Boido, E., Arrieta, Y., Curbelo, R., Barnaba, C., Larcher, R., Nardin, T., … Dellacassa, E. (2026). Comprehensive secondary metabolite analysis of underexplored Uruguayan red grape varieties: implications for oenological potential. *OENO One, 60*(3).
https://doi.org/10.20870/oeno-one.2026.60.3.9887

SUPPLEMENTARY DATA

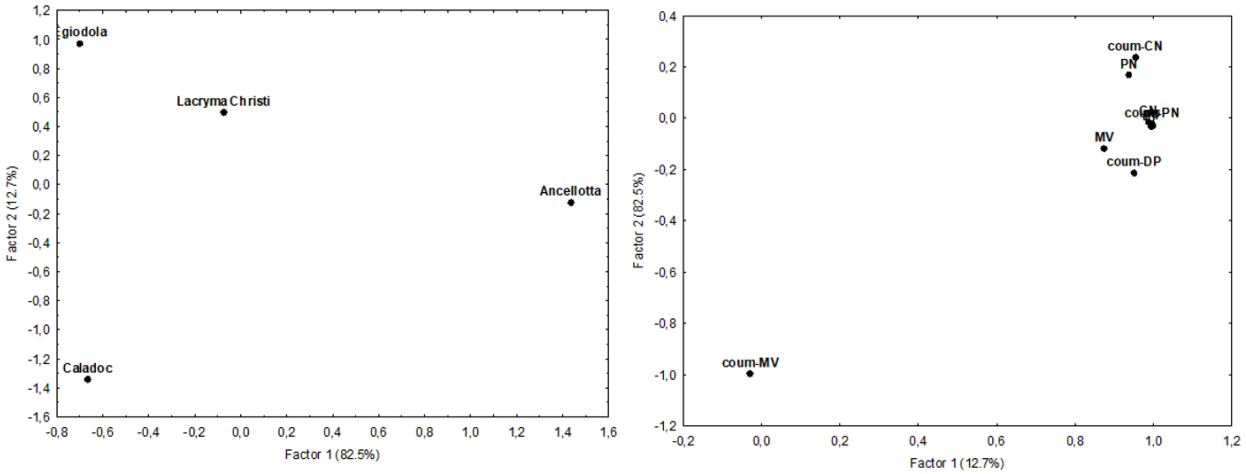


Figure S1. Score plot of the first two principal components of anthocyanin content for each selected variety.

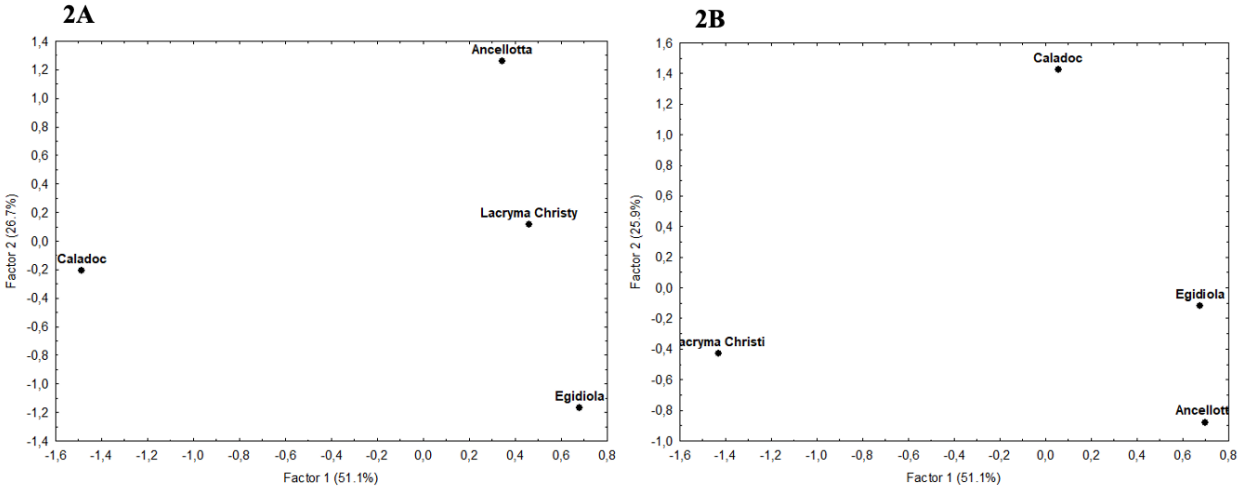


Figure S2. Score plot of the first two principal components) of skins (2A) and seeds (2B) phenolic profiles for each selected variety.

