Critical Reviews in Food Science and Nutrition

Food Safety Evaluation Based on Near Infrared Spectroscopy and Imaging: a Review

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Accepted author version posted online: 27 Jun 2014.

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Abstract:

In recent years, due to the increasing consciousness of food safety and human health, much progress has been made in developing rapid and nondestructive techniques for the evaluation of food hazards, food authentication and traceability. Near infrared (NIR) spectroscopy and imaging techniques have gained wide acceptance in many fields because of their advantages over other analytical techniques. Following a brief introduction of NIR spectroscopy and imaging basics, this review mainly focuses on recent NIR spectroscopy and imaging applications for food safety evaluation, including (1) chemical hazards detection; (2) microbiological hazards detection; (3) physical hazards detection; (4) new technology-induced food safety concerns; and (5) food traceability. The review shows NIR spectroscopy and imaging to be effective tools that will play indispensable roles for food safety evaluation. In addition, on-line/real-time applications of these techniques promise to be a huge growth field in the near future.

Keywords: Chemical hazards; Microbiological hazards; Physical hazards; Transgenic food; Food traceability; NIR

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1 Introduction

Food safety is a matter that affects anyone who eats food. Whether or not a person consciously thinks about food safety before eating a meal, a host of others has already thought about the safety of that food, from farmers to scientists to company presidents to government officials and sanitarians (Roberts, 2001). The world health organization (WHO) and its member states have recognized food safety as an essential public health function (WHO, 2002). From farm to table, there are many opportunities for disease-causing organisms and other food safety hazards to enter our food supply. Foodborne disease takes a major toll on public health. Millions of people fall ill and many die as a result of eating unsafe food. The availability of safe food improves the health of people and is a basic human right. Keeping food safe is becoming even more of a challenge (Buckley et al., 2010). People used food preservation techniques like drying to make food safer in the early days, and the food safety toolbox has now expanded to include newer methods like food irradiation or natural antimicrobials. Besides, more and more attention has been paid to food safety inspection in recent years because of numerous threats to the safety of the food supply. Ensuring the safety of food becomes a shared responsibility among producers, industry, government, and consumers.

Among many available food safety inspection techniques, rapid and nondestructive methods like spectroscopy and imaging techniques are preferable. In particular, near infrared spectroscopy

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(NIRS) has gained wide acceptance within the food industry for food safety monitoring, including adulteration detection, origin tracing, pesticide residue detection, etc. The growing interest in NIRS for food safety evaluation is probably a direct result of its major advantages over other analytical techniques, including non-invasive/non-destructive sampling and testing, minimal/no sample preparation requirements, fast measurement, the capacity for prediction of physical and chemical parameters from one single spectrum, and the possibility of at-line, on-line and in-line analysis by use of fiber optic probes and other adaptable instrumentation.

The near infrared (NIR) region of the electromagnetic spectrum, adjacent to the visible and mid-infrared regions, covers the wavelength range of 780-2526 nm (12820-3959 cm^{-1}) according to the definition by ASTM (American Society of Testing and Materials). In 1800, F.W. Herschel separated the electromagnetic spectrum with a prism and discovered that the temperature increased markedly towards and beyond the red, i.e., in the region that is now called the near infrared (Reich, 2005). In NIR spectroscopy, an object is irradiated with NIR light and then the reflected or transmitted radiation is measured. Changes in the measured radiation depend on the chemical and physical properties of the object, like composition and structure.

The potential of NIR spectroscopy technique was first recognized by K. Norris, who introduced "modern NIRS" into agricultural practice to measure moisture in grain (Williams et al, 1982). From then on, the breakthrough of this spectroscopy method as a rapid and nondestructive tool proceeded in jumps coupled with the development of computer science and

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chemometric data processing techniques, as well as developments in fiber optic instrumentation. Many other applications have followed since then. There have been several literature reviews focused on NIR spectroscopy and its applications in pharmacy (Reich, 2005; Roggo et al, 2007; Luypaert et al., 2007), wood and paper (Tsuchikawa, 2007), animals (Landau et al., 2006), etc. In particular, reviews have shown NIR spectroscopy successfully applied in food quality detection applications for fruits and vegetables (Nicolaï et al., 2007), meat and meat products (Prieto et al., 2009; Prevolnik et al., 2004), and other foods and beverages (Huang et al., 2008).

Beside food quality, food safety has also become an issue of extremely high concern even by ordinary people around the world. This paper is dedicated to food safety applications of NIR spectroscopy and imaging. A brief introduction of NIR spectroscopy is provided to help readers to fully comprehend this spectroscopic technique, including theory and principles of the technique (Section 2.1), NIR spectral instruments (Section 2.2), NIR spectral imaging (Section 2.3) and chemometrics methods commonly used in NIR spectral analysis (Section 2.4). Section 3 focuses on important current and possible future applications of NIR spectroscopy for food safety monitoring, including chemical hazards detection (Section 3.1), microbiological hazards detection (Section 3.2), physical hazards detection (Section 3.3), new technologies induced food safety concerns (Section 3.4), and food traceability (Section 3.5). The last section briefly discusses the future potential of NIR spectroscopy and imaging technique in food industry and gives a short summary.

2 Near infrared spectroscopy

Papers and reviews related to NIR usually include a review of essential basics of NIR technique. For example, Blanco and Villarroya (2002) and Bosco (2010) described the NIR foundation, background and history in great detail, and also the instrumentation and chemometrics. Considering the integrity of a review paper, a very brief introduction of NIR basics will still be given as below.

