

We will start momentarily at 2pm ET



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East Brunswick Board of Education



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Q: “Hungry for a brain snack?”

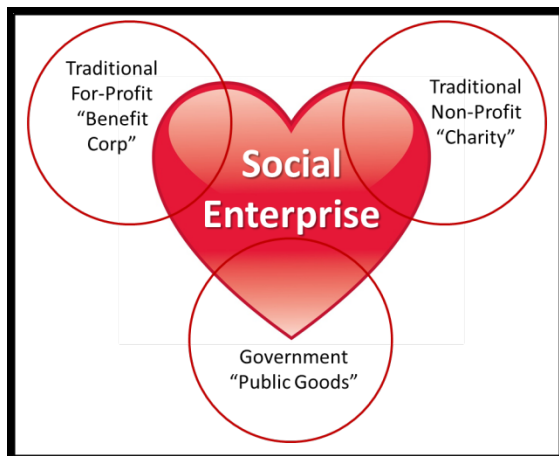
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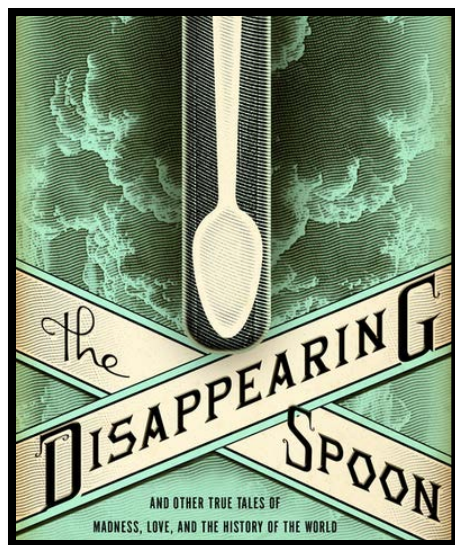


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StrangeTales from the Periodic Table

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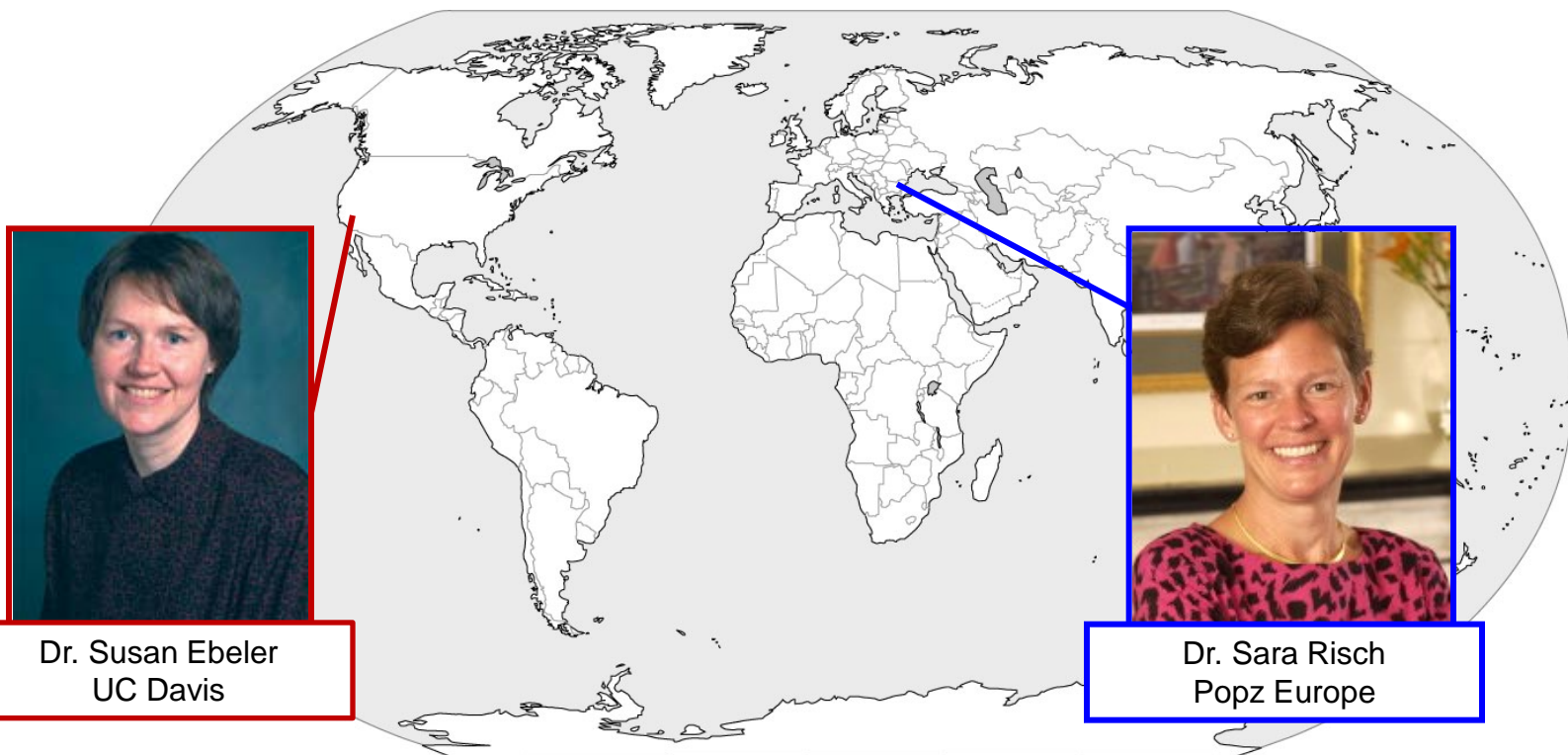


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Barrels of Chemistry: Decoding How Oak Affects Wine Flavor



