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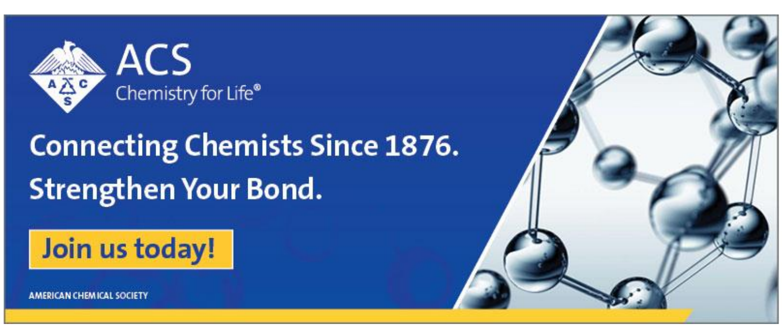

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"A very fine ACS Webinar: Andrew Waterhouse was able to capture the essence of wine reactions throughout the winemaking process and present these in a highly condensed but effective webinar."

http://bit.ly/WineKeyReactions

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Culinary Chemistry Archive: 29 Delicious Recordings and Counting!

What Makes Wine Tick: Key Reactions that Create this Delightful Beverage
Andrew Waterhouse delves into the two types of phenolic compounds that give wine much of its taste and health benefits.

How to Make Chocolate for your Special Valentine: Flowers Bloom, Chocolate Shouldn't
Rich Hartel is returning to share how to properly make chocolate and avoid the moldy looking "bloom" that can occur when it is done incorrectly.

Kitchen Chemistry: We've Got a Lot to Learn from Professional and Recreational Cooks
Join Matt Hartings a Professor of Chemistry at American University as he explains some of the intricate chemical transformations through various cooking techniques and food preparation.

Thanksgiving Chemistry for your Family's Feast
Guy Crosby returns to show how a little chemistry can improve your holiday meal.

Ice Cream Chemistry
Rich Hartel returns to explain the surprisingly complex chemistry of everyone's favorite summer treat.

Halloween Candy Chemistry: Caramels, Gummies, Jellies, and Candy Corn
Join us as Rich Hartel returns to dive deeper in to the chemistry of your favorite sweet treats!

Garlic and Other Alliums: The Lore and the Science
Eric Block explains the colorful history of alliums as well as the science of why they make us cry, give us horrible breath and taste so wonderful.

Color Chemistry: Red and White Beer for St. George's Day
Learn what determines the color of beer and how color is measured in the brewing industry.

The Chemistry of Cocktails: Bruising and Louching and Fire Oh My!
Dr. Darcy Gentleman discusses the chemistry of cocktails and quenches your thirst for knowledge.

Wine Science: Designing Great Wines
Join Dr. Susan Ebeler as she explains the chemistry of wine, from the vineyard to your palate.

Barrels of Chemistry: Decoding How Oak Affects Wine Flavor
Learn how the hints of cream, smoke, spice and vanilla that hide in your wine have less to do with the grape and more to do with the wood.

Sous Vide Cooking and Chemistry
Discover a form of cooking that can make the toughest cuts of meat come out tender, juicy and medium rare with Douglas Baldwin.

https://www.acs.org/content/acs/en/acs-webinars/culinary-chemistry.html

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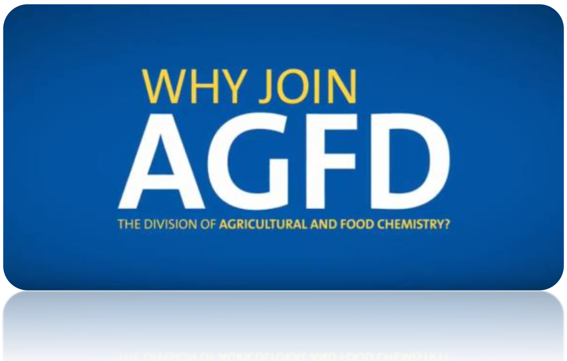
ACS Division of Agricultural & Food Chemistry



AGFD brings together persons particularly interested in the chemistry of agricultural and food products, both raw and finished; to foster programs of general papers and symposia on special topics dealing with this field of chemistry; to promote such other activities as will stimulate activity in and emphasize the importance of research in agricultural and food chemistry.

Find out more about the ACS AGFD! http://agfd.sites.acs.org

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Upcoming ACS Webinars
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Thursday, May 31, 2018

Advanced Nano-Delivery Systems: *Facilitating Tumor Delivery and Mitigating Resistance*

Co-produced with the ACS Division of Medicinal Chemistry and the American Association of Pharmaceutical Scientists

Experts

Mansoor Amiji
Northeastern University

Venkat Krishnamurthy
AstraZeneca

Thursday, June 6, 2018

Refugees, Displaced Scientists, and Chemistry Communities: *Creative Approaches to Support Chemical Practitioners*

Co-produced with ACS International Activities as part of the ACS Science and Human Rights Initiative

Experts

Jeff Wilkesman
University of Carabobo

Admir Masic
Massachusetts Institute of Technology

Robin Perutz
The University of York

Dorothy Phillips
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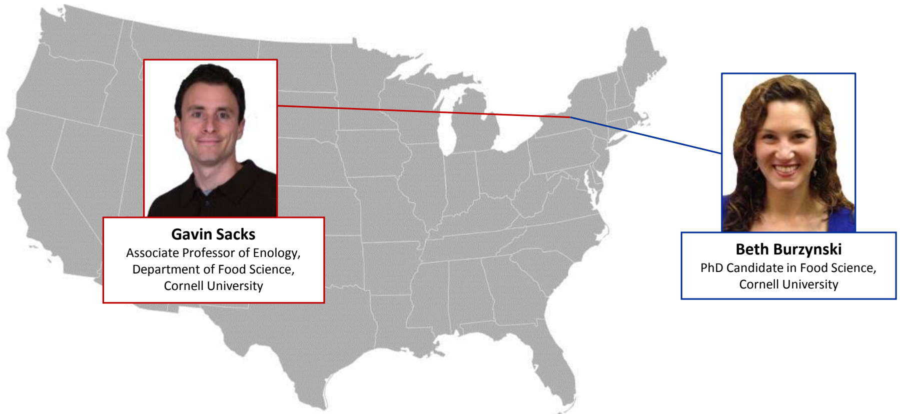
*"**Ready to Drink Yet?** The Chemistry of How Wine Flavor Changes During Aging"*



Slides available now and an invitation to view the recording will be sent when available.