2.1 Theory and principals

Normally, when light irradiates a sample, the incident light may be reflected, absorbed or transmitted (Figure 1) and the relative contribution of each phenomenon depends on the sample properties, including both chemical composition and physical structure (Zhou, 1994). Not all molecules can be studied by NIR, as most absorption bands in this region correspond to overtones and combinations of fundamental vibrations of C-H, O-H, and N-H chemical functional groups. Overtone bands appear between 780 nm and 2000 nm, depending on the overtone order and the bond nature, and are much weaker than those for fundamental frequency and strength. NIR combination bands appear between 1900-2500 nm (Blanco and Villarroya, 2002). Table 1 shows the approximate positions of combination bands and overtones of main functional groups and water (Yan et al., 2005).

Figure 1

Table 1

NIR spectra always contain broad, often overlapping peaks, because any molecule will have the potential for many types of combinations (Bosco, 2010). This is especially obvious for large molecules and complex mixtures, such as foods. The multiple bands and effect of peak broadening result in NIR spectra that have broad envelopes with few sharp peaks (Nicolaï, 2007). Typical NIR reflectance spectra of some foods are shown in Figure 2. The spectrum of fruit is dominated by the water absorption with overtone bands of the O-H bonds at 960 nm, 1440 nm, and a combination band at 1940 nm. For grain and tea spectra, the 2nd overtone of water and O-H bond are too weak to be seen. This illustrates why sophisticated multivariate statistical techniques are essential to extract useful information from NIR spectra.

Figure 2

2.2 NIR spectral Instruments

Generally, an NIR spectrometer is composed of a light source, a monochromator, a sample holder or a sample presentation interface, and a detector. The light source usually used in NIR spectrometers is a tungsten halogen lamp. Sometimes, light-emitting diodes (LEDs) are used for discrete-wavelength spectrometers. The monochromator is essential for NIR instruments to separate the polychromatic spectral regions into monochromatic frequencies. There are a number of optical configurations for this purpose, including the use of diffraction gratings, interferometers, diode-arrays, acousto-optic tunable filters (AOTF), etc. Instruments with

different light source and monochromator types provide different spectral frequencies and spectral ranges covered. There are three NIR measuring modes, including reflectance, transmittance, and transflectance. These different measuring modes are suitable for different samples according to the sample status and optical properties. To measure good NIR spectra, the proper sample presentation or sample holder is very important. Modern NIR instruments always offer several special accessories for spectra measurement. Detectors used for NIR spectrometers include silicon (Si), lead sulfide (PbS) and indium gallium arsenide (InGaAs). Si detectors are used for measuring spectra from the visible region to 1100 nm. PbS detectors are sensitive from 1100 to 2500 nm. InGaAs detectors can cover the wide range of 800-2500 nm, but are more expensive compared to Si and PbS detectors. Blanco and Villarroya (2002) drew a chart of principal features of NIR spectroscopy equipment, as shown in figure 3. There is great flexibility in the wide array of available NIR instruments that can be chosen, depending on the sample properties and analytical needs.

Figure 3

2.3 NIR Spectral imaging

Spectral imaging is an emerging technique that combines conventional imaging and spectroscopy to obtain both spectral and spatial information of a sample. A spectral image is a stack of images of the same object at different spectral bands. Commonly used NIR spectral imaging techniques are multispectral images and hyperspectral images. Multispectral images

contain only a selection of spectral points, rather than a real, full spectrum, for every image pixel, while each pixel in a hyperspectral image has a full spectrum (Ariana and Lu, 2008). Hyperspectral imaging has served as an invaluable research tool for finding a few select wavelengths with which to develop simpler (multispectral) image processing/analysis methods for adaptation to rapid online processing applications (Kim et al., 2011). A hyperspectral image is a three-dimensional block comprised of two spatial dimensions and one spectral dimension. There are three approaches for building hyperspectral images, whiskbroom, pushbroom, and tunable filter imaging, which differ in the method by which the spatial and spectral information is acquired and are also known as point scanning, line scanning, and area (plane) scanning, respectively. In food inspection experiments, the line scanning approach employing the pushbroom method is very popular. Typical pushbroom hyperspectral imaging systems consist of a CCD or CMOS camera, a spectrograph coupled with a C-mount lens, an illumination unit, and a computer equipped with image acquisition software (Elmasry et al., 2012). NIR spectral imaging systems allow experiments to be performed on very irregular samples, since NIR imaging systems perform well in reflectance mode with large depths-of-field and an excellent signal-to-noise ratio of the arrays (Reich, 2005).

2.4 Chemometrics methods

As described in Section 2.1, NIR absorption bands are typically broad and extensively overlapped. Moreover, they are 10 to 100 times weaker than their corresponding fundamental

mid-infrared absorption bands. Therefore, the analytical information contained in NIR spectra is hardly selective because of its multivariate nature, and it is impossible to distinguish the very slight spectral differences between samples (vulnerable to a number of physical, chemical and structural variables) by the naked eye. In order to extract useful information from vast amounts of spectral data speedily and efficiently, chemometrics (mathematical and statistical methods) are required not only for data preprocessing but also for quantitative or qualitative analysis.

Selecting suitable pre-processing methods should always be considered in relation to the successive modeling stage. There are two categories of most widely used pre-processing techniques in NIR spectroscopy (in both reflectance and transmittance mode): scatter correction methods and spectral derivatives. Scatter corrective pre-processing methods includes multiplicative scatter correction (MSC), inverse MSC, extended MSC (EMSC), extended inverse MSC, de-trending, standard normal variate (SNV) and normalization. Norris-Williams (NW) derivatives and Savitzky-Golay (SG) polynomial derivative filters are two representative techniques of spectral derivation. A detailed description of data pre-processing methods can be found elsewhere (Chu et al., 2004; Rinnan et al., 2009).

Principal component analysis (PCA) is used as a tool for compressing multivariate data for both quantitative and qualitative analysis. It resolves the spectral data into orthogonal components whose linear combinations approximate the original data. A number of multivariate regression and classification methods often rely on PCA data.

