Electronic Supplementary Information

Discrimination of Flavonoids and Red Wine Varietals by Arrays of Differential Peptidic Sensors

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Table S1. MS analysis and yields of peptides

Peptide	Sequence	% Yield	MS (Calc'd)	MS (Found)
1	IHIGHHI	95.8	825.46 (M^+)	826, $M+2H^+$
2	WAHEDEFF	47.2	1080.44 (M^+)	1081, $M+H^+$; 1103, $M+Na^+$
3	FHFPHHF	60.0	968.45 (M^+)	969, $M+H^+$; 485, $M+2H^+$
4	WGHGGHHG	57.0	844.36 (M^+)	845, $M+H^+$; 866, $M+Na^+$
5	WDHHHD	35.6	846.33 (M^+)	846.55, $M+H^+$
6	WEHHHE	75.0	874.36 (M^+)	438, $M+2H^+$
7	WDDHDD	70.5	802.26 (M^+)	402, $M+2H^+$
8	WEEHEE	66.7	858.33 (M^+)	430, $M+2H^+$
9	PHGGGWGQ	40.3	795.45 (M^+)	795.54 $M+H^+$ 398.70 $M+2H^+$
10	WHCCHDHCD	30.5	1155.36 (M^+) 578.18 ($M + 2H^+$)	578.59, $M + 2H^+$

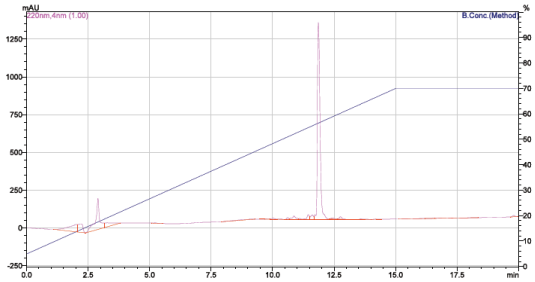


Figure S1. HPLC chromatogram of **1** (220 nm)

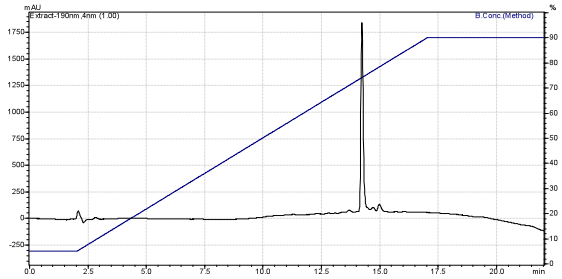


Figure S2. HPLC chromatogram of **2** (190 nm)

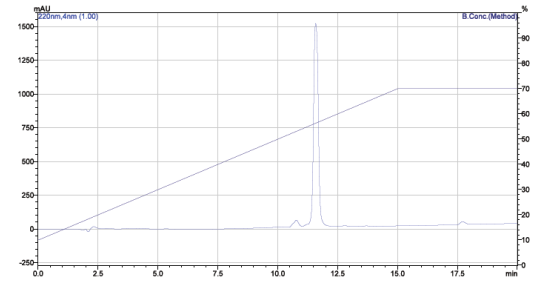


Figure S3. HPLC chromatogram of **3** (220 nm)

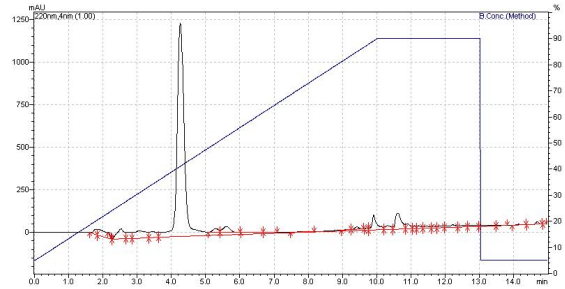


Figure S4. HPLC chromatogram of **4** (220 nm)

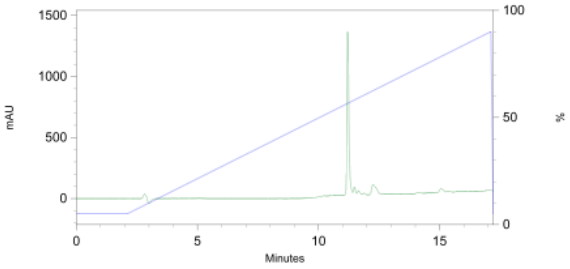


Figure S5. HPLC chromatogram of **5** (220 nm)

