

# A Metabolomics based Approach to Characterize Differences in Wine Volatiles Caused due to Rootstocks and Irrigation

**Mani Awale**

**Show me Grape and Wine Symposium**

**March 3rd, 2020**

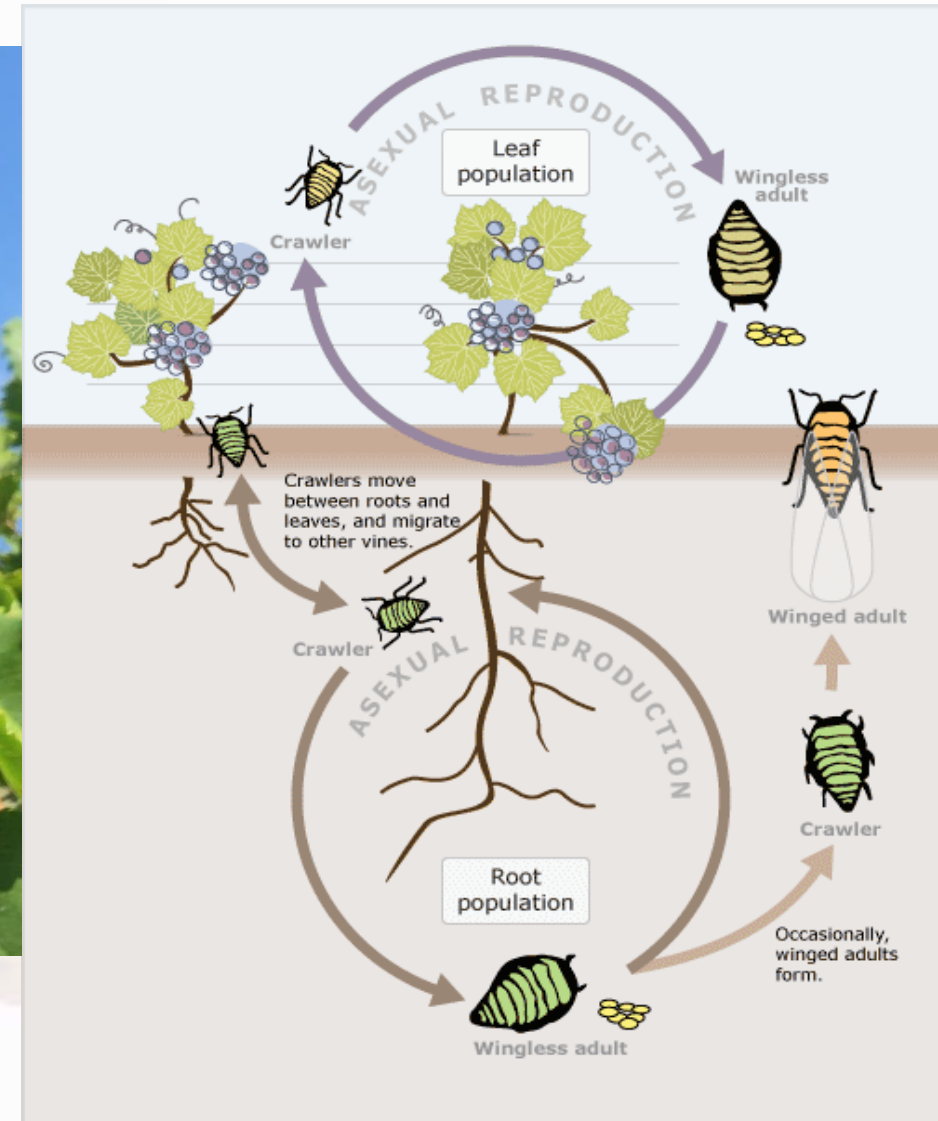
**Advisor: Dr. Misha Kwasniewski**

**Rootstock**

- 1103P
- 3309C
- own
- so4

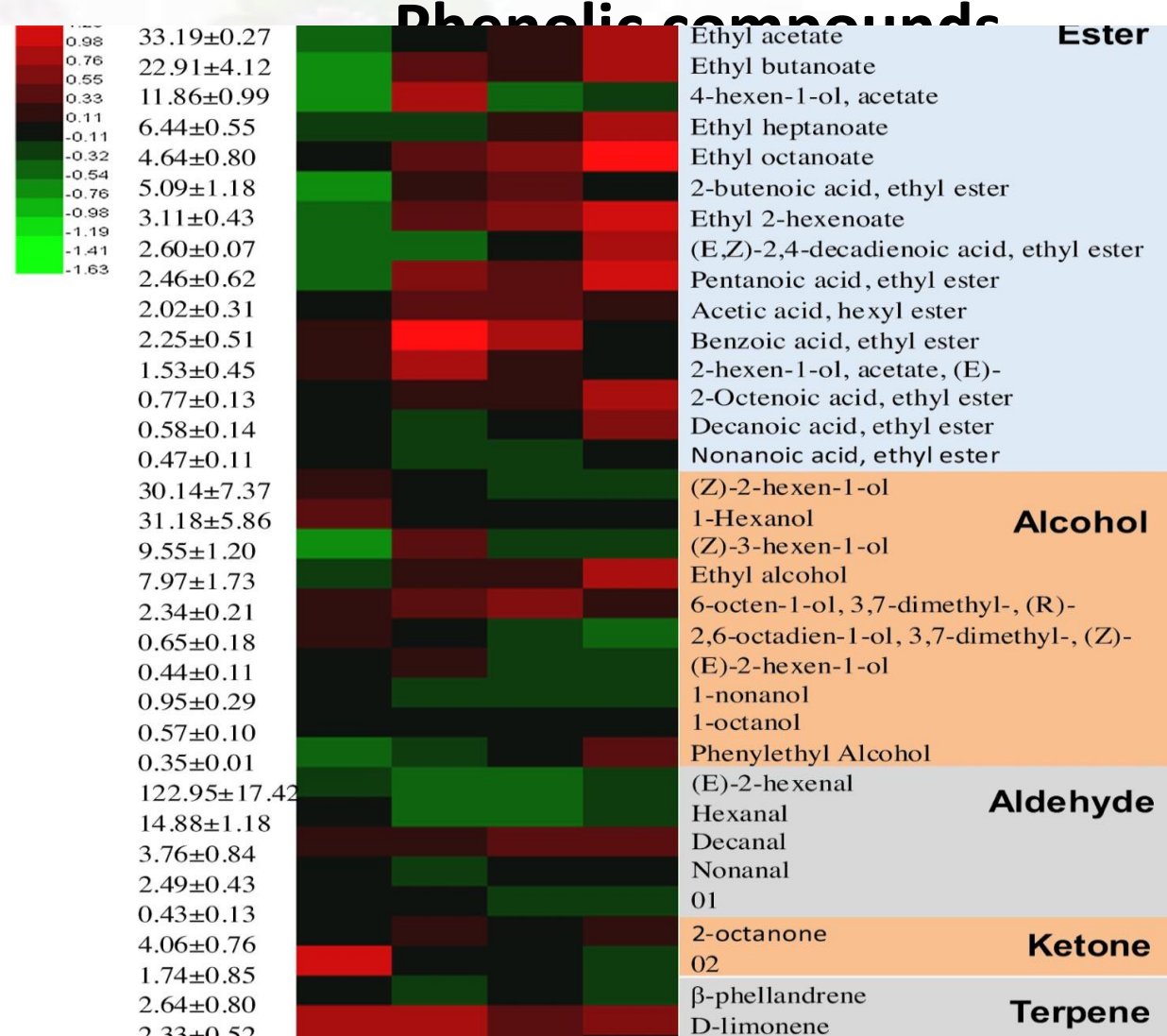
# Grafting in grapevines:

