From Vine to Vintage: NMR Metabolomics of Young and Mature Wine and Grape Ale

Dessislava Gerginova [1], Plamen Chorbadzhiev [1,2] and Svetlana Simova [1,*]

[1] Bulgarian NMR Centre, Institute of Organic Chemistry with Centre of Phytochemistry, Bulgarian Academy of Sciences, Acad. G. Bonchev str. Bl. 9, 1113 Sofia, Bulgaria; dessislava.gerginova@orgchm.bas.bg (D.G.), plamen.chorbadzhiev@orgchm.bas.bg (P.C.)
[2] University of Chemical Technology and Metallurgy, 8 St Kliment Okhridski blvd, 1756 Sofia, Bulgaria
* Correspondence: svetlana.simova@orgchm.bas.bg (S.S.)

SUPPORTING INFORMATION

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Table S1a. Sample abbreviations, grape varieties, vineyards, and years of production for young and mature wines.

Code	Grape variety	Origin	Year
Mature wine			
mr_m1	Merlot	"Katarzyna" Estate – Mezzek	2013
mr_m2	Merlot	"Villa Vinifera"	2015
mr_m3	Merlot	"Vinprom Karnobat" – Chateau Karnobat	2015
mv_m1	Mavrud	"Villa Vinifera"	2015
mv_m2	Mavrud	"Vinzavod" – Mavrud KNP	2014
mv-m3	Mavrud	Domaine "Menada"	2018
sb_m1	Sauvignon blanc	Chateau "Burgozone"	2016
sb_m2	Sauvignon blanc	**"**Villa Vinifera"	2016
sb_m3	Sauvignon blanc	"Minkov brothers" – Le Photographe	2017
Young wine			
mr_y1	Merlot	" Noya" Winery	2023
mr_y2	Merlot	"Grandfather Plamen" Winery	2023
mr_y3	Merlot	Villa "Bassarea"	2023
mv_y1	Mavrud	Chateau "Copsa"	2023
mv_y2	Mavrud	"Rosalea"	2023
mv-y3	Mavrud	"Dimitrovi" Winery	2023
sb_y1	Sauvignon blanc	**"**Dzhinvira" Winery	2023
sb_y2	Sauvignon blanc	Villa "Bassarea"	2023
sb_y3	Sauvignon blanc	" DeVina – Vineyards & Wine"	2023

Table S1b. Manufacturer, aging, grape variety, part of grape used, vintage and country of origin for the grape ale samples measured.

	Beer name	Barrel aged	Grape variety	Part of grape used	Vintage	Country of origin
ga_1	MONYO Brewing Co. - Hungarian Terroir: Szekszárd Kékfrankos Barrel Aged Wild Grape Ale	yes	Kékfrankos (Blaufränkisch)	Grape skins, must, and juice	2020	Hungary
ga_2	MONYO Brewing Co. - Hungarian Terroir: Balatonboglár Sauvignon Blanc	yes	Sauvignon blanc	Grape skins, must, and juice	2021	Hungary
ga_3	Kykao - Handcrafted - Reverse Engineered Malagouzia	on lees	Malagouzia	Grape skins	2020	Greece
ga_4	Kykao - Handcrafted - Kykao × Patraiki Wines - Reverse Engineered Pet Nat	no	Muscat	Grape skins	2023	Greece

Table S2. Misclassification table for the OPLS-DA model assessing the botanical origin of young and mature wines - Merlot, Mavrud, Sauvignon blanc.

	Members	Correct	merlot mature	mavrud mature	sauvignon mature	merlot young	mavrud young	sauvignon young
merlot - mature	3	100%	3	0	0	0	0	0
mavrud - mature	3	100%	0	3	0	0	0	0
sauvignon - mature	3	100%	0	0	3	0	0	0
merlot - young	3	100%	0	0	0	3	0	0
mavrud - young	3	100%	0	0	0	0	3	0
sauvignon - young	3	100%	0	0	0	0	0	3

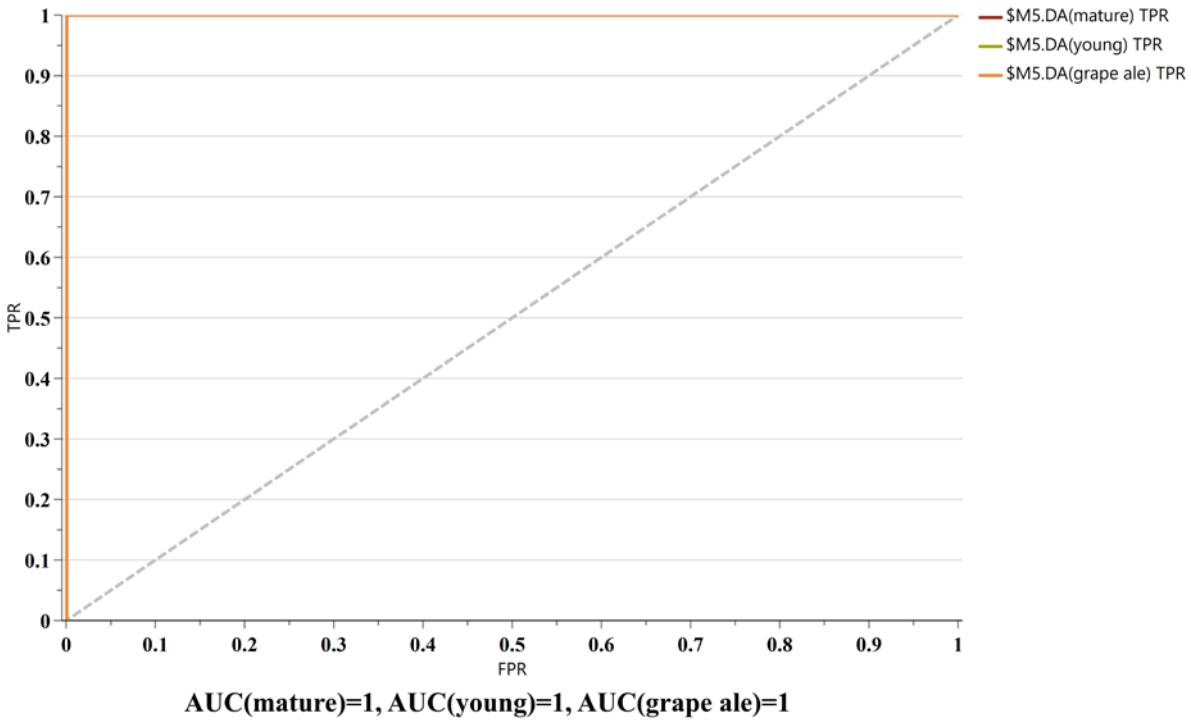

Figure S1. Receiver operating characteristic (ROC) curve employed to assess the classification performance of the orthogonal partial least squares-discriminant analysis (OPLS-DA) model in differentiating between grape ales, young wines, and mature wines.

Figure S2.
Contribution plots illustrating the key compounds that distinguish young and mature wines across three grape varieties (Merlot – light blue and blue, Mavrud – pink and red violet, and Sauvignon blanc – yellow and orange).