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A Review on the Applications of Portable Near-Infrared Spectrometers in the Agro-Food Industry

Industry has created the need for a costeffective and nondestructive quality-control analysis system. This requirement has increased interest in near-infrared (NIR) spectroscopy, leading to the development and marketing of handheld devices that enable new applications that can be implemented in situ. Portable NIR spectrometers are powerful instruments offering several advantages for nondestructive, online, or in situ analysis: small size, low cost, robustness, simplicity of analysis, sample user interface, portability, and ergonomic design. Several studies of on-site NIR applications are presented: characterization of internal and external parameters of fruits and vegetables: conservation state and fat content of meat and fish: distinguishing among and quality evaluation of beverages and dairy products; protein content of cereals; evaluation of grape ripeness in vineyards; and soil analysis. Chemometrics is an essential part of NIR spectroscopy manipulation because wavelength-dependent scattering effects, instrumental noise, ambient effects, and other sources of variability may complicate the spectra. As a consequence, it is difficult to assign specific absorption bands to specific functional groups. To achieve useful and meaningful results, multivariate statistical techniques (essentially

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tions concerning quality, convenience, diversity, and health. Simultaneously, there is a need to meet health and safety requirements; increasingly demanding environmental legislation; and security, ethics, and sustainable production requirements. The quality of agricultural and food products is classified according to internal and external parameters.¹

spectral preprocessing) are therefore required to extract the information hidden in the spectra. This work reviews the evolution of the use of portable near-infrared spectrometers in the agro-food industry.

involving regression techniques coupled with

Index Headings: Near-infrared spectroscopy; NIR; Portable instruments; Agro-food industry; In situ analysis; Chemometrics.

INTRODUCTION

he agro-food industry has a significant role in the world economy. In the last decades, it has followed this revolution to meet increasing consumer needs and expecta-However, several analytical techniques have been applied to assess those parameters; the invasive, destructive, and time-consuming nature of the reference methods has spurred efforts toward

the development of nondestructive methods such as spectroscopic techniques. Several studies have been published concerning the application of these techniques to the agro-food industry.² Near-infrared (NIR) spectroscopy has received particular attention since the pioneering work of Norris and Hart,³ and the contributions of Williams,4 McClure et al.,5 and Norris et al.6 Several studies emerged from Karl Norris's work, applying NIR spectroscopy to the rapid analysis of the moisture, protein, and fat content of a wide range of agricultural and food products.^{7,8} Early applications of this technique included determinations of dry matter content in onions,9 soluble solids content (SSC) in apples,10 and water content in mushrooms.11 This technique was also used to perform microstructural measurements of stiffness,12 internal damage,13,14 and even sensory attributes.¹⁵ Numerous studies have been published involving NIR spectroscopy and its usefulness in the agro-food industry. ^{2,16–18}

Recently, considerable attention has been given to the miniaturization and portability of spectroscopic devices. 19 The use of portable instruments for infield measurements offers interesting

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TABLE I. Specifications of the most commonly found literature reported portable NIR instruments.^a

Commercial name	Manufacturer	Models available	Spectral range (nm)	Resolution (nm)	Light source	Signal to noise
AgriSpec	ASD	Not applicable	350–2500	3 at 700; 10 at 1400/2100	Halogen	14 500 S/N at 1400 nm
FieldSpec4	ASD	a. FieldSpec4 Standard- Resb. FieldSpec4 Hi-Resc. FieldSpec4 Wide-Resd. FieldSpec Handheld 2	a, b, c, 350–2500 d, 325–1075	a, d, 3 at 700; 10 at 1400/2100 b, 3 at 700; 8 at 1400/2100 c, 3 at 700; 30 at 1400/2100	Halogen	Not specified
LabSpec4	ASD	e. LabSpec4 Standard- Res f. LabSpec4 Hi-Res	350–2500	e, 3 at 700; 10 at 1400/2100 f, 3 at 700; 6 at 1400/2100	Halogen	Vis-NIR 9000:1 at 700 nm SWIR 1 9000:1 at 1400 nm SWIR 2 4000:1 at 2100 nm
AvaSpec	Avantes	Not applicable	200-1100	0.05-20	Not specified	200:1
Luminar 5030	Brimrose	Not applicable	600–1100, 850–1700, 900–1800, 1100–2300	2–10	Not specified	Not specified
microPHAZIR	Thermo Scientific	Not applicable	1600–2400	Not specified	Tungsten light bulb	Not specified
Phazir	Polychromix	g. DTS-Phazir-1016 h. DTS-Phazir-1624	g, 1000–1600 h, 1600–2400	Not specified	Tungsten light bulb	g, 8 nm h, 12 nm
USB	Ocean Optics	USB 4000 VIS-NIR	Grating dependent	~1.5	Tungsten light bulb	300:1 (at full signal)

^a AC/DC, alternating current/direct current; SWIR, short wave infrared; USB universal serial bus.

possibilities by allowing direct measurement of important parameters. These devices have several advantages, including reduced cost, increased safety for the environment and operators, and the improved accuracy of the method by preserving the sample and avoiding its transport. In recent years, several efforts have been made to apply this technique to solid-sample analysis. Salvador Garrigues and Miguel de la Guardia recently summarized studies using portable instruments and their wide use in a vast field of applications.²

This study provides an overview of the more recent applications of portable NIR instruments in the agro-food sector. These applications have been divided into fruits and vegetables, meat and fish, beverages and dairy, cereals and feedstock, soils and manures, and viticulture and olive growing. Descriptions of the applications are provided, highlighting the potential of this method in terms of its versatility.

NEAR-INFRARED SPECTROSCOPY

Near-infrared radiation ranges from 780 to 2500 nm of the electromagnetic spectrum.^{20,21} The measurement of the interaction between this radiation and a sample results in a spectrum characterized by weak absorption bands that are

broad and superimposed.²² The fundamentals of vibrational spectroscopy provide the theory necessary to interpret this characteristic spectrum.²³ The typically observed bands in NIR spectra correspond to bonds containing the hydrogen atom, such as C-H, N-H, O-H, and S-H, that are frequently present in most organic and some inorganic compounds.¹⁷ A NIR spectrum is essentially composed of overtones and combination bands containing useful chemical and even physical information. The literature on NIR spectroscopy and its applications in different fields is extensive and can be found elsewhere.17

Portable Near-Infrared Spectrometers. Industrial applications created the need for a cost-effective and nondestructive quality-control system. This requirement increased the interest in NIR spectroscopy, leading to the transformation of large, stationary analytical instruments into lightweight tools that enabled new applications to be implemented in situ at an industrial level.24 Although these portable NIR spectrometers offer several advantages, such as nondestructive and in situ analyses, their development must consider some critical factors, such as cost, size, weight, power consumption, robustness, safety, userfriendliness, durability, accuracy of measurement, and high performance reliability. Another important characteristic to be taken into account is instrument design. An ergonomic design should make these portable devices handheld, thus enhancing their ease of use. While some devices are sold as closed instruments (and cannot be adapted), others offer the possibility of interchanging measurement accessories so that the same instrument can be used for different sample requirements.²⁵ Several portable NIR spectrometers are currently available in the marketplace, varying in cost and purpose. Table I lists some of the most important specifications of the portable NIR instruments most commonly found in the literature with reported applications in the agrofood industry.

Near-Infrared Spectral Processing. Chemometrics, usually described as the application of mathematics, multivariate statistics, and computer science, ¹⁸ plays a fundamental role in the extraction of all-important relevant information hidden in NIR spectra. Because a NIR spectrum consists of weak and broad absorption bands, a straightforward interpretation is often not possible. Furthermore, there are several other factors that increase the complexity of the spectra: water absorption bands, scattering effects, instrumental noise,

TABLE I. Extended.