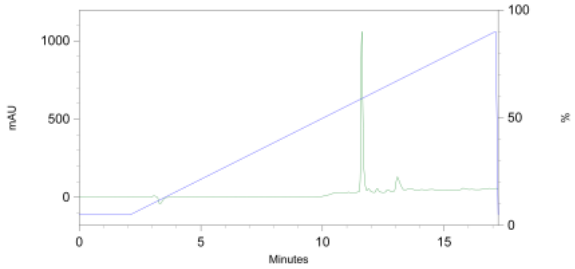


Figure S6. HPLC chromatogram of **6** (220 nm)

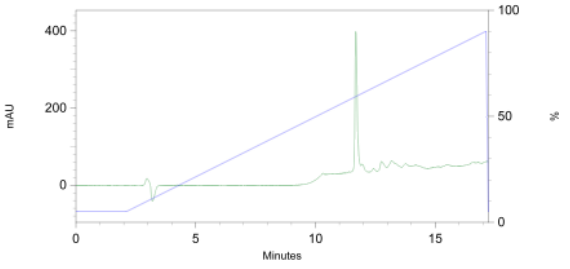


Figure S7. HPLC chromatogram of **7** (220 nm)

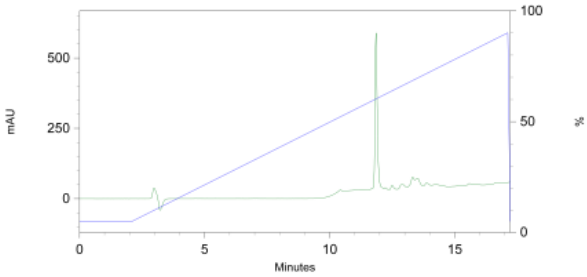


Figure S8. HPLC chromatogram of **8** (220 nm)

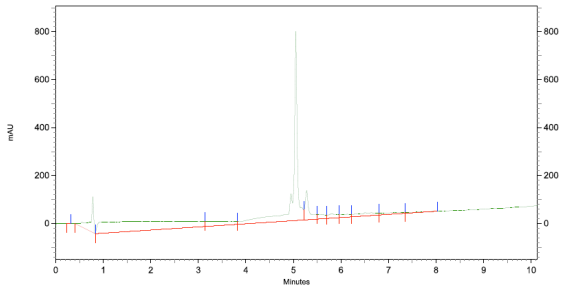


Figure S9. HPLC chromatogram of **9** (220 nm)

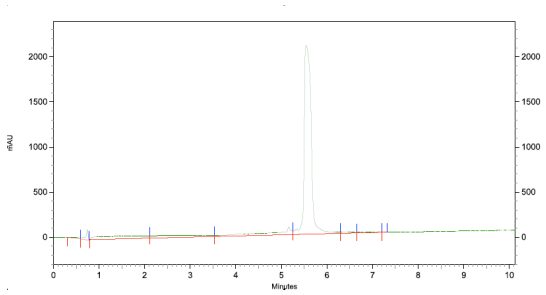


Figure S10. HPLC chromatogram of **10** (220 nm)

Table S2. Conditions for the binding assay between Cu^{2+} and PCV

	Solution in cuvette	Titrant
[HEPES], mM (in 1:1 ethanol:H_2O, v/v)	50	50
[PCV], mM	0.075	0.075
[Cu^{+2}], mM	0	0.750
pH	7.4	7.4
Total volume (μL)	2000	2000

Table S3. Conditions for the binding assays for peptides and Cu^{2+}:PCV complex

	Solution in cuvette	Titrant
[HEPES], mM (in 1:1 ethanol:H_2O, v/v)	50	50
[PCV], mM	0.075	0.075
[Cu^{+2}], mM	0.075	0.075
[Peptide], mM	0	Varied from 0.2 to 0.4
pH	7.4	7.4
Total volume (μL)	2000	2000

Table S4. Concentrations of solutions for cuvette assays to determine the optimal concentrations of peptides, metals and indicators composing the sensing ensemble