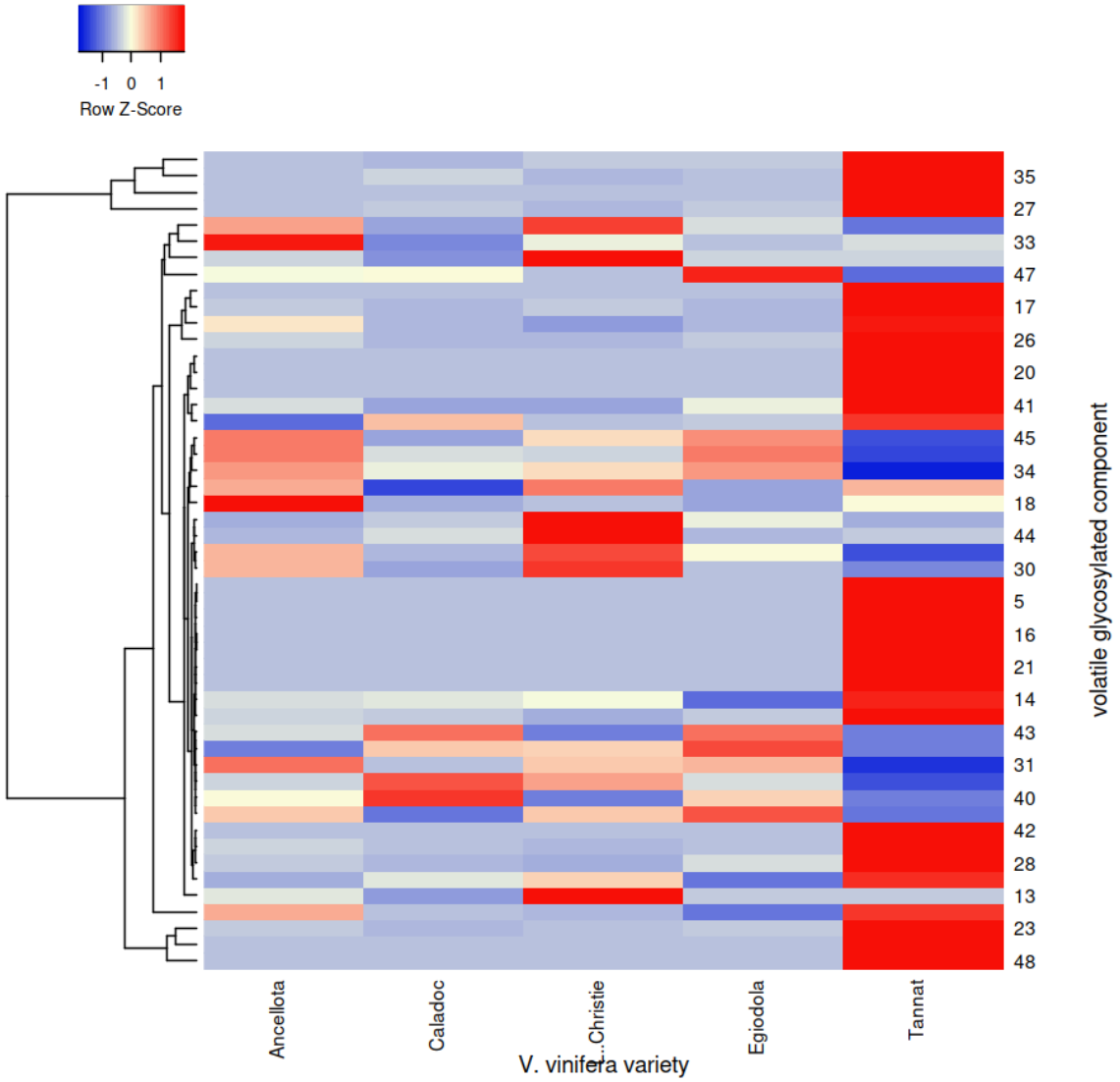


Figure S3. Heat map showing the distribution of the major glycosylated volatile compounds according to the grape variety studied.

SUPPLEMENTARY DATA
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Table S1. Polyphenols found by untargeted approach for the grape seeds of the varieties studied.

