

Table S2 UPLC-ESI-HR/MS comparison of main leaf-epigenetic profiles of *lex* aquifolium cultivars, *lex* × meserveae cultivars and reference commercial *lex* paragonensis (DMS).
RT—retention time, RA%—the relative area of peak, when the area of the target one in the sample is calculated as 100%.

No.	Compound name [M] ⁺ , RT [min]	Cpd. neutral formula	MW/Ms fragments [proposed pathway]	MW/Ms aglycone	Measured [M] ⁺ , m/z	Err. [ppm]	Occurrence frequency	Min RA %	Average RA % ± SD	SD RA %	AM RA %	HMS RA %	HPT RA %	BT RA %	BO RA %	PA ref. RA %
1	1235.01, 6.05 min	C5H9O22	911 [M-(HexHex)-H] ⁺ 765 [M-(HexHex)-diHex-H] ⁺ 749 [M-(HexHex)-Hex-H] ⁺ 603 [M-(HexHex)-diHexHex-H] ⁺ 471 [M-(HexHex)-HexHex-Hex-H] ⁺	471	1235.6103	-3.0	6	5.0	3.4 ± 0.9	4.1	3.9	5.0	3.0	3.2	1.4	—
2	927, 6.08 min	C4H7O18	—	—	927.4975	-1.8	2	3.1	2.2 ± 0.9	—	1.3	3.1	—	—	—	—
3	1089, 6.09 min	C5H9O23	—	—	1089.5201	-3.1	3	4.9	2.6 ± 1.5	2.2	0.7	4.9	—	—	—	—
4	927, 6.17 min	C4H7O18	—	—	927.4980	-2.2	3	3.1	2.3 ± 0.5	—	2.4	1.5	3.1	—	—	—
5	1089.5, 6.27 min	C5H9O23	—	—	1089.5332	-1.0	1	3.8	3.8 ± 0.0	—	—	3.8	—	—	—	—
6	1113.16, 6.35 min	C5H9O24	—	—	1113.5625	-2.3	3	6.2	2.6 ± 2.4	0.5	1.0	6.2	—	—	—	—
7	927, 6.36 min	C4H7O18	—	—	927.4976	-1.8	4	9.0	6.9 ± 3.1	0.7	—	9.0	9.8	7.2	—	—
8	1089.5, 6.35 min	C5H9O23	—	—	1089.5515	0.6	1	3.6	3.6 ± 0.0	—	—	—	—	3.6	—	—
9	781, 6.4 min	C4H6O14	—	—	781.4387	-0.9	3	6.1	4.7 ± 1.4	—	—	2.6	6.1	5.3	—	—
10	1235.01, 6.48 min	C5H9O22	—	—	1235.6108	1.4	1	1.7	1.7 ± 0.0	—	—	—	—	1.7	—	—
11	1001, 6.48 min	C4H7O22	—	—	1001.4616	-1.7	2	0.9	0.7 ± 0.1	—	0.6	0.9	—	—	—	—
12	927, 6.54 min	C4H7O18	—	—	927.4962	-0.3	2	1.5	1.0 ± 0.6	1.5	0.4	—	—	—	—	—
13	1131.56, 6.55 min	C5H9O24	—	—	1131.5624	-2.8	2	4.1	2.6 ± 1.5	1.1	—	4.1	—	—	—	—
14	1235.01, 6.62 min	C5H9O22	911 [M-(HexHex)-H] ⁺ 765 [M-(HexHex)-diHex-H] ⁺ 749 [M-(HexHex)-Hex-H] ⁺ 603 [M-(HexHex)-diHexHex-H] ⁺ 471 [M-(HexHex)-HexHex-Hex-H] ⁺	471	1235.6109	-3.5	3	23.1	11.8 ± 7.5	—	11.5	23.1	0.9	—	—	—
15	1001, 6.67 min	C4H7O22	—	—	1001.4638	-3.9	6	13.7	5.0 ± 3.3	5.2	0.8	2.9	1.6	13.7	6.0	—
16	927, 6.68 min	C4H7O18	—	—	927.4994	-3.8	4	3.7	2.4 ± 0.8	2.5	0.7	3.7	2.7	—	—	—
