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## Near-infrared spectroscopy in process control and quality management of fruits and wine

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### Summary

Recently, rapid quality assessment of food is an increasingly important topic. The rising demand of consumers for high quality products generates a need to establish fast and suitable analytical methods. Near-infrared (NIR) spectroscopy has turned out to be a time-saving, cheap, easy-to-use and environmentally friendly technique, which can be applied for the determination of manifold quality attributes in various kinds of food matrices. This article gives overview of the basic principles of near-infrared measurements and describes the immense field of applications, with the main focus on fruits, grapes and wine and the evaluation of wine aroma.

**Keywords:** near-infrared spectroscopy, NIR, process control, quality management, fruit analysis, grape and wine analysis, wine aroma

### Introduction

The safety and accurate quality assessment of food is becoming increasingly important in the last decades. Various affairs in food safety and quality (e.g. BSE, horse meat in ready meals, Fipronil in eggs) (EUROPEAN FOOD SAFETY AUTHORITY; WORLD HEALTH ORGANIZATION) trigger development and continuous improvement of control systems for food safety and food quality with consumer protection as a main goal. A set of methods has been evolved in the last decades including improved classical wet-lab methods or quick methods.

Most classical wet-lab methods give precise and accurate results, but assets and drawbacks may come along. High-performance liquid chromatography (HPLC) or gas chromatography (GC), often coupled with mass spectrometry (MS), require experienced users, expensive technical equipment and ultrapure, high priced chemicals, which additionally hold the risk of harming the user's health and/or may affect the environment if not used adequately. Another main shortcoming is the time requirement for those methods, which may take several hours or even days to produce results.

NIR spectroscopy increasingly gains attention, because it is easy to use, cheap, provides results quickly and direct implementation in production processes is possible. Thus, the delay of time caused by sampling, analysis and evaluation can be avoided, so immediate intervention in case of irregularities is possible, which reduces the waste of resources and economic losses. Furthermore, the consumer's awareness for quality characteristics of food (presence/absence of various ingredients, origin of the product, cultivation technique or manufacturing process) is growing. The use of NIR spectroscopy enables continuous monitoring of these attributes to meet consumer's expectations and prevent food fraud.

Development of instrumentation and industrial applications of NIR spectroscopy began to increase in the second half of the 20<sup>th</sup> century. First applications to agricultural products were done in 1964 by Norris who recognized the potential of this technique already at the

early stages of development (SIESLER, 2002). Since then, the field of application has expanded (> 700,000 results for NIR analysis of food, Google Scholar, July 2020) just as the diversity of instrumentation, for instance on-line measurements and portable devices (ALEIXANDRE-TUDO et al., 2019; AMUAH et al., 2019; FERNÁNDEZ-NOVALES et al., 2019; BEĆ et al., 2020).

The objective of this article is (i) to review the basic principles of near-infrared measurements and (ii) to give a detailed overview of applications with the main focus on fruit, grape and wine quality control and the option to evaluate wine aroma by the use of NIR spectroscopy.

### Basic principles of near-infrared measurements

Near-infrared radiation was discovered by Friedrich Wilhelm Herschel in the year 1800 (HERSCHEL, 1800) and covers the range between mid-infrared and visible light in the electromagnetic spectrum (780 to 2500 nm). When near-infrared radiation hits a sample, the radiation is absorbed, transmitted or reflected, which in each of the three cases depends on the chemical composition and the physical properties of the sample (NICOLAÏ et al., 2007).

The near-infrared spectrum is dominated by overtone and combination bands of CH, OH and NH functionalities and, in case of moist samples, water, which shows two very strong and broad absorption bands in the near-infrared region (SIESLER, 2002; BURNS and CIURCZAK, 2008; BEĆ and HUCK, 2019). The absorption bands often overlap, which results in very low structural selectivity and impedes the interpretation of spectra and especially qualitative evaluation (NÆS et al., 2004). For this reason, it is necessary to use multivariate statistical techniques (often called chemometrics) to extract the information linked directly to the desired compounds for the development of calibration models. Additionally, irrelevant information has to be suppressed in the spectra, which can be achieved by various preprocessing techniques (NICOLAÏ et al., 2007). Even within the same matrix, the use of different preprocessing techniques can result in varying effects on the resulting calibration models (PURWANTO et al., 2015; KHODABAKHSHIAN et al., 2016; XU et al., 2017) just as the use of different calibration techniques (GIOVENZANA et al., 2015; ALTIERI et al., 2017; MALEGORI et al., 2017). The validation of calibration models is essential to assure their prediction accuracy and can either be performed internally (cross-validation) or with an independent set of samples. Statistic values, which are often used to describe the accuracy of a model, are the root mean square error (RMSE), the correlation coefficient ( $r$ ) or the multiple correlation coefficient ( $R^2$ ) (NÆS et al., 2004).