Dr. Susan Ebeler
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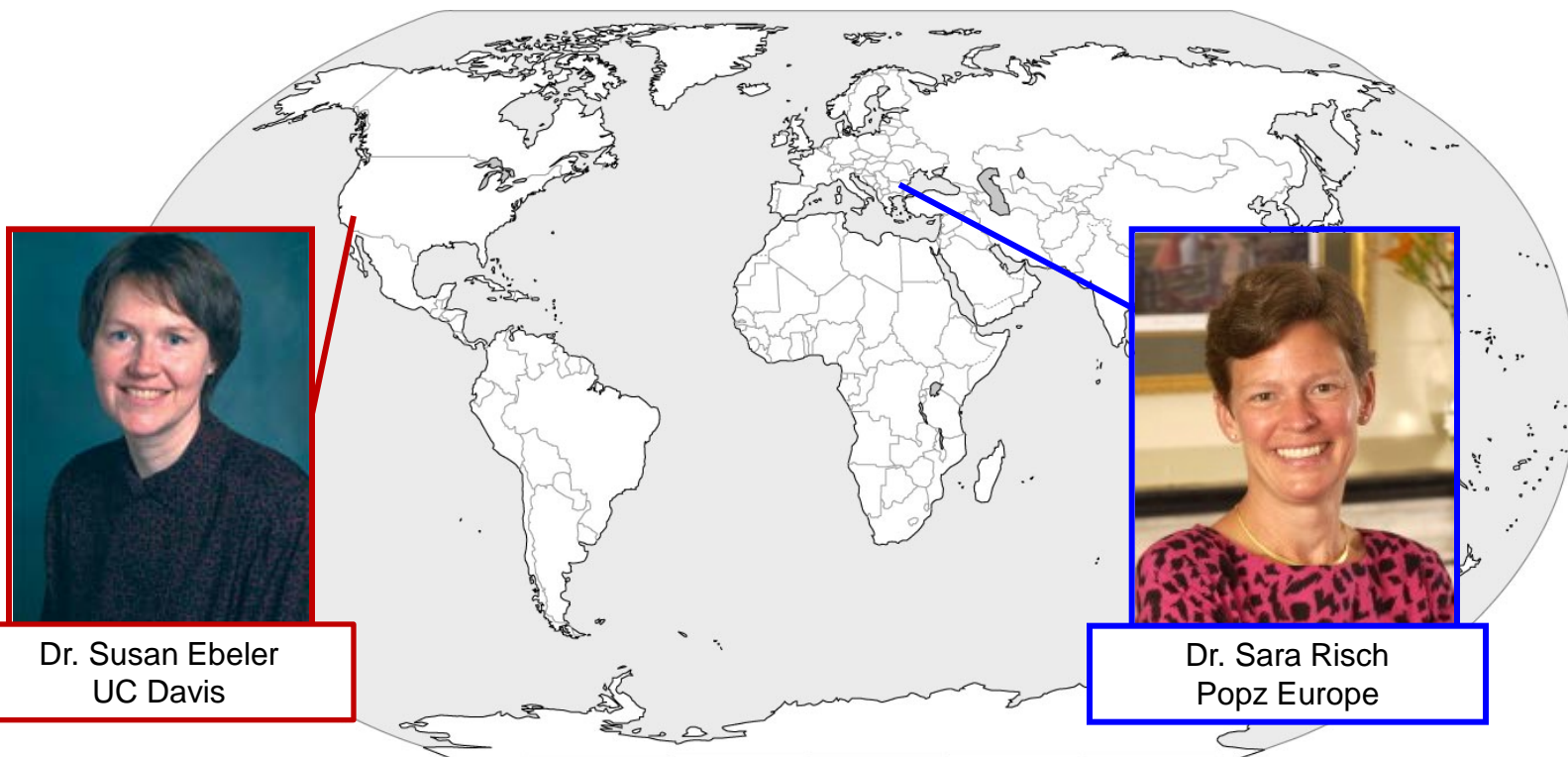


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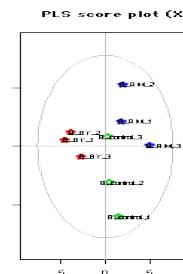
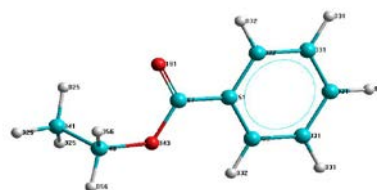
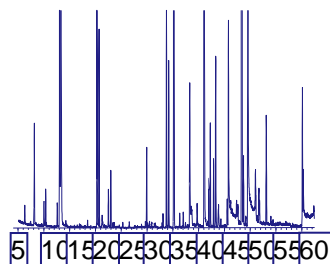
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Barrels of Chemistry: Decoding How Oak Affects Wine Flavor



Susan E. Ebeler
Department of Viticulture and Enology
University of California, Davis, CA



Why Barrels?

- ◆ **Vessel for fermentation**
- ◆ **Storage container**
- ◆ **Impacts flavor**
 - Flavor compounds extracted from wood
 - Evaporation
 - Oxygenation



Type of Wood

◆ Oak

- *Quercus robur*
- *Quercus petraea*
- *Quercus alba*

◆ Note: Cork Oak = *Quercus suber*



Type of Wood

◆ Oak

- *Quercus robur*
- *Quercus petraea*
- *Quercus alba*

◆ Sources

- France
- US
- Slavonia (Croatia)
- Canada
- Russia



Poll Question

◆ **What other types of woods have been used for wine barrels?**

- **Chestnut**
- **Redwood**
- **Acacia**
- **Cedar**
- **Pine**

Barrel Making and Toasting

- ◆ **Harvesting, drying, seasoning, barrel-forming, toasting**



Barrel Making and Toasting

- ◆ Thermal degradation and formation of new flavor compounds



Toasted Oak Flavor

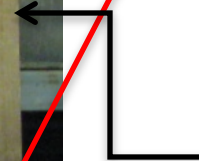
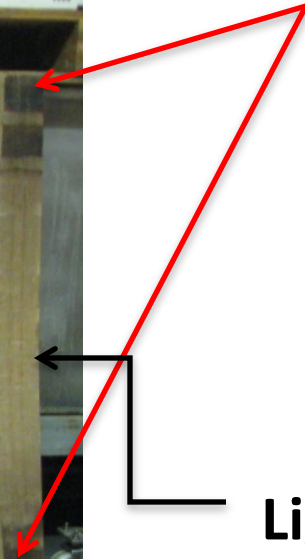
- ◆ Evaluate variability in toasting process--within a barrel and between barrels
- ◆ Volatiles and nonvolatiles