Sensing ensemble	[Metal^{2+}], mM, in cuvette	[Indicator], mM, in cuvette	Composition of sensing ensemble chosen (peptide:metal:indicator)
PCV-Cu^{2+}-**3**	0.075	0.075	1:1:1
PCV-Cu^{2+}-**4**	0.075	0.075	0.5:1:1
PCV-Cu^{2+}-**2**	0.075	0.075	0.5:1:1
PCV-Cu^{2+}-**1**	0.075	0.075	1:1:1
PCV-Cu^{2+}-**5**	0.075	0.075	0.5:1:1
PCV-Cu^{2+}-**6**	0.075	0.075	0.25:1:1
PCV-Cu^{2+}-**7**	0.075	0.075	0.5:1:1
PCV-Cu^{2+}-**8**	0.075	0.075	0.5:1:1
PCV-Cu^{2+}-**9**	0.075	0.075	0.5:1:1
PCV-Cu^{2+}-**10**	0.075	0.075	0.125:1:1
CAS-Cu^{2+}-**3**	0.060	0.060	0.5:1:1
CAS-Cu^{2+}-**8**	0.060	0.060	0.4:1:1
BPR-Ni^{2+}-**3**	0.018	0.018	0.75:1:1
BPR-Ni^{2+}-**8**	0.018	0.018	1:1:1

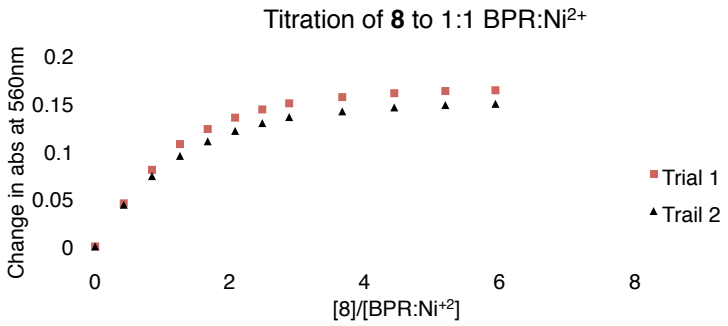


Figure S11. Binding curve from the titration of **8** to 1:1 **NB** (Ni^{2+}-bromopyrogallol red complex)

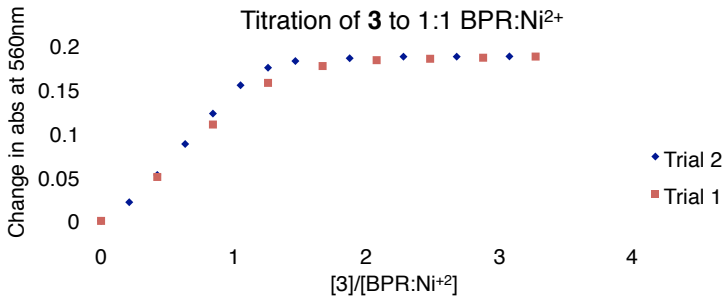


Figure S12. Binding curve from the titration of **3** to 1:1 **NB** (Ni^{2+}-bromopyrogallol red complex)

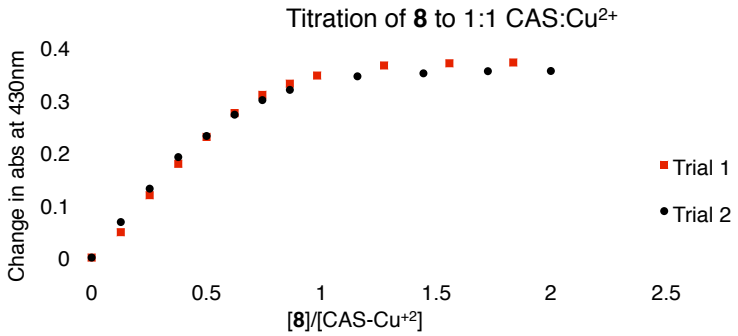


Figure S13. Binding curve from the titration of peptide **8** to **CC** (Cu^{2+}-chromazurol S complex)

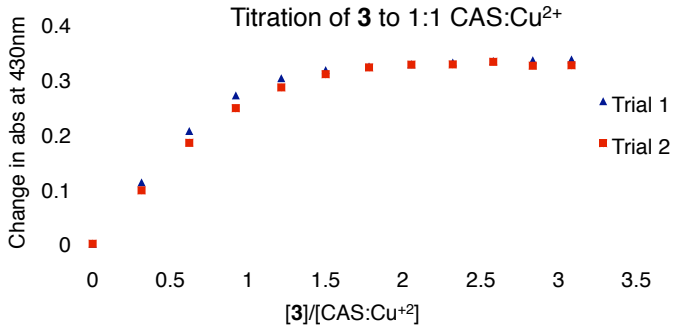


Figure S14. Binding curve from the titration of peptide **3** to **CC** (Cu^{2+}-chromazurol S complex)