- The invasion of European grape industry by the soil-borne aphid-like insect phylloxera (*Daktuloasphaira vitifoliae* Fitch)
- Rootstocks from North American species were grafted
- *V. riparia*, *V. rupestris* and *V. berlandierii*
- 80% of all vineyards grow grafted grapevines



# Rootstocks can impact scion phenotypes

- ❑ Water and nutrients uptake
- ❑ Vine vigor and canopy configuration
- ❑ Fruit ripening
- ❑ Yield
- ❑ Berry composition





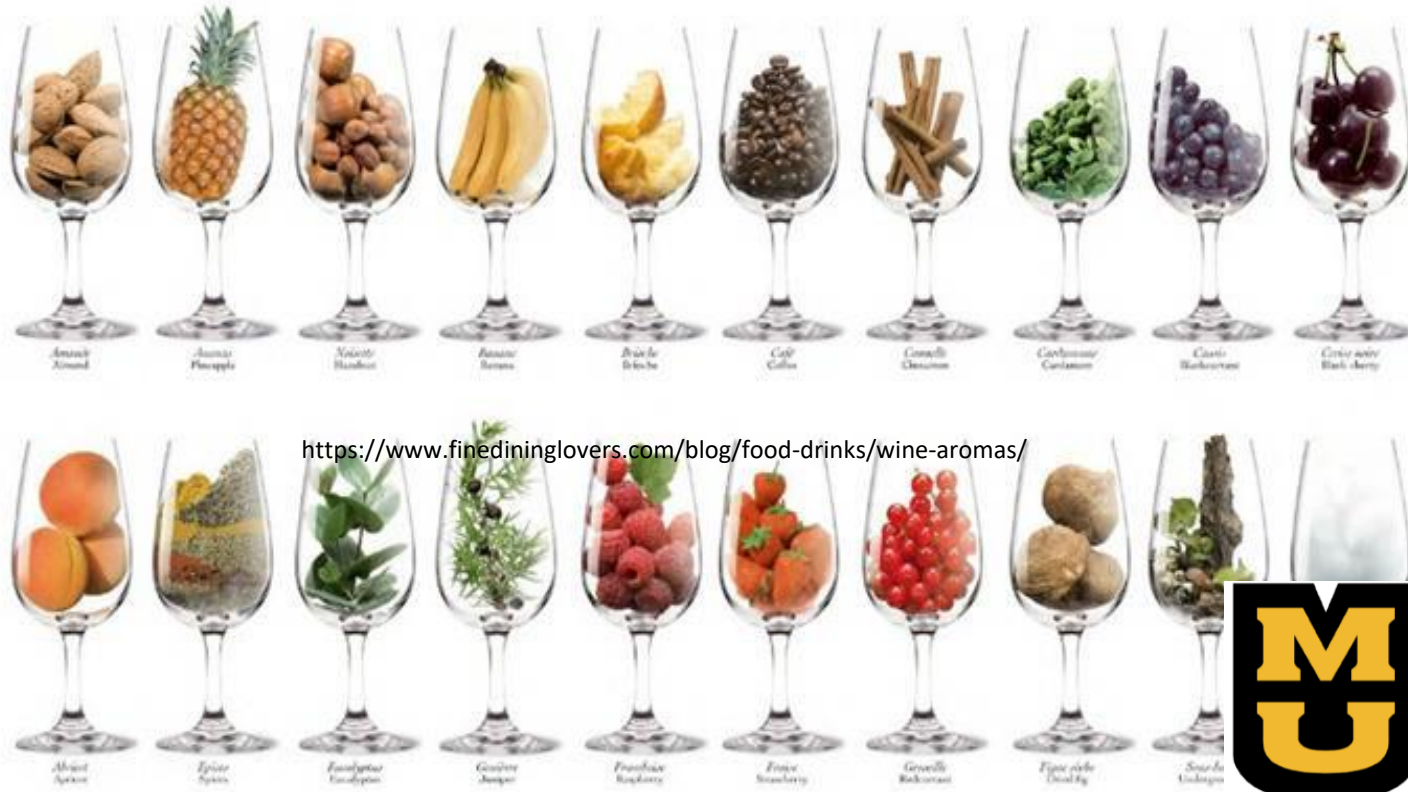
# Rationale for this study:

- Hybrid grapes are mostly grown own-rooted (ungrafted)
- Besides tolerance to phylloxera, rootstocks confer many advantages including biotic and abiotic advantages
- The impact on hybrid wine volatiles due to rootstocks is not well explored
- How irrigation and rootstocks impact wine volatiles?



