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Using IR spectroscopy as a holistic monitoring approach in winemaking: A review

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ABSTRACT

Wine matrix is composed of a vast number of compounds that depend on a wide range of factors associated with the raw material, such as grape variety and vineyard location, and processing, such as the winemaking protocol and barrel ageing. Monitoring all aspects of winemaking from grape to wine is a technically challenging task, as different key compounds are related to each step, requiring different analytical methods for their estimation. Nowadays, efforts are made to avoid the use of chemical reagents that can be harmful to the environment and lower the energy consumption during chemical analyses. Ideally, analyses should be performed using a single instrument, without the need for solvents or lengthy preparatory steps. In the past few years, due to its cost-effectiveness and the speediness of the analyses while using low sample volumes, IR spectroscopy has been effectively applied in grape and wine analyses, from compound identification and quantification to wine profile characterisation and authentication. One of its most advantageous features is that it can produce a spectral fingerprint that is unique to each sample, making it highly efficient, especially for authentication purposes. This review examines the feasibility of employing IR spectroscopy for the assessment of all steps required in winemaking, from grape to wine, and its ability to produce integrated results.

KEYWORDS: holistic monitoring, FTIR, wine analysis, grape analysis

INTRODUCTION

Wine is the result of a series of operations that start with the selection of fruit and the harvest date and conclude with the wine bottling and winery waste management. Choice of operations depends on the type of wine to be produced and they are all based on a "skeleton" set of winemaking procedures; *i.e.*, the winemaking protocol. Due to the unique characteristics of each vintage, every step of vinification needs to be monitored to avoid deviations from the expected style and a degradation in wine quality. Consequently, a wide variety of analyses are performed on both fruit and wine (Zoecklein *et al.,* 1999). Nowadays, most wineries have in-house labs that perform some of the most basic analyses. However, specialised analyses are rarely performed, due either to a lack of sophisticated equipment or to the high costs associated with external laboratories (Jacobson, 2006). Moreover, when carrying out grape analyses, sample preparation can be so burdensome and lengthy that a winery will rarely performs any other grape analyses other than those that ensure appropriate sugar accumulation before harvesting; *e.g.*, Brix measurements. For this reason, there is a great need for fast and simple analyses that can be performed on site and in a holistic manner.

In recent years, infrared spectroscopy has proven to be quite efficient for use in the vitivinicultural sector, being fast, accurate, versatile and, most importantly, capable of integrating different types of analyses and providing results for various wine or grape parameters through one single measurement. This feature has already been used in the development of wine analysers that can quantify more than 10 basic wine parameters (Moreira *et al.,* 2002). Today, there is a renewed interest in IR spectroscopy, as it can be adapted for use in more sustainable winemaking approaches and in green chemistry; *i.e.*, performing analyses via chemical processes that use the minimum quantity of hazardous substances (Comuzzo *et al.,* 2022; Nowak *et al.,* 2021). For this reason, IR spectroscopy is the focus of the present review.

IR spectroscopy is a "vibrational spectroscopy" technique that is based on the ability of molecules to vibrate after being exposed to infrared radiation. The vibrational spectrum produced after energy has been absorbed is unique to each molecule and can thus be used as a fingerprint for identification purposes (Coates, 2000). This type of spectroscopy is known as Fourier transform IR spectroscopy (FTIR) when the spectrum is depicted once the signal that represents light intensity has undergone Fourier transformation. Different parts of the spectrum may be used in analyses, such as mid IR (MIR, 4,000 to 400 cm^{-1}) or near IR (NIR, 12,500 to 4,000 cm^{-1}), and FTIR spectrometers can produce results in both these parts (Abo, 2007). In each case, the resulting spectrum provides information on the type of bonds in the sample, with most information being recorded in the region called the "fingerprint" region (Figure 1), from 1,500 to 400 cm^{-1} (Basalekou *et al.,* 2020). Different modes of FTIR techniques (*e.g.*, attenuated total reflection "ATR" and diffuse reflectance infrared Fourier transform "DRIFT") exist, with the IR beam being either reflected or transmitted through the sample, thus allowing high-quality spectra to be collected based on the properties of each sample.

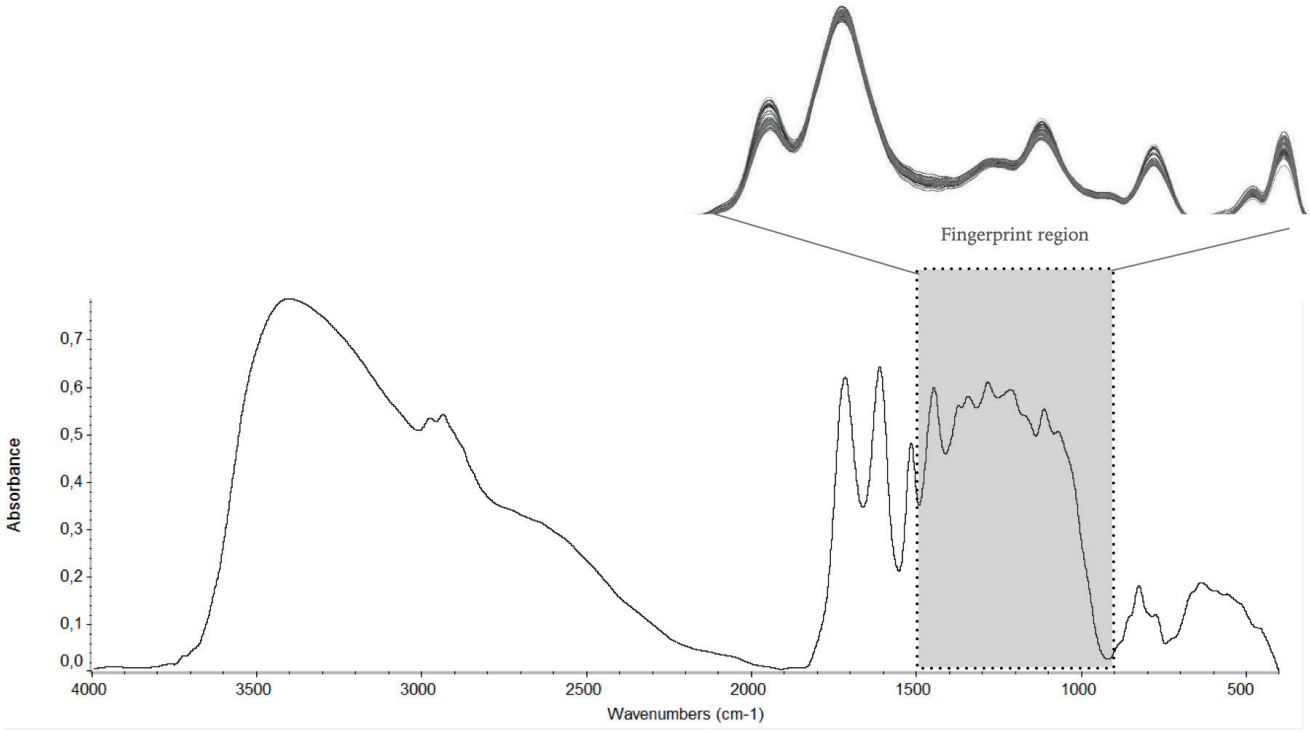


FIGURE 1. Typical wine spectrum and overlay of several wine spectra in the fingerprint region.

Peaks and spectral bands are assigned to functional groups instead of chemical compounds due to the recorded spectra translating to types of bonds. Consequently, compound identification is based on fluctuations in different parts of the whole spectrum rather than in specific peaks, thus generating a large amount of data which can only be assessed through statistical analysis. Several techniques can be applied to facilitate this task, and sample pretreatment (Table 1) is carried out to suppress large bands considered as noise in the spectrum (noise in must and wine samples usually originates from water or ethanol). Apart from sample pretreatment, noise can also be lowered through spectra-processing techniques, such as smoothing, while derivatisation and deconvolution can further assist by resolving overlapping peaks (Zou & Ma, 2014). Finally, information recorded on the spectrum can be assessed through multivariate statistical techniques, which univariately assess spectral fluctuations and can lead to compound determination or model development. Advanced techniques, such as hyperspectral imaging (which combines spectroscopy with digital imaging), can also be employed for the optimisation of spectra collection (hyperspectral imaging divides the spectrum further into more bands, thus enhancing resolution) (Xu *et al.,* 2022). It should be noted that statistical analysis can be applied to either selected regions based on their affinity to the compound(s) of interest or to the whole spectrum, in which case the regions of interest may be later revealed (*e.g.*, in unsupervised statistical analyses, such as PCA, the regions or peaks of interest are revealed based on their participation in the formation of groups that separate the samples). Therefore, regions used for model development may not always coincide with the regions where functional groups of interest are recorded, while bands regarded as noise might also be included in statistical analysis (Figure 2).

