SUPPLEMENTARY DATA

Table S1. Correlation analysis between variables.

		Correlation analysis		
Variable A	Variable B	Correlation coefficient	Sig. (2-tailed)	Correlation test
Palate acidity	Total acids content	0.549*	0.018	Spearman's
Visual hue	a*	0.871**	<0.001	Pearson's
	b*	0.591**	0.010	Pearson's
	Hue	– 0.893**	<0.001	Pearson's
	ABS <420 nm>	0.613**	0.007	Pearson's
	ABS <520 nm>	0.777**	<0.001	Spearman's
	Tonality	– 0.846**	<0.001	Spearman's
	Yellow [%]	– 0.766**	<0.001	Pearson's
	Red [%]	0.784**	<0.001	Spearman's
Acetaldehyde	Nose: Biological *vs* Oxidative notes	– 0.310	0.210	Spearman's
Ethyl acetate	Nose: Biological *vs* Oxidative notes	0.603**	0.008	Spearman's
	Nose ageing notes + Palate ageing notes	0.637**	0.004	Spearman's
	Palate: Biological *vs* Oxidative notes	0.776**	<0.001	Pearson's
	Nose: Amontillado *vs* Oloroso	0.529*	0.024	Spearman's

The table reports correlation coefficients (r) and corresponding p-values obtained between selected sensory and instrumental variables. Pearson's or Spearman's correlation tests were applied depending on data distribution. Asterisks indicate levels of statistical significance ($p < 0.05$; ** $p < 0.01$).*

Table S2. Rotated component matrix for FTIR variables.

Rotated Component Matrix

	Component		
	1	2	3
Total acidity	0.925	– 0.226	– 0.046
Volatile acidity	0.055	– 0.077	0.708
Density	0.288	0.139	0.748
Reductive sugars	– 0.124	0.919	0.099
Malic acid	0.882	0.043	0.187
Lactic acid	0.459	– 0.09	0.22
IPT	– 0.012	0.262	0.71
Glucose	0.763	0.484	– 0.025
Fructose	0.04	0.966	0.139

Principal Component Analysis (PCA) was performed using Varimax rotation with Kaiser normalisation. Values are expressed as factor loadings. Higher absolute values indicate a stronger contribution of each variable to the corresponding principal component.

