SUPPLEMENTARY DATA
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Supplementary Material

SUPPLEMENTARY TABLE S1. Analyte name, precursor and product ions, declustering potential (DP), entrance potential (EP), collision energy (CE), Collision CellExitPotential (CXP), retention time and Q2/Q1 used in the LC-MS/MS analysis of MeSA glycosides.

Name	Molecular Formula	Precursor ion	Q1 Product Ion	DP	EP	CE	CXP	Q2 Product ion	DP	EP	CE	CXP	t_R	Q2/Q1
MeSAG	$C_{14}H_{18}O_8$	337.0	337.0	80	10	10	15	185.2	80	10	24	15	15.6	17
MeSA-violutoside	$C_{19}H_{26}O_{12}$	469.1	469.1	80	10	10	15	337.2	80	10	38	15	15.2	108
MeSA-primeveroside	$C_{19}H_{26}O_{12}$	469.1	469.1	80	10	10	15	337.2	80	10	38	15	15.7	108
MeSA-canthoside A	$C_{19}H_{26}O_{12}$	469.1	469.1	80	10	10	15	337.2	80	10	38	15	14.9	108
MeSA-rutinoside	$C_{20}H_{28}O_{12}$	483.1	483.1	80	10	10	15	337.1	80	10	35	15	16.8	60
MeSA-gentiobioside	$C_{20}H_{28}O_{13}$	499.1	499.1	80	10	10	15	347.2	80	10	31	15	13.6	20
MSTG-A	$C_{24}H_{34}O_{16}$	601.1	601.1	80	10	10	15	449.2	80	10	38	15	14.5	14

SUPPLEMENTARY TABLE S2. MeSA glycosides concentration (average ± standard deviation) as µg/L in the 18 single-cultivars considered.

CULTIVAR	TOTAL AMOUNT	MONOGLYCOSIDE	DIGLYCOSIDES				
		MeSAG	MeSA-gentiobioside	MeSA-violutoside	MeSA-rutinoside	MeSA-primeveroside	MeSA-canthoside A
ALBANA	167.8 ± 98.9	50.9 ± 37.5	77.7 ± 50.1	25.1 ± 14.6	5.1 ± 4.1	5.9 ± 3.3	2.7 ± 3.7
ARNEIS	120.3 ± 62.4	28.2 ± 13.7	13.3 ± 9.7	33.1 ± 16.5	41.4 ± 22.6	3.1 ± 2.3	1.1 ± 1.6
CORTESE	211.3 ± 103.4	58.8 ± 26.5	77.6 ± 48.8	64.1 ± 36.3	3.2 ± 1.6	5.7 ± 3.2	1.6 ± 2.9
ERBALUCE	674.9 ± 257.9	204.4 ± 87.5	334.4 ± 159.5	92.5 ± 42.9	21.1 ± 10.1	17.1 ± 6.8	5.2 ± 7.8
FALANGHINA	36.5 ± 27.2	14.4 ± 8.9	5.8 ± 4.2	11.9 ± 11.6	0.3 ± 0.5	2.4 ± 2.4	1.5 ± 2.6
FIANO	146.4 ± 48.9	74.9 ± 18.6	24.1 ± 21.9	27.3 ± 14.3	2.1 ± 0.9	14.1 ± 3.8	3.8 ± 6.4
GARGANEGA	328.3 ± 138.6	136.4 ± 66.6	107.3 ± 58.8	67.1 ± 30.1	3.3 ± 3.9	13.2 ± 5.3	0.9 ± 1.1
GRECO DI TUFO	113.6 ± 38.5	29.7 ± 17.1	15.9 ± 10.5	52.6 ± 20.7	5.4 ± 2.2	6.7 ± 1.8	3.1 ± 3.4
GEWÜRZTRAMINER	29.5 ± 12.7	8.9 ± 4.7	7.1 ± 5.7	12.3 ± 5.1	0.3 ± 0.6	0.2 ± 0.3	0.4 ± 0.5
LUGANA	1286.3 ± 453.6	504.3 ± 150.9	561.2 ± 304.9	145.1 ± 45.1	38.6 ± 34.9	34.4 ± 11.9	2.7 ± 4.3
MÜLLER THURGAU	50.7 ± 17.6	20.5 ± 9.7	17.3 ± 9.7	11.2 ± 4.2	1.1 ± 1.9	0.4 ± 0.6	0.2 ± 0.6
NOSIOLA	53.3 ± 19.7	16.2 ± 10.6	14.8 ± 8.6	14.5 ± 4.8	3.1 ± 1.4	1.7 ± 1.4	2.6 ± 3.6
PALLAGRELLO	60.4 ± 61.1	28.6 ± 36.2	9.4 ± 9.3	13.6 ± 7.7	3.3 ± 2.3	2.9 ± 4.4	2.3 ± 5.7
PINOT GRIGIO	76.7 ± 79.4	29.8 ± 37.8	23.1 ± 23.9	21.2 ± 15.5	0.7 ± 2.2	1.7 ± 2.6	0.2 ± 0.6
RIBOLLA GIALLA	150.8 ± 94.8	52.1 ± 35.9	43.3 ± 32.1	49.3 ± 30.3	1.5 ± 1.4	4.4 ± 3.4	0.1 ± 0.1
VERMENTINO	34.1 ± 17.1	13.8 ± 7.1	5.8 ± 3.4	13.2 ± 7.3	0.3 ± 0.3	0.7 ± 0.6	0.1 ± 0.1
VERNACCIA	59.3 ± 17.3	26.8 ± 7.5	8.4 ± 4.1	15.3 ± 4.1	0.3 ± 0.5	3.7 ± 2.1	4.6 ± 6.2
VERDICCHIO	1101.6 ± 591.9	452.1 ± 157.6	461.3 ± 392.1	115.2 ± 60.6	36.7 ± 23.9	31.3 ± 16.9	4.7 ± 4.2

