

Characterization of the compounds in Negative mode

No.	Compound Name	Formula	Mass error (ppm)	Mass
1	Geniposide	C ₁₇ H ₂₄ O ₁₀	2.25	388.1369
2	Genipin	C ₁₁ H ₁₄ O ₅	1.22	226.0841
3	Nevadensin	C ₁₈ H ₁₆ O ₇	1.67	344.0896
4	Mannitol	C ₆ H ₁₄ O ₆	-1.12	182.079
5	Tiglyl tiglate	C ₁₀ H ₁₆ O ₂	4.45	168.115
6	6alpha-Hydroxygeniposide	C ₁₇ H ₂₄ O ₁₁	0.17	404.1319
7	Crocin	C ₄₄ H ₆₄ O ₂₄	2.48	976.3788
8	4'-Hydroxywogonin	C ₁₆ H ₁₂ O ₆	3.75	300.0634
9	Onopordin	C ₁₆ H ₁₂ O ₇	-2.73	316.0583
10	5,3'-Dihydroxy-6,7,4',5'-tetramethoxyflavone	C ₁₉ H ₁₈ O ₈	-4.97	374.1002
11	3',4',5'-Trihydroxywogonin	C ₁₆ H ₁₂ O ₈	0.9	332.0532
12	5,7,3',5'-Tetrahydroxy-8,4'-dimethoxyflavone	C ₁₇ H ₁₄ O ₈	2.86	346.0689
13	5,7,3'-Trihydroxy-8,4',5'-trimethoxyflavone	C ₁₈ H ₁₆ O ₈	-3.58	360.0845
14	Gardenin A	C ₂₁ H ₂₂ O ₉	0.28	418.1264
15	Ixoroside	C ₁₆ H ₂₄ O ₉	1.64	360.142
16	Gardoside	C ₁₆ H ₂₂ O ₁₀	0.03	374.1213
17	[1S-(1alpha,4aalpha,7aalpha)]-7- [(acetyloxy)methyl]-1-(beta-D- glucopyranosyloxy)-1,4a,5,7a- tetrahydrocyclopenta[c]pyran-4-carboxylic acid	C ₁₉ H ₂₆ O ₁₁	2.55	430.1475
18	Mussaenosidic acid	C ₁₆ H ₂₄ O ₁₀	0.78	376.1369
19	Shanzhiside	C ₁₆ H ₂₄ O ₁₁	1.75	392.1319
20	2-Hydroxyethyl gardenamide A	C ₁₃ H ₁₇ N O ₅	4.73	267.1107
21	6'-O-Sinapoyljasminoside C	C ₂₇ H ₃₄ O ₁₁	1.33	534.2101
22	Jasminodiol	C ₁₀ H ₁₆ O ₃	1.12	184.1099
23	Jasminoside A	C ₁₆ H ₂₆ O ₇	1.86	330.1679
24	Jasminoside B	C ₁₆ H ₂₆ O ₈	2.98	346.1628
25	Jasminoside I	C ₂₂ H ₃₆ O ₁₂	2.09	492.2207
26	Secaubryolide	C ₃₁ H ₄₄ O ₅	-3.26	496.3189
27	Gardaloside	C ₁₆ H ₂₂ O ₉	1.77	358.1264
28	Genipin-1-β-gentiobioside	C ₂₃ H ₃₄ O ₁₅	-0.36	550.1898
29	Scortechinone H	C ₃₄ H ₄₀ O ₈	-2.56	576.2723
30	Scortechinone P	C ₃₄ H ₄₂ O ₁₀	3.2	610.2778
31	Coronalolide	C ₃₀ H ₄₂ O ₅	-3.98	482.3032
32	Sootepin D	C ₃₁ H ₄₈ O ₄	-0.45	484.3553
33	Sootepdienone	C ₁₅ H ₂₂ O ₂	2.87	234.162
34	Methyl dihydrojasmonate	C ₁₃ H ₂₂ O ₃	3.2	226.1569
35	Methyl propyl disulfide	C ₄ H ₁₀ S ₂	-1.33	122.0224

Characterization of the compounds in Positive mode

No.	Compound Name	Formula	Mass error (ppm)	Mass
1	Geniposide	C ₁₇ H ₂₄ O ₁₀	0.35	388.1369
2	Genipin	C ₁₁ H ₁₄ O ₅	-1.64	226.0841
3	Nevadensin	C ₁₈ H ₁₆ O ₇	1.26	344.0896
4	Mannitol	C ₆ H ₁₄ O ₆	-0.53	182.079
5	Tiglyl tiglate	C ₁₀ H ₁₆ O ₂	-0.12	168.115
6	6alpha-Hydroxygeniposide	C ₁₇ H ₂₄ O ₁₁	-0.67	404.1319
7	Gardenin B	C ₁₉ H ₁₈ O ₇	-0.11	358.1053
8	Onopordin	C ₁₆ H ₁₂ O ₇	0.06	316.0583
9	5,3'-Dihydroxy-6,7,4',5'-tetramethoxyflavone	C ₁₉ H ₁₈ O ₈	0.55	374.1002
10	5-Hydroxy-7,2',3',4',5'-pentamethoxyflavone	C ₂₀ H ₂₀ O ₈	-0.19	388.1158
11	5,7,3'-Trihydroxy-8,4',5'-trimethoxyflavone	C ₁₈ H ₁₆ O ₈	1.27	360.0845
12	Gardenin C	C ₂₀ H ₂₀ O ₉	-1.87	404.1107
13	5,7,4'-Trihydroxy-3,6-dimethoxyflavone	C ₁₇ H ₁₄ O ₇	-0.4	330.074
14	Ixoroside	C ₁₆ H ₂₄ O ₉	1.9	360.142
15	Gardoside	C ₁₆ H ₂₂ O ₁₀	-1.19	374.1213
16	Mussaenosidic acid	C ₁₆ H ₂₄ O ₁₀	-2.53	376.1369
17	2-Hydroxyethyl gardenamide A	C ₁₃ H ₁₇ NO ₅	-0.98	267.1107
18	6'-O-Sinapoyljasminoside C	C ₂₇ H ₃₄ O ₁₁	0.54	534.2101
19	Jasminoside A	C ₁₆ H ₂₆ O ₇	-0.53	330.1679
20	Jasminoside B	C ₁₆ H ₂₆ O ₈	1.39	346.1628
21	Jasminoside I	C ₂₂ H ₃₆ O ₁₂	1.66	492.2207
22	Secaubrytriol	C ₃₀ H ₅₀ O ₅	1.58	490.3658
23	Genipin gentiobioside	C ₂₃ H ₃₄ O ₁₅	0.68	550.1898