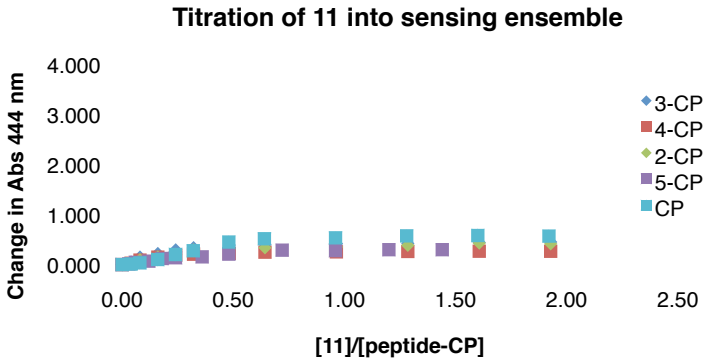


Figure S15. Titration of peptide **11** into peptide-**CP** complexes

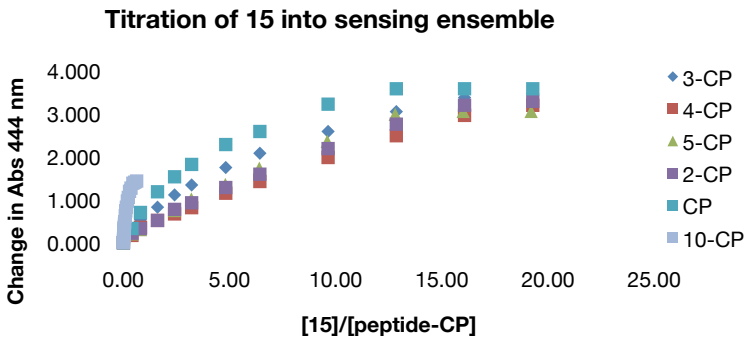


Figure S16. Titration of peptide **15** into peptide-**CP** complexes

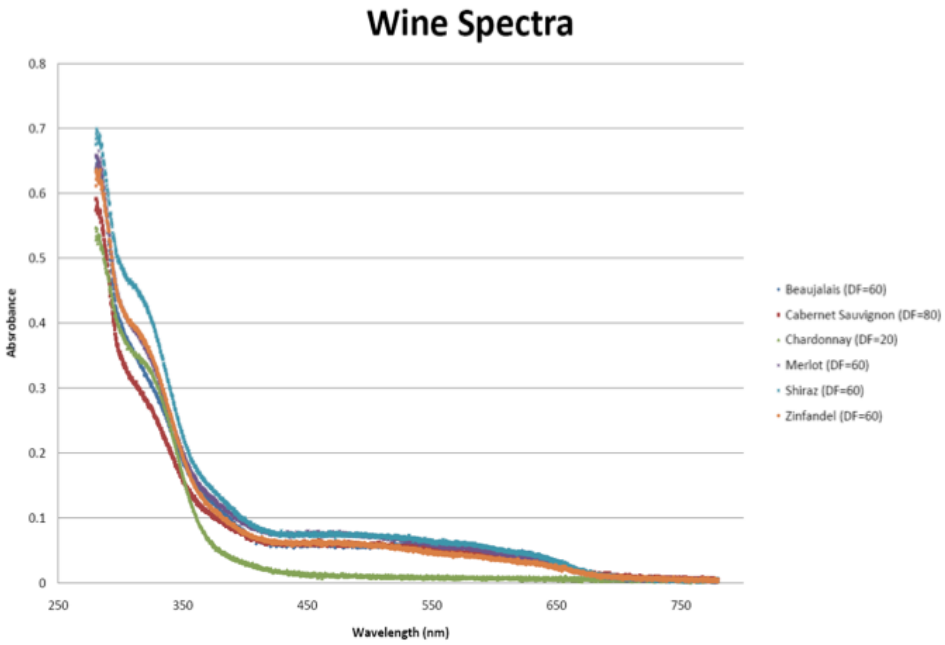


Figure S17. Spectra of different wines at pH 7.4. Wines were in 50 mM HEPES dissolved in 1:1 ethanol:water.