Commercial name	Sampling mode	Scanning time (ms)	Communications interface	Power supply	Operating temperature (°C)	Weight (kg)	Size (mm)
AgriSpec	Customizable	100	Ethernet, RJ-45, Wifi	AC/DC, battery (2 h)	0–40	5.4	$127 \times 368 \times 292$
FieldSpec4	Customizable	a, b, c, 100 d, Not specified	a, b, c, Ethernet, Wifi d, USB	` /	0–40	a, b, c, 5.44 d, 1.2	a, b, c, 127 × 368 × 292 d, 90 × 140 × 215
LabSpec4	Customizable	100	Ethernet, Wifi	AC/DC, battery	0–40	5.44	127 × 368 × 292
AvaSpec Luminar 5030	Customizable Diffuse reflectance	1.8 16 000 wavelength/s	USB, RS-232 Ethernet	USB, AC/DC AC/DC	Not specified Not specified	0.716 Not specified	175 × 110 × 44 Not specified
microPHAZIR	Diffuse reflectance		USB	Battery (3 h)	5-50	1.8	$266\times109\times251$
Phazir	Diffuse reflectance	1–2 s	USB	Battery (5-8 h)	5–45	1.7	$254\times292\times152$
USB	Customizable	>5 ms	USB	AC/DC	Not specified	0.190	89.1 × 63.3 × 34.3

sample complexity, and matrix/environmental effects. 16 Therefore, multivariate analysis methods coupled with spectral preprocessing techniques are the fundamentals of chemometrics for the appropriate treatment of analytical information contained in NIR spectra.²⁶ Essentially, spectral information captured with portable instruments is processed using standard chemometric methods that have been thoroughly described in the literature.²⁷ Reducing instrumental noise or background information is usually performed using smoothing techniques. A detrending preprocessing technique is sometimes used to remove the effects of accumulating data sets from a trend, so that only the absolute changes are shown.²⁸ Derivatives are a common method used to eliminate unimportant baseline signals from samples.²⁹ Orthogonal signal correction (OSC) was developed to reduce light-scattering effects, among other general types of interference (not interfering with the correlation with reference values). Path length effects, scattering effects, source or detector variations, and other general instrument sensitivity effects are usually corrected using normalization preprocessing methods, such as standard normal variate (SNV)²⁸ and multiplicative signal correction (MSC).^{30,31} Consequently, preprocessing techniques, have been developed to unlock spectral data and enhance the robustness and predictive ability of the calibration model.²² Chemometric methods most commonly used to process NIR spectral information and build calibrations are available in the literature and are not developed here.^{18,32,33} In terms of their purposes and their algorithms or computational procedures, the most commonly used multivariate analysis methods are listed in Table II. The results presented here use the root mean square error of

TABLE II. Classification of the major qualitative and quantitative multivariate-analysis methods used in NIR spectroscopy applied to the agro-food industry.^{17,a}

Quantitative
Non-linear methods
Linear methods
ANN, non-linear PLS
MLR, PCR, PLS, LS-SVM
Qualitative
Unsupervised methods
Supervised methods
Cluster analysis, ANN (e.g., Kohonen networks), PCA
FDA, KNN, LDA, SIMCA

prediction (RMSEP) or root mean square error of cross-validation (RMSECV) as indicators of NIR-based model accuracy. The equation for root mean square error (RMSE) is

$$RMSE = \sqrt{\frac{\sum_{i=1}^{i=n} (y_i - \hat{y}_i)}{n}}$$
 (1)

where \hat{y}_i is the prediction value of the *i*th observation, y_i is the measured value of the observation, and n is the number of the observations. Equation 1 can be used to compute the root mean square error of calibration (RMSEC), RMSECV, and RMSEP.²⁷

APPLICATIONS IN THE AGRO-FOOD INDUSTRY

In the following sections a full description is given of the applications of portable NIR spectrometers in the agro-food industry including the type of sample and its attributes, and, when available, the spectrometer used, its acquisition mode, and its spectral range (in most studies the visible spectral region was also included). This review considers the application of portable NIR instruments in the agro-food industry independently of the application conditions. It is clear that the great advantage of these systems is the

^a FDA, Fisher discriminant analysis; KNN, k-nearest neighbor; LDA, linear discriminant analysis; LS-SVM, least squares support vector machines; MLR, multiple linear regression; PCA, principal component analysis; PCR, principal component regression; PLS, partial least squares; SIMCA, soft independent modeling of class analogy.

TABLE III. Reported applications of portable NIR instruments for fruit and vegetable analysis.^a

Species	Attributes	Spectrometer, spectral range (nm), acquisition mode	Multivariate analytical methods	Results	Reference
Mandarin	Firmness (N)	Phazir 2400	MPLS	RMSECV = 2.96	
Ivianuarin	MPF (N)	(Polychromix), 1600–	MIFLS	RMSECV = 2.90 $RMSECV = 8.07$	
	Pericarp thickness (mm)	2400, reflectance		RMSECV = 0.57 $RMSECV = 0.53$	
	Juice weight (g)	2400, reflectance		RMSECV = 0.33 $RMSECV = 14.15$	
	Juice content (%)			RMSECV = 14.13 $RMSECV = 5.45$	
	SSC (%)			RMSECV = 0.76 $RMSECV = 0.76$	
	pH			RMSECV = 0.70 $RMSECV = 0.09$	
	TA (% of citric acid)			RMSECV = 0.09 $RMSECV = 0.14$	
	Maturity index			RMSECV = 0.14 $RMSECV = 1.16$	
	Weight (g)			RMSECV = 1.10 $RMSECV = 24.31$	
	Equatorial diameter (mm)			RMSECV = 5.63	
	Axial diameter (mm)			RMSECV = 3.21	
	Color index			RMSECV = 2.62	
Apricot (on tree)	SSC (%)	Phazir (Polychromix),	PLS	RMSEP = 7.4	48
ripriest (on tiee)	Firmness (%)	940–1797, reflectance	1 25	RMSEP = 7.7	10
	TA (%)	3.0 1737, Tellectance		RMSEP = 13.2	
	Color (%)			RMSEP = 11.6	
Tomato	SSC (%)	I.N.A., 690-1700, I.N.A.	PLS	RMSECV < 0.4	49
10111110	Firmness (DI)	111 (11 11) (350 17 00) 111 (11 11	125	RMSECV = 5.9	.,
	Color			RMSECV = 2.26	48 49 50 51 52 53 37
Orange	SSC (°Bx)	I.N.A., 200-1100, I.N.A.	LS-SVR	RMSEP = 0.321	50
Orange	SSC (°Bx)	I.N.A., 350–2500,	PCR, PLS	RMSEP = 0.47	
8-	TA (g malic acid/L)	transmittance	,	RMSEP = 0.25%	
Apple ('Golden	SSC (°Bx)	AvaSpec 2048 (Avantes),	PLS	RMSECV = 6.2%	52
delicious')	TA (g malic acid/L)	450-980, reflectance		RMSECV = 6.6%	
,	Firmness (N)	, , , , , , , , , , , , , , , , , ,		RMSECV = 9.1%	
	Chlorophyll (nmol/cm ²)			RMSECV = 17.2%	
	Ascorbic acid (mg/100 g)			RMSECV = 15.5%	
	Carotenoids (nmol/cm ²)			RMSECV = 10.6%	
	Total phenols (mg catechin/g)			RMSECV = 20.0%	
Apple ('Stark Red	SSC (°Bx)			RMSECV = 6.9%	
Delicious')	TA (g malic acid/L)			RMSECV = 4.2%	
	Firmness (N)			RMSECV = 7.9%	
	Chlorophyll (nmol/cm ²)			RMSECV = 9.4%	
	Ascorbic acid (mg/100 g)			RMSECV = 18.4%	
	Carotenoids (nmol/cm ²)			RMSECV = 7.7%	
	Total phenols (mg catechin /g)			RMSECV = 1.8%	
	Total anthocyanins (mg			RMSECV = 35.3%	
	malvidin/g)				
	Total flavonoids (mg catechin/g)			RMSECV = 5.0%	
	Non-anthocyanic flavonoids (mg			RMSECV = 6.3%	
	catechin/g)				
Apple	Acidity (g H ₂ SO ₄ /L)	I.N.A., 600-1100, I.N.A.	GRNN	RMSEP = 0.0558	53
	Ascorbic acid (mg/100 g)			RMSEP = 4.0431	
Mandarin ('Page')	SSC (°Bx)	I.N.A., 310–1100,	PLS	RMSECV = 0.45	37
	TA (g malic acid/L)	reflectance		RMSECV = 0.09	
Mandarin ('Miho')	SSC (°Bx)			RMSECV = 0.59	
	TA (g malic acid/L)			RMSECV = 0.07	
Nectarine	Weight (g/fruit)	Phazir 2400	MPLS	RMSECV = 31.34	54
	Diameter (cm)	(Polychromix), 1600–		RMSECV = 0.63	
	SSC (%)	2400, reflectance		RMSECV = 0.69	
	Firmness (N)			RMSECV = 13.45	
Pear	SSC (°Bx)	VISNIR USB 4000,	PLS, MLR,	$0.48 < RMSEP < 0.67^{b}$	38
		(Ocean Optics), 800–	LS-SVM		
	GGG (0D.)	950, diffuse reflectance	D	D1607D 007	
Orange	SSC (°Bx)	LabSpec (ASD), 500–	PLS	RMSEP = 0.87	55
	Acidity (g H ₂ SO ₄ /L)	2300, reflectance		RMSEP = 0.13	
	TA (g malic acid/L)			RMSEP = 2.47	
	Maturity index			RMSEP = 1.54	
	Firmness (N)			RMSEP = 1.82	
	Juice volume (mL)			RMSEP = 8.38	
	Fruit weight (g)			RMSEP = 43.51	
	Rind weight (g)			RMSEP = 16.07	
	Fruit color index			RMSEP = 6.48	
	Juice color index			RMSEP = 55.69	

TABLE III. Continued.

