

Supplementary Data

S1.1. Used Red wine

Table S1: Variety, Origin, and Vintage of the used red wines

| Number | Variety | Country | Vintage |
|---------------|---------------------------|----------------|----------------|
| 1 | Cabernet Sauvignon | France | 2018 |
| 2 | Cabernet Sauvignon | Italy | 2018 |
| 3 | Cabernet Sauvignon | USA | 2014 |
| 4 | Cabernet Sauvignon | Germany | 2018 |
| 5 | Cabernet Sauvignon | Australia | 2016 |
| 6 | Cabernet Sauvignon | Spain | 2016 |
| 7 | Cabernet Sauvignon | Italy | 2019 |
| 8 | Merlot | Italy | 2018 |
| 9 | Merlot | France | 2018 |
| 10 | Merlot | USA | 2018 |
| 11 | Merlot | France | 2016 |
| 12 | Merlot | New Zealand | 2018 |
| 13 | Merlot | France | 2019 |
| 14 | Merlot | USA | 2017 |
| 15 | Pinot Noir | France | 2019 |
| 16 | Pinot Noir | Germany | 2019 |
| 17 | Pinot Noir | Germany | 2013 |
| 18 | Pinot Noir | Germany | 2017 |
| 19 | Pinot Noir | Germany | 2018 |

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|-----------|--------------------|-------------|------|
| 20 | Pinot Noir | New Zealand | 2018 |
| 21 | Pinot Noir | New Zealand | 2019 |
| 22 | Primitivo | Italy | 2020 |
| 23 | Primitivo | Italy | 2017 |
| 24 | Primitivo | Italy | 2020 |
| 25 | Primitivo | Italy | 2019 |
| 26 | Primitivo | Italy | 2017 |
| 27 | Primitivo | USA | 2018 |
| 28 | Primitivo | USA | 2017 |
| 29 | Syrah | Australia | 2018 |
| 30 | Syrah | Italy | 2019 |
| 31 | Syrah | USA | 2017 |
| 32 | Syrah | France | 2019 |
| 33 | Syrah | New Zealand | 2019 |
| 34 | Syrah | France | 2020 |
| 35 | Syrah | France | 2019 |
| 36 | Tempranillo | Spain | 2015 |
| 37 | Tempranillo | Spain | 2015 |
| 38 | Tempranillo | Spain | 2018 |
| 39 | Tempranillo | Spain | 2019 |
| 40 | Tempranillo | Spain | 2017 |
| 41 | Tempranillo | Spain | 2018 |
| 42 | Tempranillo | Spain | 2012 |
| 43 | Vernatsch | Germany | 2018 |

| | | | |
|-----------|------------------|---------|------|
| 44 | Vernatsch | Germany | 2018 |
| 45 | Vernatsch | Italy | 2019 |
| 46 | Vernatsch | Italy | 2019 |
| 47 | Vernatsch | Italy | 2019 |
| 48 | Vernatsch | Italy | 2019 |
| 49 | Vernatsch | Germany | 2018 |
| 50 | Lemberger | Austria | 2018 |
| 51 | Lemberger | Germany | 2018 |
| 52 | Lemberger | Austria | 2017 |
| 53 | Lemberger | Germany | 2019 |
| 54 | Lemberger | Germany | 2016 |
| 55 | Lemberger | Germany | 2019 |
| 56 | Lemberger | Germany | 2019 |

S1.2. Used White wines

Table S2: Variety, Origin, and Vintage of the used white wines

| Number | Variety | Country | Vintage |
|---------------|-------------------|----------------|----------------|
| 1 | Chardonnay | France | 2018 |
| 2 | Chardonnay | Italy | 2020 |
| 3 | Chardonnay | Germany | 2018 |
| 4 | Chardonnay | Spain | 2019 |
| 5 | Chardonnay | Germany | 2016 |

