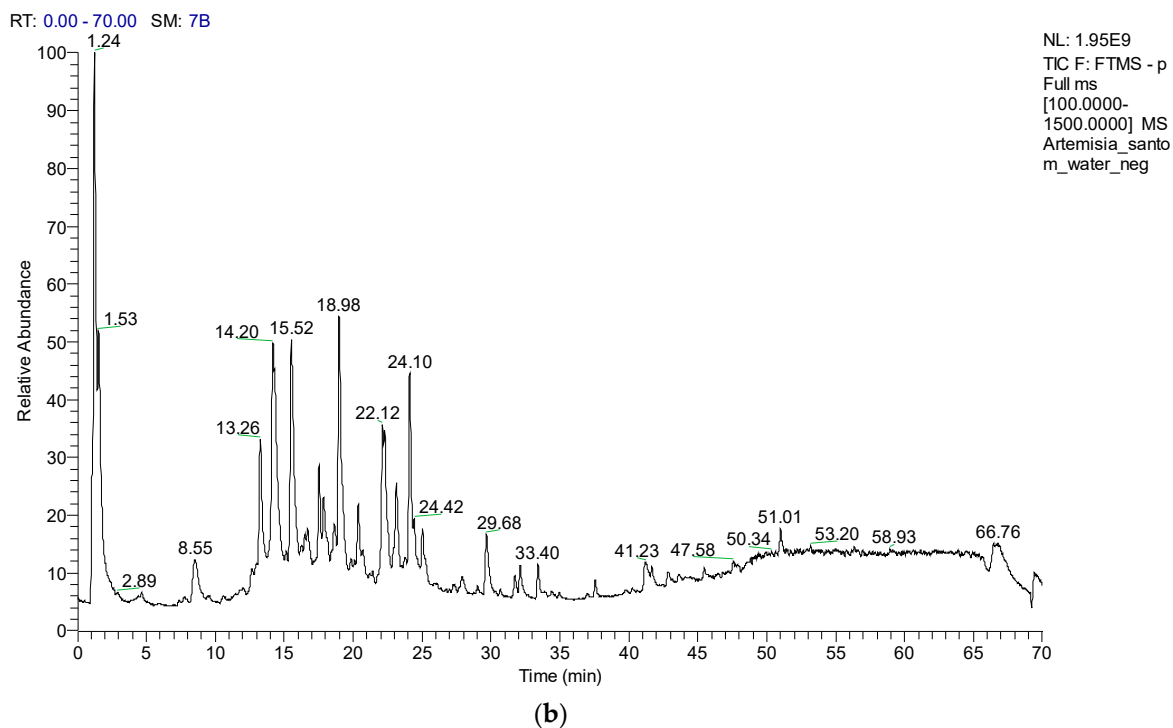


Figure S4. Chromatogram of the water extract from *Artemisia santonicum* in positive (a) and negative (b) mode.

Table S1. Chemical composition of ethyl acetate extract.

	Name	Formula	Rt	[M + H] ⁺	[M – H] [–]	Fragment 1	Fragment 2	Fragment 3	Fragment 4	Fragment 5
1 ¹	Chlorogenic acid (3-O-Caffeoylquinic acid)	C ₁₆ H ₁₈ O ₉	14.23	355.10291		163.0389	145.0284	135.0442	117.0337	89.0388
2	Caffeic acid	C ₉ H ₈ O ₄	14.27		179.03444	135.0439	107.0491			
3 ¹	Vanillin	C ₈ H ₈ O ₃	15.42	153.05517		125.0598	111.0443	93.0339	65.0392	
4	Chryptochlorogenic acid (4-O-Caffeoylquinic acid)	C ₁₆ H ₁₈ O ₉	15.46	355.10291		163.0389	145.0285	135.0441	117.0338	89.0388
5	Fraxetin (7,8-Dihydroxy-6-methoxycoumarin)	C ₁₀ H ₈ O ₅	16.94	209.04500		194.0210	181.0497	163.0391	149.0233	135.0443
6	Tuberonic acid glucoside	C ₁₈ H ₂₈ O ₉	17.50		387.16551	207.1021	163.1119	101.0230	89.0229	59.0123
7	5-O-Feruloylquinic acid	C ₁₇ H ₂₀ O ₉	17.91		367.10291	193.0501	191.0555	173.0445	134.0361	93.0331
8	Scopoletin (7-Hydroxy-6-methoxycoumarin)	C ₁₀ H ₈ O ₄	18.41	193.05009		178.0260	165.0544	149.0598	137.0597	133.0285
9	Unidentified terpene	C ₁₅ H ₂₀ O ₃	18.94	249.14908		231.1378	203.1431	185.1326	157.1012	
10	Isofraxidin (6,8-Dimethoxy-7-hydroxycoumarin)	C ₁₁ H ₁₀ O ₅	19.16		221.04500	206.0215	190.9980			
11 ¹	Taxifolin (Dihydroquercetin)	C ₁₅ H ₁₂ O ₇	19.22		303.05048	285.0409	217.0508	199.0390	175.0389	125.0230
12	Methoxy-pentahydroxy(iso)flavone-O-pentosylhexoside	C ₂₇ H ₃₀ O ₁₇	21.95		625.14047	330.0389	315.0150	287.0202		
13	Di-O-caffeoylquinic acid isomer 1	C ₂₅ H ₂₄ O ₁₂	22.27		515.11896	353.0880	191.0554	179.0340	173.0445	135.0439
14 ¹	Isoquercitrin (Hirsutrin, Quercetin-3-O-glucoside)	C ₂₁ H ₂₀ O ₁₂	22.83		463.08765	301.0358	300.0278	271.0255	255.0297	151.0027
15 ¹	Rutin (Quercetin-3-O-rutinoside)	C ₂₇ H ₃₀ O ₁₆	22.91	611.16122		465.1030	303.0499	129.0546	85.0284	71.0496
16	Methoxy-pentahydroxy(iso)flavone-O-hexoside	C ₂₂ H ₂₂ O ₁₃	23.08		493.09822	331.0462	330.0382	316.0226	315.0150	287.0199
17	Artemisin	C ₁₅ H ₁₈ O ₄	23.13	263.12834		245.1171	227.1064	217.1222		
18	Methoxy-pentahydroxy(iso)flavone-O-deoxyhexosylhexoside	C ₂₈ H ₃₂ O ₁₇	23.17		639.15613	331.0464	330.0383	316.0233	315.0151	287.0201
19	Methoxy-tetrahydroxy(iso)flavone-O-hexoside	C ₂₂ H ₂₂ O ₁₂	23.18		477.10330	315.0483	313.0351	300.0272	299.0189	
20	Di-O-caffeoylquinic acid isomer 2	C ₂₅ H ₂₄ O ₁₂	24.11		515.11896	353.0880	191.0554	179.0340	173.0445	135.0440
21	α-Santonin	C ₁₅ H ₁₈ O ₃	24.25	247.13342		201.1274	173.0961	158.0725	145.1013	135.0806
22 ¹	Isorhamnetin-3-O-glucoside	C ₂₂ H ₂₂ O ₁₂	24.81		477.10330	315.0519	314.0436	299.0203	285.0407	271.0255
