Analytical chemistry strategies in the use of miniaturised NIR instruments: an overview

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Abstract

Miniaturised NIR instruments have been increasingly used in the last years, and they have become useful tools for many applications on a broad variety of samples. This review focuses on miniaturised NIR instruments from an analytical point of view, to give an overview of the analytical strategies used in order to help the reader to set up their own analytical methods, from the sampling to the data analysis. It highlights the uses of these instruments, providing a critical discussion including current and future trends.

Keywords: analytical methods, miniaturised devices, handheld devices, near-infrared spectroscopy, chemometrics

1. Introduction

Near-infrared (NIR) spectroscopy is a well-established and mature technique [1] that has become the preferred tool in many fields of applications [2–4] since it was first applied in the 1960s for analytical purposes in the grain industry [5]. NIR equipment, as most of the analytical instrumentation, has evolved from large, benchtop-based instruments through on-line and in-line instruments for industry, and finally to miniaturised portable lab-on-a-chip devices. One of the outcomes of this change to smaller equipment is the increasing portability of analytical instrumentation. Portability is not a newcomer in analytical instrumentation and it has been a fashionable topic for many years [6], although recent developments, among others, in MEMS (micro-electro-mechanical systems) and MEOMS (micro-opto-electro-mechanical systems), have boomed the use of portable analytical instrumentation: total portable analytical instrumentation market was estimated at USD 13.06 billion in 2020 and is expected to grow at a compound annual growth rate of 8.11% from 2020 to 2026 [7]. There is not a clear consensus in the literature about the distinction between portable and miniaturised NIR devices [8]. Globally speaking, miniaturised instruments seem to include new technological solutions [9], including improved light sources, miniaturised wavelength selection techniques (with techniques based on MEMS or MOEMS [10]) and more sensitive detectors. Focusing on the size of the device, field spectrometers (to be differentiated from benchtop instruments) may be divided into transportable (deployable on field while mounted in a car), portable in a suitcase (>4 kg of total weight) and handheld (<1 kg) ones [11]. Miniaturised instruments would be those having the size of a book or less.

The main characteristics and technical parameters for the most used miniaturized NIR spectrometers according to the literature are summarized in Table 1. The spectrometers cover different spectral regions according to the different wavelength selectors and to detector they use, as is discussed by Chai et al [10]. A first group of sensors allows the acquisition of spectra in the NIR spectral range related to the 2nd overtone, 1st overtone and combinations (about from 900 to 2500 nm); a second group considers the 1st overtone and combinations region (about from 1300 to 2500 nm) and a third group allows only the acquisition in the 3rd overtone region (about around 700-1000 nm). Almost all the instruments use tungsten halogen lamps, what may cause heating problems of the instrument and, in some cases, also of the samples. The SCiO spectrometer (Consumer Physics), besides the issues related to its restricted range of acquisition and to the reduced number of variables (wavelengths), is the only commercial sensor that uses light-emitting diodes (LED) what implies that the instrument is more cost-effective with low power consumption. Concerning the connectivity system, which is strictly related to its portability, security and also to maintenance costs, some spectrometers need an external working platform to connect using a USB system, while other ones are equipped with Bluetooth and use local storage or cloud services with different pricing plans.

Several benefits arise from this portability and reduced dimensionality of the instruments. On one hand, portability itself means that instead of taking the sample to the lab, the lab goes to the sample, being able to increase the in-field measurements and the achievement of rapid results. Another consequence is the price reduction of these instruments. If a typical laboratory NIR instrument can cost between EUR 30-40,000, miniaturised NIR instruments for a few thousand euros can be found, meaning a decrease of at least one order of magnitude in the price. It should be noted that this decrease in price and size is usually related to a logical decrease in the performance of quality parameters associated with the analytical methods using these instruments [12]. Despite this, a good number of applications suitable for their use have been found and reviewed in this work.

The last years have seen excellent reviews dealing with general spectroscopic [11] or specific NIR miniaturised instrumentation [8, 9]. However, these reviews are mainly centred in the technical parts of the instruments, describing in a detailed way the different parts and components of miniaturised instrumentation. Other recent reviews are focussed on specific fields of applications such as forensic [13], environment [14], natural medicines [15] or meat [16]. This overview is focused on practical issues related to analytical chemistry using miniaturised NIR devices to give to the readers an overview of the broad range of samples that can be analysed with these instruments, giving an idea of their applicability and of their current increasing use in different fields of applications. The different strategies of analysis used in the reviewed papers will be discussed to help to the reader to set up their own analytical methods, from the sampling to the data analysis.

This review has been therefore considered from an analytical point of view, primarily focussing on the type of samples (solid samples, liquid and fluid samples, gas samples), on the pretreatments (if any) and on the type of analysis (including parameters such as the number of replicates, number of scans, use of specific containers or sample holders …) made to the different type of samples.

The strategy of analysis greatly depends on the sample but also on the miniaturised NIR device used. The different miniaturised NIR devices that can be found on the market share some similarities but they may also be very different among them. For example, some of the miniaturised NIR devices have a small scanning spot and work well for homogeneous samples since they scan a small part of the sample. Some other devices have a larger spot so they also can work well for more heterogeneous samples, even if sample pretreatment is often performed as described in the following sections of the manuscript to overcome heterogeneity issues. Despite these differences, the miniaturised NIR devices have in common the logic of analytical setup since most of them have been designed to analyse rigid solids (not powders or liquids), although with a suitable analytical strategy other types of sample than rigid solids can be successfully analysed, as it will we shown in this paper.

From the optimised analysis for a given sample using a given instrument, interesting ideas can be taken for the design of the analysis of a different problem, giving to researchers useful inputs from the work of other colleagues in a new world of instruments that is growing very rapidly. This is the focus of this overview.

After the section covering the different type of samples, the paper focuses on instrumental calibration during the analysis, trying to understand the instrumental steps that need to be carried out to obtain successful measurements. Finally, the focus is set on spectral interpretation and data analysis, including data preprocessing and chemometric methods used to extract the useful information obtained with NIR miniaturised instruments.

Since there is an increasing number of publications and citations including miniaturised NIR spectroscopy [12], this review focusses on the papers covering the most interesting analytical applications reported in the last 5 years up to summer-fall 2021. The criteria of maintaining the name of the instruments and companies as they literally appear in the reviewed papers has been followed, despite some companies may have change their legal status: for instance, former JDSU (Milpitas, CA, USA) is currently Viavi Solutions (Scottsdale, AZ, USA).

2. Sample pretreatments and analysis

2.1 Solid samples

Solid samples have been divided into two main categories. The first one, named “Powder and ground samples” (section 2.1.1 of the manuscript), includes all samples that are analysed in the form of powder: samples that for their own nature are already powder or are typically marketed in powder form, or solid samples which, after being pretreated, become powdery. The remaining solid samples have been revised in the paragraph “Other solid samples” (section 2.1.2 of the manuscript).

2.1.1 Powder and ground samples

Several applications of miniaturised NIR instruments involving the analysis of powder and ground samples have been found and reviewed. Table 2 summarizes the articles. In the table, samples are listed according to the sample type, in alphabetical order.

Sample pretreatment

In applications where miniaturised instruments are used, one would expect to find analytical strategies in which the sample is analysed as it is, with no or almost no manipulation in order to obtain maximum portability. However, one of the first things that emerge from the reviewed articles is that in some cases samples are not analysed in their own form, but authors performed sample pretreatment steps before the spectroscopic analysis. Sample pretreatment often means the need for specific apparatus or reagents, and results of the analysis are not immediately obtained as the speed of a NIR analysis suggests, due to the time needed for the pretreatment step. The need for a sample pretreatment also leads to an interesting question: can the proposed analytical method be considered portable? This probably depends on the type of the sample pretreatment and on the possibility to perform the pretreatment directly in the field.

Forensic and pharmaceutical industry are the fields of application in which less sample pretreatment is observed. In the first area, the challenge is to fill the gap between police forces on the streets and the forensic laboratories, and thus to develop tools for police agents to produce immediate answers to forensic questions directly at the point of seizing [17]. For instance, cannabinoids in hemp flours [18] and illicit drug street samples [19] were both analysed without any sample pretreatment, proposing even in the latter case a mobile application that allows to classify illicit drugs and to quantify them in presence of adulterant or dilution agents[19]. In another application, a method for the detection of cocaine and its quantification was optimised [20], developing a very huge database (more than 10.000 spectra) using 15 NIR sensors (SCiO, Consumer Physics) and a multistage machine learning algorithm, allowing not only to make qualitative and quantitative analyses, but also to adapt the database in case of samples not yet analysed since the illicit drugs market is constantly evolving.

Regarding the pharmaceutical field, the process analytical technology (PAT) approach is surely the driving force for the development of real-time process monitoring strategies, where sample pretreatment is usually not possible. NIR spectroscopy has already been an adopted tool for PAT [1], and the rise of portable and miniaturised NIR instruments in the market has prompted researchers to test the use of these instruments within pharmaceutical processes. MicroNIR (MicroNIR PAT-U Viavi) was tested [21] in a pharmaceutical powder blend application, in which three active ingredients (ibuprofen, paracetamol and caffeine) and five excipients were present. Measurements were conducted at-line (in static conditions) and in-line (dynamic conditions) interfacing the instrument with a blender (Figure 1). Results obtained were satisfactory, but the authors reported lower performances with respect to a benchtop instrument. It is not surprising that the lower performances were attributed to the more representative transmission spectra and the improved spectral resolution of the benchtop instrument. The same miniaturised equipment was employed in another blending process [22] to perform a direct bilastine drug assay in mixtures. The authors developed a laboratory scale equipment and a manufacturing equipment, and in both cases successful results were obtained. A system to monitor the moisture content and the mass transfer rate in a fluidised bed using a sensor from Spectral Engines (model N—Series 2.2) connected to a NIR reflectance probe directly inserted in the fluidised bed drier was developed [23]. The sensor was shown to be a robust alternative for process monitoring, being robust to vibration and temperature changes, and straightforward to install. Another sensor from Spectral Engines was integrated into a software platform to monitor a solid-gas-liquid process for the production of saturated polyester resins [24].

Not only forensic and pharmaceutical samples have been analysed without any sample pretreatment. As shown in Table 2, the analysis of powder samples is often performed without any sample pretreatment.

It is worthwhile to notice that humidity absorbed from the air may affect the measurement of strongly hygroscopic samples. As an example, the determination of the moisture content in dried plant extracts with three handheld and two benchtop instruments was carried out [25]. Samples were analysed both in their native form and laced with a drying agent to oppress the strong hygroscopic properties of the dried extracts. The authors noticed, for native samples, a decrease in the prediction power obtained with all the spectrometers, probably due to the aggregation of the sample particles due to humidity absorbed from the air during the handling and the measurement steps. The addition of a dry agent represents an extra step compared to the analysis of the sample as it is, with an increase in time, cost and waste generated by the analysis, important factors when performing measurements with a portable instrument.

Drying through air is a common pretreatment in the case of soil analysis (see e.g. [26, 27]), but often samples are also crushed, grounded and sieved before the analysis. In an interesting application, spectra of soil samples were acquired in diffuse reflectance mode using a reflectance fiber optical probe directly immersed into the soil sample, immediately after the sampling [28]. Different soils were collected at 0–5 cm depth using a cylinder in the characterization of soil carbon and nitrogen [29]. Soil samples were subsequently air dried and sieved before measuring with a JDSU MicroNIR 2200 device. In other papers dealing with soils [30], the samples were air-dried (40 °C), crushed, and passed through a 2-mm sieve before spectra acquisition, or washed and sieved [31] to ensure homogeneous samples.

In another application, [32] water content was determined in fresh mulberry leaves. In the quantification of crude protein and soluble sugar, the leaves were dried, pulverised and sifted before the analysis. Whole and milled black pepper grains were analysed [33] with one benchtop and three handheld spectrometers, in order to quantify piperine in the samples. The authors concluded that only one of the three considered spectrometers, the MicroNIR 2200, was able to reliably measure piperine content in whole black pepper seeds. They hypothesized that the limiting factor for the other miniaturised sensors were the very inhomogeneous size and surface of the whole pepper seeds. Hom Mali rice was analysed [34] with the aim to classify samples according to the geographical provenance. In this case the authors tested ground and whole samples and found that whole dehulled polished rice was successfully classified without the need for any pretreatment.

Other authors faced the problem of sample inhomogeneity. This issue is very interesting to comprehend and face. Benchtop NIR instrumentation succeeds in the direct analysis of samples without the need for any preparation even in the case of inhomogeneous samples, due to the use of optimized diffuse reflectance accessories combined with sample spinners. Measurements are made during the spinner rotation and different parts of the sample are scanned, averaging out the inhomogeneities. In the case of portable instruments, dealing with inhomogeneous samples is not trivial, because such accessories are not available and the advantages of using them are therefore lost. Moreover, very often the area of measurement is very small (a few mm in some cases) making measurements even more complicated. The analytical strategies that have to be employed for inhomogeneous sample analysis with portable sensors may be very different from the ones for benchtop instruments.

Globally speaking, grinding into powder is the more common pretreatment that was found reading the literature, as shown in Table 2. For instance, tea was ground into powder and sifted [35, 36] in order to classify tea types and predict compounds related to the quality and taste of the investigated samples (catechin, caffeine, theanine and epigalloncatechin gallate). *Rosmarini folium* was milled before spectroscopic analysis [37] to predict rosmarinic acid in samples, and also whole coriander seed samples were ground to a homogeneous powder with the aim to classify authentic samples from adulterated ones [38]. Mechanical preparation (milling) was applied to black tea, with the conclusion that it likely removes spectral obstruction due to physical reasons (e.g. scattering) [39]. Even if milled samples are more homogeneous, in some cases the milling process may change the properties of the samples, as reported in the analysis of gluten-free grains in order to predict their antioxidant capacity [40]. The authors found that, in general, analysis of non-milled samples yielded better results. They hypothesized that the milling process made samples more vulnerable towards external influences, as their protective husk was removed through the milling process. The same authors [41] also compared a benchtop NIR instrument with 3 miniaturised NIR devices in the determination of protein content in millet samples. Samples were analysed with and without pretreatment. Due to the small size of millet, a cylindrical quartz cuvette was used to contain the samples. In this case, the best results were obtained with the benchtop device.

A quite large pretreatment for the analysis of peanut seed in order to quantify the chemical composition of the samples was presented [42]. The authors called the method rapid in the article title, but only the sample preparation step required 24h of drying before the grounding step, and the obtained powder was dried up for 20h at 41°C to remove moisture before spectroscopic analysis.

Sample analysis

In some commercial instruments, the miniaturised spectrometer is equipped with a sampler holder for powder or ground samples. For instance, MicroNIR Pro 1700 Viavi used for pharmaceutical raw material identification [43], is equipped with a vial holder.

Powder and ground samples often require a container. The fifth column of Table 2 reports the containers used in the revised articles. Cuvettes, vials and petri dish made of borosilicate, quartz or glass having no effect on the spectra [38] are the most used containers. Kibble (dog food) was directly analysed in a plastic bag (the material is not specified) by applying the scanning head of the SCiO at 1 cm above the surface [44]. It is worth noticing that using a container may affect the sample spectra. The most appropriate container will therefore be the one that will not affect the ability of the method to see differences between samples.

Depending on the used sensor, several parameters like the number of scans or the scanning time needed to be optimised, as well as the distance between the sample and the sensor, to name a few parameters. But in most of the reviewed articles, the authors did not describe how did they optimize the instrumental parameters. A good description of the sensor configuration and experimental setup can be found using a S2.2 sensor (Spectral Engines) [27] for the estimation of soil properties. The authors considered the distance between the sensor and the sensed surface, and the light intensity of the device, evaluating ten different configurations. They concluded that the experimental configuration affected the measurements, and thus this kind of optimization is strongly recommended when using sensors that allow the instrumental parameters to be set, and that can scan the sample at different geometries.

Similarly, replicate measurements were typically performed to take representative measurements from the sample. The authors reported in many cases how many replicates did they perform on the sample, without however describing how did they determine such optimal number. When dealing with homogenous samples, miniaturised NIR devices with small or with large scanning spots may be used, but when dealing with heterogenous samples, devices with large scanning spots should be preferably used to account for information from different parts of the sample.

What emerged from the literature is that measurements were often taken rotating the petri dish or the cuvette containing the sample, in an attempt to increase the representativity of the measurements. For instance, flour samples were analysed [45] placing them in a rotating dish and smoothing the surface of the sample. In this case, the spectrometers (MicroNIR 1700 Viavi, NR 2.0-W Spectral Engines, and Si-Ware NeoSpectra), were mounted above the sample surface (1-2 mm distance) and during the measurements the dish rotated at 2 revolutions per minute to eliminate sample heterogeneity and to capture a larger sample area. An average spectrum was then obtained for every sample. It is worth noting that in the study, as in other reviewed articles, the instruments needed to be fixed to a support system to standardise the acquisition stage and distance from the samples (Figure 2). In another example, a quartz container was used to analyse green tea for quality control purposes [46]. In this case, the quartz container filled with tea was placed over the sensor, and each sample was scanned three times after a rotation of 120° to eliminate the scattering error caused by the nonuniformity of the sample. The average spectra were then calculated. Better spectral replication was obtained positioning the sensor under a petri dish containing the sample in an interlaboratory study [47], in which oregano adulteration was detected using a SCiO device. Milk powder was analysed [48] with two miniaturised spectrometers to quantify melamine using a cylindrical cuvette (no references about the material of the cuvette) as the sample container. Two different measurement procedures are described for each of the two spectrometers, both considering replicate measurements in different spots of the cuvette. Only in one of them the cuvette was refilled with the same sample for three times, and the averages of the obtained signals were considered as the sample spectrum. The authors used a temperature control device to increase the signal to noise ratio. A thermoelectric cooling appliance was employed in another application [37] to maintain the temperature of the spectrometer (in this case a MicroNIR 2200 was used) between 28 and 30°C.

2.1.2 Other solid samples

Miniaturised NIR instruments have also been applied to the analysis of a variety of solid samples. Table 3 summarizes the reviewed articles. In the table, samples are listed according to the sample type, in alphabetical order.

Sample pretreatment

In the articles reviewed in this chapter most of the solid samples have been analysed without any pretreatment. Therefore, this type of samples seems to be the most prone to be used in truly miniaturised analytical methods, without the need for any other step.

Foods are the most analysed type of solid samples without pretreatments, aiming to a rapid check of quality parameters, including classification or assessment of freshness. Among foods, fruits have been widely analysed with miniaturised NIR instruments. Some examples of fruit analysis include the determination of four fruit quality parameters in apples with Viavi MicroNir 1700 [49] obtaining similar predictive performances to the benchtop spectrometer in comparison, the determination of dry matter content in avocado fruit as an index of eating quality of ripened fruit [50], the analysis of different horticultural products (kiwifruit, apple, feijoa and avocado) to predict their quality by developing prediction or classification models showing the applicability of miniaturised NIR instruments to different types of fruits [51], or the determination of quality parameters such as dry matter and total soluble solids in peach and table grape [52], obtaining good correlation using one miniaturised instrument and one portable device (Consumer Physics SCiO and Felix Instruments F-750) with the reference values. Two miniaturised NIR instruments (with some degree of wavelength overlapping) and the use of sophisticated chemometric techniques such as data fusion were used for the prediction of moisture and soluble solids in pear fruit [53]. Miniaturised NIR instruments have also been used in field analysis: grape was analysed in commercial vineyards using Thermo Scientific MicroPhazir successfully assessing the water status and total soluble solids under field conditions [54, 55]. Small fruits similar to grape have also been successfully analysed with miniaturised NIR instruments [56]: titratable acidity and ascorbic acid content in acerola fruit during ripening were assessed, obtaining with Viavi MicroNir 1700 comparable results to the ones obtained with a FT-IR spectrometer. A miniaturised NIR system was fabricated from two commercially integrated modules to measure the total soluble solids as a way to assess the quality in sweet cherries obtaining satisfactory results [57] and several nutritional parameters were quantified in mulberry fruits [58] using the DLP NIRscan Nano. All these papers analysing fruits prove that miniaturised NIR instruments can successfully be applied to the rapid analysis of different quality parameters in fruits of different sizes, provenances, composition, and even in field analysis in the absence of lab-controlled conditions.

Among food, not only fruit has been the objective of the analysis of miniaturised NIR devices without the need for pretreatments. Eggs have also been analysed using different miniaturised instruments to estimate their freshness or to predict the storage time [59–61]. In all cases, and similarly to the case of measuring entire fruits, contact measurements were made.

Samples with some degree of heterogeneity are challenging samples to be analysed without pretreatments because there is always the analytical need to obtain representative measurements of the globality of the sample. Meat can be seen as a heterogeneous sample, but some papers have analysed this type of sample without the need for pretreatments. In the analysis of meat samples, samples are typically scanned at different points and then the spectra are usually averaged. Some examples include assessing chicken meat authenticity [62], monitoring the processing of dry fermented sausages [63], assessing the quality of Iberian hams [64] or detecting pork adulteration in sausages [65], although in this latter case better results regarding fat adulteration were obtained with NIR laboratory equipment.

Fish samples may present a similar degree of difficulty to meat when being analysed by NIR miniaturised instruments. Several papers directly analyse fish samples without the need for pretreatments. For instance, the assessment of the authenticity of fish fillets and patties using a Viavi MicroNIR OnSite (distinguishing fillets and patties of Atlantic cod from those of haddock) [66] can be mentioned.

Other food samples have also been analysed without the need for pretreatments. Viavi MicroNIR 1700 was used in the successful identification of adulterants (corn and peels/sticks) and in the distinction of roasting level between Arabica and Robusta coffees [67]. Consumer Physics SCiO was used in the analysis of single grains to successfully discriminate cultivars of barley, chickpea and sorghum in Ethiopia [68]. In this paper it is not clear how many spectra were obtained from each grain and if the spectra of the different grains were then averaged. In another application, several parameters for routine quality control in compound feeds for a wide variety of animals and using different presentation forms (crumbs, pellets and meals) were determined [69]. The authors used two different NIR miniaturised devices (Polychromix Phazir 1624 and JDSU MicroNIR 1700) and the external validation resulted in satisfactory results to attempt a compound feed control. However, all the samples analysed were certified reference materials from different proficiency test programs, and certified reference materials are homogeneous samples by default, remaining doubts about the performance of these instruments in commercial samples probably presenting a higher degree of heterogeneity. 200 walnuts were individually assessed [70] at 6 different locations of the nut for varietal discrimination. The authors concluded that the results obtained seem to be useful for the discrimination. The direct analysis with Consumer Physics SCiO of 50 g of rice into glass containers (rotating the container three times) was used [71] for the detection of rice authenticity and quality, obtaining more than 90% classification rate for all the categories of rice samples studied. 150 varieties of peanuts were analysed with a benchtop and a miniaturised NIR device (Viavi MicroNIR 1700) in an attempt to differentiate peanuts according to the high oleic acid content and major fatty acids [72]. The results obtained with both instruments were found to be similar, and the authors claimed that that the miniaturised device can substitute the benchtop device to make raw material purchase and breed variety faster and more efficient. A rotating sample holder was used in a system based on the Texas Instrument NIRscan Nano module to analyse the quality of dairy farm forage by analysing nutritional parameters such as crude protein, acid detergent fibre and neutral detergent fibre, obtaining a method for the evaluation of the quality of forage in real time [73].

Other papers deal with already preprocessed samples such as ground or minced meat [74–76], chicken parts [77] or grated cheese [78], with the analytical method not adding any extra pretreatment step to the samples.

Other solid samples than foods have also been analysed with miniaturised NIR instruments without the need for pretreatments. Pharmaceutical goods probably benefit from the homogeneity of most of their products in the search for a rapid and simple quality control or for the detection of counterfeit products [79]. The performance of two NIR devices (a benchtop FT-NIR and the miniaturised device Tellspec NIR-S-G1) was compared with two handheld Raman systems in the detection of falsified pharmaceutical products (including artemether-lumefantrine, paracetamol and ibuprofen) [80]. The NIR products offered more reliable performances than their Raman counterparts, with the low-cost devices offering promising performances almost comparable to benchtop systems. Interestingly, all the tablets and capsules were directly scanned through their blister, making the process faster and prone to automatization. A somewhat different kind of pharmaceutical products that have also been analysed with miniaturised NIR devices are orodispersible films [81, 82]. These films are single or multilayer sheets of suitable materials intended to liberate rapidly the active substance in the mouth without the need for administration with water. These films may be an option for extemporaneous preparations or for personalised medicines. They are flat films with a moderate surface, which makes them very good samples to be directly analysed covering all the window of the miniaturised instrument. Related to pharmaceutical products, ThermoScientific MicroPhazir and a benchtop NIR device were compared in the prediction of the optimum harvest time of *Verbena officinalis*, a herb listed in European Pharmacopoeia and which extract is used in the fabrication of medicines [83]. The benchtop instrument showed slightly better prediction performances of the active compounds present in the herb, but both instruments demonstrated the ability of performing direct measurements on pharmaceutically relevant fresh plant material.