Species	Attributes	Spectrometer, spectral range (nm), acquisition mode	Multivariate analytical methods	Results	Reference
	SSC (°Bx) Acidity (g H ₂ SO ₄ /L) TA (g malic acid/L) Maturity index Firmness (N) Juice volume (mL) Fruit weight (g) Rind weight (g)	Luminar 5030 (Brimrose), 1100– 2300, reflectance		RMSEP = 1.12 RMSEP = 0.40 RMSEP = 2.07 RMSEP = 2.57 RMSEP = 1.53 RMSEP = 12.13 RMSEP = 32.63 RMSEP = 14.71	
Plum	SSC (°Bx) Firmness (N) Correct classification according to the variety	Phazir 2400 (Polychromix), 1600– 2400, reflectance	PLS-DA	RMSECV = 1.39 RMSECV =2.76 96.5%	56
Apple	SSC (°Bx)	I.N.A., I.N.A., I.N.A.	LS-SVM	RMSEP = 0.82	57
Orange ('Gannan navel')	SSC (°Bx)	I.N.A., 551–950, I.N.A.	LS-SVM	RMSEP = 0.55	39
Mandarin ('Nanfeng')	SSC (°Bx) TA (g malic acid/L) Ascorbic acid (mg/100 g) Surface color (ΔΕ)	VISNIR USB 4000 (Ocean Optics), 400– 1040, transmittance	SVM, BPNN, PLS	$0.64 < RMSEP < 0.65^{b}$ $RMSEP = 0.09^{b}$ $2.7 < RMSEP < 2.8^{b}$ $0.81 < RMSEP < 0.82^{b}$	40
Apricot ('Bergaroug,' 'Harostar,' 'Kioto') Bergarouge Harostar	SSC (°Bx) TA (g malic acid/L) Firmness (N) Correct classification according to variety	S-2000 (Ocean Optics), 650–1200, reflectance	PLS FDA	5.7 < RMSECV < 9.3%° 7.1 < RMSECV < 17.7%° 6.2 < RMSECV < 24.1%° 86% 97%	58
Kioto, 1st harvest	to variety			96% 92%	
Kioto, 2nd harvest Blueberry	SSC (°Bx) Total anthocyanins (mg malvidin/g) Total flavonoids (mg catechin/g) Total polyphenols (mg catechin/g)	D.N.I., 450–980, reflectance	PLS	92% RMSECV = 0.79 RMSECV = 0.31 RMSECV = 0.37 RMSECV = 0.20	34
	Ascorbic acid (mg/100 g)			RMSECV = 1.02	
Mango	SSC (°Bx)	Fruit Tester 20 (Fantec), 850–1000, interactance	PLS	RMSEP = 0.40	59
Apple	SSC (°Bx)	D.N.I., 200–1000, diffuse reflectance	Multiple regression analysis	RMSEP = 0.52	35
Apples 'Golden Delicious' 'Jonagold'	SSC (°Bx) SSC (°Bx) SSC (°Bx)	SD-1000 (Ocean Optics), 350–999, reflectance	MLR	RMSEP = 1.14 $RMSEP = 1.10$ $RMSEP = 1.18$	41
Strawberry	Firmness (N) MPF (N) SSC (%) TA (% citric acid) pH	Phazir 2400 (Polychromix), 1600– 2400, reflectance	MPLS	$\begin{array}{l} {\rm RMSECV} = 0.17 \\ {\rm RMSECV} = 0.48 \\ {\rm RMSECV} = 0.66 \\ {\rm RMSECV} = 0.07 \\ {\rm RMSECV} = 0.09 \end{array}$	60
'Antilla Fnm' 'Camarosa' 'Coral' 'Florida Fortuna' 'Primoris Fnm'	Correct classification according to variety (%)		PLS-DA	78% 57% 68% 67% 75%	
Orange	Acidity	I.N.A., I.N.A., I.N.A.	I.N.A.	RMSEP = 0.08165	66
Tomato (after harvesting)	Firmness (MPa) Lycopene (mg/g) Firmness (MPa)	FQ-NIRGUN (Fantec), 600–1100, I.N.A.	PLS PCR	RMSEP = 0.0989 RMSEP = 0.0835 RMSEP = 0.0999	67
Tomato (on vine)	Lycopene (mg/g) Firmness (MPa)		PLS	RMSEP = 0.0999 RMSEP = 0.0833 RMSEP = 0.0998	
X - 9	Lycopene (mg/g) Firmness (MPa)		PCR	RMSEP = 0.0827 $RMSEP = 0.1011$	
Pear	Lycopene (mg/g) Firmness (N)	I.N.A., I.N.A., diffused	PLS, MLR	RMSEP = 0.0827 $7.74 < RMSEP < 8.08^{b}$	42
Nectarine, 1st harvest	Full irrigation (correct classification) (%)	transmittance Phazir 2400 (Polychromix), 1600–	PLS2-DA	96.3%	68
	Regulated deficit irrigation (correct classification) (%)	2400, reflectance		91.6%	

TABLE III. Continued.

Species	Attributes	Spectrometer, spectral range (nm), acquisition mode	Multivariate analytical methods	Results	Reference
Nectarine, 2nd harvest	Full irrigation (correct classification) (%)			85.6%	
	Regulated deficit irrigation (correct classification) (%)			92.4%	
Tomato leaf	Nitrogen concentration	I.N.A., 310–1100, reflectance	PLS	RMSECV = 0.5120	69
Orange leaf	N P K Ca Mg Fe Mn Zn	I.N.A., 310–1100, reflectance	PLS	RMSECV = 0.129 RMSECV = 0.010 RMSECV = 0.144 RMSECV = 6.709 RMSECV = 0.101 RMSECV = 9.675 RMSECV = 3.449 RMSECV = 2.873	70
Pear	SSC (°Bx)	S-2000 (Ocean Optics), 620, 850, 880, 940, diffuse reflectance	PLS, MLR, ANN	$0.54 < RMSEP < 0.64^{b}$	71
Blueberry	Correct classification according to ripeness stage	I.N.A., 445–970, diffuse reflectance	PCA	>93%	61
Tomato	Dry matter (% w/w) (results depend on the tomato position or combination of positions)	MMS1 (Zeiss), 305–1100, interactance	PLS	0.34 < RMSEP < 0.57	72

^a BPNN, back-propagation neural network; DI, Durofel index; D.N.I., development of a new instrument; FDA, Fisher discriminant analysis; GRNN, generalized regression neural network; H₂SO₄, sulfuric acid; I.N.A., information not available; LS-SVM, least squares support vector machines; LS-SVR, least squares support vector regression; MLR, multiple linear regression; MPF, maximum penetration force; MPLS, multiblock partial least squares; PCA, principal component analysis; PCR, principal component regression; PLS, partial least squares; PLS-DA, partial least squares discriminant analysis; SSC, soluble solids content; TA, titratable acidity

possibility of using them under real production conditions; however, many of the studies considered here were actually performed under laboratory conditions (involving sampling and transportation of the samples to the laboratory). Therefore, these studies do not actually assess the performance of the systems under real production conditions and are not examples of taking direct in situ measurements under the uncontrolled conditions typical of production sites.

