ANDREW L. WATERHOUSE
GAVIN L. SACKS
DAVID W. JEFFERY

UNDERSTANDING WINE CHEMISTRY

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Andrew L. Waterhouse
University of California
Department of Viticulture and Enology
Davis, CA, USA

Gavin L. Sacks
Cornell University
Department of Food Science
Ithaca, NY, USA

David W. Jeffery
The University of Adelaide
Department of Wine and Food Science
Urrbrae, SA, Australia

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Foreword

In vino, veritas…a Latin phrase meaning "in wine, truth." Its sentiments, however, are certainly not unique to Roman society. Indeed, numerous civilizations throughout history have similar phrasings given the prominence that wine has played, and continues to play, in diverse religious, cultural, and social events. Yet, despite its nearly seven millenia as part of the human experience, our understanding of this beverage and all of its truths remains woefully incomplete, even in light of the prowess of modern science. The reasons for this state of affairs are complicated, perhaps justifiably so given that it is the complexity of wine that draws many to its taste and to learning the art of its production.

At its most basic level, wine is a mixture of hundreds of different molecules in a constant state of flux, a feature that gives it the quality of being a living, breathing thing. The identity and concentration of these varied compounds at any given time depends on every factor conceivable, from the vine and the soil, to the weather that season, to the full production process, to how a bottle has been stored, to how long a poured glass or opened bottle has had a chance to breathe before being enjoyed. Our perception of its taste is equally fluid, dependent on its temperature, our mood, what else we have recently consumed, and how well our receptors can distinguish those hundreds of molecules in the first place. Thus, if we are even to consider how to unlock the complexity of wine, we must start by understanding this beverage from the standpoint of its chemistry, since it is molecules and what they can do that is at the heart of the matter.

This text by Waterhouse, Sacks, and Jeffery is an excellent starting point for such investigations. Chemistry on its own can seem hopelessly complex, but what these leading scholars have managed to accomplish seemlessly over the course of 33 chapters is the means not only to appreciate, but also to understand the relevant chemistry and chemical phenomena that impact every element of wine from an analytical, organic, and physical perspective. That success results from an approach that first details all of the different compound classes that are found in wine, their reactivities, and how they can contribute to its final taste profile. The text then moves on to the production process and explains, at an appropriately detailed chemical level, not only the fermentation and production process overall, but how each of its steps and certain decisions along the way can impact what molecules, and how much of them, end up in the final product. Finally, by presenting the latest scholarship, the authors highlight the frontiers of wine chemistry research, indicating opportunities for readers to pursue further avenues of discovery if so inclined.

Whether a neophyte, a connoisseur, a production hobbyist, or an aspiring professional, this carefully crafted text offers all readers an opportunity to enhance their knowledge of and appreciation for this wonderful beverage, along with the potential to contribute to enhancements in its future enjoyment. It is certainly hoped that these authors will continue to supplement and refine this already excellent work in the years to come through further editions as the knowledge of wine chemistry continues to grow. However, for now, congratulations are due for their efforts in successfully distilling diverse knowledge drawn from many different disciplines of chemistry into a fully accessible, engaging, and pedagogically powerful approach to the science of wine.

Scott A. Snyder
University of Chicago, Illinois, USA
January 2016

Preface

Having backgrounds in traditional branches of chemistry (organic, analytical, physical), we now feel privileged to be writing about wine chemistry. Not only is wine chemistry a subject that inspires and challenges, it is also a wonderful vehicle for conversation – we often encounter colleagues, visitors and acquaintances who remark on how much they love wine and its complexity. That complexity can be intriguing but it can also be a barrier to further understanding, whether wine is a hobby or an occupation.

Wine chemistry is taught in a growing number of institutions as part of enology and viticulture curricula, as well as in traditional undergraduate chemistry departments as an elective course. Furthermore, there are many individuals in wine production and allied fields (e.g., suppliers) who expect to make science-based decisions or recommendations. With this in mind, we identified the need for a book that could demonstrate to a reader how to utilize a basic knowledge of chemistry to rationally explain – and, better yet, predict – the diversity observed among wines.