# What are Aroma compounds:

- Low molecular weight compounds
- Contribute to the complexity of the wine flavor
- Floral, fruity, nutty, spicy or herbaceous aromas
- Aldehydes, alcohols, esters, hydrocarbons, ketones, furans and unidentified compounds
  - Grape-derived volatiles
  - Oak-derived compounds
  - Fermentation- derived compounds

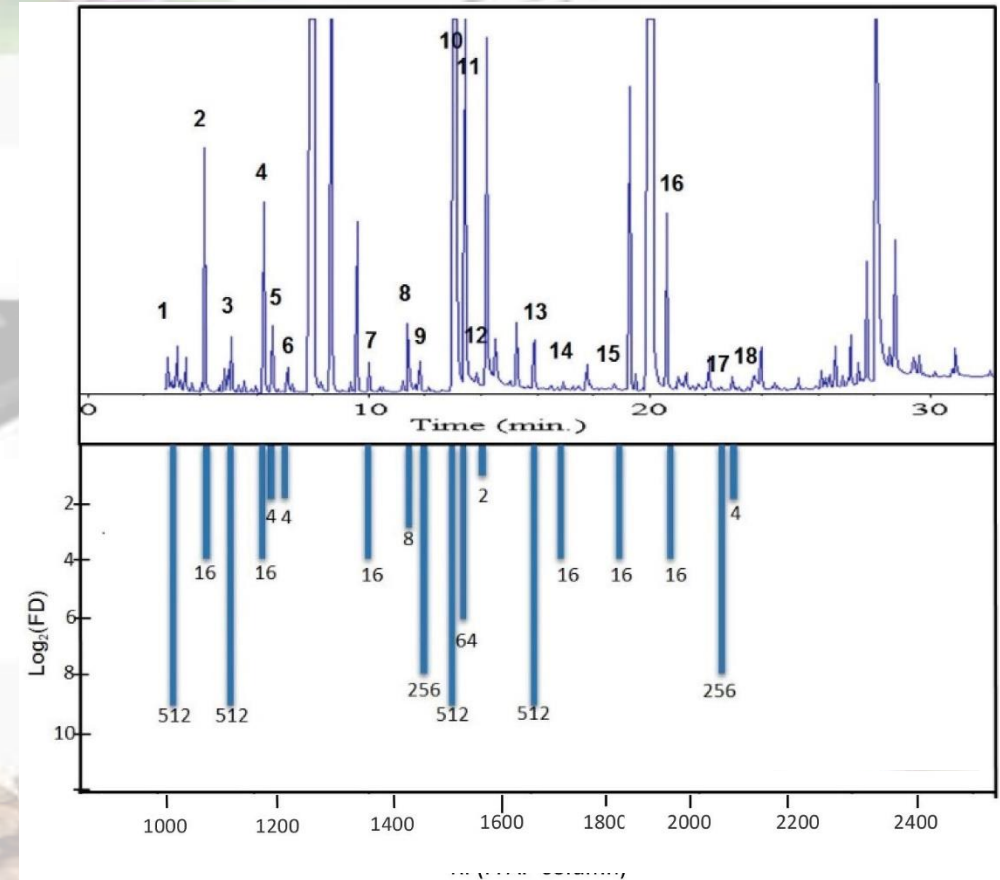


<https://www.finedininglovers.com/blog/food-drinks/wine-aromas/>





# How do we measure aromas?



Gas Chromatography Mass Spectrometry (GC-MS)

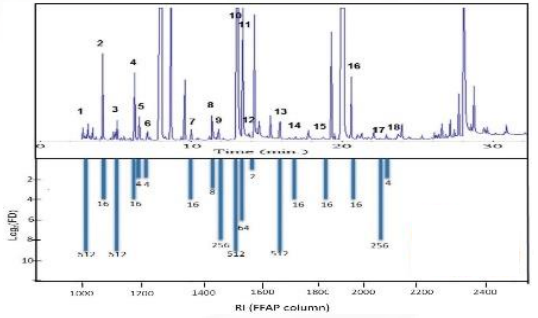
## Untargeted metabolomics:

- Global profiling of the metabolome
- Extraction and detection of as many metabolites as possible
- Qualitative and relative quantification

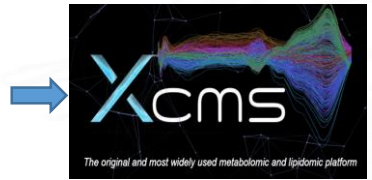
## Targeted metabolomics:

- Accurate quantifications of a select group of intended metabolites
- Time consuming

# Metabolomics workflow:



.D files from GCMS

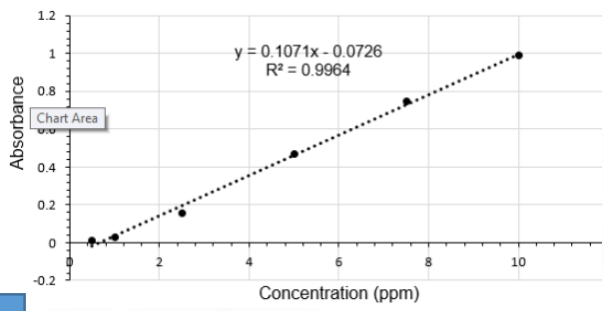
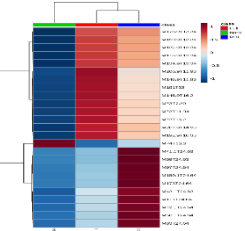


Feature detection,  
baseline correction,  
retention time correction

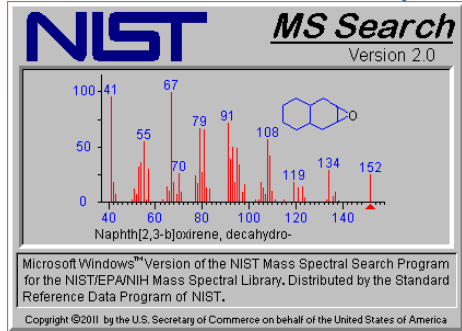


Features were processed using

- Normalization by sum
- Log-transformation
- Autoscaling



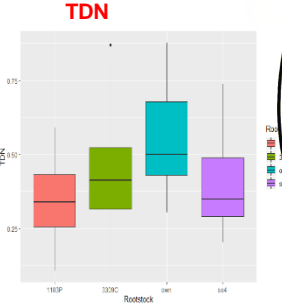
Confirmation and quantitation  
of compounds with authentic  
standards and calibration curve



Identification  
of  
compounds  
from the  
features with  
Retention  
index and  
NIST library