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"Ready to Drink Yet?"

The Chemistry of How Wine Flavor Changes During Aging

Gavin L. Sacks
Associate Professor of Enology
Department of Food Science
Cornell University

Moderator: Beth Burzynski, PhD Candidate in Food Science, Cornell University

Cornell CALS College of Agriculture and Life Sciences

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Let's get started . . . consider the range of wine labels available to US consumers

This is a wine label

So are all these

Wine labels can include info on

- Producer/brand
- Production region (e.g. Bordeaux)
- Grape variety (e.g. Chardonnay)
- Vintage year
- Alcohol content, "contain sulfites", government warnings

In the US, wine labels must be pre-approved prior to bottling or importation by the Tax and Trade Bureau (TTB)

Audience Challenge Question

ANSWER THE QUESTION ON BLUE SCREEN IN ONE MOMENT

How many different wine labels are approved for sale each year in the United States?

- 2,000 to 4,000
- 6,000 to 10,000
- 15,000 to 30,000
- 40,000 to 60,000
- 75,000 to 125,000

Image: mnn.com

Premium wine is a "craft" product, not a "commodity" Variation in sensory (and thus chemistry) is expected

Taste (Gustation)

salty**, bitter, sweet, acidic**, and umami compounds

Touch (Chemesthesis)

Compounds responsible for **pungency**, cooling, **astringent**, viscous and related tactile sensations

Smell (Olfaction)

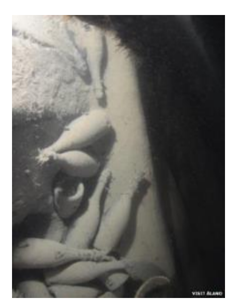
Volatile compounds, of which 50-75 create most wine-like aromas

Appearance

Pigments (mostly red and yellow) or light-scattering haze particles

Popular appeal of wine - Explanations

- Its variation
- Its deliciousness, particularly with food
- Its sense of place
- It contains ethanol
- Its mystique, including its longevity



The reputation for "age-ability" persists even though the majority of wines are meant to be, and are, consumed within 0.5-2 years of production

(the occasional bottle of 170-year old shipwrecked Champagne excepted)

"Age-worthy" does not have a well agreed upon definition among enologists

Working definition: "assuming two wines (A and B) are equally liked at some time point, Wine A 'ages better' if it is better liked than Wine B at a later time point."

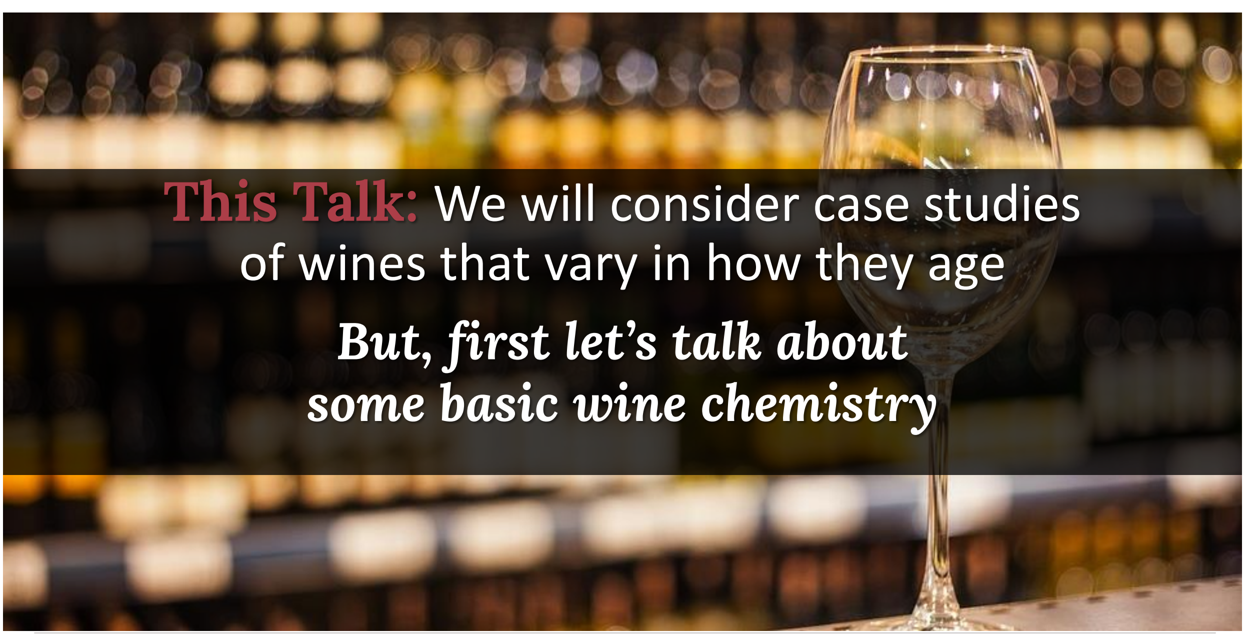
Maybe, youthful characteristics are preserved in Wine A