23 ¹	Eriodictyol	C ₁₅ H ₁₂ O ₆	24.83		287.05556	151.0024	135.0439	125.0227	107.0124	83.0123
24	Dimethoxy-trihydroxy(iso)flavone-O-hexoside	C ₂₃ H ₂₄ O ₁₂	24.84	493.13461		331.0811	316.0577	301.0356		
25	Isorhamnetin-3-O-rutinoside (Narcissin)	C ₂₈ H ₃₂ O ₁₆	25.13		623.16122	315.0517	314.0428	300.0263	299.0201	271.0250
26 ¹	Quercetin	C ₁₅ H ₁₀ O ₇	26.90		301.03483	273.0411	178.9977	151.0024	121.0281	107.0124
27	Methoxy-pentahydroxy(iso)flavone	C ₁₆ H ₁₂ O ₈	26.98		331.04540	316.0225	209.0076	181.0138	165.9897	
28 ¹	Naringenin	C ₁₅ H ₁₂ O ₅	27.12		271.06065	227.0700	177.0186	165.0189	151.0025	119.0488
29	Homoeriodictyol (3'-Methoxy-4',5,7-trihydroxyflavanone)	C ₁₆ H ₁₄ O ₆	27.19		301.07122	151.0025	149.0596	134.0361	83.0123	

30 ¹	Luteolin (3',4',5,7-Tetrahydroxyflavone)	C ₁₅ H ₁₀ O ₆	27.74		285.03991	217.0497	199.0396	175.0391	151.0025	133.0283
31	Methoxy-tetrahydroxy(iso)flavone	C ₁₆ H ₁₂ O ₇	27.86		315.05048	300.0277	243.0298	227.0341		
32	Dimethoxy-tetrahydroxy(iso)flavone	C ₁₇ H ₁₄ O ₈	28.00		345.06105	330.0382	315.0149	287.0200		
33 ¹	Apigenin (4',5,7-Trihydroxyflavone)	C ₁₅ H ₁₀ O ₅	29.55		269.04500	225.0552	201.0550	151.0025	149.0232	117.0331
34	Chrysoeriol (Scoparol, 3'-Methoxy-4',5,7-trihydroxyflavone)	C ₁₆ H ₁₂ O ₆	29.66		299.05556	284.0329	256.0372	227.0338		
35	Dimethoxy-trihydroxy(iso)flavone	C ₁₇ H ₁₄ O ₇	29.83		329.06613	314.0435	313.0356	299.0200	285.0407	271.0252
36	Trihydroxy-trimethoxy(iso)flavone	C ₁₈ H ₁₆ O ₈	30.60	361.09235		346.0681	345.0602	331.0441		
37	Dihydroxy-dimethoxy(iso)flavone isomer 1	C ₁₇ H ₁₄ O ₆	31.15		313.07122	298.0483	297.0403	283.0250	269.0456	255.0296
38	Dihydroxy-trimethoxy(iso)flavone	C ₁₈ H ₁₆ O ₇	31.66	345.09743		330.0732	315.0496	287.0541		
39	Dihydroxy-dimethoxy(iso)flavone isomer 2	C ₁₇ H ₁₄ O ₆	31.67		313.07122	298.0484	297.0407	283.0251	269.0462	255.0301
40	Pinocembrin (5,7-Dihydroxyflavanone)	C ₁₅ H ₁₂ O ₄	32.14		255.06573	213.0535	151.0025	145.0649	107.0125	83.0124
41	Dihydroxy-tetramethoxy(iso)flavone	C ₁₉ H ₁₈ O ₈	32.41	375.10800		360.0837	345.0598	299.0548		
42	Dihydroxy-dimethoxy(iso)flavone isomer 3	C ₁₇ H ₁₄ O ₆	33.90		313.07122	298.0485	297.0391	283.0251	269.0461	255.0299
43	Dihydroxy-dimethoxy(iso)flavone isomer 4	C ₁₇ H ₁₄ O ₆	34.30		313.07122	298.0485	297.0387	283.0249	255.0296	
44	Genkwanin (Puddumetin, Apigenin-7-O-methyl ether)	C ₁₆ H ₁₂ O ₅	34.38	285.07630		270.0521	242.0573	225.0544	197.0596	167.0339
45	Dimethoxy-hydroxy(iso)flavone	C ₁₇ H ₁₄ O ₅	38.03	299.09195		284.0678	256.0727			

¹ Confirmed by standard

Table S2. Chemical composition of methanol extract.