Rather than providing only a description of wine constituents, or focusing on sensory characteristics, analytical aspects, or processing issues, we tackle the types of chemical and biochemical reactions that commonly occur in wine – in other words, we interpret winemaking outcomes through the lens of chemical principles. In doing this, we aim to assist students, winemakers, and others in predicting the effects of wine treatments and processes, or interpreting experimental results, based on an understanding of the major reactions that can occur in wine. We assume only a minimal prior knowledge of wine and winemaking, but do expect basic chemistry knowledge including organic chemistry, though we anticipate that our readers may have forgotten a lesson (or three) from these courses. At times we have relied on recent reviews rather than providing extensive citations to the literature, so we encourage the reader to seek out the primary sources of information to enhance their knowledge of any of the topics we have covered.

We approach our objectives by segregating the book into three parts.

- Part A, Wine Components
  To begin, we review the compound classes found in wine, their typical concentrations, their basic chemical reactivities, and their contribution to wine stability or sensory characters. This first part also considers the types of reactions that components can undergo in a wine environment, and is designed to be used as a reference for subsequent sections. Key chemical concepts involving electrophiles and nucleophiles, and electrophilic aromatic substitution are featured in Chapters 10 and 14, respectively.
- Part B, Chemistry of Winemaking
  Following a brief overview of grape composition and wine production practices, we describe the key reactions that occur during and after fermentation. In particular, we highlight how decisions made during winemaking will favor or disfavor certain chemical reactions leading to differences in wine composition.

We expect that this part can be used to generate hypotheses regarding the effect of unfamiliar winemaking processes or changes in juice components on final wine composition. A feature on different bottle closures appears in Chapter 25.

- Part C, Special Topics
  To conclude, we present several case studies that relate the preceding sections to current or emerging areas of wine chemistry. With these examples we aim to demonstrate representative examples of the challenges – and opportunities – facing those who are interested in this amazing natural product called wine.

In preparing such a book we anticipate there will be gaps and errors, and we encourage the reader to send us comments with regard to anything. From simple typographical errors, to missing topics or citations, errors in data or interpretation, and even suggestions for new approaches to explaining wine chemistry, all suggestions are encouraged. We are planning to follow up with a second edition and any comments or ideas for improvement are most welcome. Please send your ideas to: winechem@ucdavis.edu.

In closing, we acknowledge the work of the many researchers in the international wine science community that we have drawn upon in formulating this book, and also appreciate the feedback from our students who helped shape the book by reading draft chapters along the way. We also thank the grapegrowers and winemakers of the world for producing wines in a breathtaking range of styles – and thus chemistries – without which this topic and book would not exist. Lastly, we are eternally grateful to our partners and families who put up with our absence, or absentmindedness, and supported us throughout the process of publishing this book.

Introduction

The chemical diversity of wine

How many choices does a consumer have when they buy a wine? In the United States, all wines sold must have a Certificate of Label Approval (COLA) from the Alcohol and Tobacco Tax and Trade Bureau (TTB), and in 2013 the TTB approved over 93 000 COLA requests.[1] Because many wines are vintage products, that is, a new label will be produced for each harvest year, the true number of wines available in wine stores throughout the United States may be closer to 250 000.[2] In contrast to commodity products where producers strive for homogeneity (e.g., soybeans, milk), variation in specialty products like wine is not only tolerated – it is appreciated and celebrated. Consumers expect that wines with different labels should smell different, taste different, and look different; from a chemist's perspective, consumers expect wines to have different chemical compositions. The study of wine chemistry is the study of these differences – explaining how there can be hundreds of thousands, if not millions, of different wine compositions, and contributing to a winemaker's understanding of how the myriad of choices they are faced with can lead to these differences.

What is wine?

To a first-order approximation, a dry table wine is a mildly acidic (pH 3–4) hydroalcoholic solution. The two major wine components are water and ethanol, typically accounting for about 97% on a weight-for-weight (w/w) basis. The remaining compounds – responsible for most of the flavor and color of wine – are typically present at <10 g/L (Figure I.1), and many key odorants are found at part-per-trillion (ng/L) concentrations! Notably, none of these compounds appear to be unique to wine – compounds present in wine can also be found in coffee, beer, bread, spices, vegetables, cheese, and other foodstuffs.[3] What distinguishes different wines from other products (and each other) is differences in the relative concentrations of compounds, rather than the presence of unique components.