- Desirable sensory compounds could be more stable
- Fewer undesirable compounds could form

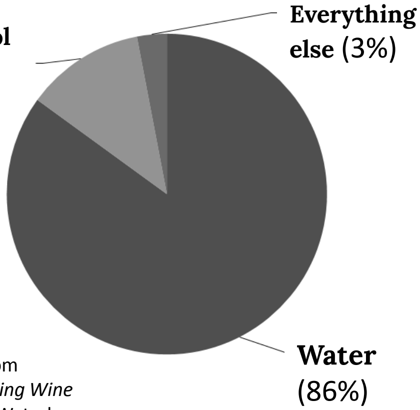
Or, new "aged" characteristics appear in Wine A

- Undesirable sensory compounds could be lost more rapidly during storage
- More desirable compounds could form

Image: istockphoto.com;
(WP:NFCC#4), Fair use, https://en.wikipedia.org/w/index.php?curid=40373629



Chemically, what's in a typical dry red wine?



Adapted from *Understanding Wine Chemistry*; Waterhouse, Sacks, and Jeffery. **2016**

Everything else, a non-comprehensive list

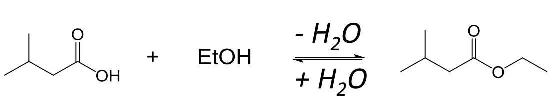
- Glycerol (6-12 g/L)
- Organic acids (5-8 g/L) → **wine pH is 3-4**
- Hexose sugars (0.5-3 g/L)
- Minerals, e.g. K^+ (0.5-2 g/L)
- Important odorants (ng/L to mg/L)
- Phenolics (0.5-2 g/L)
  - Anthocyanins [color]
  - Tannins [astringency]
- Sulfur dioxide (20-40 mg/L)
- Glutathione (15-100 mg/L)

Reducing compounds (nucleophiles)

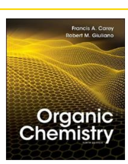
What reactions can happen at pH 3-4, 10-12% EtOH, reducing conditions, 20 °C, over 6-24 months?

Reactions involving water or ethanol, often acid catalyzed

- Hydrolysis, ethanolysis (below)
- H_2O/EtOH addition or elimination



Other textbook reactions, e.g. Grignard? Not likely ☺



Reactions between wine nucleophiles and electrophiles

- Example nucleophiles = SO_2/HSO_3^- H_2S, thiols, polyphenols
- Example electrophiles = carbonyls (e.g. acetaldehyde); tannin hydrolysis products; quinones

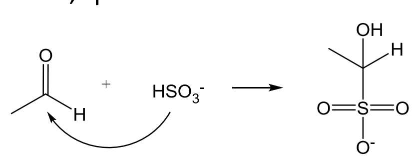


Image: mcgrawhill.com

Case Study 1: Varietal wines "not aging well" due to loss of desirable compounds

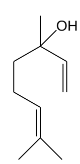
Muscat-type wines vs. *Gewürztraminer*

Both types of wines have floral aromas when young, but they have different reputations for aging

Consider two monoterpene-rich, "floral" smelling grape varieties, with dissimilar fates during aging

Muscat-type grapes,
e.g. Moscato bianco from Asti

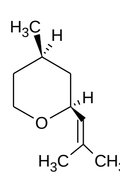
"Serving recommendations [for Moscato d'Asti] . .drink it young and fresh!" - winefolly.com



Key odorant = **linalool**
("lily-of-the-valley")

Gewürztraminer

"While you often can drink Gewürztraminers young, some benefit from 2-4 years worth of aging." - wineintro.com



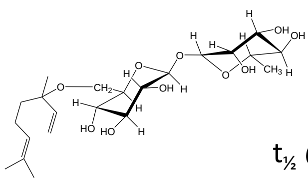
Key odorant =
***(-) cis*-rose oxide**
"rose/litchee"

Image: Wikimedia Commons

The key “floral” monoterpenes in Muscat-type wines, e.g. linalool, are unstable in wine matrix

Linalyl glycosides

Non-odorous precursors

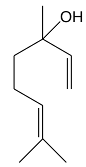


Partial release during fermentation

Slow non-enzymatic release during storage

$t_{½}$ @ wine pH = <u>months</u>

Linalool
“lily-of-the-valley”
Threshold = 50 ppb



Acid catalyzed ring closure

$t_{½}$ @ wine pH = <u>weeks</u>

α-Terpeniol
“resin, pine”
Threshold = 400 ppb

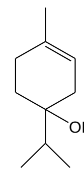
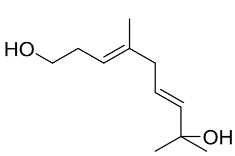


Image: Wikimedia Commons

By comparison, the key Gewürztraminer monoterpene is stable or increases during storage

Monoterpene diol precursors

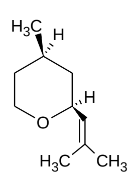
Odor threshold = very high



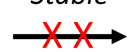
Enzymatic reduction

Acid-catalyzed ring closure

(-) cis-rose oxide
“rose/litchee”
Threshold = 0.5 ppb



Stable



Koslitz, et al *JAFC* **2008**
Belitz, Grosch, Schieberle **2004**

Recap: Wines with strong floral aromas often do not "age well" if you desire the odor to stay floral

- **Monoterpenes, particularly linalool, contribute "floral" aromas, but are not stable in aqueous acidic matrices** (WINE!)
  - In particular, Muscat-type varieties (e.g. Muscat bianco)
  - Stonefruit notes of some wines (e.g. Viognier) do not persist
- **A monoterpene exception: *cis*-rose oxide**
  - Gewürztraminer can continue to have "litchee" aromas, even with age

Case Study 2: Production practices lead to desirable odorants that are readily lost during storage