Fruits and Vegetables. Most of the studies in this area were performed in the laboratory, applying NIR spectroscopic instruments to intact harvested fruits (in some cases, spectra were collected from the same fruit in more than one position or using spinning accessories). There are, however, a significant number of applications involving the direct use of the equipment in the field, where measurements were made directly of on-tree fruits under varying weather conditions. There are numerous studies highlighting the po-

tential of NIR spectroscopy as applied to fruit and vegetables 16 and about enhancing its use as a rapid and nondestructive analytical technique useful for determining internal and external characteristics, either quantitative or qualitatively. However, the fruit and vegetable sector demands field NIR spectroscopy equipment capable of performing in situ analyses to allow producers to establish the most suitable harvest dates, consequently ensuring the best possible crop quality, while avoiding waste and loss. Table III summarizes portable NIR spectroscopy applications to fruit. Promising results have been achieved when portable NIR spectroscopy has been applied in this sector, indicating the successful use of NIR spectroscopic measurements in nondestructively evaluating and monitoring fruit-quality parameters.^{34–36} The potential of this technique has been highlighted for assessing the internal quality of fruits nondestructively in the field under different weather conditions,^{37–47} usually with

the goal of predicting whether the fruit was ready to be harvested. Most studies in this area model parameters commonly used as maturity indicators, such as soluble solids content (SSC), 34,35,37–41,43–65 titratable acidity, 37,40,48,51–53,55,58,60,62,64,66 and pH.55,60,62 External quality parameters were also investigated, with special attention given to color; 40,44,48,49,62,67 weight, ^{44,62} and size. ^{54,62} Among the physical parameters considered, firmness was the most common, 42,44,47–49,52,54,56,62,67 with some attention also paid to juice content and juice weight,62 pericarp thickness, 58,62 and maximum penetration force.62 In addition, Beghi et al.52 and Guidetti et al.34 explored some nutraceutical parameters: total anthocyanin, total phenol, total flavonoid, nonanthocyanic flavonoid, carotenoid, chlorophyll, and ascorbic acid content.

The correlation of the measured chemical and physical parameters with the environmental conditions to which fruits were exposed was often evaluated. 65,68 Environmental factors are

^b Results vary according to the calibration method

^c Results vary according to the species

TABLE IV. Reported applications of portable NIR devices for meat and fish product analysis.^a

Species	Attributes	Spectrometer, spectral range (nm), acquisition mode	Multivariate analytical methods	Results	Reference
Swordfish	Correct classification according to the preservation status	MMS1 (Zeiss), 380– 1080, reflectance	PLS-DA, PCA	≥96.7% correctly classified	81
Pork meat in gas A ^b	Am (log cfu/g) En (log cfu/g) Lab (log cfu/g) pH	Phazir 2400 (Polychromix), 1600– 2400, reflectance	PLS, MPLS	RMSECV = 1.063 RMSECV = 1.198 RMSECV = 1.256 RMSECV = 0.100	73
Pork meat in gas B ^c	Am (log cfu/g) En (log cfu/g) Lab (log cfu/g) pH			RMSECV = 1.079 RMSECV = 1.153 RMSECV = 1.296 RMSECV = 0.117	
Pork meat in gas $A^b + gas \ B^c$	Am (log cfu/g) En (log cfu/g) Lab (log cfu/g) pH			RMSECV = 0.817 RMSECV = 0.342 RMSECV = 0.982 RMSECV = 0.039	
Duroc pork and Iberian pork	M. masseter muscle (correct classification of different breeds of pork)	FieldSpec (ASD), 350–2500, reflectance	ANN	95 %	74
Rabbit False flax seeds: 0% (C) 10% (M) 15% (H)	In vivo, live rabbits LD muscle (in ethanol) Fatty acids (perirenal fat)	LabSpec-Pro (ASD), 350–2500, reflectance	Cluster hierarchical analysis	$R^2 = 0.316$ $R^2 = 0.374$ $R^2 = 0.86$ (M vs. C) $R^2 = 0.90$ (H vs. C) $R^2 = 0.29$ (M vs. H)	77
Tuna	Fat content (%), frozen, glazed tuna Fat content (%), frozen,	Fruit Tester 20 (Fantec), 600–1000 transmittance	PLS	$5.14 < \text{RMSEP} < 9.42^{d}$ $3.23 < \text{RMSEP} < 5.08^{d}$	79
	nonglazed tuna Fat content (%), thawed tuna			$2.09 < RMSEP < 3.80^{d}$	
	Fat content (%) (with temperature compensation)			$3.18 < RMSEP < 4.72^{d}$	
Skipjack fish	Fat content (%)	Fruit Tester 20 (Fantec), 600–1000, I.N.A.	PLS	$1.06 < RMSEP < 3.42^{d}$	80
Meat	Fat (%) Moisture (%) Protein (%)	Phazir 1624 (Polychromix), 1600– 2400, reflectance	MPLS	RMSEP = 4.34 $RMSEP = 0.63$ $RMSEP = 2.57$	82
Pig	Intact carcass fat; correct classification according to feeding regimes (%)	Phazir 1624 (Polychromix), 1600– 2400, reflectance	PLS2-DA	60.6 < 93.9 < 96.4	75

^a Am, aerobic mesophiles; ANN, artificial neural networks; cfu, colony-forming units; En, Enterobacteriaceae; INA, information not available; Lab, lactic acid bacteria; LD, longissimus dorsi; MPLS, multiblock partial least squares; PCA, principal component analysis; PLS, partial least squares; PLS-DA, partial least squares discriminant analysis.

known to be greatly responsible for variability in fruit quality. Portable NIR spectroscopy could be a solution to the problem of fruit selection, assessing the individual quality characteristics of the fruits to match them to the required internal quality standards. One of the main concerns of fruit growers and distributors is fruit quality after harvest. The shelf-life and storage conditions of various fruit were evaluated to understand the influence of such crop practices as irrigation, fertilization, thinning, and pruning on the quality of the

harvested fruit and on the loss of quality during storage. ^{56,68} Research was also focused on the plant leaves, not just the fruit. There the nutritional status of a plant was mainly determined as a function of its concentration of nitrogen ⁶⁹ and other chemical elements, such as P, K, Ca, Mg, Fe, Zn, and Mn. ⁷⁰ The studies showed that NIR spectroscopy is highly efficient for determining nitrogen concentration.

The performance of different types of spectrometers was also tested, determining that the results obtained using portable devices are comparable to those achieved using bench-top spectrometers. 52,55,56,59,68 Cayuela and Weiland compared the performance of two different portable NIR spectrometers and found that the success of this technique is related to the selection of the most suitable instrument for a particular parameter. 55 Some of the weaknesses of the NIR spectroscopy method include the need to find a proper calibration method and the constant need to keep it updated (especially when the samples involved may be subject to periodical or

^b FreshlineTM 3MIX (30:40:30 O₂/CO₂/N₂).

^c FreshlineTM 3MIX 20/5 (5:20:75 O₂/CO₂/N₂).

^d Results vary according to the measured portion and/or wavelength selection.

TABLE V. Reported applications of portable NIR devices for beverage and dairy-product analysis.^a

Species	Attributes	Spectrometer, spectral range (nm), acquisition mode	Multivariate analytical methods	Results	Reference
Milk (with adulterants: tap water, whey, synthetic milk, synthetic urine, urea, H ₂ O ₂)	Fluid milk (% v/v)	MicroPHAZIR (Polychromix), 1600– 2400, diffuse reflectance	PLS	RMSEP = 4.74	89
Milk	Fat (%) Protein (%) DM (%)	INA, 600–1100, diffuse reflectance	PLS	RMSEP = 0.187 $RMSEP = 0.120$ $RMSEP = 0.296$	88
Milk	Fat (%) Protein (%) Lactose (%) Moisture (%) Temperature (%)	INA, 800–1080 DNI, 1050–1650, transflectance, reflectance	PLS	$0.066 < RMSECV < 3.62^{b}$) $0.078 < RMSECV < 1.87^{b}$ $RMSECV = 0.081^{b}$ $0.09 < RMSECV < 0.25^{b}$ $3.01 < RMSECV < 3.30^{b}$	90
Rice wine	Alcohol (%) Nonsugar solids (%)	DNI, 1100–2150, reflectance	PLS	RMSEP = 0.259 RMSEP = 0.0134	86
Tea drinks	Tea polyphenols Free amino acids	DNI, 1100–2150, reflectance	PLS	RMSECV = 0.059 $RMSECV = 0.005$	85
Beer	Bitterness (IBU) Total polyphenol (mg/L) Total nitrogen (%) pH Beer color (EBC) Apparent extract (%) Alcohol (%) Beer distinction	PlaScan-SH (OPT Research Inc.), 1200– 2400, diffuse reflectance	MLR PCA	$R^2 = 0.67$ $R^2 = 0.64$ $R^2 = 0.69$ $R^2 = 0.64$ $R^2 = 0.34$ $R^2 = 0.53$ $R^2 = 0.76$ Beers were clustered into three groups	83

^a DM, dry matter; DNI, development of a new instrument; EBC, European Brewing Convention; H₂O₂, hydorgen peroxide; IBU, international bitterness unit; INA, information not available; MLR, multiple linear regression; PCA, principal component analysis; PLS, partial least squares.