No.	Name	Formula	Rt	[M + H] ⁺	[M – H] [–]	Fragment 1	Fragment 2	Fragment 3	Fragment 4	Fragment 5
1	Neochlorogenic acid (5-O-Caffeoylquinic acid)	C ₁₆ H ₁₈ O ₉	8.65	355.10291		163.0390	145.0285	135.0443	117.0337	89.0390
2	Syringic acid glucoside isomer 1	C ₁₅ H ₂₀ O ₁₀	10.28		359.09783	197.0450	182.0214	153.0545	138.0311	123.0073
3	Syringic acid glucoside isomer 2	C ₁₅ H ₂₀ O ₁₀	10.58		359.09783	197.0449	182.0213	153.0546	138.0310	123.0074
4	Dihydroxycoumarin-O-hexoside	C ₁₅ H ₁₆ O ₉	12.07	341.08726		179.0340	151.0392	135.0443	133.0286	123.0443
5	Dihydroxycoumarin isomer 1	C ₉ H ₆ O ₄	13.86	179.03444		151.0389	135.0445	133.0286	123.0442	
6 ¹	Chlorogenic acid (3-O-Caffeoylquinic acid)	C ₁₆ H ₁₈ O ₉	14.15	355.10291		163.0389	145.0285	135.0442	117.0337	89.0388
7	Dihydroxycoumarin isomer 2	C ₉ H ₆ O ₄	14.28	179.03444		151.0389	135.0440	133.0286	123.0443	105.0340
8	Caffeic acid	C ₉ H ₈ O ₄	14.30		179.03444	135.0439	107.0489			
9	Methylcoumarin	C ₁₀ H ₈ O ₂	15.13	161.06026		133.0650	115.0546	105.0703	103.0547	91.0547
10 ¹	Vanillin	C ₈ H ₈ O ₃	15.43	153.05517		125.0599	111.0444	93.0340	65.0393	
11	Chryptochlorogenic acid (4-O-Caffeoylquinic acid)	C ₁₆ H ₁₈ O ₉	15.50	355.10291		163.0389	145.0285	135.0442	117.0337	89.0390
12	Naringenin-6,8-di-C-glucoside	C ₂₇ H ₃₂ O ₁₅	16.87		595.16630	475.1268	415.1013	385.0919	355.0827	

13	Fraxetin (7,8-Dihydroxy-6-methoxycoumarin)	C ₁₀ H ₈ O ₅	16.99	209.04500	194.0214	181.0497	163.0392	149.0235	135.0441
14	Tuberonic acid glucoside	C ₁₈ H ₂₈ O ₉	17.52	387.16551	207.1022	163.1121	101.0231	89.0229	59.0123
15	5-O-Feruloylquinic acid	C ₁₇ H ₂₀ O ₉	17.90	367.10291	193.0500	191.0555	173.0445	134.0362	93.0331
16	Scopoletin (7-Hydroxy-6-methoxycoumarin)	C ₁₀ H ₈ O ₄	18.45	193.05009	178.0263	165.0549	149.0596	137.0597	133.0286
17	Hexosyl-2-coumarate	C ₁₅ H ₁₈ O ₈	18.75	325.09235	163.0389	119.0488	71.0124		
18	Vicenin-2 (Apigenin-6,8-di-C-glucoside)	C ₂₇ H ₃₀ O ₁₅	18.92	593.15065	503.1197	473.1097	383.0775	353.0672	297.0769
19	Unidentified terpene	C ₁₅ H ₂₀ O ₃	18.97	249.14908	231.1380	203.1433	185.1327	157.1012	
20	Isofraxidin (6,8-Dimethoxy-7-hydroxycoumarin)	C ₁₁ H ₁₀ O ₅	19.18	221.04500	206.0216	190.9980			
21 ¹	Taxifolin (Dihydroquercetin)	C ₁₅ H ₁₂ O ₇	19.22	303.05048	285.0410	217.0495	199.0397	175.0388	125.0231
22	Caffeoyl-syringoylglucose isomer 1	C ₂₄ H ₂₆ O ₁₃	19.72	521.12952	323.0776	221.0440	179.0341	161.0232	153.0546
23	Apigenin-C-hexoside-C-pentoside isomer 1	C ₂₆ H ₂₈ O ₁₄	19.97	563.14009	503.1164	473.1078	443.0949	383.0776	353.0672
24	Apigenin-C-hexoside-C-pentoside isomer 2	C ₂₆ H ₂₈ O ₁₄	20.26	563.14009	503.1201	473.1092	443.0980	383.0778	353.0671
