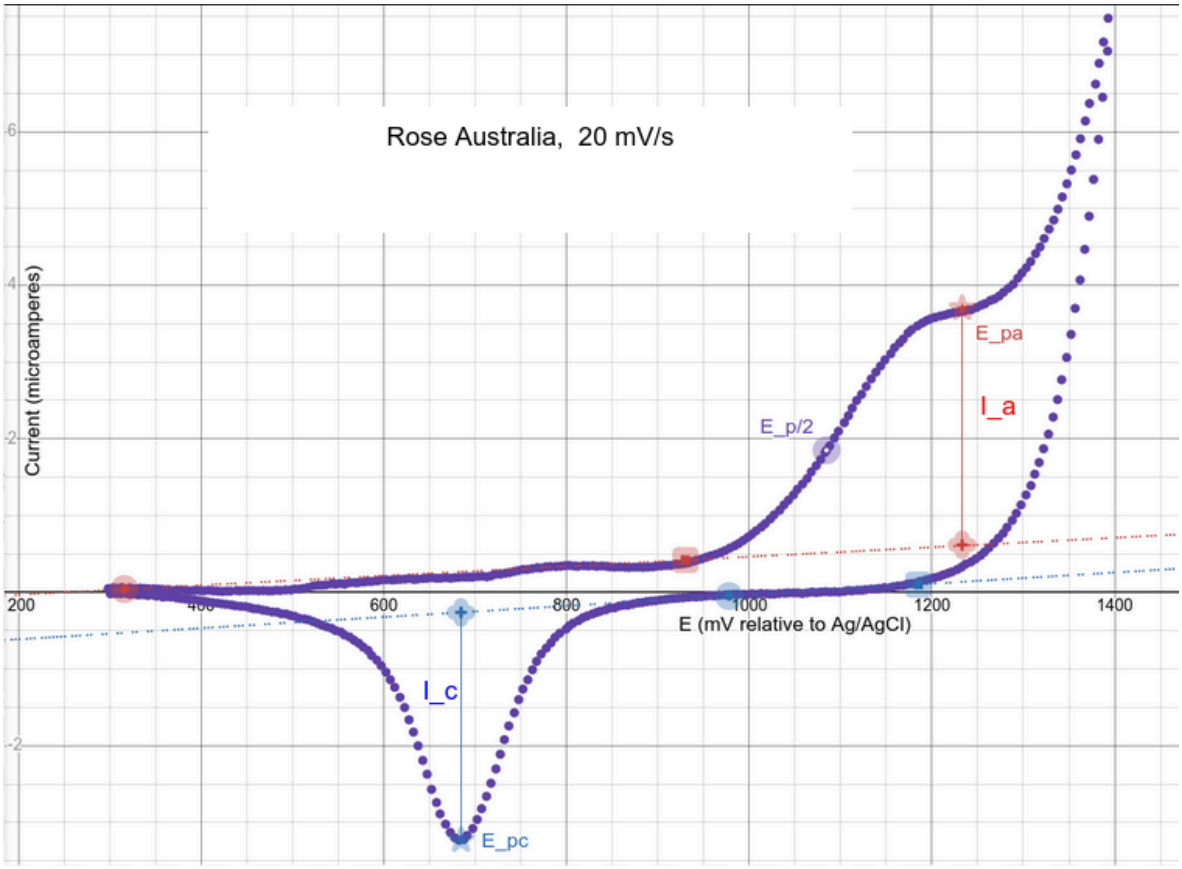
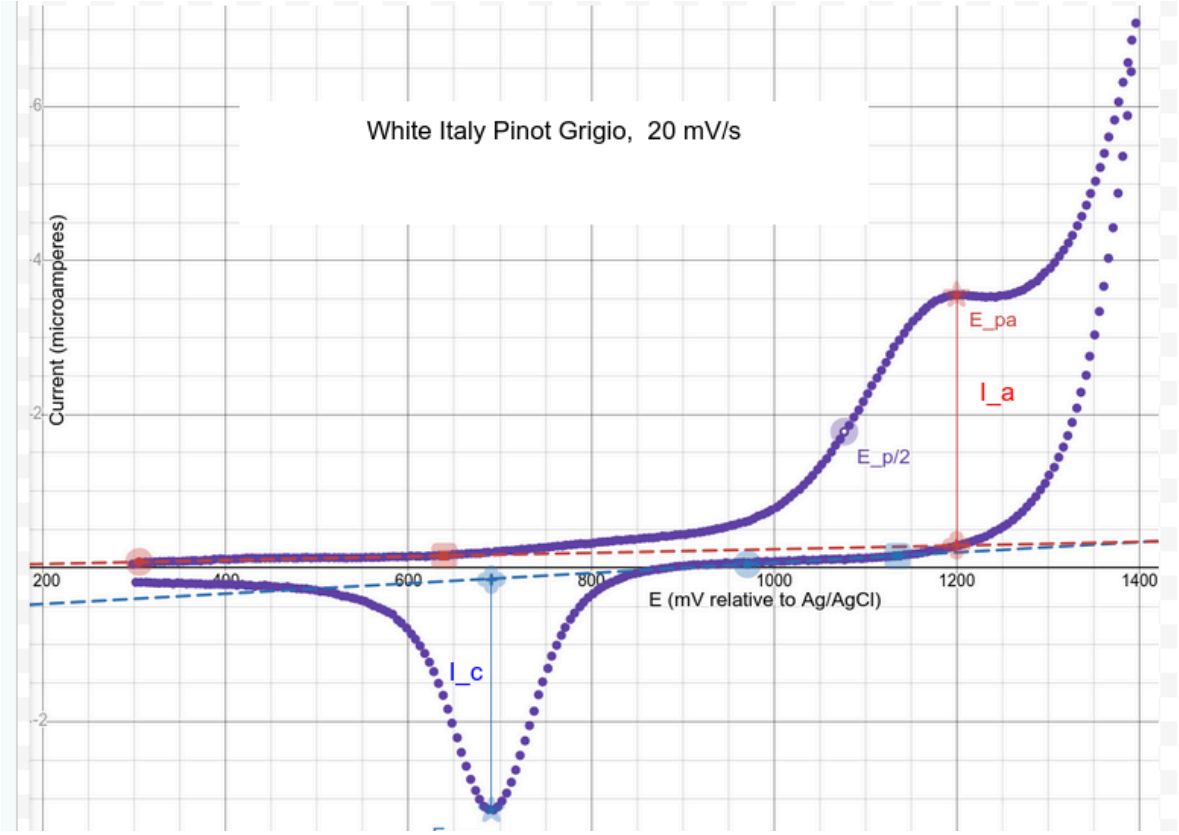
Lab 9: Analysis of Wine Using PCA