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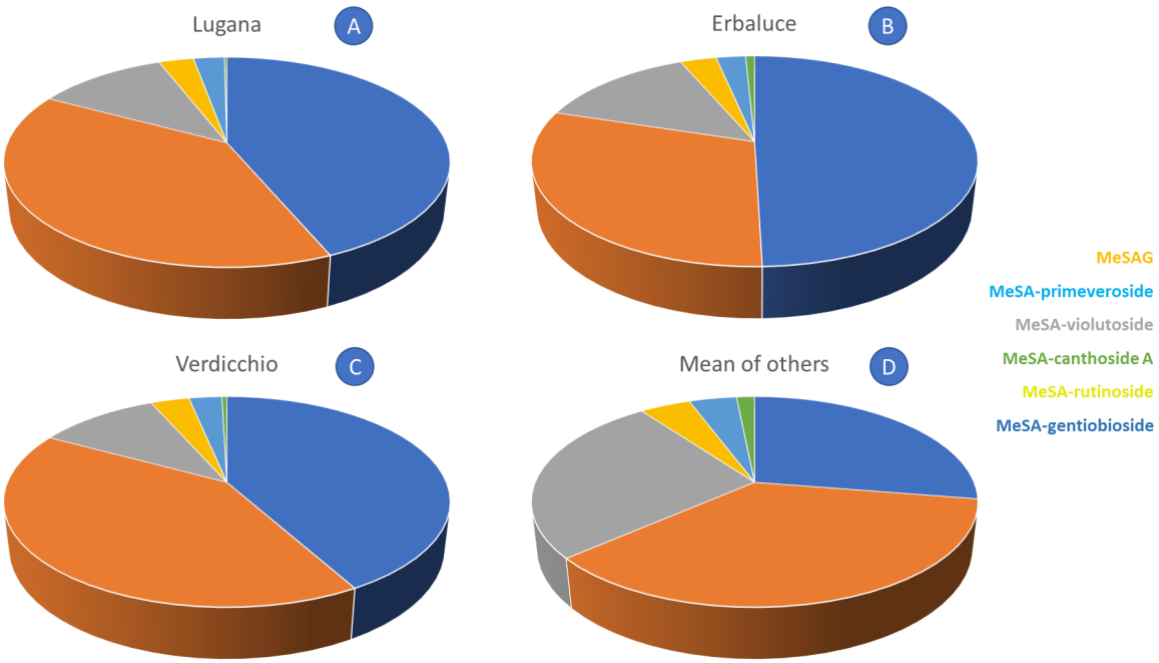

FIGURE S1. Pie charts of the relative MeSA distributions over its glycosylated forms in the 3 richest cultivars (Lugana – A, Erbaluce – B, Verdicchio – C) and a mean of the other 15 (D).