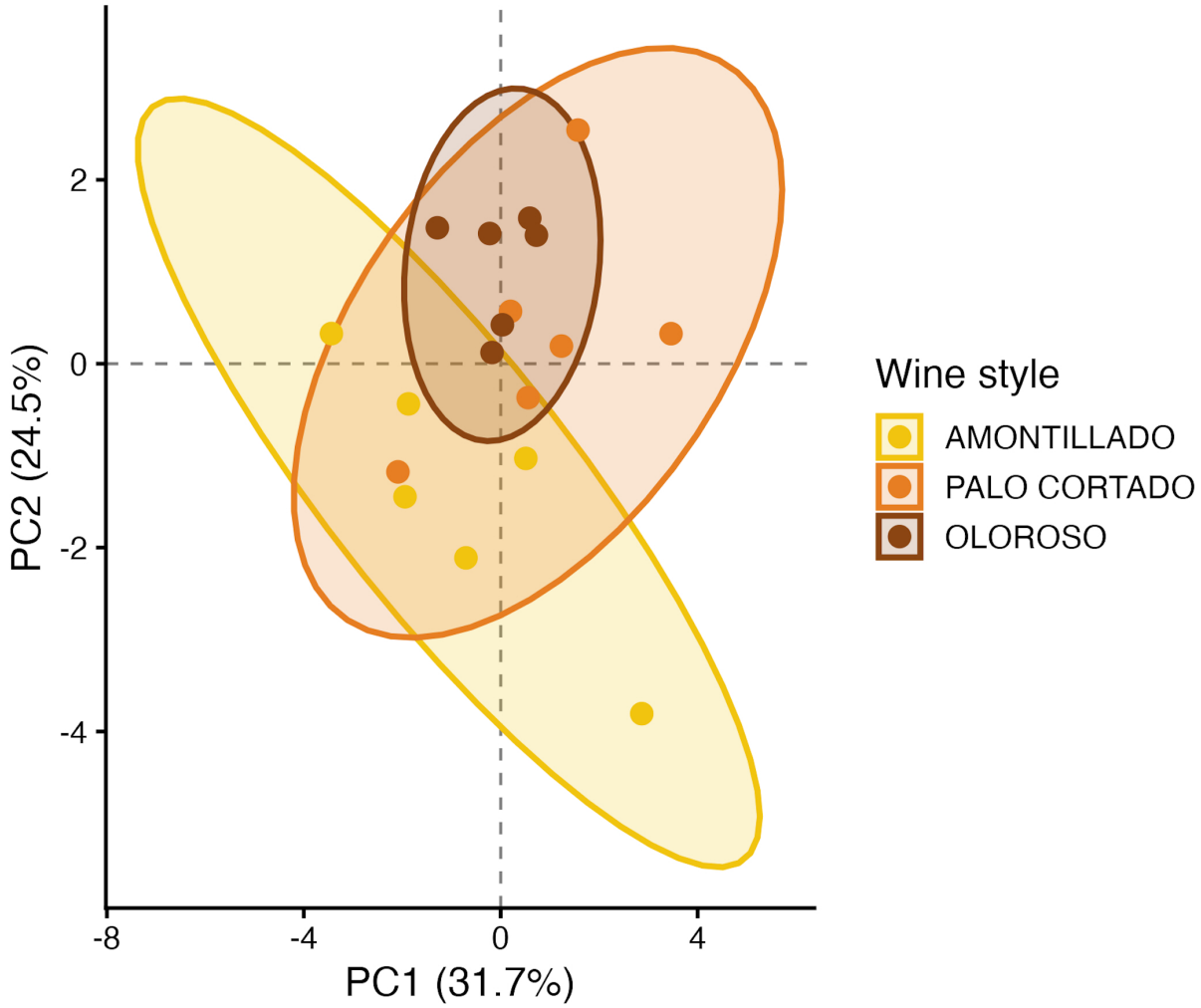


Figure S1. Principal Component Analysis (PCA) scores plot of oenological parameters.

Samples are coloured according to wine style, and ellipses represent the dispersion within each group.

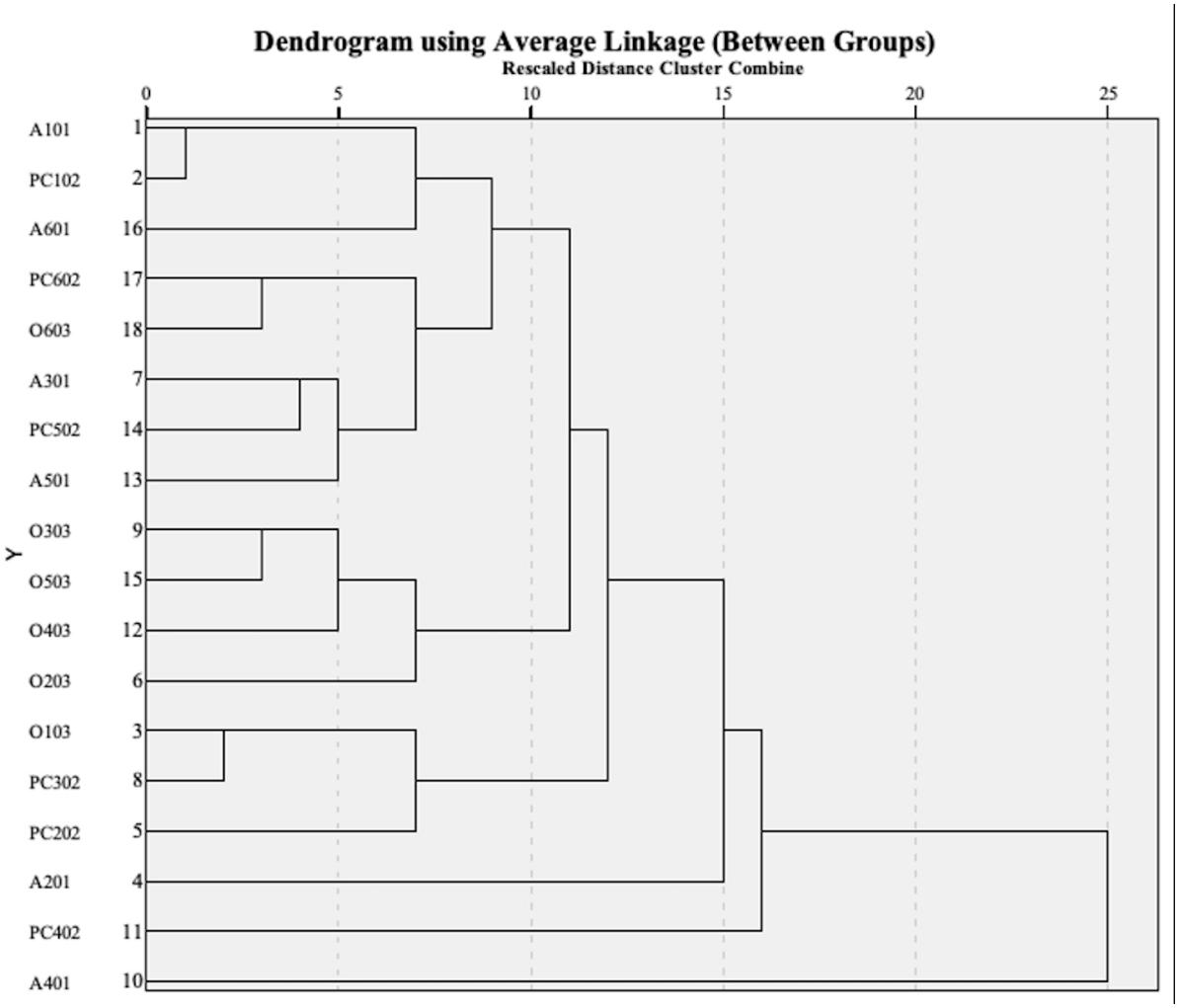


Figure S2. Hierarchical clustering dendrogram based on the FTIR-derived parameters of the wines.

Clustering was performed using squared Euclidean distance and the between-groups linkage method.