17	1089, 6.72 min	C5H9O23	765 [M-(HexHex)-H] ⁺ 603 [M-(HexHex)-diHex-H] ⁺ 471 [M-(HexHex)-HexHex-Hex-H] ⁺	471	1089.5514	-2.5	3	12.8	5.7 ± 4.7	—	1.4	12.8	3.0	—	—	—
18	781, 6.74 min	C4H6O14	—	—	781.4391	-1.4	3	2.3	2.0 ± 0.2	—	—	—	1.8	2.3	2.0	—
19	1235.01, 6.79 min	C5H9O22	911 [M-(HexHex)-H] ⁺ 765 [M-(HexHex)-diHex-H] ⁺ 749 [M-(HexHex)-Hex-H] ⁺ 603 [M-(HexHex)-diHexHex-H] ⁺ 471 [M-(HexHex)-HexHex-Hex-H] ⁺	471	1235.6116	-4.0	6	100.0	40.5 ± 28.7	13.6	32.2	67.0	24.6	100.0	5.6	—
20	836, 6.85 min	C42H6O17	—	—	839.4082	-1.4	6	3.8	2.0 ± 0.7	3.8	1.3	1.8	1.8	2.1	0.9	—
21	1089, 6.88 min	C5H9O23	825 [M-(Hex)-H] ⁺ 663 [M-(Hex)-Hex-H] ⁺ 487 [M-(Hex)-HexHex-Hex-H] ⁺	487	1089.5516	-2.6	6	10.2	5.6 ± 2.8	2.8	2.5	10.2	6.6	8.5	3.2	—
22	927, 6.9 min	C4H7O18	—	—	927.4998	-4.2	5	6.7	3.7 ± 1.3	—	2.0	3.4	4.0	6.7	2.6	—
23	825, 6.9 min	C42H6O16	—	—	825.4294	-1.9	3	3.4	2.3 ± 0.7	2.2	1.3	3.4	—	—	—	—
24	779, 6.91 min	C4H6O14	—	—	779.4227	-0.4	3	2.1	1.5 ± 0.4	1.4	0.8	2.1	—	—	—	—
25	825, 7.01 min	C42H6O16	—	—	825.4289	-1.3	3	3.3	1.9 ± 1.0	3.3	1.1	1.3	—	—	—	—
26	839, 7.03 min	C42H6O17	663 [M-(Hex)-H] ⁺ 501 [M-(Hex)-Hex-H] ⁺	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
27	1089, 7.07 min	C5H9O23	—	—	1089.5516	-2.7	6	6.7	3.7 ± 2.4	1.2	0.5	2.3	5.3	6.3	6.7	—
28	837, 7.07 min	C42H6O17	765 [M-(Hex)-H] ⁺ 603 [M-(Hex)-diHex-H] ⁺ 487 [M-(Hex)-HexHex-Hex-H] ⁺	487	837.4907	-3.8	6	21.9	8.1 ± 5.6	4.0	0.9	3.6	11.6	12.4	15.6	—
29	1131.56, 7.08 min	C5H9O24	—	—	1131.5629	-3.2	2	30.9	17.7 ± 13.2	—	4.4	30.9	—	—	—	—
30	1073, 7.09 min	C5H9O23	—	—	1073.5377	-3.6	3	7.4	4.4 ± 1.0	—	—	7.4	4.1	1.6	—	—
31	839, 7.12 min	C42H6O17	663 [M-(Hex)-H] ⁺ 501 [M-(Hex)-Hex-H] ⁺	501	839.4090	-2.3	7	8.7	4.0 ± 1.8	2.4	1.5	5.7	2.2	8.7	3.7	3.5
32	1235.01, 7.13 min	C5H9O22	—	—	1235.6111	-3.6	2	2.7	2.2 ± 0.5	—	—	—	2.7	—	1.7	—
33	781, 7.13 min	C4H6O14	—	—	781.4394	-1.8	6	11.7	6.7 ± 2.8	11.7	1.9	9.8	4.0	7.1	5.9	—
34	825, 7.15 min	C42H6O16	—	—	825.4302	-1.7	1	3.1	3.1 ± 0.0	—	—	3.1	—	—	—	—
35	927, 7.18 min	C4H7O18	—	—	927.4993	-3.7	7	19.6	6.9 ± 3.7	3.9	2.3	19.6	6.0	6.7	7.1	2.7
36	1089, 7.19 min	C5H9O23	—	—	1089.5511	-2.2	6	9.0	3.5 ± 1.9	1.1	1.1	9.0	2.8	3.6	3.3	—
37	823, 7.24 min	C4H6O15	—	—	823.4493	-0.9	2	4.7	2.7 ± 2.0	—	0.7	4.7	—	—	—	—