Questions

1. https://docs.google.com/spreadsheets/d/11nICFs_IWLvptGVQwJOkuhFIGhMHvmXj-roou_IRF8I/edit?usp=sharing
2. 



3. Voltages given relative to SHE

Wine type and name	Scan Rate (mV/s)	Epa (mV)	Epc (mV)	Ep/2 (mV)	Emid (mV)	(Epa+Ep/2)/2 (mV)	Epa-Ep/2	Ipa (A)	Ipc (A)	Ipc/Ipa (A)
White Italy Pinot Grigio B	20	1419.7	910.5	1297	1165.1	1358.35	122.7	3.25E-06	-3.00E-06	-0.92
Rose Australia	20	1453	913	1308	1183	1380.5	145	3.12E-06	-2.96E-06	-0.95
Unknown	20	1421.6	927	1313	1174.3	1367.3	108.6	-3.06E-06	-3.06E-06	1.00

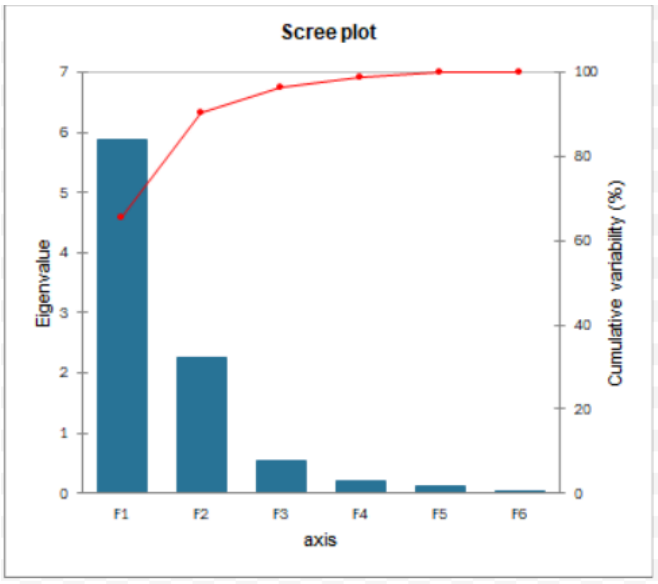
4. Given that we only have three data points for each category, there is insufficient power to determine based on our samples alone which characteristics are the same or different between the wine samples. All observed and computed values are relatively similar to roughly the same extent. The unknown wine is closer to the white wine for cathodic measurements and closer to the Rose for anodic measurements.

