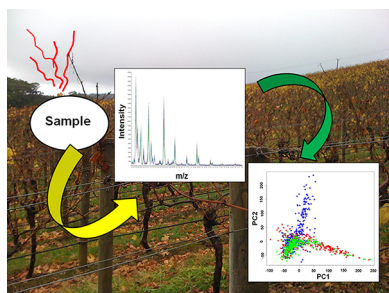


# Instrumental Methods (Spectroscopy, Electronic Nose, and Tongue) As Tools To Predict Taste and Aroma in Beverages: Advantages and Limitations

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## 1. INTRODUCTION

The human senses have always been used to assess food quality. Although the senses of sight, hearing, taste, smell, and touch are used daily in all aspects of our lives, their analytical applications to evaluate food properties are relatively recent.<sup>1,2</sup> The sensory systems of *Homo sapiens* are the product of millions of years of evolution where natural selection has resulted in our capacity to detect a wide range of compounds present in the environment, advantageous to our survival, allowing hedonistic evaluation of our environment.<sup>2</sup>

Many features of food can be studied analytically using sensory methods and techniques (e.g., taste, aroma, texture, and

color), and they can be integrated to provide the overall sensory evaluation of food.<sup>1–15</sup> Additionally, the human senses have the ability to “focus” or concentrate on specific attributes (e.g., sweetness or bitterness of a beverage). It is only recently (compared to the evolutionary time scale) that instrumental methods have reached a level of sophistication which enables investigation of the properties of food. For example, recent advances in chromatographic separation, coupled with sensitive detection systems, can be used to obtain qualitative and quantitative data to assess food composition.<sup>1,2,12–15</sup>

Overall two main types of methods for evaluation of the quality of beverages and foods can be used, namely, subjective and objective. Subjective methods are those based on human assessment of the quality characteristics of the food.<sup>5–7,14</sup> These methods involve perception of texture, flavor, odor, color, and touch by a panel of experts or consumers.<sup>7,8,10,15</sup> However, even though human evaluators can be highly trained, their opinions might vary due to psychological and physical variability.<sup>6,7</sup> Subjective sensory methods are also time consuming and susceptible to large sources of variation. By nature, such assessments can be biased by individual preferences and may be subject to day-to-day variations.<sup>7–10,15</sup>

In contrast, objective methods for assessment of quality include instrumental analysis and could be very beneficial for numerous reasons as they are nonsubjective, highly repeatable, and reproducible and, most of all, the fact that instruments do not suffer from fatigue or adaptation.<sup>7–15</sup>

Given the complex nature of alcoholic beverages, there are many advantages to developing instrumental methods to describe their quality or sensory profile. However, to be of practical use by the beverage industry, instrumental methods must be cost effective and provide rapid, reproducible results with continuous operation.

To date, instrumental methods for sensory analysis have lacked the ability to consistently perceive all of the key sensory attributes of interest and have been inconsistent in predicting relationships between sensory and instrumental measurements, depending on the attribute and food matrix analyzed.<sup>7,8,10–15</sup>

Existing analytical methods used to measure wine and alcoholic beverages composition and quality are not adequate for the demands of production in a global market due to their high cost and slow turnaround time. Factors like promptness

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and low cost of analysis, minimal sample preparation, and environmentally friendly methods are of paramount importance in the modern and sustainable wine and alcoholic beverage industries.<sup>16</sup>

In order to enable the beverage (and other food applications) industry to rapidly respond to the changing demands of both consumers and the market, it is important to have a quantitative means for assessing sensory properties by means of objective measurements (e.g., analysis of volatile compounds) which can provide reliable information about the quality of the food.<sup>17</sup> However, many of these methods are unsuitable to be used or adopted by the industry for rapid analysis of quality. For example, analysis of volatile compounds in wine to assess wine aroma by gas chromatography–mass spectrometry (GC-MS) involves expensive instrumentation and time-consuming sample preparation using solvents as well as analysis (from a few to several minutes).<sup>7,10,12–14,17,18</sup>

In the last 20 years increasing interest on the use of rapid screening techniques or instrumental methods to determine quality characteristics of foods and beverages has been of great interest to the food industry. These techniques are relatively inexpensive and easy to operate, often require little or no sample preparation, and can be used in-line or at-line to obtain results quickly. Such techniques or sensors can be grouped into electronic noses (EN),<sup>18–20</sup> optical methods based in vibrational spectroscopy (e.g., infrared, UV), and more recently the so-called electronic tongue instruments that were developed to characterize complex food or beverage samples in order to replace or reduce the use of sensory analysis using human subjects.

### 1.1. Aroma

Flavor is complex, and many different sensory modalities and chemical compounds influence flavor perception. Aroma (or smell) is the major contributor to overall flavor perception in wine and other beverages, and it is largely related to the volatile aroma compounds that contribute to the overall flavor of the sample.<sup>10</sup>

Many of the analytical methods used to study aroma typically involve preparation of an extract (or collection of volatiles on traps) followed by chromatographic separation and detection.<sup>1,2,5,10–15</sup> Other aspects of the analysis, such as the temporal dimension of the eating/drinking process, which includes the effect of release and transport of the aroma compounds to the olfactory epithelium, are not considered in such analyses, although the temporal dimension is a central feature of the eating/drinking process.<sup>1,2,10–15</sup>

Typically, the human senses do not react to the absolute intensity of a stimulus but to the rate of change in a stimulus. The temporal dimension can be measured sensorially using methods that can relate time and intensity odor of the compounds, and mathematical models have been developed to describe how perception is affected by temporal changes in breath aroma concentration.<sup>1,2,10–15</sup>

Ideally, instrumental methods should be able to follow changes in the temporal dimension, making objective measurements that can be related to perception. In order to achieve this fast, sensitive analytical systems which have a selectivity and sensitivity comparable with the human olfactory receptor are needed.<sup>1,2,10</sup> For example, use of electroencephalography (EEG) and magnetic resonance imaging (MRI) can both be used to study brain activity directly but are not practical from an industrial point of view.<sup>1,2,10</sup>