25	Caffeoyl-syringoylglucose isomer 2	C ₂₄ H ₂₆ O ₁₃	20.53	521.12952	323.0775	221.0450	179.0340	161.0232	135.0439
26	Apigenin-C-hexoside-C-pentoside isomer 3	C ₂₆ H ₂₈ O ₁₄	20.63	563.14009	473.1083	443.0987	383.0774	353.0669	297.0771
27	Feruloylpentose	C ₁₅ H ₁₈ O ₈	20.74	325.09235	193.0500	149.0597	134.0361	117.0332	
28	Caffeoyl-syringoylglucose isomer 3	C ₂₄ H ₂₆ O ₁₃	21.36	521.12952	323.0775	221.0458	182.0214	179.0342	161.0233
29	Quercetin-O-pentosylhexoside	C ₂₆ H ₂₈ O ₁₆	21.70	595.12991	301.0355	300.0278	271.0253	255.0298	
30	Luteolin-O-pentosylhexoside	C ₂₆ H ₂₈ O ₁₅	21.79	579.13500	285.0407	284.0332	175.0390	151.0025	
31	Methoxy-pentahydroxy(iso)flavone-O-pentosylhexoside	C ₂₇ H ₃₀ O ₁₇	21.98	625.14047	330.0384	315.0151	287.0202		
32	Isovitexin (Avroside, Homovitexin, Saponaretin, Apigenin-6-C-glucoside)	C ₂₁ H ₂₀ O ₁₀	22.21	433.11348	415.1024	397.0919	337.0704	313.0705	283.0602
33	Di-O-caffeoylquinic acid isomer 1	C ₂₅ H ₂₄ O ₁₂	22.29	515.11896	353.0880	191.0555	179.0341	173.0447	135.0440
34 ¹	Isoquercitrin (Hirsutrin, Quercetin-3-O-glucoside)	C ₂₁ H ₂₀ O ₁₂	22.86	463.08765	301.0357	300.0277	271.0252	255.0301	151.0025
35 ¹	Rutin (Quercetin-3-O-rutinoside)	C ₂₇ H ₃₀ O ₁₆	22.95	611.16122	465.1035	303.0500	129.0550	85.0290	71.0498
36	Methoxy-pentahydroxy(iso)flavone-O-hexoside	C ₂₂ H ₂₂ O ₁₃	23.09	493.09822	331.0464	330.0383	316.0224	315.0151	287.0198
37	Artemisin	C ₁₅ H ₁₈ O ₄	23.17	263.12834	245.1173	227.1069	217.1224		
38	Methoxy-pentahydroxy(iso)flavone-O-deoxyhexosylhexoside	C ₂₈ H ₃₂ O ₁₇	23.19	639.15613	331.0463	330.0383	316.0223	315.0152	287.0198
39	Methoxy-tetrahydroxy(iso)flavone-O-hexoside	C ₂₂ H ₂₂ O ₁₂	23.19	477.10330	315.0453	313.0349	300.0279	299.0197	
40	Caffeoyl-feruloylquinic acid isomer 1	C ₂₆ H ₂₆ O ₁₂	23.76	529.13461	367.1033	353.0887	193.0501	179.0341	173.0446
41	Caffeoyl-feruloylquinic acid isomer 2	C ₂₆ H ₂₆ O ₁₂	23.99	529.13461	367.1035	353.0879	193.0499	179.0344	173.0445
42	Di-O-caffeoylquinic acid isomer 2	C ₂₅ H ₂₄ O ₁₂	24.10	515.11896	353.0879	191.0553	179.0340	173.0445	135.0439

43	Caffeoyl-feruloylquinic acid isomer 3	C ₂₆ H ₂₆ O ₁₂	24.24		529.13461	367.1034	353.0876	193.0499	179.0340	173.0445
44	α-Santonin	C ₁₅ H ₁₈ O ₃	24.49	247.13342		201.1275	173.0961	158.0726	145.1012	135.0806
45	Caffeoyl-feruloylquinic acid isomer 4	C ₂₆ H ₂₆ O ₁₂	24.50		529.13461	367.1033	353.0881	193.0500	179.0340	173.0446
46	Tetrahydroxyflavone-O-deoxyhexosylhexoside	C ₂₇ H ₃₀ O ₁₅	24.78		593.15065	285.0408	284.0329	255.0300	227.0345	
47 ¹	Isorhamnetin-3-O-glucoside	C ₂₂ H ₂₂ O ₁₂	24.82		477.10330	315.0508	314.0436	299.0200	285.0409	271.0251