^b Results vary according to the type of spectrometer used.

TABLE VI. Reported applications of portable NIR instruments for cereal and feedstock analysis.^a

Species	Attributes	Spectrometer, spectral range (nm), acquisition mode	Multivariate analytical methods	Results	Reference
Wheat leaf	Nitrogen content (fresh leaves)	FieldSpec (ASD), 350-	PLS	RMSECV = 0.372	97
	(% DM) Nitrogen content (dried leaves) (% DM)	2500, reflectance		RMSECV = 0.268	
	Nitrogen content (all leaves) (% DM)			RMSECV = 0.352	
	$LMA(g/m^2)$			RMSECV = 6.300	
Maize silage	DM (%)	INA, 960–1700, I.N.A.	MPLS	RMSECV = 0.97	100
	CP (%)			RMSECV = 0.12	
	NDF (%)			RMSECV = 0.40	
Noodle wheat flours (whole	Moisture (%)	PlaScan-SH (OPT	PLS	RMSEP = 0.351	99
noodles)	Protein (%)	Research Inc.), 1200–		RMSEP = 0.526	
	Ash (%)	2400, diffuse		RMSEP = 0.397	
	Fat (%)	reflectance		RMSEP = 0.087	
	Carbohydrate (%)			RMSEP = 0.681	
Noodle wheat flours	Moisture (%)			RMSEP = 0.321	
(powder)	Protein (%)			RMSEP = 0.426	
	Ash (%)			RMSEP = 0.402	
	Fat (%)			RMSEP = 0.091	
	Carbohydrate (%)			RMSEP = 0.458	
Rice	Low-level cadmium-polluted	INA, 1200–2400, diffuse	CDA	86.7%	96
	Medium-level cadmium-polluted	reflectance		83.9%	
	High-level cadmium-polluted			87.5%	
	Overall correct classification rate			85.2%	
Rice	Protein content (%) Amylose content (%)	INA, INA, transmittance	PLS	RMSEP = 0.279 $RMSEP = 0.52$	95

^a CDA, canonical discriminant analysis; CP, coat protein; DM, dry matter; INA, information not available; LMA, leaf mass per unit area; MPLS, multiblock partial least squares; NDF, neutral detergent fibers; PLS, partial least squares.

seasonal changes). Consequently, some studies focused on finding the calibration models, testing and comparing several different preprocessing techniques, and optimizing regression methods. 50,54,58,71,72

Meat and Fish. Almost all the meat analyses in this sector were performed on slaughtered animals. Fish analyses were normally performed on frozen samples. Spectra were collected in reflectance mode from different sections of the body. The published research in this field indicates that the NIR spectroscopy technique could work as an analytical sensor, establishing the state of meat conservation, although further work remains to be done to develop more robust models (Table IV).73 The potential of this technique to distinguish between pork from different pig breeds confirms that it is a rapid and objective method for identification and authentication.74 A portable NIR device was also tested as a way to make in situ classifications of individual pig carcasses as a function of the pigs' feeding regimes. The portable device enabled individual in situ inspections and successfully classified Iberian pig carcasses into three commercial categories. To achieve these results, some instrumental optimizations were required, especially in the wavelength range, the spectral resolution, and the sampling area. Additional recommendations for new instrumental designs to be used in the meat sector were also proposed.⁷⁵ A similar experiment was tried using lamb carcasses, but despite the correct classification of more than 90% of the samples, researchers rated the performance of the equipment as low.⁷⁶ Masoero et al. applied this technique not only to rabbit meat but also to live rabbits, showing that the feeding regime produced real differences in groups of experimental live rabbits and in rabbit meat samples. Correlations between the rabbit samples and their feeding regimen were obtained, although with limited success.77,78

Portable NIR spectrophotometers were also used for the analysis of fish samples. Most of these studies were aimed at determining fish fat content. Results showed that this technique is dependent on the fish-body section

analyzed as well as on the sampling conditions. 79,80 A portable visible NIR (Vis-NIR) device was determined to efficiently distinguish between fresh and frozen fish samples. 81

The problem of calibration is usually considered one of the biggest weaknesses of NIR spectroscopy. However, an interesting study proved that the successful transfer of calibration models from large, previously collected databases to new devices more suitable for in situ analysis is possible.⁸²

Beverages and Dairy. In studies of the beverages sector, NIR spectra were usually collected in transmittance or transflectance mode. The samples were placed in specifically designed sample chambers or in common quartz cells to be read by the equipment. In some cases, the analyses were executed using dispersive handheld NIR equipment equipped with a liquids adaptor or accessory. Portable NIR devices have been applied to the analysis of beverages and dairy products, and several successful applications have been reported (Table V). Portable devices seemed to be a promising technique for distinguishing between types of beer and for evaluating beer quality in terms of total polyphenols and total nitrogen. The differences in raw material and production processes seemed to be the most common source of variability among beers.⁸³ Similar results were achieved when NIR spectroscopy was applied to Japanese sake. This technique enabled researchers to distinguish among different samples and could be a tool for the improvement of Japanese sake quality.84 In tea drinks, polyphenols and free amino acids were shown to be the most important quality indicators, and portable NIR spectroscopy proved to be a fast and reliable technique for testing the quality of tea drinks.85 Rice wine was also the target of NIR spectroscopy applications for determining the concentrations of alcohol and non-sugar solids. A portable NIR rice-wine analyzer was successfully developed. The results of these studies suggest that this portable apparatus (which is user friendly and pollution-free) could be an efficient, fast, and reliable alternative way to analyze rice-wine quality.86,87

Good calibrations were also found

when spectroscopy was used to analyze milk for fat protein and dry matter content,88 as well as to detect and quantify adulterated milk samples. The research suggested that this method could potentially be used as an alternative to traditional analysis methods because of its simplicity, sensitivity, low energy cost, and portability. Nevertheless, the studies also revealed that portable mid-infrared (mid-IR) systems have better discriminant power and reliability of predictions than the NIR systems tested.89 Analyses of milkpowder samples were also made, which compared the results using two different types of portable NIR and Vis-NIR spectrometers. Once again, the success of the technique was determined to be closely related to the selection of the most suitable instrument.90

Cereals and Feedstock. In this area, the included spectroscopy studies have mainly been of wheat, rice, and corn, with the protein concentration being the parameter that was most often investigated (Table VI). The studies demonstrated that portable NIR spectroscopy is suitable for performing nondestructive, in-field measurements of the protein content of wheat,91-94 corn,91 and rice.95 In-field NIR spectroscopy also proved to be useful as a rapid, nondestructive, and convenient analytical method for the primary screening and detection of cadmium-polluted rice.⁹⁶ The investigation of wheat-plant leaves to determine the nitrogen content or the leaf mass showed promising results as well. Consequently, this technique represents a solution to the problem of finding a required rapid and nondestructive method that can be applied during plant-growing cycle.⁹⁷

A portable NIR spectrometer was also used to predict the water content of rice crackers, in an attempt to understand their hygroscopic behavior. 98 It was also used to determine the moisture content of noodles. 99 The texture of noodles is dependent on the type of wheat flour as well as on mixing ratios used to make them, while another study used spectroscopy to discriminate between noodle flours by describing the relationship between the NIR spectra and the chemical-analysis data. 98