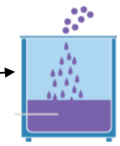
Beaujolais Nouveau vs. *Standard red wines*

Beaujolais Nouveau is known for intense "cherry, banana" type aromas and is intended for sale within weeks of fermentation

Red winemaking: The 30 second story

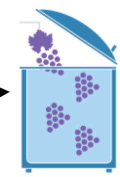
Standard Red Wine Maceration

Grapes are crushed and fermented by yeast in the presence on skins and seeds



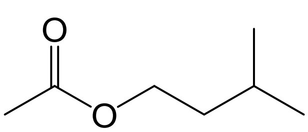
Carbonic Maceration (common for Beaujolais Nouveau)

Whole grape clusters are blanketed in CO_2, grapes auto-ferment to ~2% alcohol. Then, grapes are pressed, and juice is fermented to dryness by yeast



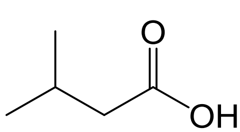
Images adapted from by John Blanchard, SF Chronicle; https://www.sfchronicle.com/wine/article/California-taps-into-bright-young-things-of-10607345.php

Several differences in odorant concentrations between carbonic (CM) and standard maceration, including…



Isoamyl acetate
"Cherry/banana"

↑ Higher in CM wines



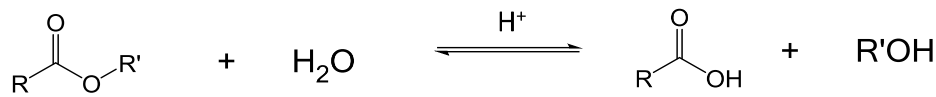
Isovaleric acid
"Cheesy, sweaty"

↓ Lower in CM wines

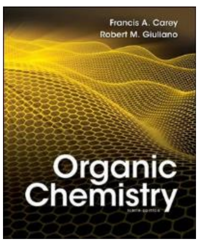
(although, below sensory threshold in most wines)

Data from Antalick, et al. AJEV 2014.

Ester hydrolysis / Esterification in Wine Just like in your Organic Chem I Class



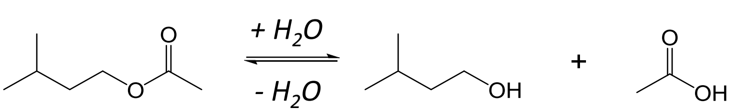
Ester **Fatty acid** **Alcohol**



$$K_{eq} = \frac{[\text{alcohol}][\text{fatty acid}]}{[\text{ester}][H_2O]} \sim 0.25$$

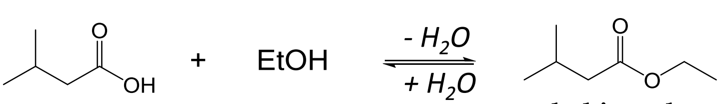
← **Literature estimate**

Working through the math…and assuming [EtOH] = ~2M or 12% v/v, acetic acid = ~5 mM, $[H_2O]$ = ~50M



Isoamyl acetate "banana" **Isoamyl alcohol** **Acetic acid**

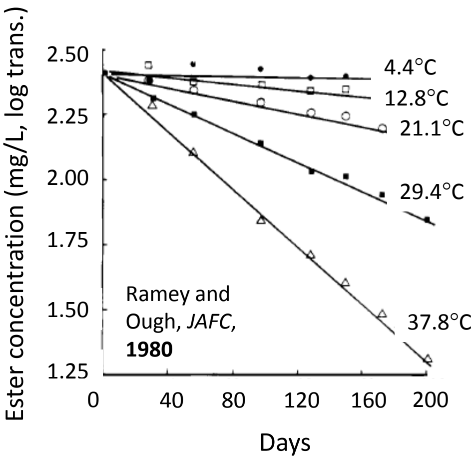
Isoamyl acetate and other <u>acetate esters decrease</u> during storage



Isovaleric acid **Ethanol** **Ethyl isovalerate** "strawberry"

Ethyl isovalerate and some other <u>ethyl esters can increase</u> during storage

Organic Chem I, cont., kinetics



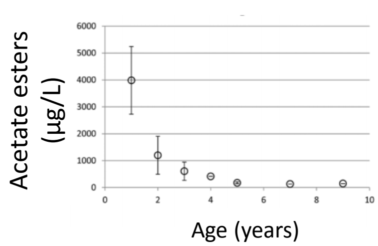
Ester hydrolysis/esterification follow pseudo-first order kinetics in wines

At pH 3.6, T=25°C,
$t_{1/2}$ for hydrolysis of an ester is **3-5 months**
$t_{1/2}$ for esterification of a fatty acid **is 1-2 yrs**

How to slow down ester reactions?

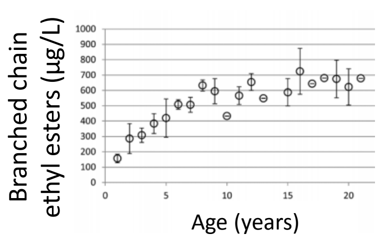
- Raise pH (causes other problems)
- Store cold, especially during transit
- **Drink quickly!**
  - *Beaujolais on Thanksgiving*

Recap: wines which rely heavily on acetate esters will likely “not age well”



Examples of wines with high acetate esters

- Beaujolais Nouveau and other carbonic wines
- ‘Tropical fruity’ whites, e.g. many Pinot Grigio, Sauvignon blanc, and stainless steel Chardonnay



Standard red winemaking

= more branched chain fatty acids
= more branched chain ethyl ester formation during storage

Fruity or other aromas?