An alternative option is to use purely instrumental techniques to follow changes in breath volatile concentration during eating or drinking and to relate the patterns observed to sensory perception. Examples of such instruments are the so-called electronic noses (EN).<sup>15–23</sup> EN employ arrays of sensors (in much the same way as the olfactory epithelium has arrays of receptors) which can be used to monitor volatile compounds.<sup>1,2,10–15,22</sup> All sensors have a certain amount of specificity, such that one particular sensor may respond more to esters than aldehydes, whereas the opposite might be true for another type of sensor. However, the sensors do not respond in a manner comparable with that of the human olfactory system. They lack sensitivity (parts per million concentration) and selectivity, while their slow response rate makes them unsuitable for following rapid changes in breath volatile concentration.<sup>14,20–27</sup> Real-time detection of volatile concentration can be achieved using an electron impact source with a membrane separator between the source and the external environment.<sup>1,2</sup> The mass spectrometer has advantages (relative to the electronic nose) owing to its fast response rate and greater sensitivity. However, the membrane reduces the overall sensitivity of the method, and its selective permeability reduces its potential application. Other mass spectrometer systems, atmospheric pressure chemical ionization mass spectrometry (APCI-MS) and proton transfer reaction mass spectrometry (PTR-MS), are being developed and can be used for real-time detection of compounds at parts per billion concentrations.<sup>1,2,22,29</sup>

### 1.2. Taste

Taste-related compounds (tastants) also show changes in concentration over time, and their solubility will depend on the release from the matrix and rate of clearance by saliva. Like aroma compounds, tastants have different detection thresholds and qualities, factors that need to be taken into account in methods that assess taste.<sup>1,2,10</sup> Typically, only rough estimates of the acid/sugar balance are necessary for natural products. However, increasing use of intense sweeteners and nonsweet sugars in manufactured food products makes it difficult to provide a simple analytical estimation of overall taste.<sup>5–7,10–15</sup> It might prove easier to develop instrumental methods for assessment of tastants owing to the fact that these compounds are present at higher concentrations in food samples and have fewer descriptors compared to aroma compounds. Instrumental methods available for analysis of taste include the electronic tongue, which is based on an array of lipid or polymer membranes. In the presence of tastants the electrical properties of the membranes changed, resulting in a modification in electrical output relative to a reference electrode. Compounds with similar taste properties typically produce patterns of electrical output from the sensors which are also similar.<sup>5–7,10–15</sup>

The electronic tongue can be used to discriminate between the taste properties (e.g., bitter, sweet, sour, umami) of amino acids. The electronic tongue appears to be a useful tool for profiling of foods (particularly beverages); however, like many analytical techniques, it does not measure the release and persistence of compounds in vivo during eating or drinking.<sup>5–7,20,24–30</sup>

This review discusses recent applications of instrumental methods based in spectroscopy (e.g., infrared) and other sensor systems (e.g., electronic noses and tongues) as tools to predict taste and aroma in wine and other alcoholic beverages.

## 2. ELECTRONIC NOSES

The most sensitive and broader range odor detector is undoubtedly the mammalian olfactory system, whose high complexity and efficiency derive from millions of years of evolutionary development.<sup>22,25,27,29</sup> The limits of traditional instrumental techniques in the matter of odors have led to growing attention to odor measurement procedures relying on the use of the human nose as a detector, in compliance with the scientific method.<sup>23,22,25,27,29</sup>

For many years sensory evaluation of smells by means of panels of sensory trained evaluators has been the main odor assessment and quantification tool in the beverage and food industries called dynamic olfactometry.<sup>23,26–28</sup> This is a standardized method used for determining the concentration of odors and evaluating odor complaints.<sup>23,26–28</sup> This methodology is based on the use of a dilution instrument, called olfactometer, which presents the odor sample diluted with odor-free air at precise ratios, to a panel of human assessors.<sup>23</sup> The examiners are selected in compliance with a standardized procedure performed using reference gases; only assessors who meet predetermined repeatability and accuracy criteria are selected as panelists.

Perception of odors is a logarithmic phenomenon, and for this reason, in this kind of measurement it is necessary to take into account the fact that odor concentration is associated with odor intensity through a defined logarithmic relation.<sup>23,26–31</sup> Using other sensorial methods, subjective parameters, such as the hedonic tone or the perceived odor strength, could be also assessed.<sup>23,26–31</sup>

An improvement in odor determination consists of a GC-MS coupled with olfactometric detection (GC-MS/O). Gas chromatographic separation of an odorous air sample could be useful for identifying specific odorant components. Use of GC-MS/O allows a deeper understanding of the odorant composition as concerns compound identification and quantification, offering the advantage of a partial correlation between the odorant chemical nature and the perceived smell.<sup>10,15,23,26–31</sup> This instrumental approach allows solving the odor complexity issue, which is also the main reason for the careful procedures required for sampling of odors in the atmosphere or air.<sup>23</sup> Overall, odor detection remains linked to human perception. Although careful choice of panel members and use of standard procedures for odorous sample collection and analysis allow obtaining reliable and repeatable olfactometric measures, thus overcoming the subjectivity due to the human olfaction variability, increasing attention is being paid to the availability of more objective odor evaluation methods.<sup>10,15,23,26–31</sup>

Discovery of materials with chemo-electronic properties has provided the opportunity for development of artificial olfactory instruments mimicking the biological system.<sup>19–21,23,26–31</sup> In the past decade a large field of scientific research has been devoted to development of electronic noses (EN). These kinds of sensors are the so-called olfaction instruments capable of discriminating between a variety of simple and complex odors. Like human olfaction, EN are based on an array of electronic-chemical sensors with partial specificity to a wide range of odorants and an appropriate pattern recognition system.<sup>19–21,23,26–31</sup> In contrast to the ideal gas sensors, which are required to be highly specific to a single chemical species, sensors for EN need to give broadly tuned responses like the olfactory receptors in the human nose: in both cases odor

quality information and recognition is ensured by the entire pattern of responses across the sensors array rather than the response of any one particular sensor. Furthermore, mimicking data processing in the biological systems, the incoming chemo-electronic signals are processed through the use of data reduction techniques (e.g., principal component analysis) in both human and EN devices, the function of odor recognition is finally achieved by means of some form of associative memory for storage and recall of previously encountered odors.<sup>19–21,23,26–31</sup> A wide variety of competing sensor technologies (conducting polymers, piezoelectric devices, electrochemical cells, metal oxide sensors [MOX], and metal-insulator semiconductor field effect transistors [MIS-FETs]) are currently available: independent of the considered device, sensor elements have to show fast, reproducible, and reversible responses to odor samples.<sup>23,26–39</sup>

The classical EN, consisting of an array of sensors, is still the most common approach, although new technologies have recently entered the market.<sup>27,29,30</sup> A diverse number of technologies has been used such as metal oxide sensors (MOX),<sup>31,32</sup> mass spectrometry (MS), ion mobility spectrometry (IMS), and gas chromatography (GS) sensors.<sup>19–21,27,30,33–39</sup>

Nowadays, EN instruments are extensively used to measure the headspace of a food or beverage sample to obtain a 'fingerprint' measurement of the volatiles in the headspace and relate this information to the volatile compounds which may be responsible for the aroma sensory properties of that sample. A number of food and beverage studies demonstrated the relationship between EN measurements and the rating of sensory properties by sensory panelists. The term EN is often associated with detection of odors or an attempt to smell with an electronic device.<sup>19–21,27</sup> The EN offers the capability to detect some gases with no odor activity and is not necessarily adapted only to substances of importance to mammalian life such as the scent of other animals, foodstuff, food ingredients, and food samples or food spoilage.<sup>19–21,27</sup>