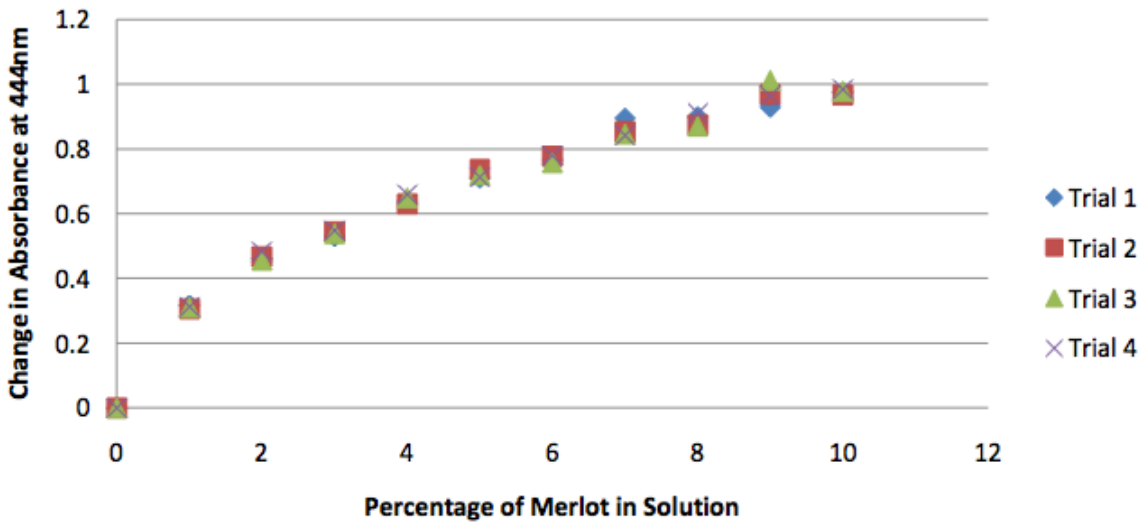


Figure S18. Binding curve of Merlot with PCV-Cu^{2+}.

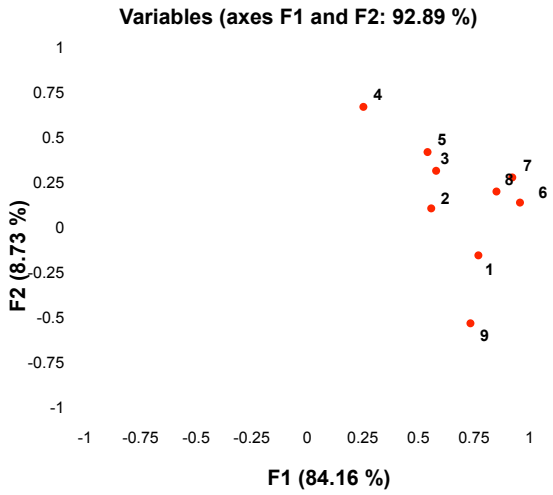
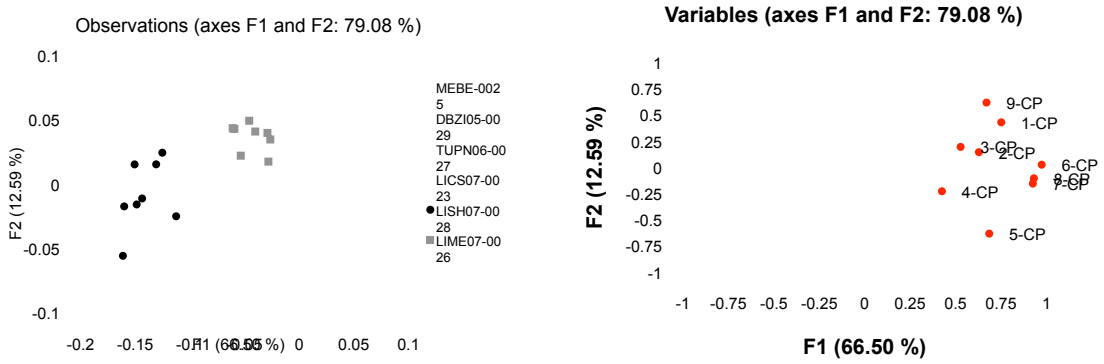
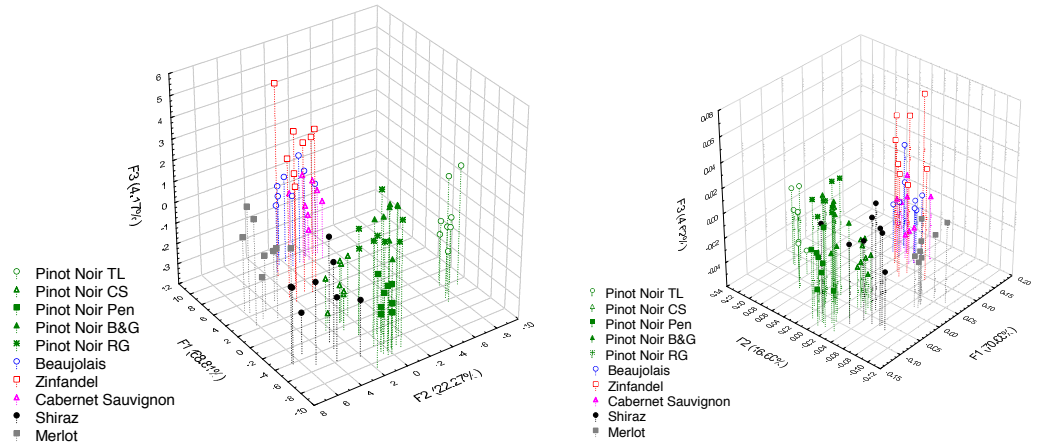