[1] As a caveat, a COLA is a pre-approval process, and not all will become commercial wines.

[2] Furthermore, data based on TTB COLAs only captures those wines approved for sale in the US, which represents only a fraction of wines produced commercially – the wine-searcher.com database reports tracking over 400 000 wines available for sale worldwide as of April 2016.

[3] One compound that is somewhat unique to grape juice and wine is tartaric acid, which is undetectable in most other fruits and vegetables (although it is at a very high concentration in tamarind). Tartaric acid also belongs to the short list of compounds that was first discovered in wine or grapes, and later discovered elsewhere; the monoterpenes wine lactone and Riesling acetal are also on this list, as are some anthocyanin-derived pigments (vitisins and pinotins).

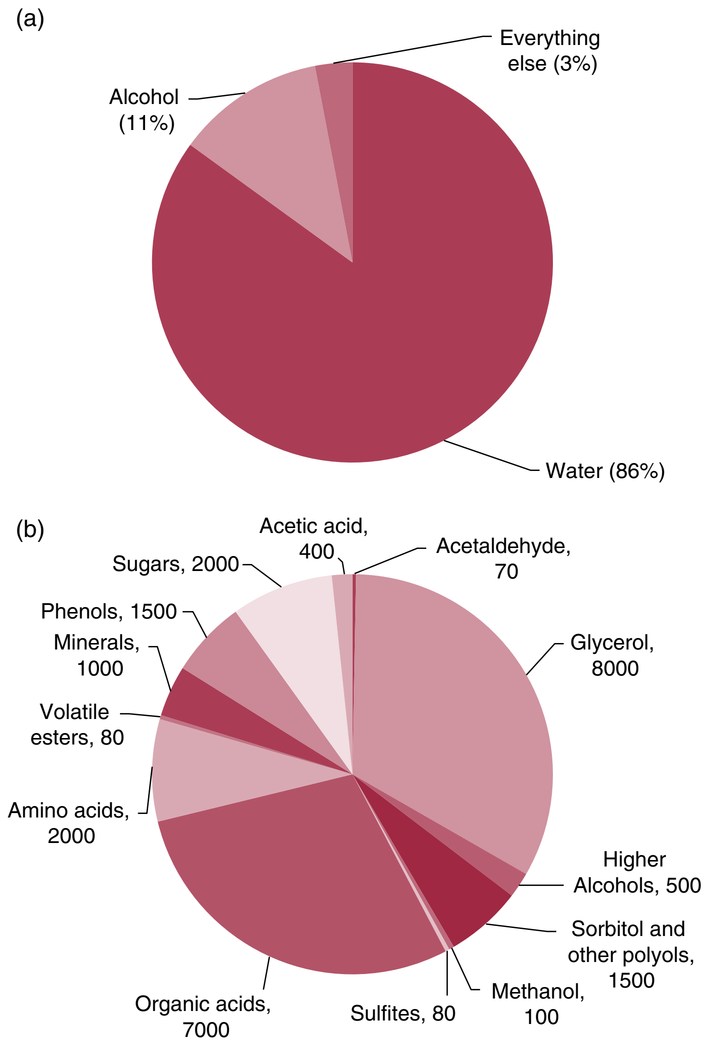

Figure I.1 *Composition of a representative dry red table wine (a) on a % w/w basis and (b) typical concentrations (mg/L) of major wine components excluding water and ethanol, that is, the main contributors to "Everything Else." Key trace components (0.1 ng/L–10 mg/L) would not be visible and are therefore not included*

Wine is produced by the alcoholic fermentation of grape juice or must (juice and solids), which results in the complete or partial transformation of grape sugars to ethanol and CO_2. However, winemaking and wine storage result in many chemical changes beyond simply the consumption of sugars and formation of alcohol. This is readily exemplified by the volatile composition of a wine, which is far more complex than that of grape juice (Figure I.2). These volatile components can contribute to the aroma of wine and such odorants are often classified based on when they are formed; that is, in the grape (*primary*), during fermentation (*secondary*), or during storage (*tertiary*) (Table I.1).