For the nature and the value of their samples, cultural heritage specimens should ideally be treated in the less invasive possible way. A miniaturised NIR prototype developed in collaboration with Viavi was used to analyse archaeological bones, cinematographic films and bronze patinas to enable rapid information acquisition to guide restoration strategies (Figure 3) [84]. Paper in ancient documents was analysed as a non-destructive way to investigate paper ageing and solving dating problems [85]. In a related field, three non-commercial miniaturised NIR devices covering different wavelength ranges were used to assess elephant ivory provenance by analysing raw ivory [86]. Regarding cultural heritage, in which infrared spectroscopy is largely used especially in the mid-infrared (MIR) region [87], it is worthwhile to recall that NIR radiation penetrates more into the sample, because it is a more energetic radiation than MIR radiation. NIR radiation may therefore not be suitable for the analysis of very thin surface layers (e.g. paintings) because it may penetrate too much and collect information from the bulk of the sample.

In other cases, only small pretreatments like washing fruit [88, 89], mixing and transferring to a sample container in the case of forage samples [90], or flattening/partially flattening plastic samples [91] were applied. Probably these pretreatments would not prevent the analytical measurement from being considered portable.

However, in some cases other steps than the direct instrumental measurement from the solid sample were applied. In these cases, laboratories can benefit from the low cost of miniaturised NIR devices compared to benchtop instruments, but depending on the number and type of pretreatments, some analytical measurements involving miniaturised NIR devices may not be considered as totally portable. Not surprisingly due to the specific nature or degree of homogeneity of some of the samples, food and soil samples are included into the ones that may need pretreatment steps prior to spectroscopic analysis. In this way, grape skins were separated from whole grapes for the determination of extractable polyphenols in red grape [92], and the grape skins were soft-pressed inside the bottom of a quartz cuvette and measured using a Viavi

MicroNIR Pro Lite 1700. This was made to avoid differences in reflectance due to different grape curvature. In another application, the performance of a miniaturised NIR spectrometer, Texas Instruments NIRscan Nano, was evaluated for the prediction of intramuscular fat in lamb [93]. In this study, lamb meat, devoid of any subcutaneous fat, was minced and frozen at −18 °C followed by freeze drying for 72 h. The authors compared the miniaturised NIR device with benchtop instruments and they concluded that the miniaturised device can be a potential alternative to benchtop spectrometers for rapid and real-time classification of fresh lamb meat. In another food application, slices of potatoes were analysed to identify sprouting activity in potatoes during storage [94]. Finally, in another application dealing with food, cheddar cheese was analysed with Consumer Physics SCiO aiming to predict total protein and intact casein content [95]. The authors reported that shredding cheese provided the most consistent and repeatable NIR spectra.

An interesting paper [96] deals with the detection of wood defects as an alternative to visual grading of wood quality. Two prototypes and one commercial miniaturised NIR device were developed for this task. They used wood disks cut from trees, with the future aim to implement NIR spectroscopy for automatic grading of logs directly in the forest.

Sample analysis

Because of the nature of solid samples, reflectance measurements are typically done using miniaturised NIR devices. Only a few studies reported spectra acquired in transflectance mode [82, 84, 97] using a reflector behind the samples (Figure 4). Most of the miniaturised NIR instruments require or have better performances with direct contact between the solid samples and the scanning window. It is important to mention that several papers do not describe the type of measurement (contact or distance), and sometimes this is an information that must be derived from the type of sample and the specific instrument. Most of the previously reviewed solid samples (with or without pretreatment) are analysed with contact scanning. Instruments requiring or preferably working at contact distance are useful to directly analyse samples that are big and flat enough to cover the scanning window without the use of any special sample holder or container. Instruments also able to make non-contact measurements may offer a higher degree of versatility towards the sample to be measured, also decreasing the possibility to damage the scanning window. To mention some examples of non-contact measurements, Viavi MicroNIR 1700 was used to measure ready-to-eat pasta with sauce [98] by scanning at a distance of 1–2 mm above the sample surface and SCiO was used to predict the quality of horticultural products with the illuminator pointing at the fruit skin [51].

Smaller samples, or samples not fully covering the scanning window, may require a sample holder or container in order to have the scanning window fully covered with the sample (for instance 50 g of rice were collected into glass containers and further scanned with Consumer Physics SCiO [71]) or to increase the homogeneity of the measured samples, although SCiO has also been used in the analysis of single grains [68] using the SCiO sample holder. In the case of forages, a plastic container was used to contain 2-3 g of forages prior to the analysis in the comparison of four different instruments (benchtop and miniaturised) with different spectral ranges [90]. The authors pointed out the importance of selecting an instrument with the right wavelength interval.

Instrumental parameters such as the number of scans or scanning time (in case these options are available in the configuration of the measurement, which is not always the case) are typical key parameters that should be optimised to obtain the best instrumental response. But in most of the reviewed papers, the authors simply present the used configuration without describing the optimization process. Nevertheless, some authors [64, 73] used different scanning approaches to find the best analytical results.

A challenging analytical problem is measuring solid samples with some degree of heterogeneity, where the number and position of replicates may be a critical point when trying to obtain representative measurements. Typically, the spectra are acquired at different positions of the sample, usually between two and four, normally averaging then the acquired spectra. But even 11 different scanning points were selected to discriminate between authentic and counterfeit banknotes [99] or 50 spectra were taken for each sample of animal feed at different sampling points [69]. An example of these strategies is the analysis of eggs with DLPR NIRscan Nano [59], in which spectra were acquired at three different locations of the eggshell, and then different combinations of the locations were tested in order to find the best prediction ability of the freshness of the eggs. Also within food samples, spinaches are a good example of this type of samples. Different strategies involving measurements at different points of a leaf and at different leaves of a plant using a Viavi MicroNIR 1700 were developed [100, 101] for the direct and rapid measurement using miniaturised NIR instruments.

2.2 Liquid and fluid samples

The application of handheld and miniaturised spectrometers to the analysis of liquid and fluid samples that were considered in this manuscript are reported in Table 4. In the table, samples are listed according to the sample type, in alphabetical order.

Sample pretreatment

Liquid and fluid samples are often analysed in their own form. Bovine milk is one of the most analysed liquid samples, and this is not surprising given its nutritional importance all around the world. Several authors did not perform any sample pretreatment before the spectroscopic measurements. For instance, samples were hand mixed or gently shaken before the analysis of raw milk [102, 103] and commercial milk samples [104]. Raw goat milk samples were analysed to detect adulteration with cow milk, and before the analysis both type of samples were subjected to a heat treatment of 65°C for 30 min with subsequent cooling at 4°C [105]. A more complex sample pretreatment was carried out [106] studying the lipid degradation during the time of storage of human milk.

Concerning fluid samples, resin was directly analysed [107] through the sealed bags employed for the sampling using an accessory provided by the Consumer Physics SCiO manufacturer to avoid ambient light interferences. In another application, honey was analysed to detect frauds and to verify authenticity [108]. Before the spectroscopic analysis, non-filtered samples were incubated in an air-oven overnight at 55°C to dissolve any crystal present in the sample and they were left to equilibrate to ambient temperature before the analysis. A heating treatment at 70°C was also applied to homogenize crude palm oil samples before the spectroscopic analysis [109].

Sample analysis

How to measure liquid samples is not obvious when dealing with miniaturised NIR spectrometers. While some devices are equipped with accessories that facilitate the analysis, in some cases the authors had to design and optimize an analytical strategy to perform the measurements.

Viavi MicroNIR 1700 Pro was used [110] to analyse adulteration of extra virgin olive oil with vegetable oils. Two accessories, for transmission and reflectance modes, were named in the article. The same sensor and accessories were used [111] to detect the presence of lard adulteration in palm oil. Again the same sensor, equipped with the vial holder and the droplet accessories, was used to analyse fuels and oils [112]. In particular, the last accessory allowed measurements simply putting a droplet of sample on the sapphire window of the accessory.

Very interesting strategies have been found during the bibliographic research when miniaturised devices were not equipped with specific accessories for the analysis. A filter paper was used as the media to contain beer samples [113, 114]. The paper was soaked with the sample and immediately measured to avoid any loss of volatile compounds. All the readings were performed placing the filter (with or without sample) in between the spectrometer and the white background, in order to avoid the signal noise due to environmental factors.

The blank filter was also analysed, and its signal was subtracted from the sample signals. The calibration of the system was performed every 15 minutes with the white background. A low-cost in-house developed accessory (patent pending) was built to analyse organic solvents using the Consumer Physics SCiO sensor [115]. The accessory that the authors developed allowed the analysis of transparent liquids and the determination of low water concentration (approx. 0.01 wt%) in organic solvents, paving the way for other industrial and research applications. Potato chip frying oil was analysed putting a drop directly on the sensor surface (Si-Ware NeoSpectra Micro), and the oil was covered with a reflectance accessory [116]. A flow microreactor was coupled to a miniaturised sensor (Viavi MicroNIR) with the aim to in-line monitor the dehydration of D-fructose to 5-hydroxymethylfurfural [117]. A flow cuvette between the lamp and the sensor was used (transmittance mode), and the authors declared that the sensor gave excellent responses to different flow rates (Figure 5).

Liquid samples are often analysed with the use of cuvettes or Petri dishes. According to the scope of the research, different configurations have been used to obtain suitable spectra. It is worthwhile to note that, in some cases (see e.g. Si-Ware NeoSpectra development kit), the sample container must cover all the sensor surface.

When Viavi devices were employed, the transmission mode can easily be used thanks to the accessories supplied by the manufacturer. But most of the spectrometers are not equipped with a transmission accessory, and home-made solutions must be found in these cases. As an example, a system to perform measurements of vinegar samples in a 2 mm pathlength transmission cell was developed [118], using the empty cell as the reference spectrum.

Some strategies were proposed to perform transflectance measurements. This way of measure is a good alternative when transmission is not feasible. For instance, milk was analysed with the aim to classify samples according to the presence or absence of lactose [119]. The authors placed the sample in a petri dish, and an aluminium diffuse reflector was placed over the petri dish, with the sensor on the opposite side. The beam passed through the sample and then it was reflected back again through the sample towards the detector (5 mm pathlength). An opaque liquid cap that allowed to perform transflectance measurements (17 mm path length) was employed in the monitoring of fatty acid profile in raw milk [103]. In a paper describing a very detailed optimization of the measurements for milk analysis (protein, fat and solids-non-fat), the authors concluded that they needed to use a 17 mm sample thickness cuvette with an aluminium backside to obtain satisfactory results using a Thermo Scientific Microphazyr device [102], while in another paper [120], some of the same authors with the same spectrometer, quantified the same parameters in reflectance mode using a non-linear approach for the data modelling. A transflection strategy was used to determine the main sugars in syrup formulations, using a quartz cuvette equipped with a stainless steel reflector (path length of 0.6 mm) [121]. A transflectance home-made cell was also proposed [122] in the quantification of biodiesel and adulteration with vegetable oils in diesel/biodiesel blends.

Concerning milk analysis, several authors analysed milk in reflectance mode. Several adulterants in milk samples were tried to quantify and it was observed that, as the adulterants were mainly liquids (e.g. tap water, hydrogen peroxide, synthetic urine) the adulteration included a dilution process which drove to the clustering of samples according to the type of adulterants [123]. So, the authors decided to model the dilution level instead of the concentration of specific adulterants. Fat content in milk samples were also quantified using two miniaturised devices in reflectance mode using a quartz cuvette of 10 mm path length [104]. But when the authors tried to quantify the protein content, the results were not so good. Probably in this case the authors were able to take advantage of the concentrations of fat (low, medium and high concentration) in a sort of 'dilution' of fat globules in milk samples. The reflectance mode was also successfully used [105, 124] in milk classification issues. It is worthwhile to note that some authors rotate the sample holder during the measurements to catch the sample variability, similarly as the case previously seen for powder and ground samples (see e.g. [125]).

In a very interesting application concerning on-line monitoring of biodiesel production (see [126] and references therein), the authors made an accessory that was used for transmittance measurements, allowing to set the optical path length. The authors prepared synthetic blends using a mixture design approach in order to optimize this experimental variable and to build and validate the multivariate calibration models. The conclusion was that the results were satisfactory and comparable with the gas chromatography results, although there were adverse conditions in the monitoring processes ascribable to the high amount of ethanol in the reaction mixture.

2.3 Gas samples

A few applications have been found in gas analysis. Acetylene, carbon dioxide and water vapor gases were detected with a home-made sensor [127]. The sensor covered the MIR and the NIR spectral ranges, but NIR resulted in the best sensitivity. A cheap handheld NIR spectrometer (Texas Instruments NanoNIR) and a tungsten lamp were coupled to a lab-made NIR flow cell for the automatic quantification of methane, ethane, and propane in natural gas and biogas samples [128]. The analysed mixtures were prepared following an experimental design strategy and obtained good results without any pretreatment of the NIR signal. A recently published application [129] reports about using Si-Ware NeoSpectra micro-FT-NIR OEM version for the analysis of methane, ethane, propane, butane, CO_2 and N_2O. The authors, in a way to acquire NIR spectra of gaseous samples by means of diffuse reflectance, mixed the sample with a dense medium (polytetrafluoroethylene) to promote light scattering since gas samples do not reflect the NIR radiation that could be detected using this type of geometry.

3. Instrument calibration

A small number of articles describe how the instruments were calibrated, and if further calibration was needed during the analytical session. Perhaps the authors take this for granted, as the manufacturer often provides the necessary details (typically the use of a blank or black reflectance standards). Some authors (see e.g. [38, 104, 130, 131]) reported the need to warm up the spectrometer lamp before the use, as one might expect since the used lamps are typically tungsten lamps (see Table 1). Wang et al. [132] optimised the warm-up time repeatedly measuring a reflectance standard until the spectral measurement was stabilised: the device (Si-Ware NeoSpectra micro) required 5 minutes of warm up time. Concerning the heating of the lamp, tungsten lamps (like the ones used in Viavi MicroNIR or Si-Ware NeoSpectra Micro development kit) emit heat, which may affect the stability of the investigated samples. For this reason, some authors proposed a solution involving LED lamps [133]. In some cases, a background (Spectralon was the most used reflectance standard, although some devices such as SCiO come with their own integrated standard) was conducted at the beginning of each measurement day [51] or it was repeated during the analytical session at different intervals. Typically, the manufacturers provide recommendations about the frequency of calibration, including (for instance for Si-Ware NeoSpectra Micro development kit) the requirement for a warming time (see the discussion above about the warm-up for tungsten lamps). The frequency of calibration depends therefore on each individual instrument and this is a parameter to be optimised. Interestingly, some authors [62, 70, 72, 92] used a two-point reflectance calibration, corresponding the reflectance standard to 100% reflectance, and the 0% reflectance was obtained by taking a measurement placing the device 50 cm away from any object. There is also described a more sophisticated system that includes measurements of internal soil standards [27].

It is well known that the effective pathlength of NIR radiation for diffuse reflection measurements varies depending on the wavelength and on the material, and it may vary from several hundred micrometres to millimetres [98]. In order to better understand the measuring process and the obtained signal, the penetration of NIR radiation into mango pericarp tissue [89] and into umbu [88] using a Viavi MicroNIR 1700 were evaluated to estimate the effective sampling volume of the fruit observed by the instrument.

A very reduced number of articles reported data concerning the long-term stability of the sensors. An experiment over a period of 5 days (8h/day) in a process control context using the Viavi MicroNIR was conducted [117]. The authors noticed that the spectra presented an offset in the baseline, that they attributed to variation in the temperature of the radiation source and of the detector, typical for single-beam equipments. This variation can be corrected easily with the application of derivative data pretreatments. The repeatability and reproducibility of Felix F-750 (a portable equipment), Tellspec and Consumer Physics SCiO (miniaturised devices) were evaluated [88] at selected wavelengths, obtaining different repeatability and reproducibility values for the three devices. Nevertheless, the multivariate calibration models developed with the three devices showed similar predictive performances and accuracies in the determination of umbu quality parameters.

In another paper, the instrumental calibration of DLP NIRscan Nano engine was verified [134] according to a well-established calibration verification procedure outlined by the USP (US Pharmacopeia) < 1119>. The authors tested the photometric linearity, performed a wavelength verification by scanning a standard material as suggested by USP < 1119>, and determined the signal-to-noise ratio. The authors stated that the handheld NIR device passed the instrumental verification procedure.

4. Spectra interpretation and data analysis

As reported in the fifth column of Table 1 or in the third column of Tables 2-4, and in more detail in the review published by Bec et al. [8], the handheld and miniaturised NIR instruments show a limited wavelength range if compared with benchtop NIR instrumentation. This leads, in some cases, to a reduced performance depending on the application considered. As an example, three miniaturised instruments were employed to predict several properties in dried, ground forage samples, and the authors concluded that the miniaturised instruments had no comparable performances with respect to the benchtop device [90]. It is important to mention that the wavelength ranges were quite different between the tested instruments. Several papers [25, 33, 38–40] reported interesting images in which the signals collected by different miniaturised and benchtop instruments are compared, and quantum mechanically simulated NIR spectra are also given.

Focussing on Consumer Physics SCiO, it is worthwhile to note that the spectra are presented to the user only after preprocessing, and for this reason the comparison of these spectra with raw spectra recorded with other instruments [33] needs to be done with care. It is worthwhile to note that the SCiO spectral range (740-1070 nm) reaches into the visible region. This can be an advantage, if the lightness or the darkness of a sample strongly correlates with the analyte or the property under study. Otherwise, this may be a source of noise, and the elimination of the visible parts of the spectra may improve the performance of the sensor. Moreover, the lower the wavelength, the higher the penetration into the sample. This is quite irrelevant in truly homogeneous samples, but it may be an advantage when outer layers are contaminated [40]. It is also important to mention that chemical signatures are more intense at higher wavelengths [135], what should also be taken into account when deciding the wavelength range and hence the specific instrument to use.

Some authors found in their analysis discrepancies between the working regions described by the manufacturers and the experimentally determined working regions. Both Viavi MicroNIR 2200 and Thermo Scientific MicroPhazir gave wrongly measured spectra in the lower wavenumber regions in the analysis of *Theae nigrum folium* if compared with the reference benchtop equipment (Buchi NIRFlex N-500) [39]. Almost the same distortion was observed in the analysis of piperine content in *Piper nigrum* [33] (Figure 6) and in the determination of moisture in plant matrices [25]. No specific details about the measurements in Figure 6 are provided (e.g. use of cuvettes, contact or distance measurements) what can also contribute to the differences among the recorded spectra. Another way to compare spectra from different devices was using two-dimensional correlation spectroscopy (2D – COS) to identify discrepancies between the signals recorded [37]. A wavelength-by-wavelength comparison between the two tested instruments (Felix F-750, a portable equipment and SCiO, a miniaturised sensor) and a standard solid object (white Teflon sphere) at different room conditions was made, observing strong differences between the devices [52]. However, the fact that the spectrum recorded by a portable sensor does not exactly match with the theoretical one or with the spectrum measured by a benchtop instrument, cannot negatively influence the possibility of developing reliable analytical methods with portable sensors. On one hand, if the difference between the spectra of the different samples is maintained, even small deviations from the theoretical spectrum would not significantly affect the performance. On the other hand, when the deviations observed from the theoretical spectrum make different samples to appear similar, then it is useful (or necessary in some cases) to remove that spectroscopic zone in order not to add noise to the data. What certainly creates complications when observing deviations between the spectrum of a portable instrument and a benchtop one, is in the transfer of calibrations, a topic that has not yet been extensively treated in the literature as commented in the conclusions of this paper.

From Figure 6 is interesting to remark the short wavelength range of SCiO compared with most of the reported miniaturized NIR devices (what can also be seen in Table 1). This short wavelength range is typically associated to a low information content. Nevertheless, for certain applications the use of proper chemometric techniques on the SCiO data is able to produce reliable qualitative and quantitative results as it is shown in the different reviewed papers.

Spectra were recorded in replicates in almost all the revised papers. Replicates were then averaged to obtain a spectrum representative for each sample, and multivariate modelling was employed mainly for classification or prediction purposes. Some authors [101] checked the quality of the measured spectra by using the root mean square (RMS) statistic [136] in an attempt to obtain representative spectra for a given sample. As it is well known, spectra preprocessing is essential in NIR calibration (see [137, 138] and references therein) as it allows to remove unwanted signals in spectroscopic data. Smoothing, baseline correction, derivatives, standard normal variate (SNV) and multiplicative scatter correction (MSC) are the most used data pretreatments, mainly in combination between them (SNV and MSC both correct scattering, and thus they are never used simultaneously). It is clear that these transformations may affect the interpretation of the outcomes and so they have to be carefully selected [139].

Once suitable spectra are obtained, explorative, classification and prediction modelling can be developed. A crucial point in multivariate modelling is the choice of samples to be used in the calibration and validation steps, and thus the choice of the validation system. Concerning this topic, a very interesting tutorial [140] illustrates how the level of validation and the choice of the methods for analysing data may impact the conclusions and the chemical insight gained in analytical problems.

Calibration samples used to build the multivariate models should include all the sample variability. Ideally, the more samples analysed, the more variability included, but if the variability sources are known, experimental design can be successfully used to choose the calibration samples. For instance, D-optimal design was used (see [21] and references therein) to choose 31 different formulations to be used as the calibration set to predict content uniformity in a blend monitoring. A ternary mixture design was employed [48] to choose 10 milk powders (infant formula) samples to buy in supermarkets including the maximum variability, and to be used as the base for a series of melamine artificially adulterated samples with 11 levels of adulteration.

In most of the revised articles, the authors did not report in detail how the samples were divided into calibration and validation sets. The two data sets should be independent, but often this is not possible due to limitations in the collection of samples. The choice of a sample selection method and the limitations of the chosen method should be therefore carefully considered. Some authors specify that a random choice was performed (see e.g. [38, 42, 44, 52, 60, 64, 69, 70, 86, 103, 113, 120] – reporting in [120] a double external validation) while other ones used mathematical algorithms to choose the calibration and the validation samples. This means that they made this choice driven by the chemical features of the samples, which are reflected in the spectral shape or in the chemical property used as the reference value in the case of prediction models. The two datasets are therefore not strictly independent from each other, what can be even more important for small data sets. A comparison between the prediction error obtained by models built by random selection of the calibration set and by selection driven by a mathematical model, may give to the researcher useful information on the data and on the robustness of the chosen method. Resampling of the calibration set may give also interesting information. Only a few articles reported cross-validation as the only validation method, and for this reason the results presented could be considered only a proof-of-concept, as external validation is mandatory to obtain definitive models.

The Kennard-Stone (K-S) algorithms was surely the most used algorithm (see e.g. [25, 39, 40, 53, 76, 104, 105, 125, 133, 141]) to find the calibration and validation sets. The algorithm selects, for the validation set, samples that best represent the average samples, according to the Euclidian distance from a given sample to all the other samples in the data set. Samples with the highest distance to the average are then included in the calibration set. This ensures that the test set variance is fully contained in the calibration set and that it can lead to better calibration results if compared with the random sample selection (see e.g. [33] and references therein). However, sometimes the Kennard-Stone algorithm leads to over-optimistic results. To avoid this problem, the Duplex algorithm can be used (see e.g. [48, 62, 76, 107, 108, 142]). This algorithm overcomes the problem of obtaining over-optimistic results by distributing the variance in a more balanced way between the calibration and the validation sets [140].

While the Kennard-Stone or Duplex algorithms divide the samples according to the spectroscopic features, in another paper samples were selected for the calibration and validation sets according to the value of ***y***, the property to predict [143]. In this article, describing the prediction of fatty acid in wheat flour, the authors chose the validation samples so that they were homogeneously distributed with respect to the fatty acid content determined by the reference method. A similar approach was used in [37, 46]. These splitting methods are described in column eleven of Tables 2-4 as semi-random. Another algorithm often used to select datasets is the Sample Set Partitioning based on joint X-y distances (SPXY), employed to select samples according to their differences in both **X** (instrumental responses) and ***y*** (predicted parameter) spaces [144].

Another important issue that should be considered when performing a multivariate model is to catch all the system variability, collecting measurements in different conditions (environment, operator, day…). As an example [145], measurements on commercial milk powder were performed in different days to include the potential day-to-day variance into the model. Samples for external validation were analysed in multiple days of the collection, two days of which were completely independent of the calibration days, to evaluate the robustness of the developed model. Catching all the system variability should always be the way to develop a reliable chemometric model. Related to considering the different conditions when building the model, it is worthwhile to recall that chemometric models need a maintenance. They should be periodically updated to reflect the variation of samples during time, as e.g. in the case of the market of illicit drugs which is in continuous evolution [19] or even food, where the authors proposed an interesting discussion on the calibration model maintenance [45].