The above-described features of IR spectroscopy allow it to be used for the analysis of intact grapes and must, as well as wine; it can be used to assist with analyses during winemaking. In order to better describe the steps of the winemaking process, from grape to wine by-products, the term 'wine' needs to be defined. According to the International Organisation of Vine and Wine, "wine is the beverage resulting exclusively from the partial or complete alcoholic fermentation of fresh grapes – crushed or not – or of grape must, and its actual alcohol content should not be less than 8.5 % vol" (OIV, 2015). The definition of type of raw material (only grapes or grape must) to be used in winemaking is one of many sets of legislative guidelines aiming to protect both producer and consumer through regulation of production and minimisation of adulteration. The characteristics of the grapes determine the type of wine to be produced, and different winemaking processes may be employed, depending on the style of wine.

A basic red and white wine making protocol – variations of which give all other wine types, such as rosé, sparkling and sweet – is shown in Figure 3. According to this protocol, wine production commences at harvest with the arrival of the grapes in the winery, and ends with wine bottling. The grapes should meet certain criteria defined by the type of wine to be produced (*e.g.*, grapes of a certain variety and colour) and the winemaker's standards for fruit (*e.g.*, sugar accumulation or/and phenolic maturity). In red winemaking a maceration step (skin contact) is necessary prior to pressing in order to extract colour from grape skins, while in white winemaking grapes are immediately pressed and the must is then clarified. Subsequently, alcoholic fermentation takes place, sometimes followed by malolactic fermentation (MLF). Even though barrel ageing is more common in red wines, there are several white wine styles that incorporate wood contact, but for a shorter duration than in red winemaking. In order to obtain specific wine styles, different steps of the protocols for red and white winemaking can be repeated, combined or even altered. Variations to the protocol include second fermentation and/or added or forced carbonation (sparkling wines), adjusting maceration length (rosé wines), ending fermentation before total consumption of sugars or by using late harvested or botrytised grapes (sweet wines), adding spirit to increase alcoholic strength (fortified wines) and increased contact with oxygen after fermentation (sherry type wines).

In this review, the analyses performed on grapes, fermenting must and finished wine (outlined in Figure 1) are described and the feasibility of using IR spectroscopy for their implementation is discussed based on information available in the literature to date (2024). This review explores the question of whether alternatives to wet chemistry methods are a viable means of monitoring the quality of the winemaking procedure from grape to wine.

GRAPE

Knowing the type of grape variety prior to vinification is important for both the optimum management of the vineyard and the optimum handling of fruit, and its verification is particularly important in the case of newly acquired but already established vineyards (Murru *et al.,* 2019). Protected Designation of Origin (PDO) wines are also required by legislation to meet certain criteria during their production, including, among others, the use of specific varieties (Corsinovi & Gaeta, 2019). Certain guidelines must also be followed in the case of organic wines (Laureati & Pagliarini, 2016). In winemaking, grape monitoring is carried out to identify key compounds and observe how they evolve, as well as to determine the colour, sensory profile and sanitary status of the grapes and thus ensure quality. Most grape-related analyses focus on determining the optimal date of harvest; *i.e.*, the date on which grapes have achieved optimum maturation. The ultimate goal of all vineyard analyses is to facilitate the selection of the harvest date, while ensuring that the grapes are healthy and meet the winemaking standards.

1. Authentication

Grape variety authentication can be successfully achieved with IR spectroscopy on vine leaves, grape skins, seeds, pulp or juice (Table 1). Using grape leaves and a thin skin layer cut from grapes from five different grape varieties,

TABLE 1. Types of sample preparation used for the spectroscopic analyses of grapes.

Category	Parameter of interest	Type of spectroscopy	Sample	Reference
Authentication	Variety	ATR-FIR	Leaves and a thin grape skin layer	Murru *et al.* (2019)
	Maturity, variety, and origin	NIR	Whole grapes	Arana *et al.* (2005)
	Variety	ATR-FTIR NIR	Grape juice	Cozzolino *et al.* (2012a)
	Variety and clone	ATR-FIR	Leaves	Álvarez *et al.* (2020)
	Clone	NIR hyperspectral imaging	Leaves	Fernandes *et al.* (2015)
	Type of farming	ATR-FTIR	Seeds, pulp, or skins (skins and seeds dried, pulp frozen)	Radulescu *et al.* (2021)
	Type of juice (organic or conventional)	FTIR	Heated juice	Junges *et al.* (2022)
Disease monitoring	*Botrytis* bunch rot	MIR	Grape bunch	Hill *et al.* (2013)
	Botrytis bunch rot and sour rot	ATR-FTIR	Grape must	Cornelissen *et al.* (2023)
	Aspergillus spp., *Botrytis cinerea*, and *Penicillium expansum*	ATR-FTIR	Grape berries	Schmidtke *et al.* (2019)
	Virus infections	ATR-FTIR	Leaves	Topala *et al.* (2017)
	Grapevine leafroll disease	Hyperspectral imaging	Grape berries	Gao *et al.* (2020)
Maturity	Sugar to acid ratio	FT-NIR	Grape berries	Daniels *et al.* (2019)
	TSS	NIR	Grapes under field conditions	Urraca *et al.* (2016)
Sensory profile	Sweetness and acidity	FT-NIR	Grape berries	Basile *et al.* (2020)
	Taste, texture and visual, and olfactory attributes	NIR	Skins and seeds	Ferrer-Gallego *et al.* (2013)
	"Fruity", "floral", "green", and "microbiological" aroma descriptors	NIR	Grape juice with sodium azide	Gehlken *et al.* (2023)
	Smoke taint	NIR	Grape berries	Summerson *et al.* (2020)
Quality at receival	Phytosanitary status	Vis/NIR	Grape bunch	Beghi *et al.* (2017)
	TSS and phenolic content	Vis/NIR	Grape berries	Xiao *et al.* (2019)
Polyphenol determination	Phenolic acids, anthocyanins, flavan-3-ols, and flavonols	NIR	Grapes and grape skins	Ferrer-Gallego *et al.* (2011)
	Anthocyanins	NIR hyperspectral imaging	Grape berries	Chen *et al.* (2015)
Polyphenol extractability	Total phenolic content	NIR hyperspectral imaging	Grape seeds	Baca-Bocanegra *et al.* (2018)
	Polysaccharides	ATR-FTIR	Skins	Nogales-Bueno *et al.* (2017)
	Pectin esterification	Raman	Skins	Nogales-Bueno *et al.* (2017)