### Applications of near-infrared spectroscopy

#### *Applications in process control and quality management of fruit and wine industry*

For the successful application of NIR spectroscopy, a number of conditions has to be fulfilled. First, the compound or property has to have an influence on the NIR spectrum. In case of such an influence

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mostly a relationship exists between intensity of absorption bands and concentrations. Relationships can also be indirect, when a compound or property is correlated with another one, which is directly related to the spectrum. The samples for building the model must be selected according to the concentration range of the examined compound and must cover all sources of variability, *e.g.* different seasons or cultivars. Furthermore, the sources of error have to be identified to evaluate and to improve the precision of the model. Finally, the validity over time needs to be given by regular maintenance (MACHO and LARRECHI, 2002). Qualitative analysis is based on grouping samples according to selected properties and is mainly used for identification purposes and quality judgement. Classification by NIR spectroscopy can be more precise than by mid-infrared (MIR) spectroscopy, but appropriate mathematical operations are needed for every model to minimize misclassifications. For quantitative analysis, Lambert-Beer's law is applied, which describes a linear relationship between concentration and absorbance at a given wavelength (SIESLER, 2002). Quantitative analysis often shows very good and reliable performance for compounds present in high amounts, but often decreases for lower concentrations (NICOLAI *et al.*, 2007). In general, the detection limit is about 0.1% (m/m), however, lower values can be reached in some cases, depending on the application and the characteristics of sample and analyte matrix (PASQUINI, 2003).

The main areas of application of NIR spectroscopy are petrochemistry, environmental analysis, the clinical and pharmaceutical sector and the agricultural food sector (BLANCO and VILLARROYA, 2002). The food sector represents a very extensive field of raw materials, intermediates and products. Therefore, the establishment of a uniform procedure for quality assessment would be of great interest for producers and consumers. For instance, grain and grain products belong to the earliest applications of NIR spectroscopy for quality control in the food sector (WILLIAMS *et al.*, 1985). Most applications to grain and grain products such as flour focus on the determination of compounds like protein content, moisture, ash (MANLEY *et al.*, 2013) or dietary fiber content (KAYS *et al.*, 1996; ARCHIBALD and KAYS, 2000; KAYS and BARTON, 2002; ZÖRB *et al.*, 2018), which all represent important quality parameters. Nowadays, for the determination of the protein content, a portable NIR spectrometer can be used (BHANDARI *et al.*, 2004). Many but not all quality characteristics of bread are correlated with the protein content (ZÖRB *et al.*, 2018). Moreover, the suitability of NIR spectroscopy as a determination method for contaminants in grains was shown for ergot bodies in cereals (VERMEULEN *et al.*, 2013).

Other application examples for meat, milk and their derived products as well as for vegetables are described elsewhere (HUANG *et al.*, 2008; QU *et al.*, 2015).

#### **Applications for fruit analysis**

The NIR spectroscopy is a suitable method for the determination of fruit maturity, scheduling of harvesting time, quality assessment of fruit products or the detection of possible contaminations. Tab. 1 gives an overview of current applications of NIR spectroscopy in fruit analysis.

The application of NIR spectroscopy may start at the field for monitoring plant nutrient status, for instance the leaf nitrogen status in pear orchards (WANG *et al.*, 2017). It was also possible to monitor the infestation of two different species of larvae, which can affect apples by NIR spectroscopy (SIEGWART *et al.*, 2015). In affected fruits, two larva species could be differentiated. The method can help to reduce pesticides and might serve for the development of alternative crop protection methods. Even fruits grown at the same site, under similar conditions and harvested similarly can vary in size, color, shape and biochemical composition, which may result in a different inner and

outer quality. To avoid harvesting of fruits, which have not reached criteria for maturity, adequate parameter determination of the best time for harvesting can be achieved quickly and simultaneously by NIR spectroscopy. Some of those measurements in the field were available using special portable devices, *e.g.* for blueberries (RIBERA-FONSECA *et al.*, 2016b).

To protect the post-harvest quality of fruits within a possible storage or transport time, it is important to know the optimum conditions for storage and for transport (KIENZLE *et al.*, 2011). Post-harvest quality has to be controlled constantly depending on fruit characteristics, for example when fruits are climacteric, or in case of differing marketing destination, such as direct or later sale, food processing or export. Besides visible changes like shape or color, changes in biochemical composition can occur, which may also affect consumer's acceptance. Fruits for immediate sale must be free of damages and spoilage. In various studies (LORENTE *et al.*, 2015; FOLCH-FORTUNY *et al.*, 2016; WEDDING *et al.*, 2019), damages and infections were identified by NIR spectroscopy even if barely visible. For example, based on NIR measurements, peaches were classified due to different susceptibility to brown rot (SPADONI *et al.*, 2016). Moreover, the number of days before the decay of peaches could be determined (HUANG *et al.*, 2017). Therefore, recommendations for the best time to eat the fruit can be provided based on the results of NIR measurements. Furthermore, the results can help to optimize storage conditions and to decide on marketing destinations to avoid economic losses and minimize food waste, *e.g.* in case of damages or short shelf-life.