## 3. INFRARED SPECTROSCOPY

Chemical bonds present in the organic matrix of beverages vibrate at specific frequencies, which are determined by the mass of the constituent atoms, the shape of the molecule, the stiffness of the bonds, and the periods of the associated vibrational coupling.<sup>40–43</sup> A specific vibrational bond absorb in the infrared (IR) spectral region where diatomic molecules have only one bond that may stretch (e.g., the distance between two atoms may increase or decrease). More complex molecules have many bonds; vibrations can also be conjugated, leading to two possible modes of vibration: stretching and bending. Despite these potential problems, absorption frequencies may be used to identify specific chemical groups, and this capability has traditionally been the main role of Fourier transform (FT) midinfrared (MIR) (FT-MIR) spectroscopy.<sup>40–43</sup> The MIR region of the electromagnetic spectrum lies between 4000 and 400  $\text{cm}^{-1}$  and can be segmented into four broad regions: the X–H stretching region (4000–2500  $\text{cm}^{-1}$ ), the triple-bond region (2500–2000  $\text{cm}^{-1}$ ), the double-bond region (2000–1500  $\text{cm}^{-1}$ ), and the fingerprint region (1500–400  $\text{cm}^{-1}$ ).<sup>40–43</sup> Characteristic absorption bands are associated with major components of food. Water is a significant absorber in the MIR spectral region and can interfere with determination of other components present in beverages. Absorptions in the fingerprint region are mainly caused by bending and skeletal



vibrations, which are particularly sensitive to large wavenumber shifts, thereby minimizing against unambiguous identification of specific functional groups.<sup>40–43</sup> Even in this region, however, the spectrum may be used as a fingerprint of a sample such as a food product or food ingredient. Analysis of such fingerprints forms the basis of many applications of MIR spectroscopy in food analysis. Broad fields of application include constituent quantification and qualification issues for food and food ingredients; substance identification and authentication are included in the latter field.<sup>40–43</sup>

Other types of sensors based on vibrational spectroscopy in the IR region are those based sensors in the near-infrared (NIR). In the last 40 years NIR spectroscopy has become one of the most attractive and used methods of analysis which provides a simultaneous, rapid, and nondestructive way to quantify major components in many agriculture-related products and plant materials.<sup>43</sup> Use of NIR for analysis of beverages is characterized by low molar absorptivities and scattering, which leaves a nearly effortless evaluation of pure materials. Although Herschel discovered light in the NIR region as early as 1800, spectroscopists of the first half of the last century ignored it in the belief that it lacked analytical interest.<sup>43–47</sup> More than 100 years later, the NIR region of the electromagnetic spectrum has become one of the most promising techniques in molecular spectroscopy.

Spectral 'signatures' in the MIR result from the fundamental stretching, bending, and rotating vibrations of the sample molecules, while NIR spectra result from complex overtones and high-frequency combinations at shorter wavelengths.<sup>40–47</sup> Spectral peaks in the MIR frequencies are often sharper and better resolved than in the NIR domain; the higher overtones of the O–H (oxygen–hydrogen), N–H (nitrogen–hydrogen), C–H (carbon–hydrogen), and S–H (sulfur–hydrogen) bands from the MIR wavelengths are still observed in the NIR region, although much weaker than the fundamental frequencies in the MIR. In addition, the existence of combination bands (i.e., CO stretch and NH bend in protein) gives rise to a crowded NIR spectrum with strongly overlapping bands.<sup>40–47</sup>

A major disadvantage of this characteristic overlap and complexity in the NIR spectra has been the difficulty of quantification and interpretation of data from NIR spectra. On the other hand, the broad overlapping bands can diminish the need for using a large number of wavelengths in calibration and analysis routines. In recent years, new instrumentation and computer algorithms have taken advantage of this complexity and made the technique much more powerful and simple to use. However, the advent of inexpensive and powerful computers has contributed to the surge of new NIR applications.<sup>40–47</sup>

#### 4. ELECTRONIC TONGUES

Electronic tongues (E-tongues) are sensor arrays capable of distinguishing very similar liquids employing the concept of global selectivity, where the difference in the electrical response of different materials serves as a fingerprint for the analyzed sample.<sup>48–55</sup> They have been widely used for analysis of wines, fruit juices, coffee, milk, and beverages in addition to detection of trace amounts of impurities or pollutants in waters.<sup>50,52–55</sup> Among the various principles of detection, electrochemical measurements and impedance spectroscopy are the most widely used. With regard to the materials for the sensing units, in most cases use is made of ultrathin films produced in a layer-by-layer fashion to yield higher sensitivity with the

advantage of control of the film molecular architecture. The concept of E-tongues has been extended to biosensing using sensing units capable of molecular recognition, as in films with immobilized antigens or enzymes with specific recognition for clinical diagnosis.<sup>50,52–55</sup> Identification of samples is basically a classification there has been a trend to use artificial intelligence and information visualization methods to enhance the performance of E-tongue devices.<sup>50,52–55</sup>

Briefly, the E-tongue is constituted by sensing units formed by ultrathin films of distinct materials deposited on gold interdigitated electrodes, which are immersed in liquid samples, followed by impedance spectroscopy measurements.<sup>50,52,54,55</sup> The E-tongue sensor is based on the global selectivity concept, for example, materials forming the sensing units are not selective to any substance in the samples; therefore, it allows grouping of information into distinct patterns of response, enabling distinction of complex liquid systems using conventional polyelectrolytes such as poly(sodium styrene sulfonate) (PSS) and poly(allylamine) hydrochloride (PAH), chitosan, and poly(3,4-ethylenedioxythiophene) (PEDOT).<sup>50,53–55</sup>

Table 1 summarizes the sensory modality measured (e.g., aroma or taste) and instrumental methods available, providing an overall overview of how they operate.

**Table 1. Sensory Modality or Characteristic (Aroma and Taste) and Generic Instrumental Method**

sensory modality	generic instrumental method or sensor	principle
aroma	electronic nose	polymer sensor metal oxides sensors mass spectrometry head space traps
taste	electronic tongue	voltametric potentiometric amperometric
aroma, taste and visual characteristics (color)	near and midinfrared, combination of sensors	molecular/ vibrational spectroscopy

#### 5. CHEMOMETRICS AND DATA MINING

Chemical information contained in such instrumental methods resides in the occurrence of peaks, band positions, intensities, and shapes. The most successful approach to extracting quantitative, qualitative, or structural information from such spectra is to use multivariate mathematical analysis or chemometrics.<sup>56–62</sup> These powerful methods and the computer technology necessary to use them have only become readily available in recent years, but their use has become a significant feature on the development of instrumental applications.