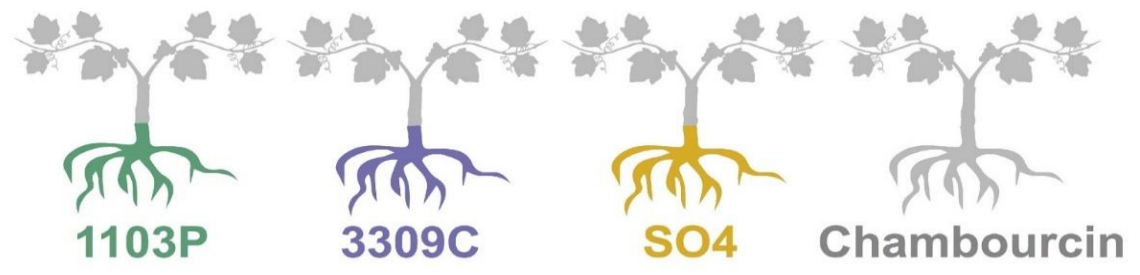
Statistical analysis  
using R studio



Analysis and  
Interpretation



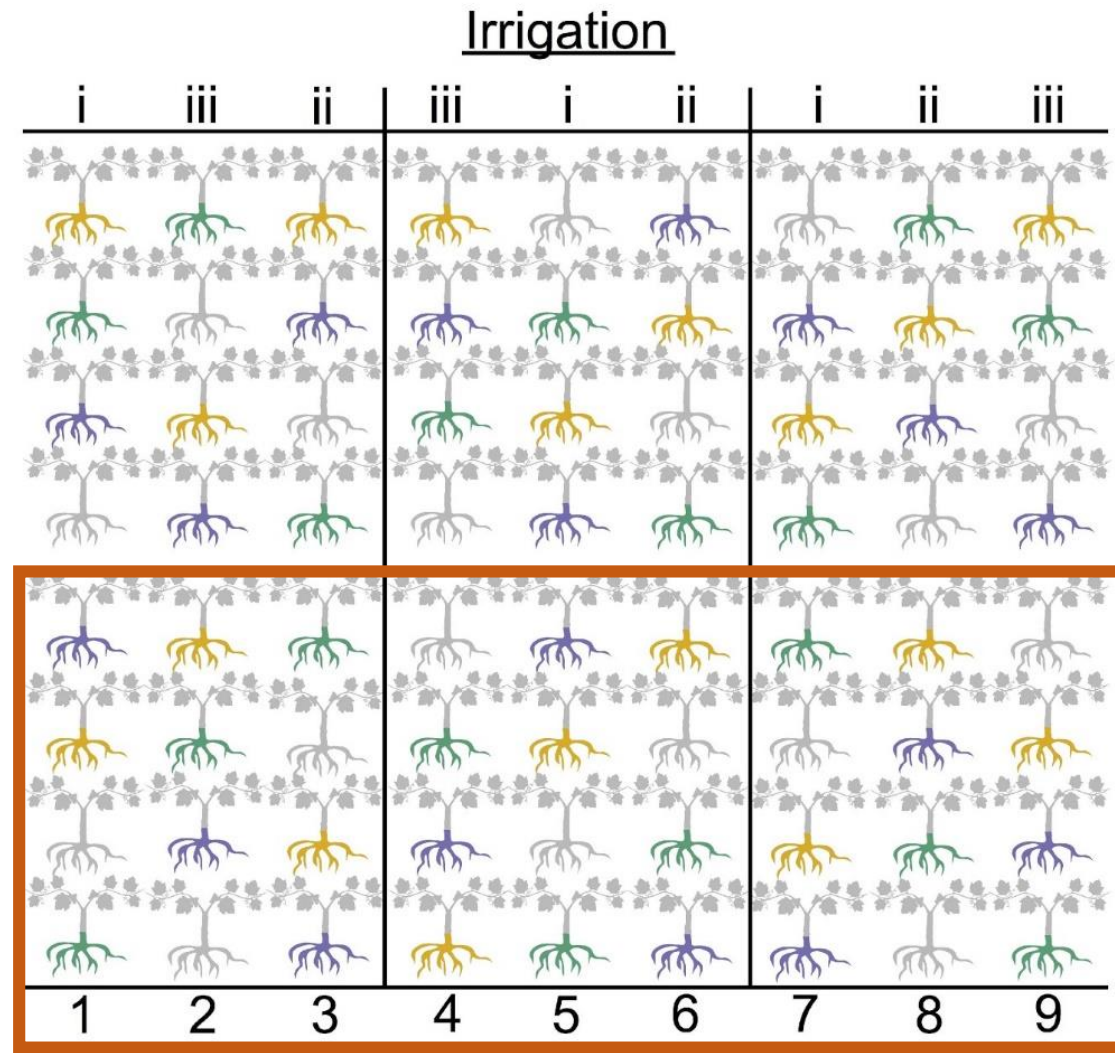
# Scion: Chambourcin (a French American grape)



Rootstock	Parentage	Characteristics
Own rooted Chambourcin	<i>Vitis vinifera</i> , <i>V. cinerea</i>	
3309C	<i>V. riparia</i> X <i>V. rupestris</i>	suitable for wetter environments
1103P	<i>V. rupestris</i> X <i>V. berlandieri</i>	suitable for drier environments, especially for the hot, Mediterranean climate
SO4	<i>V. riparia</i> X <i>V. berlandieri</i>	Tolerant to wet soil