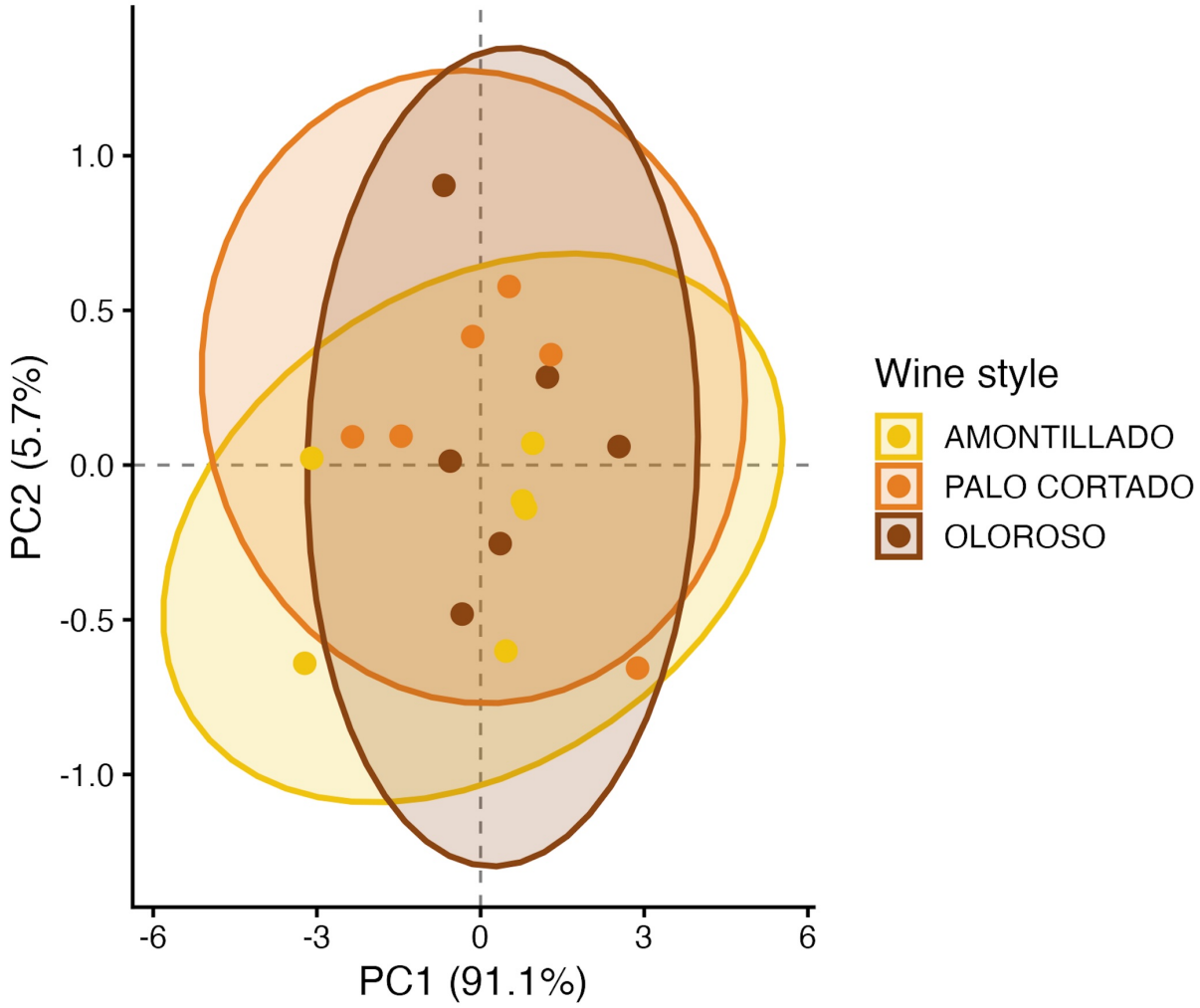


Figure S3. Principal Component Analysis (PCA) scores plot of absorbance parameters.

Samples are coloured according to wine style, and ellipses represent the dispersion within each group.

Table S3. Rotated component matrix for colour-related variables.

Rotated component matrix		
	Component	
	1	2
ABS 420 nm	0.48	0.87
ABS 520 nm	0.75	0.61
ABS 620 nm	0.88	0.45
L	– 0.86	– 0.44
a*	0.92	0.32
b*	0.38	0.93

Principal Component Analysis (PCA) was performed using Varimax rotation with Kaiser normalisation. Values are expressed as factor loadings. Higher absolute values indicate a stronger contribution of each variable to the corresponding principal component.