From Antalick, et al AJEV 2014

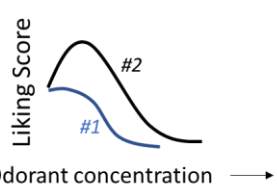
An aside on additional hydrolytic reactions, before returning to case studies…

"Is it good aging? Or bad aging"?

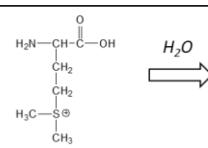
Dimethyl sulfide (DMS) and 1,1,6-trimethyldihydronaphthalene (TDN)

DMS, TDN . . . do we want these forming in our wines?

Hypothetical responses of two consumers (#1, #2) to spiked wine



> *"only the dose makes a thing not a poison"*
> - **Paracelsus**



CH_3-S-CH_3

S-methylmethionine (SMM)

Higher in riper grapes

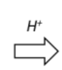
Dimethyl sulfide (DMS)

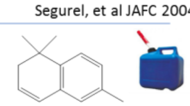
"canned corn, truffle, asparagus"

Segurel, et al JAFC 2004

Glycosylated C_{13}-norisoprenoids

Higher in Riesling, sun exposed grapes





1,1,6-trimethyldihydro-naphthalene (TDN)

"kerosene"

Understanding Wine Chemistry

Image from jcsmith.com and Wikimedia Commons

Cornell CALS College of Agriculture and Life Sciences

Audience Challenge Question

ANSWER THE QUESTION ON BLUE SCREEN IN ONE MOMENT

Which of these approaches to accelerated aging have been patented?

More than one correct answer may exist

- Agitation
- High-temperature
- Ionizing radiation
- Ultrasound
- Electric Currents

Image: Wikimedia Commons

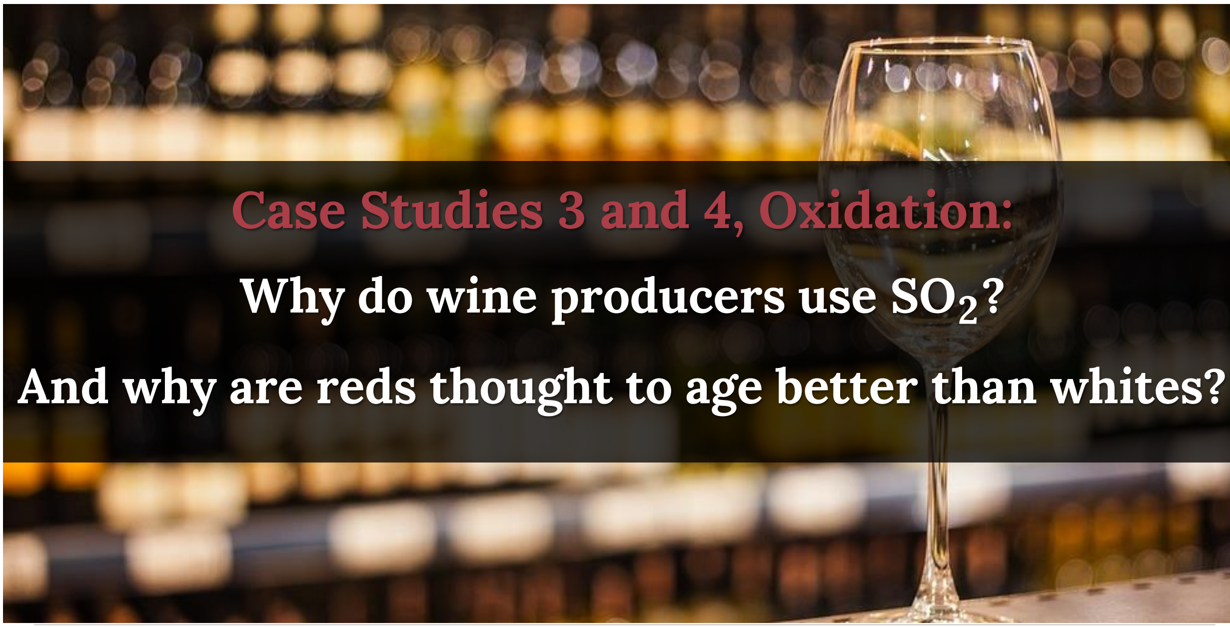
"Rapid aging" approaches do not appear to duplicate conventional aging (say, in a 12 °C cellar)

Example 1: UV or gamma ray irradiation generates free radicals
→ volatile sulfur compound formation → "burnt hair" aromas

Example 2: High temperature storage promotes different reactions at different rates
→ Wine reactions differ in activation energies

Unfortunately, higher temperatures often accelerate unwanted reactions to a greater extent!

Reaction in beverage model system	Activation energy, E_a (kJ/mol)	Fold-increase in reaction rate compared to 12 °C: At 30 °C	At 50 °C	
Acid hydrolysis of proanthocyanidins (tannins)	45	3	9	**Possibly desirable**
Esterification or ester hydrolysis	62	5	22	
Hydrolysis of SMM to DMS	186	106	10250	
Acid hydrolysis of anthocyanin pigment	118	19	350	**Unlikely to be desirable**
Formation of ethyl carbamate from urea and ethanol	118	19	350	



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Audience Challenge Question

ANSWER THE QUESTION ON BLUE SCREEN IN ONE MOMENT

In the current model of wine oxidation, which wine component directly reacts with O_2?