| | | | |
|-----------|-------------------|-----------|------|
| 6 | Chardonnay | Australia | 2019 |
| 7 | Chardonnay | USA | 2018 |
| 8 | Riesling | Germany | 2015 |
| 9 | Riesling | France | 2017 |
| 10 | Riesling | USA | 2013 |
| 11 | Riesling | Germany | 2018 |
| 12 | Riesling | Germany | 2019 |
| 13 | Riesling | Germany | 2020 |
| 14 | Riesling | Germany | 2020 |
| 15 | Riesling | Germany | 2019 |
| 16 | Riesling | Germany | 2018 |
| 17 | Riesling | Germany | 2019 |
| 18 | Riesling | Germany | 2019 |
| 19 | Riesling | Germany | 2018 |
| 20 | Riesling | Germany | 2019 |
| 21 | Riesling | Germany | |
| 22 | Pinot gris | Italy | 2019 |
| 23 | Pinot gris | Italy | 2020 |

| | | | |
|-----------|------------------------|-------------|------|
| 24 | Pinot gris | France | 2017 |
| 25 | Pinot gris | New Zealand | 2018 |
| 26 | Pinot gris | Germany | 2019 |
| 27 | Pinot gris | Germany | 2019 |
| 28 | Pinot gris | Germany | 2019 |
| 29 | Sauvignon blanc | France | 2019 |
| 30 | Sauvignon blanc | Germany | 2019 |
| 31 | Sauvignon blanc | Italy | 2019 |
| 32 | Sauvignon blanc | USA | 2019 |
| 33 | Sauvignon blanc | New Zealand | 2020 |
| 34 | Sauvignon blanc | France | 2018 |
| 35 | Sauvignon blanc | Germany | 2018 |
| 36 | Pinot blanc | Germany | 2019 |
| 37 | Pinot blanc | Germany | 2020 |
| 38 | Pinot blanc | Germany | 2018 |
| 39 | Pinot blanc | Germany | 2017 |
| 40 | Pinot blanc | Germany | 2020 |
| 41 | Pinot blanc | Italy | 2019 |

| | | | |
|-----------|-----------------------|---------|------|
| 42 | Pinot blanc | France | 2017 |
| 43 | Gewürztraminer | Germany | 2016 |
| 44 | Gewürztraminer | Germany | 2018 |
| 45 | Gewürztraminer | France | 2019 |
| 46 | Gewürztraminer | Germany | 2019 |
| 47 | Gewürztraminer | France | 2019 |
| 48 | Gewürztraminer | Spain | 2019 |
| 49 | Gewürztraminer | Germany | 2019 |
| 50 | Gewürztraminer | Italy | 2019 |
| 51 | Gewürztraminer | Italy | 2019 |
| 52 | Gewürztraminer | Spain | 2018 |
| 53 | Gewürztraminer | Germany | 2019 |
| 54 | Gewürztraminer | France | 2018 |
| 55 | Gewürztraminer | Germany | 2019 |
| 56 | Gewürztraminer | Germany | 2020 |

S1.3. Photometer settings

Table S3: Photometer comparison regarding sipper and photometer configuration

| Parameter | JASCO V-730 | Varian Cary 100 |
|-----------------------------|--------------------|------------------------|
| Sipper configuration | 1 mm flow cuvette | |

| | | |
|---------------------------------|--|--------------------------------------|
| Suction time | 3 sec | 8 sec |
| Flow time | 0 sec | 0 sec |
| Wait time | 1 sec | 5 sec |
| Drain time | 5 sec | 8 sec |
| Photometer configuration | | |
| Photometric mode | Absorption | Absorption |
| Bandwidth | 1 nm | 2 nm |
| Response time | 0.96 sec | 0.03-0.6 sec (depends on scan speed) |
| Correction mode | Baseline | Baseline |
| Light source > 340 nm | Tungsten lamp | Tungsten lamp |
| Light source < 340 nm | Deuterium lamp | Deuterium lamp |
| Filter exchange | Stepwise | n. A. |
| Monochromator system | Single monochromator in Rowland off-circle arrangement | Czerny-Turner monochromator |
| Detector system | Si-Photodiode (S1337) | Photomultiplier tube (R928) |