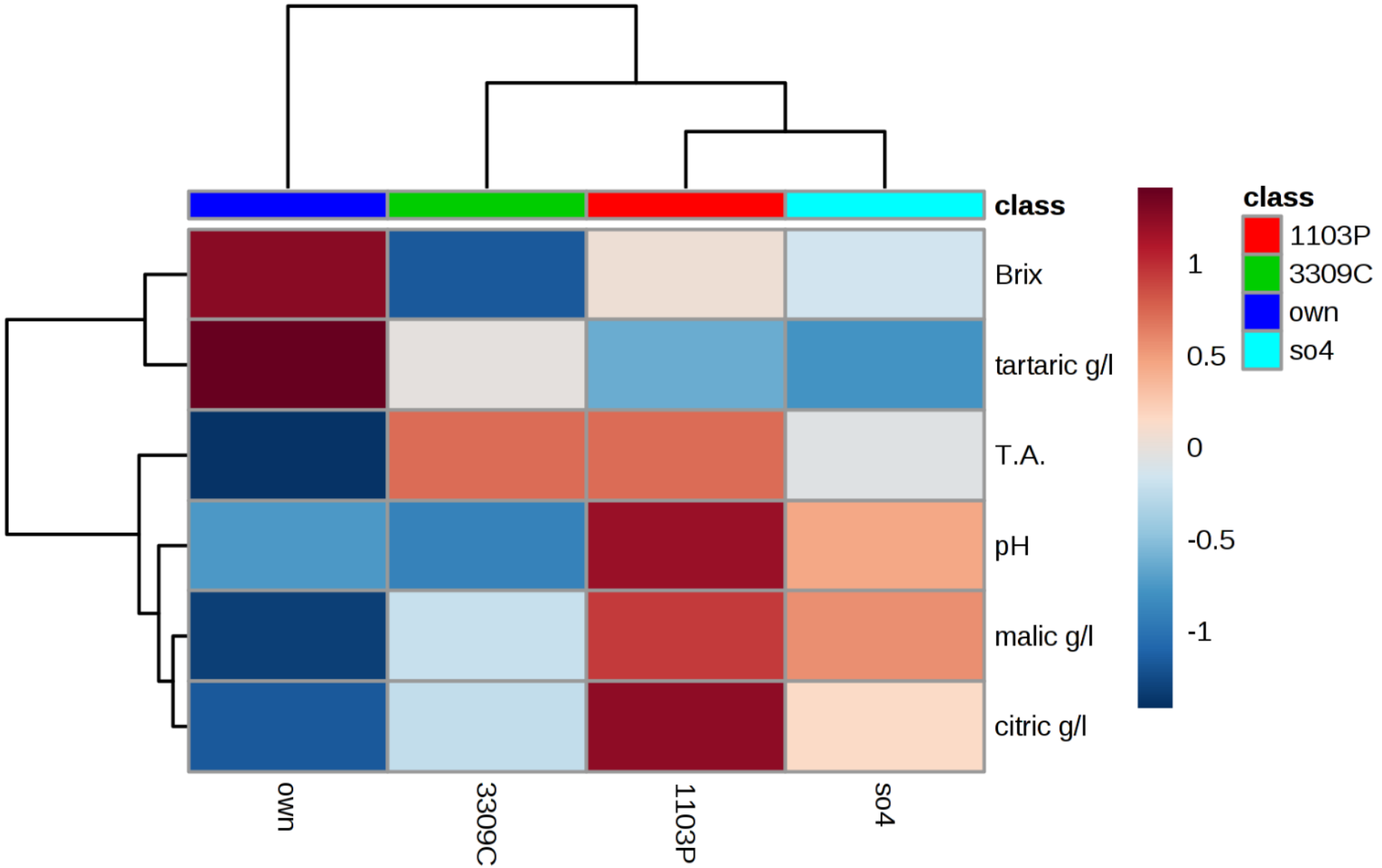
## 3 irrigation treatments:

- Full irrigation (Full)-100% ET
- Regulated Deficit irrigation (RDI)-50% ET
- No irrigation (None)-Rainfed

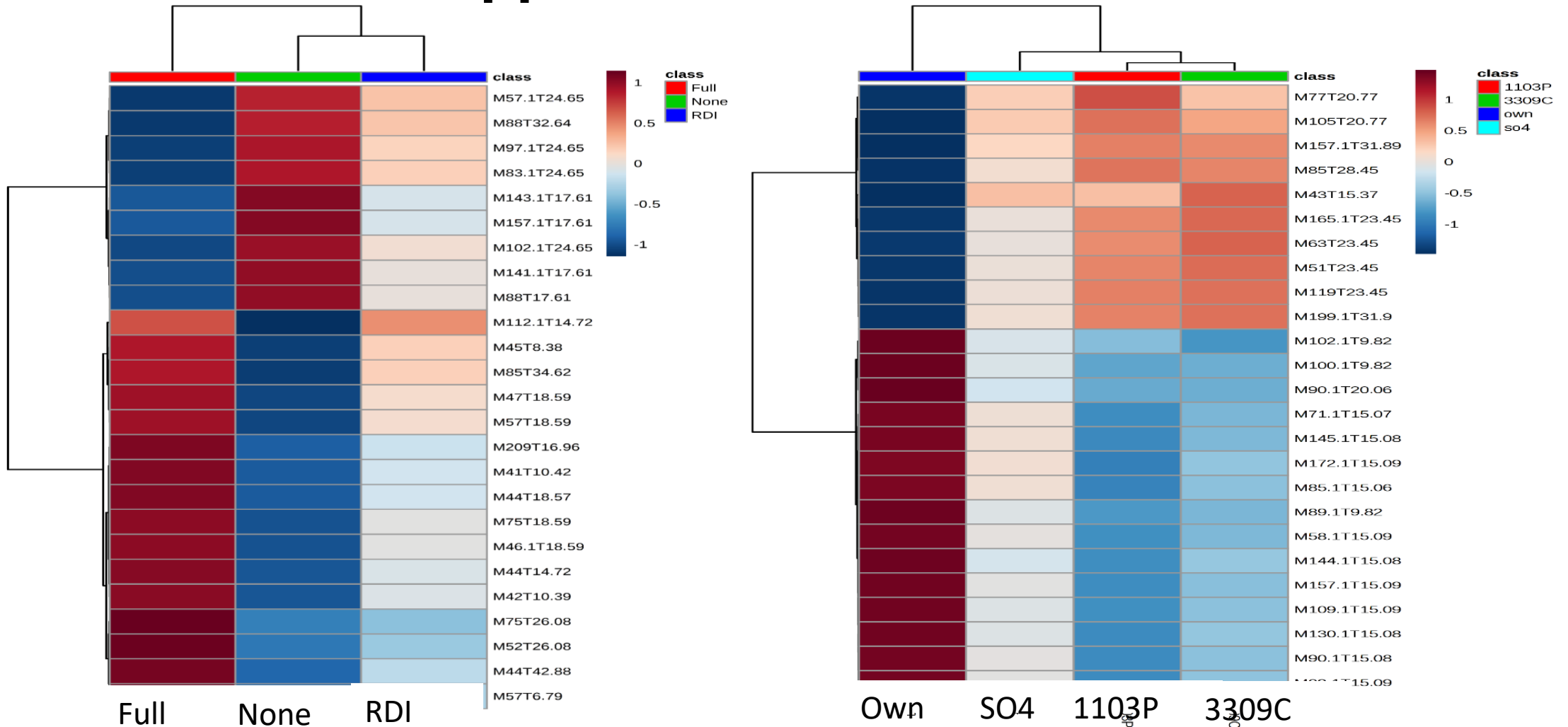


Block  
 = 4 replicate vines  
 288 vines total  
 i = Full water  
 ii = Partial water  
 iii = No irrigation