Oak Volatiles



Darker ends



**Lighter
middle**

Variability in the toasting process—Jupilles forest, medium plus toast

Oak Flavor

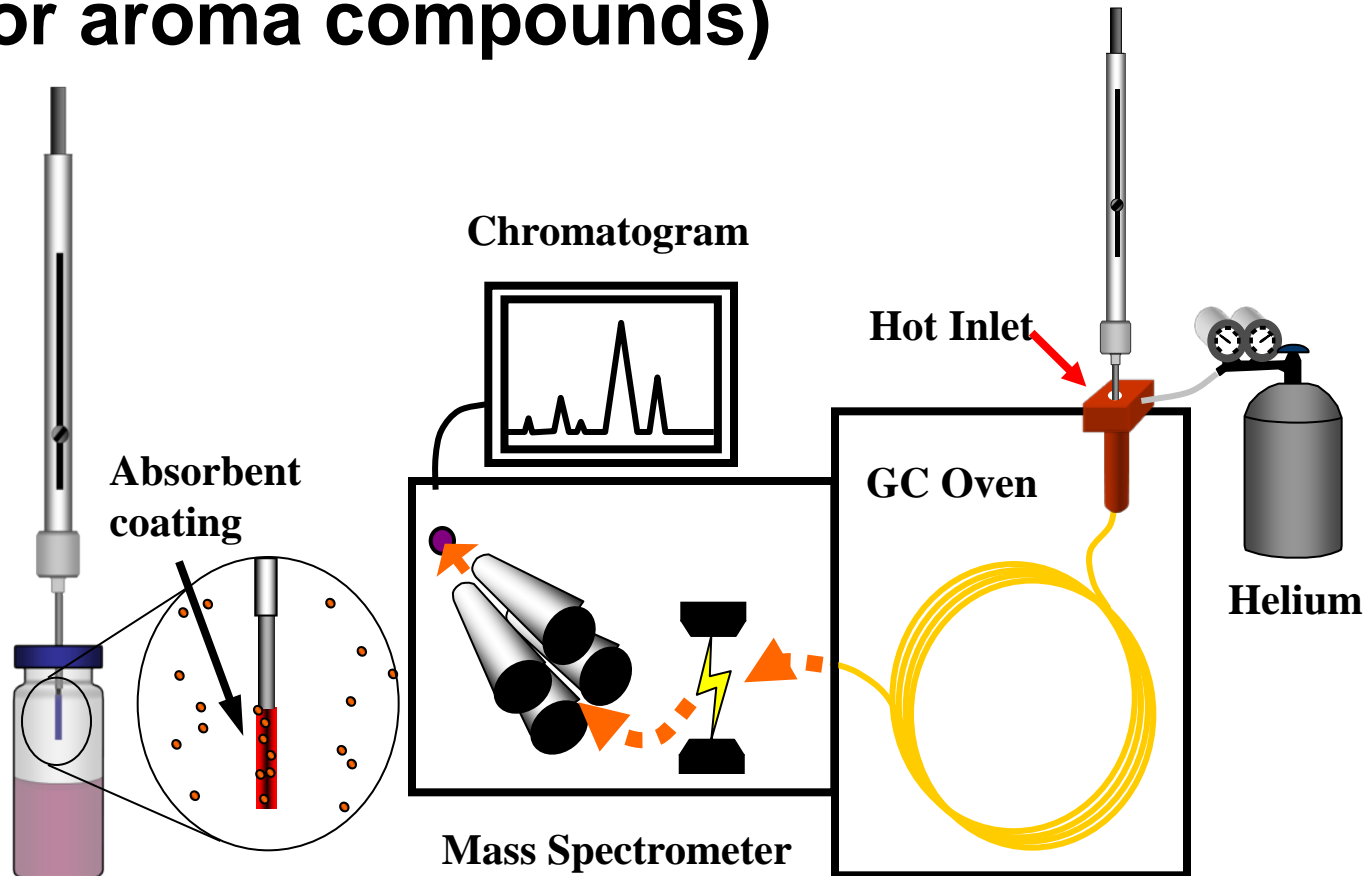
- ◆ **Volatiles (influence aroma)**
 - ◆ **Carbohydrate derived:** Furfural, 5-methyl furfural
 - ◆ **Lignin derived:** Guaiacol, 4-methyl guaiacol, 4-ethyl guaiacol, 4-vinyl phenol, 4-ethyl phenol, eugenol, isoeugenol, vanillin, syringol
 - ◆ **Lipid derived:** *cis*- β -methyl- γ -octalactone, *trans* β -methyl- γ -octalactone (oak lactones)

Oak Flavor

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 - ◆ **Lipid derived:** *cis*- β -methyl- γ -octalactone, *trans* β -methyl- γ -octalactone (oak lactones)
- ◆ **Non-volatiles (influence taste and mouthfeel)**
 - ◆ Monomeric and polymeric phenols

How do we measure flavor?

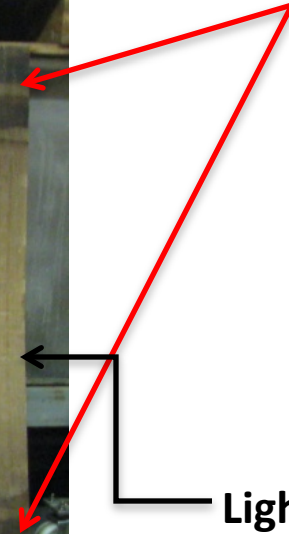
- ◆ Chemical analysis (gas chromatography for aroma compounds)



