

Table S2 UHPLC-ESI-MS/MS comparison of main leaf-sap profiles of five aquifolium cultivars, five *mesocroce* cultivars and reference commercial *isoparagossium* (Data).

No.	Compound name (RT [min])	Cdk. neutral formula	MS/MS fragments (proposed pathway)	MS/MS signature	Measured [M] ⁺ m/z	Err. [ppm]	Occurrence frequency	Max RA %	Average RA % ± SD	SD RA %	AM RA %	MS RA %	HP RA %	BP RA %	PS RA %	PA/MS RA %	Compound name (RT [min])	Cdk. neutral formula	MS/MS fragments (proposed pathway)	MS/MS signature	Measured [M] ⁺ m/z	Err. [ppm]	Occurrence frequency	Max RA %	Average RA % ± SD	SD RA %	AM RA %	MS RA %	HP RA %	BP RA %	PS RA %	PA/MS RA %									
																																	No.	Compound name (RT [min])	Cdk. neutral formula	MS/MS fragments (proposed pathway)	MS/MS signature	Measured [M] ⁺ m/z	Err. [ppm]	Occurrence frequency	Max RA %
1	1235.61, 6.05 min	C5H9O2	911 [M-HeHex-H] ⁺ 705 [M-HeHex-H] ⁺ 749 [M-HeHex-H] ⁺ 603 [M-HeHex-H] ⁺ 471 [M-HeHex-H] ⁺	MS/MS signature	471	1235.6103	-3.0	6	5.0	3.4 ± 0.9	4.1	3.9	5.0	3.0	3.2	1.4	91	1235.61, 9.97 min	C5H9O2	911 [M-HeHex-H] ⁺ 705 [M-HeHex-H] ⁺ 749 [M-HeHex-H] ⁺ 603 [M-HeHex-H] ⁺ 471 [M-HeHex-H] ⁺	MS/MS signature	471	1235.6103	-3.4	1	1.7	1.7 ± 0.0	—	—	—	—	—	—	1.7	—						
2	927.6, 6.08 min	C4H7O2	—	—	—	927.6075	-1.8	2	3.1	2.2 ± 0.9	—	1.3	3.1	—	—	—	—	92	909.9, 9.08 min	C4H7O2	—	—	—	909.9044	-2.2	6	23.7	6.0 ± 6.2	7.1	0.2	23.7	2.1	1.2	1.9	—						
3	1009.6, 6.09 min	C5H9O2	—	—	—	1009.6021	-3.1	3	4.9	2.6 ± 1.5	2.2	0.7	4.9	—	—	—	—	—	93	1009.6, 9.09 min	C5H9O2	—	—	—	1009.6021	-2.8	1	3.5	3.5 ± 0.0	—	—	—	—	—	3.5	—					
4	927.6, 6.17 min	C4H7O2	—	—	—	927.6000	-2.2	3	3.1	2.3 ± 0.5	—	—	2.4	1.5	3.1	—	—	—	94	927.6, 9.17 min	C4H7O2	—	—	—	927.6000	-4.0	5	1.6	0.9 ± 0.5	1.1	0.3	—	1.6	1.1	0.2	—					
5	1009.6, 6.27 min	C5H9O2	—	—	—	1009.5332	-1.0	1	3.8	3.8 ± 0.0	—	—	3.8	—	—	—	—	—	95	979.3, 10.1 min	C5H9O2	—	—	—	979.3018	-3.5	2	1.7	0.9 ± 0.8	1.7	0.1	—	—	—	—	—					
6	1131.56, 6.3 min	C5H9O2	—	—	—	1131.5625	-2.8	3	6.2	2.8 ± 2.4	0.5	1.0	6.2	—	—	—	—	—	96	807.5, 10.13 min	C5H9O2	—	—	—	807.5010	-1.8	3	18.2	6.8 ± 7.6	—	—	—	—	—	—	—					
7	927.6, 6.36 min	C4H7O2	—	—	—	927.6076	-1.8	4	9.9	6.9 ± 3.1	—	—	—	9.9	9.8	7.2	—	—	—	97	927.6, 10.21 min	C4H7O2	—	—	—	927.6076	-0.8	1	4.6	4.6 ± 0.0	—	—	—	—	—	—	4.6	—			