Linear multivariate models are the most employed models to analyse spectroscopic data. Depending on the research purpose, principal component analysis (PCA) as exploratory analysis, partial least square regression

(PLSR) as regression method and partial least-squares discriminant analysis (PLS-DA) and soft independent modelling of class analogies (SIMCA) as classification methods, were the most used techniques as shown in Tables 2-4, column nine. Only a few articles reported better results using non-linear methods.

It is worthwhile to recall that when the predictors influence the response in a direct way, a linear multivariate method should work if the experiment is properly set and the analyte to be predicted lays above the detection limit. But the predictors may also influence the response in an indirect way, and therefore non-linear data may be produced. In this case, non-linear methods should be employed. Although non-linear methods have been widely applied in spectroscopic calibration since 1990s, their application has some disadvantages that should be considered when choosing the multivariate method to use. Among the disadvantages, we can mention the enlarged risk of over-fitting that leads to require very large data sets [146]. To mention some examples using non-linear methods, pharmaceutical raw materials were identified with supervised pattern recognition using support vector machine (SVM) [43] or a correct classification rate of 98.33% was obtained for different tea types using nonlinear radial basis function-support vector machine (RBF-SVM) [35]. The same research group detected green tea adulterants: a qualitative discrimination of 97.47% for the prediction set was achieved with SVM, and also the quantification of the adulterants gave good results with a support vector machine regression model (SVR) [46]. In both cases, the Innospectra Corporation NIR-S-R2 spectrometer was used. SVM was also used to classify and predict quality and freshness of eggs [59], obtaining similar classification and prediction rates than using linear models. Artificial neural networks were also used to predict the egg storage time [60], obtaining better results than using PLSR techniques. Extreme learning machine (ELM) was successfully employed to predict fatty acids in wheat flour [143], while artificial neural networks allowed the determination of moisture in a complex plant matrix outperforming benchtop devices [25]. A neural network based-model was also used [120], in which the authors developed a mobile application to be connected with the miniaturised spectrometer to get in situ real-time estimation of chemical quality control parameters of cow milk. SVM was also used to build a calibration transfer model between a benchtop instrument and Viavi MicroNIR 1700 [49], successfully using a historical and very large database acquired using the benchtop spectrometer for the determination of several parameters in apples.

A few articles reported multivariate models built following a data fusion approach. Data fusion methodology can be briefly described as a system that allows to combine the results from multiple sources (instrumental sources are typically used, but other type of data such as e.g., sensory data, may be used), thus from different blocks of data. The combined data can be used for classification and/or prediction purposes. For an in-depth study of these techniques, this literature is suggested [147, 148]. The increase in information due to the simultaneous use of different data blocks can help to reduce the impact of spurious sources of variability, obtaining lower errors in the models. To obtain this result, the different data blocks should bring complementary information. In the reviewed papers, authors mainly coupled sensors with different spectroscopic range to increase the information hidden in the spectra. For instance, a prototype was designed including a miniaturised NIR sensor developed in-house (939–1833 nm), a miniaturised commercial UV-Vis spectrometer (320–889 nm) and a miniaturised RGB camera [149]. High-level data fusion was then applied to the obtained data to detect food fraud in extra virgin olive oil. The same system was applied to detect fraudulent additions in skimmed milk powder (the UV-VIS spectrometer was used for both fluorescence and diffuse reflectance VIS spectroscopy) [150], while two commercial sensors were coupled to improve the prediction error in the quantification of macronutrients in commercial milk samples [104].

In the reviewed literature, very often a variable selection step was performed. Variable selection can lead to several advantages, like the improvement of model predictions, a better interpretation of the data, or a lower measurement cost. It is mainly used when the number of variables is much larger than the number of samples. For an overview of this topic, references [151–154] are suggested to the reader. In the case of miniaturised NIR spectrometers, there are usually not many more variables than samples, but the evidence is that the variable selection step in many cases allowed to obtain better models. Again, model validation is crucial: if the selected variable set represents only the calibration set, predictions may be very poor since the validation set may contain conditions not included in the calibration set. It is worthy to recall that the variable selection should be done on the calibration set, and the model build with the reduced number of variables must be validated on an independent set of samples.

Concerning Consumer Physics SCiO, it is worthwhile to mention that the recorded spectra can be directly managed using the software 'The Lab', which is a cloud-based application that allows to create chemometric models by Consumer Physics proprietary algorithms. Several authors tried to model data both with 'The Lab' and with other software, and usually the best results were obtained with other software, since 'The Lab' cloud-application offers limited possibilities (see e.g. [47]).

Regarding prediction models, globally speaking more efforts should be done to validate the models calculating the figures of merit, since these parameters help to characterize the performance of the models. [155]. Most of the authors determined several parameters that describe the goodness of the model in terms of prediction error, being the root mean square error of prediction -RMSEP- [156] and the R^2 statistic associated to the calibration line of the multivariate model the most used (root mean square of cross-validation – RMSECV is also used, but it cannot be considered a definitive estimation of the prediction error since it does not account for an external validation as is in the case of RMSEP). Less articles reported the SEP (standard error of prediction) value, which is very useful to comprehend the causes of the differences between the real and the estimated values (the difference between RMSEP and SEP gives the bias of the model). But only a few reported the limit of detection (LOD) or quantification (LOQ) of the proposed analytical methods. These parameters are fundamental to understand the applicability of an analytical protocol, since they provide especially important information when working at low concentrations. The approach described by Allegrini and Olivieri [157, 158] was employed in several papers [40, 48, 110], while other authors [38] calculated the LOD and LOQ with the software TQ Analyst 8 without specifying the approach used. The LOD and LOQ was also calculated considering the estimation of the noise level in the dataset and on the regression coefficients determined in the regression models [131], while other authors [112] did not describe in detail how did they calculate them. The LOD was also calculated [104] using the approximate expression for the sample-specific standard error of prediction (SEP), as derived by Faber and Bro [159].

Process control application always reports multivariate control charts [160], which are often used to address the presence of abnormal variation in the monitored system. Multivariate control charts are obtained after a variable reduction step, and PCA may be an option to reduce the data dimensionality. Multivariate control charts are constructed thus using Hotelling's T^2 or Q residuals, as presented in different papers [24, 117].

5. Conclusions and prospects

In this overview, covering about the last five years, excellent scientific papers are reported, proving that miniaturised NIR sensors are assuming an important role within analytical chemistry and that they are applied in a broad variety of fields. The manufacturers have subjected the sensors to continuous optimization, making them increasingly robust and reliable instruments suitable for the analysis of many analytes (or sample properties) in various fields. In parallel, researchers have developed analytical strategies and data treatments optimised to the characteristics of the miniaturised sensors on the market.

As emerged from the literature, miniaturised NIR devices are spreading according to different logics. On the one hand, they are employed as portable tools that can be used directly in the field. The portability of an analytical method using miniaturised NIR devices is in most cases directly related to the complexity of the pretreatments: if the pretreatments are not user-friendly or require the use of complex equipment, despite the use of miniaturised instrumentation the portability may be compromised. Especially in food analysis, but also in other contexts, miniaturised NIR devices are often used without any sample pretreatment (see Tables 2-4). Sometimes miniaturised instrumentation gives only a preliminary screening of the sample before laboratory analysis but, in several cases, these instruments provide performances comparable to benchtop instruments. Some of them are even designed to be used by non-experts end users: they can obtain information on a sample in a few seconds of analysis without any knowledge in analytical chemistry or data processing, using mathematical models directly available in the cloud and developed by the manufacturer. It would not be surprising if these tools, in the near future, turn into smartphone accessories linked to specific mobile applications capable of managing the combined system, allowing analytical measurements on demand. Some of the revised works already go in this direction (see e.g. [19, 120]).

On the other hand, some companies are starting to test the possibility of implementing miniaturised NIR devices to monitor and control their processes. Being much smaller than benchtop NIR spectrometers and much cheaper, they can potentially be introduced at many points in an industrial process allowing a more detailed control of it. Moreover, they can allow even small businesses to start controlling their processes thanks to the reduced cost. A small number of process control studies have been found in the literature and it is probably understandable: the sensor cannot be used as it is, but it must be integrated into the process line, and this requires a further optimization step. Another limiting factor may be inherent to the different performances offered by miniaturised devices if compared with benchtop instruments.

In the reviewed literature, very often the authors compared the results obtained using the miniaturised NIR instruments with the results obtained with a benchtop instrument, used as the reference. Some studies considered to rotate the sample holder to obtain representative spectra as is commonly done in benchtop analysis but clearly the number of rotations when using portable spectroscopy is limited. Another issue for comparison purposes is related to the definition of replicates. Some authors intended as replicates subsequent acquisition of spectra (which is commonly known as instrumental replicates and that do not provide an estimation of the heterogeneity of the sample), while others considered the displacement of the sample, the refilling of the sample holder or more in general the analysis of different aliquots of the sample (analytical replicates). Some authors even did not describe the type of measurement (contact or distance). This may lead to difficulties in comparison between instruments because results contain different sources of errors (for a more advanced discussion on replicates and errors see [161]). Moreover, this comparison is often carried out between the average errors of prediction or classification, in a univariate way, and it is worthwhile to note that such errors come from multivariate statistical analysis. Multivariate criteria should then be used to determine the figures of merit of the proposed analytical methods and to compare the results obtained between different instrumentations. Only a few number of articles calculated multivariate figures of merit as mentioned in the previous section, or compared the results obtained by the miniaturised instruments with the reference value in a statistical way (e.g. [104, 162, 163]).

Chemometric models developed in quality and process control have to be maintained to retain or improve their prediction performances [164]. The long-term prediction performance of spectroscopic calibration or classification models is a critical factor as new sources of variation that deteriorate the performance may emerge. In the literature, a very few numbers of articles consider this aspect. Only some authors performed analysis over time to include variabilities due to changes in the instrumental features or sample characteristics (see e.g. [45, 145]). Concerning this aspect, it is worthwhile to note that there is no literature about the life of a miniaturised sensor. No information has been found concerning the deterioration of the sensors, and this is a good point to be considered when deciding to develop a chemometric model in a quality or control process. The development of a good model often requires many samples and sample replicates, and these models often need a constant update trying to catch the variability of samples over time (e.g. the market of illegal drugs is continuously evolving). Few authors proposed a solution to this issue ([20]). When developing a model, a fair amount of effort in terms of money and time is required, and the model is strictly related to the instrument used. How many years will the sensor last (and consequently the model built with it)? At the moment, there is no answer to this question in the literature. Will it be possible to transfer the multivariate model built to another sensor? A few number of articles compare instruments of the same type, to investigate if changing the device may lead to a change in the performance of the models, or to test if the models could be transferable between sensors (see e.g. [47, 102]) or between a portable instrument and a benchtop one [49, 165, 166] . Despite good results are obtained, studies are still few, probably because the commercialised spectrometers are still young and constantly evolving, or due to the discrepancies or distortions between the signal recorded with portable sensors with respect to the theoretical spectra or with the spectra recorded with benchtop instruments reported by some authors.

When dealing with NIR measurements, it is also important to remind the inherent limitations associated to this type of spectroscopy: due to the intrinsic characteristics of NIR spectra, NIR measurements cannot separate most of the individual compounds (e.g. individual fatty acids) to be used in multivariate analysis. This implies that in these cases, calibration models aimed to predict individual compounds are based on the correlation to other compounds of the sample (collinearity between the analytes of interest and interfering compounds) [167, 168]. This degree of collinearity may compromise the robustness and the validity of the calibration model when it has to be applied to future samples [169]. This fact reinforces the need for a proper validation of the models, as we have pointed out previously.

In choosing a miniaturised NIR sensor, the application for which it is intended is a fundamental aspect to be considered. The spectrometers, as already discussed previously in this paper and in other excellent papers [8], cover different spectroscopic ranges, and radiation thus penetrates differently in the samples. Moreover, they are able to scan different sample areas, and this is a key point when dealing with inhomogeneous samples. Other strategies such as nested ANOVA [170] may also be used to have an estimation of the variability in and between the samples and to find the most suitable sampling procedure to have a correct estimation of the number of samples and replicates to be performed.

Another aspect to consider is the way in which miniaturised NIR devices transfer the data to the computer for the multivariate modelling. In our experience, the data transfer may not be as rapid as is required in e.g., process control optimization. In some cases, the devices directly communicate with the PC, while in some other cases the devices store the spectra in an internal memory, and then the user must manually transfer the data into the PC or into the cloud. Automation is not obvious in some cases and takes time. Another important aspect to consider is that some articles reported the heating of the acquisition window or the heating of the sensor itself after multiple analysis. In view of a continuous application, this can affect the variability of the spectra and is noteworthy in case of thermolabile samples.

In conclusion, the use of a miniaturised NIR device may be a good choice in a broad range of applications as demonstrated by the impressive numbers of papers published in the last years, even though there is the need for the design of the optimised analytical strategy adapted to each sample and to each miniaturised device. The use of these tools follows the principles of green analytical chemistry in the drastic reduction of costs due to reagents, time, transportation to the lab and wastes, to name a few. Above all, it should be considered the cost of the instrument itself, which is orders of magnitude lower than a benchtop spectrometer, and the minimum quantity of material to be disposed when the instrument itself ends its life cycle. Some of the commercialised miniaturised spectrometers have a cost that can often be faced also by small companies or by a single person, who could use it in everyday life. Each one of us could potentially have a small laboratory at home.

Of course, not all that glitters is gold. Several drawbacks emerged from the revised articles as argued in this article. This can be a stimulus for manufacturers to further improve their products, but also for analytical chemists who must face new challenges.

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7. Conflict of interest

The authors declare that they have no conflict of interest.

8. References

[1] Pasquini, C. Near Infrared Spectroscopy: A Mature Analytical Technique with New Perspectives – A Review. *Anal. Chim. Acta*, **2018**, *1026*, 8–36. DOI:10.1016/j.aca.2018.04.004.

[2] *Near-Infrared Spectroscopy Theory, Spectral Analysis, Instrumentation, and Applications*; Ozaki, Y., Huck, C., Tsuchikawa, S., Engelsen, S. B., Eds.; Springer: Singapore, 2021.

[3] *Handbook of Near-Infrared Analysis*; Ciurczak, E. W., Igne, B., Workman, J., Burns, D. A., Eds.; CRC Press: Boca Raton, FL, 2021.

[4] *Near-Infrared Spectroscopy in Food Science and Technology*; Ozaki, Y., McClure, W. F., Christy, A. A., Eds.; John Wiley & Sons, Inc.: Hoboken, NJ, 2007.

[5] Agelet, L. E.; Hurburgh, C. R. A Tutorial on near Infrared Spectroscopy and Its Calibration. *Crit. Rev. Anal. Chem.*, **2010**, *40*, 246–260. DOI:10.1080/10408347.2010.515468.

[6] McMahon, G. *Analytical Instrumentation A Guide to Laboratory, Portable and Miniaturized Instruments*; John Wiley & Sons Ltd.: Chichester, UK, 2007.

[7] Portable Analytical Instruments Market Research Report by Product, by Technology, by End User, by Region - Global Forecast to 2026 - Cumulative Impact of COVID-19 https://www.globenewswire.com/news-release/2021/08/09/2277228/0/en/Portable-Analytical-Instruments-Market-Research-Report-by-Product-by-Technology-by-End-User-by-Region-Global-Forecast-to-2026-Cumulative-Impact-of-COVID-19.html (accessed Sep 8, 2021).

[8] Beć, K. B.; Grabska, J.; Huck, C. W. Principles and Applications of Miniaturized Near-Infrared (NIR) Spectrometers. *Chem. - A Eur. J.*, **2021**, *27*, 1514–1532. DOI:10.1002/chem.202002838.

[9] Yang, Z.; Albrow-Owen, T.; Cai, W.; Hasan, T. Miniaturization of Optical Spectrometers. *Science (80-.).*, **2021**, *371*, eabe0722. DOI:10.1126/science.abe0722.

[10] Chai, J.; Zhang, K.; Xue, Y.; Liu, W.; Chen, T.; Lu, Y.; Zhao, G. Review of Mems Based Fourier Transform Spectrometers. *Micromachines*, **2020**, *11*, 214. DOI:10.3390/mi11020214.

[11] Crocombe, R. A. Portable Spectroscopy. *Appl. Spectrosc.*, **2018**, *72*, 1701–1751. DOI:10.1177/0003702818809719.

[12] Beć, K. B.; Grabska, J.; Siesler, H. W.; Huck, C. W. Handheld Near-Infrared Spectrometers: Where Are We Heading? *NIR news*, **2020**, *31*, 28–35. DOI:10.1177/0960336020916815.

[13] de Araujo, W. R.; Cardoso, T. M. G.; da Rocha, R. G.; Santana, M. H. P.; Muñoz, R. A. A.; Richter, E. M.; Paixão, T. R. L. C.; Coltro, W. K. T. Portable Analytical Platforms for Forensic Chemistry: A Review.

Anal. Chim. Acta, **2018**, *1034*, 1–21. DOI:10.1016/j.aca.2018.06.014.

[14] Gałuszka, A.; Migaszewski, Z. M.; Namieśnik, J. Moving Your Laboratories to the Field - Advantages and Limitations of the Use of Field Portable Instruments in Environmental Sample Analysis. *Environ. Res.*, **2015**, *140*, 593–603. DOI:10.1016/j.envres.2015.05.017.

[15] Beć, K. B.; Grabska, J.; Huck, C. W. NIR Spectroscopy of Natural Medicines Supported by Novel Instrumentation and Methods for Data Analysis and Interpretation. *J. Pharm. Biomed. Anal.*, **2021**, *193*, 113686. DOI:10.1016/j.jpba.2020.113686.

[16] Kademi, H. I.; Ulusoy, B. H.; Hecer, C. Applications of Miniaturized and Portable near Infrared Spectroscopy (NIRS) for Inspection and Control of Meat and Meat Products. *Food Rev. Int.*, **2019**, *35*, 201–220. DOI:10.1080/87559129.2018.1514624.

[17] Hespanhol, M. C.; Pasquini, C.; Maldaner, A. O. Evaluation of a Low-Cost Portable near-Infrared Spectrophotometer for in Situ Cocaine Profiling. *Talanta*, **2019**, *200*, 553–561. DOI:10.1016/j.talanta.2019.03.091.

[18] Risoluti, R.; Gullifa, G.; Battistini, A.; Materazzi, S. Monitoring of Cannabinoids in Hemp Flours by MicroNIR/Chemometrics. *Talanta*, **2020**, *211*, 120672. DOI:10.1016/j.talanta.2019.120672.

[19] Coppey, F.; Bécue, A.; Sacré, P. Y.; Ziemons, E. M.; Hubert, P.; Esseiva, P. Providing Illicit Drugs Results in Five Seconds Using Ultra-Portable NIR Technology: An Opportunity for Forensic Laboratories to Cope with the Trend toward the Decentralization of Forensic Capabilities. *Forensic Sci. Int.*, **2020**, *317*, 110498. DOI:10.1016/j.forsciint.2020.110498.

[20] Kranenburg, R. F.; Verduin, J.; Weesepoel, Y.; Alewijn, M.; Heerschop, M.; Koomen, G.; Keizers, P.; Bakker, F.; Wallace, F.; van Esch, A.; et al. Rapid and Robust On-Scene Detection of Cocaine in Street Samples Using a Handheld near-Infrared Spectrometer and Machine Learning Algorithms. *Drug Test. Anal.*, **2020**, *12*, 1404–1418. DOI:10.1002/dta.2895.

[21] Casian, T.; Gavan, A.; Iurian, S.; Porfire, A.; Toma, V.; Stiufiuc, R.; Tomuta, I. Testing the Limits of a Portable Nir Spectrometer: Content Uniformity of Complex Powder Mixtures Followed by Calibration Transfer for in-Line Blend Monitoring. *Molecules*, **2021**, *26*, 1129. DOI:10.3390/molecules26041129.

[22] Biagi, D.; Nencioni, P.; Valleri, M.; Calamassi, N.; Mura, P. Development of a Near Infrared Spectroscopy Method for the In-Line Quantitative Bilastine Drug Determination during Pharmaceutical Powders Blending. *J. Pharm. Biomed. Anal.*, **2021**, *204*, 114277. DOI:10.1016/j.jpba.2021.114277.

[23] Avila, C. R.; Ferré, J.; de Oliveira, R. R.; de Juan, A.; Sinclair, W. E.; Mahdi, F. M.; Hassanpour, A.; Hunter, T. N.; Bourne, R. A.; Muller, F. L. Process Monitoring of Moisture Content and Mass Transfer Rate in a Fluidised Bed with a Low Cost Inline MEMS NIR Sensor. *Pharm. Res.*, **2020**, *37*, 84. DOI:10.1007/s11095-020-02787-y.

[24] Avila, C.; Mantzaridis, C.; Ferré, J.; Rocha de Oliveira, R.; Kantojärvi, U.; Rissanen, A.; Krassa, P.; de Juan, A.; Muller, F. L.; Hunter, T. N.; et al. Acid Number, Viscosity and End-Point Detection in a Multiphase High Temperature Polymerisation Process Using an Online Miniaturised MEMS Fabry-Pérot Interferometer. *Talanta*, **2021**, *224*. DOI:10.1016/j.talanta.2020.121735.

[25] Mayr, S.; Beć, K. B.; Grabska, J.; Wiedemair, V.; Pürgy, V.; Popp, M. A.; Bonn, G. K.; Huck, C. W. Challenging Handheld NIR Spectrometers with Moisture Analysis in Plant Matrices: Performance of PLSR vs. GPR vs. ANN Modelling. *Spectrochim. Acta - Part A Mol. Biomol. Spectrosc.*, **2021**, *249*, 119342. DOI:10.1016/j.saa.2020.119342.

[26] Sharififar, A.; Singh, K.; Jones, E.; Ginting, F. I.; Minasny, B. Evaluating a Low-Cost Portable NIR Spectrometer for the Prediction of Soil Organic and Total Carbon Using Different Calibration Models.

Soil Use Manag., **2019**, *35*, 607–616. DOI:10.1111/sum.12537.

[27] Karyotis, K.; Angelopoulou, T.; Tziolas, N.; Palaiologou, E.; Samarinas, N.; Zalidis, G. Evaluation of a Micro-Electro Mechanical Systems Spectral Sensor for Soil Properties Estimation. *Land*, **2021**, *10*, 63. DOI:10.3390/land10010063.

[28] Lopo, M.; Páscoa, R. N. M. J.; Graça, A. R.; Lopes, J. A. Classification of Vineyard Soils Using Portable and Benchtop Near-Infrared Spectrometers: A Comparative Study. *Soil Sci. Soc. Am. J.*, **2016**, *80*, 652–661. DOI:10.2136/sssaj2015.09.0324.

[29] Barthès, B. G.; Kouakoua, E.; Clairotte, M.; Lallemand, J.; Chapuis-Lardy, L.; Rabenarivo, M.; Roussel, S. Performance Comparison between a Miniaturized and a Conventional near Infrared Reflectance (NIR) Spectrometer for Characterizing Soil Carbon and Nitrogen. *Geoderma*, **2019**, *338*, 422–429. DOI:10.1016/j.geoderma.2018.12.031.

[30] Tang, Y.; Jones, E.; Minasny, B. Evaluating Low-Cost Portable near Infrared Sensors for Rapid Analysis of Soils from South Eastern Australia. *Geoderma Reg.*, **2020**, *20*, e00240. DOI:10.1016/j.geodrs.2019.e00240.

[31] Thomas, F.; Petzold, R.; Becker, C.; Werban, U. Application of Low-Cost Mems Spectrometers for Forest Topsoil Properties Prediction. *Sensors*, **2021**, *21*, 3927. DOI:10.3390/s21113927.

[32] Ma, Y.; Zhang, G. Z.; Rita-Cindy, S. A. A. Quantification of Water, Protein and Soluble Sugar in Mulberry Leaves Using a Handheld near-Infrared Spectrometer and Multivariate Analysis. *Molecules*, **2019**, *24*, 4439. DOI:10.3390/molecules24244439.

[33] Mayr, S.; Beć, K. B.; Grabska, J.; Schneckenreiter, E.; Huck, C. W. Near-Infrared Spectroscopy in Quality Control of Piper Nigrum: A Comparison of Performance of Benchtop and Handheld Spectrometers. *Talanta*, **2021**, *223*, 121809. DOI:10.1016/j.talanta.2020.121809.

[34] Srinuttrakul, W.; Mihailova, A.; Islam, M. D.; Liebisch, B.; Maxwell, F.; Kelly, S. D.; Cannavan, A. Geographical Differentiation of Hom Mali Rice Cultivated in Different Regions of Thailand Using FTIR-ATR and NIR Spectroscopy. *Foods*, **2021**, *10*, 1951. DOI:10.3390/foods10081951.

[35] Wang, Y.; Li, M.; Li, L.; Ning, J.; Zhang, Z. Green Analytical Assay for the Quality Assessment of Tea by Using Pocket-Sized NIR Spectrometer. *Food Chem.*, **2021**, *345*, 128816. DOI:10.1016/j.foodchem.2020.128816.