A broad range of techniques is now available including data reduction tools, regression techniques, and classification methods. Principal component analysis (PCA) is a commonly used data compression and visualization tool, reducing a spectral data set into a small (generally less than 20) number of new, orthogonal (e.g., noncorrelated) variables on each of which a score (or value) for each sample is calculated.<sup>56–62</sup> Graphical display of these scores can often reveal patterns or clustering within a data set because similar samples are expected to locate close to each other; unexpected sample locations in this hyperspace may alert the analyst to unusual or outlying samples, which may be reanalyzed or, as a final resort, deleted from the data set prior to further data processing. Principal

component (PC) scores may be used in further mathematical operations to classify samples into different, naturally occurring groups.<sup>56–62</sup> A number of procedures are available for sample classification or discrimination; soft independent modeling of class analogy (SIMCA) is an example of a popular class-modeling method, while linear discriminant analysis (LDA), hierarchical cluster analysis (HCA), factorial discriminant analysis (FDA), artificial neural networks (ANN), and partial least-squares (PLS) discriminant analysis (DA) are examples of much used discriminant methods.<sup>56–62</sup> Class-modeling methods focus on characterizing each of the classes of sample being analyzed and involve calculation of a model and boundaries within which samples of each particular type may be expected to be found.<sup>56–62</sup>

Discriminant methods focus on characterizing the boundaries between samples of different classes and do not involve calculation of statistically robust confidence limits for each class.<sup>40,41,56–62</sup> Application of artificial neural networks (ANN) is a more recent technique for data and knowledge processing that is characterized by its analogy with a biological neuron.<sup>57–59,61</sup> When the firing frequency of a neuron is compared with that of a computer, then for a neuron this frequency is rather low.<sup>57–59,61</sup> In the biological neuron the input signal from the dendrites travels through the axons to the synapse. There the information is transformed and sent across the synapse to the dendrites of the next neuron.<sup>57–59,61</sup> For fuller coverage of chemometric tools and procedures, the interested reader is referred to other sources.<sup>56–62</sup>

## 6. APPLICATIONS OF INSTRUMENTAL METHODS

### 6.1. Electronic Noses

The matrix of alcoholic beverages is made up of a complex mixture of chemicals including water, alcohol, phenolic compounds, organic acids, sugars, and volatile aroma compounds, all of which can contribute to the sensory characteristics of the food.<sup>11,15,47,63–66</sup> Those components responsible for aroma and flavor are not only involved in complex interactions with each other, resulting in masking and additive effects, but also involved in complex interactions with nonflavor active components in alcoholic beverages matrix (e.g., water, alcohol, nonvolatile compounds). Due to these complex interactions, it might not be simple to obtain a robust prediction of sensory properties through measurement of just a small number of volatile or chemical components, without taking into account the matrix of beverages.<sup>11,15,16,47,63–66</sup>

Few studies have examined the use of EN or gas sensors to characterize the aroma of wine, mainly due to major compounds in the samples headspace, such as ethanol, causing interference with the gas sensor.<sup>33–39,69,70</sup> However, this limitation does not exist with mass spectrometry (MS)-based EN instruments where the alcoholic-based beverage headspace is monitored and the whole spectra are analyzed.<sup>67–74</sup> Recent studies have shown that rapid analysis of wine volatiles by MS-EN produces signals containing information that even without chromatographic separation can be used to determine a fingerprint of wine based on its aroma profile.<sup>67–74</sup>

A benefit of MS-EN instruments over other EN sensors is that they detect mass fragments formed during ionization of volatile compounds. Some of these volatiles can be directly responsible for the sensory differences between samples, and measuring the mass fragments of these compounds can provide some understanding of the chemical basis for sensory

differentiation as well as basis for varietal discrimination.<sup>30,37</sup> Furthermore, MS-EN instruments are based on the very well-known and commonly used technology of MS, and the stability, sensitivity, and reproducibility of this technique has long been established.<sup>7</sup>

While the benefits of quick classification and differentiation of wines without the need of determining the chemical composition of the gaseous phase are undisputable, it has to be taken into account that EN is a nonselective technique, that is, it detects the major volatiles of the headspace regardless of whether those volatiles are actively contributing to the aroma of the wine or not.<sup>7,16</sup> The volatile compounds responsible for the characteristic aromas of wine are often not quantitatively the major volatile components in the headspace of wine; rather they are usually minor constituents present at microgram or nanogram per liter levels.<sup>7</sup> Consequently, those volatile compounds at higher concentrations in the headspace, which are not contributing to the aroma of the wines, may be dominating the spectral data obtained from EN and introducing noise to the regression models developed. Furthermore, the EN method is not likely to be sensitive enough to detect all of the most important volatile aroma compounds which are present at trace levels which would further impact on the ability of the EN profile to predict the sensory properties of the sample.

Metal oxide sensor (MOX) instruments were tested for the ability to characterize Ontario-produced fruit wines.<sup>70</sup> Both fruit wines (blueberry, cherry, raspberry, blackcurrant, elderberry, cranberry, apple, and peach) and grape wines (red, Chardonnay, Riesling, and ice wine) were obtained from several Ontario wineries. Replicates of each wine sample were dried onto membrane filters to remove ethanol and analyzed by a commercially available instrument.<sup>70</sup> Results show that MOX sensors can discriminate between fruit and grape wines and may become an important tool for standardization of wine quality.<sup>70</sup>

Application tin oxide–array sensors for identification of typical aromatic compounds present in white and red wines was evaluated to detect different aroma attributes (e.g., fruity, floral, herbaceous, vegetative, spicy, smoky).<sup>71,72</sup> Comparison of both PCA and LDA chemometric techniques shows that compounds responsible for the aroma in red and white wines were clearly separated. From the results obtained, the authors concluded that the system evaluated could correctly discriminate the aromatic compounds added to wine samples.<sup>71,72</sup>

Combination of an EN device based on resistive MOX sensors, an E-tongue (based on voltametric sensors), and an e-eye (based on CIE Lab coordinates) has been used to monitor the aging of a red wine.<sup>73</sup> The changes in the chemical composition of wines that occur during maturing have permitted the system to discriminate among wine samples collected after 1, 3, 6, and 10 months of aging. The discrimination capability of the electronic panel test obtained by means of PCA, PLS-DA is even higher than the discrimination achieved by means of traditional chemical analysis. After 10 months of aging it has been possible to discriminate between the wine aged in a French oak barrel and the same wine soaked with oak chips of the same origin and toasting level and treated with micro-oxygenation.<sup>73</sup>