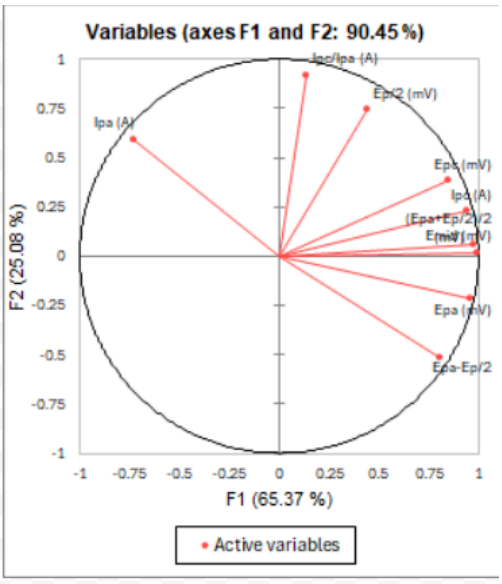
The potential for ferricyanide vs Ag/AgCl can be computed from literature as 360 mV - 220 mV = 140 mV. It was not recorded experimentally during this lab due to explicit instruction by a TA.

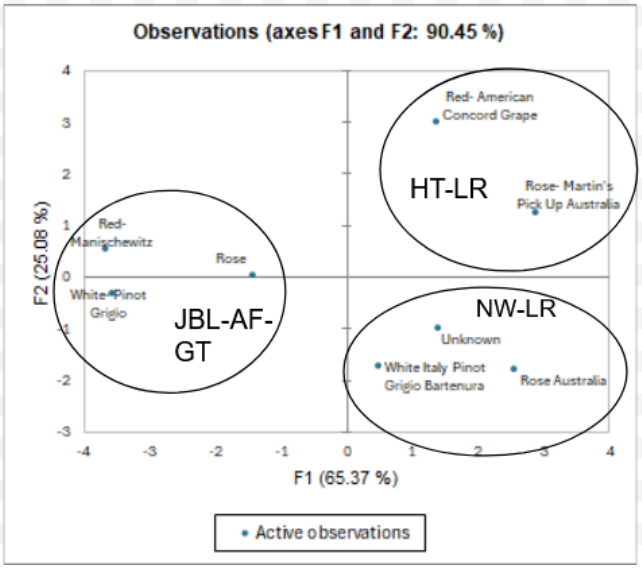
Our blank reading showed strong repeated evidence of contamination with observed peaks similar to our voltammograms for the wine sample, thus we did not subtract our blank for our data analysis.

Conclusion

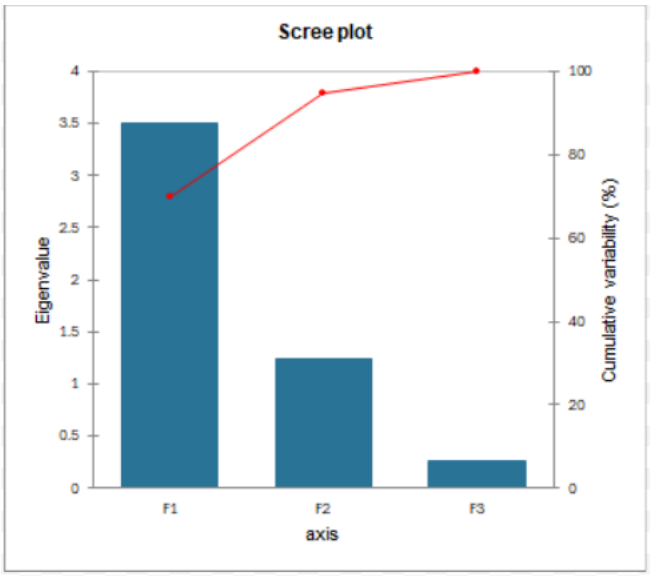
1. Regardless of the choice of all features, just the reduction features, or just the oxidation features, the clustering cleanly appears around the lab group which conducted the analysis, not the color or country of the wine. These clusters have been circled and labeled with the intials of the lab group which contributed the sample.

