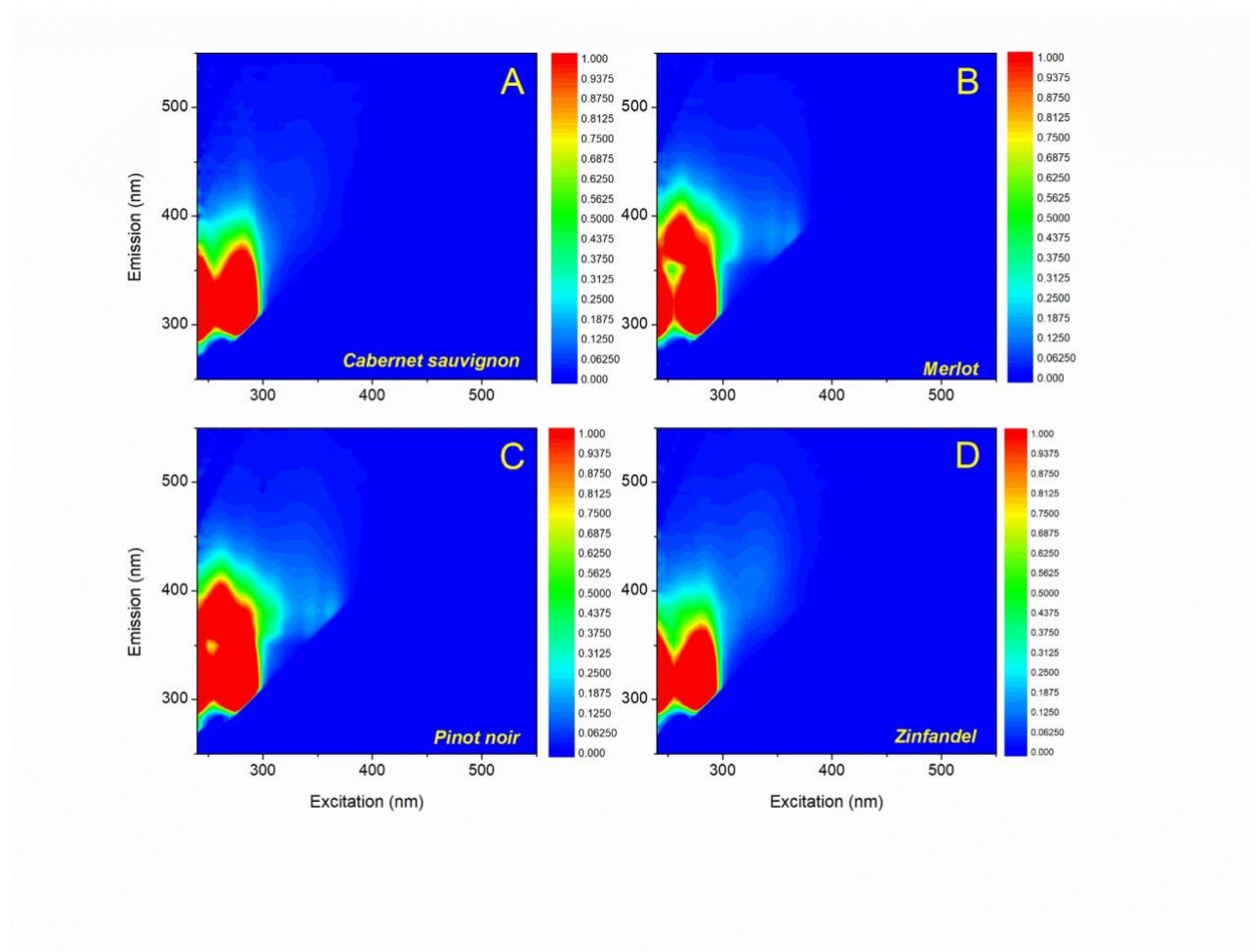


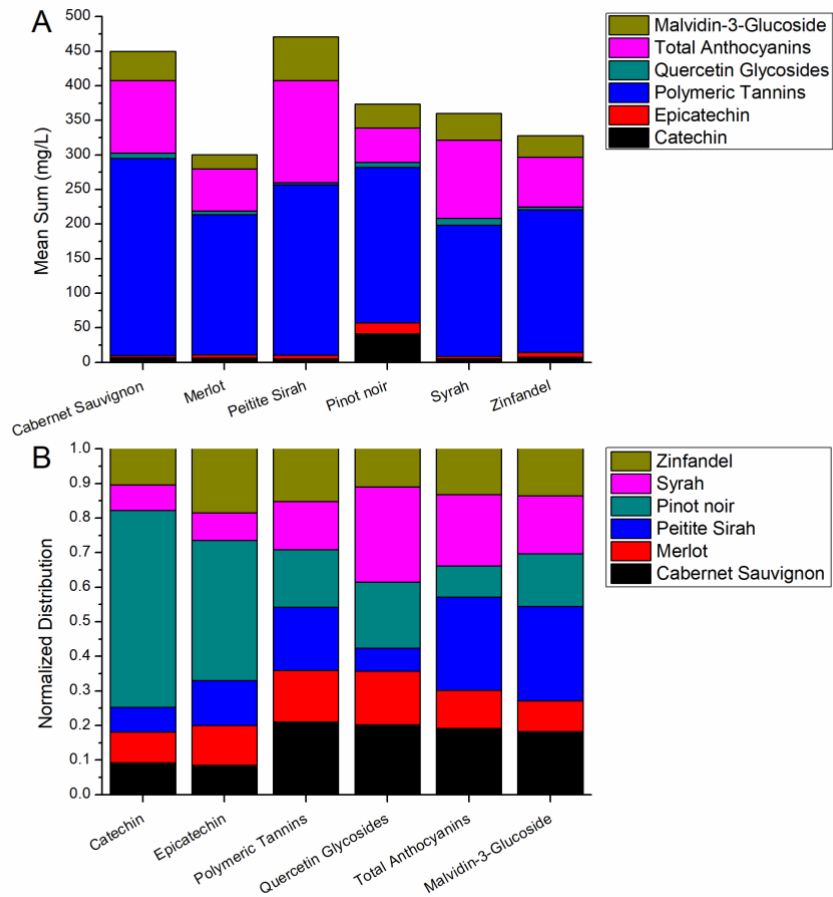
## Supplemental Material



**FIGURE S1.** Fluorescence Excitation-Emission matrix contour plots for the same typical Cabernet-Sauvignon (A), Merlot (B), Pinot noir (C) and Zinfandel (D) grape extract samples shown in Figure 1 with peak contours scaled to a value of 1.

**SUPPLEMENTARY DATA**

Gilmore, A. M., Sui, Q., Blair, B., & Pan, B. S. (2022). Accurate varietal classification and quantification of key quality compounds of grape extracts using the absorbance-transmittance fluorescence excitation emission matrix (A-TEEM) method and machine learning. *OENO One*, 56(4). <https://doi.org/10.20870/oeno-one.2022.56.4.5561>



**FIGURE S2.** Panel A shows the Mean Sum distribution comprising the six quality compound marker concentrations listed in the legend plotted as the averages from the validation data set organised of the six varieties tested on the x-axis. Panel B shows the same data as Panel A organised as the normalised distribution of each of the six quality marker compounds on the x-axis for the six varieties listed in the legend.

**TABLE S1.** Multivariate model configurations for Solo V8.9.2 and V9.0 used for Varietal Clustering, Classification and Phenolic Regression Models.

Model Parameter	Pre-processing X-block	Pre-processing Y-block	Model Options
			Agglomerative HCA Options
Varietal HCA	CCCR Offset = 0.1 EMM Filter Full Rank	NA	Ward's Method Use Manhattan Distance
			**XGBDA Model Options
Varietal XGBDA	GLSW = 0.048 CCCR Offset = 0.04	NA	Max depth = 1 Num round = 1000 ETA = 0.02 PLS Compression LV = 7
Regression			XGB Model Options
Polymeric Tannins	GLSW = 0.22 CCCR Offset = 0	Mean Centring Variance (Std) Scaling	Max depth = 6 Num round = 300 ETA = 0.05 PLS Compression LV = 5