Besides outside appearance, taste plays a key role in the consumer's acceptance. The contents of sugar and acid often determine whether the taste is conceived as pleasant. In addition, the sugar/acid ratio and the BrimA (Brix minus acids) value (JORDAN *et al.*, 2001) can serve as flavor indices (NCAMA *et al.*, 2017). Fruits with high contents of dry matter are often preferred by the consumers, which has been observed in sensory evaluation of mangos (DOS SANTOS NETO *et al.*, 2018) and pears (SERRA *et al.*, 2019) classified by their dry matter content using NIR spectroscopy. Due to the increasing interest in foods with health benefits, the consumers may pay more attention to the content of various compounds, which are claimed to have positive health effects. Therefore, it is favorable to implement rapid and precise methods for non-destructive analysis of those valuable substances. Despite the low concentration of several of these interesting compounds, good or excellent results could be achieved by the use of NIR spectroscopy to monitor the quality of fruits and fruit products. Climate change aspects and environmental pollution may further intensify the consumer's awareness for food derived from sustainable cultivation or of regional origin. Simultaneously, this trend may enhance the risk of food fraud further making it necessary to establish a fast and easy method for supervision. In several studies, *e.g.* origin discrimination of Chinese quince fruits (SHAO *et al.*, 2017), discrimination between different farming systems for strawberries (AMODIO *et al.*, 2017) and pineapples (AMUAH *et al.*, 2019) and discrimination between naturally and artificially ripened mangos (LAKADE *et al.*, 2019) was possible with high accuracies by the use of NIR spectroscopy. Despite these examples, it might further be difficult to determine the origin of production of diverse plant products and one has to be further critical with these reports.

As shown in Tab. 1, NIR spectroscopy is widely used in fruit and fruit product analysis and numerous studies on manifold quality attributes are available. However, in many cases the calibration needs to be further validated by larger sets of samples to stabilize the calibration and improve prediction accuracy. Additionally, a larger variety of properties should be examined to check, in which cases global or separated calibration models are needed for analysis. Specific spectroscopy-based devices, such as the DA-meter, show the potential of NIR technique for the food sector. The DA-meter is a portable spectrometer, which measures the index of absorbance difference ( $I_{AD}$ ).

**Tab. 1:** Applications of NIR spectroscopy in fruit analysis

	<b>Fruit</b>	<b>Parameters/Properties</b>	<b>R<sup>2</sup></b>	<b>Reference</b>	
<b>Fruit Maturity</b>	Acerola <sup>a</sup>	Titrateable acid Ascorbic acid	0.66 – 0.74 0.40 – 0.65	MALEGORI et al., 2017	
	Avocado	Moisture content Dry matter Mesocarp oil content	0.91 – 0.95 0.91 – 0.95 0.67 – 0.71	OLAREWAJU et al., 2016	
	Mango <sup>a</sup>	Total soluble solids Dry matter Titrateable acid Firmness	0.92, 0.87 0.67, 0.84 0.50, - 0.72, -	NASCIMENTO MARQUES et al., 2016; DOS SANTOS NETO et al., 2017	
	Peach <sup>a</sup>	Flesh firmness Water soluble pectin	0.80 0.82	UWADAIRA et al., 2018	
	Pomegranate	Total soluble solids Titrateable acid pH value	0.93 (r) 0.94 (r) 0.84 (r)	KHODABAKHSHIAN et al., 2017b	
	<b>Fruit Quality</b>	Avocado	Bruises Rot	60 – 100 <sup>b</sup> 65 – 84 <sup>b</sup>	WEDDING et al., 2019
		Citrus fruits	Decay lesions Fungal infections	90 – 96 <sup>b</sup> 98 <sup>b</sup>	FOLCH-FORTUNY et al., 2016 LORENTE et al., 2015
		Date Fruit	Total soluble solids Moisture content Colour (b*)	0.97 0.94 0.64	ALHAMDAN and ATIA, 2017
		Kiwifruit	Total soluble solids Flesh firmness	0.58 – 0.83 0.30 – 0.60	LI et al., 2017
		Mango <sup>a</sup>	Dry matter Internal browning	0.75 83.1 <sup>b</sup>	DOS SANTOS NETO et al., 2018 GABRIÉLS et al., 2020
Peach		Days before decay	82.26 <sup>b</sup>	HUANG et al., 2017	
Pear		Maturity stage	97.2 <sup>b</sup>	XU et al., 2017	
Persimmon		Soluble tannins	0.92	CORTÉS et al., 2017	
Strawberry		Storage time	97.4 <sup>b</sup>	SHEN et al., 2018	
<b>Fruit Compounds</b>		Açaí	Anthocyanins	0.74	DE ALMEIDA TEIXEIRA et al., 2015
	Apple (peel/flesh)	Phenolic compounds	0.91/0.84	PISSARD et al., 2018	
	Berry fruits	Phenolic compounds Antioxidant activity	0.98 0.99	GAJDOŠ KLJUSURIĆ et al., 2016	
	Blackberry	Carotenoids Phenolic compounds	0.71 0.65	TOLEDO-MARTÍN et al., 2018	
	Castanhola	Anthocyanins Phenolic compounds	0.80 0.82	CÂMARA COSTA et al., 2017	
	Juçara	Anthocyanins	0.73	DE ALMEIDA TEIXEIRA et al., 2015	
	Jujube	Total sugar Total acid Phenolic compounds Antioxidant activity	0.90 0.98 0.94 0.96	GUO et al., 2016	
	Mango	Soluble solids content Titrateable acid	0.68 0.69	PURWANTO et al., 2015	
	Persimmon	Colour index Firmness Soluble solids content Titrateable acid Soluble tannins	0.99 0.99 0.98 0.98 0.99	ALTIERI et al., 2017	
	Pineapple <sup>a</sup>	Total soluble solids	0.85	AMUAH et al., 2019	
	Pomegranate	Firmness Total soluble solids Titrateable acid pH value	0.94; - 0.94; 0.97 -; 0.93 0.88; 0.94	KHODABAKHSHIAN et al., 2016; KHODABAKHSHIAN et al., 2017a	
	Strawberry	Soluble solids content Firmness	0.83 0.54	MANCINI et al., 2020	