Feedstock has also been analyzed using NIR spectroscopy. Animal health

TABLE VII. Reported applications of portable NIR devices for soil and manure analysis.a

Species	Attributes	Spectrometer, spectral range (nm), acquisition mode	Multivariate analytical methods	Results	Reference
Soil	Total N content (%)	DNI, 940, 1050, 1100, 1200, 1300, and 1550, reflectance	BPNN	RMSEP = 0.019	91
Soil	Soil moisture content (%)	DNI, 1450, INA	Linear regression method	RMSEP = 0.85	109
Soil	Total N content (%)	DNI, 940, 1050, 1100, 1200, 1300, and 1550, reflectance	BPNN	RMSEP = 0.043	110, 111
Soil	Total N Total organic matter	DNI, 800–2500, reflectance	PLS	$R^2 = 0.8324$ $R^2 = 0.8833$	103
Soil	Organic matter (%) pH Ammonium nitrogen Nitric nitrogen Total kalium	Luminar 5030 (Brimrose), 1100– 2300, reflectance	PLS	RMSEP = 13.353 RMSEP = 1.1126 RMSEP = 23.2595 RMSEP = 106.285 RMSEP = 10.1516	104
Soil	Organic C (%) Moisture content (%) Clay content (%)	DNI, 1600–3100, reflectance	PLS, SMLR	0.18 < RMSEP < 0.27 ^b 1.7 < RMSEP < 1.9 ^b 3.6 < RMSEP < 4.4 ^b	105
Soils	Organic C (%) Cation exchange capacity (mEq/100 g) Moisture content (%)	DNI, 1640–2640, reflectance	PLS	0.23 < RMSEP < 0.28° 3.59 < RMSEP < 3.91° 1.59 < RMSEP < 1.88°	106
Cattle manure	Total C (mg/g) Organic C (mg/g) Total N (mg/g) C:N (mg/g) K (mg/g) S (mg/g) P (mg/g) pH	INA, 360–1690, INA	PCA/PLS	RMSEP = 23.4 RMSEP = 0.91 RMSEP = 0.74 RMSEP = 0.87 RMSEP = 0.83 RMSEP = 0.73 RMSEP = 0.61 RMSEP = 0.89	115
Compost (moist) Compost (oven-dried)	Organic matter (%)	AgriSpec (ASD), 350– 2500, diffuse reflectance	PLS, PCR	$10.1 < \text{RMSECV} < 25.7^{\text{b}}$	116

^a BPNN, back-propagation neural network; DNI, development of a new instrument; INA, information not available; MLR, multiple linear regression; PCA, principal component analysis; PCR, principal component regression; PLS, partial least squares; SMLR, stepwise multiple linear regression.

is directly related to diet. Therefore, to meet the requirements of animals and for maximum production, diets must be optimized. A study on the performance of portable NIR spectroscopy instruments when applied to the analyses of maize silage. The accuracy of the results was very close to that obtained using a laboratory NIR instrument. 100 Once again, a comparison was made of various regression techniques used during the cereal analysis, and the results favored the artificial neural networks (ANN) technique.⁹³ Studies of the development of new portable NIR spectroscopy devices were also done on cereals. It was concluded that the portable equipment (which had a simple structure, low-power consumption, and small size) provided a low-cost solution to the problem of determining wheat and corn quality in complex environments. 91,92,94,101

Soils and Manures. Studies of soil samples have also used NIR spectroscopy (Table VII). Soil samples for these studies were usually collected at the surface or at known depths. In those situations, samples were first sieved and/or dried (either oven- or air-dried) and then analyzed. Different types of soils were investigated and compared. Some reports have been made of researchers attempting in-field soil analyses using specific contact probes. The measurement and control of soil characteristics are particularly important for the proper development of the agricultural prod-

ucts. Soil organic matter is one of the most studied parameters. 102-108 Some experiments using spectroscopy showed a good correlation between the spectral data and data obtained using standard chemical methods, whereas others suggested the need for further verification of results over a wider range of soil samples. Gomez et al. exposed for the first time the potential of satellite hyperspectral data for the prediction of the organic carbon content of soil. They demonstrated good accuracy of the model no matter what number or range of soil samples used. 108 Soil moisture was also a commonly studied parameter, 105,106,109 and one of these studies used spectroscopy to generate spatial distribution maps. 109 Total nitrogen

^b Results vary according to the calibration method.

^c Results vary according to the data set and moisture content.

TABLE VIII. Reported applications of portable NIR devices in viticulture and olive oil production.^a

Species	Attributes	Spectrometer, spectral range (nm), acquisition mode	Multivariate analytical methods	Results	Reference
Grapes (fresh berries)	SSC (°Bx) TA (g tartaric acid/dm³) pH	AvaSpec-2048 (Avantes), 400–1000, reflectance	PLS	RMSEP = 1.48 RMSEP = 1.48 RMSEP = 0.15	117
Grapes (homogenized samples)	PA (mg/dm³) EA (mg/dm³) SSC (°Bx) TA (g tartaric acid/dm³) pH PA (mg/dm³)			RMSEP = 133.90 RMSEP = 81.87 RMSEP = 0.95 RMSEP = 1.12 RMSEP = 0.13 RMSEP = 129.00	
Grapes (fresh berries)	EA (mg/dm³) SSC (°Bx) TA (g tartaric acid/dm³)		PLS-DA	RMSEP = 77.70 77.1% 68.6%	
Grapes (homogenized samples)	SSC (°Bx) TA (g tartaric acid/dm³)			88.7% 83.1%	
Grapevine leaf ('Syrah,' 'Merlot,' 'Cabernet Sauvignon') Grapevine leaf ('Cabernet	Water potential	Luminar 5030 (Brimrose), 1100–2300 transmittance	PLS	RMSECV = 1.48 $RMSECV = 1.08$	126
Sauvignon')					
Grapes ('Cabernet Sauvignon') Grapes ('Cabernet Sauvignon,' 'Sangiovese,' 'Merlot')	SSC (°Bx) TA (g tartaric acid/dm³) Maturity index (sugar/acidity	INA, 590–1090, INA INA, 400–1000, reflectance	PLS PLS	0.61 < RMSECV < 1.15 ^b 0.2 < RMSEP < 0.4 ^b 2.8 < RMSEP < 6.0 ^b	118 119
	ratio) PA (mg/L) pH Reductant sugars (g/L)			$101.3 < RMSEP < 125.7^{b}$ $0.0 < RMSEP < 0.1^{b}$ $6.6 < RMSEP < 12.2^{b}$	
Grapes ('Cabernet Sauvignon,' 'Carménère,' 'Merlot,' 'Pinot Noir,' 'Chardonnay')	SSC (°Bx) pH Anthocyanin concentration (mg/g)	USB 2000 (Ocean Optics), 640–1300, INA	PLS	1.010 < RMSEP < 1.267 ^c 0.088 < RMSEP < 0.159 ^c 0.183 < RMSEP < 0.315 ^c	120
Grapes	SSC (*Bx) pH TA (g/L) Anthocyanin concentration (mg/g)	Luminar (Brimrose), 1100–2300, transmittance	PLS	$\begin{array}{l} \text{RMSECV} = 1.9 \\ \text{RMSECV} = 0.16 \\ \text{RMSECV} = 1.89 \\ \text{RMSECV} = 0.11 \end{array}$	121
Grapes	SSC (°Bx) Acidity (g H ₂ SO ₄ /L) Water content (%)	INA, 400–1100, interactance	MLR	RMSECV = 1.12 $RMSECV = 1.35$ $RMSECV = 1.89$	127
Olives ('Moraiolo,' 'Dolce di Andria,' 'Nocellara Etnea')	Total phenols Verbascoside Oleuropein 3,4 DHPEA-EDA	Luminar 5030 (Brimrose), 1100– 2300, transmittance	PLS	0.451 < RMSECV < 1.672° 0.074 < RMSECV < 0.210° 0.175 < RMSECV < 0.365° 0.237 < RMSECV < 1.138°	128
Olives ('Arbequina,' 'Picual,' 'Verdial de Huévar,' 'Manzanilla de Sevilla')	Oil content (%) Moisture (%)	Luminar 5030 (Brimrose), 1100– 2300, transmittance	PLS	1.52 < RMSECV < 1.99° 1.65 < RMSECV < 2.26°	129
Olives	Fruit moisture (%) DM (%) Oil content (fresh weight) (%)	LabSpec (ASD), 350– 2500, reflectance	PLS	$\begin{aligned} & \text{RMSECV} = 1.741 \\ & \text{RMSECV} = 1.710 \\ & \text{RMSECV} = 0.901 \end{aligned}$	130
A DIM I A DA DIMENTEN FOR A STATE OF THE STA	Oil content (DM) (%) Fruit maturity index (%) Oil-free acidity (%)			RMSECV = 1.619 RMSECV = 0.465 RMSECV = 0.030	