The number of compounds identified in wine follows advances in analytical technology. A survey from 1969 reported that wine and other alcoholic beverages contained 400 volatiles, while a later book from 1983

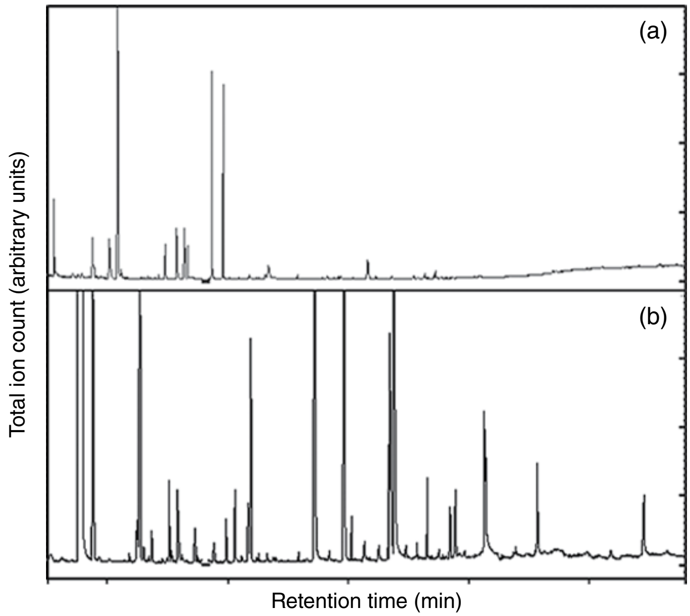

Figure I.2 Comparison of GC-MS chromatograms for (a) a grape juice and (b) a wine produced from that grape juice. Every peak in the chromatograms represents at least one unique volatile compound

Table I.1 Primary, secondary, and tertiary classifications of wine odorants

Compound classification	Description	Examples (Part and Chapter)
Primary	Compounds present in the grape that persist unchanged into wine	Methoxypyrazines (A.5), rotundone (A.8)
Secondary	Compounds formed as a result of alcoholic or malolactic fermentation due to either i) Normal metabolism of sugars, amino acids, etc. ii) Transformation of grape-specific precursors	i) Ethyl esters (B.22.2), fusel alcohols (B.22.3) ii) Varietal thiols (B.23.2)
Tertiary	Compounds formed during wine storage, for example, as a result of i) Extraction from oak ii) Microbial spoilage or chemical tainting iii) Abiotic transformation of precursor compounds in wine	i) Oak lactones (B.25) ii) Trichloroanisole (A.18) iii) TDN (B.23.1)

reported over 1300 volatiles [1]. A more recent analysis of wines using a state-of-the-art mass spectrometry system (FT-ICR-MS) was able to detect tens of thousands of unique chemical signals across a set of wines, and assign chemical formulae to almost 9000 components [2]. However, the advanced instrumentation in this last report would not distinguish structural isomers – for which there may be billions for a condensed tannin

Table I.2 *Summary of major functional classes of interest to wine chemists. Note that compounds may fit into more than one category*

Compound functions	Description	Examples (Part and Chapter)
Organoleptic	Compounds that contribute to the taste, odor, or tactile sensations of a wine	Acids (A.3), monoterpenes (A.8), tannins (A.14)
	Compounds that affect wine color or cause a visible haze	Anthocyanins (A.16), proteins (B.26.2)
	Compounds that act as precursors of organoleptically active compounds	Glycosides (B.23.1), *S*-conjugates (B.23.2)
Stability	Compounds that inhibit or promote microbial or abiotic changes during storage	Organic acids (A.3), sulfur dioxide (A.17)
Bioactive	Compounds that may positively or negatively affect human health	Phenolic compounds (A.11), biogenic amines (A.5), ethyl carbamate (A.5)
Matrix	Compounds that affect the speciation or activity of other compounds, usually through non-covalent interactions	Water and ethanol (A.1)
Authenticity	Markers that help distinguish authentic products from fraudulent products	Artificial colors (C.28)

consisting of 30 monomers (Chapter 15). Thus, the number of chemical compounds in wine, like most natural products, is essentially uncountable.