Figure S19. Variable correlation plot from the LDA of spectroscopic data from the discrimination of wine varietals using array **Y**. Sensing ensembles are represented by the peptide number.



A B

Figure S20. PCA score plot (A) and loading plot (B) from the evaluation of different wine varietals using array **Y**. Numbers represent the peptides in the peptide:Cu^{2+}:pyrocatechol violet complex



A B

Figure S21. LDA (A) and PCA (B) plots from the evaluation of Pinot Noir wines and other wine varietals using array **Y**.

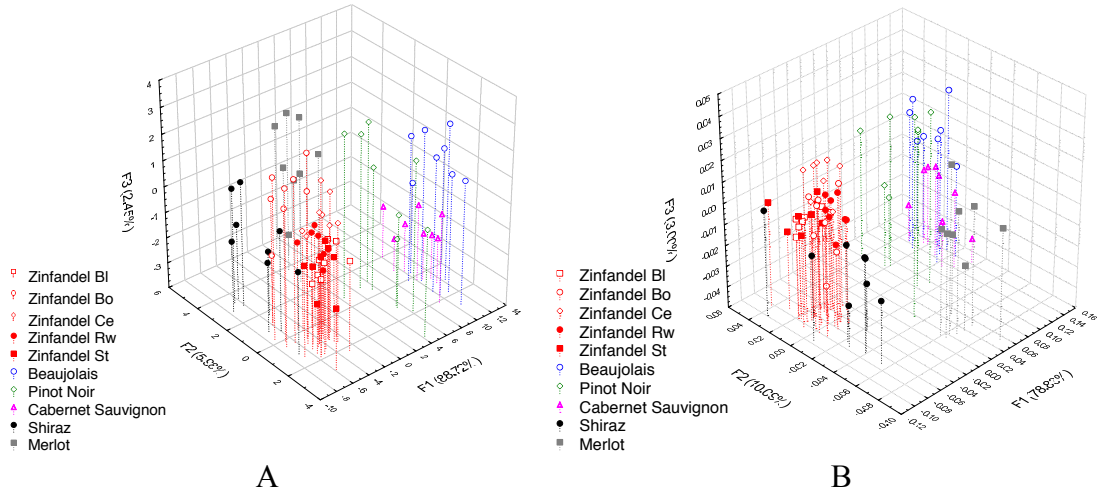


Figure S22. LDA (A) and PCA (B) plots from evaluation of Zinfandel wines and other varietals evaluated with array **Y**.