Multivariate regression techniques (quantitative analysis) aim to establish a relationship between the observed response values and spectral matrix (Nicolaï et al., 2007). Multiple linear regression (MLR) is the simplest, in which the response (Y variable) is approximated by a linear combination of the spectral values at every single wavelength. However, MLR models typically do not perform well because of the often high co-linearity of the spectra and easily lead to over-fitting and loss of robustness of the calibration models (Saranwong et al., 2001). Principal component regression (PCR) uses a small number of principal components (PCs) instead of the original variables as predictors to fit a MLR model (Naes et al., 2002). Partial least squares (PLS) regression is the most widely used compared to other multivariate regression methods. Unlike MLR, PLS can analyze data with strongly collinear (correlated), noisy and redundant variables (X variables or wavelengths) and also model several characteristics (Y values) at the same time (Cozzolino et al., 2009). Artificial neural networks (ANN) and least squares support vector machines (LS-SVM) can deal with non-linear relationships between variables.

Multivariate classification techniques (qualitative analysis) can be divided into two categories: unsupervised and supervised ones. Samples are classified without a prior knowledge except the spectra when unsupervised classification is concerned. Supervised classifications are techniques in which a prior knowledge is required (Roggo et al., 2007). The classical methods for supervised classification are soft independent modeling of class analogy (SIMCA), discriminant analysis (DA), k-nearest-neighbor (KNN) classifier, and partial least squares discriminant

analysis (PLSDA). Classical unsupervised methods are PCA and cluster analysis. Spectra similarity analysis methods based on correlation, distance, and angle can also be regarded as qualitative analysis. A detailed description of multivariate data analysis techniques (both quantitative and qualitative) can be found elsewhere (Siesler et al., 2007).

Figure 4

3 Applications of NIR spectroscopy and imaging in food safety evaluation

3.1 Overview

A large portion of food safety history is concentrated on scientific discoveries from the 1600s to modern times. The concept of safe and wholesome food encompasses many diverse elements. From a food safety aspect, safe food is free not only from toxins, pesticides, and chemical and physical contaminants, but also from microbiological pathogens such as bacteria and viruses that can cause illness. Experts describe food safety problems in terms of hazards, with those hazards categorized as chemical, microbiological, or physical (Roberts, 2001). Foodborne illness can be caused by these hazards. The nature and extent of these risks are being elucidated by an increasing body of scientific data. There is also mounting concern about new technologies and especially the introduction of genetically modified organisms into the food supply. Additionally, the ability to trace and authenticate a food product also has become a major food safety concern.

3.2 Chemical hazards detection

Chemical hazards include agricultural chemicals such as pesticides (including insecticides and rodenticides), herbicides, fertilizers, antibiotics and other animal drugs, cleaning residues, naturally occurring toxins, food additives, allergens, and toxic chemicals from industrial processes that can enter the food chain directly during processing or indirectly from the environment through plants and animals (Roberts, 2001.). NIR spectroscopy and imaging technique has been used in several kinds of chemical hazards detection.

3.2.1 Pesticides

Pesticides are chemical compounds widely used in farming during production to control pests, which directly results in pesticide residues on fruits and vegetables during growing stages (Knezevic et al., 2009). Over 1000 chemical products are currently used to control plant pests and diseases (Ortelli et al., 2006). Food safety issues have caused increasing consumer awareness and prompted an urgent need to develop analytical methods enabling swift screening for pesticide residues in foods. Traditional analytical methods for pesticide measurement are time consuming, costly and contaminated. Therefore, rapid and non-destructive NIR spectroscopy techniques provide a potential replacement means for such traditional analysis. Zhou et al. (2009) presented a multivariate method of rapidly determining chlopyrifos residue in white radish, based on near infrared spectroscopy and partial least squares (PLS) regression. Their results showed that NIRS with interval PLS algorithm could be used successfully to analyze

chlorpyrifos residue in white radish. Shen et al. (2009) applied NIR spectra (11000-4000 cm^{-1}) to detect pesticide phoxim residues. They introduced a sample pretreatment method of mixing samples with silica gel, which was employed as a sorbent to extract and enrich the low-concentration samples. Their experiments proved that this sample pretreatment method was effective to enrich the analyte's concentration. Sánchez et al. (2010) used a diode-array spectrometer for intact raw peppers and two scanning monochromators fitted with different sample-presentation accessories (transport and spinning modules) for crushed peppers and for a dry extract system for infrared analysis (DESIR) to measure the measurement of pesticide residues in peppers. PLS2-DA models correctly classified samples by presence/absence of pesticides between 62% and 68%. For validation, the highest percentage of correctly classified samples was 75 and 82% for pesticide-free and pesticide-containing samples, respectively. Wang et al. (2012) used the first time Fourier transform NIR spectroscopy combined with PLS-DA to determine the presence of dichlorvos, a broad-spectrum pesticide used worldwide, directly in water samples. They found that over 9000–8333 cm^{-1} (1111-1200 nm), NIR spectroscopy had good performance with a classification accuracy of 100% and a correlation coefficient of 0.92. Although, pesticide residues always occur in foods in trace amounts, the above results showed that NIRS technology can be used with suitable sample pretreatments to provide swift, non-destructive preliminary screening for trace pesticide residue.

3.2.2 Food additives

Food additives, as commonly defined, are any substance added to a food either directly or indirectly through production, processing, storing, or packaging. Different countries have different restrictions on food additives. Therefore, the number of food additives legitimately used by manufacturers differs in different countries. Approved food additives are safe; however, greedy manufactures sometimes add illegal and harmful additives in food in order to increase profits.