Oak Volatiles



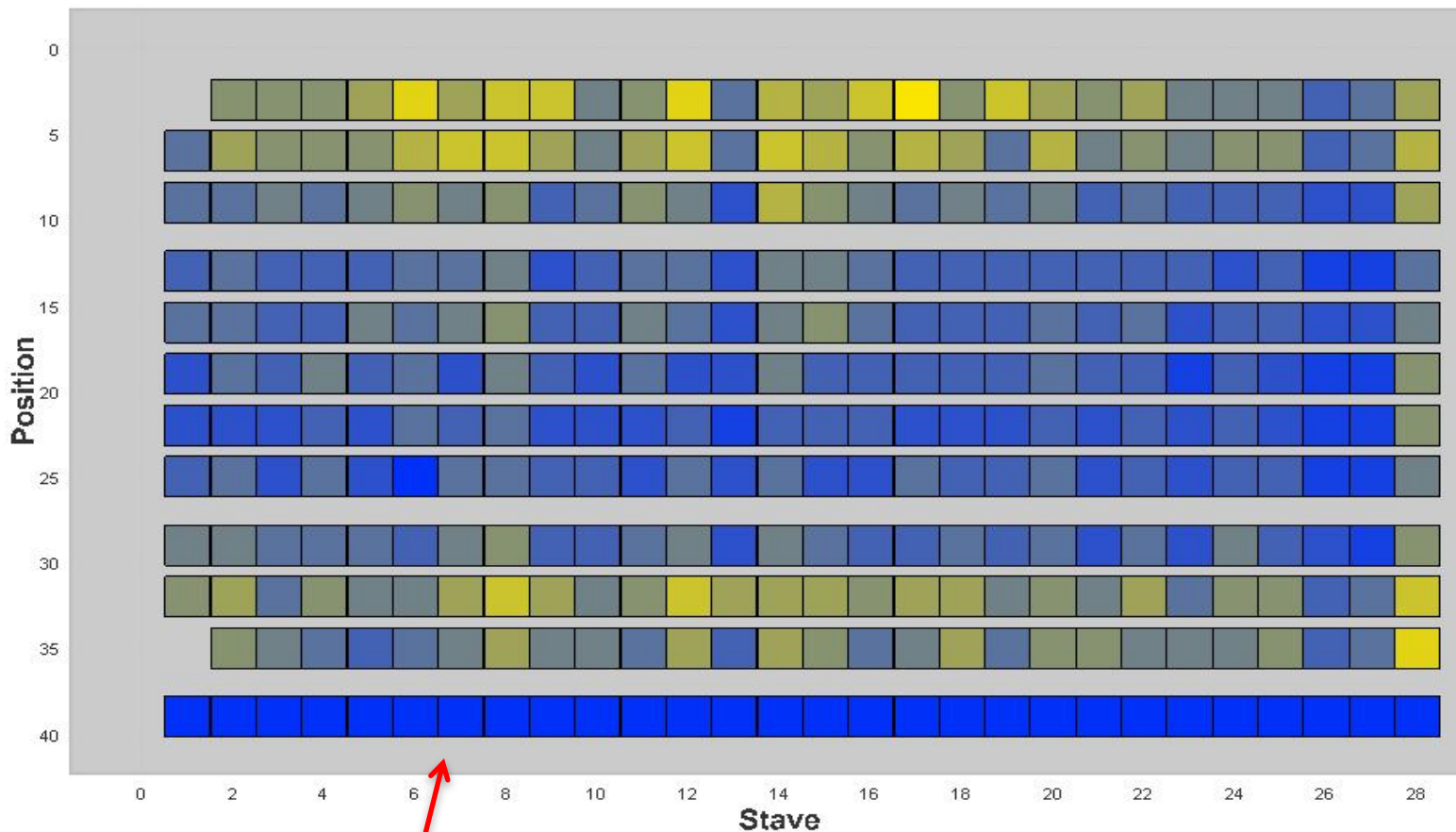
Darker ends



Lighter
middle

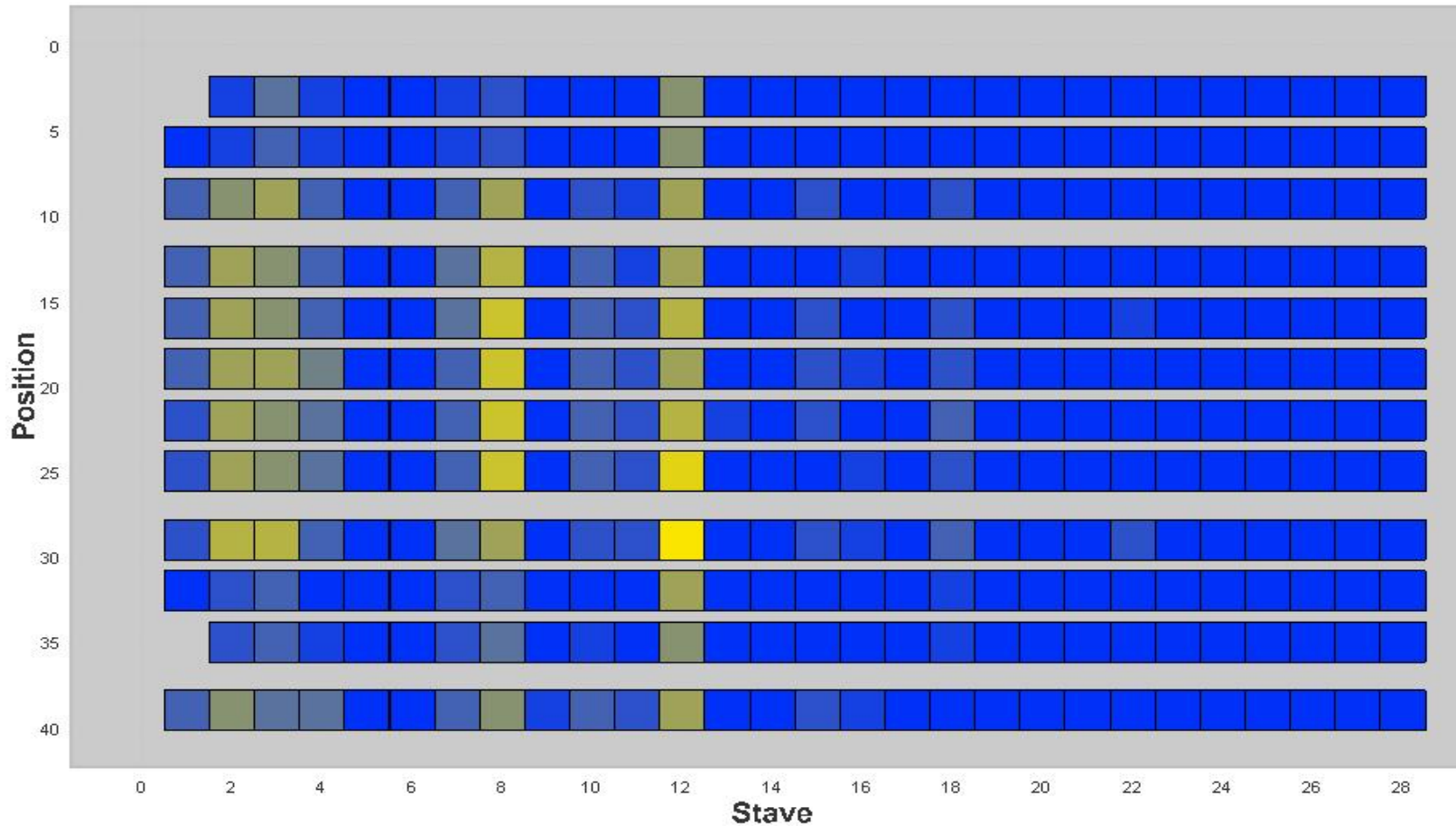
Variability in the toasting process—Jupilles forest, medium plus toast

Full barrel map—4-methyl guaiacol



Samples from outside face of stave

Full barrel map—*trans*-oak lactone



Polling question

◆ A person who makes wine barrels is called:

–Luthier

–Cooper

–Wainwright

–Crocker

–Tonellier

Toasted Oak Composition: Nonvolatile Profiling

- ◆ UHPLC-qTOF/MS
- ◆ Non-targeted analysis
- ◆ Characterize variability in composition between barrels and within a barrel (along position of stave)
- ◆ Identify components-- accurate mass and MS/MS for structural information