	Watermelon	Total soluble solids	0.71	TAMBURINI et al., 2017
		Lycopene	0.81	
	Wax jambu	$\beta$ -Carotene	0.74	VIEGAS et al., 2016
		Anthocyanins	0.98	
		Phenolic compounds	0.94	
Fruit Product Quality	Apple juice	<i>Z. rouxii</i> contamination	0.99	NIU et al., 2018
	Cashew apple nectar	Total sugar	0.71	CARAMÉS et al., 2017
		Total soluble solids	0.62	
		Titrateable acid	0.75	
		pH value	0.75	
	Guava nectar	Ascorbic acid	0.84	CARAMÉS et al., 2017
		Total sugar	0.82	
		Total soluble solids	0.88	
		Titrateable acid	0.79	
	Guava pulp	pH value	0.76	ALAMAR et al., 2016
		Ascorbic acid	0.86	
		Total sugar	0.72	
		Total soluble solids	0.66	
	Kiwi juice	Titrateable acid	0.79	NIU et al., 2018
		Moisture	0.94	
		Ascorbic acid	0.85	
		<i>Z. rouxii</i> contamination	0.99	
	Strawberry juice	Soluble solids content	0.98	WŁODARSKA et al., 2019
		Phenolic compounds	0.84	
	Strawberry powder	Freshness of fruits	97 <sup>b</sup>	WANG et al., 2019
Various fruit juices	Saccharin adulteration	98 <sup>b</sup>	MABOOD et al., 2018	
Yellow passion fruit pulp	Total sugar	0.90	ALAMAR et al., 2016	
	Total soluble solids	0.54		
	Titrateable acid	0.59		
	pH value	0.61		
	Moisture	0.93		

<sup>a</sup> Portable NIR spectrometer used

<sup>b</sup> Classification rate [%]

The  $I_{AD}$  describes the difference in chlorophyll absorbance at 670 nm and 720 nm and can be used to pre-estimate fruit ripeness (ZIOSI et al., 2008).

### Applications for grape and wine analysis

As well as for other fruits, NIR spectroscopy may be used for monitoring grape quality and the following steps of winemaking. Tab. 2 shows various applications in viticulture, grape quality and wine analysis.

In vineyards, water availability is an important aspect for grapevine growth. Due to climate change, irrigation becomes increasingly important in viticulture to avoid negative effects of water stress for plant vigor and the resulting wine quality. To measure plant water status, NIR spectroscopy can be used directly in the vineyard (GIOVENZANA et al., 2018). NIR spectroscopy was used as an on-the-go spectral measurement to obtain information about the leaf water status of vines (DIAGO et al., 2018). The spectrometer with an operation wavelength from 1100-2100 nm was mounted on an all-terrain vehicle with a motion speed of 5 km/h in the vineyard. To prove the data set from the NIR spectrometer, the stem water potential was used for correlation purpose. This study showed two absorption peaks at about 1450 nm, which corresponded to the first overtone of the symmetric and asymmetric hydroxyl (OH) bond stretching and/or combination bands and around 1940 nm, which can be assigned to the combination of the OH stretching and bending bands of water (DIAGO et al., 2018). Those stretching, bending and combinations are vibrational reactions of the organic groups provoked by the electromagnetic excitation of the NIR spectroscopy. Due to the fact that

leaves have high water content, the prevalence of the OH group absorbance and the corresponding NIR spectra is proven (NICOLAÏ et al., 2007). Other literature shows water-related bands at 975, 1200, 1470, 1930 and 2500 nm (CLEVERS et al., 2010; CAO et al., 2013). The results may contribute to the development of better irrigation scheduling to reach higher irrigation efficiency. In addition to water, the grapevine requires a number of mineral elements to grow, flower and to produce fruit (WHITE, 2015). For instance, the concentration of nitrogen, sulfur and the C/N-ratio in vine leaves and grape berries was determined by NIR spectroscopy (CUQ et al., 2020). However, calibration models with high accuracy were reported for nitrogen ( $R^2 = 0.95$ ) and for the C/N-ratio ( $R^2 = 0.87$ ) in leaves and berries. Based on these results, sustainable fertilization strategies for plant nutrients might be improvable.