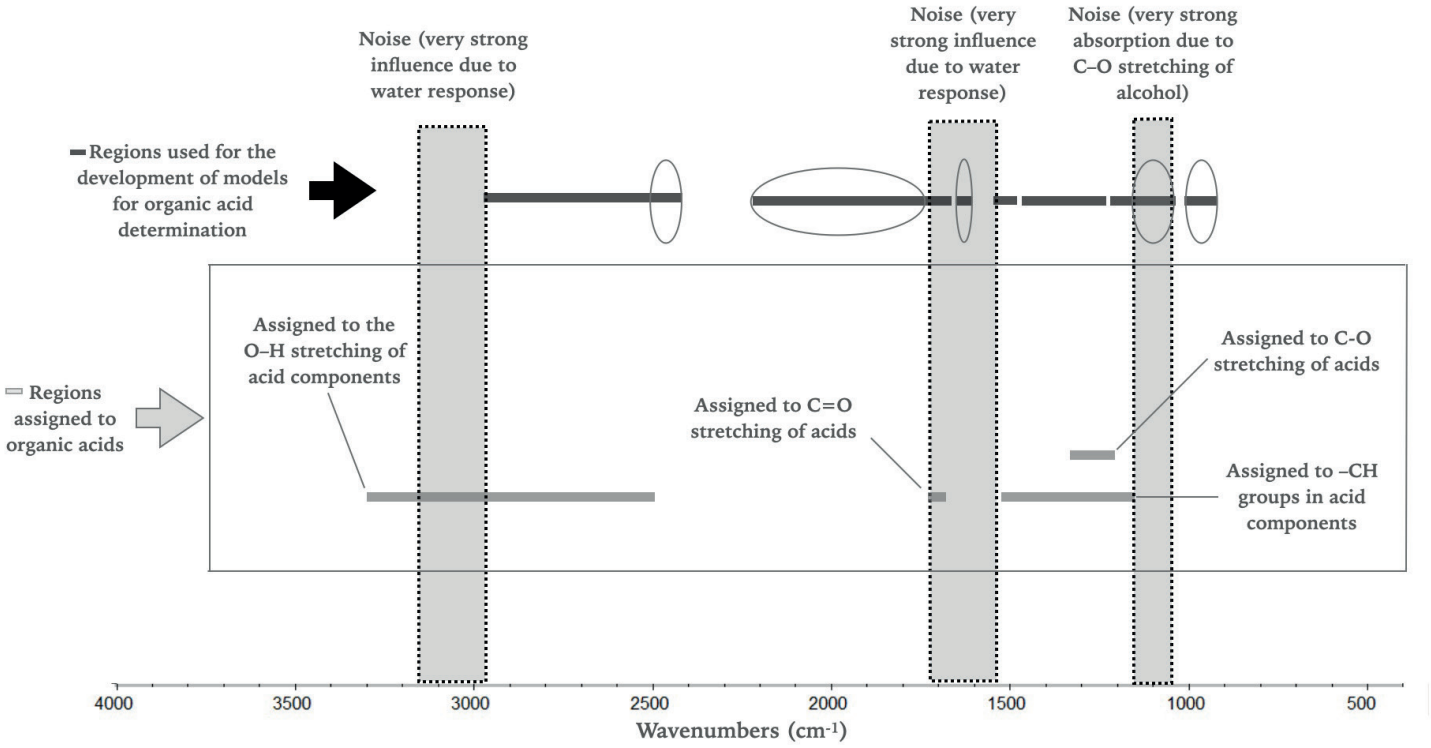


FIGURE 2. Spectral regions used for the development of models for the determination of organic acids (black horizontal lines) and spectral regions assigned to types of bonds relating to organic acids (grey horizontal lines) in Regmi *et al.* (2012). Vertical grey bars indicate regions considered as noise, circles indicate regions not including functional groups of interest but used in model development.

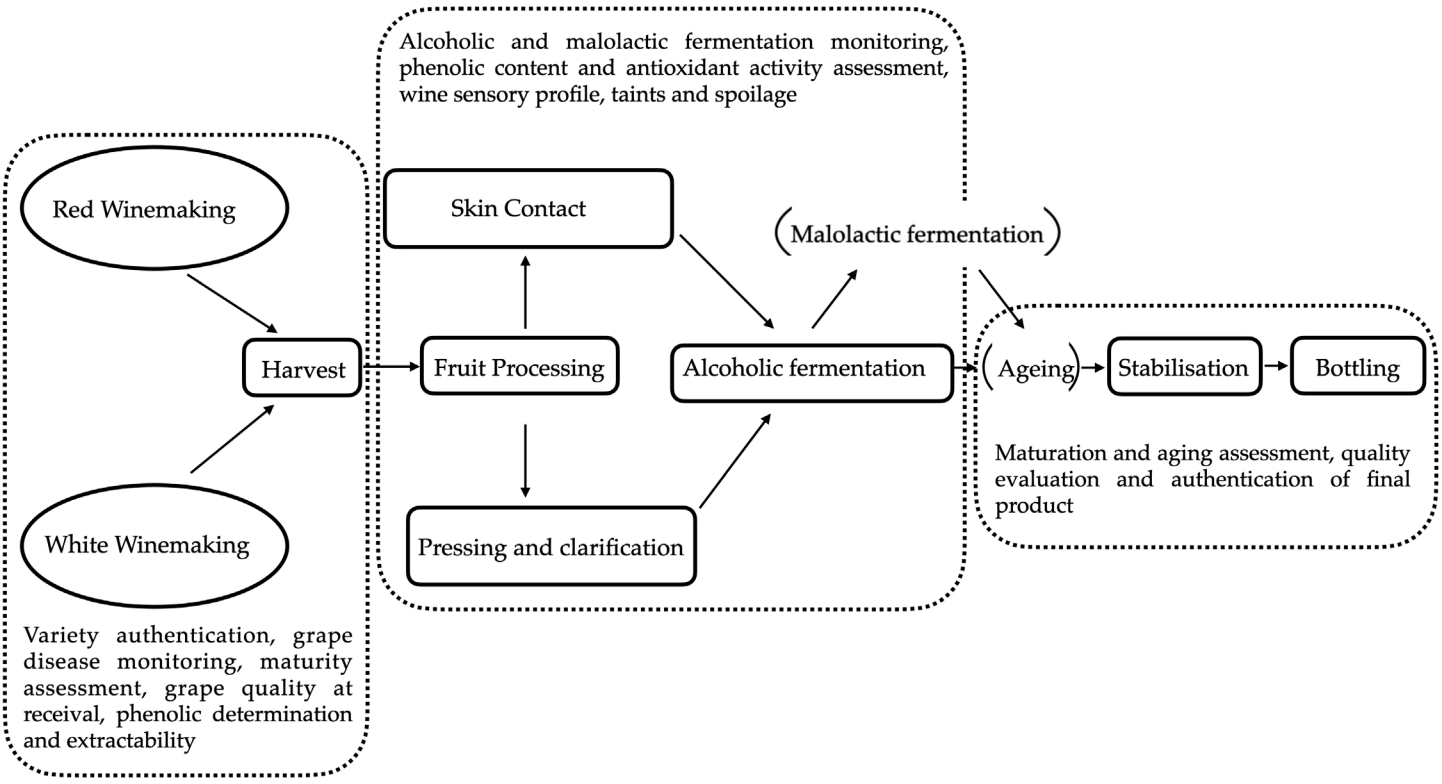


FIGURE 3. Basic protocol for winemaking and analyses that are outlined in the present review.

ATR-FTIR coupled with artificial neural networks was able to identify the grape variety based on the spectral region from 4,000 to 600 cm^{-1} with a 91.2 % correct classification (Murru *et al.,* 2019). The analysis could be performed independently of any structural changes to the samples, requiring no pre-treatment steps, and the models that were produced were based on chemical compounds, such as polyphenols and fructose (Murru *et al.,* 2019). Using whole grapes, variety determination of two white grape varieties was successful using NIR spectroscopy (spectral region from 15,000 to 12,500 cm^{-1}), with the development of regression models (Arana *et al.,* 2005); the percentage of correct classification was higher (97.2 %) but not comparable to the study of Murru *et al.* (2019). The use of grape juice has been found to produce lower classification efficiency by coupling MIR spectroscopy with linear discriminant analysis (LDA) (86 %, for the discrimination of two grape varieties, Chardonnay and Riesling) (Cozzolino *et al.,* 2012a).

Even though IR spectroscopy is able to produce a chemical fingerprint of the grapes, discrimination between sibling varieties or clones is more difficult to achieve, for which viticulturists must rely on ampelographic data. Using leaves and direct ATR-FTIR measurements, Álvarez *et al.* (2020) succeeded in discriminating not only the variety between five different varieties but also the clone between two different clones of the Pinot noir variety. The spectral area used was 1,700-700 cm^{-1} and the predictive models were developed employing SIMCA and PLS-DA analysis. NIR hyperspectral imaging coupled to PLS analysis has already been used for the discrimination of four clones of Cabernet-Sauvignon with a correct classification rate of 97.8 % (Fernandes *et al.,* 2015). Although research on clone differentiation is limited, there is great potential for further development through the enlargement of the clone dataset, as well as the employment of different statistical techniques.

Authentication is also essential for the verification of type of farming in the case of organically grown grapes. ATR-FTIR along with chemometrics has been able to identify farming type (organic *vs* conventional) in red grape extracts, showing good potential, with the models obtained by PCA analysis showing 100 % correct classification using seeds or pulp, and 85 % correct classification when skins were used (Radulescu *et al.,* 2021). Recently, Junges *et al.* (2022) also achieved a 100 % correct classification using LDA on a larger set of samples (45 samples obtained from 11 varieties as opposed to 8 samples from 4 grape varieties in the study of Radulescu *et al.* (2021)) and a different sample pretreatment, as the juice was obtained by heating.

2. Disease monitoring

Grape quality can be altered by diseases, which are of either fungal, bacterial or viral origin (Pearson & Goheen, 1989). However, not all diseases have direct effects on grape and thus wine quality.

Botrytis, caused by the fungus *Botrytis cinerea*, is among the most significant diseases of wine grapes and is usually identified visually by the percentage of affected (rotting) grapes in the vineyard. Hill *et al.* (2013) tested the feasibility of using NIR and MIR spectroscopy for the quantification of *Botrytis* bunch rot in grapes, producing successful PLS prediction models based on both the MIR and NIR spectral regions. However, the highest predictive ability was observed using first derivative spectra from the MIR region (1,100 to 1,050 cm^{-1}).

Grapevine bunch rot detection has recently been achieved through ATR-FTIR analysis, based on a very narrow spectral area, specifically 1,734 cm^{-1} to 1,722 cm^{-1} (Cornelissen *et al.,* 2023). In this study, functional data analysis (FDA) was employed for the statistical analysis, and the discrimination of samples according to their rot degree was achieved. This method shows good potential, nevertheless there is room for improvement especially for samples showing rot < 40 %.