^a DM, dry matter; 3,4 DHPEA-EDA, 3,4-dihydroxyphenolethanol-elenolic acid di-aldehyde; EA, extractable anthocyanins; H_2SO_4 , sulfuric acid; INA, information not available; MLR, multiple linear regression; PA, potential anthocyanins; PLS, partial least squares; PLS-DA, partial least squares discriminant analysis; SSC, soluble solids content; TA, titratable acidity.

content, 103,104,110,111 pH, 104 soil color and mineral composition, 112 and clay content have also been predicted. 105,112 Viscarra Rossel et al. compared models for clay content using field-collected

spectra and laboratory-collected spectra (after drying the samples). Surprisingly, and contrary to what was expected, the field-collected spectra provided better predictions of clay content.¹¹² Haché et

al. simultaneously investigated the spectral properties of soil and wheat, with the aim of discriminating between conventional and conservation agricultural practices. The soil spectra were useful

^b Results vary according to the calibration method.

^c Results vary according to the species.

in discriminating among tillage practices, whereas the wheat spectra were more suitable for discriminating among nutrient sources.113 In the detection of cyanide concentrations, portable NIR spectrometers were considered to be reliable instruments. Although spectrometers could not replace traditional laboratory analysis because of their limited detection in this instance, they could be very useful in the detection of contaminated areas.114 Portable soil analytical instruments based on NIR spectroscopy have also been developed. Those systems presented several advantages, such as stable performance and high precision. Nevertheless, soil moisture seemed to influence the accuracy of the detector, and measurement corrections were required. 103,105,107,109–111

Manures and composts are also included in this section. However, even though the analyses done in the studies were performed using portable NIR-based devices, the experiments were done in the laboratory. Nevertheless, studies have concluded that field-portable NIR spectroscopy is suitable for manure and compost analysis and that, despite the influence that environmental changes may have on instrument performance, the devices would be more useful applied in the field. 115,116 A detailed list of these applications is provided in Table VII.

Viticulture and Olive Growing. Viticulture is one of the sectors that has been studied most using portable NIR devices (Table VIII). These experiments were done using samples in several ways, both in the field and in the laboratory. While some researchers analyzed grapes by the bunch (usually divided into sections), others focused on individual berries. Other studies compared whole berries to homogenized samples. Picked grapevine leaves were also analyzed. Conversely, studies of olives were performed on the intact fruit on the tree. The parameters analyzed were similar to those employed for fruits and vegetables, with the aim being to determine the stage of maturity. The parameters considered most often were the SSC (in degrees Brix [°Bx]) and pH,^{117–123} titratable acidity,^{117,121,122} reducing sugars, 119,122 and tartaric and malic acids. 122 Phenol ripening parameters such as the concentration of anthocyanins^{117,119–121,123} and polyphenols¹¹⁷ were also studied.

The viticulture studies concluded that Vis-NIR portable devices could be suitable, rapid, and nondestructive tools for assessing and monitoring grape ripeness directly in the field. Sethuramasamyraja et al. used a portable NIR spectrometer for measuring anthocyanin and Brix parameters in a geo-referenced field of wine grapes. Those quality indicators were then subjected to geospatial modeling, resulting in the spatial distribution of wine quality variability across the field (anthocyanin-content data were used to form a quality zone, whereas the Brix data set facilitated the prediction of the harvest timing). 123 The influence of bunch position and orientation on grape ripeness was also investigated to allow the selective harvesting of grape bunches depending on the type of wine to be made. 122 Susceptibility of the grapevines to disease was a factor of great concern; Calcante et al. tested spectroscopy as a way to detect different levels of grapevine downy mildew symptoms. 124,125 Laboratory and field tests of grapevine leaves demonstrated that NIR spectroscopy can be used to quantify the water potential of grapevine leaves, revealing that the best predictive models are those specific to the variety and maturity phase. 126 In this area, once again, the performance of different spectrophotometers¹²⁵ and modeling techniques¹¹⁸ was compared. A low-cost portable apparatus was designed and built with the aim of accurately measuring the ripeness parameters (previously mentioned) under in situ conditions. Researchers used spectral preprocessing techniques to diminish the effects of error sources, such as temperature and humidity, thus achieving the desired robustness of the model.127

The quality of olive oil depends directly on the quality of the olives. Among the studied parameters of olives were the predicted phenol compound content, ¹²⁸ oil and moisture contents, ^{129–131} dry matter, and oil-free acidity. ¹²⁶ The studies demonstrated that portable NIR instruments were feasible tools for in situ, nondestructive measurements of total phenols in olives. The same parameters were also studied by

León-Moreno; he concluded that portable NIR spectroscopy could be used to evaluate oil content and moisture during different selection steps of olive-breeding programs, providing accurate results for the selection of genotypes. ¹³¹ Nevertheless, researchers suggested that further work was necessary to develop the calibration of the devices and, thus, to make the models more robust.

Other Applications. Other applications of portable NIR spectroscopy included studies of several plants or plant leaves. Portable NIR instruments were developed and employed to determine leaf water content 132–134 and chlorophyll content. 133,134 They were also used to determine the total nitrogen content of fresh tea leaves, to monitor plant growth, and to manage fertilization. 135 Portable NIR instruments are still being evaluated for possible use in collecting signature spectra from vegetation. 136

Some recent papers described results comparing the performance of different NIR spectrometers when applied to the same problem. Rotbart et al. compared the performance of three different NIR spectrometers, including portable instruments, in determining the nitrogen content of olive tree leaves. ¹³⁷

Other applications include the differentiation of some plastics and foodstuffs using portable NIR spectroscopy instruments, relying not only on a statistical and mathematical approach but also on a chemical interpretation of the NIR spectra. Researchers intended to continue the basic interpretation of NIR spectra by focusing on various foodstuffs and, thus, to provide a useful analytical technique for many industrial needs. 138

PORTABLE VERSUS LABORATORY NEAR-INFRARED INSTRUMENTS

Portable instruments have been reported as having some limitations when compared with state-of-the-art lab bench-top NIR instruments, which are often equipped with interferometers and better optical properties (e.g., better signal-to-noise ratio, sensitivity, and optical resolution). Essentially, laboratory instruments with interferometers (e.g., the Michelson interferometer) have

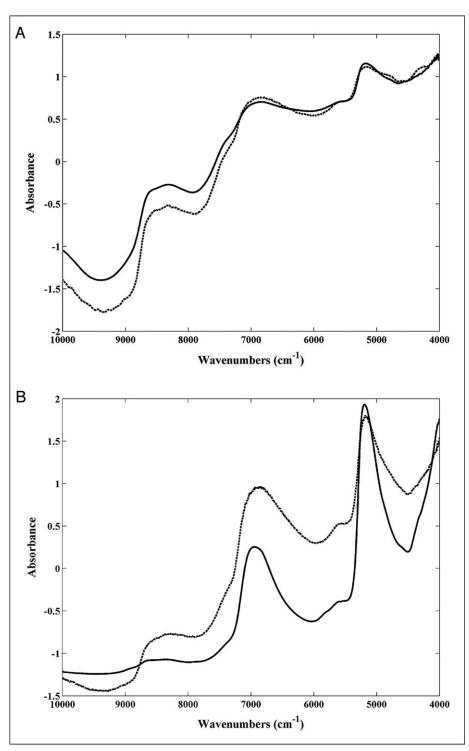


Fig. 1. Comparison of NIR spectrum obtained on a NIR portable instrument (FieldSpec 4, ASD, USA) and a NIR bench-top instrument (FTLA2000,ABB, USA). (A) For grape berries. (B) For grapevine leaves. Black line, portable instrument; gray dotted line, bench-top instrument.

several advantages over dispersive instruments based on different technologies (e.g., interference filters, diffraction grating, and acousto-optical diffraction gratings): the optical throughput advantage (Jacquinot advantage), the multiplexing advantage (Fellgett advantage), and resolution (Connes advantage).¹⁹

Portable instruments have the obvious advantage of possible field-use because of an absence of moving parts. Technological innovations in dispersive portable instruments have been reducing the advantages of laboratory instruments. Figure 1 compares the performance of a laboratory Fourier transform (FT)-NIR instrument (FTLA2000, ABB) to a dispersive portable NIR instrument (FieldSpec 4, ASD) when measuring grapes (Fig. 1a) and grapevine leaves (Fig. 1b) using approximately the same 8 cm⁻¹ resolution. As shown, the performance of the two devices is comparable under the same measurement conditions. Nevertheless, depending on the measurement conditions and sample characteristics, the field operation of NIR spectrometers may encounter additional problems inherent to the in situ measurements, which may introduce unwanted variability into the spectra,.