[36] Wang, Y. J.; Li, T. H.; Li, L. Q.; Ning, J. M.; Zhang, Z. Z. Evaluating Taste-Related Attributes of Black Tea by Micro-NIRS. *J. Food Eng.*, **2021**, *290*, 110181. DOI:10.1016/j.jfoodeng.2020.110181.

[37] Kirchler, C. G.; Pezzei, C. K.; Beć, K. B.; Mayr, S.; Ishigaki, M.; Ozaki, Y.; Huck, C. W. Critical Evaluation of Spectral Information of Benchtop vs. Portable near-Infrared Spectrometers: Quantum Chemistry and Two-Dimensional Correlation Spectroscopy for a Better Understanding of PLS Regression Models of the Rosmarinic Acid Content in Rosmarin. *Analyst*, **2017**, *142*, 455–464. DOI:10.1039/c6an02439d.

[38] Mcvey, C.; Gordon, U.; Haughey, S. A.; Elliott, C. T. Assessment of the Analytical Performance of Three Near-Infrared Spectroscopy Instruments (Benchtop, Handheld and Portable) through the Investigation of Coriander Seed Authenticity. *Foods*, **2021**, *10*, 956. DOI:https://doi.org/10.3390/foods10050956.

[39] Mayr, S.; Schmelzer, J.; Kirchler, C. G.; Pezzei, C. K.; Beć, K. B.; Grabska, J.; Huck, C. W. Theae Nigrae Folium: Comparing the Analytical Performance of Benchtop and Handheld near-Infrared Spectrometers. *Talanta*, **2021**, *221*, 121165. DOI:10.1016/j.talanta.2020.121165.

[40] Wiedemair, V.; Huck, C. W. Evaluation of the Performance of Three Hand-Held near-Infrared Spectrometer through Investigation of Total Antioxidant Capacity in Gluten-Free Grains. *Talanta*,

2018, *189*, 233–240. DOI:10.1016/j.talanta.2018.06.056.

[41] Wiedemair, V.; Mair, D.; Held, C.; Huck, C. W. Investigations into the Use of Handheld Near-Infrared Spectrometer and Novel Semi-Automated Data Analysis for the Determination of Protein Content in Different Cultivars of Panicum Miliaceum L. *Talanta*, **2019**, *205*, 120115. DOI:10.1016/j.talanta.2019.120115.

[42] Bilal, M.; Xiaobo, Z.; Arslan, M.; Tahir, H. E.; Azam, M.; Junjun, Z.; Basheer, S.; Abdullah. Rapid Determination of the Chemical Compositions of Peanut Seed (Arachis Hypogaea.) Using Portable near-Infrared Spectroscopy. *Vib. Spectrosc.*, **2020**, *110*, 103138. DOI:10.1016/j.vibspec.2020.103138.

[43] Sun, L.; Hsiung, C.; Pederson, C. G.; Zou, P.; Smith, V.; Von Gunten, M.; O'Brien, N. A. Pharmaceutical Raw Material Identification Using Miniature Near-Infrared (MicroNIR) Spectroscopy and Supervised Pattern Recognition Using Support Vector Machine. *Appl. Spectrosc.*, **2016**, *70*, 816–825. DOI:10.1177/0003702816638281.

[44] Goi, A.; Simoni, M.; Righi, F.; Visentin, G.; De Marchi, M. Application of a Handheld Near-Infrared Spectrometer to Predict Gelatinized Starch, Fiber Fractions, and Mineral Content of Ground and Intact Extruded Dry Dog Food. *Animals*, **2020**, *10*, 1660. DOI:10.3390/ani10091660.

[45] Chen, X.; Siesler, H. W.; Yan, H. Rapid Analysis of Wheat Flour by Different Handheld Near-Infrared Spectrometers: A Discussion of Calibration Model Maintenance and Performance Comparison. *Spectrochim. Acta - Part A Mol. Biomol. Spectrosc.*, **2021**, *252*, 119504. DOI:10.1016/j.saa.2021.119504.

[46] Li, L.; Jin, S.; Wang, Y.; Liu, Y.; Shen, S.; Li, M.; Ma, Z.; Ning, J.; Zhang, Z. Potential of Smartphone-Coupled Micro NIR Spectroscopy for Quality Control of Green Tea. *Spectrochim. Acta - Part A Mol. Biomol. Spectrosc.*, **2021**, *247*, 119096. DOI:10.1016/j.saa.2020.119096.

[47] McGrath, T. F.; Haughey, S. A.; Islam, M.; Elliott, C. T. The Potential of Handheld near Infrared Spectroscopy to Detect Food Adulteration: Results of a Global, Multi-Instrument Inter-Laboratory Study. *Food Chem.*, **2021**, *353*, 128718. DOI:10.1016/j.foodchem.2020.128718.

[48] Henn, R.; Kirchler, C. G.; Grossgut, M. E.; Huck, C. W. Comparison of Sensitivity to Artificial Spectral Errors and Multivariate LOD in NIR Spectroscopy – Determining the Performance of Miniaturizations on Melamine in Milk Powder. *Talanta*, **2017**, *166*, 109–118. DOI:10.1016/j.talanta.2017.01.035.

[49] Pissard, A.; Marques, E. J. N.; Dardenne, P.; Lateur, M.; Pasquini, C.; Pimentel, M. F.; Fernández Pierna, J. A.; Baeten, V. Evaluation of a Handheld Ultra-Compact NIR Spectrometer for Rapid and Non-Destructive Determination of Apple Fruit Quality. *Postharvest Biol. Technol.*, **2021**, *172*, 111375. DOI:10.1016/j.postharvbio.2020.111375.

[50] Subedi, P. P.; Walsh, K. B. Assessment of Avocado Fruit Dry Matter Content Using Portable near Infrared Spectroscopy: Method and Instrumentation Optimisation. *Postharvest Biol. Technol.*, **2020**, *161*, 111078. DOI:10.1016/j.postharvbio.2019.111078.

[51] Li, M.; Qian, Z.; Shi, B.; Medlicott, J.; East, A. Evaluating the Performance of a Consumer Scale SCiO^{TM} Molecular Sensor to Predict Quality of Horticultural Products. *Postharvest Biol. Technol.*, **2018**, *145*, 183–192. DOI:10.1016/j.postharvbio.2018.07.009.

[52] Donis-González, I. R.; Valero, C.; Momin, M. A.; Kaur, A.; Slaughter, D. C. Performance Evaluation of Two Commercially Available Portable Spectrometers to Non-Invasively Determine Table Grape and Peach Quality Attributes. *Agronomy*, **2020**, *10*, 148. DOI:10.3390/agronomy10010148.

[53] Mishra, P.; Marini, F.; Brouwer, B.; Roger, J. M.; Biancolillo, A.; Woltering, E.; Echtelt, E. H. van. Sequential Fusion of Information from Two Portable Spectrometers for Improved Prediction of Moisture and Soluble Solids Content in Pear Fruit. *Talanta*, **2021**, *223*, 121733. DOI:10.1016/j.talanta.2020.121733.

[54] Tardaguila, J.; Fernández-Novales, J.; Gutiérrez, S.; Diago, M. P. Non-Destructive Assessment of Grapevine Water Status in the Field Using a Portable NIR Spectrophotometer. *J. Sci. Food Agric.*, **2017**, *97*, 3772–3780. DOI:10.1002/jsfa.8241.

[55] Urraca, R.; Sanz-Garcia, A.; Tardaguila, J.; Diago, M. P. Estimation of Total Soluble Solids in Grape Berries Using a Hand-Held NIR Spectrometer under Field Conditions. *J. Sci. Food Agric.*, **2016**, *96*, 3007–3016. DOI:10.1002/jsfa.7470.

[56] Malegori, C.; Nascimento Marques, E. J.; de Freitas, S. T.; Pimentel, M. F.; Pasquini, C.; Casiraghi, E. Comparing the Analytical Performances of Micro-NIR and FT-NIR Spectrometers in the Evaluation of Acerola Fruit Quality, Using PLS and SVM Regression Algorithms. *Talanta*, **2017**, *165*, 112–116. DOI:10.1016/j.talanta.2016.12.035.

[57] Wang, T.; Chen, J.; Fan, Y.; Qiu, Z.; He, Y. SeeFruits: Design and Evaluation of a Cloud-Based Ultra-Portable NIRS System for Sweet Cherry Quality Detection. *Comput. Electron. Agric.*, **2018**, *152*, 302–313. DOI:10.1016/j.compag.2018.07.017.

[58] Yan, H.; Xu, Y. C.; Siesler, H. W.; Han, B. X.; Zhang, G. Z. Hand-Held Near-Infrared Spectroscopy for Authentication of Fengdous and Quantitative Analysis of Mulberry Fruits. *Front. Plant Sci.*, **2019**, *10*, 1548. DOI:10.3389/fpls.2019.01548.

[59] Brasil, Y. L.; Cruz-Tirado, J. P.; Barbin, D. F. Fast Online Estimation of Quail Eggs Freshness Using Portable NIR Spectrometer and Machine Learning. *Food Control*, **2022**, *131*, 108418. DOI:10.1016/j.foodcont.2021.108418.

[60] Coronel-Reyes, J.; Ramirez-Morales, I.; Fernandez-Blanco, E.; Rivero, D.; Pazos, A. Determination of Egg Storage Time at Room Temperature Using a Low-Cost NIR Spectrometer and Machine Learning Techniques. *Comput. Electron. Agric.*, **2018**, *145*, 1–10. DOI:10.1016/j.compag.2017.12.030.

[61] Cruz-Tirado, J. P.; Lucimar da Silva Medeiros, M.; Barbin, D. F. On-Line Monitoring of Egg Freshness Using a Portable NIR Spectrometer in Tandem with Machine Learning. *J. Food Eng.*, **2021**, *306*, 110643. DOI:10.1016/j.jfoodeng.2021.110643.

[62] Parastar, H.; van Kollenburg, G.; Weesepoel, Y.; van den Doel, A.; Buydens, L.; Jansen, J. Integration of Handheld NIR and Machine Learning to “Measure & Monitor” Chicken Meat Authenticity. *Food Control*, **2020**, *112*, 107149. DOI:10.1016/j.foodcont.2020.107149.

[63] González-Mohino, A.; Pérez-Palacios, T.; Antequera, T.; Ruiz-Carrascal, J.; Olegario, L. S.; Grassi, S. Monitoring the Processing of Dry Fermented Sausages with a Portable NIRS Device. *Foods*, **2020**, *9*, 1294. DOI:10.3390/foods9091294.

[64] Piotrowski, C.; Garcia, R.; Garrido-Varo, A.; Pérez-Marín, D.; Riccioli, C.; Fearn, T. Short Communication: The Potential of Portable near Infrared Spectroscopy for Assuring Quality and Authenticity in the Food Chain, Using Iberian Hams as an Example. *Animal*, **2019**, *13*, 3018–3021. DOI:10.1017/S1751731119002003.

[65] Schmutzler, M.; Beganovic, A.; Böhler, G.; Huck, C. W. Methods for Detection of Pork Adulteration in Veal Product Based on FT-NIR Spectroscopy for Laboratory, Industrial and on-Site Analysis. *Food Control*, **2015**, *57*, 258–267. DOI:10.1016/j.foodcont.2015.04.019.

[66] Grassi, S.; Casiraghi, E.; Alamprese, C. Handheld NIR Device: A Non-Targeted Approach to Assess Authenticity of Fish Fillets and Patties. *Food Chem.*, **2018**, *243*, 382–388. DOI:10.1016/j.foodchem.2017.09.145.

[67] Correia, R. M.; Tosato, F.; Domingos, E.; Rodrigues, R. R. T.; Aquino, L. F. M.; Filgueiras, P. R.; Lacerda, V.; Romão, W. Portable near Infrared Spectroscopy Applied to Quality Control of Brazilian Coffee. *Talanta*, **2018**, *176*, 59–68. DOI:10.1016/j.talanta.2017.08.009.

[68] Kosmowski, F.; Worku, T. Evaluation of a Miniaturized NIR Spectrometer for Cultivar Identification: The Case of Barley, Chickpea and Sorghum in Ethiopia. *PLoS One*, **2018**, *13*, 1–17. DOI:10.1371/journal.pone.0193620.

[69] Modroño, S.; Soldado, A.; Martínez-Fernández, A.; de la Roza-Delgado, B. Handheld NIRS Sensors for Routine Compound Feed Quality Control: Real Time Analysis and Field Monitoring. *Talanta*, **2017**, *162*, 597–603. DOI:10.1016/j.talanta.2016.10.075.

[70] Nogales-Bueno, J.; Feliz, L.; Baca-Bocanegra, B.; Hernández-Hierro, J. M.; Heredia, F. J.; Barroso, J. M.; Rato, A. E. Comparative Study on the Use of Three Different near Infrared Spectroscopy Recording Methodologies for Varietal Discrimination of Walnuts. *Talanta*, **2020**, *206*, 120189. DOI:10.1016/j.talanta.2019.120189.

[71] Teye, E.; Amuah, C. L. Y.; McGrath, T.; Elliott, C. Innovative and Rapid Analysis for Rice Authenticity Using Hand-Held NIR Spectrometry and Chemometrics. *Spectrochim. Acta - Part A Mol. Biomol. Spectrosc.*, **2019**, *217*, 147–154. DOI:10.1016/j.saa.2019.03.085.

[72] Yu, H.; Liu, H.; Wang, Q.; van Ruth, S. Evaluation of Portable and Benchtop NIR for Classification of High Oleic Acid Peanuts and Fatty Acid Quantitation. *Lwt*, **2020**, *128*, 109398. DOI:10.1016/j.lwt.2020.109398.

[73] Rego, G.; Ferrero, F.; Valledor, M.; Campo, J. C.; Forcada, S.; Royo, L. J.; Soldado, A. A Portable IoT NIR Spectroscopic System to Analyze the Quality of Dairy Farm Forage. *Comput. Electron. Agric.*, **2020**, *175*, 105578. DOI:10.1016/j.compag.2020.105578.

[74] Nolasco-Perez, I. M.; Rocco, L. A. C. M.; Cruz-Tirado, J. P.; Pollonio, M. A. R.; Barbon, S.; Barbon, A. P. A. C.; Barbin, D. F. Comparison of Rapid Techniques for Classification of Ground Meat. *Biosyst. Eng.*, **2019**, *183*, 151–159. DOI:10.1016/j.biosystemseng.2019.04.013.

[75] Silva, L. C. R.; Folli, G. S.; Santos, L. P.; Barros, I. H. A. S.; Oliveira, B. G.; Borghi, F. T.; Santos, F. D. do.; Filgueiras, P. R.; Romão, W. Quantification of Beef, Pork, and Chicken in Ground Meat Using a Portable NIR Spectrometer. *Vib. Spectrosc.*, **2020**, *111*, 103158. DOI:10.1016/j.vibspec.2020.103158.

[76] Kartakoullis, A.; Comaposada, J.; Cruz-Carrión, A.; Serra, X.; Gou, P. Feasibility Study of Smartphone-Based Near Infrared Spectroscopy (NIRS) for Salted Minced Meat Composition Diagnostics at Different Temperatures. *Food Chem.*, **2019**, *278*, 314–321. DOI:10.1016/j.foodchem.2018.11.054.

[77] Nolasco Perez, I. M.; Badaró, A. T.; Barbon, S.; Barbon, A. P. A.; Pollonio, M. A. R.; Barbin, D. F. Classification of Chicken Parts Using a Portable Near-Infrared (NIR) Spectrophotometer and Machine Learning. *Appl. Spectrosc.*, **2018**, *72*, 1774–1780. DOI:10.1177/0003702818788878.

[78] Wiedemair, V.; Langore, D.; Garsleitner, R.; Dillinger, K.; Huck, C. Investigations into the Performance of a Novel Pocket-Sized near-Infrared Spectrometer for Cheese Analysis. *Molecules*, **2019**, *24*, 428. DOI:10.3390/molecules24030428.

[79] Guillemain, A.; Dégardin, K.; Roggo, Y. Performance of NIR Handheld Spectrometers for the Detection of Counterfeit Tablets. *Talanta*, **2017**, *165*, 632–640. DOI:10.1016/j.talanta.2016.12.063.

[80] Ciza, P. H.; Sacre, P. Y.; Waffo, C.; Coïc, L.; Avohou, H.; Mbinze, J. K.; Ngono, R.; Marini, R. D.; Hubert, P.; Ziemons, E. Comparing the Qualitative Performances of Handheld NIR and Raman Spectrophotometers for the Detection of Falsified Pharmaceutical Products. *Talanta*, **2019**, *202*, 469–478. DOI:10.1016/j.talanta.2019.04.049.

[81] Vakili, H.; Wickström, H.; Desai, D.; Preis, M.; Sandler, N. Application of a Handheld NIR Spectrometer in Prediction of Drug Content in Inkjet Printed Orodispersible Formulations Containing Prednisolone and Levothyroxine. *Int. J. Pharm.*, **2017**, *524*, 414–423. DOI:10.1016/j.ijpharm.2017.04.014.

[82] Foo, W. C.; Widjaja, E.; Khong, Y. M.; Gokhale, R.; Chan, S. Y. Application of Miniaturized Near-Infrared Spectroscopy for Quality Control of Extemporaneous Orodispersible Films. *J. Pharm. Biomed. Anal.*, **2018**, *150*, 191–198. DOI:10.1016/j.jpba.2017.11.068.

[83] Pezzei, C. K.; Schönbichler, S. A.; Kirchler, C. G.; Schmelzer, J.; Hussain, S.; Huck-Pezzei, V. A.; Popp, M.; Krolitzek, J.; Bonn, G. K.; Huck, C. W. Application of Benchtop and Portable Near-Infrared Spectrometers for Predicting the Optimum Harvest Time of Verbena Officinalis. *Talanta*, **2017**, *169*, 70–76. DOI:10.1016/j.talanta.2017.03.067.

[84] Catelli, E.; Sciutto, G.; Prati, S.; Chavez Lozano, M. V.; Gatti, L.; Lugli, F.; Silvestrini, S.; Benazzi, S.; Genorini, E.; Mazzeo, R. A New Miniaturised Short-Wave Infrared (SWIR) Spectrometer for on-Site Cultural Heritage Investigations. *Talanta*, **2020**, *218*, 121112. DOI:10.1016/j.talanta.2020.121112.

[85] Risoluti, R.; Materazzi, S.; Tau, F.; Russo, A.; Romolo, F. S. Towards Innovation in Paper Dating: A MicroNIR Analytical Platform and Chemometrics. *Analyst*, **2018**, *143*, 4394–4399. DOI:10.1039/c8an00871j.

[86] Chaitae, A.; Rittiron, R.; Gordon, I. J.; Marsh, H.; Addison, J.; Pochanagone, S.; Suttanon, N. Shining NIR Light on Ivory: A Practical Enforcement Tool for Elephant Ivory Identification. *Conserv. Sci. Pract.*, **2021**, *3*, e486. DOI:10.1111/csp2.486.

[87] Rosi, F.; Cartechini, L.; Sali, D.; Miliani, C. Recent Trends in the Application of Fourier Transform Infrared (FT-IR) Spectroscopy in Heritage Science: From Non-Invasive FT-IR. In *Chemical Analysis in Cultural Heritage*; Sabattini, L., Dorothé van der Werf, I., Eds.; De Gruyter: Berlin (Germany), 2020; pp 121–150. DOI:10.1515/psr-2018-0006.

[88] Marques, E. J. N.; de Freitas, S. T. Performance of New Low-Cost Handheld NIR Spectrometers for Nondestructive Analysis of Umbu (Spondias Tuberosa Arruda) Quality. *Food Chem.*, **2020**, *323*, 126820. DOI:10.1016/j.foodchem.2020.126820.

[89] Marques, E. J. N.; De Freitas, S. T.; Pimentel, M. F.; Pasquini, C. Rapid and Non-Destructive Determination of Quality Parameters in the “Tommy Atkins” Mango Using a Novel Handheld near Infrared Spectrometer. *Food Chem.*, **2016**, *197*, 1207–1214. DOI:10.1016/j.foodchem.2015.11.080.

[90] Berzaghi, P.; Cherney, J. H.; Casler, M. D. Prediction Performance of Portable near Infrared Reflectance Instruments Using Preprocessed Dried, Ground Forage Samples. *Comput. Electron. Agric.*, **2021**, *182*, 106013. DOI:10.1016/j.compag.2021.106013.

[91] Rani, M.; Marchesi, C.; Federici, S.; Rovelli, G.; Alessandri, I.; Vassalini, I.; Ducoli, S.; Borgese, L.; Zacco, A.; Bilo, F.; et al. Miniaturized Near-Infrared (MicroNIR) Spectrometer in Plastic Waste Sorting. *Materials (Basel).*, **2019**, *12*, 2740. DOI:10.3390/ma12172740.

[92] Baca-Bocanegra, B.; Hernández-Hierro, J. M.; Nogales-Bueno, J.; Heredia, F. J. Feasibility Study on the Use of a Portable Micro near Infrared Spectroscopy Device for the “in Vineyard” Screening of Extractable Polyphenols in Red Grape Skins. *Talanta*, **2019**, *192*, 353–359. DOI:10.1016/j.talanta.2018.09.057.

[93] Dixit, Y.; Pham, H. Q.; Realini, C. E.; Agnew, M. P.; Craigie, C. R.; Reis, M. M. Evaluating the Performance of a Miniaturized NIR Spectrophotometer for Predicting Intramuscular Fat in Lamb: A Comparison with Benchtop and Hand-Held Vis-NIR Spectrophotometers. *Meat Sci.*, **2020**, *162*, 108026. DOI:10.1016/j.meatsci.2019.108026.

[94] Rady, A. M.; Guyer, D. E.; Donis-González, I. R.; Kirk, W.; Watson, N. J. A Comparison of Different Optical Instruments and Machine Learning Techniques to Identify Sprouting Activity in Potatoes during Storage. *J. Food Meas. Charact.*, **2020**, *14*, 3565–3579. DOI:10.1007/s11694-020-00590-2.

[95] Ma, Y. B.; Babu, K. S.; Amamcharla, J. K. Prediction of Total Protein and Intact Casein in Cheddar Cheese Using a Low-Cost Handheld Short-Wave near-Infrared Spectrometer. *Lwt*, **2019**, *109*, 319–

326. DOI:10.1016/j.lwt.2019.04.039.

[96] Sandak, J.; Sandak, A.; Zitek, A.; Hintestoisser, B.; Picchi, G. Development of Low-Cost Portable Spectrometers for Detection of Wood Defects. *Sensors (Switzerland)*, **2020**, *20*, 545. DOI:10.3390/s20020545.

[97] Hespanhol, M. C.; Souza, J. C.; Pasquini, C. Feasibility of a Portable, Low-Cost near-Infrared Spectrophotometer for the Quality Screening of Omega-3 Dietary Supplements. *J. Pharm. Biomed. Anal.*, **2020**, *189*, 113436. DOI:10.1016/j.jpba.2020.113436.

[98] Neves, M. D. G.; Poppi, R. J.; Siesler, H. W. Rapid Determination of Nutritional Parameters of Pasta/Sauce Blends by Handheld near-Infrared Spectroscopy. *Molecules*, **2019**, *24*, 2029. DOI:10.3390/molecules24112029.

[99] Correia, R. M.; Domingos, E.; Tosato, F.; Aquino, L. F. M.; Fontes, A. M.; Cáo, V. M.; Filgueiras, P. R.; Romão, W. Banknote Analysis by Portable near Infrared Spectroscopy. *Forensic Chem.*, **2018**, *8*, 57–63. DOI:10.1016/j.forc.2018.02.003.

[100] Entrenas, J. A.; Pérez-Marín, D.; Torres, I.; Garrido-Varo, A.; Sánchez, M. T. Simultaneous Detection of Quality and Safety in Spinach Plants Using a New Generation of NIRS Sensors. *Postharvest Biol. Technol.*, **2020**, *160*, 111026. DOI:10.1016/j.postharvbio.2019.111026.

[101] Torres, I.; Sánchez, M. T.; Pérez-Marín, D. Integrated Soluble Solid and Nitrate Content Assessment of Spinach Plants Using Portable NIRS Sensors along the Supply Chain. *Postharvest Biol. Technol.*, **2020**, *168*, 111273. DOI:10.1016/j.postharvbio.2020.111273.

[102] de la Roza-Delgado, B.; Garrido-Varo, A.; Soldado, A.; González Arrojo, A.; Cuevas Valdés, M.; Maroto, F.; Pérez-Marín, D. Matching Portable NIRS Instruments for in Situ Monitoring Indicators of Milk Composition. *Food Control*, **2017**, *76*, 74–81. DOI:10.1016/j.foodcont.2017.01.004.