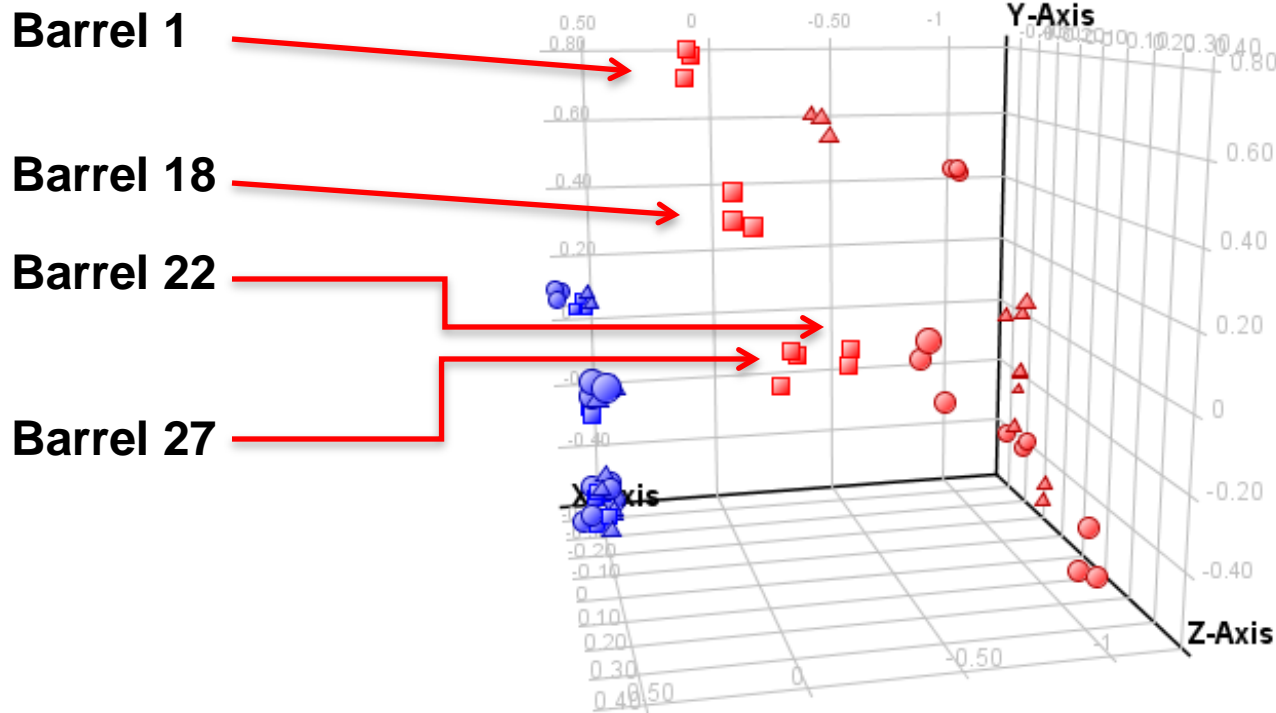
Toasted Oak Nonvolatile Profiling

- ◆ **Develop a set of “entities” with:**
 - Accurate mass
 - Retention time
 - Abundance or intensity
- ◆ **Multivariate statistics to evaluate relationships across the sample set**

Mass	Retention Time	p-value
250.0808	2.50	0.001
258.0863	4.49	0.001
262.0810	3.36	0.001
264.0493	3.07	0.001
276.0969	4.28	0.001
278.0652	2.62	0.001
280.0262	3.07	0.001
280.0277	1.99	0.010
280.0453	2.64	0.001
280.0556	1.78	0.001
290.0598	3.82	0.010

Variation Among Four Different Barrels

Principal Component Analysis (PCA): Inside faces of staves



X-axis Component 1 (69.95%)

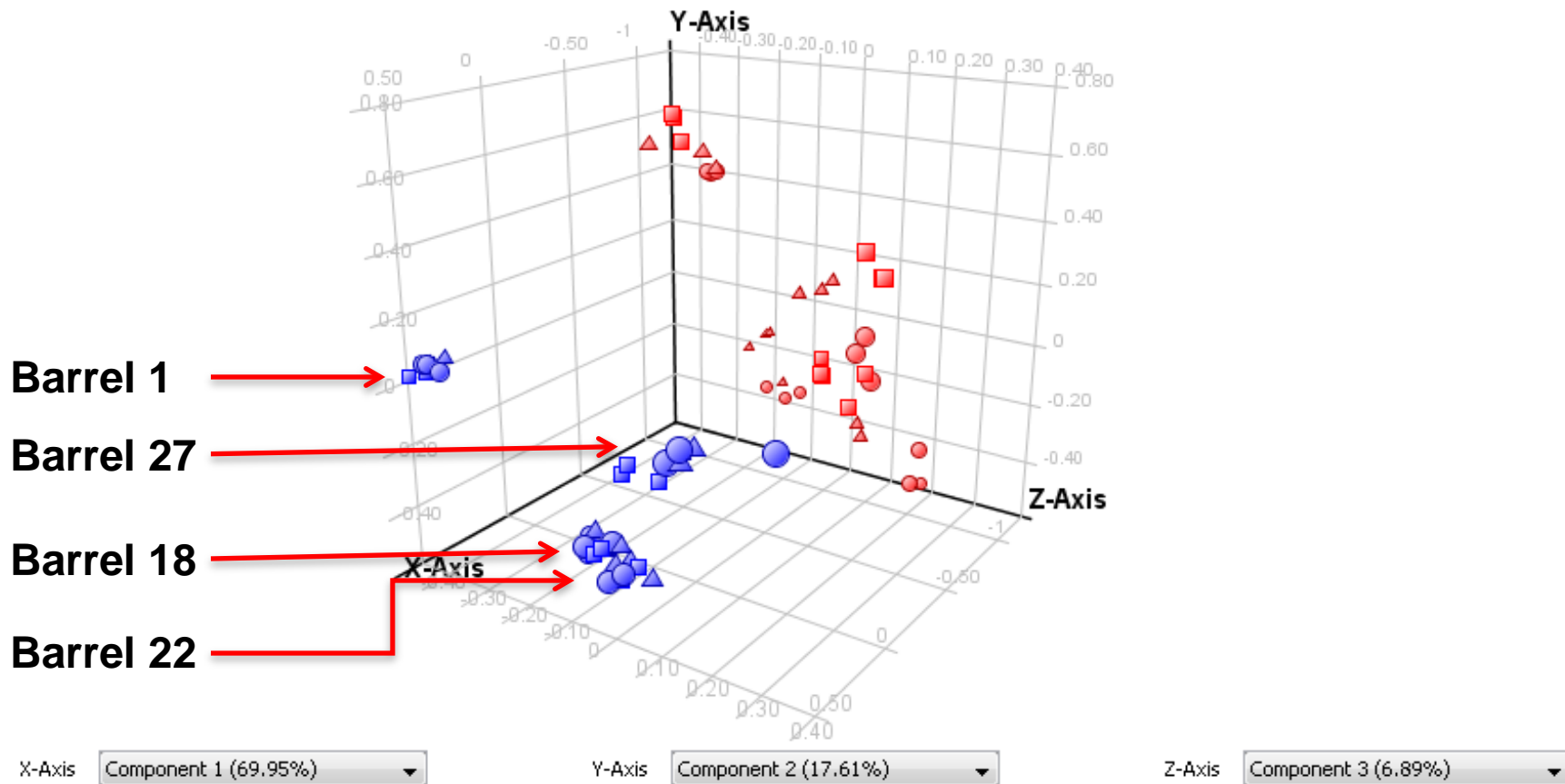
Y-axis Component 2 (17.61%)