38	781, 7.24 min	C4H6O14	—	—	781.4383	-0.4	5	10.0	3.2 ± 2.7	—	0.9	10.0	1.5	2.1	1.5	—
39	971, 7.29 min	C4H7O20	647 [M-(HexHex)-H] ⁺ 471 [M-(HexHex)-Hex-H] ⁺ 765 [M-(HexHex)-diHex-H] ⁺ 747 [M-(HexHexAc)-H2O-H] ⁺ 603 [M-(HexHexAc)-Hex-H] ⁺ 471 [M-(HexHexAc)-HexHex-Hex-H] ⁺	471	971.4887	-3.1	3	6.5	3.6 ± 2.0	—	—	—	6.5	2.3	1.9	—
40	1131.56, 7.31 min	C5H9O24	765 [M-(HexHex)-H] ⁺ 747 [M-(HexHexAc)-H2O-H] ⁺ 603 [M-(HexHexAc)-Hex-H] ⁺ 471 [M-(HexHexAc)-HexHex-Hex-H] ⁺	471	1131.5629	-3.2	3	39.4	15.4 ± 16.0	0.7	6.1	39.4	—	—	—	—
41	1235.01, 7.3 min	C5H9O22	—	—	1235.6119	-3.5	1	2.1	2.1 ± 0.0	—	—	—	—	2.1	—	—
42	1073, 7.41 min	C5H9O22	749 [M-(HexHex)-H] ⁺ 765 [M-(HexHex)-diHex-H] ⁺ 301 [M-(HexHex)-CO2-HexHex-H] ⁺ 453 [M-(HexHex)-CO2-HexHex-HCOOH-H] ⁺	453	1073.5563	-2.3	4	18.6	9.1 ± 4.9	—	—	7.1	18.6	9.4	1.2	—
43	823, 7.43 min	C4H8O15	781 [M-(Hex)-H] ⁺ 619 [M-(Hex)-Hex-H] ⁺ 487 [M-(Hex)-HexHex-Hex-H] ⁺	487	823.4490	-0.6	3	6.7	2.7 ± 2.7	6.7	0.6	0.8	—	—	—	—
44	1235.01, 7.51 min	C5H9O22	911 [M-(HexHex)-H] ⁺ 765 [M-(HexHex)-diHex-H] ⁺ 749 [M-(HexHex)-Hex-H] ⁺ 603 [M-(HexHex)-diHexHex-H] ⁺ 471 [M-(HexHex)-HexHex-Hex-H] ⁺	471	1235.6104	-3.6	4	28.1	10.1 ± 9.9	1.3	—	—	28.1	11.1	8.9	—
45	971, 7.48 min	C4H7O20	—	—	971.4880	-2.4	6	7.2	4.1 ± 1.8	4.2	1.8	2.6	2.5	6.2	7.2	—
46	1131.56, 7.54 min	C5H9O24	765 [M-(HexHex)-H] ⁺ 747 [M-(HexHexAc)-H2O-H] ⁺ 603 [M-(HexHexAc)-Hex-H] ⁺ 471 [M-(HexHexAc)-HexHex-Hex-H] ⁺	471	1131.5626	-2.9	3	26.4	10.2 ± 10.9	2.1	2.0	26.4	—	—	—	—
47	823, 7.54 min	C4H8O15	781 [M-(Hex)-H] ⁺ 619 [M-(Hex)-Hex-H] ⁺ 487 [M-(Hex)-HexHex-Hex-H] ⁺	487	823.4499	-1.6	3	9.6	4.6 ± 3.3	3.2	1.1	9.6	—	—	—	—
48	1089, 7.64 min	C5H9O23	—	—	1089.5516	-2.7	1	4.2	4.2 ± 0.0	—	—	—	—	—	4.2	—
49	927, 7.68 min	C4H7O18	—	—	927.4990	-3.4	2	5.7	4.4 ± 1.3	3.1	—	5.7	—	—	—	—
50	855, 7.75 min	C4H6O16	663 [M-(Hex)-H] ⁺ 501 [M-(Hex)-Hex-H] ⁺ 487 [M-(Hex)-HexHex-Hex-H] ⁺	487	855.4277	-1.3	7	48.7	19.5 ± 38.3	6.5	2.1	1.5	48.7	11.1	9.8	9.4
51	1073, 7.78 min	C5H9O22	911 [M-(HexHex)-H] ⁺ 765 [M-(HexHex)-diHex-H] ⁺ 749 [M-(HexHex)-Hex-H] ⁺ 603 [M-(HexHex)-diHexHex-H] ⁺ 471 [M-(HexHex)-HexHex-Hex-H] ⁺	471	1073.5567	-2.7	3	6.2	5.4 ± 0.6	—	6.2	5.5	4.4	—	—	—
52	1235.01, 7.9 min	C5H9O22	—	—	1235.6098	-2.6	1	2.3	2.3 ± 0.0	—	—	—	2.3	—	—	—