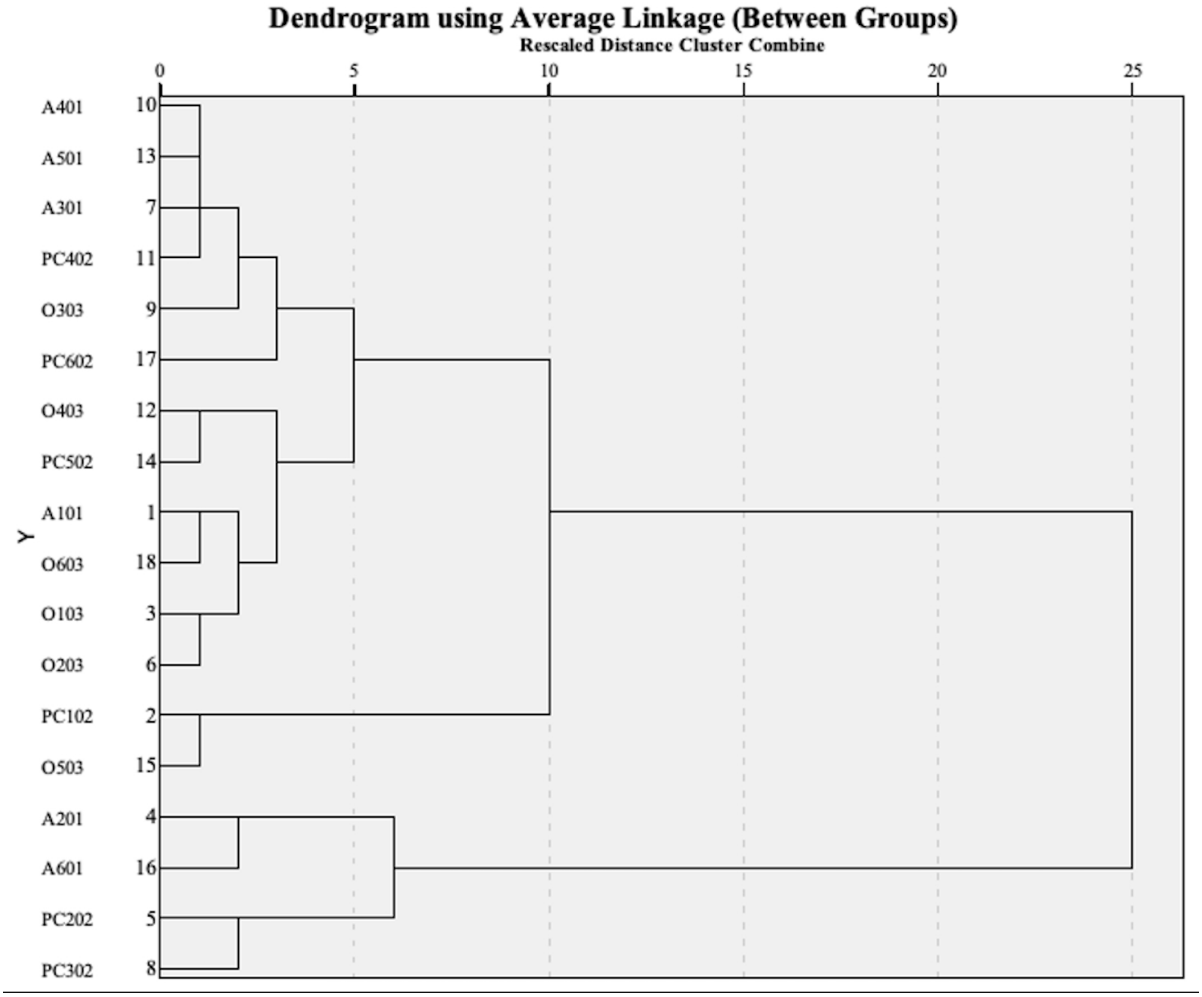


Figure S4. Hierarchical clustering dendrogram based on absorbance parameters of the wines.

Clustering was performed using squared Euclidean distance and the between-groups linkage method.