An electronic panel created by an EN, E-tongue, and electronic eye has been successfully used to evaluate the organoleptic characteristics of red wines produced using different extraction techniques and micro-oxygenation methods and bottled using closures of different oxygen transmission

rates (OTR).<sup>74</sup> Use of PLS-DA has allowed one to establish prediction models based on the type of closure, the polyphenol content, or the effect of micro-oxygenation. The best correlations were found using the e-eye and the EN related to the OTR of the closure, while the E-tongue was more sensitive to changes in the polyphenol content of the wine samples analyzed. The discrimination and prediction capabilities of the system are significantly improved when signals from each module are combined. Overall, it was concluded by the authors that the electronic panel can be a useful tool for characterization and control of oxygen and antioxidant capability of red wines.<sup>74</sup>

The ability of two EN systems (conducting polymer and surface acoustic wave based) to differentiate volatiles of grapes and wines treated with an aqueous ethanol spray (5% v/v) at veraison was evaluated.<sup>75</sup> EN evaluation of grape volatiles was compared with Cabernet Franc and Merlot chemical composition with the aroma of the wine measured by GC (volatiles) and sensory data. Canonical discriminant and PCA found that both EN systems and the chemical measures (e.g., Brix, TA, pH, color intensity and hue, total phenols, glycosides, and berry weight) were able to discriminate between ethanol-treated and untreated grapes and wines for both cultivars. According to the authors, grape differences were due mainly to variations in hue, phenolic-free glycosides, and total phenols.<sup>75</sup> Aroma sensory evaluations using a consumer panel differentiated between ethanol treatments and controls for Merlot but not for Cabernet Franc wines.<sup>75</sup>

Some special sweet wines are obtained by partial fermentation of musts from off-vine dried grapes containing large amounts of sugars. This process is very slow and subject to serious stop problems that can be avoided using osmo-ethanol-tolerant yeasts.<sup>68</sup> Musts containing 371 g L<sup>-1</sup> of sugars were partially fermented with selected *Saccharomyces cerevisiae* strains, namely, X4 and X5, to 12% (v/v), and the wines obtained with X5 strain exhibited a higher volatile acidity but lower concentrations of higher alcohols, carbonyl compounds, and polyols than those obtained with X4 strain.<sup>68</sup> Use of PCA of the data provided by an EN system afforded discrimination between fermented and unfermented musts but not between wines obtained with X4 or X5 strains. The PCA applied to the major volatile compounds and polyols shows similar results, but a clear discrimination between wines is obtained by removing the polyols glycerol and 2,3-butanediol from the PCA models developed.<sup>68</sup>

A comparative study between the perception and the recognition thresholds of volatile components calculated from an EN system and from a human sensory panel was reported.<sup>76</sup> The EN system was home developed; based on a thin film semiconductor a sensor was used, while the human sensory panel is formed by 25 tasters with previous experience in wine tasting. Both systems were trained in parallel to detect 17 volatile compounds involved in aromatic and off-flavor notes (grouped under 9 aromatic descriptors) from the threshold concentrations found in the literature (called T) to increasing concentrations (T, 2T, and 4T). The results showed that the perception level of the human nose was superior in comparison to the results obtained from the EN system. However, the EN system gave better results in the recognition threshold in some aroma compounds associated with off-flavor notes in the set of wine analyzed. According to these results, the authors concluded that the EN system could be a useful complementary

tool to sensory human panels.<sup>76</sup> Similar results were reported by other authors.<sup>77</sup>

## 6.2. Infrared Spectroscopy

It has been demonstrated that wine-quality rankings (as the score or allocation assigned to wines by sensory panels) for red and fortified wines could be discriminated by visible (VIS) and NIR spectroscopy.<sup>16,78–80</sup> Studies carried out in a commercial winery in Australia demonstrated that vis–NIR spectroscopy can predict wine quality as judged by both commercial wine-quality rankings and wine show scores.<sup>16,78–80</sup> Correlations between NIR spectra and sensory data obtained using wine show samples were less significant in general in comparison with the commercial grading data. The coefficient of determination ( $R^2$ ) and the standard error in cross validation (SECV) obtained to predict tawny port wine score were 0.84 and 0.97, respectively (see Table 2).<sup>78–80</sup>

**Table 2. Examples on the Application of Electronic Noses, Electronic Tongues, and Other Instrumental Methods To Quantify Aroma and Taste Characteristics in Beverages<sup>a</sup>**

aroma or taste characteristic	method	range	R	RMSEP	ref
pencil shaving	E-tongue	0.3–3.95	0.83	0.81	99
vegetal		1.3–3.75	0.85	0.39	
spice		0.98–3.92	0.90	0.47	
4-EG	EN	0–290 ( $\mu\text{L}^{-1}$ )	0.51	38.8	32
4-EP		0–1710 ( $\mu\text{L}^{-1}$ )	0.52	241.3	
estery	NIR	1.1–4.8	0.64	0.55 <sup>a</sup>	78
lemon		0.6–3.2	0.50	0.48	
passionfruit		0.1–5.2	0.45	0.98	
honey		0.4–4.3	0.70	0.58	
developed	NIR + EN		0.91	0.66	65
floral			0.73	0.84	
green			0.66	0.64	
tropical			0.43	0.98	

<sup>a</sup> $R^2$ : coefficient of determination. RMSEP: root mean square of the standard error of prediction. SEP: standard error of prediction. EN: electronic nose. NIR: near-infrared. 4-EG: four ethylguaicol. 4-EP: four ethylphenol.

Grading of wine by vis–NIR spectroscopy provides a rapid assessment or prescreening tool to add to the range of analyses available to winemakers. It could allow preliminary blend allocation of large numbers of batches of wines prior to sensory assessment. Winemakers may be able to develop 'profiles' for their blends as in-house vis–NIR calibrations. Calibrations based on sensory scores will tend to be difficult to obtain due to variation between individual wine tasters and may not pick up compounds that are present at low concentrations yet have strong sensory properties. Nevertheless, interpretation of spectral data may provide valuable insight into the more abundant parameters affecting wine quality and highlight the interactions that occur within the complex wine matrix in governing sensory properties.<sup>78–80</sup>

Recent studies have demonstrated the ability of vis–NIR spectroscopy to predict quality scores derived from a panel of winemakers in a set of red wine samples. Most of the NIR calibrations developed accounted for more than 70% ( $R^2 > 0.70$ ) of the variation described by the sensory panel.<sup>79,80</sup> Use of vibrational spectroscopy, in particular, use of vis–NIR to



measure aroma (honey, estery, lemon, caramel, toasty, perfumed floral, passionfruit) and palate properties (overall flavor and sweetness) in commercial available bottles of Australian Riesling and unwooded Chardonnay wines was reported (see Table 2).<sup>78</sup> The results showed good correlation between spectra and sensory properties ( $R > 0.70$ ) for estery, honey, toasty, caramel, perfumed floral, and lemon, while poor correlations ( $R < \text{about } 0.55$ ) were found in most of the cases for passionfruit, sweetness, and overall flavor.<sup>78</sup>