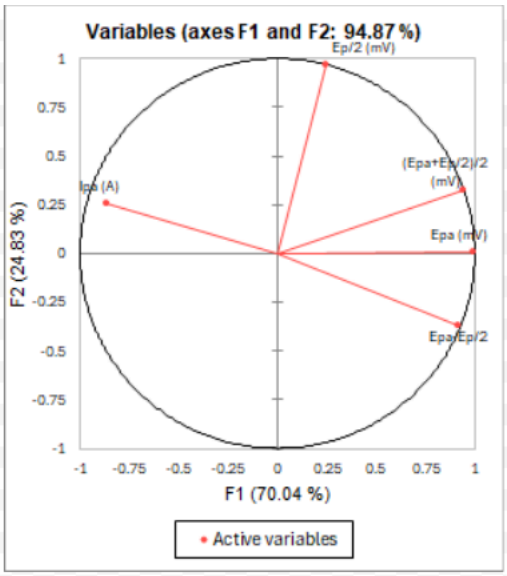

Scree plot
Eigenvalue
Cumulative variability (%)
F1
F2
F3
F4
F5
F6
axis

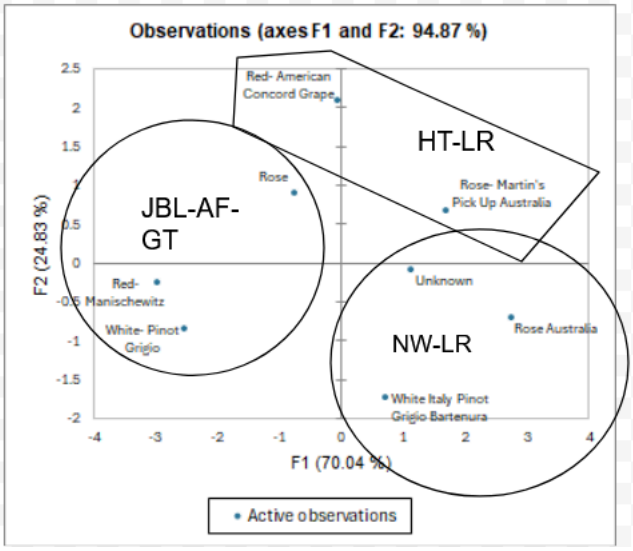

Variables (axes F1 and F2: 90.45 %)
Ipc/Ipa (A)
Epc/2 (mV)
Ipa (A)
Epa (mV)
Ipc (A)
(Epa+Epc/2)/2
Epa-Epc/2
F2 (25.08 %)
F1 (65.37 %)
Active variables


Observations (axes F1 and F2: 90.45 %)
Red- American Concord Grape
HT-LR
Rose- Martin's Pick Up Australia
Red- Manzschewitz
Rose
White Pinot Grigio
JBL-AF-GT
NW-LR
Unknown
White Italy Pinot Grigio Bartenura
Rose Australia
F2 (25.08 %)
F1 (65.37 %)
Active observations