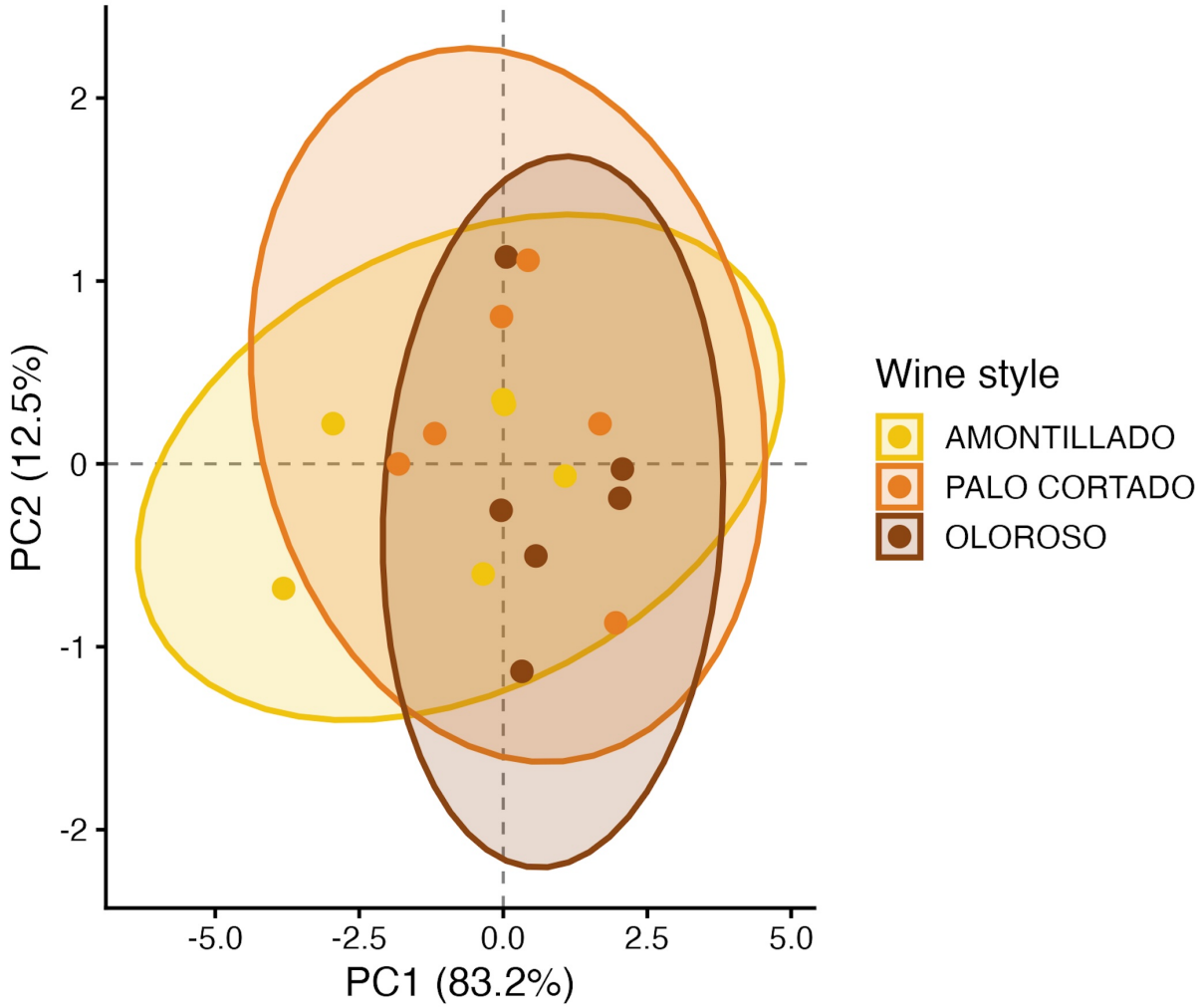


Figure S5. Principal Component Analysis (PCA) scores plot of CIELAB parameters.

Samples are coloured according to wine style, and ellipses represent the dispersion within each group.