i.d.	Compound*	RT (min)	Accurate mass (*m/z*)	Fragments (*m/z*)	Note
1	trihydroxybenzoyl hexose conjugate 1	3.00	331.0671	169.0143,125.0244	ester; isomer of gallic acid
2	hydroxyethylbenzenediol hexose conjugate	4.28	315.1085	153.0193,123.0437	isomer of hydroxytyrosol
3	gallic acid	4.50	169.0142	125.0244	
4	hydroxymethoxybenzoic acid hexose conjugate 1	5.13	329.0878	167.035,152.0114,123.0452	isomer of vanillic acid
5	trihydroxybenzoic acid hexose conjugate 2	5.50	331.0671	169.0143,125.0244	isomer of gallic acid
6	Hydroxytyrosol	5.50	153.0557	123.0437, 95.0487	
7	hydroxymethoxyphenylacetic acid hexose conjugate	6.10	343.1035	181.0506,137.0617,122.0373	isomer of homovanillic acid
8	tetrahydroxyflavan-3-ol hexose conjugate (2RA + 2RB) 1	6.42	451.1246	179.035,167.035,151.0401,137.0244, 121.0295,109.0295	isomer of catechin glucoside
9	hydroxymethoxybenzoylhexose conjugate 2	8.36	329.0878	269.0666,239.0561,209.0455,167.035, 152.0114,123.0452,119.0349	ester; isomer of vanillic acid
10	protocatechuic acid	9.40	153.0193	109.0294	
11	Tyrosol	9.50	137.0608	119.0502, 106.0426	
12	dihydroxycinnamic acid hexose conjugate 1	10.56	341.0878	179.035,135.0452	isomer of caffeic acid
13	methylphenol hexose-pentose conjugate	12.30	401.1453	269.1031,161.0455,119.0349,101.0244, 89.0244,71.0138,59.0138	isomer of cresol
14	tetrahydroxyflavan-3-ol hexose conjugate (2RA + 2RB) 2	12.30	451.1246	179.035,167.035,151.0401,137.0244, 121.0295,109.0295	isomer of catechin glucoside
15	dihydroxycinnamoyl hexose conjugate 2	13.33	341.0878	179.035,135.0452	ester; isomer of caffeic acid
16	hydroxymethoxycinnamic acid hexose conjugate	13.36	355.1035	193.0506,178.0268,149.0608	isomer of ferulic acid
17	ethoxymethylmethoxyphenol hexose conjugate	14.42	343.1398	181.087,166.0633,153.0656	isomer of vanillyl ethyl ether
18	tetrahydroxyflavan-3-ol hexose conjugate (2RA + 2RB) 3	14.70	451.1246	179.035,167.035,151.0401,137.0244, 121.0295,109.0295	isomer of catechin glucoside
19	syringic acid	15.30	197.0455	182.0216, 166.9984	
20	vanillic acid	15.50	167.0350	152.0114, 123.0452	

21	Aesculetin	16.00	177.0193	133.0296, 105.0345	
22	Catechin	16.20	289.0717	245.0805, 221.0812	
23	monohydroxycinnamoylhexose conjugate	16.50	325.0929	265.0717,235.0612,205.0506,163.04, 119.0349,101.0244,89.0244	isomer of cinnamic acid
24	*p*-carboxyphenol acid	17.90	137.0244	93.0646	
25	*o*-vanillina	18.00	151.0401	136.0152, 123.0083	
26	gentisic acid	18.50	153.0193	109.0295, 108.0217	
27	trihydroxyflavanonol hexose conjugate (1RA + 2RB)	19.50	449.1089	177.0193,151.0401,151.0036,125.0244, 107.0138	isomer of aromadendrin glucoside
28	Epicatechin	20.00	289.0718	245.0805, 221.0812	
29	caffeic acid	20.00	179.0350	135.0452	
30	Isoacetovanillone	20.80	165.0557	150.0321, 122.0371	
31	sinapic acid	24.30	223.0611	208.0373, 179.0714	
32	ferulic acid	26.00	193.0506	178.0268, 149.0608	
33	tetrahydroxyflavanonol hexose conjugate (2RB+2RA)	26.98	465.102	177.0193,151.0401,151.0036,125.0244, 107.0138	isomer of taxifolin glucoside
34	Tryptophol	28.50	160.0767	142.0659, 130.0660	
35	*p*-coumaric acid	28.50	163.0401	119.0502, 93.1266	
36	trihydroxyflavanone hexose conjugate (2RA + 1 RB) 1	28.98	433.1140	151.0036,135.0452,123.0088,107.0138	isomer of naringenin glucoside
37	methyl vanillate	30.50	181.0506	166.0268, 151.0036	
38	trihydroxyflavanone hexose conjugate (2RA + 1 RB) 2	30.60	433.1140	151.0036,135.0452,123.0088,107.0138	isomer of naringenin glucoside
39	pentahydroxyflavonol hexose conjugate (3RB + 2RA) 1	30.89	479.0831	178.9985,151.0036,137.0244,107.0138	isomer of myricetin glucoside
40	pentahydroxyflavonol hexose conjugate (2RA+3RB) 2	31.57	479.0821	178.9985,151.0036,137.0244,107.0138	isomer of myricetin glucoside
41	tetrahydroxyflavonol hexose conjugate (2RB+2RA) 1	31.83	463.0882	178.9985,151.0036,121.0295,107.0138	isomer of quercetin glucoside
42	salicylic acid	32.30	137.0244	93.0346, 122.0374	
43	tetrahydroxyflavonol deoxyhexose-hexose conjugate (2RB+2RA)	34.10	609.1483	178.9985,151.0036,121.0295,107.0138	isomer of quercetin ramnoside-glucoside