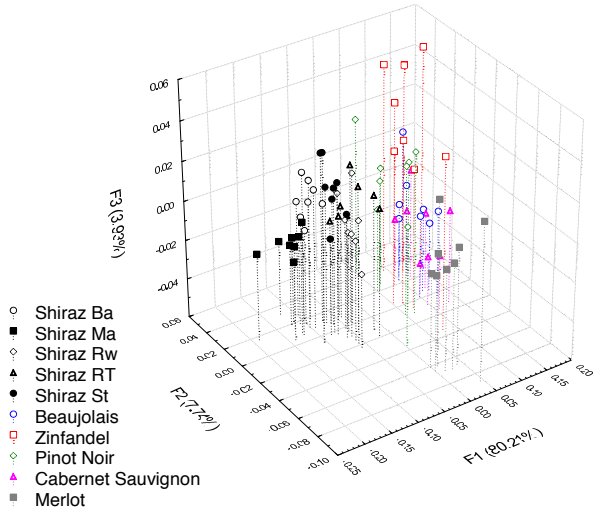
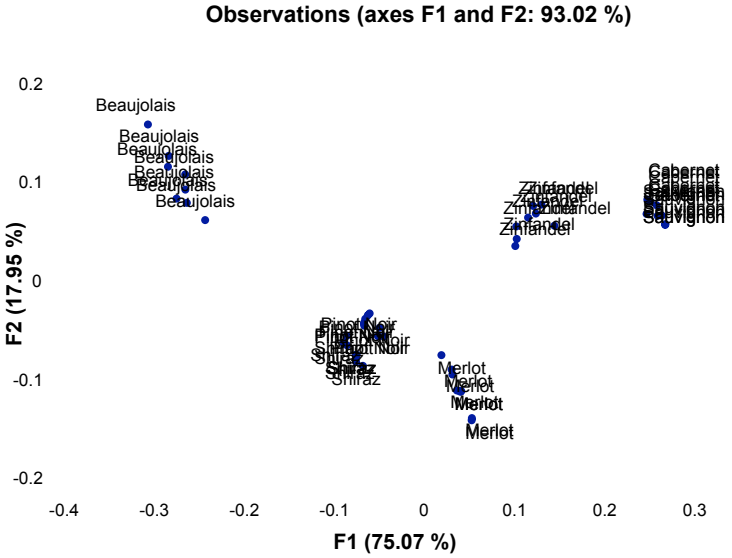


Figure S23. PCA from the evaluation of Shiraz wines and other varietals using array **Y**

A



B

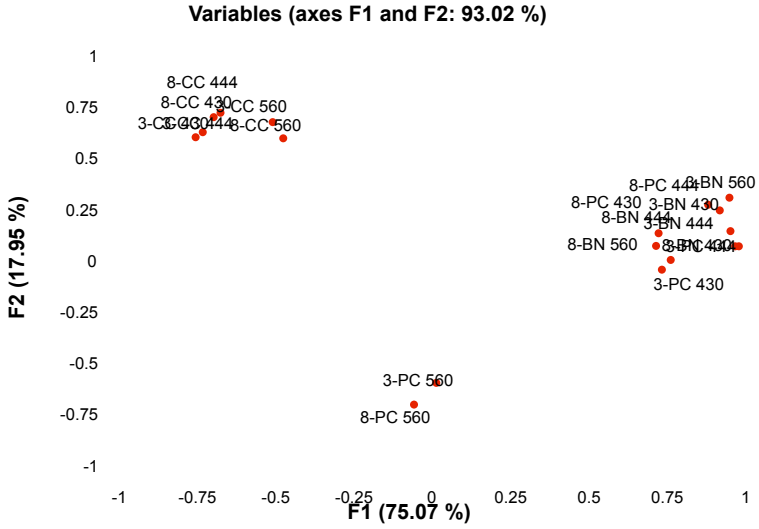
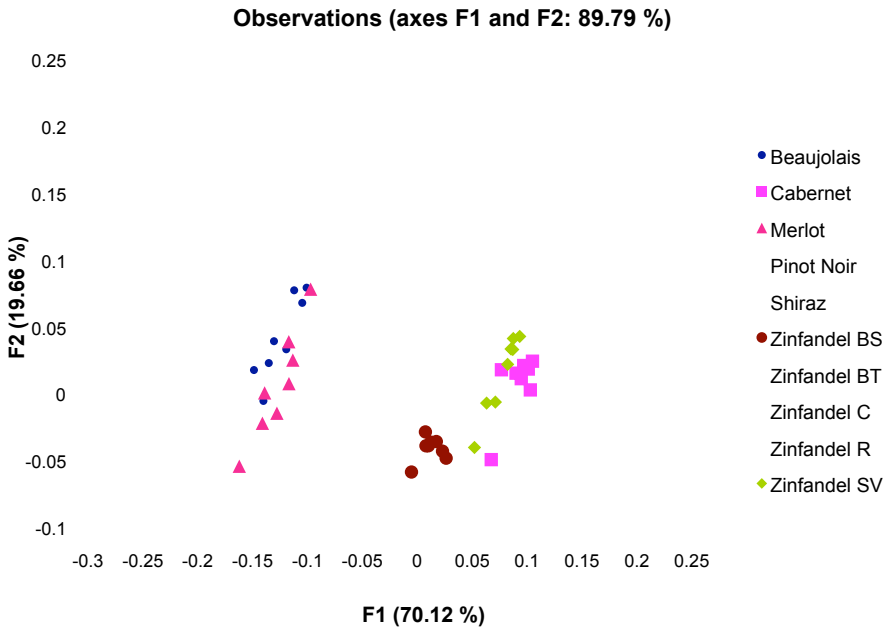