Grape maturity estimation is mainly based on the development of sugar and acid concentrations, which both can be determined by NIR spectroscopy as demonstrated in various studies. The sugar concentration decides on the potential alcoholic strength while pH value and titrateable acid help to control wine quality, e.g. red wine color (NOGALES-BUENO et al., 2014). Further maturity parameters (maturity index, various organic acids) were examined by NIR spectroscopy in grape berries at different stages of development (FERNÁNDEZ-NOVALES et al., 2009a; MUSINGARABWI et al., 2016). In addition to these technological ripening parameters such as sugar and acid content, the phenolic maturity of the grapes may play an important role for the resulting wine quality due to its influence on organoleptic properties (FERRER-GALLEGO et al., 2011). The anthocyanin contents were examined in grapes of different ripening times by the use of NIR spectroscopy. Although the contents could be determined re-

liably, a separation for the different ripening times only based on the anthocyanin content was not possible, probably due to different varieties examined (HERNÁNDEZ-HIERRO et al., 2013). Portable devices for infield measurements can save time, because it is still a huge effort to sample enough grapes to achieve representative results for the whole vineyard (FERNÁNDEZ-NOVALES et al., 2019). Total soluble solids, anthocyanins and total polyphenols were examined using a device mounted on an all-terrain-vehicle (FERNÁNDEZ-NOVALES et al., 2019). The results show that the method has great potential for mapping the grape composition in the vineyard and harvest scheduling based on these results.

Besides the technological and phenolic maturity, the phytosanitary status of the grapes is of particular importance for the quality of the resulting wine. One of the most common grape diseases is grape rot caused by *Botrytis cinerea* which negatively affects taste and color of the resulting wine (MORALES-VALLE et al., 2011) (except of “noble rot”) and can also affect food safety (SERRA et al., 2005). Both in the vineyard and at delivery at the winery the phytosanitary status of the grapes is estimated visually, which makes the results subjective. NIR spectroscopy was shown to be suitable to quantify *Botrytis* bunch rot, although further calibration is needed (HILL et al., 2014). Direct application of NIR technology in the vineyard would be advantageous, such as a device mounted on a grape harvester for sorting purposes. A real-time analysis of crushed grapes upon delivery at wineries was executed for the determination of ten different parameters (POREP et al., 2015a). The prediction accuracy of a global calibration model was insufficient for quantitative purposes ( $0.2 < R^2 < 0.7$ ), but could be improved by the development of separate calibration models for different grape colors, vintages and wineries. Commonly, glycerol, gluconic acid and acetic acid contents are used to receive information about the phytosanitary status of the grape (STURM, 2009). Ergosterol, a sterol occurring in fungi but not in plant or animal tissue, was determined in grape mashes to prove the suitability of NIR spectroscopy for the detection of grape rot (POREP et al., 2014). Good results were achieved ( $R^2 = 0.841$  for cross-validation), which allow at least a semi-quantitative determination. In-line determination under industrial conditions confirmed the results (POREP et al., 2015b). A real-time objective method for wineries may further improve wine quality and safety and moreover enables fair pricing of delivered grapes due to their phytosanitary status.

Wine fermentation is a very complex process, which requires detailed knowledge about the chemical composition of the fermenting mixture. For a non-viscous fermentation process, the content of yeast assimilable nitrogen plays an important role in avoiding sluggish or stuck fermentations (GARDNER et al., 2002). The grape must or mash undergoes many changes during fermentation, e.g. degradation of sugar and formation of ethanol. NIR spectroscopy can be used in white grape must to pre-estimate the potential alcoholic strength and the wine quality due to the contents of sugar and acid (WU et al., 2010). Time-related changes in the fermentation process can be monitored, which enables to classify different fermentation stages (COZZOLINO et al., 2006a) and to predict the stage of fermentation due to the concentration of different compounds such as sugars, alcohols and secondary metabolites (DI EGIDIO et al., 2010). The whole fermentation process can be monitored and critical points can be identified (BURATTI et al., 2011), also regarding further treatment of the wine, such as the calcium content in must and ground wine for sparkling wine production (VÉSTIA et al., 2019). During wine production some by-products remain, such as grape pomace, which is rich in phenolic compounds (KAMMERER et al., 2004). NIR spectroscopy can be used to easily determine its content, so grape pomace may be used as a natural source for extracting phenolic compounds for further use i.e. in bioeconomy instead of disposing of it directly (PÁSCOA et al., 2015).