With this in mind, the goal of a wine chemist is not to enumerate every compound, but rather to identify compounds, or in many cases classes of compounds, that will directly or indirectly control key quality aspects of the wine such as organoleptic properties (aroma, flavor, appearance), safety, and stability. Alternatively, compounds may be of interest because they can be used to detect the presence of fraud. These categories, and examples, are summarized in Table I.2.

Chemical reactions in wine

The complexity of its composition would suggest that the range of chemical reactions in wine is limitless. However, as noted above, wine is ~97% ethanol and water, which precludes the large number of reactions in introductory organic chemistry texts that require the absence of protic solvents (e.g., no Grignard reactions). Similarly, the mildly acidic conditions of wines (typically, pH ~3.5) mean that base-catalyzed reactions are usually of low importance (e.g., aldol condensations are unlikely).

As with all chemistry, the key to predicting reactions is to define the components of wine that can react with each other. Many of these reactions will be familiar to students of organic chemistry, and include:

- Reactions between nucleophiles and electrophiles, for example, bisulfite and carbonyls
- Hydrolytic reactions, usually acid-catalyzed, for example, of esters, interflavan bonds, and glycosides
- Addition and elimination reactions, again usually acid-catalyzed.

These reactions and many more are the very essence of this book, and are presented in detail throughout the following chapters. One uniquely challenging aspect of wine chemistry as compared to the organic chemistry lab (and most other foodstuffs) is that reactions are allowed to take place for months, years, or even decades, often at ambient temperatures and in a reductive environment. These conditions can lead to unexpected reaction products – this is especially important since a part-per-trillion of certain compounds may be enough to affect flavor.

Chemistry as a historical record

Many chapters of this text, particularly in Part A, contain tables of "typical concentrations" of various wine components, usually from peer-reviewed reports published since 2000.[4] However, grapegrowing and winemaking practices are not static [3], and typical values may change dramatically with changes in fashion or technology – not to mention climate [4]. In some cases, the analysis of aged wine reveals changes in typical wine composition and lends insight to changes in production practices. For instance, in the nineteenth century, wine drinkers used to prefer much sweeter wines – premium Champagnes would have over 140 g/L of sugars, as compared to < 10 g/L in most modern versions [5]. Control of spoilage organisms like acetic acid bacteria through the use of sulfur dioxide and anaerobic storage during this period was still primitive – a survey of Greek wines from 1872 reported acetic acid concentrations in the range of 1.5 to 3.6 g/L [6], all in excess of modern legal limits. Wine tanks from this era also typically had lead-containing bronze valves (no longer used today), which could be leached under acidic conditions to result in relatively high lead concentrations in wine [5]. Differences in mineral content could also arise from viticulture practices – grapegrowers in the nineteenth and early twentieth century routinely used arsenic to ward off insects and mold [7].[5]

In summary, the values provided in this text should be seen as a snapshot of wine composition circa the early twenty-first century, rather than as fundamental constants. A modern consumer's expectation of a high-quality wine is a reflection of both improved technical capacities as well as accumulated traditions, which in the year 2016 means (for the majority of internationally known premium wines) fermenting with selected strains of *Saccharomyces cerevisiae*, aging in oak barrels, and storing wine in glass bottles with corks. Presumably, the pursuit of different options in the past might have led to alternative perspectives on the idea of wine "perfection" and target chemical compositions. Similar statements can be made about the future of wine, and we expect that the numbers provided here will provide some amusement to the wine chemists of the year 2100.

The chemical senses and wine flavor

The majority of compounds discussed in this text have a role in wine flavor. Because the lexicon used to discuss flavor in scientific publication differs from that used in casual conversation, this introduction will conclude with a brief review of key flavor terminology.

Flavor is defined as the "perception resulting from stimulating a combination of the taste buds, the olfactory organs, and chemesthetic receptors within the oral cavity" [10] – in other words, everything a taster can perceive in the mouth, for example, olfaction, taste, and chemesthesis.

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[4]These surveys also predominantly consider wines from countries with scholarly activity in enology and viticulture – several European countries, the United States and Canada, South Africa, Australia and New Zealand.