Figure S24. (**A**) Score plot and (**B**) corresponding loading plot of PCA of UV-vis response from the evaluation of different wine varietals using array **Z**.

A



B

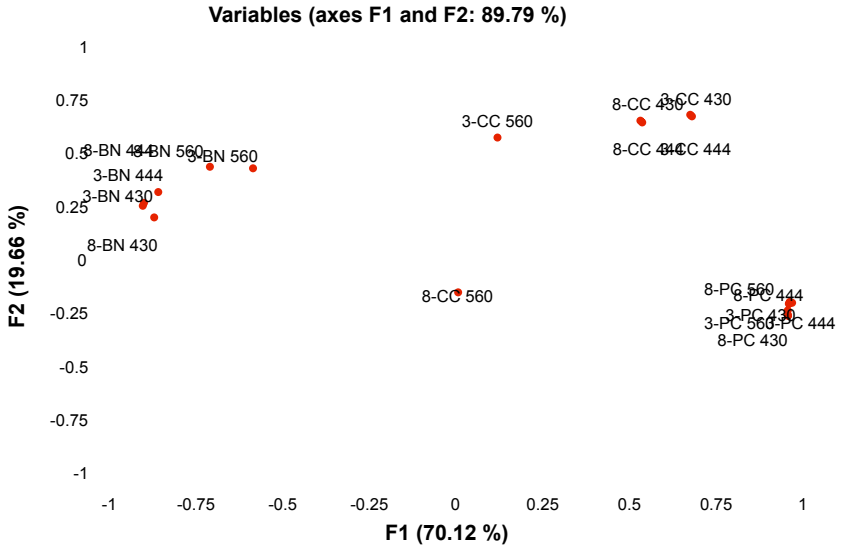


Figure S25. (**A**) Score plot and (**B**) corresponding loading plot of PCA of UV-vis response from the evaluation of different wine varietals and different brands of Zinfandel wines BS, BT, C, R, and SV with array **Z**.

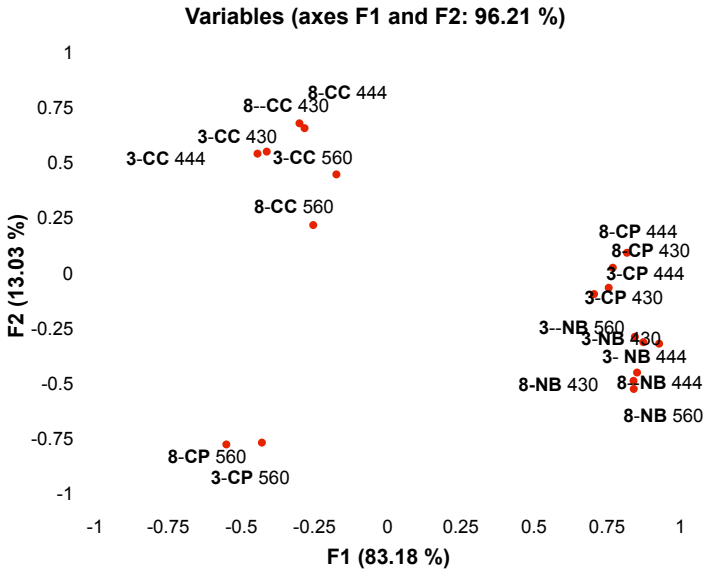


Figure S26. Variable correlation plot from the LDA of spectroscopic data from the discrimination of Zinfandel wines and other wine varietals using array **Z**.