A variety of different pathogens, including *Aspergillus carbonarius, Penicillium expansum*, and *Botrytis cinerea,* have also been differentiated in infected grape berries *via* ATR-FTIR coupled with chemometrics and machine learning (Schmidtke *et al.,* 2019): *Aspergillus carbonarius* has been identified as the key species responsible for producing ochratoxin A (OTA, a toxic fungal metabolite that is detrimental to human health) in grapes (Paola & Marco, 2015), *Penicillium* has been linked to patulin formation, and bunch rot caused by *Botrytis cinerea* has been associated with a decrease in grape quality. The method developed by Schmidke and colleagues also allowed them to differentiate the grapes affected by *Botrytis* from all *Aspergillus* and *Penicillium* species, thus showing high potential for use in the assessment of the phytosanitary condition of grapes.

Grapevine fleck virus**,** fanleaf virus and leafroll associated virus type 1 + 3 were found to alter the IR spectra of infected vine leave samples, especially at 1,185-1,000 cm^{-1}, within which carbohydrates are assigned (Topala *et al.,* 2017). Fleck virus is considered a mild disease (Mannini & Digiaro, 2017), but fanleaf (Jackson, 2014) and leafroll (Song *et al.,* 2021) affect grape quality more severely.

Hyperspectral imaging and chemometrics are now also used for the detection of grapevine diseases (Gao *et al.,* 2020; Kunduracioglu & Pacal, 2024; Ryckewaert *et al.,* 2023; Zhu *et al.,* 2020). Using these techniques, grapevine leafroll-associated virus 3 has been successfully detected in the leaves of Cabernet-Sauvignon, even during the asymptomatic stages of the disease, with wavelengths of 690, 715, 731, 1,409, 1,425 and 1,582 nm contributing the most to its detection (Gao *et al.,* 2020). Chemometric approaches (LDA dimensionality reduction with Random Forest classifiers and spatial distribution with Support Vector Machine classifier) have also been successfully used for the early detection of grape powdery and downy mildew (Knauer *et al.,* 2017; Lacotte *et al.,* 2022).

3. Maturity

Grapes reach physiological maturity when the seeds attain the ability to germinate, which occurs immediately after veraison (Keller, 2010). However, the definition of grape maturity from a winemaking perspective is a rather more complex task due to the temporal disconnect between the ripeness of flavour characteristics and sugar accumulation in the fruit (Zoecklein *et al.,* 2010). For this reason, different indices of maturity have been proposed based on the desired type of wine, such as technological maturity (based on sugar accumulation) and phenolic maturity (Picque *et al.,* 2010).

Technological maturity is routinely used for the selection of harvest date, and it can be defined by sugar accumulation as well as by the grape sugar to acid ratio. Internal maturity parameters, including sugar accumulation and acidity, have been estimated using FT-NIR spectroscopy, contactless in grape berries (Daniels *et al.,* 2019). For this method, maturity signalling attributes were used as the training parameters through which PLS regression models were built, using the region from 12,000 to 4,000 cm^{-1}. The root mean square error of prediction (RMSEP) was low for most parameters, indicating the model's good predictive ability.

Sugar concentration in grapes is frequently estimated by total soluble solids (TSS) analysis. Since grape sugars are the substrate for the subsequent fermentation, their concentration will be reflected in the wine's final ethanol level, which is very important in winemaking. The estimation of the exact sugar concentration is routinely performed three to four weeks before harvest, but it is impossible to obtain representative samples from a vineyard. A handheld NIR spectral analyser was successfully used to estimate the TSS in grapes under field conditions using the region from 6,300 to 4,200 cm^{-1} (Urraca *et al.,* 2016). The calibration for the model required 700 intact berry samples of different total soluble solid concentrations, after which the analysis was performed in a non-destructive manner.

4. Grape sensory profile

Because the sensory properties of grapes indicate their ripening status, the aroma evolution of berries and organoleptic status of seeds have been used for the development of a grape tasting protocol (Winter *et al.,* 2004) for optimum selection of harvest date. As well as ripening, grape sensory characteristics have a direct influence on the wine sensory profile.

The physicochemical properties of the parameters considered important for determining maturity are sugar content (sweetness) and acidity (sourness), which are closely related to the sensory profile of the grapes. Intact grape berries have therefore also been used for sensory data and FT-NIR spectra correlation (Basile *et al.,* 2020). The region used was from 9,400 to 7,500 cm^{-1} but two different models were built for the prediction of sugar (57.32 % correct classification) and acidity (83.04 % correct classification), and each of the model's selected spectral regions was pre-processed differently. There are many difficulties associated with sensorial correlations, and it should be noted that the sensory classification of berries in the study of Basile *et al.* (2020) did not include their astringency or aromatic profiles, which also have an effect on the consumer/taster evaluation of the intensity of acidity and sweetness.

In another study, Ferrer-Gallego *et al.* (2013) were able to predict grape (seeds and skins) taste and texture and visual and olfactory attributes using NIR spectroscopy. These sensory attributes are routinely used for the organoleptic evaluation of seed ripeness degree by trained tasters; however, as a trained panel is not always available throughout maturation, the development of an analytical tool for selecting harvest date is also important. Using the region from 9,100 to 4,000 cm^{-1}, Ferrer-Gallego and colleagues developed calibration models by PLS regression analysis, which showed high potential for the prediction of grape skin and seed sensory attributes. As this study used grapes belonging to the same variety, samples were taken from two different vineyards in two different vintages (2008 and 2009) in order to maximise variability; nonetheless, the authors suggest that other grape varieties and production areas be used to further evaluate the model's predictive ability.

Recent studies have further explored the feasibility of grape sensory data prediction. Gehlken *et al.* (2023) achieved a prediction accuracy with a correlation coefficient of calibration $r_C \geq 0.976$ for the descriptors "fruity", "floral", "green", and "microbiological". However, due to the addition of sodium azide for the preservation of the juice samples, they could not be sensorially evaluated. Instead, sensory evaluation was performed on model wine solutions to which the aromas detected by GC-MS in the homogenised grape mash had been added. It should be noted that tannins, which are known to influence the perception of several compounds that contribute to flavour, were absent from the model solutions.

Along with machine learning, NIR allowed smoke contamination (or smoke taint) to be detected in vine leaves and grape berries (Summerson *et al.,* 2020). Wildfires are an increasing problem worldwide, and the exposure of vineyards to smoke can attribute undesirable and even unpalatable aromas and flavours to affected grapes. Even though smoke aromas from wildfires are a taint, the aforementioned study was based on the determination of volatile phenols (smoke aroma compounds), which are usually detected through sensory testing, showing great potential for the development of models to assess these aromas non-destructively. Neural network based on the region from 6,300 to 4,200 cm^{-1} was able to produce models of high accuracy (97.4 %) using intact berries (Summerson *et al.,* 2020).

5. Quality at receival

The possibility of mature but low-quality fruit arriving at the winery cannot be eliminated. For this reason, almost all wineries have a sorting table in order to discard grapes that do not meet the winemaker's standards. Beghi *et al.* (2017) developed a Vis/NIR spectroscopy-based method coupled with PLS-DA for the detection of the phytosanitary status of

the grapes. The spectral range used was 400-1,650 nm and the highest accuracy obtained by the validation set was 94 %. The method is able to detect grapes infected by *Botrytis*, powdery mildew and sour rot, as well as sunburned fruit.

Sorting can also be based on the grape's quality parameters, such as phenolic load and total soluble solids, a task that further accommodates the needs of the winemaker. Xiao *et al.* (2019) used the Vis/NIR spectrum along with PLS-DA for the development of models that correctly classified grapes according to their TSS and phenolic content with an accuracy higher than 77 %. The grapes used for the calibration of the model were of good sanitary health and were collected randomly in order to increase sample variability.

Several IR based techniques enable prediction of quality parameters in intact berries (Chariskou *et al.,* 2022; dos Santos Costa *et al.,* 2019; Wang *et al.,* 2022; Wen *et al.,* 2024; Ye *et al.,* 2022), and based on the new capabilities of many sorting tables as well as the portability of many IR devices (Schaare *et al.,* 2012; Wang *et al.,* 2022), sorting at the winery could be further improved, incorporating more quality parameters such as anthocyanin content which in the case of red wine grapes is very important, but also help discard fruit that does not conform to the variety and the type of cultivation specifications.