48 ¹	Eriodictyol	C ₁₅ H ₁₂ O ₆	24.84		287.05556	151.0025	135.0439	125.0230	107.0125	83.0123
49	Dimethoxy-trihydroxy(iso)flavone-O-hexoside	C ₂₃ H ₂₄ O ₁₂	24.89	493.13461		331.0812	316.0578	301.0337		
50	Isorhamnetin-3-O-rutinoside (Narcissin)	C ₂₈ H ₃₂ O ₁₆	25.14		623.16122	315.0515	314.0438	300.0278	299.0200	271.0250
51	Dimethoxy-tetrahydroxy(iso)flavone-O-deoxyhexosylhexoside	C ₂₉ H ₃₄ O ₁₇	25.26		653.17177	345.0619	344.0541	330.0376	301.0358	287.0209
52	Caffeoyl-feruloylquinic acid isomer 5	C ₂₆ H ₂₆ O ₁₂	25.67		529.13461	367.1033	353.0879	193.0499	179.0340	173.0445
53	Caffeoyl-feruloylquinic acid isomer 6	C ₂₆ H ₂₆ O ₁₂	25.90		529.13461	367.1035	353.0880	193.0500	179.0340	173.0445
54	Caffeoyl-feruloylquinic acid isomer 7	C ₂₆ H ₂₆ O ₁₂	26.46		529.13461	367.1035	353.0880	193.0501	179.0340	173.0445
55 ¹	Quercetin	C ₁₅ H ₁₀ O ₇	26.91		301.03483	273.0405	178.9976	151.0025	121.0281	107.0124
56	Methoxy-pentahydroxy(iso)flavone	C ₁₆ H ₁₂ O ₈	27.00		331.04540	316.0226	209.0093	181.0134	165.9896	
57 ¹	Naringenin	C ₁₅ H ₁₂ O ₅	27.15		271.06065	227.0702	177.0183	165.0178	151.0025	119.0488
58	Homoeriodictyol (3'-Methoxy-4',5,7-trihydroxyflavanone)	C ₁₆ H ₁₄ O ₆	27.22		301.07122	151.0025	149.0596	134.0361	83.0123	
59 ¹	Luteolin (3',4',5,7-Tetrahydroxyflavone)	C ₁₅ H ₁₀ O ₆	27.76		285.03991	217.0504	199.0400	175.0391	151.0024	133.0282
60	Methoxy-tetrahydroxy(iso)flavone	C ₁₆ H ₁₂ O ₇	27.88		315.05048	300.0278	243.0288	227.0352		
61	Dimethoxy-tetrahydroxy(iso)flavone	C ₁₇ H ₁₄ O ₈	28.03		345.06105	330.0384	315.0151	287.0202		
62 ¹	Apigenin (4',5,7-Trihydroxyflavone)	C ₁₅ H ₁₀ O ₅	29.58		269.04500	225.0549	201.0551	151.0025	149.0233	117.0332
63	Chrysoeriol (Scoparol, 3'-Methoxy-4',5,7-trihydroxyflavone)	C ₁₆ H ₁₂ O ₆	29.70		299.05556	284.0329	256.0380	227.0342		
64	Dimethoxy-trihydroxy(iso)flavone	C ₁₇ H ₁₄ O ₇	29.86		329.06613	314.0436	313.0353	299.0199	285.0409	271.0252
65	Trihydroxy-trimethoxy(iso)flavone	C ₁₈ H ₁₆ O ₈	30.64	361.09235		346.0683	345.0606	331.0446		
66	Dihydroxy-dimethoxy(iso)flavone isomer 1	C ₁₇ H ₁₄ O ₆	31.18		313.07122	298.0486	297.0406	283.0251	269.0451	255.0296
67	Dihydroxy-dimethoxy(iso)flavone isomer 2	C ₁₇ H ₁₄ O ₆	31.69		313.07122	298.0485	297.0406	283.0251	269.0459	255.0297
68	Dihydroxy-trimethoxy(iso)flavone	C ₁₈ H ₁₆ O ₇	31.71	345.09743		330.0733	315.0494	287.0543		
69	Pinocembrin (5,7-Dihydroxyflavanone)	C ₁₅ H ₁₂ O ₄	32.15		255.06573	213.0535	151.0025	145.0649	107.0125	83.0124
70	Dihydroxy-tetramethoxy(iso)flavone	C ₁₉ H ₁₈ O ₈	32.45	375.10800		360.0842	345.0601	299.0555		
71	Dihydroxy-dimethoxy(iso)flavone isomer 3	C ₁₇ H ₁₄ O ₆	33.91		313.07122	298.0486	297.0414	283.0251	269.0472	255.0300