For the resulting wines, the chemical composition can be examined

similarly. In an extensive study 15 parameters in red, white and rosé wines of different ages and from different origins were determined (URBANO-CUADRADO et al., 2004). With the intention to facilitate the quality evaluation of wines, different types of wines were measured in their bottles (COZZOLINO et al., 2007). Even though no exact quantitative evaluation was possible, however, the technique is suitable for qualitative evaluation and screening. An important aspect for the control of wine quality is the verification of the geographic origin, which is closely linked to climate, fertilization and soil characteristics affecting quality and taste of the wine (FISCHER et al., 1999). By the use of NIR spectroscopy, wines from different countries could be differentiated with higher accuracy than wines from different regions in the same country, which may be caused by more similar growing conditions within the same country (RIOVANTO et al., 2011). The contents of stable isotopes of mineral elements can serve as indicators for authenticity, but cannot be determined by NIR spectroscopy because no specific isotope absorption is present in the NIR spectrum. Indirect estimation might only be possible due to association with organic functional groups (COZZOLINO et al., 2008c). Furthermore, the variety of a wine is an important aspect since it is linked to sensory and chemical characteristics. Grape varieties could successfully be differentiated by NIR spectroscopy (COZZOLINO et al., 2003). Moreover, wines made from a single variety may be distinguished from blends. For the determination of the single varieties in blended wines difficulties may occur for low contents and with an increasing number of varieties in the blend.

Wine aroma and flavor are very complex issues, which are influenced by a large number of aspects, among them the selected yeast strain and bacteria (BOIDO et al., 2009). Different *Oenococcus oeni* strains for malolactic fermentation in red and white wines could be differentiated by NIR spectroscopy (COZZOLINO et al., 2012). Depending on the bacteria strain, classification rates up to 100% could be obtained. This way, potentially useful commercial wine strains can be identified, which cause different aroma and flavor profiles.

In grape and wine analysis, NIR spectroscopy is widely used with promising results. Main compounds like ethanol or sugar content can be determined with very high accuracy. For components being present in lower or trace amounts, such as polyphenolic compounds, it is difficult to obtain exact results, because their concentration is probably too small to affect the NIR spectrum significantly. Indirect determination is possible with good results due to correlation with compounds in higher concentration, but model robustness might be low for different batches (NICOLAÏ et al., 2007). Problems may also occur due to interferences (MARTELO-VIDAL and VÁZQUEZ, 2014b, 2015). Furthermore, differentiation between various attributes showed difficulties in some cases with NIR spectroscopy giving only medium results.

#### **Applications in the evaluation of wine aroma**

The decision to buy a wine is based on outer influences, e.g. design of the bottle, name, variety, marketing or recommendations. For the motivation to buy the same wine again, the most important aspect is the taste and the aroma. The personal impression always remains subjective, although individual wines are closely linked to certain taste and flavor attributes depending on different characteristics like grape variety or wine style (CAYUELA et al., 2017). The large number of compounds contributing to wine aroma and their low concentrations require very complex analyses. The most current method for the analysis of aroma compounds is gas-chromatography, often coupled with mass spectrometry as a detector (GC-MS). This way, many different classes of compounds can be analyzed precisely even if they only occur in trace amounts.

Tab. 3 gives an overview of the applications in grape and wine aroma evaluation using NIR spectroscopy. To obtain an objective opinion on