Z-axis Component 3 (6.89%)

94.45% of variance explained in 1st three dimensions

Variation Between Four Different Barrels

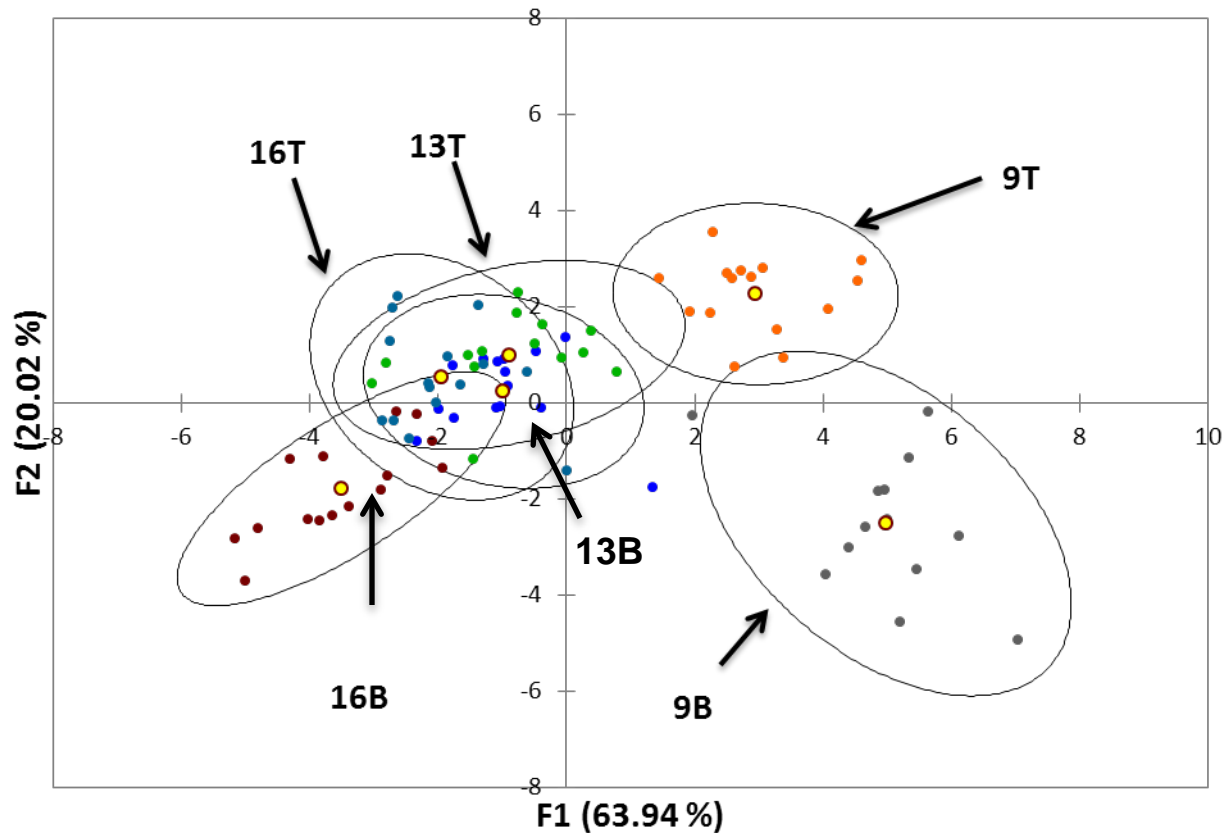
Principal Component Analysis (PCA): Outside faces of staves



Variation Along Stave

Discriminant Analysis

Observations (axes F1 and F2: 83.96 %)



Toasted Oak Nonvolatile Profiling

- ◆ **Composition is different between staves/barrels**
- ◆ **Composition is different along the length of the staves**
- ◆ **Differences between staves/barrels > differences along the length of the stave (after toasting)**

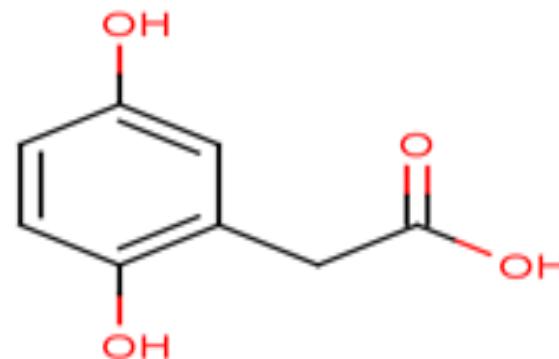
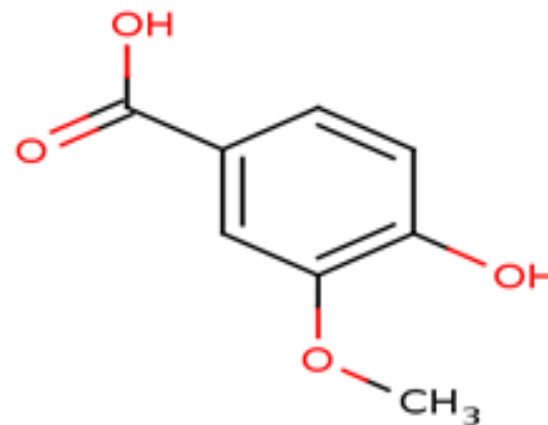
Identifying Compounds

- ◆ **Accurate mass used to generate formulas**
- ◆ **Search Metlin Metabolomics Database to obtain potential structures**
- ◆ **MS/MS for further determination of structures (in progress)**