72	Dihydroxy-dimethoxy(iso)flavone isomer 4	C ₁₇ H ₁₄ O ₆	34.32		313.07122	298.0485	297.0395	283.0252	255.0298	
73	Genkwanin (Puddumetin, Apigenin-7-O-methyl ether)	C ₁₆ H ₁₂ O ₅	34.44	285.07630		270.0521	242.0573	225.0560	197.0604	167.0340
74	Dimethoxy-hydroxy(iso)flavone	C ₁₇ H ₁₄ O ₅	38.09	299.09195		284.0679	256.0730			

¹ Confirmed by standard**Table S3.** Chemical composition of water extract.

No.	Name	Formula	Rt	[M + H] ⁺	[M – H] [–]	Fragment 1	Fragment 2	Fragment 3	Fragment 4	Fragment 5
1	Neochlorogenic acid (5-O-Caffeoylquinic acid)	C ₁₆ H ₁₈ O ₉	8.57	355.10291		163.0390	145.0285	135.0442	117.0337	89.0390
2	Syringic acid glucoside	C ₁₅ H ₂₀ O ₁₀	10.57		359.09783	197.0450	182.0213	153.0546	138.0311	123.0074
3	Dihydroxycoumarin-O-hexoside	C ₁₅ H ₁₆ O ₉	12.09	341.08726		179.0340	151.0392	135.0443	133.0286	123.0442
4	Dihydroxycoumarin isomer 1	C ₉ H ₆ O ₄	13.89	179.03444		151.0392	135.0443	133.0286	123.0443	
5 ¹	Chlorogenic acid (3-O-Caffeoylquinic acid)	C ₁₆ H ₁₈ O ₉	14.15	355.10291		163.0390	145.0285	135.0443	117.0338	89.0389
6	Dihydroxycoumarin isomer 2	C ₉ H ₆ O ₄	14.25	179.03444		151.0389	135.0440	133.0286	123.0443	105.0340
7	Caffeic acid	C ₉ H ₈ O ₄	14.32		179.03444	135.0440	107.0490			
8	Methylcoumarin	C ₁₀ H ₈ O ₂	15.15	161.06026		133.0650	115.0544	105.0703	103.0547	91.0548
9 ¹	Vanillin	C ₈ H ₈ O ₃	15.46	153.05517		125.0599	111.0444	93.0340	65.0393	
10	Chryptochlorogenic acid (4-O-Caffeoylquinic acid)	C ₁₆ H ₁₈ O ₉	15.51	355.10291		163.0390	145.0285	135.0443	117.0337	89.0389
11	Fraxetin (7,8-Dihydroxy-6-methoxycoumarin)	C ₁₀ H ₈ O ₅	16.99	209.04500		194.0212	181.0503	163.0390	149.0234	135.0442
12	Tuberonic acid glucoside	C ₁₈ H ₂₈ O ₉	17.52		387.16551	207.1025	163.1118	101.0230	89.0229	59.0123
13	5-O-Feruloylquinic acid	C ₁₇ H ₂₀ O ₉	17.90		367.10291	193.0499	191.0555	173.0445	134.0362	93.0331
14	4-O-Feruloylquinic acid	C ₁₇ H ₂₀ O ₉	18.43		367.10291	193.0501	191.0557	173.0447	134.0362	93.0331
15	Scopoletin (7-Hydroxy-6-methoxycoumarin)	C ₁₀ H ₈ O ₄	18.45	193.05009		178.0263	165.0547	149.0595	137.0599	133.0286
16	Hexosyl-2-coumarate	C ₁₅ H ₁₈ O ₈	18.76		325.09235	163.0390	119.0489	71.0124		
17	Vicenin-2 (Apigenin-6,8-di-C-glucoside)	C ₂₇ H ₃₀ O ₁₅	18.92		593.15065	503.1202	473.1103	383.0775	353.0670	297.0771
18	Unidentified terpene	C ₁₅ H ₂₀ O ₃	19.00	249.14908		231.1380	203.1433	185.1327	157.1012	
19	Isofraxidin (6,8-Dimethoxy-7-hydroxycoumarin)	C ₁₁ H ₁₀ O ₅	19.19		221.04500	206.0216	190.9980			
20	Caffeoyl-syringoylglucose isomer 1	C ₂₄ H ₂₆ O ₁₃	19.72		521.12952	323.0776	221.0449	179.0340	161.0233	153.0545
21	Apigenin-C-hexoside-C-pentoside isomer 1	C ₂₆ H ₂₈ O ₁₄	19.98		563.14009	503.1212	473.1082	443.0979	383.0778	353.0674