As in other foods, it is likely that no single compositional characteristic explains the differences in sensory properties between wines; rather a combination of different variables such as grape- and yeast-derived compounds (e.g., volatile and nonvolatile compounds), oxidation products, and other constituents present in the wine matrix should be used. However, no information is currently available concerning possible correlations between spectral data and volatile components in the wine varieties analyzed. Therefore, these methods (vis, NIR, and MIR) might indirectly explain the variations in the sensory characteristics of the wines analyzed. Taking into account the nature of the characteristics measured, such calibrations might be useful as rapid instrumental screening tools when a large number of wines need to be rated for quality prior to formal sensory analysis in order to reduce the cost and resources required for such analyses, particularly for those assessments where the purpose is to assess the degree and incidence of bottle aged development in a set of wines.<sup>78–80</sup>

Use of FT-MIR spectroscopy in combination with multivariate data analysis has been introduced for quality and authenticity assessment of spirit drinks and beer in official food control. PCA was applied to the FT-MIR data from a reduced set of authentic Mexican tequilas ( $n = 14$ ) and commercially available samples purchased in Mexico and Germany ( $n = 24$ ) of the same spirit beverage. Use of FT-MIR allowed a rapid screening of density and ethanol as well as the volatile compounds methanol, ethyl acetate, propanol-1, isobutanol, and 2-/3-methyl-1-butanol using PLS regression (SEP ranging from 5.3% to 29.3%), while using PCA a differentiation between tequila derived from “100% agave” (Agave tequilana Weber var. Azul, Agavaceae) and tequila produced with other fermentable sugars (“mixed” tequila) was possible.<sup>81</sup>

Overall, the practical implications for the alcoholic beverage industry are that instrumental measurements such as vis, NIR, and MIR spectroscopy are complementary to sensory analysis and can facilitate the task at early stages of product development, making high-throughput screening of novel products feasible or able to maintain the consistency of high-value products. Alternatively, spectroscopy may be useful as a rapid screening method for determination of approximate quality category estimation as a prescreening mechanism (low, medium, and high) of some sensory properties in wine shows.<sup>16,79,80</sup>

### 6.3. Electronic Tongues

An electronic tongue system based on poly(3,4-ethylenedioxythiophene)-modified electrode has been reported as a potentially useful amperometric sensor to use either alone or in the frame of a set of sensors bearing complementary information.<sup>82</sup> The sensor was proposed in blind analysis of red wines from Italy (Sangiovese, Primitivo, and Montepuciano) for classification and calibration purposes.<sup>82</sup> Data obtained from voltammetric measurements have been treated using PLS

regression. A calibration procedure has been performed to correlate results from analyses of wines, analyzed with traditional analytical methods, with the corresponding voltammetric responses. Results showed that development of electrochemical sensors also allows fast identification of samples exceeding threshold limits of meaningful parameters for quality control in the wine industry, such as  $\text{SO}_2$ , color intensity, and total polyphenols.<sup>82</sup> Application of the system within a sensor array (electronic tongue) to a fast prescreening routine control procedure is proposed.<sup>82</sup>

A low-cost method was also proposed to classify wine and whisky samples using a disposable voltammetric electronic tongue that was fabricated using gold and copper substrates and a pattern recognition technique such as PCA.<sup>83</sup> The proposed device was successfully used to discriminate between expensive and cheap whisky samples and to detect adulteration processes using only a copper electrode. For wines, the electronic tongue was composed of copper and gold working electrodes and able to classify three different brands of wine and make distinctions regarding the wine type (dry red, soft red, dry white, and soft white brands).<sup>83</sup>

A voltammetric E-tongue system was developed to discriminate between Chinese rice wines. Three types of Chinese rice wine with different marked ages (1, 3, and 5 years) were classified by the E-tongue by PCA and CA analysis.<sup>84</sup> The E-tongue systems consisted of six working electrodes (gold, silver, platinum, palladium, tungsten, and titanium) in a standard three-electrode configuration.<sup>84</sup> Multifrequency large amplitude pulse voltammetry (MLAPV), which consisted of four segments of 1, 10, 100, and 1000 Hz, was applied as the potential waveform. The three types of Chinese rice wine could be classified accurately by PCA and CA, and some interesting regularity is shown in the score plots with the help of PCA. Partial least-squares (PLS) and a back-error propagation-artificial neural network (BP-ANN) were used to predict wine age. Regression results showed that the marked ages of the three types of Chinese rice wine were successfully predicted using PLS and BP-ANN.<sup>84</sup>

Use of a voltammetric E-tongue system formed by five modified graphite–epoxy electrodes in the qualitative and quantitative analysis of cava wines was reported.<sup>85</sup> Different samples were analyzed using cyclic voltammetry without any sample pretreatment. Recorded data were evaluated using PCA and discrete wavelet transform in order to compress and extract significant features from the voltammetric signals.<sup>85</sup> The preprocessed information was evaluated by ANN, which accomplishes qualitative classification.<sup>85</sup>

An E-tongue system based on potentiometric chemical sensors was assessed as a rapid tool for quantification of bitterness in red wines. A set of 39 single-cultivar Pinotage wines comprising 13 samples with medium to high bitterness was obtained from the producers in West Cape, South Africa.<sup>86</sup> Samples were analyzed with respect to a set of routine wine parameters and major phenolic compounds using MIR spectroscopy and HPLC, respectively. A trained sensory panel assessed the bitterness intensity of 15 wines, 13 of which had a bitter taste of medium to high intensity.<sup>86</sup> Thirty-one wine samples including seven bitter-tasting ones were measured by the E-tongue system. Influence of the chemical composition of wine on the occurrence of the bitter taste was evaluated using one-way analysis of variance. It was found that bitter-tasting wines had higher concentrations of phenolic compounds (catechin, epicatechin, gallic, and caffeic acids and

quercetin) than nonbitter wines.<sup>79</sup> Sensitivity of the sensors of the array to the phenolic compounds related to bitterness was studied at different pH levels. Sensors displayed sensitivity to all studied compounds at pH 7 but only to quercetin at pH 3.5. On the basis of these findings, the pH of wine was adjusted to 7 prior to measurements. Calibration models for classification of wine samples according to the presence of the bitter taste and quantification of the bitterness intensity were calculated using PLS-DA regression. Statistical significance of the classification results was confirmed by the permutation test. Both the E-tongue system and chemical analysis data could discriminate between bitter and control wines with correct classification rates of 94% and 91%, respectively. Prediction of the bitterness intensity with good accuracy (root-mean-square error of 2 and mean relative error of 6% in validation) was possible only using data generated by the E-tongue system.<sup>86</sup>