53	927, 7.92 min	C4H7O18	765 [M-(Hex)-H] ⁺ 603 [M-(Hex)-Hex-H] ⁺ 471 [M-(Hex)-HexHex-Hex-H] ⁺	471	927.4971	-1.3	6	68.4	18.4 ± 16.7	4.5	10.8	68.4	7.0	11.5	8.0	—
54	969, 7.98 min	C4H7O19	—	—	969.5092	-2.8	1	1.5	1.5 ± 0.0	1.5	—	—	—	—	—	—
55	887.5, 7.98 min	C4H8O21	725 [M-(Hex)-H] ⁺	—	879.9133	-3.2	3	3.2	1.9 ± 1.2	3.2	2.4	0.2	—	—	—	—
56	971, 7.98 min	C4H7O20	—	—	979.4793	-0.6	2	1.5	0.9 ± 0.3	1.5	0.4	—	—	—	—	—
57	1131.56, 8.05 min	C5H9O24	—	—	1131.5614	-1.8	2	8.7	5.2 ± 3.4	1.8	—	8.7	—	—	—	—
58	1073, 8.11 min	C5H9O22	911 [M-(HexHex)-H] ⁺ 765 [M-(HexHex)-diHex-H] ⁺ 749 [M-(HexHex)-Hex-H] ⁺ 603 [M-(HexHex)-diHexHex-H] ⁺ 471 [M-(HexHex)-HexHex-Hex-H] ⁺	471	1073.5584	-4.3	7	85.7	58.3 ± 22.4	64.8	29.5	53.0	85.7	75.8	85.3	14.0
59	895, 8.11 min	C4H6O15	—	—	899.4354	-1.3	6	36.5	18.7 ± 19.5	15.2	3.4	8.6	26.5	36.5	12.8	—
60	927, 8.13 min	C4H7O18	—	—	927.4946	1.4	1	5.0	5.0 ± 0.0	—	—	—	—	—	5.0	—
61	765, 8.25 min	C4H6O13	603 [M-(Hex)-H] ⁺	—	765.4419	1.6	1	9.1	9.1 ± 0.0	—	—	—	—	—	9.1	—
62	927, 8.29 min	C4H7O18	765 [M-(Hex)-H] ⁺ 603 [M-(Hex)-Hex-H] ⁺ 471 [M-(Hex)-HexHex-Hex-H] ⁺	471	927.4964	-0.6	7	100.0	64.3 ± 28.7	100.0	26.5	100.0	77.6	80.2	59.8	6.4
63	1131.56, 8.35 min	C5H9O24	—	—	1131.5676	1.5	1	1.7	1.7 ± 0.0	—	—	—	—	—	1.7	—
64	1101, 8.5 min	C5H9O23	939 [M-(Hex)-H] ⁺	—	1101.5492	-0.4	1	2.0	2.0 ± 0.0	—	—	—	—	—	2.0	—
65	1381, 8.5 min	C6H10O23	895 [M-(HexHexHex)-H] ⁺ 733 [M-(HexHexHex)-Hex-H] ⁺ 587 [M-(HexHexHex)-HexHex-Hex-H] ⁺ 455 [M-(HexHexHex)-HexHexHex-Hex-Hex-H] ⁺	455	1381.6658	-0.9	1	13.6	13.6 ± 0.0	—	—	—	—	—	13.6	—
66	927, 8.54 min	C4H7O18	765 [M-(Hex)-H] ⁺ 603 [M-(Hex)-Hex-H] ⁺	—	927.4974	-1.7	5	9.6	6.0 ± 2.2	5.0	—	9.6	7.9	2.3	5.4	—
67	781, 8.58 min	C4H6O14	—	—	781.4398	-2.4	5	3.9	1.8 ± 1.4	3.1	0.8	3.9	—	0.8	0.3	—
68	1397, 8.63 min	C6H10O25	1077 [M-(HexHex)-H] ⁺ 911 [M-(HexHex)-Hex-H] ⁺ 749 [M-(HexHex)-HexHex-Hex-H] ⁺ 603 [M-(HexHex)-diHexHex-Hex-Hex-H] ⁺ 471 [M-(HexHex)-HexHexHex-Hex-Hex-Hex-H] ⁺	471	1397.6468	-1.9	4	39.5	12.7 ± 13.4	0.9	1.4	9.2	—	39.5	—	—
69	969, 8.63 min	C4H7O19	927 [M-(Hex)-H] ⁺ 807 [M-(Hex)-H] ⁺ 765 [M-(Hex)-Hex-H] ⁺ 603 [M-(Hex)-HexHex-Hex-H] ⁺ 471 [M-(Hex)-HexHex-HexHex-Hex-H] ⁺	471	969.5087	-2.3										