6. Grape polyphenol determination

With regard to phenolic maturity, phenols and their concentrations are very important as they have a significant impact on the grape and consequently the wine's organoleptic profile (Ferrer-Gallego *et al.,* 2011). In light of this, NIR spectroscopy was used along with chemometrics to determine the concentration of various classes of polyphenols, such as phenolic acids, anthocyanins, flavan-3-ols, and flavonols. Analyses performed directly on grapes and grape skins using the region from 9,100 to 5,000 cm^{-1} produced the most promising results (Ferrer-Gallego *et al.,* 2011).

The colour of red wines is very important, which is why viticulturists and winemakers aim to stimulate the production or optimize the extraction of anthocyanin, the compound responsible for the red colour of grapes and wines. Anthocyanins, as well as phenols in general, reach a peak around harvest, which may not, however, coincide with the optimum sugar level; therefore, a rapid method that can detect anthocyanin content in grapes would be very useful, especially when deciding the harvest date. Anthocyanins were successfully assessed with the help of hyperspectral imaging on grape berries and a spectral range of 928-1695 nm of the NIR (Chen *et al.,* 2015). Support vector regression led to the development of a predictive model with a coefficient of validation of 0.9414 and a RMSEP of 0.0046. This method could provide a fast alternative for the measurement of anthocyanins during ripening and contribute to the selection of the optimum harvest date, especially for red wine grape varieties.

7. Polyphenol extractability

Polyphenols originate from the skins and seeds of berries and are extracted in the wine during maceration. Their extractability levels in wine are influenced by the maturity level of the grape: when grapes reach maturity, phenolic extractability in skins increases, while in seeds it decreases (Des Gachons & Kennedy, 2003; Hanlin *et al.,* 2010). In winemaking, the extractability of phenols is important as their presence in wines influences their ageing ability and sensory qualities (Baca-Bocanegra *et al.,* 2018). NIR hyperspectral imaging and chemometrics have been found to provide good results for the screening of grape seed total phenolic content, and to also correctly identify samples with low or high extractability levels. The obtained models had a 76.9 % correct classification in a data set with external validation, and the method has the advantages of speed and relatively low analysis costs (Baca-Bocanegra *et al.,* 2018). ATR-FTIR and Raman spectra have recently been linked to phenolic extractability through the amount of polysaccharides and the degree of pectin esterification in grape skin samples (Nogales-Bueno *et al.,* 2017). The basis of selecting polysaccharides and pectins for their analysis was their influence on cell wall degradation. For example, low levels of galactose, mannose and cellulose, and a low degree of pectin methylation (which correlates with high sugar content which in turn coincides with ripening) are connected to higher cell wall degradation, leading to a higher phenol extraction degree. However, it should be noted that this evidence only corresponds to the internal surface of the grape skin (Nogales-Bueno *et al.,* 2017).

WINEMAKING

Winery-related analyses are carried out to monitor fermentation, as well as to ensure grape polyphenols are efficiently extracted from the must or wood phenols and flavour compounds from barrels during ageing. The final goal of all wine analyses is to ensure the finished wine's quality.

1. Alcoholic fermentation

During alcoholic fermentation, yeasts – whether selected or autochthonous – convert sugars to ethanol and CO_2. This is the most critical stage of winemaking, as it can either highlight the sensory identity of the fruit and its quality or downgrade it. Therefore, fermentation is closely monitored *via* both tasting and chemical analyses in order to prevent deviations, such as stuck or sluggish fermentations, and to ensure a high-quality product is obtained. Stuck and sluggish fermentations are mostly the result of inappropriate temperature changes, nutrient deficiencies or undesired yeast imposition; the resulting metabolic products may in turn lead to the undesirable synthesis of compounds that deteriorate quality and lead to spoilage, such as acetic acid (Cavaglia *et al.,* 2020). Critical fermentation parameters that are routinely monitored are temperature, pH, sugars, and titratable acidity (Wang *et al.,* 2014). FT-NIR and FTIR have been found to provide information on sugar

consumption and alcohol determination during fermentation; moreover, when they were combined with electronic nose and tongue, modifications to aroma and taste that take place during fermentation were also revealed (Buratti *et al.,* 2011). Electronic noses and tongues have been developed for quality determination in foods and beverages, and when combined with pattern recognition data they can help discriminate or classify samples (Rodríguez-Méndez *et al.,* 2016). In terms of compound determination, NIR combined with electronic nose has been found to provide a successful PLSR model (R = 0.999, RMSEC 0.206 and RMSEP 0.205) for alcohol prediction in must (Zhang *et al.,* 2012).

Sugar and alcohol content in must are representative of substrate and product concentrations, and thus their evaluation can be an indicator of fermentation status. The use of selected industrial yeast strains ensures high productivity and fermentative efficiency and is generally preferred to using wild yeasts. However, since the latter have been shown to offer diversity in flavour, many winemakers opt for spontaneous fermentations, regardless of associated high risks (dos Santos *et al.,* 2021). In this case, it is necessary to monitor fermentation kinetics in order to avoid problematic fermentations. ATR-MIR spectroscopy had been found to predict the time course of wild fermentations with high accuracy (Cozzolino & Curtin, 2012) ; and is thus a valuable montioring tool. The predictive model was built using PLS discriminant analysis (PLS-DA) and showed a R^2 and standard error of cross validation of 0.94 and 1.29 respectively, while the validation statistics showed a R^2 and standard error of prediction (SEP) of 0.93 and 1.21. The fermentation profile of yeasts can also be screened using FTIR by evaluating their major fermentation products (*i.e.*, alcohol or CO_2) (Nieuwoudt *et al.,* 2006).

2. Malolactic fermentation

As well as alcoholic fermentation in which sugars are converted to ethanol and carbon dioxide, malolactic fermentation (MLF) can also be used in wineries, especially when acidity needs to decrease in order to improve the wine's organoleptic profile. In MLF, the sharp-tasting L-malic acid is converted to the milder L-lactic acid and carbon dioxide. This conversion is performed by lactic acid bacteria (LAB), and it is accompanied by an increase in pH, which most winemakers monitor almost daily, not only to ensure the onset of MLF but also to detect any potential LAB spoilage as early as possible. The onset of MLF has been assessed in model wine using infrared spectroscopy in the near- and mid-regions (Vigentini *et al.,* 2014). These results confirmed the feasibility of using IR spectroscopy as a supporting but not stand-alone tool for both the detection of the start of MLF and the autolysis of LAB.

Detection of the metabolic activity of malolactic bacterial strains in winemaking is important as it can contribute to the selection of strains that impart desirable traits to wine aroma and flavour profile. Both mid- and near- IR spectroscopy have been used successfully to differentiate wines produced with different *Oenococcus oeni* (LAB species linked to MLF in wine) strains with the help of LDA (Cozzolino *et al.,* 2012b). The authors propose a model for the rapid initial clustering of strains that are produced based on the similarity of their metabolomes, and they highlight the importance of speed in such analyses over any variations in the results.

3. Wine phenolic content and antioxidant activity

Phenolic content and antioxidant capacity are routinely analysed as they contribute to the longevity and quality status of the wine, as well as to its positive health effects (German & Walzem, 2000).

Due to the fact that phenols act as antioxidants (Dávalos & Lasunción, 2009), many methods for predicting antioxidant activity are based on the detection of phenolic compounds, thus allowing a correlation with existing assays for antioxidant capacity to be plotted. Rapid screening of phenolic and antioxidant content has been successfully carried out by Silva *et al.* (2014) with the help of FTIR and chemometrics (PLS). The method showed potential for total phenol estimation, but it only provided rough estimations of antioxidant capacities; *i.e.*, the determination coefficients indicated a low correlation between DPPH and FRAP for the models built. Models with higher predictive ability were developed by Grijalva-Verdugo *et al.* (2018) based on DPPH and ABTS assays using Mexican Cabernet-Sauvignon wines (including samples from different vineyards, vintages and wineries). The spectral range selected for the statistical analysis was 1,550 and 824 cm^{-1} (Figure 4) and the coefficient of determination R^2 for validation of DPPH and ABTS were 0.9460 and 0.9396 respectively.

NIR spectroscopy also shows potential for the estimation of antioxidant capacity. Hristova-Avakumova *et al.* (2018) developed a model based on DPPH and ABTS assays using a region of 900-1,700 nm and PLS regression. The wines used for the calibration of the method were those available on the market at the time, and they comprised several different varieties. The coefficients of correlation of validation were 0.97 and 0.94 for DPPH and ABTS respectively. The low number of studies that have estimated antioxidant activity using NIR spectroscopy may be due to the spectral region used for analysis being dominated by -OH bonds from the water in the wine matrix. However, newer studies are working towards the elimination of this problem (Páscoa *et al.,* 2020).