8	1009.6, 6.35 min	C5H9O2	—	—	—	1009.5515	0.6	1	3.6	3.6 ± 0.0	—	—	—	—	3.6	—	—	—	98	779.1, 10.24 min	C5H9O2	—	—	—	779.1243	-2.5	3	6.0	3.1 ± 1.9	2.2	1.1	6.0	—	—	—	—	—				
9	978.1, 6.4 min	C4H6O2	—	—	—	978.1387	-0.9	3	6.1	4.7 ± 1.4	—	—	—	2.6	6.1	5.3	—	—	—	99	809.1, 10.27 min	C4H6O2	—	—	—	809.1348	-2.4	4	6.0	2.6 ± 1.7	2.2	—	—	6.0	1.2	1.1	—	—			
10	1235.61, 6.48 min	C5H9O2	—	—	—	1235.6108	1.4	1	1.7	1.7 ± 0.0	—	—	—	—	1.7	—	—	—	100	851.1, 10.36 min	C4H6O2	—	—	—	851.1449	-1.6	6	5.3	2.4 ± 1.0	2.5	1.6	5.3	1.6	2.0	1.3	—	—				
11	1001.6, 6.48 min	C4H7O2	—	—	—	1001.4636	-1.7	2	0.9	0.7 ± 0.1	—	—	0.6	0.9	—	—	—	—	—	101	1247.1, 10.47 min	C5H9O2	—	—	—	1247.1079	-1.0	1	12.6	12.6 ± 0.0	—	—	—	—	—	—	12.6	—			
12	927.6, 6.54 min	C4H7O2	—	—	—	927.4962	-0.3	2	1.5	1.0 ± 0.6	1.5	0.4	—	—	—	—	—	—	—	102	1115.1, 10.48 min	C5H9O2	—	—	—	1115.1678	-3.1	3	32.8	12.6 ± 13.4	2.3	2.9	32.8	—	—	—	—	—			
13	1131.56, 6.55 min	C5H9O2	—	—	—	1131.5624	-2.8	2	4.1	2.6 ± 1.5	1.1	—	4.1	—	—	—	—	—	—	103	1235.58, 10.56 min	C5H9O2	—	—	—	1235.5877	-3.4	7	6.0	2.4 ± 1.8	1.3	0.5	1.2	5.2	1.8	0.7	6.0	—			
14	1235.61, 6.62 min	C5H9O2	911 [M-HeHex-H] ⁺ 705 [M-HeHex-H] ⁺ 749 [M-HeHex-H] ⁺ 603 [M-HeHex-H] ⁺ 471 [M-HeHex-H] ⁺	MS/MS signature	471	1235.6109	-3.5	3	23.1	13.8 ± 7.5	—	11.5	23.1	0.9	—	—	—	—	—	104	851.1, 10.66 min	C4H6O2	—	—	—	851.1443	-1.0	6	13	0.9 ± 0.3	1.1	0.3	0.9	1.1	1.3	0.8	—	—			
15	1001.6, 6.67 min	C4H7O2	—	—	—	1001.4638	-3.9	6	11.7	5.0 ± 3.3	5.2	0.8	2.9	1.6	13.7	6.0	—	—	—	105	1235.58, 10.77 min	C5H9O2	—	—	—	1235.5917	-5.1	7	5.3	1.9 ± 1.2	1.4	0.3	2.3	2.1	1.3	0.3	5.3	—			
16	927.6, 6.68 min	C4H7O2	—	—	—	927.4994	-3.8	4	3.7	2.4 ± 0.8	2.5	0.7	3.7	2.7	—	—	—	—	—	106	887.5, 10.71 min	C4H6O2	—	—	—	887.5126	-2.4	6	100.0	38.9 ± 32.2	74.4	100.0	14.5	11.9	30.6	1.8	—	—	—	—	
17	1009.6, 6.72 min	C5H9O2	705 [M-HeHex-H] ⁺ 603 [M-HeHex-H] ⁺ 471 [M-HeHex-H] ⁺	MS/MS signature	471	1009.5514	-2.5	3	12.8	5.7 ± 4.7	—	1.4	12.8	3.0	—	—	—	—	—	107	839.1, 10.74 min	C5H9O2	—	—	—	839.1088	-2.0	2	9.8	8.5 ± 1.3	—	—	—	—	—	—	9.8	—			
18	781.7, 6.76 min	C4H6O2	—	—	—	781.4991	-1.4	3	2.3	2.0 ± 0.2	—	—	—	1.8	2.3	2.0	—	—	—	108	927.1, 10.9 min	C4H6O2	—	—	—	927.4993	-3.6	3	2.8	1.9 ± 0.6	—	—	—	—	—	—	2.8	2.7	—		
19	1235.61, 6.79 min	C5H9O2	911 [M-HeHex-H] ⁺ 705 [M-HeHex-H] ⁺ 749 [M-HeHex-H] ⁺ 603 [M-HeHex-H] ⁺ 471 [M-HeHex-H] ⁺	MS/MS signature	471	1235.6116	-4.0	6	100.0	40.5 ± 28.7	13.6	32.2	67.0	24.6	100.0	5.6	—	—	—	—	109	1057.1, 10.89 min	C5H9O2	—	—	—	1057.1602	-1.2	7	83.7	36.1 ± 21.9	12.4	1.7	17.6	37.9	83.7	50.3	49.3	—		