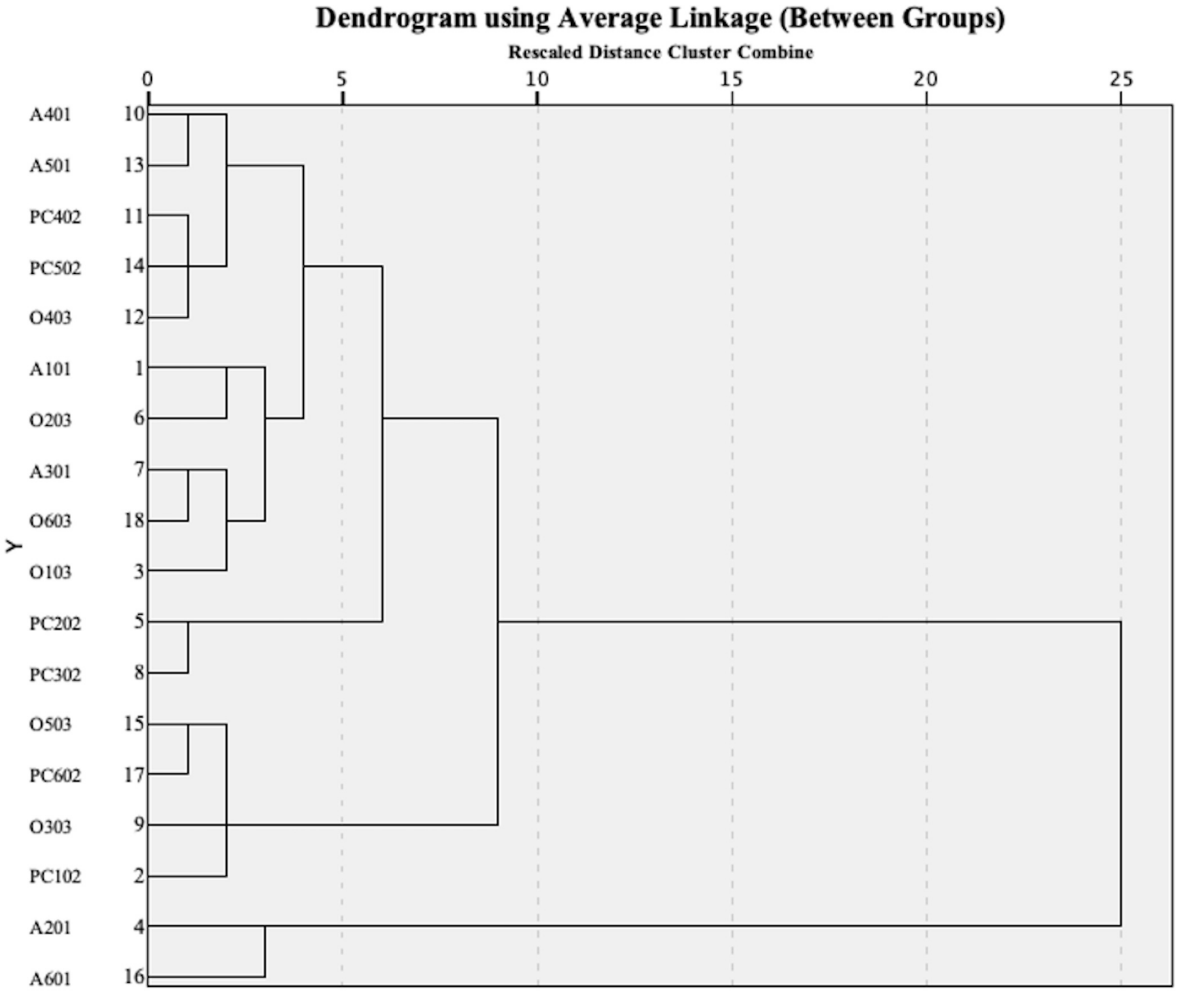


Figure S6. Hierarchical clustering dendrogram based on CIELAB parameters of the wines.

Clustering was performed using squared Euclidean distance and the between-groups linkage method.

Table S4. Rotated component matrix for volatile compounds.

Rotated component matrix						
	Component					
	1	2	3	4	5	6
Acetaldehyde	0.553	– 0.145	– 0.053	0.754	0.128	– 0.091
Methanol	0.232	0.242	– 0.228	0.810	– 0.153	0.029
1-propanol	0.885	– 0.055	0.139	0.008	0.031	– 0.109
Diacetyl	0.334	0.038	– 0.095	0.175	– 0.806	– 0.099
Ethyl acetate	0.003	0.437	– 0.298	– 0.768	0.070	0.016
Isobutanol	0.804	– 0.047	– 0.049	0.449	– 0.169	0.192
Acetic acid	– 0.240	0.805	– 0.062	– 0.106	– 0.006	0.322
1-butanol	0.105	0.932	0.029	0.106	0.072	0.045
Acetoin	0.363	0.188	– 0.063	0.057	0.203	0.787
3-methyl-1-butanol	0.816	– 0.065	0.018	0.231	0.005	0.351
2-methyl-1-butanol	0.679	– 0.108	0.397	– 0.034	– 0.119	0.503
Ethyl butyrate	0.320	– 0.185	0.700	0.101	0.355	– 0.427
Ethyl lactate	– 0.043	0.380	0.211	0.573	0.366	0.358
2,3-butanediol	0.357	0.366	– 0.205	0.166	0.758	0.054
Hexanol	0.066	– 0.111	0.962	– 0.048	– 0.083	0.112
2-phenylethanol	– 0.130	0.943	0.073	– 0.060	0.107	– 0.069
2-phenylethyl acetate	0.005	0.463	0.817	0.039	– 0.030	– 0.021

Principal Component Analysis (PCA) was performed using Varimax rotation with Kaiser normalisation. Values are expressed as factor loadings. Higher absolute values indicate stronger contributions to the corresponding principal component.