4. Wine sensory profile

Phenolic compounds are also responsible for astringency, one of the most characteristic organoleptic properties of wine. The compounds linked to this sensation are proanthocyanidins, which mainly originate from the grape skin and seeds. The polymerisation degree of procyanidins is correlated with the level of astringency, and has also been linked to wine age, as younger wines tend to have higher mean degree of polymerisation (mDP) (Basalekou *et al.,* 2019b). FTIR has been used to estimate the average degree of polymerisation of procyanidins, with the help of PLS regression analysis by Passos *et al.* (2010). For this study, analyses were performed

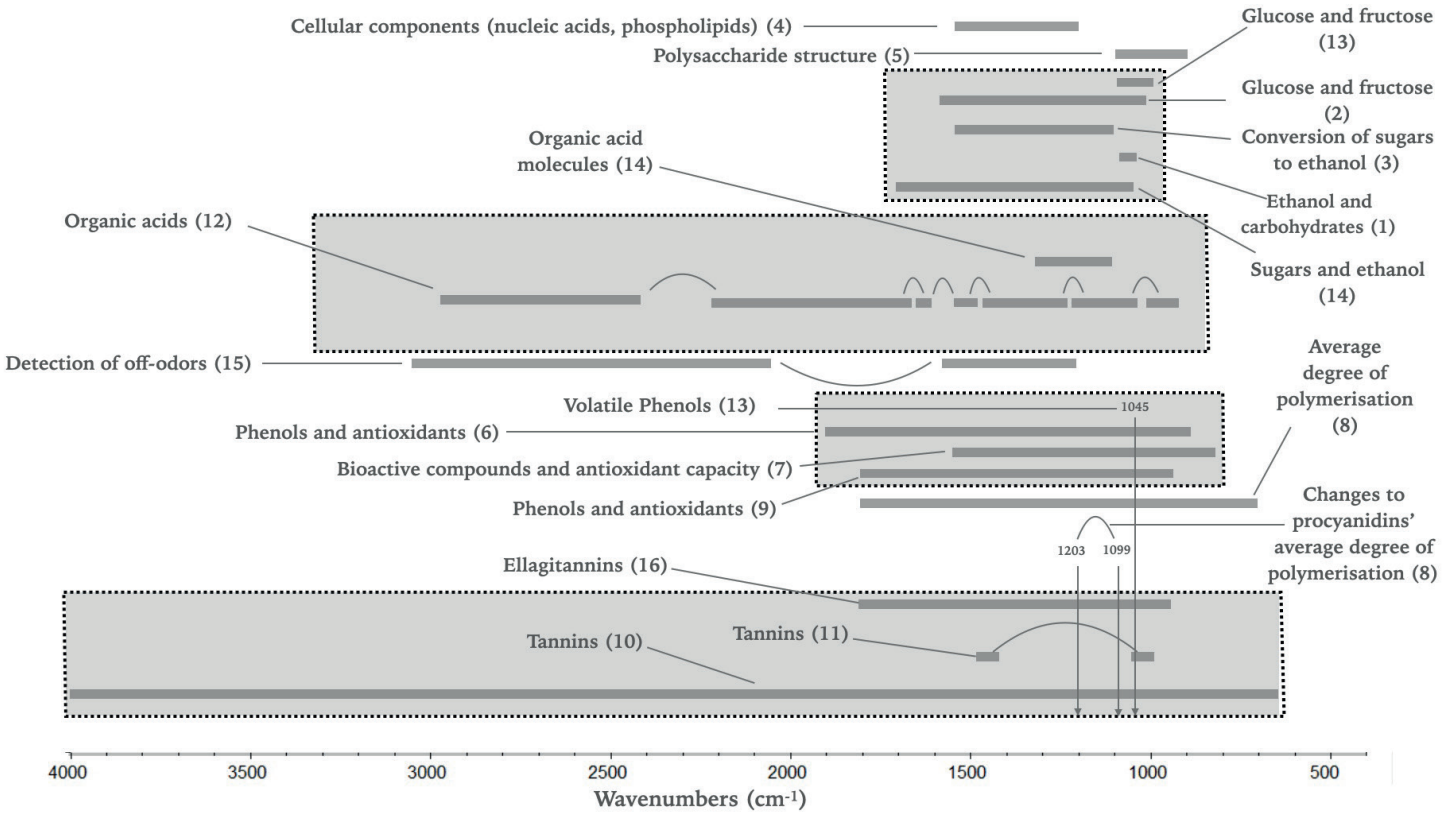


FIGURE 4. Spectral regions selected for FTIR analysis of wine compounds. Horizontal bars determine the spectral limits for each compound; curves signify that bands are used for the analysis of the same compound; dashed rectangles enclose bands that relate to the same groups of compounds.

1: Buratti *et al.* (2011); 2, 3: Cozzolino and Curtin (2012); 4, 5: Cozzolino *et al.* (2012b); 6: Silva *et al.* (2014); 7: Grijalva-Verdugo *et al.* (2018); 8: Passos *et al.* (2010); 9: Simoes Costa *et al.* (2015); 10: Fernandez and Agosin (2007); 11: Jensen *et al.* (2008); 12: Regmi *et al.* (2012); 13: Fudge *et al.* (2012); 14: Cavaglia *et al.* (2020); 15: Teixeira dos Santos *et al.* (2024); 16: Basalekou *et al.* (2019a).

on fractions of procyanidins extracted from seeds, and the methodology was based on the differences in solubility of procyanidins in methanol/chloroform solutions.

As well as mDP correlation with astringency, other indexes have been used, as procyanidins are not the only compounds responsible for this complex sensation. One of the most basic methods for assessing astringency uses the gelatin index (Glories, 1984). Simoes Costa *et al.* (2015) correlated the gelatin index of red and rosé wines with FT-MIR data using PLS regression analysis. However, no meaningful models could be obtained in the case of white wines, for which the gelatin index itself did not provide reproducible results.

Because the perception of astringency is highly subjective, even in sensory evaluations carried out by experienced tasters, there is ongoing interest in the development of an instrumental alternative for its assessment (Simoes Costa *et al.,* 2015). Protein precipitation methods, such as the gelatin index (Glories, 1984), BSA method (Hagerman & Butler, 1978), and the phloroglucinolysis HPLC-based method (Basalekou *et al.,* 2019b) are routinely used for astringency estimation. However, the selection of the most appropriate one will depend on the purpose of the study, as the results obtained by these methods are not correlated (Kallithraka *et al.,* 2011). Calibration models based on protein precipitation, phloroglucinolysis as the reference methods and FT-MIR were built by Fernandez and Agosin (2007), with promising results for tannin concentration estimation. The most accurate (root mean square error of calibration and prediction RMSEC 2.6 % and RMSEP 9.4 % respectively, and r 0.995) prediction was achieved by the calibration models using the full range of the spectrum (4,000-650 cm^{-1}) in its second derivative form and phloroglucinolysis as the reference method. The most important spectral regions for the quantification of tannins were later investigated by Jensen *et al.* (2008), who highlighted two regions (1,485-1,425 cm^{-1} and 1,060-995 cm^{-1}) for the development of the calibration models (Figure 4).

The overall sensory perception of wines is difficult to measure, even with sophisticated instrumentation such as GC-MS, due to the wine's complex nature and the synergistic effects between volatile compounds. For this reason, the most appropriate technique for the assessment of wine aroma is tasting by a trained panel (Basalekou *et al.,* 2023). Based on the evaluation by a trained panel of 13 red and 12 white wines from different

grape varieties, Cayuela *et al.* (2017) were able to predict several sensory attributes, such as 'Flavour intensity', 'Astringency', and 'Colour intensity', by correlating the tasting panel's results with Vis/NIR. The results obtained with PLS showed correlation coefficients (r) of between 0.87 and 0.92 for all three sensory attributes.

5. Taints and spoilage

Most types of spoilage occurring in wine are the result of microbiological/bacterial contaminations. However, wine deterioration can be manifested through a series of different alterations including the production of excessive volatile acidity (*i.e.*, in levels exceeding the limits set by legislation) and the oxidation/deterioration of colour and/or aroma (Basalekou *et al.,* 2023). Increased volatile acidity (VA) is regarded as the most defining spoilage in wines; however, IR determination of acetic acid, the compound responsible for VA, has not been the focus of many studies, probably due to the difficulty in distinguishing it from the multitude of other organic acids present in wine, all of which exhibit strong similarities in their recorded spectra. Regmi *et al.* (2012) examined the feasibility of using FTIR for the determination of acetic acid in wine samples with very good results (85 % acceptable predicted results).

As well as grapes, smoke taint can be detected in wines with the use of MIR spectroscopy. For this purpose, Fudge *et al.* (2012) employed LDA, yet the correct classification for smoke-affected wines was lower than that of grapes (70 % correct classification as opposed to 97.4 % in the study of Summerson *et al.* (2020)).