44	tetrahydroxyflavanonol deoxyhexose conjugate (2RA + 2RB) 1	34.80	449.1089	177.0193,151.0401,151.0036,125.0244, 107.0138	isomer of taxifolin ramnoside
45	tetrahydroxymethoxyflavonol hexose conjugate (2RA + 3RB, CH_3 on B)	34.87	493.0988	193.0142,178.9985,163.0036,151.0036, 107.0138	isomer of laricitrin glucoside
46	tetrahydroxyflavanonol deoxyhexose conjugate (2RA + 2RB) 2	35.11	449.1089	177.0193,151.0401,151.0036,125.0244, 107.0138	isomer of taxifolin ramnoside
47	tetrahydroxyflavonol hexose conjugate (2RA + 2RB) 2	35.39	463.0882	178.9985,151.0036,121.0295,107.0138	isomer of quercetin glucoside
48	tetrahydroxyflavonol hexose conjugate (2RA + 2RB) 3	35.90	463.0882	178.9985,151.0036,121.0295,107.0138	isomer of quercetin glucoside
49	tetrahydroxyflavone hexose conjugate (2RA+2RB)	35.99	447.0933	178.9985,151.0036,145.0295,121.0293, 107.0138	isomer of luteolin glucoside
50	tetrahydroxyflavanonol deoxyhexose conjugate (2RA + 2RB) 3	36.00	449.1089	177.0193,151.0401,151.0036,125.0244, 107.0138	isomer of taxifolin ramnoside
51	tetrahydroxymethoxyflavonol glucuronide (2RA+3RB, 1 CH_3 on B)	36.34	507.0776	193.0142,178.9985,163.0036,151.0036, 107.0138	isomer of laricitrin glucuronide
52	trihydroxydimethoxyisoflavonol hexose conjugate (2RA + 3RB, 2CH_3 on B)	37.43	507.1144	492.0917,477.0685,193.0142,165.0193, 163.04,149.0244,137.0244	isomer of syringetin glucoside
53	trihydroxyflavonol hexose coniugate (2RA+1RB) 1	37.48	447.0933	177.0193,163.0036,151.0036,121.0295, 107.0138	isomer of kaempferol glucoside
54	trihydroxyflavonol hexose coniugate (2RA+1RB) 2	38.35	447.0933	178.9985,151.0036,107.0138	isomer of kaempferol glucoside
55	trihydroxyflavanonol deoxyhexose conjugate (2RA + 1RB) 1	38.69	433.1140	177.0193,151.0036,119.0502,107.0138, 93.0346	isomer of aromadendrin ramnoside
56	tetrahydroxyflavonol deoxyhexose conjugate (2RA+2RB)	39.18	447.0933	177.0193,163.0036,151.0036,121.0295, 107.0138	isomer of quercetin ramnoside
57	trihydroxyflavanonol deoxyhexose conjugate (2RA + 1RB) 2	39.58	433.1140	177.0193,151.0036,119.0502,107.0138, 93.0346	isomer of aromadendrin ramnoside
58	trihydroxyflavonol hexose coniugate (2RA+1RB) 3	39.60	447.0933	178.9985,151.0036,107.0138	isomer of kaempferol glucoside
59	tetrahydroxyflavonol hexose conjugate (2RA + 2RB) 4	40.29	463.0882	193.0142,178.9985,151.0036,149.0244, 121.0295,107.0138	isomer of quercetin glucoside
60	trihydroxymethoxyflavonol glucuronide (2RA+2RB, 1 CH_3 on B)	40.30	491.0824	193.0142,178.9985,163.0036,151.0036, 107.0138	isomer of isorhamnetin glucuronide
61	trihydroxyflavonol deoxyhexose conjugate (2RA + 1RB)	42.69	431.0984	178.9985,151.0036,107.0138	isomer of kaempferol ramnoside

62	Myricetin	44.10	317.0300	178.9985, 151.0036, 137.0240
63	Laricitrin	47.70	331.0454	193.0142,178.9985,163.0036,151.0036, 107.0138
64	Syringetin	49.50	345.0610	193.0142,165.0193,163.04,149.0244, 137.0244
65	Quercetin	49.70	301.0352	273.0399, 229.0504, 178.9985, 151.0036, 121.0295
66	Kaempferol	53.10	285.0399	178.9985,151.0036,107.0138

** in brackets the number of hydroxyl and methoxyl groups on ring A (RA) and ring B (RB).*