During the past five years, melamine (2,4,6-triamino-1,3,5-triazine) became the subject of many high profile food safety scares. In 2007, US scientists confirmed that pet food adulteration with melamine was the cause of illness and death of many companion animals (Tyan et al., 2009). In 2008, contamination of milk with melamine in China likely caused more than 51,900 infants and young children to suffer from urinary problems related to the consumption of melamine-contaminated infant formula and related dairy products, including six child deaths (Xu et al., 2009). To meet the demand for rapid and nondestructive detection, several research groups investigated the use of NIR spectroscopy to detect melamine in milk. NIR spectroscopy was evaluated to detect and quantify the melamine in ordinary milk powder (Lu et al., 2009), in infant formula powder (Mauer et al., 2009), in liquid milk (Dong et al., 2009). Balabin et al. (2011) proposed the use of NIR and mid-infrared (MIR) spectroscopy data for melamine detection in complex dairy products including liquid milk, infant formula, and milk powder. The

NIR method had an assay time of one minute, and a total time of two minutes for detection. Compared to the detection limits and total time to detection for a variety of other melamine detection methods (summarized by Mauer et al., 2009), NIR spectroscopy was more sensitive than some previously published methods like hyper performance liquid chromatography (HPLC) (NY/T 1372-2007), GC-MS (mass spectrometry) (GB/22388-2008), and LC-MS/MS (Filigenzi et al., 2008); also, the total time for melamine detection using spectroscopy methods were less than for almost all other previous methods. In addition to melamine, urea is another chemical adulterant that can be added to milk products in order to boost protein content as perceived by traditional testing methods. Yang et al. (2012) used NIR spectroscopy to discriminate urea in milk. Based on the characteristics of 2D correlation infrared spectroscopy, a 100% recognition ratio of samples was achieved by PLS-DA in their study.

3.2.3 Toxins

Research on NIR spectral detection of mycotoxins toxins, marine toxins, environmental contaminants, and naturally occurring chemicals in plants has not been as common. Only Berardo et al. (2005) applied NIR for rapid identification of mycotoxigenic fungi in maize and their toxic metabolites produced in naturally and artificially contaminated products. Their results indicated that NIR could accurately predict the incidence of kernels infected by fungi, and by F. verticillioides in particular, as well as the quantity of ergosterol and fumonisin B1 in the meal.

3.2.4 Others

Hazards yielded during food storage/process as well as hazards from food containers are considered as chemical contaminants. Tateo et al. (2007) investigated a series of disposable aluminium foil containers designed for cooking and packaging food. Using NIR spectroscopy technique (4000-10000 cm^{-1}) compared with high resolution GC (HRGC) and GC/MS, organic substances used as lubricants during the manufacturing of the aluminum containers were detected, on the container surfaces intended for coming into contact with food. The results indicated that this NIR technique allowed for a preliminary qualitative check (i.e. presence/absence) to be performed, and can be conveniently applied for quality control. Kuligowski et al. (2012) investigated NIR using PLSR modeling to determine the presence of polymerized triacylglycerides (PTG) in deep-frying vegetable oil. Four different types of oil were heated during several hours, with and without the addition of foodstuff. The researchers recommended using a global PLS model for determination of PTG in oils employed for frying different kinds of foods, leading to a prediction error of 2.28% (W/W).

3.3 Microbiological hazards detection

Microbiological hazards include disease-causing bacteria, viruses, and parasites. In recent decades, foodborne illness caused by microbiological hazards is a large and growing public health problem. Most countries with systems for reporting cases of foodborne illness have documented significant increases over the past few decades in the incidence of diseases caused

by microorganisms in food, including pathogens such as *Salmonella*, *Campylobacter jejuni* and enterohaemorrhagic *Escherichia coli,* and parasites such as *cryptosporidium, cryptospora*, *trematodes* (WHO, 2002). NIR spectroscopy has been used in bacteria detection, especially for generative sources of pathogenic bacteria like animal fecal matter.

Rodriguez-Saona (2001) and Sivakesava (2004) evaluated the use of spectroscopy techniques for the rapid detection and identification of bacteria and microorganisms. The sampling technique, spectroscopic procedure, and data evaluation strategy adopted can be extended to characterize other microorganisms, with potential extension to monitoring microorganisms in food as well as in environmental and clinical samples.

Safe disposal of manure from large-scale animal and poultry production facilities is a growing food safety problem in much of the world, as fecal matter frequently contains pathogens. To ensure a wholesome and safe meat supply for consumers, the USDA (United States Department of Agriculture) Food Safety and Inspection Service (FSIS) has established policies for meat and poultry processing in order to minimize the risks of bacterial pathogens in meat and poultry products (USDA, 1994.). For this purpose, meat and poultry processing industry are asked to seek for accurate, high speed, and non-invasive methods that can provide immediate results. To meet the needs of monitoring processing lines in real-time, the USDA Agricultural Research Service (ARS) has developed hyper/multi-spectral reflectance and fluorescence imaging techniques (in the visible and near infrared regions) for use in the detection of fecal material on

chicken carcasses. Windham et al. (2002, 2003a, 2003b) developed a transportable hyperspectral imaging system to detect fecal and ingesta contamination on the surfaces of poultry carcasses. They investigated using reflectance spectra of selected regions of interest from spectral images to determine optimal wavelengths between 400-900 nm useful for fecal detection algorithms, utilizing images of birds fed corn, wheat, and milo diets. Classification models were developed and evaluated to classify fecal-contaminated skin from the spectral data with a success rate > 95% by using algorithms of PCA and single-term linear regression (STLR). They concluded that discrimination between fecal skin and uncontaminated skin was dependent on the spectral variation related to fecal color and myoglobin and/or hemoglobin content of the uncontaminated breast skin. In another study, Chao et al. (2008) used visible and near infrared spectra to differentiate fecal contaminants, ingesta contaminates, and bare equipment surfaces at a commercial poultry processing plant. They found that a visible band ratio using a wavelength pairing of 518 nm and 576 nm, and an NIR band ratio using a wavelength pairing of 1565 nm and 1645 nm, were both able to identify 100% of fecal and ingesta contaminants. Nakariyakul and Casasent (2007) also used hyperspectral imagery to detect fecal contaminants on chicken carcasses and introduced a new improved forward floating selection (IFFS) algorithm for feature selection of the wavebands to use in hyperspectral data for classification.