Identifying Compounds

Accurate mass 168.0423

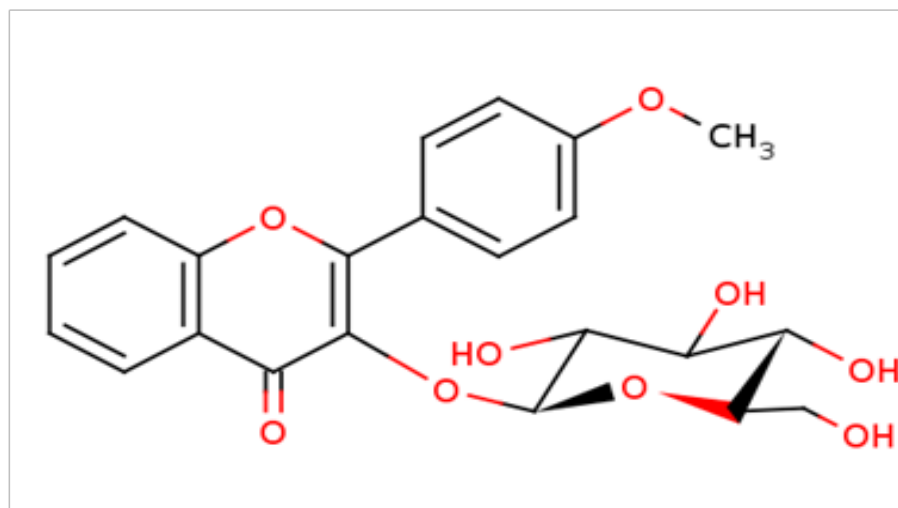
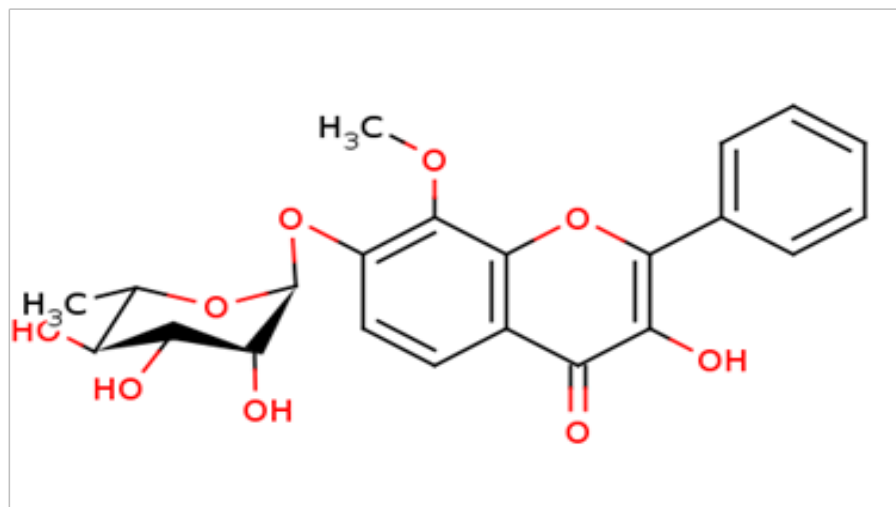
$[M+H]^+$ 169.0495	1	Vanillic acid <i>Formula:</i> C₈H₈O₄
M 168.0423		
$[M+H]^+$ 169.0495	1	Homogentisic acid <i>Formula:</i> C₈H₈O₄
M 168.0423		



Identifying Compounds

Accurate mass 430.1264

M[+H] ⁺ 431.1337 M 430.1264	5	3,7-Dihydroxy-8-methylflavone 7-rhamnoside <i>Formula:</i> C ₂₂ H ₂₂ O ₉
[M+H] ⁺ 431.1337 M 430.1264	5	3-Hydroxy-4'-methoxyflavone 3-glucoside <i>Formula:</i> C ₂₂ H ₂₂ O ₉



Toasted Oak Composition

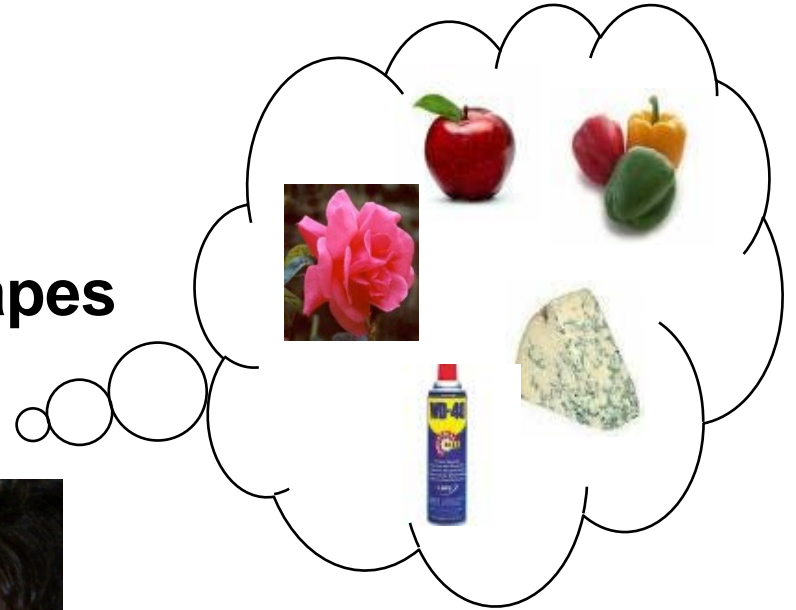
- ◆ **Combine information from volatile and nonvolatile profiles to understand and improve toasting process and to relate to effects on sensory properties**

Linking Sensory and Compositional Information

See also:

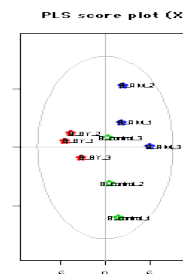
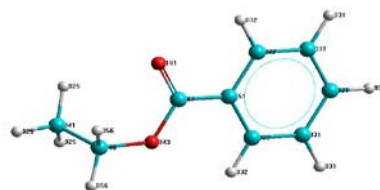
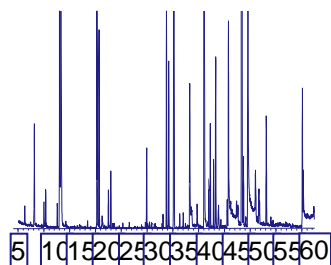
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Summary

- ◆ SPME GC-MS targeted analysis of volatile aroma compounds
- ◆ UHPLC-qTOF/MS nontargeted profiling of nonvolatiles
- ◆ There is significant variability among staves and barrels compared to within an individual stave
- ◆ Use these tools to study processing, storage, etc. effects on composition of oak barrels and wine



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References/Information Sources

- ◆ **Garde-Cerdán, T and Ancín-Azpillcueta, C. *Trends in Food Science & Technology*, 2006, 17(8): 438-447.**
- ◆ **Principles and Practices of Winemaking, Boulton et al., Chapman & Hall, 1996 (ISBN 0-412-06411-1)**
- ◆ **Chemistry of Wine Flavor, Waterhouse & Ebeler, American Chemical Society, 1998 (ISBN 0-8412-3592-9)**
- ◆ **Polaskova et al., *Chemical Society Reviews*, 2008, 37: 2478-2489, DOI: 10.1039/b714455p**
- ◆ **Ebeler and Thorngate, *J. Agric. Food Chem.*, 2009, 57: 8090-8108, DOI: 10.1021/jf9000555**
- ◆ ***Journal of Agricultural and Food Chemistry***
- ◆ ***American Journal of Enology and Viticulture***