20	839.6, 6.85 min	C4H6O2	—	—	—	839.4082	-1.4	6	3.8	2.0 ± 0.7	3.8	1.3	1.8	1.8	2.1	0.9	—	—	—	—	110	927.1, 11.04 min	C4H6O2	—	—	—	927.4988	-3.2	3	9.7	5.0 ± 3.1	—	—	—	—	—	—	—	9.7	—	
21	1009.6, 6.88 min	C5H9O2	825 [M-HeHex-H] ⁺ 603 [M-HeHex-H] ⁺ 471 [M-HeHex-H] ⁺	MS/MS signature	471	1009.5516	-2.6	6	10.2	5.6 ± 2.8	2.8	2.5	10.2	6.6	8.5	3.2	—	—	—	—	111	1235.58, 11.07 min	C5H9O2	—	—	—	1235.5889	-2.8	7	40.9	21.9 ± 10.1	31.1	7.3	29.2	18.0	40.9	7.8	19.0	—		
22	927.6, 6.9 min	C4H7O2	—	—	—	927.4998	-4.2	5	6.7	3.7 ± 1.3	—	2.0	3.4	4.0	6.7	2.6	—	—	—	—	112	1089.53, 11.14 min	C5H9O2	—	—	—	1089.5298	-2.1	4	16.0	5.1 ± 5.4	2.0	0.8	16.0	—	—	—	—	—	—	
23	825.6, 6.9 min	C4H6O2	—	—	—	825.4294	-1.9	3	3.4	2.3 ± 0.7	2.2	1.3	3.4	—	—	—	—	—	—	—	113	1115.1, 11.17 min	C5H9O2	—	—	—	1115.1666	-2.0	4	25.2	9.5 ± 7.8	6.6	1.1	25.2	—	—	—	—	—	5.2	—
24	779.6, 6.9 min	C4H6O2	—	—	—	779.4227	-0.4	3	2.1	1.5 ± 0.4	1.4	0.8	2.1	—	—	—	—	—	—	—	114	1033.5, 11.27 min	C5H9O2	—	—	—	1033.4896	-1.2	1	0.8	0.8 ± 0.0	—	—	—	—	—	—	—	—	—	
25	825.6, 7.01 min	C4H6O2	—	—	—	825.4289	-1.3	3	3.3	1.9 ± 1.0	3.3	1.1	3.3	—	—	—	—	—	—	—	115	1115.1, 11.32 min	C5H9O2	—	—	—	1115.1655	-1.1	1	36.5	36.5 ± 0.0	—	—	—	—	—	—	—	—	36.5	—
26	839.6, 7.03 min	C4H6O2	603 [M-HeHex-H] ⁺ 501 [M-HeHex-H] ⁺	MS/MS signature	501	839.4088	-2.1	7	14.8	4.3 ± 3	4.3	0.5	0.4	3.2	14.8	3.7	3.1	—	—	—	116	645.1, 11.48 min	C3H7O2	—	—	—	645.4032	-3.7	3	1.6	1.1 ± 0.6	1.5	0.1	1.6	—	—	—	—	—	—	
27	1009.6, 7.07 min	C5H9O2	—	—	—	1009.5516	-2.7	6	6.7	3.7 ± 2.4	1.2	0.5	2.3	5.3	6.3	6.7	—	—	—	—	117	777.1, 11.5 min	C4H6O2	—	—	—	777.4073	-0.8	1	39.4	39.4 ± 0.0	—	—	—	—	—	—	—	—	39.4	—
28	825.6, 7.07 min	C4H6O2	705 [M-HeHex-H] ⁺ 603 [M-HeHex-H] ⁺ 471 [M-HeHex-H] ⁺	MS/MS signature	471	825.4287	-3.1	9	25.9	8.1 ± 3.6	4.0	0.9	3.6	11.6	12.4	13.1	—	—	—	—	118	661.1, 11.53 min	C3H7O2	—	—	—	661.3757	-1.1	3	4.5	3.3 ± 1.3	—	—	—	—	—	—	—	4.5	4.0	—
29	1131.56, 7.08 min	C5H9O2	—	—	—	1131.5629	-3.2	2	30.9	17.3 ± 13.2	—	4.4	30.9	—	—	—	—	—	—	—	119	1235.58, 11.56 min	C5H9O2	—	—	—	1235.5862	-0.6	2	0.8	0.5 ± 0.3	—	—	—	—	—	—	—	—	—	
30	1033.5, 7.09 min	C5H9O2	—	—	—	1033.5177	-3.6	3	7.4	4.4 ± 1.0	—	—	7.4	4.2	1.6	—	—	—	—	—	120	781.7, 11.58 min	C4H6O2	—																	