[5]Certain chemical features of wine can also be useful to understanding its use and spread in antiquity. For example, the presence of tartaric acid in a pottery container is considered near-certain evidence that a container held wine [8]. Similarly, the presence of syringic acid was used as evidence that King Tutankhamen drank wine made from red grapes instead of pomegranates. The former contains the pigment malvidin-3-glucoside, which will degrade to the relatively stable syringic acid, while the latter does not [9].

Olfaction, or smell, involves the detection of odorants by olfactory receptors (ORs) located within the nasal cavity. Humans have approximately 700 OR, of which half are usually functioning in any individual [11]. Although each specific OR demonstrates some selectivity towards compound classes, odorants (or mixtures of odorants) typically stimulate combinations of OR, and these combinatorial patterns are associated with particular smells [12]. Olfaction requires that the odorant be volatile to reach the nasal cavity, a process that may occur through two routes:

- Orthonasal olfaction involves the detection of odorants without tasting, for example, by smelling the headspace of the wine. The perceptions arising from orthonasal olfaction are often referred to as *aroma*.
- Retronasal olfaction involves detection of odorants that travel from the oral cavity to the nasal cavity. Most commonly, this occurs following swallowing, after which exhalation drives a small amount of odorants through the nostrils [13].

Although olfaction is selective for volatile compounds, most food volatiles appear to be unimportant to odor. A recent meta-analysis estimated that of the ~10 000 volatiles detected in foodstuffs, <3% were important to food aroma [12]. The same review noted that the aromas of specific foods or beverages (including wine) could be simulated with between 4 and 44 odorants.

Taste involves the detection of small molecules by taste receptors located in the taste buds. Five classes of taste receptors have been established – "sweet," "sour," "bitter," "salty," and "umami" [14], of which only the first three appear to be routinely experienced in wine [15].

Chemesthesis involves the chemical activation of receptors responsible for sensations of pain, temperature, and touch, for example, the "heat" caused by capsaicin in hot chili peppers [16]. There are several critical distinctions between taste and chemesthesis, the most important being that taste is only sensed by the taste receptors of the tongue, while chemesthesis can be detected throughout the oral cavity – and for that matter, throughout the body.[6] The chemesthetic sensations most important to wine are those that cause:

- Pungency and irritation, which can be due to ethanol and CO_2.
- Astringency, or the perceived loss of lubrication in the mouth, which can be triggered by condensed tannins and other phenolic compounds [17].

The perception of "body" is also likely a result of chemesthesis, although the specific compounds responsible for this sensation are still unclear [18].

Classic papers on food analysis (grapes, wine, and otherwise) often focused on identifying or measuring the compounds found in high concentrations, with little emphasis on the sensory relevance of the compounds [19].[7] Since the 1990s, it has been increasingly common to identify organoleptically important compounds through the use of bioassays, for example, using a human sniffer to identify key odorants through GC-olfactometry. Candidate compounds can then be quantified and their relevance evaluated through reconstitution and omission experiments [20].

Perception of flavors. Although the eventual goal of bioassay-based approaches is to recreate the organoleptic property in a model system, a key feature is the use of *activity values* as a rough estimate of a compound's

[6] As an example, the "cooling" sensation of menthol is chemesthetic – the perception of coolness can be felt not only on the tongue but throughout the mouth, in the nose, or on tissue on to which menthol is rubbed. In contrast, a sodium chloride solution would not be perceived as salty anywhere except for the tongue.

[7] As described in Chapter 32, improvements in analytical methodology have renewed interests in using general "non-targeted" approaches to identify potentially important compounds.

Table I.3 Concentrations, odor thresholds, and calculated OAVs for five representative compounds in Sauvignon Blanc wines

Compound	Typical aromas	Concentration range (mg/L)[a]	Odor threshold (mg/L)[b]	Odor activity value, OAV
Water	–	~850 000	–	0
3-Methylbutanol (Isoamyl alcohol)	Solvent, burnt	200–250	30	6–8
1-Hexanol	Grassy	1.5–2.5	8	0.2–0.3
3-Mercaptohexanol	Passionfruit, grapefruit	0.0005–0.0038	0.000060	9–65
3-Isobutyl-2-methoxypyrazine	Bell pepper	0.000008–0.000023	0.000002	4–11

[a] Range of average values observed across 7 wine regions for 2004 and 2005 vintages [23].