Even though MLF can be beneficial to red wines by softening the acidity, in some cases it can be unnecessary and even be considered a flaw. In white wines for example, an increase in pH leads to a decrease in the perceived "freshness" of their aroma, hence LAB are considered spoilage bacteria. Recently, unwanted MLF in white wine has been detected through discrimination models using a portable ATR-MIR device. This device was able to assess alcoholic fermentation by predicting density and pH at the same time *via* regression models (Cavaglia *et al.,* 2020).

Even though aroma is rarely evaluated using IR spectroscopy, new research by Teixeira dos Santos *et al.* (2024) has examined the feasibility of detecting several off-odours that deteriorate wine quality, including compounds belonging to different classes such as higher alcohols and volatile fatty acids (the detected compounds were isoamyl alcohol, isobutanol, 1-hexanol, butyric acid, isobutyric acid, decanoic acid, ethyl acetate, furfural, and acetoin). For this reason, a single varietal wine was spiked with various concentrations of each compound and differences in FTIR spectra were detected with the help of PLS. The regression models that were developed showed excellent regression properties, with a coefficient of determination for prediction of R^2 $p > 0.90$. This is one of the first studies capable of detecting sensory taints with FTIR spectroscopy and with such high prediction accuracy.

POST-PRODUCTION

Once fermentation is completed, wines (mostly red) may undergo barrel maturation. In this process, phenols are extracted from the wood into the wine, while contact with oxygen diffused through the pores of wood leads to several types of reactions between compounds. Type of wood used in barrel ageing and several of the characteristics of the finished wine are described in legislative measures, such as PDO conformance, thus authentication is important.

1. Maturation and ageing

Wine ageing can be either oxidative (barrel ageing or maturation) or reductive (bottle ageing), depending on the amount of oxygen transferred into wine (Carpena *et al.,* 2020). During barrel ageing, the largest alteration to the wine profile results from the phenolic compounds – mostly ellagitannins – that are extracted from the wood. The concentration of ellagitannins is rarely estimated in the winery, as their analysis requires the use of sophisticated instruments and complex preparatory steps. FTIR coupled with PLS regression analysis has been found to successfully predict ellagitannin concentrations in wines aged in barrels of different woods (Basalekou *et al.,* 2019a) using the spectral range from 1,820 to 950 cm^{-1} (Figure 4): the model obtained an r of 0.93, while the Root-Mean-Square Error of Prediction, RMSEP, was 1.57.

Besides ellagitannins, several other volatiles are released from wood. Garde-Cerdán *et al.* (2010) were able to determine their concentration using NIR spectroscopy and PLS analysis in aged red wines. Calibration was obtained by correlating oak volatiles and ethylphenols from GC-MS analysis with NIR. The spectral region used was 1,200-10,000 cm^{-1}, but the water absorption regions (4,500-5,500 and 7,000-7,800 cm^{-1}) were omitted. The models that were produced showed a R^2 of 0.87, with the models explaining 86-87 % of the variation in the data.

2. Quality evaluation and authentication of the final product

FTIR has proved to be a valuable tool for authentication purposes (Basalekou *et al.,* 2020), because it allows a unique spectral profile to be produced for each wine sample, which can then be used to produce classes based on a wide set of parameters, such as origin, variety, type of wood used for maturation, length of maturation and vintage (Basalekou *et al.,* 2017a; Basalekou *et al.,* 2017b; Geana *et al.,* 2019).

Several studies have succeeded in the authentication of origin and variety, mostly using the fingerprint region of the spectrum (Figure 1) (Basalekou *et al.,* 2020). For origin authentication, various statistical approaches, such as PCA, SIMCA, and PLS, have been applied, producing models with more than 70 % correct classification; meanwhile, for grape variety authentication, LDA and artificial neural networks, among others, have been used, with equally high correct classification percentages (Basalekou *et al.,* 2016;

Basalekou *et al.,* 2020; Hu *et al.,* 2019; Riovanto *et al.,* 2011). Studies on authentication of type of wood are scarce, but FTIR have been successfully used in a study to produce a 95.4 % authentification for wood type, as well as a complete (100 %) discrimination for contact time by employing the whole spectrum (Basalekou *et al.,* 2015). More recently, NIR spectroscopy has also been employed for the discrimination of wines aged in contact with chips of various sizes and wood, producing encouraging results (> 90 % correct classification with OPLS-DA) (Nardi *et al.,* 2020); vintage authentication was based on the correlation of FTIR spectra (1,830-1,500 cm^{-1}) with the chemical age indexes of two red wines aged for two years. Chemical age indexes i and ii indicate the extent of monomeric anthocyanin displacement by anthocyanin polymers, which are formed as the wine ages (Somers & Evans, 1977). The index i r values were 0.86 and 0.90 for each variety, and the index ii r values were 0.86 and 0.97 for chemical age (Basalekou *et al.,* 2017a).

Despite the limitations of using IR spectroscopy on wine, which are mainly associated with its aqueous nature (registered in the spectrum as a very broad band of around 2900 and 3700 cm^{-1}) (Baca-Bocanegra *et al.,* 2022; Páscoa *et al.,* 2020), few studies have used sample sets consisting of non-dry or sparkling wines. Silva *et al.* (2014) were successful in discriminating dessert wines based on their type of ageing using FTIR-ATR and multivariate analysis, while Culbert *et al.* (2015) used MIR spectroscopy and the same statistical approach for the classification of sparkling wines according to their styles (white, rosé, Prosecco or Moscato) and production methods (transfer and traditional method, carbonation or Charmat).

WINERY BY-PRODUCTS

Wine production leads to the production of a large amount of waste consisting mostly of grape marc obtained after pressing. Grape marc is either used by distilleries for alcohol extraction or disposed of or recycled (Torres-Climent *et al.,* 2015).

FTIR-ATR has been used in grape-derived spirits for quality control purposes. Anjos *et al.* (2016) developed a fast methodology using the regions from 4,000 to 3,600 cm^{-1} and 3,100 to 600 cm^{-1} and PLS regression models for the prediction of alcoholic strength, methanol, acetaldehyde and fusel alcohol content of spirits made from wine and grape marc. The method was deemed acceptable for screening purposes based on a cumulative positive response to parameters, including ratio of performance to deviation (RPD) and standard error of prediction. Recently, NIR has also been successfully used to differentiate spirits based on their production technology (Anjos *et al.,* 2020). The spirits used for the calibration were aged in either wooden barrels (traditional technology group) or stainless steel tanks, in which micro-oxygenation was applied (artificial technology group). The spectral regions deemed the most important for the Principal Component Analysis (PCA) were 6,859 cm^{-1} and from 5,200 cm^{-1} to 4,200 cm^{-1}.

Many wineries use grape marc for feedstuff production, or they transform it through composting to a more stable and environmentally friendly product that can be used as fertiliser. Today, winery and distillery waste is recycled using advanced treatments into added-value products, such as grape seed oil and even cosmetics (Kalli *et al.,* 2018). As waste valorisation techniques are becoming more widespread, particularly with the shift towards sustainable production, there is a growing need for analytical methods for their quality assessment. As a result of the search for environmentally friendly techniques, IR spectroscopy has emerged as an appealing technique. It has recently been used for the discrimination of grape seeds of different origins, and thus of potentially different content of bioactive substances (Lucarini *et al.,* 2020). Distinguishing different grape seeds according to cultivar could facilitate the selection of grapes rich in bioactive substances (such as phenols) for reutilisation in nutraceuticals or food supplements, as well as for the detection of any adulteration to grape seed oils, producing lower quality oils. In this context, the feasibility of using FTIR spectroscopy's for grape seed oil characterisation has also been studied, leading to the clustering of grape seed oils according to their fatty acid profile (Vladimír *et al.,* 2021). Finally, FTIR has also enabled identification of functional groups, such as nitrates and inorganic components, in grape marc compost which are related to the compost's stability and maturity (Torres-Climent *et al.,* 2015).

METHOD ADVANTAGES AND LIMITATIONS

As has been shown here, IR spectroscopy can be used to monitor all the steps of the winemaking procedure, the biggest advantage being its ability to assess samples in various forms and at different stages; *i.e.*, whole grapes, grape skins and seeds, juice and wine, before and after fermentation, for example. Moreover, IR spectroscopy can be used for:

a) determining specific compound concentrations (ellagitannins, anthocyanins, acetic acid, and ethanol)

b) predicting parameters based on more than one factor (maturity, grape, and wine quality)

c) classifying samples based on a wide range of parameters.