- [Fe(II)] complexes
- SO_2 (in the form of bisulfite, HSO_3^-)
- Polyphenolics, particularly condensed tannins
- Glutathione and related sulfhydryls
- Alcohols, particularly ethanol

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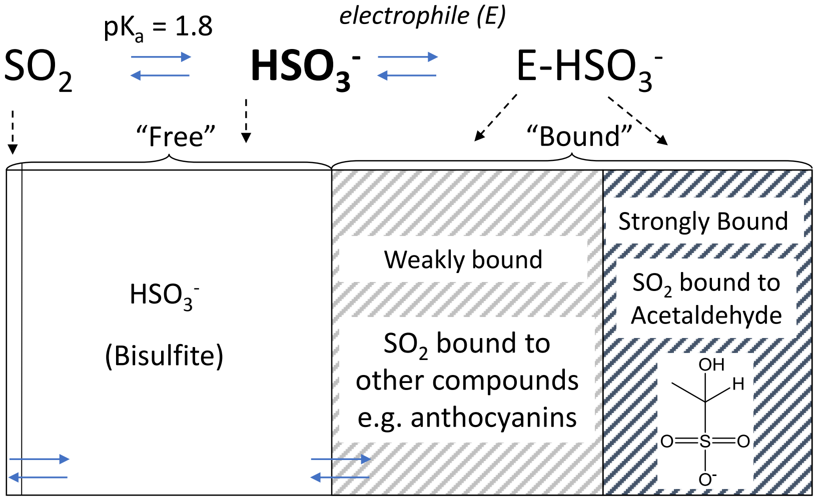
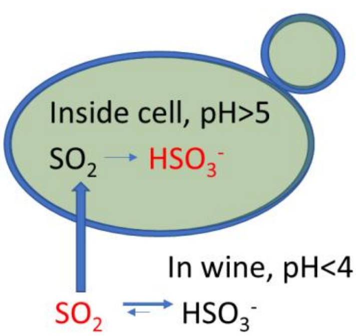
Distribution of SO_2 species in wine



- At wine pH, most SO_2 in exists as bisulfite
- Smaller portion (<5%) exists as 'molecular' SO_2
- Almost no sulfite, SO_3^{2-}
- Some bisulfite is covalently bound to wine electrophiles like acetaldehyde

Role of sulfur dioxide (SO_2) in wine

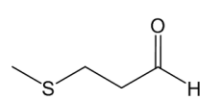
Anti-microbial: neutral, "molecular" form can cross the cell membrane



Lower pH favors molecular form

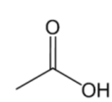
Anti-oxidant: Bisulfite (HSO_3^-) reacts with products of oxidation

Best predictor of aroma quality = low levels of off-odorants from spoilage organisms or oxidation (San Juan, et al; *JAFC* **2012**)



Methional, "baked potato"

Via abiotic oxidation



Acetic acid

Via microbial spoilage

Focus on abiotic oxidation during aging
How is O_2 getting into a bottled wine?

Same Semillon wine with one of 14 closures

Adapted from P. Godden, et al, AJWGR 2001

Oxygen can . . .

- Be present in headspace during bottling
- Migrate through or around the closure

Wine Oxidation – Production of H_2O_2

Typical wine: ~1 mg/L Fe

$$O_2 \xrightleftharpoons{[Fe(II)]} [Fe(III){-}O_2^{\bullet}]^{2+} \xrightarrow{[Fe(II)]} 2\,[Fe(III)] + H_2O_2$$

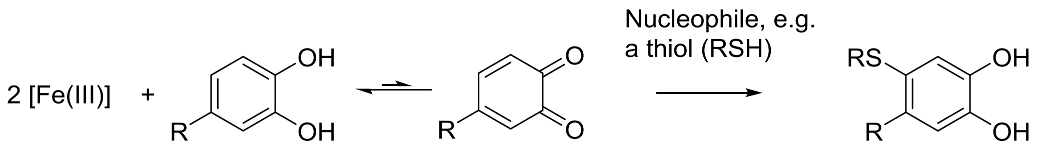
$$H_2O_2 \xrightarrow{[Fe(II)]} {}^{\bullet}OH \xrightarrow{R\text{-}OH} \text{Aldehydes, Ketones} \xrightarrow{\text{Catechin}} \text{Browning}$$

"*Fenton reaction*"

Oxidized aromas
("baked potato, bruised apple, cardboard")

Browning

Wine Oxidation – Formation of Quinones



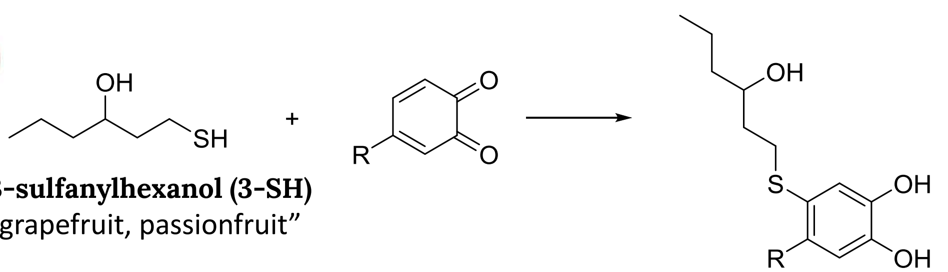
***o*-diphenol**, e.g. caffeic acid

***o*-quinone**, *e.g. caffeic acid*

Adapted from Danilewicz, AJEV 2012

- Oxidation of diphenols to quinones by [Fe(III)] is not thermodynamically favorable in wine
- Wine nucleophiles “trap” quinones and drive oxidation forward
- By comparison most distilled spirits are low in nucleophiles (and often transition metals and phenolics, too) . . Oxygen consumption is very slow

Quinones can react with many nucleophiles, including desirable “fruity” smelling thiols



3-sulfanylhexanol (3-SH)
“grapefruit, passionfruit”

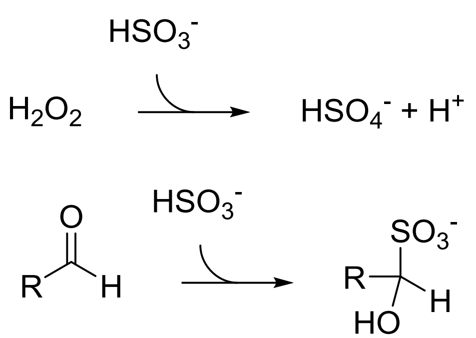
- 3-SH is critical for the fruitiness of many wines, particularly Sauvignon blanc
- Result: loss of quality, unless another nucleophile is present (enter SO_2)