Fruits and vegetables are indispensible in our daily lives. Consumers buy fruits and vegetables to maintain a healthier diet. There is often year-round availability of a large variety of domestic

and imported produce. Outbreaks of foodborne illnesses in the U.S. have been frequently associated with the consumption of fresh produce (FDA, 1998). As part of on-going food safety research at USDA, Kim et al. (2000, 2002, 2004) examined fecal contamination on apples with the use a hyperspectral imaging system in the visible to NIR region between 400-900 nm. Spectral features from both reflectance and fluorescence spectra of samples, including fecal contaminated spots, were evaluated to determine wavelengths where minima, maxima, and plateaus occur. Images at these wavelengths were used to create combinations of simple two-band ratios, second differences, normalized differences, and absorption depth images. In addition, they presented another systematic approach using hyperspectral reflectance imaging technique in conjunction with the use of PCA to define several optimal wavelength bands. Liu et al (2007) also used the same hyperspectral imaging system to detect fecal contaminants on apple surfaces. They found that large spectra differences between uncontaminated and fecal contaminated skins of two types of apples occurred in the 675-950 nm visible/NIR region and a dual-band ratio (Q722/811) algorithm could be used to identify fecal contaminated skin effectively.

Spoilage of food, which causes an increase of harmful bacteria and micro-flora, is another main factor of microbiological hazards. Lin et al. (2004) evaluated the feasibility of visible and short-wavelength near-infrared (SW-NIR) diffuse reflectance spectroscopy (600-1100 nm) to quantify the microbial loads in chicken meat and to develop a rapid methodology for monitoring

the onset of spoilage. Their results showed that visible and SW-NIR combined with PCA is capable of perceiving changes in the microbial loads in chicken muscle once the aerobic plate count (APC) increases slightly above 1 log cycle, and the PLS-based prediction method turned out more accurate quantification of the bacterial loads in chicken muscle. Fresh-cut vegetables also face the problem of bacterial contamination, which can contribute to shortened shelf life because of the rapid quality deterioration that can be caused by micro-organisms. Suthiluk (2008) measured the amount of bacterial contamination in shredded cabbage using NIR spectra in the region from 700-1100 nm. They found that NIR spectra combined with PLSR modeling was feasible for prediction of bacterial contamination in shredded cabbage.

Milk is one of the most important diet components and food ingredients for humans. Throughout the world, there are more than six billion consumers of milk and milk products. Bacteria detection in milk and milk products is essential for consumers' health. Tsenkova et al. (2006), analyzed NIR spectra of udder quarter milk samples collected continuously from individual dairy cows at various farms at different times of the year, and developed spectroscopic models for the simultaneous measurement of somatic cell count and electrical conductivity, as well as for identification of the main mastitis-causing bacteria pathogens in cow's udder quarter milk. Saranwong and Kawano (2008a, 2008b) used a NIRsystem 6500 research-type NIR spectrometer to determine the total aerobic bacteria count of raw milk, and investigated the interaction between bacterial metabolites and water absorption. Petya et al. (2010) did similar

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research in a region from 600 to 1880nm using two classification methods SIMCA and

Dneuro-fuzzy classifier. 90% of samples from class contaminated and 86% of samples from

class healthy were correct classified. The above finding present that NIR spectroscopy is a

powerful tool for bacteria detection.

3.4 Physical hazards detection

Physical hazards are foreign objects such as insects, dirt, and pieces of metal, wood, plastic,

glass, etc. that may inadvertently get into a food and could cause harm to someone eating that

food (Robert, 2001). Physical contamination can occur at any stage of the food chain. For

example, stones, bones, twigs, pieces of shell or foreign objects can enter food during harvesting,

processing, handling, or preparation. These defects should be removed, if possible, for instance

by sieving or picking out of individual items manually or using tools. However, a tougher task is

the detection of tiny objects that may hardly be seen by naked-eye. "Detecting hidden insect

infestations has been a serious problem in the grain industry," said Baker (McGraw, 1998), who

did much research on insect detection in grain with his colleagues Throne and Dowell. They used

NIRS to detect external and internal insect infestation in wheat (Dowell et al, 1998.), to identify

several Coleopteran species (Dowell et al., 1999), and to detect parasitized weevils in wheat

kernels (Baker et al., 1999). They found that NIR system is the best method to detect single

kernels of wheat that contained live or dead internal rice weevils at various life stages (Elizabeth

et al., 2002). Perez-Mendoza et al. (2005) examined the accuracy and sensitivity of NIRS for

detecting insect fragments in flour by testing three different NIR spectrometers (Perten Diode Array7000, Cognis-QTA Bruker Optics FT-NIR, and Foss NIRSystems). They concluded that NIRS is less precise than the standard flotation method, but it is rapid, nondestructive, requires no special sample preparation, and could easily be automated. Haff and Pearson (2006) used NIR spectroscopy and spectral bands selection method to determine a variety of defects and unwanted materials that commonly must be sorted out of the product at pistachio processing plants. Unwanted materials/hazards detected included adhering hulls, stick, stained or moldy product, etc. Neethirajan et al. (2007) also studied the detection of hidden insects in wheat kernels. Although NIR spectra can be used for hidden insects detection, they concluded that the soft X-ray method appeared to be better because of NIRS sensitivity to moisture in samples.

3.5 New technologies induced food safety concerns

New technologies, such as genetic engineering, irradiation of food, Ohmic heating and modified-atmosphere packaging, can be used to increase agricultural production, extend shelf life or make food safer. However, the potential public health effects of these technologies have raised concerns globally during the past decade, especially the introduction of genetically modified organisms into the food supply. In many countries, especially in Europe, transgenic foods are severely limited because many people are afraid of consuming transgenic products.