[103] Llano Suárez, P.; Soldado, A.; González-Arrojo, A.; Vicente, F.; de la Roza-Delgado, B. Rapid On-Site Monitoring of Fatty Acid Profile in Raw Milk Using a Handheld near Infrared Sensor. *J. Food Compos. Anal.*, **2018**, *70*, 1–8. DOI:10.1016/j.jfca.2018.03.003.

[104] Riu, J.; Gorla, G.; Chakif, D.; Boqué, R.; Giussani, B. Rapid Analysis of Milk Using Low-Cost Pocket-Size NIR Spectrometers and Multivariate Analysis. *Foods*, **2020**, *9*, 1090. DOI:10.3390/foods9081090.

[105] dos Santos Pereira, E. V.; de Sousa Fernandes, D. D.; de Araújo, M. C. U.; Diniz, P. H. G. D.; Maciel, M. I. S. In-Situ Authentication of Goat Milk in Terms of Its Adulteration with Cow Milk Using a Low-Cost Portable NIR Spectrophotometer. *Microchem. J.*, **2021**, *163*, 105885. DOI:10.1016/j.microc.2020.105885.

[106] dos Santos, V. J.; Baqueta, M. R.; Março, P. H.; Valderrama, P.; Visentainer, J. V. Proof-of-Concept on the Effect of Human Milk Storage Time: Lipid Degradation and Spectroscopic Characterization Using Portable near-Infrared Spectrometer and Chemometrics. *Food Chem.*, **2021**, *368*, 130675. DOI:10.1016/j.foodchem.2021.130675.

[107] Rubini, M.; Feuillerat, L.; Cabaret, T.; Leroyer, L.; Leneveu, L.; Charrier, B. Comparison of the Performances of Handheld and Benchtop near Infrared Spectrometers: Application on the Quantification of Chemical Components in Maritime Pine (Pinus Pinaster) Resin. *Talanta*, **2021**, *221*, 121454. DOI:10.1016/j.talanta.2020.121454.

[108] Guelpa, A.; Marini, F.; du Plessis, A.; Slabbert, R.; Manley, M. Verification of Authenticity and Fraud Detection in South African Honey Using NIR Spectroscopy. *Food Control*, **2017**, *73*, 1388–1396. DOI:10.1016/j.foodcont.2016.11.002.

[109] Kaufmann, K. C.; Favero, F. de F.; de Vasconcelos, M. A. M.; Godoy, H. T.; Sampaio, K. A.; Barbin, D. F. Portable NIR Spectrometer for Prediction of Palm Oil Acidity. *J. Food Sci.*, **2019**, *84*, 406–411.

DOI:10.1111/1750-3841.14467.

[110] Borghi, F. T.; Santos, P. C.; Santos, F. D.; Nascimento, M. H. C.; Corrêa, T.; Cesconetto, M.; Pires, A. A.; Ribeiro, A. V. F. N.; Lacerda, V.; Romão, W.; et al. Quantification and Classification of Vegetable Oils in Extra Virgin Olive Oil Samples Using a Portable Near-Infrared Spectrometer Associated with Chemometrics. *Microchem. J.*, **2020**, *159*, 105544. DOI:10.1016/j.microc.2020.105544.

[111] Basri, K. N.; Hussain, M. N.; Bakar, J.; Sharif, Z.; Khir, M. F. A.; Zoolfakar, A. S. Classification and Quantification of Palm Oil Adulteration via Portable NIR Spectroscopy. *Spectrochim. Acta - Part A Mol. Biomol. Spectrosc.*, **2017**, *173*, 335–342. DOI:10.1016/j.saa.2016.09.028.

[112] Santos, F. D.; Santos, L. P.; Cunha, P. H. P.; Borghi, F. T.; Romão, W.; de Castro, E. V. R.; de Oliveira, E. C.; Filgueiras, P. R. Discrimination of Oils and Fuels Using a Portable NIR Spectrometer. *Fuel*, **2021**, *283*, 118854. DOI:10.1016/j.fuel.2020.118854.

[113] Gonzalez Viejo, C.; Fuentes, S.; Hernandez-Brenes, C. Smart Detection of Faults in Beers Using Near-Infrared Spectroscopy, a Low-Cost Electronic Nose and Artificial Intelligence. *Fermentation*, **2021**, *7*, 117. DOI:10.3390/fermentation7030117.

[114] Gonzalez Viejo, C.; Fuentes, S.; Torrico, D.; Howell, K.; Dunshea, F. R. Assessment of Beer Quality Based on Foamability and Chemical Composition Using Computer Vision Algorithms, near Infrared Spectroscopy and Machine Learning Algorithms. *J. Sci. Food Agric.*, **2018**, *98*, 618–627. DOI:10.1002/jsfa.8506.

[115] van Kollenburg, G. H.; van Manen, H. J.; Admiraal, N.; Gerretzen, J.; Jansen, J. J. Low-Cost Handheld NIR Spectroscopy for Identification of Organic Solvents and Low-Level Quantification of Water Contamination. *Talanta*, **2021**, *223*, 121865. DOI:10.1016/j.talanta.2020.121865.

[116] Yao, S.; Aykas, D. P.; Rodriguez-Saona, L. Rapid Authentication of Potato Chip Oil by Vibrational Spectroscopy Combined with Pattern Recognition Analysis. *Foods*, **2021**, *10*, 42. DOI:10.3390/foods10010042.

[117] Galaverna, R.; Ribessi, R. L.; Rohwedder, J. J. R.; Pastre, J. C. Coupling Continuous Flow Microreactors to MicroNIR Spectroscopy: Ultracompact Device for Facile In-Line Reaction Monitoring. *Org. Process Res. Dev.*, **2018**, *22*, 780–788. DOI:10.1021/acs.oprd.8b00060.

[118] Sedjoah, R. C. A. A.; Ma, Y.; Xiong, M.; Yan, H. Fast Monitoring Total Acids and Total Polyphenol Contents in Fermentation Broth of Mulberry Vinegar Using MEMS and Optical Fiber Near-Infrared Spectrometers. *Spectrochim. Acta - Part A Mol. Biomol. Spectrosc.*, **2021**, *260*, 119938. DOI:10.1016/j.saa.2021.119938.

[119] de Lima, G. F.; Andrade, S. A. C.; da Silva, V. H.; Honorato, F. A. Multivariate Classification of UHT Milk as to the Presence of Lactose Using Benchtop and Portable NIR Spectrometers. *Food Anal. Methods*, **2018**, *11*, 2699–2706. DOI:10.1007/s12161-018-1253-7.

[120] Muñiz, R.; Cuevas-Valdés, M.; de la Roza-Delgado, B. Milk Quality Control Requirement Evaluation Using a Handheld near Infrared Reflectance Spectrophotometer and a Bespoke Mobile Application. *J. Food Compos. Anal.*, **2020**, *86*, 103388. DOI:10.1016/j.jfca.2019.103388.

[121] Henn, R.; Schwab, A.; Huck, C. W. Evaluation of Benchtop versus Portable Near-Infrared Spectroscopic Method Combined with Multivariate Approaches for the Fast and Simultaneous Quantitative Analysis of Main Sugars in Syrup Formulations. *Food Control*, **2016**, *68*, 97–104. DOI:10.1016/j.foodcont.2016.03.037.

[122] Paiva, E. M.; Rohwedder, J. J. R.; Pasquini, C.; Pimentel, M. F.; Pereira, C. F. Quantification of Biodiesel and Adulteration with Vegetable Oils in Diesel/Biodiesel Blends Using Portable near-Infrared Spectrometer. *Fuel*, **2015**, *160*, 57–63. DOI:10.1016/j.fuel.2015.07.067.

[123] Santos, P. M.; Pereira-Filho, E. R.; Rodriguez-Saona, L. E. Application of Hand-Held and Portable Infrared Spectrometers in Bovine Milk Analysis. *J. Agric. Food Chem.*, **2013**, *61*, 1205–1211. DOI:10.1021/jf303814g.

[124] Liu, N.; Parra, H. A.; Pustjens, A.; Hettinga, K.; Mongondry, P.; van Ruth, S. M. Evaluation of Portable Near-Infrared Spectroscopy for Organic Milk Authentication. *Talanta*, **2018**, *184*, 128–135. DOI:10.1016/j.talanta.2018.02.097.

[125] MacArthur, R. L.; Teye, E.; Darkwa, S. Predicting Adulteration of Palm Oil with Sudan IV Dye Using Shortwave Handheld Spectroscopy and Comparative Analysis of Models. *Vib. Spectrosc.*, **2020**, *110*, 103129. DOI:10.1016/j.vibspec.2020.103129.

[126] Sales, R.; da Silva, N. C.; da Silva, J. P.; França, H. H.; Pimentel, M. F.; Stragevitch, L. Handheld Near-Infrared Spectrometer for on-Line Monitoring of Biodiesel Production in a Continuous Process. *Fuel*, **2019**, *254*, 115680. DOI:10.1016/j.fuel.2019.115680.

[127] Erfan, M.; Sabry, Y. M.; Sakr, M.; Mortada, B.; Medhat, M.; Khalil, D. On-Chip Micro-Electro-Mechanical System Fourier Transform Infrared (MEMS FT-IR) Spectrometer-Based Gas Sensing. *Appl. Spectrosc.*, **2016**, *70*, 897–904. DOI:10.1177/0003702816638295.

[128] Barbosa, M. F.; Santos, J. R. B.; Silva, A. N.; Soares, S. F. C.; Araujo, M. C. U. A Cheap Handheld NIR Spectrometric System for Automatic Determination of Methane, Ethane, and Propane in Natural Gas and Biogas. *Microchem. J.*, **2021**, *170*, 106752. DOI:10.1016/j.microc.2021.106752.

[129] Paiva, E. M.; Ribessi, R. L.; Rohwedder, J. J. R. Near-Infrared Spectra of Liquid and Gas Samples by Diffuse Reflectance Employing Benchtop and Handheld Spectrophotometers. *Spectrochim. Acta Part A Mol. Biomol. Spectrosc.*, **2022**, *264*, 120302. DOI:10.1016/j.saa.2021.120302.

[130] Correia, R. M.; Domingos, E.; Tosato, F.; Dos Santos, N. A.; Leite, J. D. A.; Da Silva, M.; Marcelo, M. C. A.; Ortiz, R. S.; Filgueiras, P. R.; Romão, W. Portable near Infrared Spectroscopy Applied to Abuse Drugs and Medicine Analyses. *Anal. Methods*, **2018**, *10*, 593–603. DOI:10.1039/c7ay02998e.

[131] Correia, R. M.; Domingos, E.; Cáo, V. M.; Araujo, B. R. F.; Sena, S.; Pinheiro, L. U.; Fontes, A. M.; Aquino, L. F. M.; Ferreira, E. C.; Filgueiras, P. R.; et al. Portable near Infrared Spectroscopy Applied to Fuel Quality Control. *Talanta*, **2018**, *176*, 26–33. DOI:10.1016/j.talanta.2017.07.094.

[132] Wang, W.; Keller, M. D.; Baughman, T.; Wilson, B. K. Evaluating Low-Cost Optical Spectrometers for the Detection of Simulated Substandard and Falsified Medicines. *Appl. Spectrosc.*, **2020**, *74*, 323–333. DOI:10.1177/0003702819877422.

[133] Basri, K. N.; Laili, A. R.; Tuhaime, N. A.; Hussain, M. N.; Bakar, J.; Sharif, Z.; Abdul Khir, M. F.; Zoolfakar, A. S. FT-NIR, MicroNIR and LED-MicroNIR for Detection of Adulteration in Palm Oil via PLS and LDA. *Anal. Methods*, **2018**, *10*, 4143–4151. DOI:10.1039/c8ay01239c.

[134] Eady, M.; Payne, M.; Sortijas, S.; Bethea, E.; Jenkins, D. A Low-Cost and Portable near-Infrared Spectrometer Using Open-Source Multivariate Data Analysis Software for Rapid Discriminatory Quality Assessment of Medroxyprogesterone Acetate Injectables. *Spectrochim. Acta - Part A Mol. Biomol. Spectrosc.*, **2021**, *259*, 119917. DOI:10.1016/j.saa.2021.119917.

[135] Workman, Jr., J.; Weyer, L. *Practical Guide to Interpretive Near-Infrared Spectroscopy*; CRC Press: Boca Raton, 2008. DOI:10.1201/9781420018318.

[136] Martínez, M. L.; Garrido-varo, A.; Pedro, E. De; Sánchez, L. Effect of Sample Heterogeneity on near Infrared Meat Analysis : The Use of the RMS Statistic. *J. Near Infrared Spectrosc.*, **1998**, *320*, A313–A320.

[137] Jiao, Y.; Li, Z.; Chen, X.; Fei, S. Preprocessing Methods for Near-Infrared Spectrum Calibration. *J. Chemom.*, **2020**, *34*, e3306. DOI:10.1002/cem.3306.

[138] Rinnan, Å.; Berg, F. van den; Engelsen, S. B. Review of the Most Common Pre-Processing Techniques for near-Infrared Spectra. *TrAC - Trends Anal. Chem.*, **2009**, *28*, 1201–1222. DOI:10.1016/j.trac.2009.07.007.

[139] Oliveri, P.; Malegori, C.; Simonetti, R.; Casale, M. The Impact of Signal Pre-Processing on the Final Interpretation of Analytical Outcomes – A Tutorial. *Anal. Chim. Acta*, **2019**, *1058*, 9–17. DOI:10.1016/j.aca.2018.10.055.

[140] Westad, F.; Marini, F. Validation of Chemometric Models - A Tutorial. *Anal. Chim. Acta*, **2015**, *893*, 14–24. DOI:10.1016/j.aca.2015.06.056.

[141] Kasim, N. F. M.; Mishra, P.; Schouten, R. E.; Woltering, E. J.; Boer, M. P. Assessing Firmness in Mango Comparing Broadband and Miniature Spectrophotometers. *Infrared Phys. Technol.*, **2021**, *115*, 103733. DOI:10.1016/j.infrared.2021.103733.

[142] Pennisi, F.; Giraudo, A.; Cavallini, N.; Esposito, G.; Merlo, G.; Geobaldo, F.; Acutis, P. L.; Pezzolato, M.; Savorani, F.; Bozzetta, E. Differentiation between Fresh and Thawed Cephalopods Using Nir Spectroscopy and Multivariate Data Analysis. *Foods*, **2021**, *10*, 528. DOI:10.3390/foods10030528.

[143] Jiang, H.; Liu, T.; Chen, Q. Quantitative Detection of Fatty Acid Value during Storage of Wheat Flour Based on a Portable Near-Infrared (NIR) Spectroscopy System. *Infrared Phys. Technol.*, **2020**, *109*, 103423. DOI:10.1016/j.infrared.2020.103423.

[144] Galvão, R. K. H.; Araujo, M. C. U.; José, G. E.; Pontes, M. J. C.; Silva, E. C.; Saldanha, T. C. B. A Method for Calibration and Validation Subset Partitioning. *Talanta*, **2005**, *67*, 736–740. DOI:10.1016/j.talanta.2005.03.025.

[145] Karunathilaka, S. R.; Yakes, B. J.; He, K.; Chung, J. K.; Mossoba, M. Non-Targeted NIR Spectroscopy and SIMCA Classification for Commercial Milk Powder Authentication: A Study Using Eleven Potential Adulterants. *Heliyon*, **2018**, *4*, e00806. DOI:10.1016/j.heliyon.2018.e00806.

[146] Ni, W.; Nørgaard, L.; Mørup, M. Non-Linear Calibration Models for near Infrared Spectroscopy. *Anal. Chim. Acta*, **2014**, *813*, 1–14. DOI:10.1016/j.aca.2013.12.002.

[147] Cocchi, M. *Data Fusion Methodology and Applications*; Elsevier: Amsterdam, 2019.

[148] Borràs, E.; Ferré, J.; Boqué, R.; Mestres, M.; Aceña, L.; Busto, O. Data Fusion Methodologies for Food and Beverage Authentication and Quality Assessment - A Review. *Anal. Chim. Acta*, **2015**, *891*, 1–14. DOI:10.1016/j.aca.2015.04.042.

[149] Weesepoel, Y.; Alewijn, M.; Wijtten, M.; Müller-Maatsch, J. Detecting Food Fraud in Extra Virgin Olive Oil Using a Prototype Portable Hyphenated Photonics Sensor. *J. AOAC Int.*, **2021**, *104*, 7–15. DOI:10.1093/jaoacint/qsaa099.

[150] Müller-Maatsch, J.; Alewijn, M.; Wijtten, M.; Weesepoel, Y. Detecting Fraudulent Additions in Skimmed Milk Powder Using a Portable, Hyphenated, Optical Multi-Sensor Approach in Combination with One-Class Classification. *Food Control*, **2021**, *121*, 107744. DOI:10.1016/j.foodcont.2020.107744.

[151] Baumann, K.; Albert, H.; Von Korff, M. A Systematic Evaluation of the Benefits and Hazards of Variable Selection in Latent Variable Regression. Part I. Search Algorithm, Theory and Simulations. *J. Chemom.*, **2002**, *16*, 339–350. DOI:10.1002/cem.730.

[152] Baumann, K.; Von Korff, M.; Albert, H. A Systematic Evaluation of the Benefits and Hazards of Variable Selection in Latent Variable Regression. Part II. Practical Applications. *J. Chemom.*, **2002**, *16*, 351–360. DOI:10.1002/cem.729.

[153] Andersen, C. M.; Bro, R. Variable Selection in Regression-a Tutorial. *J. Chemom.*, **2010**, *24*, 728–737.

DOI:10.1002/cem.1360.

[154] Mehmood, T.; Liland, K. H.; Snipen, L.; Sæbø, S. A Review of Variable Selection Methods in Partial Least Squares Regression. *Chemom. Intell. Lab. Syst.*, **2012**, *118*, 62–69. DOI:10.1016/j.chemolab.2012.07.010.

[155] Olivieri, A. C. Analytical Figures of Merit: From Univariate to Multiway Calibration. *Chem. Rev.*, **2014**, *114*, 5358–5378. DOI:10.1021/cr400455s.

[156] Brereton, R. G. Introduction to Multivariate Calibration in Analytical Chemistry. *Analyst*, **2000**, *125*, 2125–2154. DOI:10.1039/b003805i.

[157] Allegrini, F.; Olivieri, A. C. IUPAC-Consistent Approach to the Limit of Detection in Partial Least-Squares Calibration. *Anal. Chem.*, **2014**, *86*, 7858–7866. DOI:10.1021/ac501786u.

[158] Olivieri, A. C.; Faber, N. M.; Ferré, J.; Boqué, R.; Kalivas, J. H.; Mark, H. Uncertainty Estimation and Figures of Merit for Multivariate Calibration: (IUPAC Technical Report). *Pure Appl. Chem.*, **2006**, *78*, 633–661. DOI:10.1351/pac200678030633.

[159] Klaas, N.; Faber, M.; Bro, R. Standard Error of Prediction for Multiway PLS 1 . Background and a Simulation Study. *Chemom. Intell. Lab. Syst.*, **2002**, *61*, 133–149. DOI:10.1016/S0169-7439(01)00204-0.

[160] Aslam, M.; Saghir, A.; Ahmad, L. *Introduction to Statistical Process Control*; John Wiley & Sons, Inc.: Hoboken, NJ, USA, 2021. DOI:10.1002/9781119528425.

[161] Wentzell, P. D. Measurement Errors in Multivariate Chemical Data. *J. Braz. Chem. Soc.*, **2014**, *25*, 183–196. DOI:10.5935/0103-5053.20130293.

[162] Escuredo, O.; Rodríguez-Flores, M. S.; Meno, L.; Seijo, M. C. Prediction of Physicochemical Properties in Honeys with Portable Near-Infrared (Micronir) Spectroscopy Combined with Multivariate Data Processing. *Foods*, **2021**, *10*, 317. DOI:10.3390/foods10020317.

[163] Patel, N.; Toledo-Alvarado, H.; Bittante, G. Performance of Different Portable and Hand-Held near-Infrared Spectrometers for Predicting Beef Composition and Quality Characteristics in the Abattoir without Meat Sampling. *Meat Sci.*, **2021**, *178*, 108518. DOI:10.1016/j.meatsci.2021.108518.

[164] Schoot, M.; Kapper, C.; van Kessel, G.; Postma, G.; Buydens, L. M.; Jansen, J. J. Cost-Benefit Analysis of Calibration Model Maintenance Strategies for Process Monitoring. *Anal. Chim. Acta*, **2021**, *1180*, 338890. DOI:10.1016/j.aca.2021.338890.

[165] da Silva, N. C.; Cavalcanti, C. J.; Honorato, F. A.; Amigo, J. M.; Pimentel, M. F. Standardization from a Benchtop to a Handheld NIR Spectrometer Using Mathematically Mixed NIR Spectra to Determine Fuel Quality Parameters. *Anal. Chim. Acta*, **2017**, *954*, 32–42. DOI:10.1016/j.aca.2016.12.018.

[166] da Silva, V. H.; da Silva, J. J.; Pereira, C. F. Portable Near-Infrared Instruments: Application for Quality Control of Polymorphs in Pharmaceutical Raw Materials and Calibration Transfer. *J. Pharm. Biomed. Anal.*, **2017**, *134*, 287–294. DOI:10.1016/j.jpba.2016.11.036.

[167] Eskildsen, C. E.; Skov, T.; Hansen, M. S.; Larsen, L. B.; Poulsen, N. A. Quantification of Bovine Milk Protein Composition and Coagulation Properties Using Infrared Spectroscopy and Chemometrics : A Result of Collinearity among Reference Variables. *J. Dairy Sci.*, **2016**, *99*, 8178–8186. DOI:10.3168/jds.2015-10840.

[168] Eskildsen, C. E.; Sanden, K. W.; Wubshet, G.; Andersen, P. V.; Øyaas, J.; Wold, J. P. Estimating Dry Matter and Fat Content in Blocks of Swiss Cheese during Production Using On-Line near Infrared Spectroscopy. *J. Near Infrared Spectrosc.*, **2019**, *27*, 293–301. DOI:10.1177/0967033519855436.

[169] Eskildsen, C. E.; Engelsen, S. B.; Dankel, K. R.; Solberg, L. E.; Næs, T. Diagnosing Indirect Relationships

in Multivariate Calibration Models. *J. Chemom.*, **2021**, *35*, e3366. DOI:10.1002/cem.3366.

[170] Mancini, M.; Rinnan, Å. Study of Variability of Waste Wood Samples Collected in a Panel Board Industry. *Front. Chem.*, **2021**, *9*, 722090. DOI:10.3389/fchem.2021.722090.

[171] Aykas, D. P.; Ball, C.; Menevseoglu, A.; Rodriguez-Saona, L. E. In Situ Monitoring of Sugar Content in Breakfast Cereals Using a Novel Ft-Nir Spectrometer. *Appl. Sci.*, **2020**, *10*, 8774. DOI:10.3390/app10248774.

[172] Risoluti, R.; Pichini, S.; Pacifici, R.; Materazzi, S. Miniaturized Analytical Platform for Cocaine Detection in Oral Fluids by MicroNIR/Chemometrics. *Talanta*, **2019**, *202*, 546–553. DOI:10.1016/j.talanta.2019.04.081.

[173] Baqueta, M. R.; Coqueiro, A.; Março, P. H.; Valderrama, P. Multivariate Classification for the Direct Determination of Cup Profile in Coffee Blends via Handheld Near-Infrared Spectroscopy. *Talanta*, **2021**, *222*, 121526. DOI:10.1016/j.talanta.2020.121526.

[174] Lan, Z.; Zhang, Y.; Zhang, Y.; Liu, F.; Ji, D.; Cao, H.; Wang, S.; Lu, T.; Meng, J. Rapid Evaluation on Pharmacodynamics of Curcumae Rhizoma Based on Micro-NIR and Benchtop-NIR. *J. Pharm. Biomed. Anal.*, **2021**, *200*. DOI:10.1016/j.jpba.2021.114074.

[175] Acosta, J. J.; Castillo, M. S.; Hodge, G. R. Comparison of Benchtop and Handheld Near-Infrared Spectroscopy Devices to Determine Forage Nutritive Value. *Crop Sci.*, **2020**, *60*, 3410–3422. DOI:10.1002/csc2.20264.

[176] Rukundo, I. R.; Danao, M. G. C.; MacDonald, J. C.; Wehling, R. L.; Weller, C. L. Performance of Two Handheld NIR Spectrometers to Quantify Crude Protein of Composite Animal Forage and Feedstuff. *AIMS Agric. Food*, **2021**, *6*, 463–478. DOI:10.3934/agrfood.2021027.

[177] Fan, L.; Liu, S.; Fan, W.; He, L.; Zhang, C.; Wu, C.; Huang, Y. Quality Assessment of Fritillariae Cirrhosae Using Portable NIR Spectrometer. *Spectrochim. Acta Part A Mol. Biomol. Spectrosc.*, **2021**, 120325. DOI:10.1016/j.saa.2021.120325.