A multiparametric system capable of characterizing and classifying white wines according to the grape variety and geographical origin was developed based on the E-tongue system.<sup>87</sup> Besides, it quantifies specific parameters of interest for quality control in wine.<sup>87</sup> The system, known as a hybrid electronic tongue, consists of an array of electrochemical microsensors-six (ISFET) based sensors, a conductivity sensor, a redox potential sensor, and two amperometric electrodes, a gold microelectrode, and a microelectrode for sensing electrochemical oxygen demand and a miniaturized optofluidic system.<sup>87</sup> The test sample set comprised 18 monovarietal white wines from four different grape varieties from Spain and two Croatian monovarietal white wines and seven bi- and trivarietal mixtures prepared from the Spanish varieties. Different chemometric tools were used to analyze and interpret the data generated by the sensors including PCA and PLS-DA analysis. Results demonstrated the usefulness of the multisensor system for analysis of wine.<sup>87,89</sup>

#### 6.4. Combination of Sensors

One of the aims of flavor chemistry is to create mathematical models that allow establishment of the existing relationships between the content of the product aroma-active compounds and the sensory properties of the sample.<sup>16,79,80</sup> In recent years, use of multivariate statistical techniques (chemometrics) on chemical and sensory data has gained increasing attention as a means to classify wines from different geographical regions and to describe similar and discriminating sensory and chemical characteristics. Knowledge about the identity of the volatile compounds that contribute to the characteristic flavor of a given style of wine is now one of the most challenging tasks for the wine industry. A great number of noninvasive and nondestructive instrumental techniques are currently available for determining the composition of food and food ingredients. Those analytical techniques are rapid and relatively inexpensive and can be applied to fundamental research in control laboratories and online. Those methods combined with multivariate data analysis such as PLS regression can be related to "hidden" chemical information.<sup>16,79,80</sup> However, such methods can not eliminate the need for more detailed laboratory analysis, but they may help to screen samples that require further examination.<sup>16,79,80</sup>

Interpretation and analysis of combining such complex and different instrumental techniques (NIR, MS-EN, E-tongue) is possible by use of multivariate statistical techniques.<sup>16,79,80,88</sup> The advantages of the combination of different rapid instrumental techniques include the possibility of obtaining

and combining information from different parts of the matrix, where the ultimate results will be the "fingerprint" of a given food under analysis. This allows the information present in the whole matrix to be unrevealed by the help of chemometrics. However, the main disadvantages of this kind of approach are that we will have the overall fingerprint; it and will be difficult to identify or relate a particular change, sensory attribute with an individual chemical compound. Few reports are found in the literature in relation to the combination of several techniques to be used together to analyze food. It has been reported by other authors that the predictive information related to a specific sensory attribute and a rapid instrumental technique did not seem to be related to a specific chemical moiety in the sample, and it is not clear which relevant information in the matrix was related to a specific sensory attribute. This is an important issue for sensory characteristics where the relationship between the sensory attributes (score) and specific chemical compounds in wine are still not clearly understood.<sup>16,79,80,88</sup>

Good correlations between NIR spectroscopy and scores for the sensory attributes might be caused by collinearity between other variables (e.g., ethanol, sugars), between wavelengths, or between other sensory properties (e.g., honey and toasty).<sup>16,79,80</sup> It is well known that many sensory attributes are not strictly associated with an identifiable chemical entity in the NIR region, requiring the use of a large number of seemingly redundant wavelengths to develop calibration models for prediction of sensory score.<sup>16,79,80</sup> On the other hand, the MS spectra based EN gives information related with the volatile compounds in the wine (headspace). Although this approach cannot give an answer about which volatile compound is responsible for the aroma of a given wine, it can be used as a rapid technique to classify or monitor changes in the wine related to aroma characteristics. Whether these changes in the wine matrix are representative of the overall changes in the wine is still unclear. In the future, combination of rapid instrumental techniques coupled with chemometrics will give the possibility to build a library of wines based on their quality attributes, in other words to build the fingerprint of a given wine. It has been demonstrated that the use of rapid instrumental techniques such as MS-based EN, vis-NIR, spectroscopy or the combination of both could be used to predict panel scores for some sensory characteristics in a set of Australian Riesling wines (Table 2).<sup>65</sup> These results proved that the relationship between MS-based EN and vis-NIR and sensory properties in wine exists. However, the relationships between chemical compounds, sensory properties, and the instrumental method were not explored. The limited number of samples and wine types available for the present study lead us to be cautious about the conclusions made from spectral data analysis.<sup>78</sup> Furthermore, the prediction ability of the PLS models needs to be evaluated with a new set of samples.<sup>65</sup>

Casale and collaborators reported the use of combining NIR, UV-vis, an EN, and an electronic tongue as a method to fingerprint Italian red wines.<sup>88</sup> Combination of such sensors with pattern recognition techniques such as LDA and PCA allow identification of red wines produced from two distinctive Italian grape varieties, namely, Barbera d'Alba and Dolcetto d'Alba.<sup>88</sup> Recently, combination of E-tongues with optical electromechanical microsensors was reported to control and monitor wine quality.<sup>88</sup> Their work demonstrated that the concatenation of sensors combined with chemometric analysis can be used to characterize and classify wine samples.<sup>88</sup>



Innovative analytical techniques, such as an amperometric E-tongue and a commercial EN, were used together with spectrophotometric methods to predict sensorial descriptors of Italian red dry wines of different denominations of origin.<sup>90</sup> Genetic Algorithms were employed to select variables and build predictive regression models. On the selected models, an accurate validation technique (the Bootstrap procedure) and a procedure for detection of outliers (Williams plot) were applied. Results obtained demonstrate the possibility of using these innovative techniques in order to describe and predict sensorial information from a panel. However, the authors reported that it was not possible to build an acceptable regression model for sourness.<sup>90</sup>