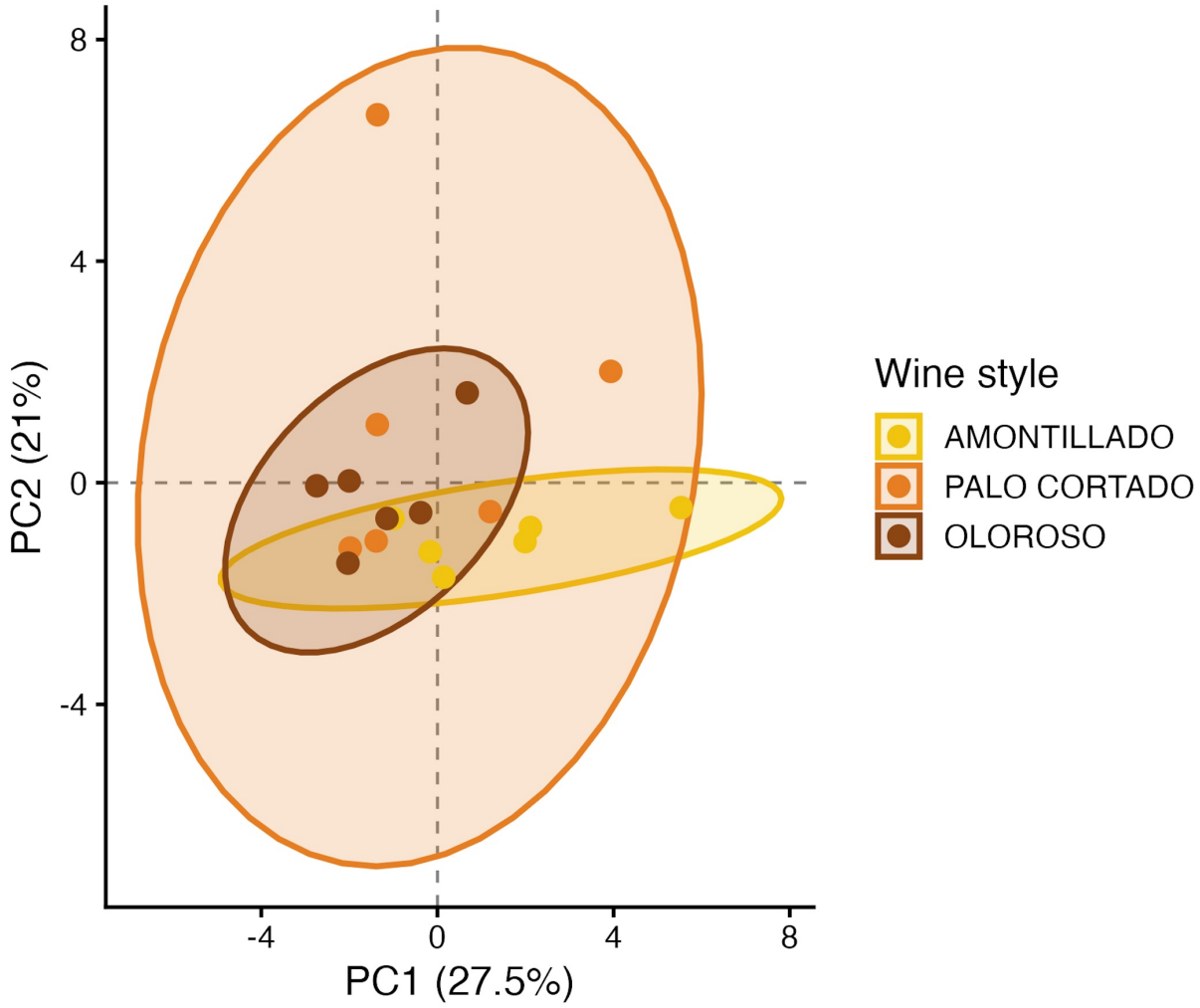


Figure S7. Principal Component Analysis (PCA) scores plot of quantification of volatile compounds.

Samples are coloured according to wine style, and ellipses represent the dispersion within each group.

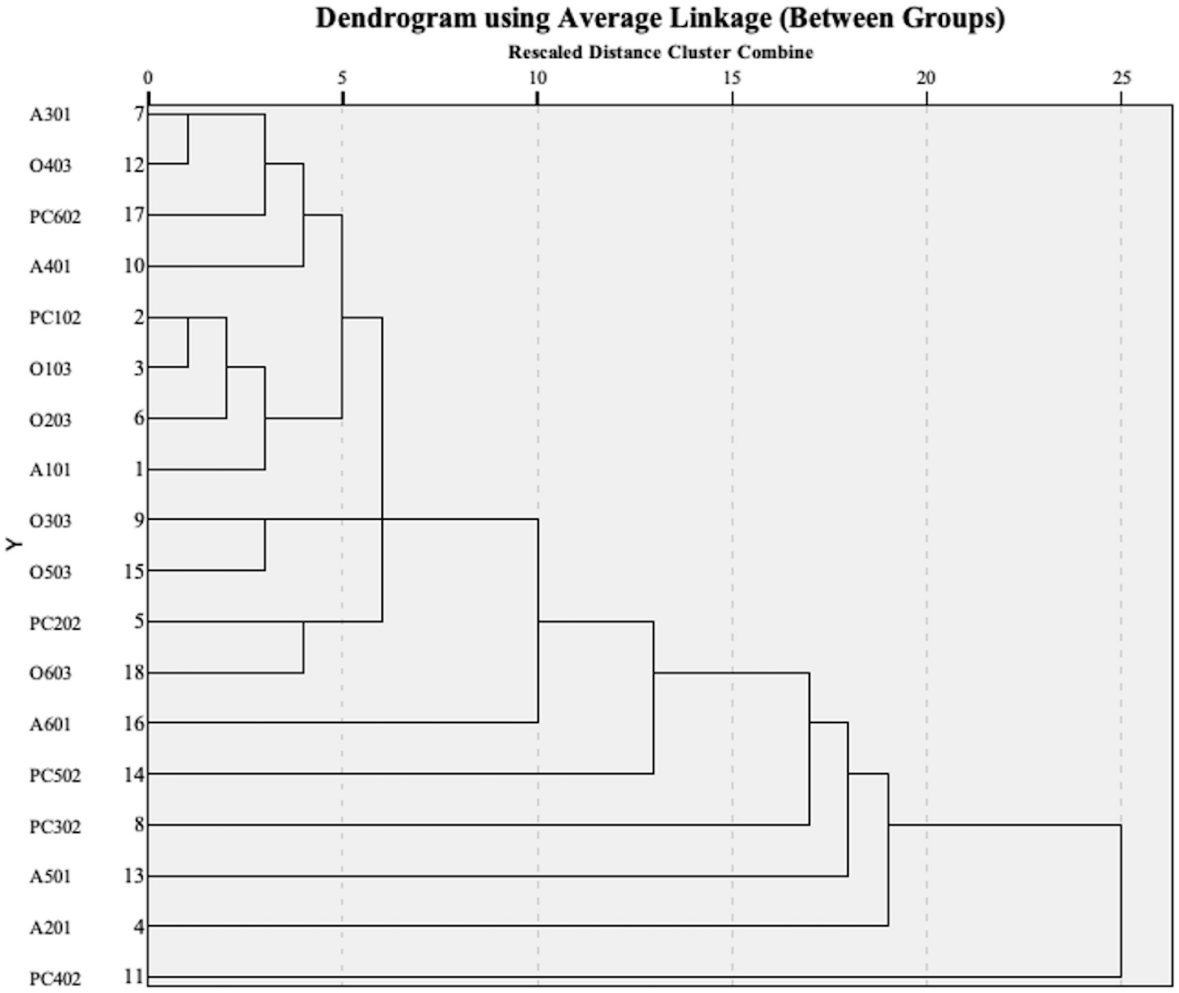


Figure S8. Hierarchical clustering dendrogram based on the volatile compound concentrations of the wines.