[178] Assi, S.; Guirguis, A.; Halsey, S.; Fergus, S.; Stair, J. L. Analysis of “legal High” Substances and Common Adulterants Using Handheld Spectroscopic Techniques. *Anal. Methods*, **2015**, *7*, 736–746. DOI:10.1039/c4ay02169j.

[179] Yan, H.; Siesler, H. W. Quantitative Analysis of a Pharmaceutical Formulation: Performance Comparison of Different Handheld near-Infrared Spectrometers. *J. Pharm. Biomed. Anal.*, **2018**, *160*, 179–186. DOI:10.1016/j.jpba.2018.07.048.

[180] Ashie, A.; Lei, H.; Han, B.; Xiong, M.; Yan, H. Fast Determination of Three Components in Milk Thistle Extract with a Hand-Held NIR Spectrometer and Chemometrics Tools. *Infrared Phys. Technol.*, **2021**, *113*, 103629. DOI:10.1016/j.infrared.2021.103629.

[181] Oliveira, M. M.; Cruz-Tirado, J. P.; Roque, J. V.; Teófilo, R. F.; Barbin, D. F. Portable Near-Infrared Spectroscopy for Rapid Authentication of Adulterated Paprika Powder. *J. Food Compos. Anal.*, **2020**, *87*, 103403. DOI:10.1016/j.jfca.2019.103403.

[182] Ng, W.; Husnain; Anggria, L.; Siregar, A. F.; Hartatik, W.; Sulaeman, Y.; Jones, E.; Minasny, B. Developing a Soil Spectral Library Using a Low-Cost NIR Spectrometer for Precision Fertilization in Indonesia. *Geoderma Reg.*, **2020**, *22*, e00319. DOI:10.1016/j.geodrs.2020.e00319.

[183] Aykas, D. P.; Ball, C.; Sia, A.; Zhu, K.; Shotts, M.-L.; Schmenk, A.; Rodriguez-Saona, L. In-Situ Screening of Soybean Quality with a Novel Handheld Near-Infrared Sensor. *Sensors*, **2020**, *20*, 6283. DOI:10.3390/s20216283.

[184] Wang, J.; Zareef, M.; He, P.; Sun, H.; Chen, Q.; Li, H.; Ouyang, Q.; Guo, Z.; Zhang, Z.; Xu, D. Evaluation

of Matcha Tea Quality Index Using Portable NIR Spectroscopy Coupled with Chemometric Algorithms. *J. Sci. Food Agric.*, **2019**, *99*, 5019–5027. DOI:10.1002/jsfa.9743.

[185] Tao, F.; Liu, L.; Kucha, C.; Ngadi, M. Rapid and Non-Destructive Detection of Cassava Flour Adulterants in Wheat Flour Using a Handheld MicroNIR Spectrometer. *Biosyst. Eng.*, **2021**, *203*, 34–43. DOI:10.1016/j.biosystemseng.2020.12.010.

[186] Zaukuu, J. L. Z.; Aouadi, B.; Lukács, M.; Bodor, Z.; Vitális, F.; Gillay, B.; Gillay, Z.; Friedrich, L.; Kovacs, Z. Detecting Low Concentrations of Nitrogen-Based Adulterants in Whey Protein Powder Using Benchtop and Handheld NIR Spectrometers and the Feasibility of Scanning through Plastic Bag. *Molecules*, **2020**, *25*, 2522. DOI:10.3390/molecules25112522.

[187] Patel, N.; Toledo-Alvarado, H.; Cecchinato, A.; Bittante, G. Predicting the Content of 20 Minerals in Beef by Different Portable Near-Infrared (NIR) Spectrometers. *Foods*, **2020**, *9*, 1389. DOI:10.3390/foods9101389.

[188] Pereira, J. F. Q.; Silva, C. S.; Vieira, M. J. L.; Pimentel, M. F.; Braz, A.; Honorato, R. S. Evaluation and Identification of Blood Stains with Handheld NIR Spectrometer. *Microchem. J.*, **2017**, *133*, 561–566. DOI:10.1016/j.microc.2017.04.038.

[189] Morillas, A. V.; Gooch, J.; Frascione, N. Feasibility of a Handheld near Infrared Device for the Qualitative Analysis of Bloodstains. *Talanta*, **2018**, *184*, 1–6. DOI:10.1016/j.talanta.2018.02.110.

[190] Barthet, V. J.; Petryk, M. W. P.; Siemens, B. Rapid Nondestructive Analysis of Intact Canola Seeds Using a Handheld Near-Infrared Spectrometer. *JAOCS, J. Am. Oil Chem. Soc.*, **2020**, *97*, 577–589. DOI:10.1002/aocs.12335.

[191] Feng, L.; Zhang, M.; Adhikari, B.; Guo, Z. Nondestructive Detection of Postharvest Quality of Cherry Tomatoes Using a Portable NIR Spectrometer and Chemometric Algorithms. *Food Anal. Methods*, **2019**, *12*, 914–925. DOI:10.1007/s12161-018-01429-9.

[192] Geronimo, B. C.; Mastelini, S. M.; Carvalho, R. H.; Barbon Júnior, S.; Barbin, D. F.; Shimokomaki, M.; Ida, E. I. Computer Vision System and Near-Infrared Spectroscopy for Identification and Classification of Chicken with Wooden Breast, and Physicochemical and Technological Characterization. *Infrared Phys. Technol.*, **2019**, *96*, 303–310. DOI:10.1016/j.infrared.2018.11.036.

[193] Anyidoho, E. K.; Teye, E.; Agbemafle, R. Nondestructive Authentication of the Regional and Geographical Origin of Cocoa Beans by Using a Handheld NIR Spectrometer and Multivariate Algorithm. *Anal. Methods*, **2020**, *12*, 4150–4158. DOI:10.1039/d0ay00901f.

[194] Huang, Y.; Sun, X.; Liao, K.; Han, L.; Yang, Z. Real-Time and Field Monitoring of the Key Parameters in Industrial Trough Composting Process Using a Handheld near Infrared Spectrometer. *J. Near Infrared Spectrosc.*, **2020**, *28*, 334–343. DOI:10.1177/0967033520939323.

[195] Mellado-Carretero, J.; Aykas, D. P.; Puxeu, M.; Varela, S.; Rodriguez-Saona, L.; García-Gonzalo, D.; de Lamo-Castellví, S. Application of Hand-Held near-Infrared and Raman Spectrometers in Surface Treatment Authentication of Cork Stoppers. *Food Packag. Shelf Life*, **2021**, *28*, 100680. DOI:10.1016/j.fpsl.2021.100680.

[196] Zumba, J.; Rodgers, J. Cotton Micronaire Measurements Using Small Portable Near-Infrared (NIR) Analyzers. *Appl. Spectrosc.*, **2016**, *70*, 794–803. DOI:10.1177/0003702816638227.

[197] Magalhães, L. de O.; Arantes, L. C.; Braga, J. W. B. Identification of NBOMe and NBOH in Blotter Papers Using a Handheld NIR Spectrometer and Chemometric Methods. *Microchem. J.*, **2019**, *144*, 151–158. DOI:10.1016/j.microc.2018.08.051.

[198] Gonçalves, D. B.; Santos, C. S. P.; Pinho, T.; Queirós, R.; Vaz, P. D.; Bloore, M.; Satta, P.; Kovács, Z.; Casal, S.; Hoffmann, I. Near Infrared Reflectance Spectroscopy Coupled to Chemometrics as a Cost-

Effective, Rapid, and Non-Destructive Tool for Fish Fraud Control: Monitoring Source, Condition, and Nutritional Value of Five Common Whitefish Species. *J. AOAC Int.*, **2021**, *104*, 53–60. DOI:10.1093/jaoacint/qsaa114.

[199] Kaur, H.; Künnemeyer, R.; McGlone, A. Comparison of Hand-Held near Infrared Spectrophotometers for Fruit Dry Matter Assessment. *J. Near Infrared Spectrosc.*, **2017**, *25*, 267–277. DOI:10.1177/0967033517725530.

[200] Gutiérrez, S.; Tardaguila, J.; Fernández-Novales, J.; Diago, M. P. Support Vector Machine and Artificial Neural Network Models for the Classification of Grapevine Varieties Using a Portable NIR Spectrophotometer. *PLoS One*, **2015**, *10*, e0143197. DOI:10.1371/journal.pone.0143197.

[201] Ni, D.; Smyth, H. E.; Gidley, M. J.; Cozzolino, D. A Preliminary Study on the Utilisation of near Infrared Spectroscopy to Predict Age and in Vivo Human Metabolism. *Spectrochim. Acta Part A Mol. Biomol. Spectrosc.*, **2021**, *265*, 120312. DOI:10.1016/j.saa.2021.120312.

[202] Wilson, B. K.; Kaur, H.; Allan, E. L.; Lozama, A.; Bell, D. A New Handheld Device for the Detection of Falsified Medicines: Demonstration on Falsified Artemisinin-Based Therapies from the Field. *Am. J. Trop. Med. Hyg.*, **2017**, *96*, 1117–1123. DOI:10.4269/ajtmh.16-0904.

[203] Yabré, M.; Ferey, L.; Sakira, A. K.; Bonmatin, C.; Fauré, C.; Somé, T. I.; Gaudin, K. Green Analytical Methods of Antimalarial Artemether-Lumefantrine Analysis for Falsification Detection Using a Low-Cost Handled NIR Spectrometer with DD-SIMCA and Drug Quantification by HPLC. *Molecules*, **2020**, *25*. DOI:10.3390/molecules25153397.

[204] Yu, Y.; Zhang, Q.; Huang, J.; Zhu, J.; Liu, J. Nondestructive Determination of SSC in Korla Fragrant Pear Using a Portable Near-Infrared Spectroscopy System. *Infrared Phys. Technol.*, **2021**, *116*, 103785. DOI:10.1016/j.infrared.2021.103785.

[205] Amuah, C. L. Y.; Teye, E.; Lamptey, F. P.; Nyandey, K.; Opoku-Ansah, J.; Adueming, P. O. W. Feasibility Study of the Use of Handheld NIR Spectrometer for Simultaneous Authentication and Quantification of Quality Parameters in Intact Pineapple Fruits. *J. Spectrosc.*, **2019**, *2019*, 5975461. DOI:10.1155/2019/5975461.

[206] Yang, Y.; Zhang, X.; Yin, J.; Yu, X. Rapid and Nondestructive On-Site Classification Method for Consumer-Grade Plastics Based on Portable NIR Spectrometer and Machine Learning. *J. Spectrosc.*, **2020**, *2020*, 6631234. DOI:10.1155/2020/6631234.

[207] Yan, H.; Siesler, H. W. Identification Performance of Different Types of Handheld Near-Infrared (NIR) Spectrometers for the Recycling of Polymer Commodities. *Appl. Spectrosc.*, **2018**, *72*, 1362–1370. DOI:10.1177/0003702818777260.

[208] Pakhomova, S.; Zhdanov, I.; van Bavel, B. Polymer Type Identification of Marine Plastic Litter Using a Miniature Near-Infrared Spectrometer (Micronir). *Appl. Sci.*, **2020**, *10*, 8707. DOI:10.3390/app10238707.

[209] Kucha, C. T.; Ngadi, M. O. Rapid Assessment of Pork Freshness Using Miniaturized NIR Spectroscopy. *J. Food Meas. Charact.*, **2020**, *14*, 1105–1115. DOI:10.1007/s11694-019-00360-9.

[210] Hao, Y.; Geng, P.; Wu, W.; Wen, Q.; Rao, M. Identification of Rice Varieties and Transgenic Characteristics Based on Near-Infrared Diffuse Reflectance Spectroscopy and Chemometrics. *Molecules*, **2019**, *24*, 4568. DOI:10.3390/molecules24244568.

[211] Cecchini, C.; Antonucci, F.; Costa, C.; Marti, A.; Menesatti, P. Application of Near-Infrared Handheld Spectrometers to Predict Semolina Quality. *J. Sci. Food Agric.*, **2021**, *101*, 151–157. DOI:10.1002/jsfa.10625.

[212] Torres, I.; Sánchez, M. T.; Vega-Castellote, M.; Luqui-Muñoz, N.; Pérez-Marín, D. Routine NIRS

Analysis Methodology to Predict Quality and Safety Indexes in Spinach Plants during Their Growing Season in the Field. *Spectrochim. Acta - Part A Mol. Biomol. Spectrosc.*, **2021**, *246*, 118972. DOI:10.1016/j.saa.2020.118972.

[213] Zontov, Y. V.; Balyklova, K. S.; Titova, A. V.; Rodionova, O. Y.; Pomerantsev, A. L. Chemometric Aided NIR Portable Instrument for Rapid Assessment of Medicine Quality. *J. Pharm. Biomed. Anal.*, **2016**, *131*, 87–93. DOI:10.1016/j.jpba.2016.08.008.

[214] Yan, H.; Siesler, H. W. Identification of Textiles by Handheld near Infrared Spectroscopy: Protecting Customers against Product Counterfeiting. *J. Near Infrared Spectrosc.*, **2018**, *26*, 311–321. DOI:10.1177/0967033518796669.

[215] Jianqiang, Z.; Panpan, Y.; Weijuan, L.; Yanmei, Y.; Tianjun, Y.; Ying, H.; Changyu, L. Rapid and Automatic Classification of Tobacco Leaves Using a Hand-Held DLP-Based NIR Spectroscopy Device. *J. Braz. Chem. Soc.*, **2019**, *30*, 1927–1932. DOI:10.21577/0103-5053.20190105.

[216] Borba, K. R.; Aykas, D. P.; Milani, M. I.; Colnago, L. A.; Ferreira, M. D.; Rodriguez-Saona, L. E. Portable near Infrared Spectroscopy as a Tool for Fresh Tomato Quality Control Analysis in the Field. *Appl. Sci.*, **2021**, *11*, 3209. DOI:10.3390/app11073209.

[217] Castrignanò, A.; Buttafuoco, G.; Malegori, C.; Genorini, E.; Iorio, R.; Stipic, M.; Girone, G.; Venezia, A. Assessing the Feasibility of a Miniaturized Near-Infrared Spectrometer in Determining Quality Attributes of San Marzano Tomato. *Food Anal. Methods*, **2019**, *12*, 1497–1510. DOI:10.1007/s12161-019-01475-x.

[218] Leoni, E.; Mancini, M.; Duca, D.; Toscano, G. Rapid Quality Control of Woodchip Parameters Using a Hand-Held near Infrared Spectrophotometer. *Processes*, **2020**, *8*, 1413. DOI:10.3390/pr8111413.

[219] Baca-Bocanegra, B.; Nogales-Bueno, J.; García-Estévez, I.; Escribano-Bailón, M. T.; Hernández-Hierro, J. M.; Heredia, F. J. Screening of Wine Extractable Total Phenolic and Ellagitannin Contents in Revalorized Cooperage By-Products: Evaluation by Micro-NIRS Technology. *Food Bioprocess Technol.*, **2019**, *12*, 477–485. DOI:10.1007/s11947-018-2225-z.

[220] de Oliveira Moreira, A. C.; de Lira Machado, A. H.; de Almeida, F. V.; Braga, J. W. B. Rapid Purity Determination of Copaiba Oils by a Portable NIR Spectrometer and PLSR. *Food Anal. Methods*, **2018**, *11*, 1867–1877. DOI:10.1007/s12161-017-1079-8.

[221] de Oliveira Moreira, A. C.; Braga, J. W. B. Authenticity Identification of Copaiba Oil Using a Handheld NIR Spectrometer and DD-SIMCA. *Food Anal. Methods*, **2021**, *14*, 865–872. DOI:10.1007/s12161-020-01933-x.

[222] Karunathilaka, S. R.; Fardin-Kia, A. R.; Srigley, C.; Chung, J. K.; Mossoba, M. M. Rapid Screening of Commercial Extra Virgin Olive Oil Products for Authenticity: Performance of a Handheld NIR Device. *NIR news*, **2017**, *28*, 9–14. DOI:10.1177/0960336016687521.

[223] Sun, Z.; Li, C.; Li, L.; Nie, L.; Dong, Q.; Li, D.; Gao, L.; Zang, H. Study on Feasibility of Determination of Glucosamine Content of Fermentation Process Using a Micro NIR Spectrometer. *Spectrochim. Acta - Part A Mol. Biomol. Spectrosc.*, **2018**, *201*, 153–160. DOI:10.1016/j.saa.2018.05.005.

[224] Silva, A. C. d.; Ribeiro, L. P. D.; Vidal, R. M. B.; Matos, W. O.; Lopes, G. S. A Fast and Low-Cost Approach to Quality Control of Alcohol-Based Hand Sanitizer Using a Portable near Infrared Spectrometer and Chemometrics. *J. Near Infrared Spectrosc.*, **2021**, *29*, 119–127. DOI:10.1177/0967033520987315.

[225] Fonseca, F. S.; e Brito, L. R.; Pimentel, M. F.; Leal, L. B. Determination of Ethanol in Gel Hand Sanitizers Using Mid and near Infrared Spectroscopy. *J. Braz. Chem. Soc.*, **2020**, *31*, 1759–1763. DOI:10.21577/0103-5053.20200115.

[226] Jahani, R.; Yazdanpanah, H.; van Ruth, S. M.; Kobarfard, F.; Alewijn, M.; Mahboubi, A.; Faizi, M.; Aliabadi, M. H. S.; Salamzadeh, J. Novel Application of Near-Infrared Spectroscopy and Chemometrics Approach for Detection of Lime Juice Adulteration. *Iran. J. Pharm. Res.*, **2020**, *19*, 34–44. DOI:10.22037/ijpr.2019.112328.13686.

[227] Risoluti, R.; Gullifa, G.; Battistini, A.; Materazzi, S. “Lab-on-Click” Detection of Illicit Drugs in Oral Fluids by MicroNIR-Chemometrics. *Anal. Chem.*, **2019**, *91*, 6435–6439. DOI:10.1021/acs.analchem.9b00197.

[228] Henrique da Silva Melo, B.; Figueiredo Sales, R.; da Silva Bastos Filho, L.; Souza Povoas da Silva, J.; Gabrielle Carolino de Almeida Sousa, A.; Maria Camará Peixoto, D.; Pimentel, M. F. Handheld near Infrared Spectrometer and Machine Learning Methods Applied to the Monitoring of Multiple Process Stages in Industrial Sugar Production. *Food Chem.*, **2022**, *369*, 130919. DOI:10.1016/j.foodchem.2021.130919.

[229] Henn, R.; Kirchler, C. G.; Huck, C. W. Miniaturized NIR Spectroscopy for the Determination of Main Carbohydrates in Syrup. *NIR news*, **2017**, *28*, 3–6. DOI:10.1177/0960336017695732.

9. Abbreviations

ANN = Artificial neural networks
BOSS = Bootstrapping soft shrinkage
BPNN = Back propagation neural network
CARS = Competitive adaptive reweighted sampling
CFS = Correlation-based feature selection
CL = Commercial language
CP-ANN = Counter-propagation neural network
CRT = Cubist regression tree
CS = Commercial software
CT = Commercial toolbox
DD-SIMCA = Data driven soft independent modelling of class analogy
DMD = Digital micromirror device
DS = Direct standardisation
ELM = Extreme learning machine
GA = Genetic algorithm
GMD = Global Mahalanobis distance analysis
GPR = Gaussian process regression
HCA = Hierarchical cluster analysis
HQI = Hit quality index (comparison with library)
HP = High performance
i-PLS = interval partial least squares
IRIV = Iteratively retaining informative variables
IVSO = Iteratively variable subset optimization
JK = Jack-knife algorithm on the regression coefficients
KNN = K-nearest neighbour
K-S = Kennard-Stone
LDA = Linear discriminant analysis

LED = Light-emitting diodes
Logistic-R = Logistic regression
LVF = Linear variable filter
LW = Loading weights
MBSD = Moving block of standard deviation method
MCC = Multivariate control chart
MCR-ALS = Multivariate curve resolution-alternating least squares
MLR = Multiple linear regression
M-PLS = Modified partial least squares
MS = Mobile sensing
MSPC = Multivariate statistical process control
MW = Moving window
MWPLS = Moving window partial least squares
NSoA = New set of acquisition
OC-PLS = One-class partial least squares
OPEN-L = Open-source programming language
OPEN-T = Open-source toolbox
OPLS-DA = Orthogonal projections to latent structures discriminant analysis
PCA = Principal component analysis
PCR = Principal component regression
PDS = Piecewise direct standardisation
PLS-DA = Partial least square discriminant analysis
PLSR = Partial least squares regression
PSI = Pearson's similarity index
QDA = Quadratic discriminant analysis
RC = Regression coefficients
RF = Random Forest
RM = Reverse method
RSDE = Random subspace discriminant ensemble
Si = Synergy interval
SIMCA = Soft independent modelling of class analogy
SMV = Spectral match value with a database
SO-CovSel = Sequential and orthogonalized covariance selection
SO-PLS = Sequential and orthogonalized partial least squares
SPA = Successive projection algorithm
SPXY = Sample set partitioning based on joint **X**-**y** distances
SRC = Sparse representation classification
SVMC = Support vector machine classification
SVMR = Support vector machine regression
SWR =Stepwise regression
UVE =Uninformation variable elimination
VCPA = Variable combination population analysis
VIP = Variable importance for projection

WM = Wrapper method
XGB = Extreme gradient boosting

Tables

Table 1 - Specification of the main technical parameters and characteristics for selected popular miniaturized NIR spectrometers. The instrument name reported is the most utilized in the literature under review. Parameters are extracted from the technical sheet of the vendors. HP: high performance, MS: mobile sensing, DMD: digital micromirror device, LED: light-emitting diodes, LVF: linear variable filter.

Spectrometer (vendor)	**Source**	**Wavelenght selector**	**Detector**	**Wavelenght region**	**Spectral resolution (at wavelength)**	**Weight (Dimension)**	**Connectivity**	**Approximate order of unit Cost**
DPL NIRscan Nano (Texas Instruments)	Tungsten halogen	Stationary dispersive grating and MEMS DMD	InGaAs (single element)	HP: 1350–2490 nm MS: 900–1700 nm	HP:12 MS:10	(6.2 x 5.8 x 3.6 cm)	Bluetooth and USB	< 5,000
MicroNIR 1700 (VIAVI)	Tungsten halogen	LVF	InGaAs (array; 128 elements)	908–1676 nm	12.5 (1000) 25 (2000)	64 g (4.5 x 5.0 cm)	USB	< 30,000
microPHAZIR (Thermo Fisher Scientific)	Tungsten halogen	MEMS Hadamard mask	InGaAs (single element)	1596–2396 nm	11	1.2 kg (24.4 x 23.2 x 9.7 cm)	USB	< 50,000
NeoSpectra development kit (Si-Ware Systems)	Tungsten halogen	MEMS Michelson interferometer	InGaAs (single element)	1350–2558 nm	16 (1550)	17 g (32. × 3.2 × 2.2 cm)	Bluetooth	< 5,000
NIRONE sensors (Spectral Engines)	Tungsten halogen	MEMS Fabry–Perot interferometer	S1.4: InGaAs (single elements) S1.7–S2.5:"extended" InGaAs (single element)	1100–1350 nm (S1.4) 1350–1650 nm (S1.7) 1550–1950 nm (S2.0) 1750–2150 nm (S2.2) 2000–2450 nm (S2.5)	12–16 13–17 15–21 16–22 18–28	15 g (2.5 × 2.5 × 1.75 cm)	Bluetooth and USB	< 5,000
NIR-S-G1 (Tellspec)	Tungsten halogen	Stationary dispersive grating and MEMS DMD	InGaAs (single element)	900–1700 nm	10	87 g (*7.6 x 8.2 x 2.7 cm*)	Bluetooth (Cloud service)	< 5,000
SCiO (Consumer Physics)	LED	Bandpass filter	Si photodiode (array, 12 elements)	740–1070 nm	N/A	35 g (0.315 × 0.95 × 2.75 cm)	Bluetooth (Cloud service)	< 1,000

Table 2 - Overview of the application of miniaturised NIR instruments on powder samples. Some information was not explicitly declared (-) in the articles. Variable selection algorithms were sometimes used only as an interpretation tool (*). The column concerning the splitting algorithms for external validation includes information related to the acquisition of new sets or batches of samples (NSoA), the use internal cross-validation (#) or no validation (//). Elaboration tools were divided into Commercial Programming Language (CL), Commercial Toolbox (CT), Commercial Software (CS), Open-source programming language (OPEN-L), Open-source toolbox (OPEN-T). Abbreviations related to the chemometrics models can be found in the list of abbreviations.