# Berry chemistry changes in different rootstocks:

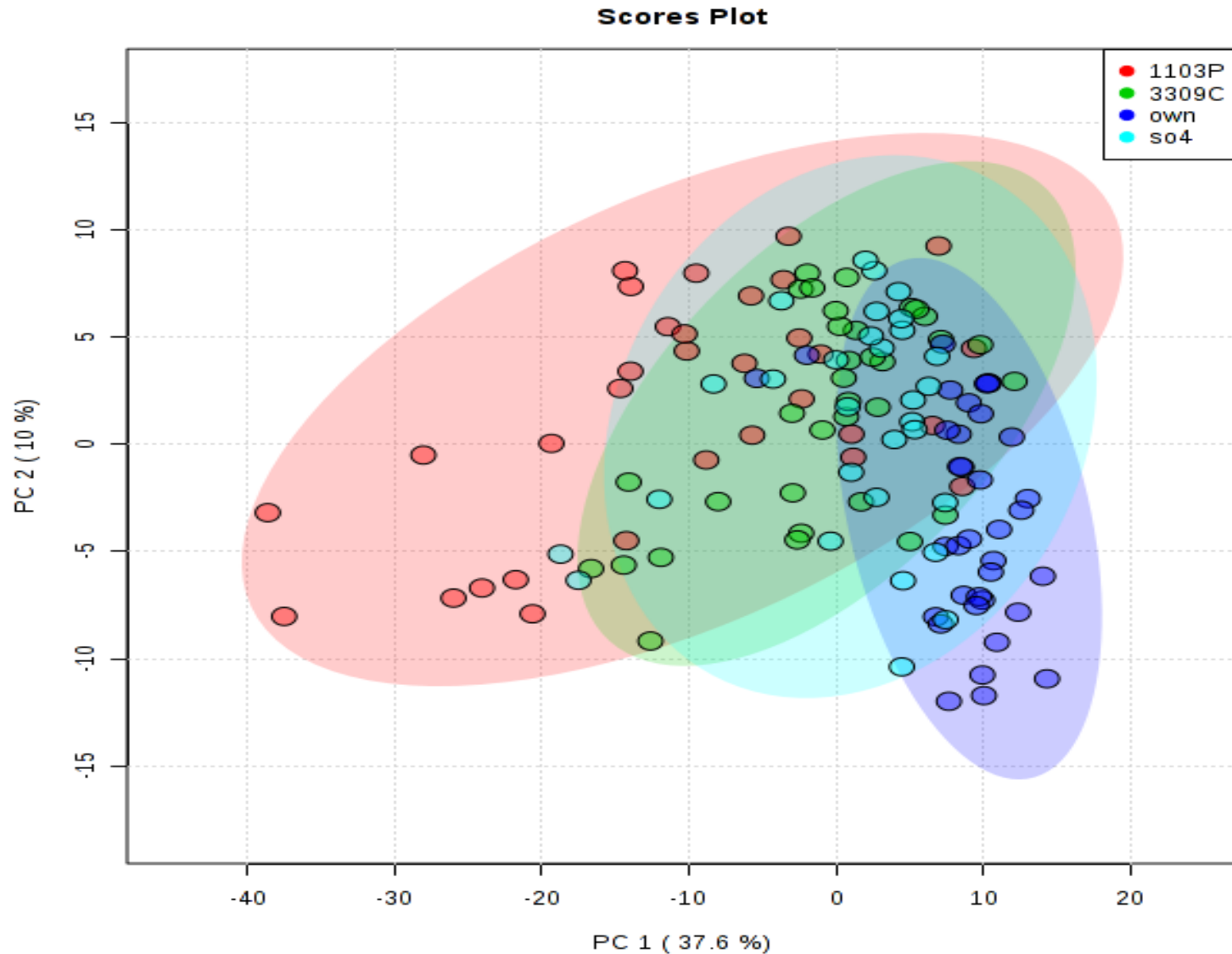


# Feature differences between rootstocks and irrigation treatments in wine 2017 using untargeted metabolomics approach:





# PCA shows differences in