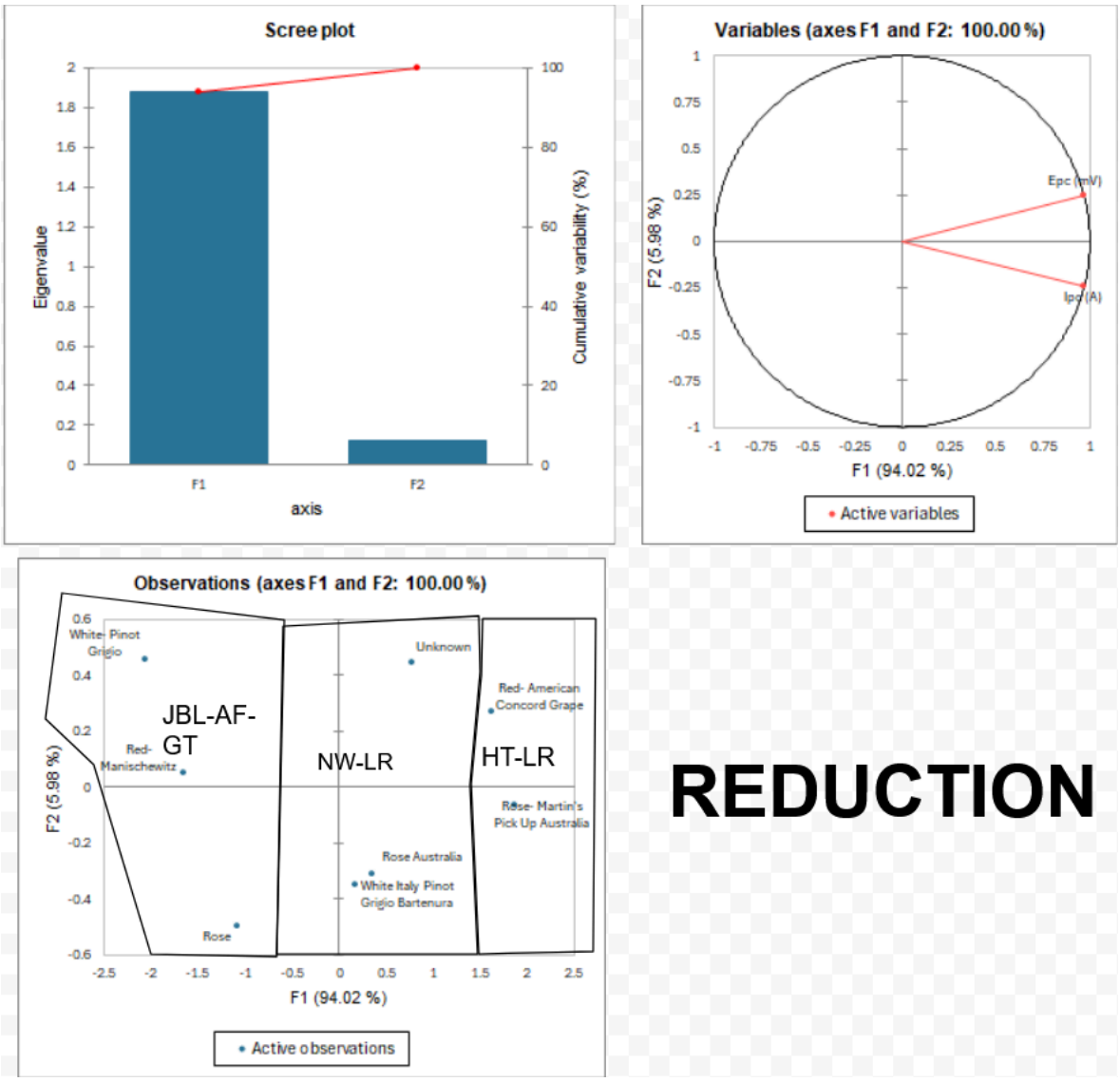
OVERALL


Scree plot
Eigenvalue
Cumulative variability (%)
F1
F2
F3
axis


Variables (axes F1 and F2: 94.87 %)
Ep/2 (mV)
Ipa (A)
(Epa+Ep/2)/2 (mV)
Epa (mV)
Epa/Ep/2
F2 (24.83 %)
F1 (70.04 %)
Active variables