Effective fermentation monitoring is a growing need due to the rapid pace of change in the wine industry, which calls for fast methods providing real-time information in order to ensure the quality of the final product.<sup>91</sup> The objective of the work was to investigate the potential of nondestructive techniques associated with chemometric data analysis to monitor time-related changes that occur during red wine fermentation. Eight microfermentation trials were conducted in the Valtellina region (Northern Italy) during the 2009 vintage and monitored using the combination of a FT-NIR and a FT-MIR spectrometer with an EN and E-tongue system. The spectroscopic technique was used to investigate molecular changes, while EN and E-tongue systems evaluated the evolution of the aroma and taste profile during the must-wine fermentation.<sup>91</sup> Must-wine samples were also analyzed by traditional chemical methods in order to determine sugars (glucose and fructose) consumption and alcohol (ethanol and glycerol) production. Use of PCA to the data generated by the instrumental methods, as an exploratory tool, allowed one to uncover molecular, aroma, and taste changes in the samples during the fermentation process.<sup>92</sup> Furthermore, the chemical data and PC1 scores from spectral, electronic nose, and electronic tongue data were modeled as a function of time to identify critical points during fermentation. The results showed that NIR and MIR spectroscopy are useful to investigate molecular changes involved in wine fermentation, while EN and E-tongue systems can be applied to detect the evolution of taste and aroma profile.<sup>92</sup> Moreover, as demonstrated through the modeling of data generated by the NIR, MIR, EN, and E-tongue systems, these nondestructive methods are suitable for monitoring of must during wine fermentation, giving important information about the quality of the final product in agreement with chemical parameters.<sup>91</sup> Although in this study measurements were carried out in off-line mode, in the future these nondestructive techniques could be valid and simple tools able to provide in-time information about the fermentation process and ensure the quality of wine.<sup>91</sup>

Other examples on the use of instrumental methods, alone or combined, are shown in Tables 2 and 3.

## 7. ADVANTAGES AND LIMITATIONS OF INSTRUMENTAL METHODS

During the past two decades, considerable effort has been made to explore the possibilities offered by instrumental methods or sensors to monitor and predict changes related with aroma and taste in alcoholic beverages.

Quantitative knowledge in relation to the main components of beverages and food products is necessary but not sufficient to predict the technological and organoleptic properties of individual labels or brands. Increased research efforts in the

**Table 3. Examples of the Application of Electronic Noses and Tongues for Determination of Aroma and Taste in Alcoholic Beverages<sup>a</sup>**

application	beverage	method/ technique	ref
aging during storage	red wine	Electronic panel/ gas sensor	73
aging wines in barrels	red wine	E-tongue	93, 95
aging	port wine, wine	E-tongue, EN	114, 115
geographical origin of wine based on aroma profiles	white wine	MOS and MS	105
classification chinese wine		E-tongue	110
wine aroma profiles		E-tongue and EN	94
analysis of taste compounds	cava wine	E tongue	85
deterioration during storage	wines	E-tongue and EN	97
wine discrimination based on taste profiles	red wines	E-tongue, vS and cP	98
profile of italian barbera wines	red wine	EN and E-tongue	92
antioxidant activity	beer	E-tongue	100
aging fingerprinting	beer	EN	101, 111
taste attributes (e.g., bitterness)	beer	E-tongue	103, 106, 108
aroma	beer	MS-EN	113
industrial applications	beer	EN	109, 111
contamination with methanol	whisky		102
micro oxygenation and aging	red wine	E-tongue	96, 99, 107
effect of temperature on the fingerprint	wine	MS-EN	104

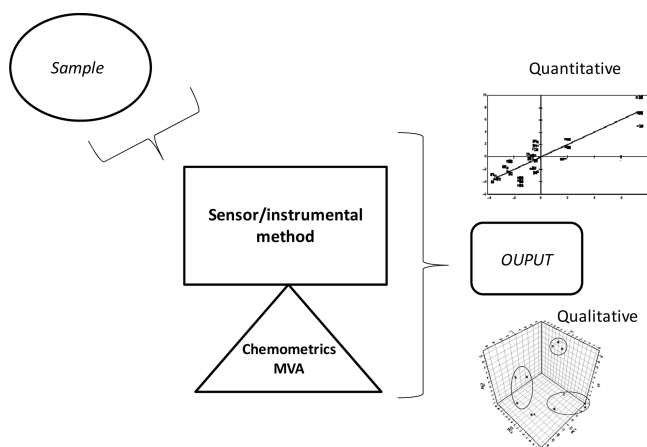
<sup>a</sup>vS: voltametric sensor. cP: conducting polymer. EN; electronic nose. E-tongue: electronic tongue. MS: mass spectrometry. MOS; metal oxidise sensors. HS: head space.

field of instrumental techniques or sensors is addressing some of the challenges of such measurements of food products and alcoholic beverages and further explore the physicochemical changes that are (i) mostly not fully understood using traditional chemistry and (ii) responsible for modification of the stability, organoleptic, and/or typicality of food products.

Development of chemometric tools combined with instrumental methods and sensors will allow the use of these methods in the near future as a tool for online determination of the overall quality of complex food systems or matrices such as beverages (Figure 1). Even though the present review focused on the alcoholic beverage industry, the principles are broader and generally applicable to other food ingredients and products.

The potential savings, reduction in time and cost of analysis, and environmentally friendly nature of the technology positioned rapid instrumental techniques as the most attractive techniques with a bright future in the field of analysis of alcoholic beverages.

There is no doubt about the great potential of instrumental techniques and sensors as a tool for rapid screening and measurement of quality parameters of alcoholic beverages. This relatively new approach to analysis of aroma and taste leads to an aromatic profile (e.g., aroma or taste fingerprint) of the whole, undivided into singular components of the gaseous and liquid phase of the sample. It can be used as a rapid technique to classify or monitor changes. However, more extensive data pretreatment and care in chemometric analysis is required mainly due to expected collinearity among variables, different scale of signal, and possible instrument drift and baseline shifts.



**Figure 1.** Integration of sample, instrumental method, and chemometrics to determine the aroma or taste profiles in beverage samples.

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### Notes

The authors declare no competing financial interest.

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Daniel Cozzolino is currently a Research Fellow with the Barley Research Laboratory with The University of Adelaide, School of Agriculture, Food and Wine. Daniel graduated from the Universidad de la Republica (Montevideo, Uruguay) as an Agricultural Engineer in 1989 and obtained his Ph.D. degree from the University of Aberdeen (Aberdeen, Scotland) in 1998. His research career started in 1993 with the development of NIR applications for a wide range of agricultural products at the National Institute for Agricultural Research (INIA-Uruguay) before joined the Australian Wine Research Institute (AWRI) based in Adelaide (South Australia) in 2002. Between 2002 and 2011, he was the Senior Research Scientist and acting Team Leader of the Rapid Analytical Methods team at the AWRI. His principal role was investigating applications of rapid methods (visible, NIR, MIR, UV, electronic noses) and chemometrics in grape and wine in collaboration with several academic and industry partners. He has published more than 120 papers in refereed journals, 10 book chapters on the application of spectroscopy and chemometrics to a diverse range of agricultural materials and commodities, and filed 1 patent.

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