

Nr	Compound class	Compound Name	Molecular formula	Retention time [min]	MS adducts	Progenesis Q1 fragmentation score	Characteristic fragments [m/z]
1	Benzoxazinoid	DHBOA-Glc	C ₁₄ H ₁₇ NO ₉	1.3	M-H, M+FA-H, 2M-H	16.5	180.0303, 162.0200
2	Benzoxazinoid	DIBOA-Glc	C ₁₄ H ₁₇ NO ₉	1.91	M-H, M+FA-H, 2M-H	2.6	180.0303, 162.0200, 134.0247
3	Benzoxazinoid	HMBOA-Glc	C ₁₅ H ₁₉ NO ₉	2.11	M-H, M+FA-H, 2M-H	10.3	194.0459, 166.0511
4	Benzoxazinoid	DIMBOA-Glc	C ₁₅ H ₁₉ NO ₁₀	2.18	M-H, M+FA-H, 2M-H	5.9	210.0406, 192.0302, 164.0356, 149.0119
5	Benzoxazinoid	DIM ₂ BOA-Glc	C ₁₆ H ₂₁ NO ₁₁	2.22	M-H, M+FA-H, 2M-H	21.7	222.0408, 194.0458
6	Benzoxazinoid	HMBOA	C ₉ H ₉ NO ₄	2.3	M-H	n/a	-
7	Benzoxazinoid	DIMBOA	C ₉ H ₉ NO ₅	2.42	M-H	n/a	164.0353, 149.0118
8	Benzoxazinoid	HDMBOA-Glc	C ₁₆ H ₂₁ NO ₁₀	2.74	M-H, M+FA-H, 2M-H	11.5	224.0564, 194.0460
9	Benzoxazinoid	HDM ₂ BOA-Glc	C ₁₇ H ₂₃ NO ₁₁	2.74	M+FA-H	n/a	254.0789
10	Organic acid	Chlorogenic acid	C ₁₆ H ₁₈ O ₉	1.77	M-H, 2M-H	24.3	191.0562
11	Organic acid	Feruloylglucose	C ₁₆ H ₂₀ O ₉	2.05	M-H	81	175.0404
12	Organic acid	Sinapoylglucose	C ₁₇ H ₂₂ O ₁₀	2.09	M-H	36.7	223.0615, 205.0507
13	Organic acid	Quinic acid	C ₁₇ H ₁₂ O ₆	0.33*	M-H, 2M-H	70.1	-
14	Organic acid	Coumaroylquinic acid isomer	C ₁₆ H ₁₈ O ₈	1.7	M-H	98	163.0409
15	Organic acid	Coumaroylquinic acid isomer	C ₁₆ H ₁₈ O ₈	2.13	M-H	51.6	191.0561, 173.0455
16	Organic acid	Feruloylquinic acid isomer	C ₁₇ H ₂₀ O ₉	2.35	M-H	46.1	191.0562
17	Organic acid	Feruloylquinic acid isomer	C ₁₇ H ₂₀ O ₉	2.61	M-H	n/a	-
18	Flavonol	Quercetin rhamnosylglucoside	C ₂₇ H ₃₀ O ₁₆	2.66	M-H	65.7	301.0353
19	Flavonol	Quercetin glucoside	C ₂₁ H ₂₀ O ₁₂	2.75	M-H	26	301.0347, 271.0252
20	Flavonol	Quercetin malonylglucoside	C ₂₄ H ₂₂ O ₁₅	2.91	M-H	75.1	505.0986, 301.0345
21	Flavonol	Kaempferol rhamnosylglucoside	C ₂₇ H ₃₀ O ₁₅	2.94	M-H	98.9	285.0412
22	Flavonol	Kaempferol glucoside	C ₂₁ H ₂₀ O ₁₁	3.04	M-H	88.6	285.0395, 255.0304
23	Flavonol	Kaempferol malonylglucoside	C ₂₄ H ₂₂ O ₁₄	3.25	M-H	96.5	489.1037, 285.0400
24	Amino acid	Leucine	C ₆ H ₁₃ NO ₂	0.8	M-H	n/a	-
25	Amino acid	Phenylalanine	C ₉ H ₁₁ NO ₂	1.1	M-H	n/a	-
26	Amino acid	Tryptophan	C ₁₁ H ₁₂ N ₂ O ₂	1.5	M-H, M+FA-H	n/a	-
27	Sugar	Monosaccharide	C ₆ H ₁₂ O ₆	0.31*	M-H	n/a	-
28	Sugar	Disaccharide	C ₁₂ H ₂₂ O ₁₁	0.34*	M-H, M+FA-H, 2M-H	3.2	-