22	Apigenin-C-hexoside-C-pentoside isomer 2	C ₂₆ H ₂₈ O ₁₄	20.26		563.14009	503.1214	473.1114	443.0987	383.0777	353.0671
23	Caffeoyl-syringoylglucose isomer 2	C ₂₄ H ₂₆ O ₁₃	20.54		521.12952	323.0780	221.0451	179.0341	161.0234	135.0440
24	Apigenin-C-hexoside-C-pentoside isomer 3	C ₂₆ H ₂₈ O ₁₄	20.65		563.14009	503.1216	473.1086	443.0984	383.0776	353.0671
25	Feruloylpentose	C ₁₅ H ₁₈ O ₈	20.73		325.09235	193.0500	149.0596	134.0361	117.0332	
26	Caffeoyl-syringoylglucose isomer 3	C ₂₄ H ₂₆ O ₁₃	21.37		521.12952	323.0777	221.0452	182.0214	179.0342	161.0233
27	Quercetin-O-pentosylhexoside	C ₂₆ H ₂₈ O ₁₆	21.70		595.12991	301.0362	300.0279	271.0250	255.0300	
28	Luteolin-O-pentosylhexoside	C ₂₆ H ₂₈ O ₁₅	21.80		579.13500	285.0409	284.0320	175.0394	151.0024	
29	Methoxy-pentahydroxy(iso)flavone-O-pentosylhexoside	C ₂₇ H ₃₀ O ₁₇	21.98		625.14047	330.0383	315.0151	287.0203		
30	Isovitexin (Avroside, Homovitexin, Saponaretin, Apigenin-6-C-glucoside)	C ₂₁ H ₂₀ O ₁₀	22.22	433.11348		415.1028	397.0917	337.0707	313.0708	283.0602

31	Di-O-caffeoylquinic acid isomer 1	C ₂₅ H ₂₄ O ₁₂	22.26		515.11896	353.0881	191.0555	179.0341	173.0446	135.0440
32 ¹	Isoquercitrin (Hirsutrin, Quercetin-3-O-glucoside)	C ₂₁ H ₂₀ O ₁₂	22.86		463.08765	301.0356	300.0278	271.0251	255.0299	151.0026
33 ¹	Rutin (Quercetin-3-O-rutinoside)	C ₂₇ H ₃₀ O ₁₆	22.95	611.16122		465.1014	303.0499	129.0549	85.0290	71.0498
34	Methoxy-pentahydroxy(iso)flavone-O-hexoside	C ₂₂ H ₂₂ O ₁₃	23.10		493.09822	331.0462	330.0385	316.0224	315.0151	287.0203
35	Methoxy-tetrahydroxy(iso)flavone-O-hexoside	C ₂₂ H ₂₂ O ₁₂	23.14		477.10330	315.0513	313.0361	300.0281	299.0201	
36	Artemisin	C ₁₅ H ₁₈ O ₄	23.17	263.12834		245.1173	227.1067	217.1223		
37	Methoxy-pentahydroxy(iso)flavone-O-deoxyhexosylhexoside	C ₂₈ H ₃₂ O ₁₇	23.19		639.15613	331.0465	330.0385	316.0228	315.0154	287.0201
38	Caffeoyl-feruloylquinic acid isomer 1	C ₂₆ H ₂₆ O ₁₂	23.74		529.13461	367.1039	353.0881	193.0500	179.0342	173.0446
39	Caffeoyl-feruloylquinic acid isomer 2	C ₂₆ H ₂₆ O ₁₂	23.89		529.13461	367.1034	353.0867	193.0500	179.0341	173.0445
40	Di-O-caffeoylquinic acid isomer 2	C ₂₅ H ₂₄ O ₁₂	24.10		515.11896	353.0882	191.0555	179.0341	173.0445	135.0440
41	Caffeoyl-feruloylquinic acid isomer 3	C ₂₆ H ₂₆ O ₁₂	24.25		529.13461	367.1035	353.0883	193.0501	179.0340	173.0446
42	α -Santonin	C ₁₅ H ₁₈ O ₃	24.50	247.13342		201.1276	173.0963	158.0727	145.1014	135.0807
43	Tetrahydroxyflavone-O-deoxyhexosylhexoside	C ₂₇ H ₃₀ O ₁₅	24.78		593.15065	285.0408	284.0331	255.0299	227.0346	
44 ¹	Isorhamnetin-3-O-glucoside	C ₂₂ H ₂₂ O ₁₂	24.83		477.10330	315.0505	314.0437	299.0203	285.0412	271.0252