Sample	**NIR Spectrometer**	**Range (nm)**	**Mode**	**Acquisition system**	**Pretreatment**	**Scope**	**Number of samples**	**Models**	**Variable Selection method**	**External validation (Splitting algorithm)**	**Elaboration system**	**Ref**
Black pepper	MicroNIR 2200 microPHAZIR SCiO	1128 – 2162 1596 – 2395 740 – 1069	Reflectance	-	None and milled	Prediction	66	PLSR	None	K-S	CS	[33]
Cannabinoids	MicroNIR	900 – 1700	Reflectance	Glass vial	Shaken	Prediction Classification	-	PCA, PLSR, PLS-DA	None	-	CS	[18]
Cereals	NeoSpectra-Micro development kit	1350 – 2560	Reflectance	Through a sample holder	None and ground	Prediction	164	PLSR	Loadings *	Random	CS	[171]
Cocaine	SCiO	740 – 1070	Reflectance	Through a vial	None	Classification	316	PCA, SIMCA, PLSR, KNN, ANN	None	Random + NSoA	CS + OPEN-L	[20]
Cocaine	MicroNIR	950 – 1650	Reflectance	Glass vial	None	Prediction	90	PCA, PLSR	None	NSoA	CS	[172]
Cocaine	DLP NIRscan Nano EVM	900 – 1700	Reflectance	Glass vial	None	Prediction	240	PCA, SIMCA, PLSR	JK	K-S	CS	[17]
Coffee	MicroNIR Pro 1700	908 – 1676	Reflectance	-	Ground	Prediction	125	PCA, PLSR	None	Real samples	CL	[67]
Coffee	MicroNIR 1700	908 – 1676	Reflectance	Glass cuvette	Homogenised	Classification	214	PCA, PLS-DA	VIP*	Random	CL + CT	[173]
Coriander seed	Ocean Insights Flame-NIR SCiO	934 – 1660 740 – 1070	Reflectance	Petri dish	Ground	Prediction Classification	290	OPLS-DA, PLSDA, RF, PLSR	None	-	CSs	[38]
Curcumae Rhizoma	NIR-S-G1	900 – 1700	Reflectance	Through plastic film	Crushed, sieved, dried	Prediction	62	PLSR	CARS, IRIV, GA	K-S	CL	[174]
Dog food	SCiO	740 – 1070	Reflectance	Plastic bag 1 cm above the surface	None and Ground	Prediction	99	PLSR	None	Random	CS	[44]
Fluid bed dryer batches	N-Series 2.2	1750 – 2150	Reflectance	Probe with a sapphire window	None	Prediction	14 batches	PLSR, PCA-based MSPC	None	NSoA	CL + CT	[23]
Forages	microPHAZIR DLP NIRscan Nano EVM	1600 – 2400 900 – 1700	Reflectance	Through a cover glass	Ground	Prediction	210	PLSR	None	Random	OPEN-L	[175]
Forages	AuroraNir NIR-S-G1 SCiO	950 – 1650 950 – 1650 740 – 1070	Reflectance	Direct contact	Dried, ground, sieved	Prediction	1128	PLSR	None	-	CSs	[90]
Forages	Tellspec Enterprise Scanner	900 - 1700	Reflectance	Through polypropylene bags	Dried and ground	Prediction	147	PCA, PLSR	None	-	CS	[176]
Fritillariae cirrhosae	PV500R-I	1353 – 1850	Reflectance	Direct contact	Weighed, crushed and sieved	Prediction Classification	72	LDA, PLSR	None	-	CSs	[177]
Gluten-free grains	MicroPHAZIR RX analyzer MicroNIR 2200 SCiO	1596 – 2396 1128 – 2162 740 – 1070	Reflectance	Quartz cuvette	None and milled	Prediction	77	PLSR	None	K-S	” The Lab” + CS	[40]

Sample	NIR Spectrometer	Range (nm)	Mode	Acquisition system	Pretreatment	Scope	Number of samples	Models	Variable Selection method	External validation (Splitting algorithm)	Elaboration system	Ref
Illegal drugs: heroin, cocaine, and cannabis	MicroNIR Onsite W 1700	950 – 1650	Absorbance	-	-	Prediction Classification	3307	PCA, PLSR, gradient-boosting classifier and regressor methods	None	K-S	OPEN-L	[19]
Illegal drugs: cocaine, phenacetin, lidocaine, caffeine, and levamisole	MicroNIR Pro 1700	908 – 1676	Reflectance	Cocaine and seal: direct contact. Ecstasy and medicines: borosilicate glass	Cocaine and seal: none. Ecstasy and medicines: macerated	Prediction Classification	64	PCA, HCA, PLSR	None	K-S	CL	[130]
Legal high substance	Thermo microPHAZIR RX NIR	1600 - 2400	-	Through vials	None	Classification	-	Library matching algorithm	None	NSoA	CS	[178]
Medicines: artemether, efavirenz, isoniazid and excipients	SCiO NIR-S-G1 Neospectra	740 – 1070 900 – 1700 1350 – 2500	Reflectance	Through a sample container	None	Prediction	-	PLSR	None	#	CL	[132]
Medicines: acetylsalicylic acid, ascorbic acid, caffeine, and excipients	(Si-Ware Systems) NR 2.0-W DLP NIRscan Nano EVM MicroNIR 1700	1298 – 2606 1550 – 1950 900 – 1701 908 – 1676	Reflectance	Petri dish	Mixed	Prediction	50	PLSR	None	-	CS	[179]
Millet	MicroPhazir RX MicroNIR 2200 SCiO	1596 – 2396 1128 – 2162 740 – 1070	Reflectance	Quartz cuvette	None and milled, shaken	Prediction	42	PLSR	MW	K-S	” The Lab” + CSs	[41]
Milk powder	microPHAZIR GP 4.0 microNIR2200	1596 – 2396 1128 – 2161	Reflectance	Cuvette	Shaken with an iron sphere	Prediction	110	PLSR	None	K-S and DUPLEX	CL + CS	[48]
Milk powder	microPHAZIR MicroNIR 2200	1596 – 2400	Reflectance	Petri dish	Homogenised	Classification	35	PCA, SIMCA	None	NSoA	CT	[145]
Milk thistle extract	MicroNIR 1700	950 – 1650	Reflectance	-	-	Prediction	78	PLSR	random frog	Hierarchical method	CS + OPEN-T	[180]
Mulberry leaves	MicroNIR 1700	950 – 1650	Reflectance	Direct contact	None and dried, pulverised and sieved	Prediction	83, 77,80	PLSR	UVE, CARS, random frog	NSoA	CL + CSs + OPEN-T	[32]
Oregano	SCiO	740 – 1070	Reflectance	Glass petri dish	None	Classification Calibration transfer	413	PLS-DA, RF, DS, PDS	None	NSoA	CSs + CL + CT	[47]
Paprika	DLP NIRscan Nano EVM	900 – 1700	Reflectance	Petri dish	Flatten	Prediction Classification	315	PLSR, PLS-DA	RC	-	CL + CS	[181]
Peanut seeds	Consisted in: Spectrometer (Ocean Optics); Optical fiber, Halogen Lamp	900 – 1700	Reflectance	Direct contact	Dried and ground	Prediction Classification	113	PLSR, PCA, LDA	Si-GA-PLS, GA-PLS, Si-PLS	Random	CL	[42]
Pharmaceutical compounds	MicroNIR Pro 1700	908 – 1676	Reflectance	Borosilicate glass vials at 3 mm distance	None	Classification	2 sets	SVMC, SIMCA, PLS-DA, LDA, QDA	None	K-S	CL	[43]
Plant extracts	MicroNIR 2200 MicroNIR 1700 ES microPHAZIR	1128 – 2162 900 – 1700 1600 – 2400	Reflectance	Quartz cuvette	Ground	Prediction	192	PLSR, GPR, ANN	None	K-S	CL + CT + CS	[25]

Sample	NIR Spectrometer	Range (nm)	Mode	Acquisition system	Pretreatment	Scope	Number of samples	Models	Variable Selection method	External validation (Splitting algorithm)	Elaboration system	Ref
Powder blend	MicroNIR PAT-W	900 – 1700	Reflectance	White PVC container	None	Prediction	42	PCA, PLSR, MBSD	Spectral observations	Plackett-Burman	CS	[22]
Powder blend	MicroNIR PAT-U	950 – 1650	Reflectance	Sample holder at an interfacing port	None	Prediction	31 formulations	PCA, PLSR	None	NSoA	-	[21]
Rosmarini folium	microPHAZIR MicroNIR 2200	1600 – 2400 1128 – 2161	Reflectance	Cuvette	Dried and milled	Prediction	60	PLSR	Uncertainty Test, RC*	Semi-Random (based on y)	CL + CS	[37]
Skimmed milk powder	In-house spectrometer	939 – 1833	Reflectance	Distance with a customised spacer	Homogenised using a spoon	Classification	168	KNN, SIMCA, PCA, Mahalanobis distance, SVMC	None	#	OPEN-L	[150]
Soils	N-Series 2.2	1750 – 2150	Reflectance	Different distances and direct contact	Cleaned from non-soil particles, air-dried, crushed, and sieved	Prediction	102	PLSR, RF	None	#	OPEN-L	[27]
Soils	NeoSpectra	1300 – 2500	Reflectance	Direct contact	Air-dried, ground, and sieved	Prediction	232 + 638	PLSR, SVMR	Cubist regression*	#	OPEN-L	[26]
Soils	(Si-Ware Systems Inc)	1350 – 2550	Reflectance	-	-	Prediction	362	Data fusion, Cubist regression, PLSR, SVMR	None	-	OPEN-L	[31]
Soils	NIR-512	866 – 1670	Reflectance	Probe	None	Classification	405	PCA, PLS-DA	None	-	CL + CT	[28]
Soils	NeoSpectra Module SWS62221	1300 – 2600	Reflectance	-	Air-dried and ground	Prediction	1601	CRT	None	-	OPEN-L	[182]
Soils	MicroNIR 2200	1151 – 2186	Reflectance	Petri dish	Air-dried, ground and oven-dried	Prediction	360	M-PLSR	None	#	OPEN-L + CS	[29]
Soils	NeoSpectra Module SWS62221 ASP-NIR-350 M-Reflect	1250 – 2500 900 – 1700	Reflectance	Direct contact	air-dried, crushed, and sieved	Prediction	392	CRT, PLSR	None	Random	OPEN-L	[30]
Soybean	NeoSpectra Micro	1350 – 2560	Reflectance	Petri dish	Ground and sieved	Prediction Classification	122	PLSR, SIMCA	None or range reduction	Random	CS	[183]
Tea	NIR-S-R2	900 – 1700	Reflectance	Quartz container	Ground and sieved	Prediction Classification	475	PCA, PLS-DA, SVMC, PLSR, SVMR	SPA, RC, IRIV	-	CL	[46]
Tea	MicroNIR 2200 microPHAZIR	1128 – 2162 1600 – 2400	Reflectance	-	Ground and milled	Prediction	65	PLSR	None	K-S	CS	[39]
Tea	NIR-S-R2	900 – 1700	Reflectance	Through a sample container	Ground and sieved	Prediction Classification	360	PLSR, PLS-DA, SVMC	CARS, VCPA, IVSO	Semi-Random (based on y)	CL + CS	[35]
Tea	DLP NIRscan Nano EVM	900 – 1700	Reflectance	Sample cup	None	Prediction	105	PLSR	Random frog, Si-PLS, GA-PLS, CARS	-	CL	[184]
Tea	NIR-S-R2	900 – 1700	Absorbance	-	Ground and sieved	Prediction	56	PLSR, MLR	SPA, CARS	-	CL	[36]
Wheat flour	NR 2.0-W MicroNIR 1700 Si-Ware Systems	1550 – 1950 908 – 1676 1298 – 2606	Reflectance	1–2 mm distance	None	Prediction	235	PLSR	None	Hierarchical method	CS	[45]
Wheat flour	In-house spectrometer	899.22 – 1724	Reflectance	Direct contact	None	Prediction	120	ELM	VCPA	Semi-Random (based on y)	CL	[143]
Wheat flour	MicroNIR 2200	1150 – 2150	Absorbance	Through a Polyvinyl chloride film	None	Classification	48	PCA-LDA, PLS-DA	None	Semi-Random (based on y)	-	[185]

Sample	NIR Spectrometer	Range (nm)	Mode	Acquisition system	Pretreatment	Scope	Number of samples	Models	Variable Selection method	External validation (Splitting algorithm)	Elaboration system	Ref
Whey Protein Powder	NIR-S-G1	900 – 1700	Reflectance	Through optical glass cuvette Through low-density polyethylene plastic bag	None	Prediction Classification	273	LDA, PLSR	None	-	OPEN-L	[186]

Table 3 - Overview of the application of miniaturised NIR instruments on other solid samples. Some information was not explicitly declared (-) in the articles. Variable selection algorithms were sometimes used only as an interpretation tool (*). The column concerning the splitting algorithms for external validation includes information related to the acquisition of new sets or batches of samples (NSoA), the use internal cross-validation (#) or no validation (//). Elaboration tools were divided into Commercial Programming Language (CL), Commercial Toolbox (CT), Commercial Software (CS), Open-source programming language (OPEN-L), Open-source toolbox (OPEN-T). Abbreviations related to the chemometrics models can be found in the list of abbreviations.

Sample	**NIR Spectrometer**	**Range (nm)**	**Mode**	**Acquisition system**	**Pretreatment**	**Scope**	**N of samples**	**Models**	**Variable Selection method**	**External validation (Splitting algorithm)**	**Elaboration system**	**Ref**
Acerola fruit	MicroNIR 1700	950 – 1650	Reflectance	-	None	Prediction	117	PLSR, SVMR	None	DUPLEX	CL + CT	[56]
Apples	MicroNIR 1700	950 – 1650	Reflectance	-	None	Prediction Calibration Transfer	866	MLR, PLSR, SVMR	None	SPXY	CS	[49]
Archaeological bones, cinematographic films, bronze patinas	Viavi prototype	1208 – 2160	Bones: Reflectance Films: Transflectance Patinas: Reflectance	Direct contact	None	Classification	Bones: 7 Film rolls: 79 Patinas: 3	PCA	None	//	CL	[84]
Avocado	MicroNIR SCiO v1.2	908 - 1676 704 - 1070	Reflectance	- Few mm distance	None and after removal of skin or equilibration at different temperatures	Prediction	1570	PLSR	None	NSoA	CS	[50]
Banknotes	MicroNIR Pro 1700	908 – 1676	Reflectance	Direct contact	None	Classification	63	PCA, PLS-DA	None	#	CL + CT + CS	[99]
Beef meat	MicroNIR Pro	905 – 1649	Reflectance	Direct contact	None	Prediction	194	PLSR	None	#	OPEN-L	[163]
Beef meat	MicroNIR Pro	905 – 1649	Reflectance	Direct contact	None	Prediction	178	PLSR	None	#	OPEN-L	[187]
Blood stains	MicroNIR 1700	908 – 1676	-	-	None	Classification	220	SIMCA, LDA, PLS-DA	SPA, GA	-	CL + CT	[188]
Blood stains	SCiO	700 – 1100	-	-	None	Classification	230	PLSR	None or range reduction	NSoA	“The Lab”	[189]
Canadian canola seeds	MicroNIR OnSite-W	908 – 1676	Reflectance	-	None	Prediction	181	PLSR	None	NSoA (2)	CSs	[190]
Cephalopods	MicroNIR Pro 1700 ES SCiO	908 – 1676 740 – 1070	Reflectance	-	None	Classification	50	PCA, PLS-DA	VIP*	DUPLEX	” The Lab” + CS + CL + CT	[142]
Cheddar cheese	SCiO	740 – 1070	Reflectance	Petri dish	Shredded and temperature equilibrated	Prediction	49	PLSR	Backward elimination, MLR-forward selection, i-PLSR	Random	OPEN-L	[95]
Cheese	SCiO	740 – 1070	Reflectance	Direct contact, quartz cuvette	None and grated	Prediction	46	PLSR	None	K-S	” The Lab” + CSs	[78]
Cherries	DLP NIRscan Nano	900 – 1700	Reflectance	-	None	Prediction	240	Logistic-R, LDA, SVMC, MLR, PCR, PLSR, SVMR	None	Random	OPEN-L	[57]

Sample	NIR Spectrometer	Range (nm)	Mode	Acquisition system	Pretreatment	Scope	N of samples	Models	Variable Selection method	External validation (Splitting algorithm)	Elaboration system	Ref
Cherry Tomatoes	(Isuzu Optics Corp)	950 – 1650	Reflectance	Optical fiber in direct contact	Thermal equilibration	Prediction	90	PLSR, SVMR, ELM, HCA	None	Random	CL + CSs	[191]
Chicken meat	MicroNIR 2200	1150 – 2150	Absorbance	Fixed distance maintained with a collar	Skin removal	Classification	80	PCA, LDA	SWR	#	CS	[192]
Chicken meat	MicroNIR Pro 1700 ES	908 – 1676	Reflectance	Direct contact Through the top of the package Through the package held bottom up	None	Classification	286	PLS-DA, CP-ANN, SVMC, RSDE	VIP	DUPLEX	CL + CT + OPEN-T	[62]
Chicken meat	DLP NIRscan Nano	900 – 1700	Absorbance	-	None and minced	Classification	137 + 90	PCA, LDA, SVMC, RF	None	K-S	CSs	[77]
Cocoa beans	Tellspec	900 – 1700	Absorbance	Through a transparent zip-locked polythene bag	None	Classification	210	PCA, LDA, SVMC	None	Random	CL	[193]
Composting process	MicroNIR PAT-U	950 – 1650	Reflectance	Direct contact	None	Prediction	100	PLSR	None	Semi - Random	CL + CT	[194]
Compound feed	MicroPHAZIR MicroNIR 1700	1600 – 2400 910 – 1676	Reflectance	Through quartz protection Spaced by a collar	None	Prediction	100	PLSR	None	Random	CS	[69]
Cork stopper	MicroPHAZIR	1600 – 2400	Reflectance	-	None	Prediction Classification	288	PLSR, SIMCA	RC*	Semi - Random	CS	[195]
Cotton fiber	MicroNIR 1700 MicroNIR 2200	950 – 1650 1150 – 2150	Reflectance	Direct contact	None	Prediction	104	PLSR	None	-	CS	[196]
Crop grains	SCiO	740 – 1070	Reflectance	Point and shoot	None	Classification	2650	AdaBoost, Naïve Bayes, PLS-DA, RF, SVMC	VIP*	Random	OPEN-L	[68]
Drug on blotter papers: NBOMe and NBOH	MicroNIR 1700	908 – 1690	Reflectance	Distance using a collar	None	Classification	101	SIMCA, PLS - DA	None	Chronological order	CL + CT	[197]
Eggs	SCiO	740 – 1070	Reflectance	10-mm distance	None	Prediction	660	PLSR, ANN	CFS	#	CL	[60]
Eggs	DLP NIRscan Nano	900 – 1700	Absorbance	Direct contact	None	Prediction	660	PCA, PLSR, SVMR, PLS-DA, SVMC	i-PLS	-	CL + CT	[61]
Elephants’ ivory	3 in-house devices	600 – 1100 700 – 1200 900 – 1700	Reflectance	Direct contact	Cleaned and temporarily marked	Classification	86	PCA, PLS-DA	None	Random	CS	[86]
Fengdous mulberry fruits	DLP NIRscan Nano EVM	909 – 1649	Reflectance	Direct contact	None	Prediction Classification	468 + 434	PLS-DA, PLSR	CARS	-	CL + CT + OPEN-T	[58]
Fish	MicroNIR OnSite	950 – 1650	Reflectance	Direct contact	None	Classification	170	LDA, SIMCA	SELECT	-	CL	[66]
Fish	Tellspec Enterprise Sensor	900 - 1700	Reflectance	-	None	Prediction Classification	805	PLSR, LDA, Logistic-R, RF, XGB, SVMC, PCA	None	-	OPEN-L	[198]

Sample	NIR Spectrometer	Range (nm)	Mode	Acquisition system	Pretreatment	Scope	N of samples	Models	Variable Selection method	External validation (Splitting algorithm)	Elaboration system	Ref
Forages	DLP NIRscan Nano	900 – 1700	-	Sample holder	None	Prediction	90	PLSR	None	None	OPEN-L	[73]
Fruits	H-100C SCiO	650 – 950 740 – 1070	Reflectance	Direct contact or close to contact Direct contact	None	Prediction	296	PLSR	None	#	CL + CT	[199]
Grape berries	MicroPHAZIR	1596 - 2396	Reflectance	Direct contact	None	Prediction	1600	PCA, PLSR	LW*, RC*	-	OPEN-L	[55]
Grapes and peach fruits	SCiO	740 – 1070	Reflectance	Direct contact	None	Prediction	Grapes: 450 Peaches: 150	PLSR	None	Random	CL + CT	[52]
Grapevine	MicroPHAZIR	1600 – 2400	Reflectance	-	None	Prediction	160	PCA, GMD, PLSR	None	#	CSs	[54]
Grapevine	MicroPHAZIR	1600 – 2400	Reflectance	Direct contact	None	Classification	400	SMVC, ANN	None	#	OPEN-L + CSs	[200]
Hamburger meat	MicroNIR Pro 1700	908 – 1676	Reflectance	-	None	Prediction	144	PLSR, SVMR	None	Rank K-S	CL	[75]
Human health	MicroNIR 1700	950 – 1600	Reflectance	Direct contact with pressure	None	Prediction	690	PCA, PLSR	Loadings *	#	CS	[201]
Iberian hams	MicroNIR OnSite Lite	900 – 1700	-	-	None	Prediction Classification	495	LDA, QDA, PLSR	None	Random	CL + CT	[64]
Kiwifruit, apple, feijoa, and avocado	SCiO	740 – 1070	Reflectance	Point and shoot	None	Prediction	Apple: 373 Kiwi: 1590 Feijoa: 296	PCA, PLSR	None	Apple: NSoA Kiwifruit: NSoA Feijoa: #	” The Lab” + CS	[51]
Lamb meat	NIRScan Nano	900 – 1700	Reflectance	Plastic weighing boat	Flattened out in a plastic weighing boat with and without temperature equilibration and ground	Prediction	609	PLSR	None	-	CS	[93]
Mango	MicroNIR 1700	950 – 1650	Reflectance	Direct contact	None Sliced	Prediction	250	PLSR	JK	SPXY	CL + CS	[89]
Mango	SCiO	740-1070	Reflectance	2 cm distance	None	Prediction	150	PLSR	BOSS	K-S	CL	[141]
Meat	SCiO Polychromix Spectral Probe	740 – 1070 940 – 1700	Reflectance	-	Minced	Prediction	328	PLSR, RF regression	None	Semi - Random K-S	OPEN-L	[76]
Meat	DLP NIRscan Nano	900 – 1700	Absorbance	Direct contact	Ground	Prediction	60 + 420	PCA, PLSR	SWR	-	CS	[74]
Medicines in tablets or capsules: paracetamol, ibuprofen and artemether-lumefantrine	NIR-S-G1	900 – 1700	Reflectance	Through the blister	None	Classification	1830	HCA, HQI, SIMCA	None	-	CL	[80]
Medicines in tablets: Artemisinin derivative-containing antimalarials	SCiO prototype	740 - 1060	Reflectance	In the integrator attachment	None	Prediction Classification	677	Library matching algorithm, APNN, PCR, PLSR	None	#	-	[202]

Sample	NIR Spectrometer	Range (nm)	Mode	Acquisition system	Pretreatment	Scope	N of samples	Models	Variable Selection method	External validation (Splitting algorithm)	Elaboration system	Ref
Medicines in tablets	SCiO prototype	740 - 1060	Reflectance	In the integrator attachment	None	Prediction Classification	677	Library matching algorithm, APNN, PCR, PLSR	None	#	-	[202]
Medicines in tablets: antimalarial artemether-lumefantrine	SCiO MicroPHAZIR RX analyzer	700 – 1100 1600 – 2400	Reflectance	Direct contact	None	Classification	304	PCA, LDA, QDA, SVMC, KNN	None	-	OPEN-L	[79]
Medicines	NIR-S-G1	900 – 1700	Reflectance	Through the blister	None	Classification	27 batches	PCA, DD-SIMCA	None	NSoA	CL + CT + OPEN-T	[203]
Omega-3 dietary supplements	DLP NIRscan Nano	900 – 1700	Reflectance	Glass cylinder	Punched and squeezed	Prediction	83	PCA, PLSR	None	Random	CS	[97]
Orodispersible formulations	MicroNIR Pro 1700 ES	950 – 1650	Transflectance	Direct contact with slight mechanical pressure	None	Prediction	720	PCA, SVMC, QDA, LDA	None	-	CS	[82]
Orodispersible formulations	NIR N2.0	1550 – 1950	Reflectance	Direct contact	None	Prediction	72	PCA, PLSR	-	NSoA	CS	[81]
Paper	MicroNIR	950 – 1650	Reflectance	Fixed distance maintained with a collar	None	Exploration	82 books or sheets	PCA	None	//	CS	[85]
Pasta/Sauce Blends	MicroNIR Pro 1700	908 – 1676	Reflectance	1–2 mm distance	None	Prediction	125	PLSR	None	Random	CL + CT	[98]
Peanuts	MicroNIR 1700	908 – 1676	Reflectance	Sample cup	Shelled	Prediction Classification	150	PCA, LDA, PLSR	None	Random	OPEN-L + CS	[72]
Pears	DLP NIRscan Nano	908 – 1676	Reflectance	Direct contact	None	Prediction	240	Data fusion, PLSR, SO-PLS	SO-CovSel	K-S	CL + OPEN-T	[53]
Pears	DLP NIRscan Nano MicroNIR Pro 1700	900 – 1700 908 – 1676	Reflectance	Near the scanning window	None	Prediction	90	PCR, PLSR	Si-PLS, GA-PLS, random frog	SPXY	OPEN-L	[204]
Pineapples	SCiO	740 – 1070	Reflectance	Contact	None	Classification	90	PCA, KNN, LDA, PLSR	LW*, RC*	-	CL	[205]
Plastic	NIR-S-G1	900 – 1700	Reflectance	As close as possible to the sample	None	Classification	-	PCA, KNN, SVMC, BPNN	None	-	OPEN-L	[206]
Plastic Waste	MicroNIR OnSite	950 – 1650	Reflectance	Point and shoot	Flattened or partially flattened	Classification	250	PCA, PLS-DA	None	-	CL + CT	[91]
Plastic waste	Si-Ware Systems NR 2.0-W DLP NIRscan Nano MicroNIR 1700	1298 – 2606 1550 – 1950 900 – 1701 908 – 1676	Reflectance	-	None	Classification	43	PCA, SIMCA	None	Random	CS	[207]
Plastic Waste	MicroNIR Pro 1700 ES	950 – 1650	Reflectance	Different distances	Several ones depending on the sample	Classification	-	SMV	None	NSoA	MicroNIR Pro software version 3.0	[208]