A specific statistical approach is applied to each of the above categories; for example, PLS models are mostly used for determination and prediction, while targeted and non-targeted approaches, such as LDA and PCA, are used for classification.

Recent research developments have shown that IR spectroscopy could further be implemented on sorting tables for quality targeted sorting, or potentially as an alternative to ampelography in the discrimination of clones; meanwhile, the assessment of the sensory profile of both grapes and wine shows very promising results as well. These developments are in part also due to the advances being made in chemometrics (neural networks, artificial intelligence) and to the various techniques that have been developed for spectra processing.

The limitations of using IR spectroscopy during winemaking are mostly associated with data handling issues, the effectiveness of selecting appropriate samples and vintage, and the influence of variety and geographical origin on the efficiency of the models produced.

IR spectroscopy is a spectral technique, which means that a vast amount of data drawn from each spectrum for processing and statistical analysis. Handling large amount of data is associated with many limitations and drawbacks, from the difficulty of many statistical software in handling such large datasets to the risk of overfitting when developing a predictive model. To avoid such data handling problems, spectroscopy-based software has been developed, and overfitting can be managed by ensuring the number of samples is larger than the number of variables. Spectra preprocessing, such as smoothing and derivatisation, can also be used to optimise the results of statistical analysis and reveal spectral differences; however, in some cases (*e.g.*, in leaf samples), they should be used cautiously to avoid losing high frequency information (Kokalj *et al.,* 2011).

When employing IR spectroscopy for the development of models to either predict compound concentrations or to assign samples to groups based on specific parameters, assigning spectra to specific compounds, rather than to types of bonds, is not possible. This inability, which in essence is the very nature of IR spectroscopy, is its biggest limitation when focusing on winemaking. For example, as was shown previously (Figure 2), models for organic acids could be successfully developed using spectra regions outside those of functional groups related to organic acids in wine, even those regarded as noise. Using assigned regions is usually expected to result in models that perform better, but this is seldom the case. Indeed, given that fluctuations can appear throughout the IR spectrum, most statistical techniques cover the whole range of the spectrum, and the differences are revealed as an unsupervised effect of the statistical analysis; for example, spectra that lead to the most accurate discrimination on a set parameter. While this may provide good statistical outcomes, it is known that correlation does not imply causation. To better illustrate this fact, in an experiment carried out by Anjos *et al.* (2020), in which NIR and PCA were successfully used to separate samples aged in chestnut and oak barrels among others, the most important spectra region for differentiation was found to be around 5176 cm^{-1}, to which water and ethanol O-H overtones are assigned. This observation, along with the fact that the higher porosity of chestnut can lead to increased ethanol evaporation, raises the question of whether ethanol alone was the cause of the separation. These types of issues underline the needs for extensive knowledge on the actual winemaking procedure in order to successfully exploit IR spectroscopy results. Indeed, in the study of Anjos *et al.* (2020) ethanol was analysed and the issue of higher porosity addressed.

Vintage, variety, and geographical origin have been found to highly affect the development of predictive models, which can only be counteracted by incorporating a large number of samples into the dataset in order to enhance its variability. This highlights the importance of selecting the most suitable samples for successful calibration development, a task overlooked in many studies and which involves selecting samples with similar qualities to those of interest for analysis. As has been seen throughout this review, samples with different parameters can be considered essential or undesirable depending on the expected outcome: samples from different varieties can be incorporated into a sample set to increase variability (as in, for example, the study of Cayuela *et al.* (2017)) or omitted from a sample set to increase accuracy (as in, for example, the study of Teixeira dos Santos *et al.* (2024)). In many cases, using a low variability sample set to increase prediction efficiency as well as the whole spectrum or wide spectral regions for classification or discrimination reasons may again increase the possibility of incorporating second degree correlations; *i.e.*, correlations not occurring through direct cause and effect. For example, when developing a model for colour intensity using one variety, the incorporation of ethanol peaks from the spectrum can lead to successful classifications, as an increase in ethanol content indicates an increase in level of maturity, which in turn indicates increased anthocyanin content and hence colour enhancement. Thus, the constructed model might be successful, but it will be difficult to use on a different variety with anthocyanin potential values lower or higher than those of the training set, or on the same variety when maceration has been extended during winemaking. It should also be noted that models are not always validated or tested to verify their outcomes.

The need for large sample sets has also been observed in already validated models, such as in commercially-produced and IR-based wine analysers. Despite being sold with a ready-to-use calibration set, these analysers need to be adjusted by measuring 10 or 20 samples that have characteristics representative of the samples to be analysed. The reason for this is that regressions are improved when restricted to a single growing region (Picque *et al.,* 2010). Thus, it is evident that none of the developed models to date can be broadly used due to the strong influence that origin and variety have on their accuracy, which also highlights the difficulties related to model transferability.

Creating an optimum sample set would require samples to be taken from all around the vine-growing world or intra-laboratory data sharing, both of which are currently not feasible. Therefore, most new methods for predicting wine parameters through IR spectroscopy have to constantly be reassessed by incorporating sample datasets from different grape varieties or geographical origins to produce new predictive models. The introduction of Neural Networks for the statistical analysis of spectra is very promising in this case, as the developed models can constantly be updated with more data – and hence improve predictive ability – rather than using new samples for the development of yet another predictive model.

The success of IR-based predictions is not only influenced by the ability of the IR spectroscopy itself but also by the group of compounds or analytical technique selected for

correlation purposes. For example, while quality cannot be assessed by carrying out a single analysis, quality prediction is feasible, even though the specific compounds responsible for classifications cannot be identified, but are rather associated with the spectral areas considered to be important for the statistical analysis. Indeed, classifications are almost always based on spectral regions rather than on single peaks. Moreover, even though specific spectral regions are designated to specific functional groups, as shown in Figures 2 and 4, there is great flexibility in spectra selection when developing a model. For example, models based on tannins may be developed using either parts of the spectrum or even the whole spectrum; the final decision made either a priori by the user, or can be revealed after the model is developed successfully, as the regions most useful in producing the most accurate model by the statistical program itself. In wine samples, selection of broad regions is common, partly due to the presence of water and alcohol absorptions which, being dominant, interfere with the determination of other compounds. The similarities of the spectra recorded from different wines (Figure 1) as well as the broad bands observed in large parts of the spectrum highlight the difficulty of assigning bands to specific functional groups.

It is interesting to note that currently most studies employing IR spectroscopy for discrimination or prediction purposes are limited to assessing the feasibility of this use, and the models that are produced do not lead to the development of repeatable methods, as in the case of GC or HPLC, for example. Different wine styles, such as sparkling, rosé or sweet wines, are also rarely assessed, even though they are of analytical interest.

It is evident that the development of a holistic approach in the future is possible, but some guidelines should be followed. First, sample selection should take into account all the potential outcomes of the analysis, meaning that the samples should be from different varieties, geographical origins, vintages and winemaking techniques. Subsets of samples can be used to increase the accuracy of specific or targeted outcomes. Moreover, samples should be in the appropriate state for each analysis; for example, grape – and not wine – samples are more appropriate for the development of models to detect grape bunch rot. As can be seen in Table 1, analyses may be performed on samples in various states (whole grape, must, wine, etc.) and following various preparatory steps (liquid, lyophilised, etc.) in order to facilitate the analytical procedure and lead to more accurate results. Sample preparation is determined by the type of parameter to be assessed. For example, lyophilisation, which lowers the noise in spectra that is caused by signals for water and ethanol, can be employed for sugar content determination. However, it is not suitable for the determination of alcoholic strength due to alterations caused to the sample by the process itself (Páscoa *et al.,* 2020). Finally, applying appropriate statistical analyses will ensure that models can be reassessed and recalibrated so that new samples can be incorporated and to obtain more accurate results. Future studies should focus on the development of multiparametric prediction models to produce a holistic representation of the status of a wine, as well as on developing models that correlate data obtained from grape analysis with the expected wine quality, while ensuring model repeatability by producing standardised calibration protocols. Speedy analyses carried out using IR spectroscopy could also further contribute to the real-time monitoring of the winemaking procedure.

CONCLUSION

IR spectroscopy-based techniques cover almost all wine related analyses, from grape quality monitoring in the vineyard to the assessment of winery by-products. All analyses are based on predictive models built with the help of chemometrics or machine learning techniques and are used to a) produce quantitative results; *e.g.*, for the determination of alcohol, b) monitor the evolution of a chemical compound or process; *e.g.*, alcoholic fermentation, and c) classify samples according to a set parameter; *e.g.*, grape geographical origin. Recent predictive models can be incorporated into already set models, while analyses require few, if any, preparatory steps. The integration of all grape- and wine-related analyses could provide a fast and efficient tool for the holistic monitoring of all winemaking processes in an accurate and environmentally friendly way.

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