Protein-based methods like enzyme-linked immunosorbent assay (ELISA), DNA-based methods like polymerase chain reaction (PCR), microscopy and chromatography are commonly

used methods for identifying transgenic products. NIRS is a very new technique in the field for identification of transgenic foods. The first application of NIR technology for transgenic food identification was reported by Hurburgh et al. (2000). NIR and PCA were successfully applied for separating non-transgenic and transgenic grain. Later, Roussel et al. (2001) in the same research group detected and segregated Roundup Ready^{TM} soybeans from conventional soybeans by NIRS using PLS, LWR and ANN models. In 2004, Munck et al. (2004) classified transgenic and non-transgenic barley by NIRS and PCR. In addition, they successfully used the NIRS technology to study the environment effects on transgenic and non-transgenic food. In 2005, Rui et al. (2005.) applied a back propagation (BP) algorithm to discriminate transgenic corn and its parents by continuous wave NIR diffuse reflectance spectroscopy in the range of 830-2500 nm. Xie et al. (2007a, 2007b, 2009, and 2010) did much research investigating NIR spectroscopy for differentiating non-transgenic and transgenic tomatoes (including fruit, juice, and leaves). Alishahi et al. (2010) appreciated Xie's research works as being among the best and most current research in the context of the application of NIR spectroscopy to differentiation of transgenic food. All these different studies showed that NIR spectroscopy may be a suitable replacement of other more complex methods for transgenic food discrimination.

3.6 Food traceability

Food traceability can help improve food safety, benefit consumers and food industry. Traceability is the ability to track any food, feed, food producing animal or substance that will be

used for consumption, through all stages of production, processing, and distribution. Analytical techniques for products and their components are essential for a food traceability system. There are many techniques available and emerging that can provide traceability information, such as stable isotope measurements, spectroscopic techniques, chromatographic techniques, mass spectrometry techniques, and so on. NIR technique becomes a powerful tool for food origin traceability due to its advantages of rapid and non-destructive sampling and measurement.

For origin traceability of plant-based food products, because food materials of different geographical origin are affected by climate, environment, and geological factors, NIR responses are different for certain organic component of plants or plant products. Wine and olive oil origin identifications are two popular research topics. In 2003, Cozzolino et al. (2003) first studied the feasibility of visible and NIR spectroscopy to discriminate commercial white wines of different varietal origins. Later, their research group used NIR spectroscopy technique to classify Tempranillo red wine from Spain and Australian (Liu et al., 2006); Riesling wines from Australia, New Zealand, France and Germany (Liu et al., 2008); Sauvignon Blanc wines from Australia and New Zealand (Cozzolino et al., 2011). They also used NIR spectra to discriminate Shiraz wines from different Australian regions (Riovanto et al., 2011). Their research results all demonstrated the potential use of NIR spectroscopy combined with chemometrics as a rapid method to classify wines according to their geographical origin. Similar research was done by Yu et al. (2007) and Shen et al. (2012), focused on the most famous Chinese rice wine (called

Shaoxing wine). A common fraudulent practice in the commercialization of Chinese rice wine is to sell wines from different geographical origins under the denomination of Shaoxing rice wine. Both their research demonstrated that NIR spectroscopy could be used as a simple and rapid technique to distinguish authentic Shaoxing wines from non-Shaoxing wines. In 2000, Bertran et al. proposed an NIR spectroscopy-based method for discriminating virgin olive oils of two very similar and geographically close denominations of origin, viz. "Siurana" and "Les Garrigues", which are made from at least 90% of olives of the Arbequina variety. In combination with two classifying methods ANNs and logistic regression (LR), they concluded that the results obtained were quite satisfactory in both cases and that the proposed method can be applied to the discrimination of other olive oils which belong to different denominations of origin. Later, NIR spectral technique was also used by other researchers to classify olive oils according to their geographical origins (Galtier et al, 2007, 2011; Casale et al, 2008, 2009, 2010; Woodcock et al, 2008; Hennessy et al, 2009; Oliveri e tal, 2010; and Bevilacqua et al, 2012). Although different NIR regions and different classification methods were used in these studies, their results all showed that NIR and chemometrics to be useful tools in the geographic traceability of olive oil. Good results were also obtained for origin traceability of other kinds of plant-based food products by using NIR spectra and chemometrics methods, including fruits such as white grapes (Arana et al., 2005), loquats (Fu et al., 2007), and citrus (Tewari et al., 2008), as well as rice

(Kim et al., 2003), honey (Henness et al., 2008; Oliveri et al., 2010; Chen et al., 2012), and tea

(Liu et al, 2010).

Comparatively, there are fewer studies on origin traceability of animal-based food products

than on plant-based food products. Xiccato et al. (2004) used NIR spectroscopy to identify the

rearing system of European sea bass caught in four Italian fish farms. Their results showed that

NIRS succeeded in giving reliable information on the sea bass rearing system, although

freeze-drying of the samples was required for correct classification by origin. They concluded

that NIRS is a promising method for sea bass characterization traceability and authentication. In

2011, Sun et al. used NIRS to trace lamb meat origin. Lamb samples were sourced from three

pasturing areas and two farming areas of China. They also concluded that NIRS combined with

chemometric analysis can be used as an effective method to classify lamb meat according to its

geographical origin.