metabolic features due to rootstock :

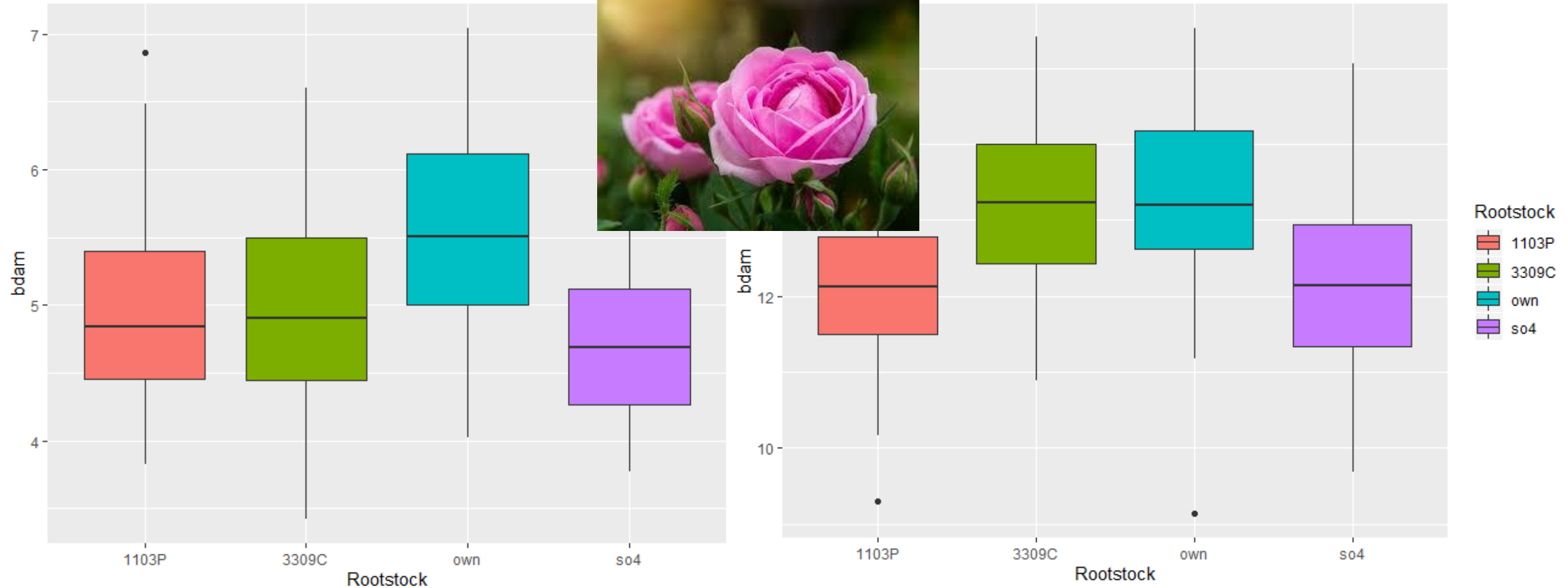


# Rootstocks decreased some compounds in wine in 2017 and 2018:

Beta Damascenone

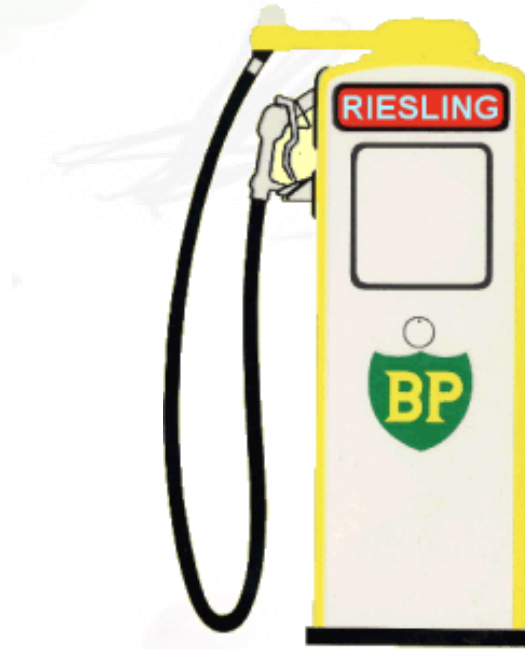
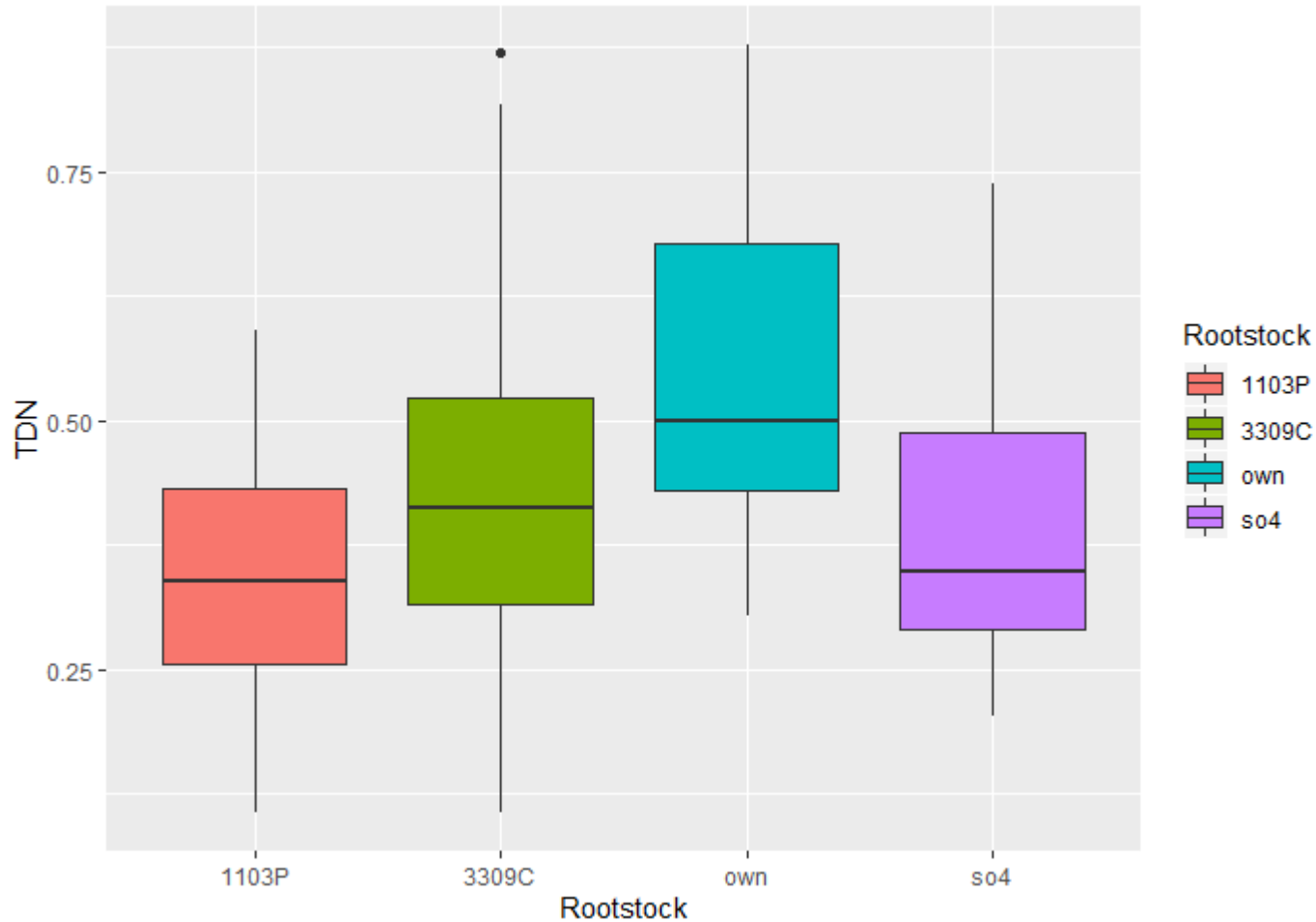
2017