45 ¹	Eriodictyol	C ₁₅ H ₁₂ O ₆	24.84		287.05556	151.0025	135.0440	125.0229	107.0125	83.0123
46	Dimethoxy-trihydroxy(iso)flavone-O-hexoside	C ₂₃ H ₂₄ O ₁₂	24.90	493.13461		331.0812	316.0579	301.0349		
47	Isorhamnetin-3-O-rutinoside (Narcissin)	C ₂₈ H ₃₂ O ₁₆	25.14		623.16122	315.0515	314.0434	300.0280	299.0201	271.0251
48	Dimethoxy-tetrahydroxy(iso)flavone-O-deoxyhexosylhexoside	C ₂₉ H ₃₄ O ₁₇	25.27		653.17177	345.0616	344.0540	330.0382	301.0367	287.0187
49	Caffeoyl-feruloylquinic acid isomer 4	C ₂₆ H ₂₆ O ₁₂	25.70		529.13461	367.1037	353.0902	193.0501	179.0341	173.0446
50	Caffeoyl-feruloylquinic acid isomer 5	C ₂₆ H ₂₆ O ₁₂	25.90		529.13461	367.1035	353.0883	193.0500	179.0341	173.0446
51 ¹	Quercetin	C ₁₅ H ₁₀ O ₇	26.92		301.03483	273.0405	178.9975	151.0024	121.0282	107.0122
52	Methoxy-pentahydroxy(iso)flavone	C ₁₆ H ₁₂ O ₈	27.01		331.04540	316.0229	209.0093	181.0134	165.9896	
53 ¹	Naringenin	C ₁₅ H ₁₂ O ₅	27.15		271.06065	227.0702	177.0185	165.0182	151.0025	119.0489
54	Homoeriodictyol (3'-Methoxy-4',5,7-trihydroxyflavanone)	C ₁₆ H ₁₄ O ₆	27.23		301.07122	151.0025	149.0595	134.0361	83.0123	
55 ¹	Luteolin (3',4',5,7-Tetrahydroxyflavone)	C ₁₅ H ₁₀ O ₆	27.77		285.03991	217.0494	199.0393	175.0392	151.0026	133.0283
56	Methoxy-tetrahydroxy(iso)flavone	C ₁₆ H ₁₂ O ₇	27.89		315.05048	300.0279	243.0302	227.0344		
57	Dimethoxy-tetrahydroxy(iso)flavone	C ₁₇ H ₁₄ O ₈	28.03		345.06105	330.0384	315.0151	287.0201		
58 ¹	Apigenin (4',5,7-Trihydroxyflavone)	C ₁₅ H ₁₀ O ₅	29.59		269.04500	225.0554	201.0549	151.0025	149.0234	117.0332
59	Chrysoeriol (Scoparol, 3'-Methoxy-4',5,7-trihydroxyflavone)	C ₁₆ H ₁₂ O ₆	29.70		299.05556	284.0330	256.0371	227.0347		
60	Dimethoxy-trihydroxy(iso)flavone	C ₁₇ H ₁₄ O ₇	29.86		329.06613	314.0437	313.0357	299.0200	285.0396	271.0250
61	Trihydroxy-trimethoxy(iso)flavone	C ₁₈ H ₁₆ O ₈	30.64	361.09235		346.0684	345.0606	331.0445		
62	Dihydroxy-dimethoxy(iso)flavone isomer 1	C ₁₇ H ₁₄ O ₆	31.19		313.07122	298.0487	297.0397	283.0251	269.0454	255.0286
63	Dihydroxy-dimethoxy(iso)flavone isomer 2	C ₁₇ H ₁₄ O ₆	31.70		313.07122	298.0485	297.0408	283.0252	269.0461	255.0300
64	Dihydroxy-trimethoxy(iso)flavone	C ₁₈ H ₁₆ O ₇	31.72	345.09743		330.0733	315.0504	287.0551		

65	Dihydroxy-dimethoxy(iso)flavone isomer 3	C ₁₇ H ₁₄ O ₆	33.92		313.07122	298.0486	297.0414	283.0250	269.0472	255.0300
66	Dihydroxy-dimethoxy(iso)flavone isomer 4	C ₁₇ H ₁₄ O ₆	34.33		313.07122	298.0490	297.0395	283.0252	255.0300	
67	Genkwanin (Puddumetin, Apigenin-7-O-methyl ether)	C ₁₆ H ₁₂ O ₅	34.46	285.07630		270.0524	242.0572	225.0549	197.0604	167.0335

¹ Confirmed by standard