Figure 5

4 Conclusion and Future outlook

This review provides evidence that NIR spectroscopy and imaging technique has considerable

potential to detect chemical hazards, microbiological hazards, and physical hazards in different

kinds of food, to discriminate food with or without processing using new technologies like

genetic modification, as well as to trace food origins. Therefore, NIR spectroscopy and imaging

technique is a feasible alternative to traditional analytical procedures that are time-consuming,

expensive, and sometimes hazardous to the environment or human health. On the other hand, NIR spectroscopy and imaging technique may sometimes have only limited ability for food safety evaluation, because hazards in food often occur in trace amounts that may be difficult to detect without special treatment/preparation. Therefore, NIR spectroscopy and imaging technique is very useful for qualitative analysis to evaluate whether food is safe or not. In order to improve the accuracy of quantitative analysis for low concentration hazards in food samples, special sample pretreatment methods are adopted sometimes, such as silica gel used as a sorbent for enriching the object's concentration of a contaminant. Chemometrics techniques are essential to extract relevant information from original spectra and to establish robust calibration models. Spectral imaging emerged out of both optical spectroscopy and traditional imaging, and has enabled better characterization of food samples with an improved description of food safety status. However, spectral imaging technique suffers from some drawbacks like long time of acquisition and processing which hindered its application and popularization for on-line detection.

In the last decades, tremendous developments and remarkable improvements in technology have occurred that will lead to NIR spectroscopy and imaging becoming more widely used in the food industry to meet the urgent needs for rapid and nondestructive testing of food products. It can be expected that this technology will undoubtedly play an indispensable role for food safety

evaluation, and on-line/real-time applications promise to be a huge growth field in the near future.

<H1>**Acknowledgements**</H1>

<H1>Funding</H1>

References

Alishahia, A., Farahmanda, H., Prietob, N., Cozzolino, D. (2010). Identification of transgenic foods using NIR spectroscopy: A review. *Spectrochimica Acta Part A*. **75**: 1-7.

Arana, I., Jarén, C., and Arazuri, S. (2005). Maturity, variety and origin determination in white grapes (Vitis Vinifera L.) using near infrared reflectance technology. *Journal of Near Infrared Spectroscopy*. **13(6):** 349-357.

Ariana, D.P., and Lu, R. (2008). Detection of internal defect in pickling cucumbers using hyperspectral transmittance imaging. Transactions of the ASABE. 51:705-713.

Baker, J. E., Dowell, F. E., and Throne, J. E. (1999). Detection of parasitized rice weevils in wheat kernels with near-infrared spectroscopy. *Biological Control*. **16**: 88-90.

Balabin, R.M., and Smirnov, S.V. (2011). Melamine detection by mid- and near-infrared (MIR/NIR) spectroscopy: a quick and sensitive method for dairy products analysis including liquid milk, infant formula, and milk powder. *Talanta*. **85**: 562-568.

Berardo, N., Pisacane, V., Battilani, P., Scandolara, A., Pietri, A., and Marocco, A. (2005). Rapid Detection of Kernel Rots and Mycotoxins in Maize by Near-Infrared Reflectance Spectroscopy. *Journal of Agricultural and Food Chemistry*. **53**: 8128-8134.

Bertran, E., Blanco, M., Coello, J., Iturriaga, H., Maspoch, S., and Montoliu, I. (2000). Near infrared spectrometry and pattern recognition as screening methods for the authentication of virgin olive oils of very close geographical origins. *Journal of Near Infrared Spectroscopy*. **8(1)**: 45-52.

Bevilacqua, M., Bucci, R., Magri, A. D., Magri, A. L., and Marini, F. (2012). Tracing the origin of extra virgin olive oils by infrared spectroscopy and chemometrics: A case study. *Analytica Chimica Acta*. **717**: 39- 51.

Blanco, M., and Villarroya, I. (2002). NIR spectroscopy: a rapid-response analytical tool. *Trends in analytical chemistry*. **21(4)**: 240-250.

Bosco, G.L. (2010). James L. Waters Symposium 2009 on near-infrared spectroscopy. *Trends in Analytical chemistry*. **29(3):** 197-208.

Buckley, M., and Reid A. (2010). Global Food Safety, Keeping food safe from farm to table. A Report from the American Academy of Microbiology.

Casale, M., Casolino, C., Ferrari, G., and Forina, M. (2008). Near infrared spectroscopy and class modelling techniques for the geographical authentication of Ligurian extra virgin olive oil. *Journal of Near Infrared Spectroscopy*. **16(1)**: 39-47.

Casale, M., Casolino, C., Oliveri, P., and Forina, M. (2010). The potential of coupling information using three analytical techniques for identifying the geographical origin of Liguria extra virgin olive oil. *Food Chemistry*. **118**: 163-170.

Casale, M., Sinelli, N., Oliveri, P., Egidiob, V. D., and Lanteri, S. (2009). Chemometrical strategies for feature selection and data compression applied to NIR and MIR spectra of extra virgin olive oils for cultivar identification. *Talanta*. **80**: 1832-1837.

Chao, K., Nou, X., Liu, Y., Kim, M. S., Chan, D. E., Yang, C. C., Patel, J., and Sharma, M. 2008. Detection of fecal/ingesta contaminants on poultry processing equipment surfaces by visible and near-infrared reflectance spectroscopy. *Applied Engineering in Agriculture*. **24(1)**: 49-55.

Chen, L., Wang, J., Ye, Z., Zhao, J., Xue, X., Heyden, Y. V., and Sun, Q. (2012). Classification of Chinese honeys according to their floral origin by near infrared spectroscopy. *Food Chemistry*. **135**: 338-342.

Chu, X., Yuan, H., and Lu, W. (2004). Progress and application of spectral data pretreatment and vavelength selection methods in NIR analytical technique. *Progress in Chemistry*. 16(4): 528-542.

Cozzolino, D., Cynkar, W.U., Shah, N., and Smith P.A. (2011). Can spectroscopy geographically classify Sauvignon Blanc wines from Australia and New Zealand? *Food Chemistry*. **126**: 673-678.

Cozzolino, D., Cynkar, W.U., Shah, N., Dambergs, R. G. and Smith P.A. (2009). A brief introduction to multivariate method in grape and wine analysis. *International Journal of Wine Research*. **1**: 123-130.

Cozzolino, D., Smyth, H.E., and Gishen, M. (2003). Feasibility Study on the Use of Visible and Near-Infrared Spectroscopy Together with Chemometrics To Discriminate between Commercial White Wines of Different Varietal Origins. *Journal of Agricultural and Food Chemistry*. **51**: 7703-7708.