Figure S1. Python Code for correlation matrices

```
#import packages
import numpy as np # numeric calculations
import pandas as pd #excel data import
import matplotlib.pyplot as plt #plotting base
import seaborn as sns #statistical plotting
import warnings
warnings.filterwarnings('ignore')
%matplotlib inline

#import excel file
df = pd.read_excel(r'Excel-file directory')
#show columns and row length
df.shape
# DataFrame optimization
df.columns = df.columns.str.strip() # delete spaces in column names
df.info()# check properties (non-null count)
df.isnull().sum() #check properties (null-count)
data= df.dropna() # drop rows without values
data.isnull().sum() # re-check null count
data = data.rename(columns={'420 nm': 'A[420 nm]', '520 nm': 'A[520 nm]', '620
nm': 'A[620 nm]'}) #rename columns
round(data.describe(),2) # describe the data count, mean, std 25%,50%,75%
quantils
#Calculate and plot Heatmap
sns.set(font_scale=1.4)#set overall font size
plt.figure(figsize=(12,8.27)) #set figure size
correlations = data.corr(method='spearman') # calculate spearman
correlation
mask = np.zeros_like(correlations) # mask the upper half of the correlation
matrix that shows the same as the down half
mask[np.triu_indices_from(mask)] = True
sns.set_style("whitegrid", {'axes.grid' : False}) # Hide Grid
#plot heatmap
sns.heatmap(round(correlations,2), cmap='RdGy', annot=True,
            annot_kws={"size": 18}, vmin=-1, vmax=1,square=True,mask=mask)
plt.yticks(rotation=0) #rotation of y ticks
plt.xticks(rotation=15) #roattion of x ticks
#save plot as vector graphic
plt.savefig(r"save directory", format='svg')
```


Figure S2. MATLAB Code for interpolation with cubic splines

```
% Cubic splines
% Enter wavelengths
x = [
380
420
460
525
590
625
675
775
];

% Enter transmission values
y = [
t_380
t_420
t_460
t_525
t_590
t_625
t_675
t_775
];

a = (y(2)-y(1))./(x(2)-x(1));
b = (y(8)-y(7))./(x(8)-x(7));

yy = spline(x,[1; y; 0]);
```

Figure S3. MATLAB code for interpolation according to Sprague

```
%%Sprague

% Enter wavelengths
x = [
380
420
460
525
590
625
675
775
];

% Enter transmission values
y = [
t_380
t_420
t_460
t_525
t_590
t_625
t_675
t_775
];

a = (884*y(1)-1960*y(2)+3033*y(3)-2648*y(4)+1080*y(5)-180*y(6))/209;
b = (508*y(1)-540*y(2)+488*y(3)-367*y(4)+144*y(5)-24*y(6))/209;
c = (-24*y(3)+144*y(4)-367*y(5)+488*y(6)-540*y(7)+508*y(8))/209;
d = (-180*y(3)+1080*y(4)-2648*y(5)+3033*y(6)-1960*y(7)+884*y(8))/209;

w = [a; b; y; c; d];

b = size(y);

e = zeros(b(1)-1,6);

%%

for i=3:9
a0 = w(i);
a1 = (w(i-2)-8*w(i-1)+8*w(i+1)-w(i+2))/12;
a2 = (-w(i-2)+16*w(i-1)-30*w(i)+16*w(i+1)-w(i+2))/24;
a3 = (-9*w(i-2)+39*w(i-1)-70*w(i)+66*w(i+1)-33*w(i+2)+7*w(i+3))/24;
a4 = (13*w(i-2)-64*w(i-1)+126*w(i)-124*w(i+1)+61*w(i+2)-12*w(i+3))/24;
a5 = (-5*w(i-2)+25*w(i-1)-50*w(i)+50*w(i+1)-25*w(i+2)+5*w(i+3))/24;

e(i-2,1)= a0;
e(i-2,2)= a1;
e(i-2,3)= a2;
e(i-2,4)= a3;
e(i-2,5)= a4;
e(i-2,6)= a5;
end
```