Clustering was performed using squared Euclidean distance and the between-groups linkage method.

Table S5. Rotated component matrix for selected sensory variables.

Rotated component matrix		
	Component	
	1	2
Nose: biological vs oxidative perception	0.75	0.39
Palate: intensity	0.65	0.63
Palate: tannins	0.26	0.90
Palate: body	0.90	0.25
Palate: biological *vs* oxidative perception	0.86	0.15
Visual: intensity	0.19	0.92
Visual: hue	0.50	0.80
Palate: complexity	0.77	0.42

Principal Component Analysis (PCA) was performed using Varimax rotation with Kaiser normalisation. Values are expressed as factor loadings. Higher absolute values indicate a stronger contribution of each variable to the corresponding principal component.

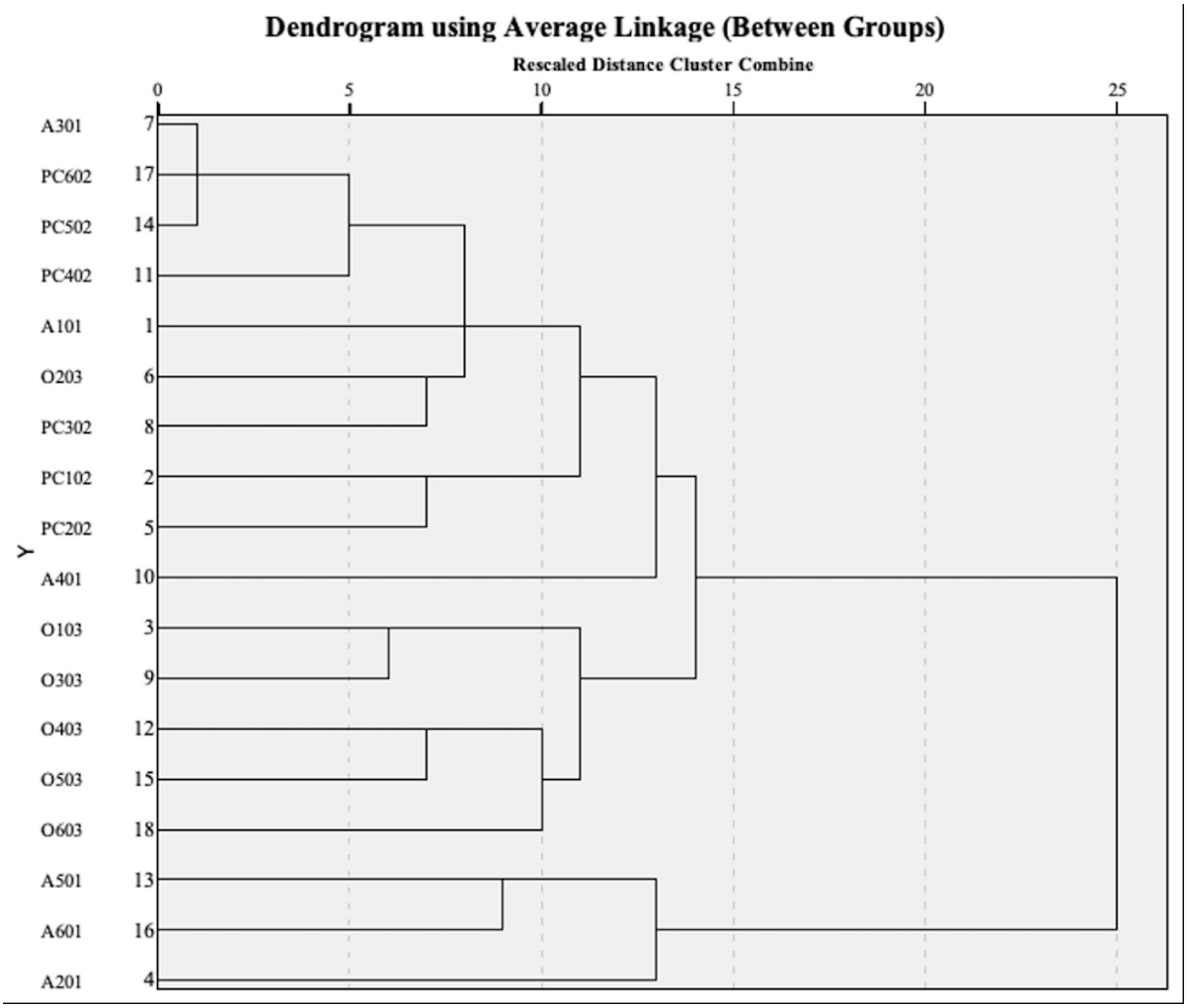


Figure S9. Hierarchical clustering dendrogram based on sensory attributes of the wines.

Clustering was performed using squared Euclidean distance and the between-groups linkage method.