Several authors in the area of agrofood products have compared the figures of merit of calibration models using portable and laboratory instruments. All these comparisons show that some limitations exist, mainly related to the sampling accessory used to measure the samples. For instance, the optical path lengths in transmittance measurements and illumination areas in reflectance mode are often different. Saranwong et al. compared the performance of a portable NIR instrument Fruit Tester 20 (Fantec, Kosai-city, Japan) with a research-type Foss NIRSystems Model 6500 (Metrohm AG, Switzerland) in measuring the sugar content (in degrees Brix) of mango fruits in diffuse reflectance mode. The two instruments shared roughly the same wavelength range, measuring-head size, and detector type, and the instruments showed similar levels of accuracy (standard error of prediction [SEP], 0.40 °Bx), despite the fact that the spectra of same sample produced using the two instruments appeared to be considerably different.⁵⁹ The main conclusion here was that a portable device was recommended for the in situ analysis of fruits similar to mangos. A similar comparison study of these two instruments, measuring fat content in frozen skipjack, showed the Foss instrument to have the superior performance.80

Two other studies, by Pérez-Marín at al., compared the performance of a handheld micro-electro-mechanical system (MEMS) spectrophotometer (Phazir 2400, Polychromix Inc., Wilmington, MA), with a diode-array Vis-NIR spectrophotometer (Perten DA-7000, Perten Instruments) in analyzing different parameters in plums⁴⁴ and nectarines.⁶⁸ The measurements were also performed in diffuse reflectance mode. In brief, the studies concluded that, although slightly better results were obtained for the diode-array instrument (for the plum and nectarine parameters), the handheld proved to be a more convenient tool for analyzing samples because it afforded the additional advantages of portability and low cost. A similar conclusion was reached by Zamora-Rojas et al. when they compared a handheld MEMS-based spectrometer (1600-2400 nm) with a high-resolution NIR spectroscopy monochromator (400-2500 nm) for the classification of individual Iberian pig carcasses into different commercial categories.⁷⁵ Although most comparison studies reported that the portable instruments had lower performance scores than the laboratory instruments, the main conclusions were that their flexibility and possibility of field-use were major advantages that made the portable options the best solution.

The selection of the most suitable portable spectrometer was also investigated. Cayuela and Weiland compared two commercially available portable spectrometers: a Labspec (Analytical Spectral Devices Inc., Boulder, CO) and a Luminar 5030 (Brimrose Corp., MD).⁵⁵ The calibration used four orange varieties, and the parameters studied are listed in Table III. According to their RMSEP values, the prediction accuracy of the two spectrometers was similar for most of the fruit-quality parameters determined. However, the Labspec device presented slightly better results for some physical parameters such as the fruit weight, rind weight, and flesh firmness. The authors suggested that the larger contact probe of the Labspec unit (with a light source of 20 mm, versus the 8 mm of the Luminar 5030) allowed the exploration of a larger portion of the fruit, consequently explaining the observed results.⁵⁵ Despite

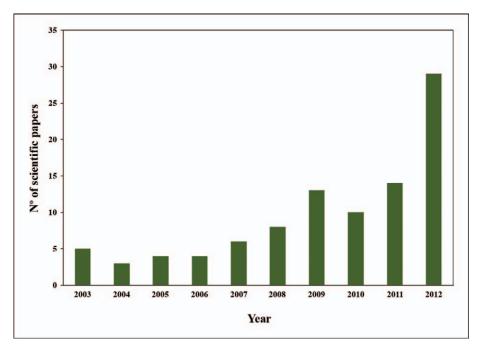


Fig. 2. Number of scientific papers involving the use of portable NIR spectrometers in the agro-food industry since 2003.

the low cost of most portable instruments compared to laboratory instruments (note that the costs of some portable instruments are still comparable to laboratory instruments), efforts to further reduce the costs of the instruments have been reported, especially by adapting instruments to specific tasks. Kalinin et al. described the performance of a specially designed instrument (designated by BIKAN-K) for measuring fat, protein, and lactose in restored milk.89 This equipment is able to measure liquid samples with a 12 mmthickness in the range 800–1080 nm. Reported results were comparable to those obtained using commercial equipment; in this case, the tested equipment was the MC-75 grating spectrometer equipped with a Si linear sensor (ILX511).

A recent paper compared the feasibility of using portable and handheld IR (both NIR and mid-IR) spectrometers for monitoring milk adulteration by tap water, whey, synthetic milk, synthetic urine, urea, and hydrogen peroxide. The portable and handheld mid-IR systems allowed the development of classification and quantification models with better discrimination power and predic-

tion ability than the NIR systems tested. 89 Attempts were made to transfer calibrations from high-performance atline NIR spectrometers to portable devices, and this was successful, as reported by Zamora-Rojas et al., for calibrations of fat, moisture, and protein in meat products. 82 The successful transfer of a previously existing calibrations database to a portable device allows a new approach for fast, low-cost, online/in situ analysis of agro-food products.

PROSPECTIVE DEVELOPMENTS

A survey of scientific papers published in the last decade (Fig. 2) shows a steady increase in the number of research and development studies being conducted using these types of portable spectrometers. They are used not only by companies to ensure process and product quality control but also by researchers, demonstrating the evolution of these devices in terms of hardware and optical systems/detector specifications. The number of scientific studies using this technology is expected to increase substantially over the coming years. In addition, the major develop-

ments in this area are expected to be in manufacturing science. The major trends are toward miniaturization, increasing the specifications quality while reducing the cost of the devices. One example of this is an increase in the range of miniaturized MicroNIR® spectrometers (JDS Uniphase [JDSU] Corporation, Milpitas, CA), which weigh less than 60 g, allow measurements from 850 to 2450 nm, and have the option of interchanging different sampling accessories. 139 As new technology is implemented in these devices, they will become more stable, more reliable, and better able to produce results that are comparable to the bench-top FT spectrometers. Another important development is the reduction in the manufacturing costs and subsequent market prices of the spectrometers overall. It is already possible to find portable NIR devices that sell for less than \$10 000 and allow full NIR spectral-region scanning, which contrasts with the situation a few years ago.

CONCLUSION

We have established that portable NIR spectroscopy is useful in a wide number of applications in the agro-food industry. The studies examined here emphasized the already-known advantages of NIR spectroscopy: lower costs; rapid, in situ, and nondestructive analyses; multi-parameter results; and environmental friendliness. Nevertheless, this technique also has drawbacks that cannot be ignored: the researcher must develop calibration models; the process is usually resource intensive, requiring not only an accurate reference analysis but also a large and updated calibration data set; the NIR devices are relatively limited in detection, which prevents their use in analyzing compounds with low concentrations (< 0.1%); and finally, to use portable NIR devices for in situ analyses, the researcher must compensate for any interfering environmental conditions (such as light and humidity).

The number of published studies in this field has been increasing in the last decade; however, there is still work to be done in the efforts to surmount these limitations. Although the examples described in this review take advantage of portable instruments, it is absolutely clear that there is still much work to be done to make these instruments easily usable in the field under production conditions. Because many of the applications surveyed here were actually performed under laboratory conditions, it is therefore not possible at the present time to evaluate the real performance of portable NIR devices under production conditions.

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