Nikolantonaki and Waterhouse, JAFC 2012

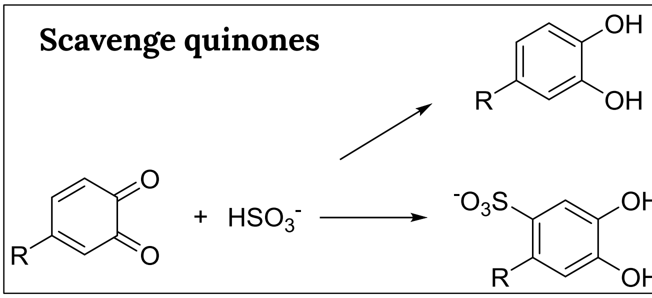
Image: Wikimedia Commons

The role of SO_2 as a wine antioxidant – Scavenge wine oxidation products

Scavenge H_2O_2 and aldehydes



Scavenge quinones



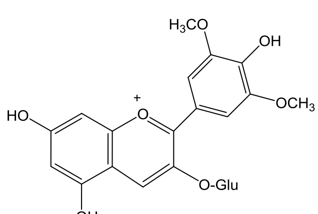
The ability to rapidly scavenge H_2O_2 is unique to HSO_3^-

Once HSO_3^- is mostly depleted (< 10 mg/L), oxidation products accumulate

So why would red wines potentially age better than white wines?

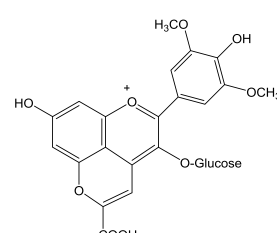
- In part, red wines are less dependent on thiols as key aroma compounds
- Also, polyphenols (anthocyanins, tannins) can react with oxidation products, e.g. malodorous carbonyls, or quinones

Ex:



Malvidin-3-glucoside
(anthocyanin)

+ Acetaldehyde ⟹

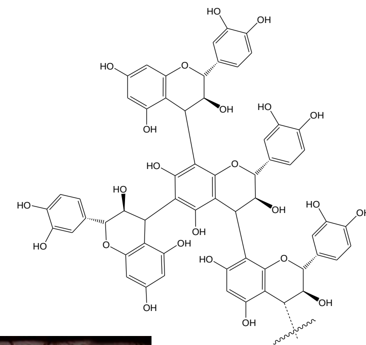


Vitisin B

Recap: Antioxidants like SO_2 and/or polyphenols may help a wine age better, but not because they directly react with O_2

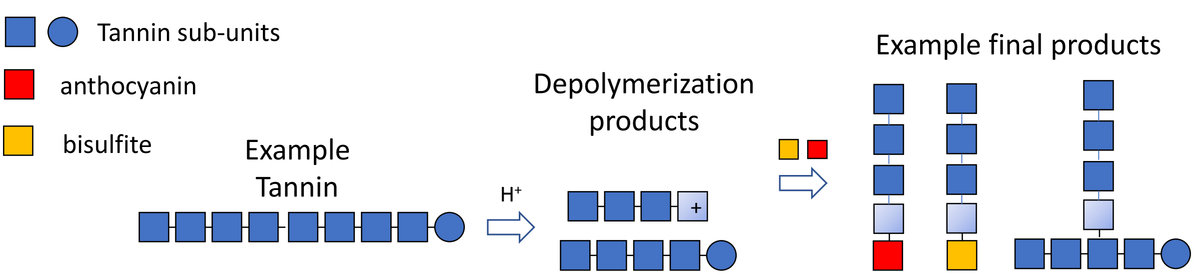
- **Oxidation of wine is catalyzed by the presence of transition metals like Fe(II)**
- **Oxidation generates H_2O_2 and polyphenol quinones.**
  - These species can result in loss of desired aroma compounds, production of oxidized aroma compounds (mostly carbonyls), and browning
  - SO_2 (as bisulfite) can react directly with H_2O_2, quinones, and carbonyls
  - Polyphenols can react with quinones and carbonyls
- **Counterintuitively, the presence of SO_2 and polyphenols increases the rate at which O_2 is consumed**

Ongoing Studies: **What happens to condensed tannins** (chemically, sensorially) **during aging?**



- **Condensed tannins, aka proanthocyanidins**
  - Polymers of flavan-3-ols, e.g. catechin
  - Present in grape skins and seeds – at higher concentrations in red wines
- **Responsible for "astringency"** (*drying, puckering sensation*) **in wines**
  - Mechanism = non-specific covalent binding of proteins, including salivary proteins

During storage, tannins can undergo both acid-catalyzed and electrophile/nucleophile reactions



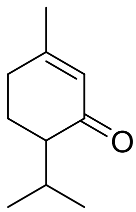
- **How do these reactions affect tannin sensory attributes?**
  - Decrease in astringency, most likely?
  - Other changes, i.e. decrease in in-mouth persistence ("stickiness")?

Waterhouse, et al 2017; Salas, et al JAFC 2003; Revelete, et al JAFC 2014

Ongoing Studies: What else forms during storage and contributes to the "bouquet" of aged wines?