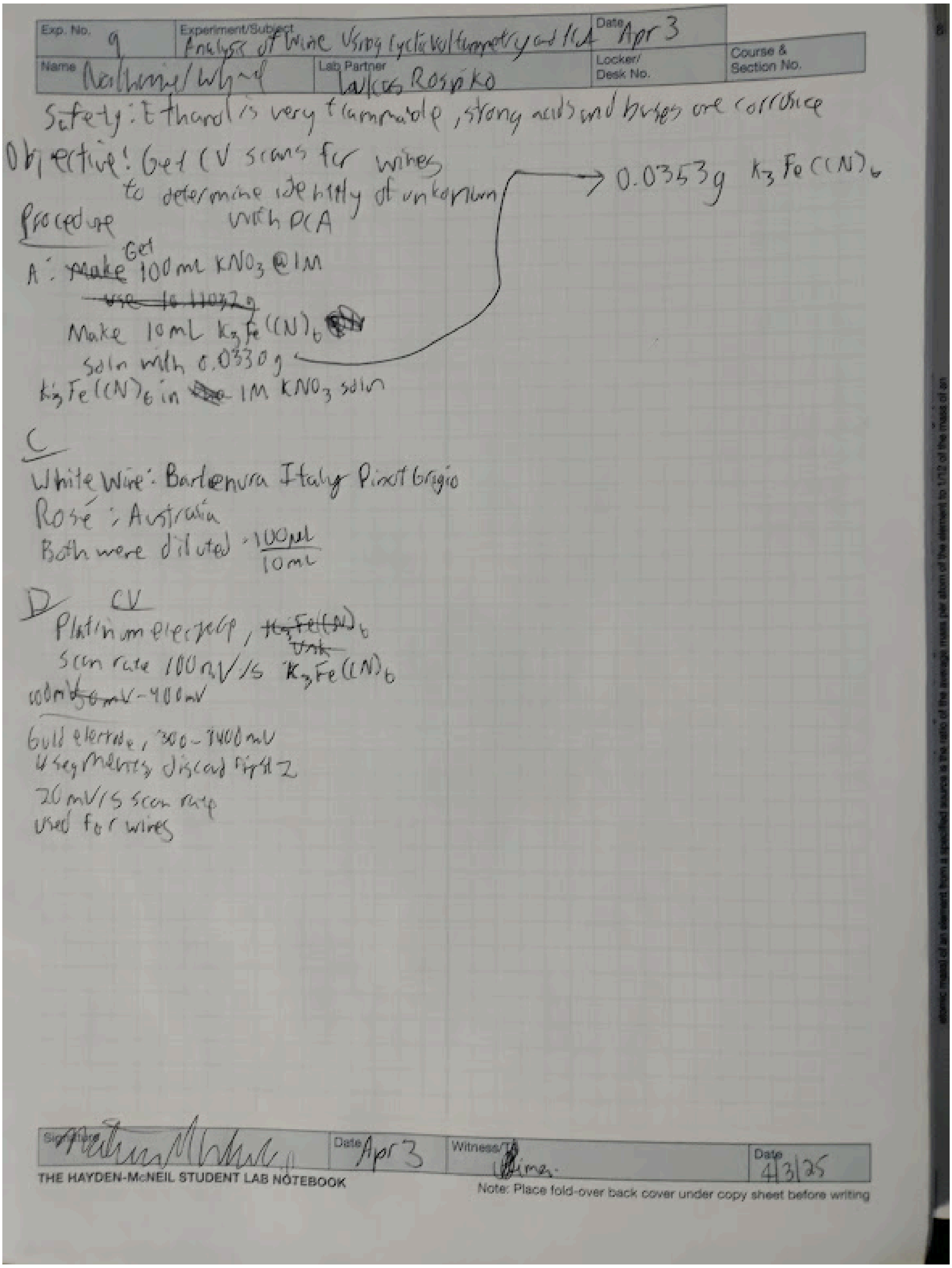

Observations (axes F1 and F2: 94.87 %)
Red- American Concord Grape
HT-LR
Rose
Rose- Martin's Pick Up Australia
JBL-AF-GT
Red- Manischewitz
White- Pinot Grigio
Unknown
Rose Australia
NW-LR
White Italy Pinot Grigio Bartenura
F2 (24.83 %)
F1 (70.04 %)
Active observations

OXIDATION



2. Our results are inconclusive. Clustering based on partner pair rather than the actual wine sample indicates the noise from instrumentation or operator error greatly outweighs the signal. We don't see in any of the observation plots the ability to neatly group data points based on color or country of origin. We also don't see the expected result of Rose between in between white wines and red wines; rather, we see that the same Rose analyzed by three different groups does not appear grouped together in any plot.
3. Both analyses were inconclusive, so no observations can be made. However, univariate analysis is generally more sensitive when there is an expected pattern, whereas multivariate analysis can identify unforseen patterns.

Lab Notebook



Exp. No. 9 | Experiment/Subject: Analysis of Wine Using Cyclic Voltammetry and PCA | Date: Apr 3

Name: Nathaniel Wheel | Lab Partner: Lukas Rospiko | Locker/Desk No. | Course & Section No.

Safety: Ethanol is very flammable, strong acids and bases are corrosive

Objective: Get CV scans for wines to determine identity of unknown with PCA

→ 0.0353g $K_3Fe(CN)_6$

Procedure

A: ~~Make~~ Get 100mL KNO_3 @ 1M

~~use 10.1103 g~~

Make 10mL $K_3Fe(CN)_6$ soln with 0.0330g $K_3Fe(CN)_6$ in 1M KNO_3 soln

C

White Wine: Bardenura Italy Pinot Grigio

Rosé: Australia

Both were diluted $\frac{100mL}{10mL}$

D CV

Platinum electrode, ~~$K_3Fe(CN)_6$~~ Unk

Scan rate 100mV/s $K_3Fe(CN)_6$

100mV ~~50mV~~ -400mV

Gold electrode, 300-1400mV

4 segments discard first 2

20 mV/s scan rate

used for wines

Signature | Date: Apr 3 | Witness | Date: 4/3/25

THE HAYDEN-McNEIL STUDENT LAB NOTEBOOK

Note: Place fold-over back cover under copy sheet before writing