[b] From References [24] to [26].

importance. Activity values are calculated as the ratio of a compound's concentration to its sensory threshold in an appropriate matrix:

$$\text{Activity value} = \frac{\text{Concentration}}{\text{Detection threshold}}$$

Typically, compounds with higher activity values have more intense flavors, but the concentration–response function varies among compounds. In simple solutions, the intensity of most taste compounds (sugars, acids) scales as a linear function of their concentration, but the intensity of most odorants increases as roughly the square root of concentration [16].

Use of activity values in evaluating the relevance of odorants to a given foodstuff dates to at least the 1960s [21, 22], and even earlier examples exist for other flavor compounds.[8] As a general rule, compounds with activity values <1 are expected to have a negligible effect on a particular sensory attribute [20]. The utility of the activity value concept can be appreciated from representative data for Sauvignon Blanc wines in Table I.3. Based strictly on concentrations, 1-hexanol appears to be a very important contributor to wine. However, conversion to odor activity values (OAVs) reveals that the "grapefruit" aroma of 3-mercaptohexanol and the "herbaceous" notes of 3-isobutyl-2-methoxypyrazine are far more likely to contribute to Sauvignon Blanc aroma – and, in fact, they do.

Activity values are useful as an initial screen to determine the likely relevance of a given compound. However, simply knowing whether a flavor compound is or is not present at suprathreshold concentrations (activity value > 1) is insufficient to determine if the compound is important to the foodstuff for several reasons:

[8] The first widespread use of activity values in food science is probably the eponymous "Scoville Unit" to describe the pungency of hot chili peppers. Originally, the Scoville value of a pepper was determined by preparing an ethanol extract and determining the dilution necessary before the heat was no longer detectable – a value of 4000 Scovilles, typical of a jalapeño, meant that the extract had to be diluted 4000-fold before the pungency was no longer detectable. Currently, Scovilles are determined indirectly by measuring capsaicin and related compounds using HPLC rather than sensory testing.

- *Masking*. The perceived intensity of a flavorant can be decreased by the presence of other flavor compounds. For example, addition of herbaceous smelling methoxypyrazines to red wine decrease the intensity of fruity aromas [27].
- *Additive or synergistic effects*. Groups of homologous compounds, that is, series of alkyl esters or ketones, can reach sensory threshold through additive effects even if all compounds individually have activity values <1 [28]. Synergism, that is, an increase in stimulus intensity beyond what is predicted for simple additive effects, can also occur, most often for taste and tactile sensations [16].
- *Matrix effects*. Differences in the matrix (pH, temperature, ethanol concentration, non-covalent interactions with macromolecules) can change the activity of flavor compounds, and particularly the volatility of odorants [29].
- *Synesthesia and confirmation bias*. The different chemosensory modalities (taste, smell, tactile) do not operate in isolation; information from these senses is integrated together. For example, panelists report that increasing the sweetness of a fruity beverage increases the intensity of fruit flavor [30]. A related concept is confirmation bias, in which prior knowledge of a product affects a panelist's perceptions; for example, white wines dyed with tasteless red food coloring are perceived as having fuller body [31].
- *Emergent properties*. Combinations of flavor compounds (particularly odorants) often elicit different percepts than individual compounds. For example, no specific wine compound has a smell exactly like wine, but the combination of odorants at appropriate concentrations allows a sniffer to know that they are smelling wine and not another beverage [32].

Finally, the use of a single value for a sensory threshold obscures the fact that individuals show considerable variation in their sensitivities to different flavor compounds, particularly odorants. One author estimated that a typical 96% confidence interval for odorant thresholds across a population spans a concentration factor of 256 [33], and individuals' thresholds and descriptors may change with repeated experiences [34]. Although this variation does not preclude studies of organoleptic properties, it does necessitate appropriate sensory practices and rigorous statistical analysis of the data (as with other studies involving human subjects). A full discussion of sensory techniques is beyond the scope of this text, but its omission should not be interpreted as trivialization of sensory science. Collecting and interpreting sensory data can be laborious and often represents a limiting step in wine chemistry. We strongly encourage the reader to consult one of the many excellent texts available on sensory science to learn more (e.g., Reference [16]).

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Part A

Wine Components and Their Reactions