**Tab. 2:** Applications of NIR spectroscopy in grape and wine analysis

	Parameters	R <sup>2</sup>	Reference
Grape Parameters For Determining Maturity	Soluble solids content <sup>a</sup>	0.94	HERRERA et al., 2003
	Reducing sugar content	0.98	FERNÁNDEZ-NOVALES et al., 2009b
	Total soluble solids <sup>a</sup>	0.91	URRACA et al., 2016
	Titrateable acid <sup>a</sup>	0.86	CHAUCHARD et al., 2004
	Soluble solids content <sup>a</sup> (berries/bunches)	0.66/0.65	GIOVENZANA et al., 2015
	Titrateable acid <sup>a</sup>	0.85	
	Sugar concentration	0.99	NOGALES-BUENO et al., 2014
	Titrateable acid	0.98	
	pH value	0.94	
	Total phenolic content	0.89	
	Soluble solids content <sup>a</sup>	0.92	RIBERA-FONSECA et al., 2016a
	Titrateable acid <sup>a</sup>	0.87	
	Firmness <sup>a</sup>	0.89	
	Total anthocyanins <sup>a</sup>	0.94	
	Monomeric anthocyanins <sup>a</sup>	0.68 – 0.96	
	Dry matter	0.88	COZZOLINO et al., 2008b
	Condensed tannins	0.81	
	Total anthocyanins	0.90	JANIK et al., 2007
	Total phenolic content (grapes/grape skins)	0.98/0.98	FERRER-GALLEGO et al., 2011
	Flavanols (grapes/grape skins)	0.93/0.99	
	Flavanols (grapes/grape skins)	0.97/0.99	
	Phenolic acids (grapes/grape skins)	0.75/0.94	
	Anthocyanins (grapes/grape skins)	0.95/0.97	
	Total anthocyanins	0.86	HERNÁNDEZ-HIERRO et al., 2013
	Non-acylated anthocyanins	0.86	
	Total phenolic content (grape seeds)	0.53 – 0.78	ROLLE et al., 2012
	Extractability	0.50	
	Extractable total phenolic content	0.82	NOGALES-BUENO et al., 2015
	Extractable flavanols	0.82	
	Extractable anthocyanins	0.79	
Total and individual anthocyanins	0.35 – 0.90	DIAGO et al., 2016	
MCP Tannins	0.67 – 0.83	ALEXANDRE-TUDO et al., 2019	
Anthocyanins	0.50 – 0.93		
Total phenols	0.61 – 0.90		
Colour density	0.59 – 0.94		
Wine Fermentation	Soluble solids content (grape juice)	0.98	WU et al., 2010
	pH value (grape juice)	0.95	
	Total yeast assimilable nitrogen	0.96	PETROVIC et al., 2020
	Free amino nitrogen	0.91	
	Ammonia	0.88	
	Volumic mass	0.99	FERNÁNDEZ-NOVALES et al., 2008
	Reducing sugars	0.99	
	Volumic mass	0.94	FERNÁNDEZ-NOVALES et al., 2011b
	Total polyphenol index	0.98	
	Colour intensity	0.98	
	Volumic mass	0.98	FERNÁNDEZ-NOVALES et al., 2011a
	Malvidin-3-glucoside	0.81 – 0.94	COZZOLINO et al., 2004
	Pigmented polymers	0.82 – 0.94	
	Tannins	0.70 – 0.90	
	Total phenolic content (grape pomace, raw/milled)	0.93/0.96	PÁSCOA et al., 2015
Total antioxidant capacity (grape pomace, raw/milled)	0.91/0.97		
Wine Compounds	Ethanol	0.67	COZZOLINO et al., 2007
	pH value	0.50	
	Free SO <sub>2</sub>	0.83	
	Total SO <sub>2</sub>	0.70	
	Polyphenolic compounds	0.41 – 1	MARTELO-VIDAL and VÁZQUEZ, 2014a

Sodium	0.92; 0.77	SAUVAGE et al., 2002
Potassium	0.89; 0.89	COZZOLINO et al., 2008c
Magnesium	0.92; 0.73	
Calcium	0.91; 0.90	
Phosphorus	-; 0.79	
Sulfur	-; 0.70	
Iron	-; 0.86	
Manganese	-; 0.78	
Boron	-; 0.81	
Grape variety	100/96 <sup>b</sup>	COZZOLINO et al., 2003
Geographic origin	93.5 <sup>b</sup>	LIU et al., 2006
	78 <sup>b</sup>	LIU et al., 2008
	76 <sup>b</sup>	COZZOLINO et al., 2011
	60 <sup>b</sup>	RIOVANTO et al., 2011
	60.4 <sup>b</sup>	TEIXEIRA DOS SANTOS et al., 2017
	95/87/84 <sup>b</sup>	HU et al., 2019

<sup>a</sup> Portable NIR spectrometer used

<sup>b</sup> Classification rate [%]

sensory characteristics of wines, evaluation needs to be carried out by a sensory panel consisting of specially trained experts. Sensory evaluations are time-consuming and despite the skills of the judging persons the results remain subjective. NIR spectroscopy has been tested as an alternative method. It could be shown that some relationship exists between the spectra and the sensory properties of a wine, even without knowledge about chemical compounds (COZZOLINO et al., 2005). The results also showed that NIR spectroscopy is a suitable method in addition to sensory evaluation (CAYUELA et al., 2017). However, total substitution of sensory evaluation by instrumental analysis is not possible because the concentration of aroma compounds does not necessarily correlate with their contribution to the overall aroma, a factor, which is not sensed by instruments. Apart from sensory characteristics, classes or single aroma compounds in wines can be analyzed by NIR spectroscopy. The detection and determination of desired aroma compounds as well as of those causing off-flavors have been examined. Despite their low concentrations, high prediction accuracies were reached in various studies (CYNKAR et al., 2007; SMYTH et al., 2008; GENISHEVA et al., 2018; FUENTES et al., 2019). In some cases, the prediction accuracy of the calibration models was good to excellent while in the vali-