- From before: certain ethyl esters, TDN, DMS
- Recent papers using **GC-O/MS** have suggested additional candidates

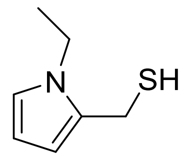
GC-Olfactometry
(GC-O)



Piperitone

"Minty"

Found in aged red wines



1-methylpyrrole-2-methanethiol

"Hazelnut"

Chardonnay

Pons, et al *Food Chem* **2016**

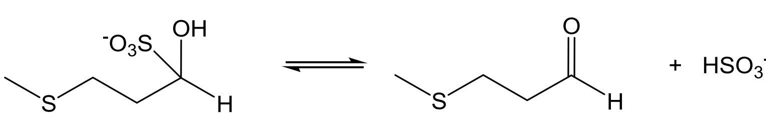
Gros, et al *JAFC* **2017**

Ongoing Studies: Why do wines differ in relative amounts of key malodorous compounds following oxidation?

Methional ("baked potato") and phenylacetaldehyde ("honey") have been implicated as key wine oxidation odorants

- Low sensory thresholds
- Relatively weak SO_2 binders as compared to other aldehydes

Wines can differ by over an order of magnitude in the amount of these aldehydes formed during oxidation and HSO_3^- loss



Bound methional

Methional

Does high bound methional explain why some wines "age badly"?

Image: Wikimedia Commons

Bueno, et al JAFC 2016

Wrapping Up: Take-Home Messages

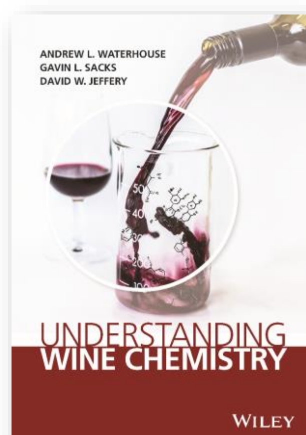
- **"Aging well" is a not single concept**
  - New desirable compounds could be formed; or else lost more slowly
  - Or, new undesirable compounds could be avoided; or else lost more quickly
  - And, what's desirable to one consumer may not be to another
- **A limited number of types of reactions can occur in aging. Key classes**
  - Solvent-mediated, such as ester hydrolysis/esterification
  - Reactions between nucleophiles and electrophiles, e.g. addition of bisulfite to oxidation products
- **There's much to learn still:** Tannin changes, odorants responsible for aged wine aroma, differences in observed oxidation products among wines

Still Thirsty?: If you like this talk, and want to learn more, consider the textbook

Understanding Wine Chemistry

Andrew L. Waterhouse, Gavin L. Sacks, and David W. Jeffery

Published in 2016 by John Wiley & Sons



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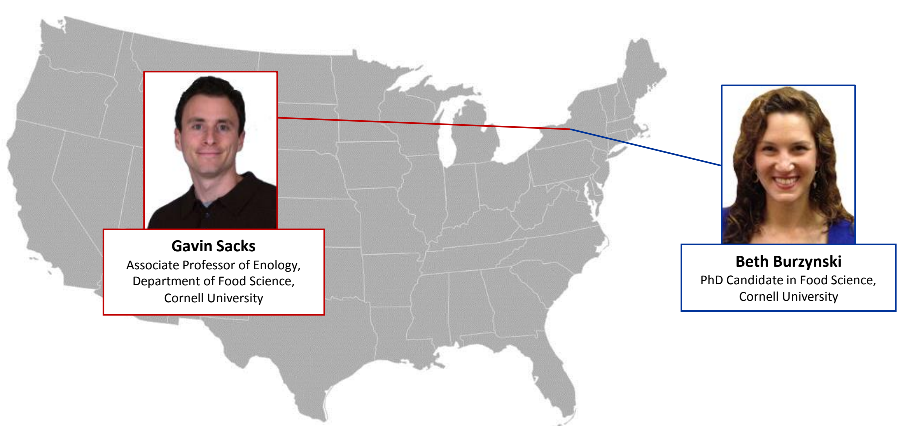

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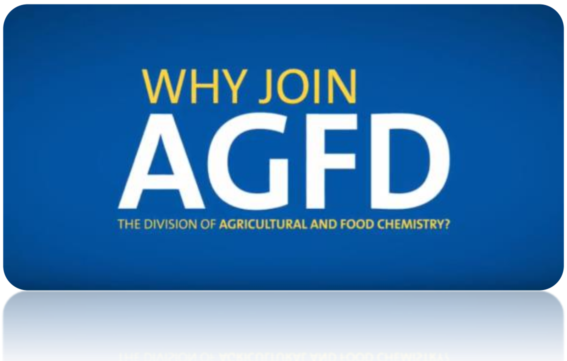

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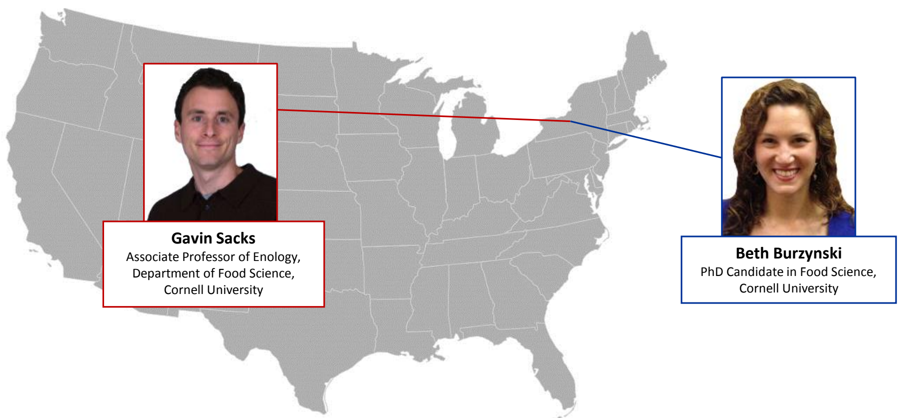

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Learn how the hints of cream, smoke, spice and vanilla that hide in your wine have less to do with the grape and more to do with the wood.

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