Sample	NIR Spectrometer	Range (nm)	Mode	Acquisition system	Pretreatment	Scope	N of samples	Models	Variable Selection method	External validation (Splitting algorithm)	Elaboration system	Ref
Polymorphs in raw materials	Port 1 Port 2 Port 3	900 – 1650 1160 – 2170 900 – 1700	Reflectance	Glass petri dish	Sieved	Prediction Calibration transfer	30	PLSR	None	SPXY	CL + CT	[166]
Pork Meat	MicroNIR 2200	1100 – 2200	Reflectance	Plastic petri dish	Minced	Prediction	80	MCR, PLSR	Weighted RC, SPA	K-S	CL + CT	[209]
Quail eggs	DLP NIRscan Nano	900 – 1700	Absorbance	Direct contact	None	Prediction	1100	PCA, PLSR, SVMR, PLS-DA, SVMC	None	-	CL + CT	[59]
Red grapes	MicroNIR Pro Lite 1700	908 – 1676	Reflectance	- Quartz cuvette	None or skin removal and soft-pressed	Prediction, Classification	400	PCA, PSI, M-PLSR, LDA, PLS-DA	None	PCA	CS	[92]
Rice	MicroNIR spectrometer	900 – 1700	Reflectance	Through samples container	None	Classification	720	PCA, PLSDA, SVMC	None	K-S	CL	[210]
Rice	SCiO	740 – 1070	Reflectance	Glass Petri dish	None	Prediction Classification	520	PCA, KNN, SVMC	None	Semi-Random	CL	[71]
Sausages	MicroNIR OnSite	950 – 1650	Absorbance	-	Usual company procedures	Classification	30	PCA, KNN, PLS-DA	None	-	CL + CT	[63]
Semolina	SCiO MicroPHAZIR RX analyzer	700 – 1100 1600 - 2400	Reflectance	Through a low reflectance glass plate	None	Prediction Classification	64	PLSR, SIMCA	None	SPXY, K-S	CL + CT	[211]
Spinach plants	MicroNIR Pro 1700	910 – 1676	Reflectance	Direct contact	None	Prediction	195	M-PLSR	None	CENTER	CL + CS	[100]
Spinach plants	MicroNIR Pro 1700	908 – 1676	Reflectance	-	None	Prediction	77	PCA, M-PLSR	None	#	CL + CS	[101]
Spinach plants	MicroNIR OnSite-W	908 – 1676	Reflectance	-	None	Prediction	261	M-PLSR	None	Mahalanobis distance ordering and Semi-Random	CL + CS	[212]
Tablets of a calcium channel blocker	MicroPHAZIR-RX	1600 – 2400	Reflectance	Through PVC blisters	None	Classification	300	PCA, SMV, DD-SIMCA	None	NSoA	CL + CS	[213]
Textile	Si-Ware Systems NR 2.0-W DLP NIRscan Nano MicroNIR 1700	1298 – 2606 1550 – 1950 900 – 1701 908 – 1676	Reflectance	-	None	Classification	72	PCA, SIMCA	None	-	CS	[214]
Textile	SCiO NIRscan Nano EVM	740 – 1070 900 - 1700	Reflectance	5 mm distance Direct contact	None	Classification	74	RF	Gini-impurity*	-	Free software	
Tobacco Leaves	DLP NIRscan Nano	900 – 1700	Absorbance	-	None	Classification	530	PCA, SRC, LDA, SVMC	None	#	-	[215]
Tomato	Neospectra-Module	1295 – 2611	Reflectance	Direct contact	None	Prediction	319	PLSR	None or range reduction	Random	CS	[216]
Tomato	MicroNIR Pro 1700	908 – 1676	Reflectance	Direct contact	Washed and stirred	Prediction	300	PLSR, PLSR2	VIP*	#	CS	[217]
Umbu	Tellspec SCiO	900 – 1700 740 – 1070	Reflectance	Direct contact	Washed	Prediction	126	PLSR	None	SPXY	CL + CSs	[88]
Veal sausage	MicroPHAZIR GP	1600 – 2400	Reflectance	Quartz cuvette Through polymer packaging	None	Prediction	84	PCA, SVMC	None	#	CS	[65]

Sample	NIR Spectrometer	Range (nm)	Mode	Acquisition system	Pretreatment	Scope	N of samples	Models	Variable Selection method	External validation (Splitting algorithm)	Elaboration system	Ref
Verbena officinalis	MicroPHAZIR	1600 - 2400	Transflectance	Direct contact Through the top of the package Through the package held bottom up	None	Prediction	75	PLSR	RC*	Semi-Random (based on y)	CS	[83]
Walnuts	MicroNIR Pro 1700	908 – 1676	Reflectance	-	None	Classification	200	PCA, LDA	None	Random	CL + CSs	[70]
Woodchip	MicroNIR OnSite	950 – 1650	Reflectance	-	None	Prediction	209	PLSR	RC*	Semi-Random (based on y)	CL	[218]
Wood	MicroNIR Pro 1700	950 – 1650	Reflectance	-	None	Classification	25	PLS-DA, SVMC	None	-	CT + CS	[96]
Wood	MicroNIR Pro Lite 1700	908 – 1676	Reflectance	-	Sieved	Prediction	200	PCA, MPLSR	None	Grouping by Mahalanobis distance and semi-random	CS	[219]

Table 4 - Overview of the application of miniaturised NIR instruments on liquids and fluids. Some information was not explicitly declared (-) in the articles. Variable selection algorithms were sometimes used only as an interpretation tool (*). The column concerning the splitting algorithms for external validation includes information related to the acquisition of new sets or batches of samples (NSoA) the use internal cross-validation (#) or no validation (//). Elaboration tools were divided into Commercial Programming Language (CL), Commercial Toolbox (CT), Commercial Software (CS), Open-source programming language (OPEN-L), Open-source toolbox (OPEN-T). Abbreviations related to the chemometrics models can be found in the list of abbreviations.

Sample	**NIR Spectrometer**	**Range (nm)**	**Mode**	**Acquisition system**	**Pretreatment**	**Scope**	**N of samples**	**Models**	**Variable Selection method**	**External validation (Splitting algorithm)**	**Elaboration system**	**Ref**
Beer	MicroPHAZIR RX analyzer	1596 – 2396	Absorbance	Filter paper	None	Classification	114	ANN	None	Random or interleaved indices	CS	[113]
Beer	MicroPHAZIR RX analyzer	1600 – 2396	-	Filter paper	None	Prediction	126	PLSR, ANN	None	Random	CS	[114]
Copoiba oil	MicroNIR 1700	908 – 1676	Transflectance	Quartz cuvette	-	Prediction	53	PLSR	None	-	CS	[220]
Copoiba oil	MicroNIR 1700	908 – 1676	Transflectance	Quartz cuvette	-	Classification	278	DD-SIMCA	None	K-S	OPEN-T	[221]
Extra virgin olive oil	MicroNIR™ Pro 1700	908 – 1676	Transmittance and reflectance	Quartz cuvette. Vial of borosilicate	None	Prediction Classification	228	PCA, SIMCA, PLSR	None	Random	-	[110]
Extra virgin olive oil	In-house spectrometer	939 – 1833	Reflectance	Customised cuvette	None	Classification	129	KNN, SIMCA, PCA, Mahalanobis distance, SVMC	None	#	OPEN-L	[149]
Extra virgin olive oil	MicroPHAZIR	1600 – 2400	Transflectance	Glass tube	None	Classification	93	SIMCA	None	NSoA	-	[222]
Fuel	MicroNIR Pro 1700	908 – 1676	Transmittance	-	Heated and temperature stabilised	Prediction	133	PLSR	VIP*	K-S	CL + CT	[131]
Fuel	MicroNIR	950 – 1650	Transflectance and transmittance/absorbance	Sample cell compartment	None	Prediction	118	PLSR	SPA, JK	SPXY	CS	[122]
Fuel	MicroNIR Pro 1700	908 – 1676	Transflectance	Quartz cuvette	None	Prediction	108	PLSR	VIP*	SPXY	CL + CT	[126]
Fuel Oil	MicroNIR Pro 1700	908 – 1676	-	Vial Holder Droplet	None	Prediction Classification	375	PLSDA, PLSR, SVMR	None	-	CL	[112]
Fuel Oil	MicroNIR 1700	950 – 1650	Transmittance	Quartz cuvette	None	Calibration Transfer	103 + 130	PLSR, DS, RM	None	SPXY	CL	[165]
N-acetyl-D-glucosamine fermentation	MicroNIR 1700	908 – 1676	Transmittance	Cuvette	None	Prediction	135	PLSR	Bi-PLS, Fi-PLS, MW-PLS, CARS	SPXY	CL + CS	[223]
Goat milk	DLP NIRscan Nano EVM NIRQuest 512 NIR	900 – 1650	Absorbance	Polystyrene Petri dishes	Heated and cooled	Classification	200	OC-PLS, PLS-DA	SPA	K-S	CL	[105]
Hand sanitizer	DLP NIRscan Nano EVM NIRQuest 512 NIR	900 – 1700	-	-	None	Classification	37	PCA, PLS–DA, LDA	SPA	K-S	CS + CL + OPEN-T	[224]
Hand sanitizer	MicroNIR Pro 1700	908 – 1676	Transmittance	Quartz cuvettes	None	Prediction	51	PLSR	VIP*	-	CL + CT	[225]
Honey	MicroNIR 1700 ES	900 – 1700	Reflectance	Borosilicate glass vials	Homogenised	Prediction Classification	100	PCA, M-PLSR, LDA	None	-	CSs	[162]

Sample	NIR Spectrometer	Range (nm)	Mode	Acquisition system	Pretreatment	Scope	N of samples	Models	Variable Selection method	External validation (Splitting algorithm)	Elaboration system	Ref
Honey	MicroNIR 1700 NIRQuest model 512-2.5	908 – 1676 860 – 2500	Reflectance	Teflon cup	Incubated and adjusted to a standard soluble solids content	Classification	84	PLS-DA	None	DUPLEX on presplitted sets	CS + CL	[108]
Human milk	MicroNIR 1700	910 – 1676	Reflectance	Glass cuvette	None and thawed Pasteurised and thawed	Prediction	918	PCA, MCR-ALS	None	//	CS + CT	[106]
Lime juice	(Tellspec)	900 – 1700	-	-	Gently squeezed and homogenised	Classification	56	PLSDA, KNN	None	K-S	CS	[226]
Medroxyprogesterone acetate injectable suspensions	Innospectra	900 – 1700	Reflectance	Glass vials	Resuspending with vortexing	Classification	227	PCA, Mahalanobis distance	Loadings*	NSoA	OPEN-L (Shiny App)	[134]
Milk	MicroPHAZIR MP	1600 – 2400	Transflectance and reflectance	Quartz cuvette. Cuvette with aluminium	Hand mixed	Prediction Calibration Transfer	552	MPLSR	None	-	CS	[102]
Milk	MicroNIR 1700	908 –1676	Reflectance	Vial	None	Classification	87	PCA, PLS-DA	None	Random	CS + OPEN-L	[124]
Milk	MicroPHAZIR 1624	1600 – 2400	Reflectance	-	None	Prediction	903	PCA, PLSR, ANN	None	NSoA	CSs	[120]
Milk	MicroPHAZIR	1600 – 2400	Reflectance	Glass vial	None	Prediction	252	SIMCA, PLSR	None	-	CS	[123]
Milk	MicroPHAZIR 1624	1600 – 2400	Transflectance	Opaque liquid cup with a quartz window and aluminium	Lightly shaken	Prediction	108	PLSR	RC*	Random	CS	[103]
Milk	SCiO Neospectra Development kit	740 – 1070 1350 – 2558	Reflectance	Silica glass beaker at a fixed distance Quartz cuvette	None	Prediction	45	Cluster analysis, PCA, PLSR	i-PLS	K-S	” The Lab” + CL	[104]
Mulberry vinegar	DLP NIRscan Nano EVM NIRQuest 512 NIR	900 – 1700 910 – 1700	Transmittance	Optical fiber	None	Prediction	97	PLSR	CARS	-	CL + CS	[118]
Oil	NeoSpectra micro-FT-NIR OEM version	1300 – 2600	Reflectance	Cell	None	Analytical Strategy	80	PLSR	-	-	CL + OPEN-T	[129]
Oral fluids	MicroNIR	900 – 1700	Reflectance	Swabs with distancing collar and an integrated antireflective-coated sapphire window	None	Prediction	50	PCA, PLSR, PLS-DA	Stepwise decorrelation of variables	.	CS	[227]
Organic Reaction: synthesis of 5-hydroxymethylfurfural	MicroNIR	1150 – 2150	-	Flow cuvettes	None	Process Monitoring	-	PCA, MCC	None	NSoA	CS	[117]
Palm oil	MicroNir LED-MicroNIR	950 – 1650 1200 +- 50 - 1450 +- 50	Transmittance	Quartz cuvette	Thawed	Classification	165	PLSR, LDA	None	K-S	CL	[133]
Palm oil	MicroNir LED-MicroNIR	950 – 1650 1200 +- 50 - 1450 +- 50	Transmittance and transflectance	Quartz cuvette	None	Prediction Classification	180	SIMCA, PLSR	CARS	K-S	CL	[111]

Sample	**NIR Spectrometer**	**Range (nm)**	**Mode**	**Acquisition system**	**Pretreatment**	**Scope**	**N of samples**	**Models**	**Variable Selection method**	**External validation (Splitting algorithm)**	**Elaboration system**	**Ref**
Palm oil	TIDA-00554 DLP	900 – 1700	-	Glass cuvette	Heated	Prediction Classification	18	PCA, SIMCA, KNN, LDA, PLSR, MLR	PCA loadings, i-PLS stepwise regression	-	CSs + CL + CT	[109]
Palm oil	SCIO model CP-SC006	740 – 1070	Reflectance	Glass cup	None	Prediction Classification	150	PCA, KNN, PCR, PLSR, SVMR	None	K-S	CS + CL	[125]
Polymerisation	N-Series 1.7	1350 – 1650	Transmittance	Immersion probe	None	Prediction	12	PLSR, PCA-based MSPC	None	NSoA	CL	[24]
Potato chip oil	NeoSpectra micro	1350 – 2552	Absorbance	Drop on the window covered with accessory	None	Prediction Classification	118	PLSR, SIMCA	None	NSoA	CS	[116]
Sugar process	MicroNIR 1700	950 – 1650	Transmittance and reflectance	Quartz cuvette Glass petri dish	Usual production procedures	Prediction	1526	PLSR, SVMR	VIP, sparse-PLS	ONION	CS + CT	[228]
Syrup	MicroPHAZIR GP 4.0	1555 – 2396	Transflectance	Quartz cuvette with stainless steel reflector	None	Prediction	116	PCA, PCR, PLSR, SVMR	Uncertainty test	K-S	CS	[121]
Syrup	MicroPHAZIR GP 4.0	1555 – 2396	-	-	-	Prediction	116	PCA, PLSR	Significance test	K-S	CS	[229]
UHT milk	MicroNIR 1700	908 – 1676	Transflectance	Glass petri dish with aluminium diffuse reflector	None	Classification	71	PCA, PLSDA, LDA	GA-PLS, SPA	K-S	CL + CT	[119]
Water contamination	SCiO	740 – 1070	Transflectance	Stainless-steel beaker	None	Prediction Classification	-	PCA, PLSR	RC*	NSoA	-	[115]

Figures

Figure 1

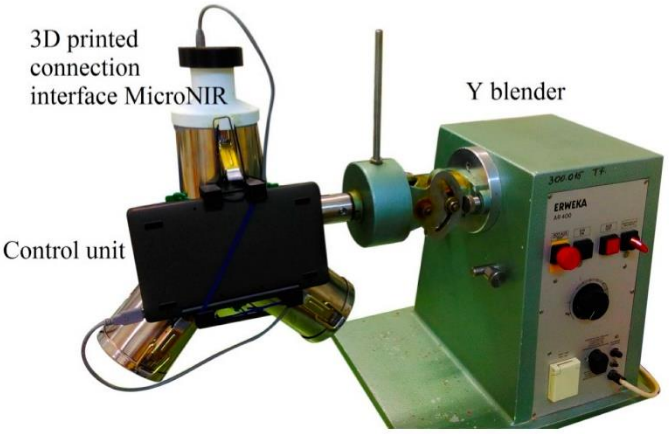

Figure 2

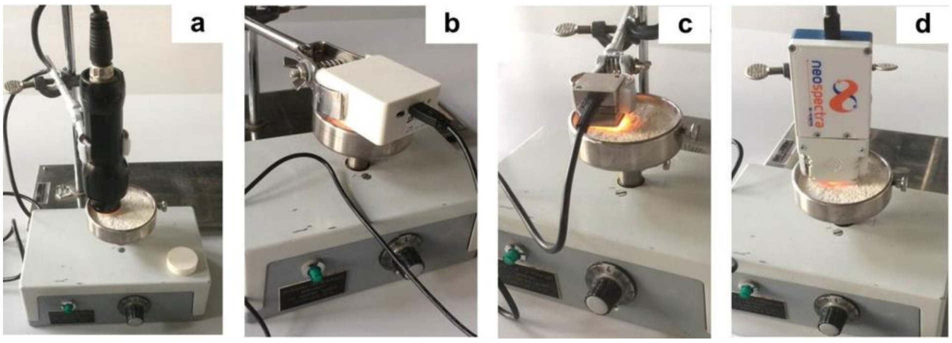

Figure 3

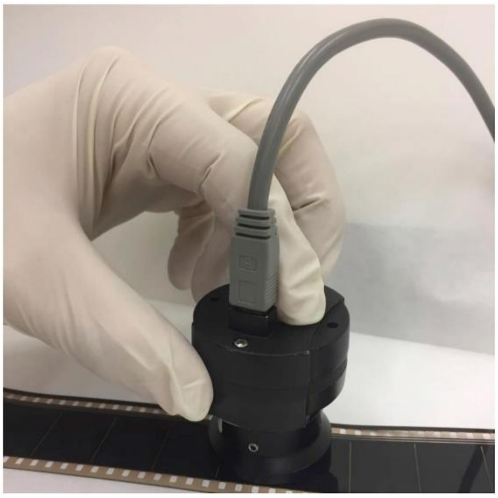

Figure 4

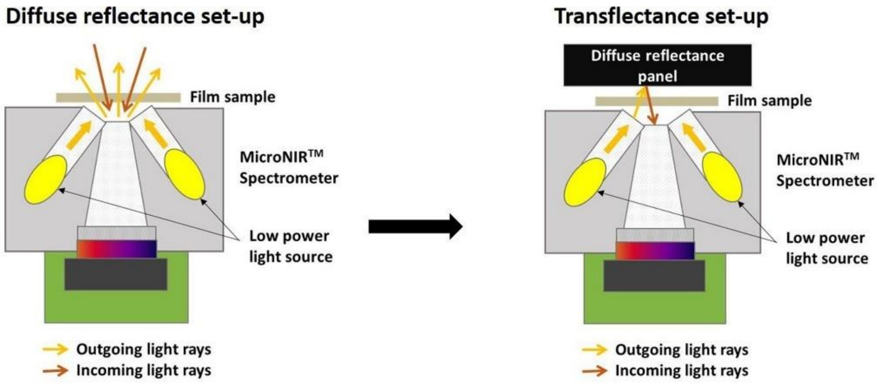
Diffuse reflectance set-up
Film sample
MicroNIRTM Spectrometer
Low power light source
Outgoing light rays
Incoming light rays
Transflectance set-up
Diffuse reflectance panel
Film sample
MicroNIRTM Spectrometer
Low power light source
Outgoing light rays
Incoming light rays

Figure 5

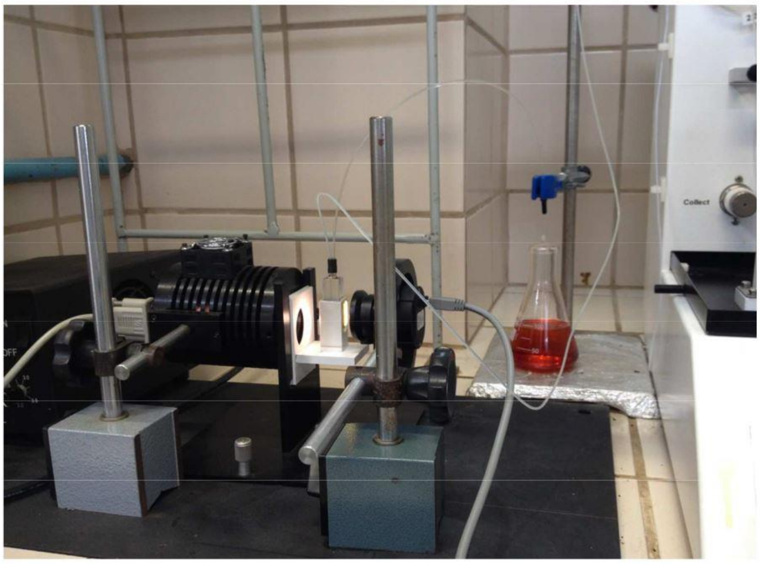

Figure 6

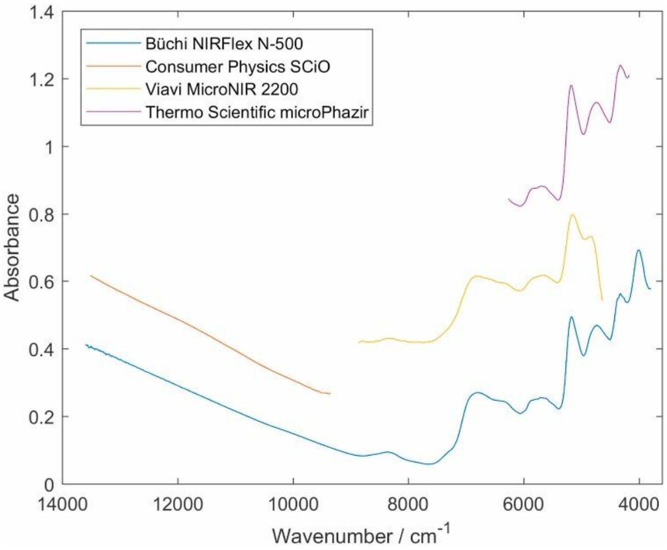
Büchi NIRFlex N-500
Consumer Physics SCiO
Viavi MicroNIR 2200
Thermo Scientific microPhazir
Absorbance
0
0.2
0.4
0.6
0.8
1
1.2
1.4
14000
12000
10000
8000
6000
4000
Wavenumber / cm-1

Figure captions

Figure 1. Example of a miniaturised instrument interfaced with a blender for on-line measurements. Reproduced with permission from Ref. [21].

Figure 2. Example of acquisition configurations for powder analysis with different miniaturised devices. Reproduced with permission from Ref. [45].

Figure 3. Example of the use of miniaturised spectrometers in thin solid samples. Reproduced with permission from Ref. [84]

Figure 4. Differences between reflectance and transflectance modes measuring thin samples. Reproduced with permission from Ref. [82].

Figure 5. Example of a miniaturised spectrometer for in-line monitoring of chemical reactions. Reproduced with permission from Ref. [117].

Figure 6. Example of spectra of a milled black pepper sample recorded with different spectrometers. Reproduced with permission from Ref. [33].