Total Anthocyanins	EPO/EMM Filter = 2 PCs CCCR Offset = 0	Mean Centring Poisson (Sqrt Mean) Scaling	Max depth = 5 Num round = 300 ETA = 0.2 PLS Compression LV = 3
Malvidin-3-Glucoside	EMM Filter (Full Rank) CCCR Offset = 0	Poisson (Sqrt Mean Scaling) Offset = 3 %	Max depth = 2 Num round = 1000 ETA = 0.08 PLS Compression LV = 5
Catechin	GLSW = 0.02 CCCR Offset = 0.12	Mean Centring Poisson (Sqrt Mean) Scaling	Max depth = 3 Num round = 500 ETA = 0.3 PLS Compression LV = 6
Epicatechin	CCCR Offset = 0 EPO/EMM Filter = 2 PCs	Poisson (Sqrt Mean Scaling) offset = 4% Mean Centring	Max depth = 4 Num round = 600 ETA = 0.4 PLS Compression LV = 6
Quercetin Glycosides	GLSW = 0.011 CCCR Offset = 0	Mean Centring Poisson (Sqrt Mean) Scaling	Max depth = 1 Num round = 400 ETA = 0.1 PLS Compression LV = 4

All terms and model settings, including those abbreviated as listed below, are defined in the Eigenvector wiki pages at the following URL: [https://www.wiki.eigenvector.com/index.php?title=Main\\_Page](https://www.wiki.eigenvector.com/index.php?title=Main_Page)

CCCR = Class Centroid Centring and Scaling including Scale Offset

EMM Filter = Extended Mixture Model

EPO Filter = External Parameter Orthogonalisation

ETA = Controls the learning rate of the XGB gradient boosting

GLSW = Generalised Least Squares Weighting

HCA = Hierarchical Cluster Analysis

Max depth = Setting to specify the maximum depth allowed for the XGB decision tree

Num round = Specifies how many rounds of XGB tree creation to perform

PLS Compression LV = Number of Latent Variables used in the X-block compression mode

All XGBDA and XGB regression models used the gbtree booster option.