dation it was considerably worse, but were improved by the separation of the sample set (LORENZO et al., 2009; GARDE-CERDÁN et al., 2010; GARDE-CERDÁN et al., 2012). Nonetheless, NIR spectroscopy showed the potential to be used at least as a screening method. Most of the evaluations in Tab. 3 have been done for sensory attributes or aroma compounds in wine. Few examinations were done regarding the aroma of grapes intended for winemaking (CYNKAR et al., 2007; BOIDO et al., 2013), which has a great influence on the aroma of the resulting wine and therefore represents an important quality prediction parameter. Many volatile compounds, which contribute to the aroma of the resulting wine are accumulated in the grapes as non-volatile glycosylated compounds but are released during winemaking and storage (aroma potential) (WIRTH et al., 2001). An early determination of the aroma potential can be helpful to decide about the best treatment of the grapes during winemaking. Although glycosylated compounds are important, they only represent a part of the grape aroma and its role in the resulting wine aroma. The determination of the whole aroma profile of grapes by NIR spectroscopy would provide a helpful tool to sort grapes before winemaking depending based on their aroma quality. Moreover, all these studies have been carried out under laboratory conditions,

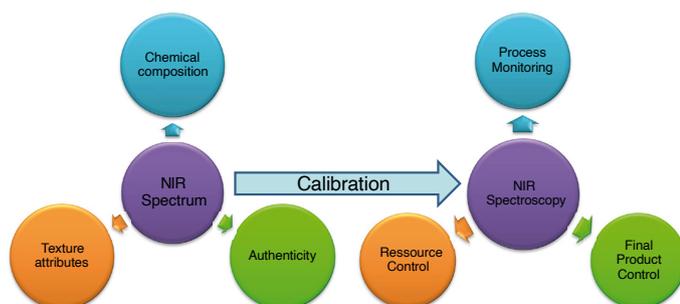
**Tab. 3:** Applications of NIR spectroscopy in the evaluation of grape and wine aroma

Samples	Compounds/Attributes	R <sup>2</sup>	Reference
Chardonnay and Riesling wines	Sensory attributes	0.68 – 0.86 (r)	COZZOLINO et al., 2005
	Overall flavor	0.56 (r)	
	Sweetness	0.60 (r)	
Riesling wines	Sensory attributes	0.38 – 0.89 (r)	COZZOLINO et al., 2006b
Red and white wines	Sensory attributes	0.73 – 0.93 (r)	CAYUELA et al., 2017
Red wines	Wine scores	0.65 (r)	COZZOLINO et al., 2008a
Tannat grapes	Glycosylated compounds	0.27 – 0.82	BOIDO et al., 2013
White grape juice	Glycosylated compounds	0.73 – 0.94	CYNKAR et al., 2007
Riesling wines	Esters	0.74	SMYTH et al., 2008
	Short-chain fatty acids	0.80	
	Monoterpenes	0.90	
White wines	Alcohols / Esters	0.94 – 0.97	GENISHEVA et al., 2018
Aged red wines	Alcohols / Esters / Short chain fatty acids	0.29 – 0.94	LORENZO et al., 2009
Barrel-aged red wines	Oak volatile compounds / Ethylphenols	0.27 – 0.84	GARDE-CERDÁN et al., 2010
Red and white grapes and wines	Guaiaicol glycoconjugates	0.97 (r)	FUENTES et al., 2019
Barrel-aged red wines	Haloanisols / Halophenols	0.22 – 0.99	GARDE-CERDÁN et al., 2012

which may cause a loss of time in practical application due to additional sampling time. The development of an in-line NIR spectroscopy measurement of grape aroma compounds would be a great progress for the evaluation of the aroma quality of grapes directly on arrival at the winery.

### Conclusions

The suitability of NIR spectroscopy has been examined and shown in numerous studies on fruits, grapes, wine, and wine aroma. Miscellaneous compounds and attributes can be obtained from the NIR spectrum in various kinds of matrices. With an adequate calibration, the NIR spectroscopy provides a wide range of applications in process control and quality management (Fig. 1). The calibration represents the most important and the most time-consuming part in establishing NIR spectroscopy as an analytical method.



**Fig. 1:** Field of applications of NIR spectroscopy

On-line determination provides similar results compared to measurements under laboratory conditions (ALEIXANDRE-TUDO et al., 2019), so NIR spectrometers can be integrated directly in the process.

However, the potential of NIR spectroscopy sometimes reaches its limits. For compounds, which are present in small amounts, semi-quantitative determination or screening is possible (POREP et al., 2014; NOGALES-BUENO et al., 2015). Nonetheless, several studies on compounds occurring in small amounts resulted in high prediction accuracy (FERRER-GALLEGO et al., 2011; GENISHEVA et al., 2018). Classification of samples can be improved by the use of MIR spectroscopy or the combination of both techniques (RIOVANTO et al., 2011; TEIXEIRA DOS SANTOS et al., 2017). With the further technical improvement of spectrometers and the development of new chemometric methods, the possibilities of determination by NIR spectroscopy may also be further improved.

In general, NIR spectroscopy provides a great variability of possible applications and an advantageous alternative to traditional analytical methods, however, in some cases its performance is not sufficient for complete substitution, but for additional evaluation.

### Conflict of interest

No potential conflict of interest was reported by the authors.

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