2018



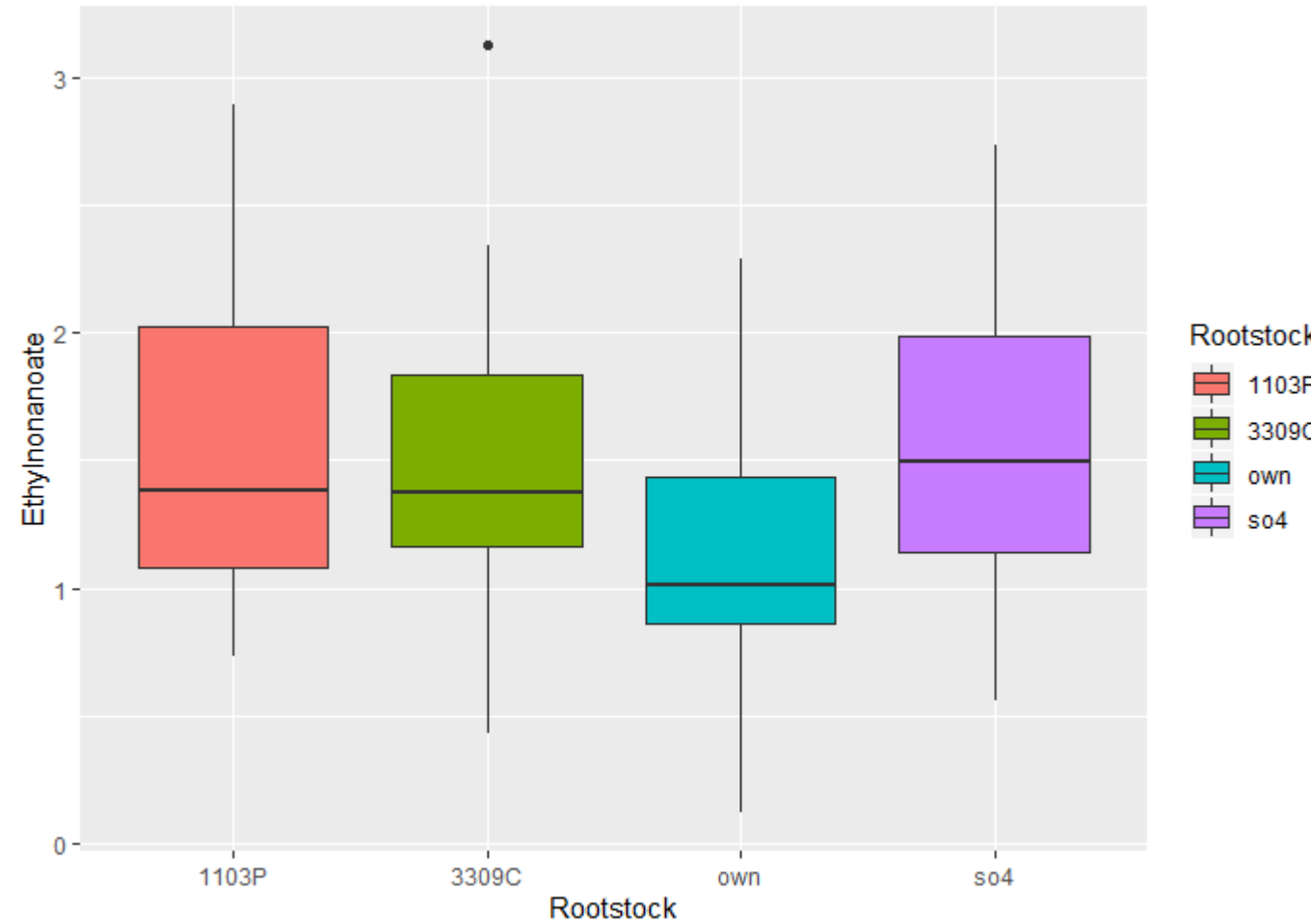
# Rootstocks decreased some compounds in wine in 2017 and 2018:

**TDN (1,1,6-trimethyl-1,2-dihydronaphthalene)**





# Rootstocks increased the levels of some compounds in wine in 2018:



# Take home messages:

- Metabolomics based approach allowed for comprehensive and unbiased identification of compounds
- Grapes and wine aroma are significantly modulated by rootstocks
- We identified more than 90 different compounds in wine and quantified 22 compounds
- Some important aroma compounds are increased by rootstocks whereas some are lowered by rootstocks
- Understanding how rootstocks impact important aroma compounds will provide important information for breeders and winemakers to produce consumer preferred high quality hybrid wines

# Acknowledgements

- Dr. Misha Kwasniewski
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- Alex
- Joe
  
- Missouri Wine and Grape Board



Grape and Wine Institute

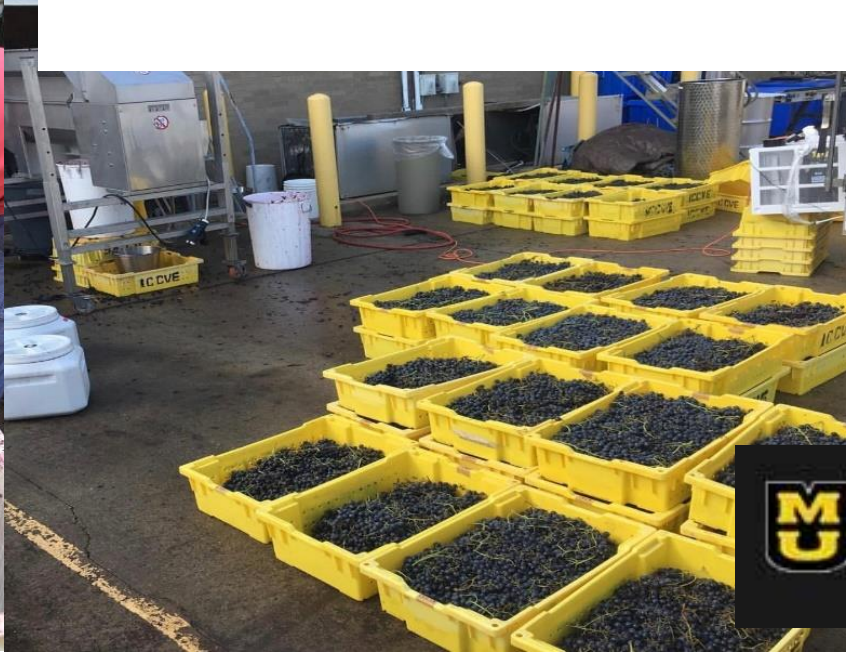
College of Agriculture, Food and Natural Resources







THANK YOU!





# Subtle Differentiation Metabolomics Workflow