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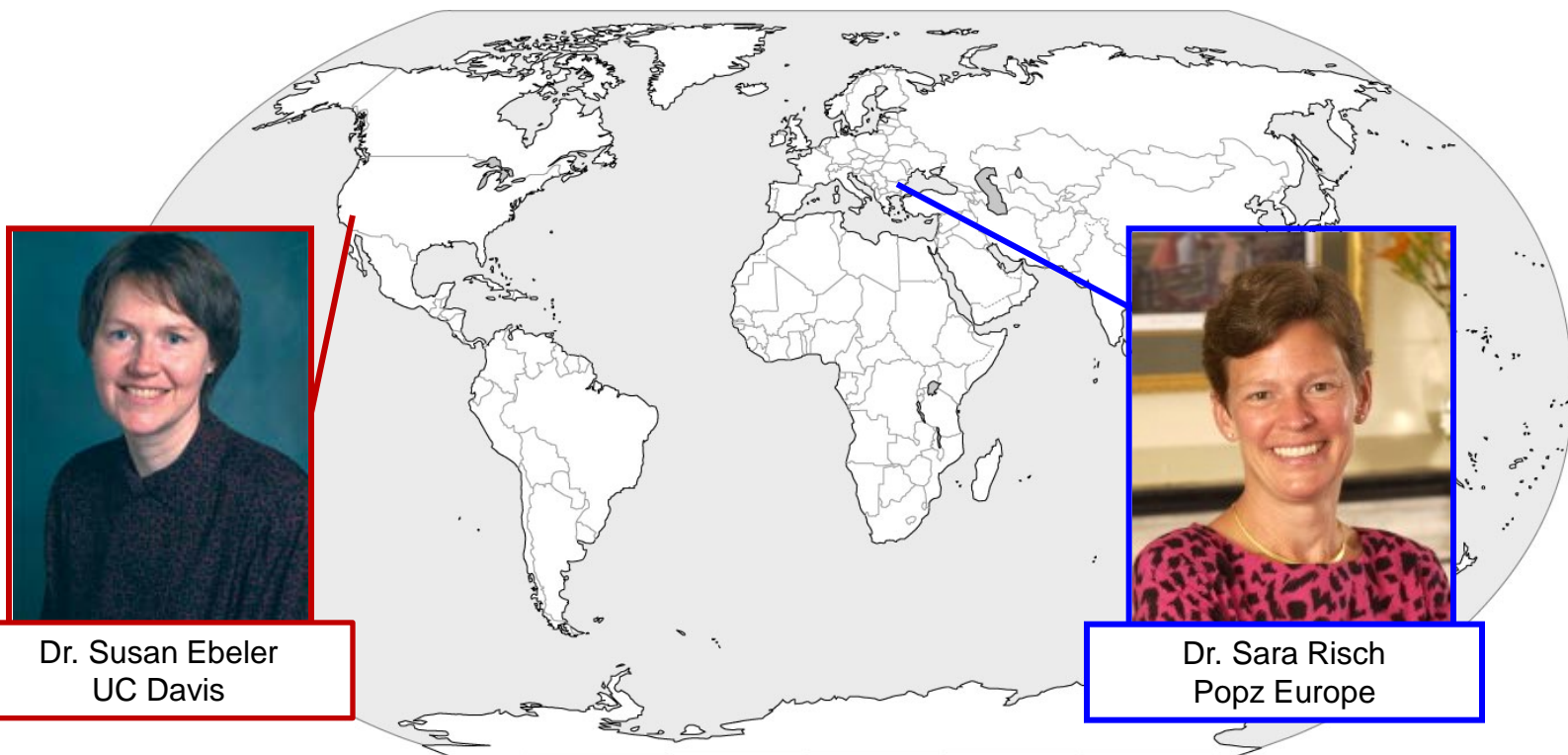


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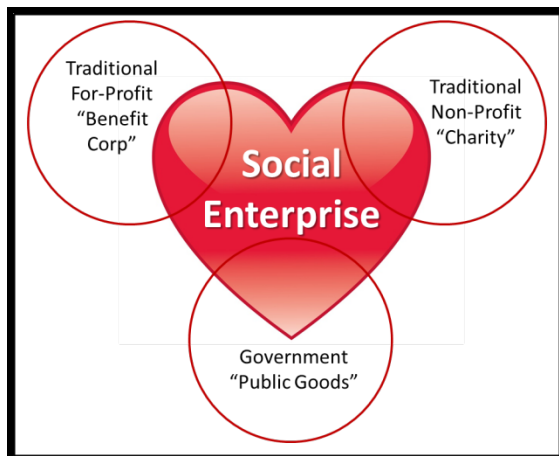
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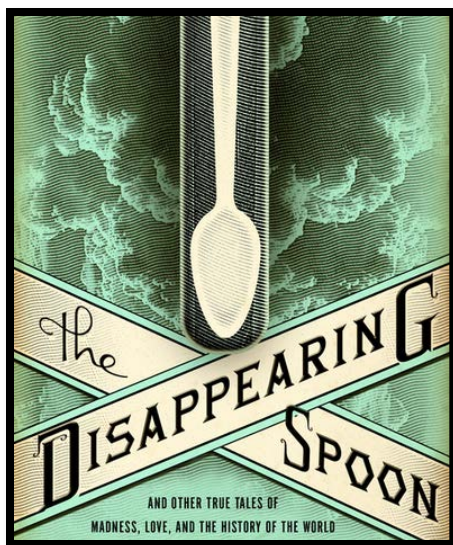


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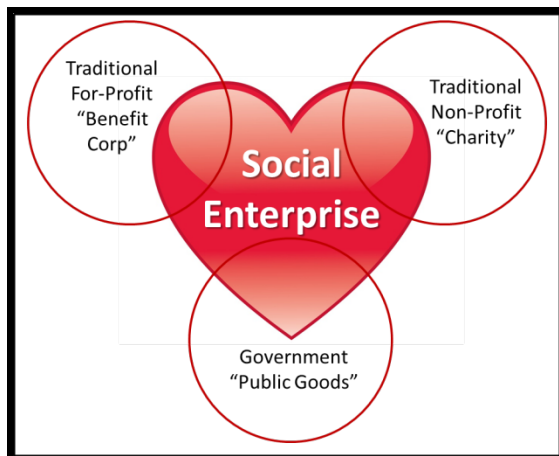
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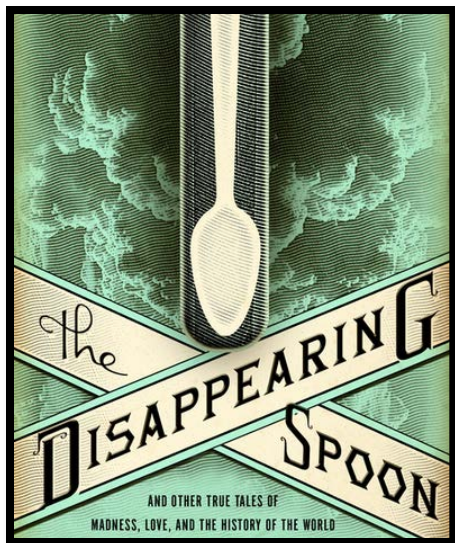
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