Dong, Y., Tu, Z., Zhu, D., Liu Y., Wang, Y., Huang, J., Sun, B., and Fan, Z. (2009). Feasibility of using NIR spectroscopy to detect melamine in milk. *Spectroscopy and Spectral analysis*. **29(11)**: 2934-2938.

Dowell, F. E., Throne, J. E., and Baker, J. E. (1998). Automated nondestructive detection of internal insect infestation of wheat kernels by using near infrared spectroscopy. *Journal of Economic Entomology*. **91**: 899-904.

Dowell, F. E., Throne, J. E., Wang, D., and Baker, J. E. (1999). Identifying stored-grain insects using near-infrared spectroscopy. *Journal of Economic Entomology*. **92**: 165-169.

Elizabeth, B. M., Dowell, F. E., Baker, J. E., and Throne, J. E. (2002). Detecting single wheat kernels containing live or dead insects using near infrared reflectance spectroscopy. ASAE Paper No. 023067. Chicago, IL.

Elmasry, G., Kamruzzaman, M., Sun, D., and Allen, P. (2012). Principles and applications of hyperspectral imaging in quality evaluation of agro-food products: a review. *Critical Reviews in Food Science and Nutrition*. **52**: 999-1023.

Filigenzi, M.S, Puschner, B., Aston, L.S., and Poppenga, R.H. (2008). Diagnostic determination of melamine and related compounds in kidney tissue by liquid chromatography/tandem mass spectrometry. *Journal of Agricultural and Food Chemistry*. **56**: 7593-7599.

Fu, X., Ying, Y., Zhou, Y., and Xu, H. (2007). Application of probabilistic neural networks in qualitative analysis of near infrared spectra: Determination of producing area and variety of loquats. *Analytica Chimica Acta*. **598**: 27-33.

Galtier, O., Abbas, O., Dréau, Y. L., Rebufa, C., Kister, J., Artaud, J., Dupuy, N. (2011). Comparison of PLS1-DA, PLS2-DA and SIMCA for classification by origin of crude petroleum oils by MIR and virgin olive oils by NIR for different spectral regions. *Vibrational Spectroscopy*. **55**:132-140.

Galtier, O., Dupuya, N., Dr´eau, Y. L., Ollivier, D., Pinatel, C., Kister, J., and Artaud, J. (2007). Geographic origins and compositions of virgin olive oils determinated by chemometric analysis of NIR spectra. *Analytica Chimica Acta*. *595*: 136-144.

GB/22388-2008. Determination of melamine in raw milk and dairy products. Chinese National Standards.

Haff, R.P., Pearson, T. (2006). Spectral band selection for optical sorting of pistachio nut defects. *Transactions of the ASABE*. **49(4)**: 1105-1113.

Hennessy, S., Downey, G., and O'Donnell, C. (2009). Confirmation of Food Origin Claims by Fourier Transform Infrared Spectroscopy and Chemometrics: Extra Virgin Olive Oil from Liguria. *Journal of Agricultural and Food Chemistry*. **57**: 1735-1741.

Hennessy, S., Downey, G., and O'Donnell, C. (2008). Multivariate Analysis of Attenuated Total Reflection-Fourier Transform Infrared Spectroscopic Data to Confirm the Origin of Honeys. *Applied Spectroscopy*. **60(10):** 1115-1123.

Huang, H., Yu, H., Xu, H., and Ying, Y. (2008). Near infrared spectroscopy for on/in-line monitoring of quality in foods and beverages: A review. *Journal of Food Engineering*. **87**: 303-313.

Hurburgh, C. R., Rippke, G. R., Heithoff, C., Roussel, S.A., and Hardy, C.L. (2000). Detection of genetically modified grains by near-infrared spectroscopy. *Proceeding Pittcon*, New Orleans, LA. March 10.

Kim, M. S., Chao, K., Chen, Y. R., Chan, D., and Mehl, P. (2000). Hyperspectral imaging system for food safety: Detection of fecal contamination an apples. Photonic Detection and Intervention Technologies for Safe Food, *Proceedings of SPIE*. **4206**: 174-184.

Kim, M. S., Lefcourt, A. M., Chao, K., Chen, Y. R., Kim, I., and Chan, D. E. (2002). Multispectral detection of fecal contamination on apples based on hyperspectral imagery: Part I. Application of visible and near-infrared reflectance imaging. *Transaction s of the ASAE*. **45(6)**: 2027-2037.

Kim, M. S., Lefcourt, A. M., Chen, Y. R., and Kang, S. (2004). Uses of Hyperspectral and Multispectral Laser Induced Fluorescence Imaging Techniques for Food Safety Inspection. *Key Engineering Materials*. **270-273**: 1055-1063.

Kim, M.S., Delwiche, S.R., Chao, K., Garrido-Varo, A., Pérez-Marín, D., Lefcourt, A.M., and Chan, D.E. (2011). Visible to SWIR hyperspectral imaging for produce safety and quality evaluation. *Sensing and Instrumentation for Food Quality and Safety*. **5**: 155-164.

Kim, S. S., Rhyu, M., Kim, J. M., and Lee, S. (2003). Authentication of Rice Using Near-Infrared Reflectance Spectroscopy. *Cereal Chemistry*. **80(3)**: 346-349.

Knezevic, Z., and Serdar, M. (2009). Screening of fresh fruit and vegetables for pesticide residues on Croatian market. *Food Control*. **20**:419-422.

Kuligowski, J., Carrión, D., Quintás, G., Garrigues, S., and Guardia M. (2012). Direct determination of polymerised triacylglycerides in deep-frying vegetable oil by near infrared spectroscopy using Partial Least Squares regression. *Food Chemistry*. **131**: 353-359.

Landau, S., Glasser, T., and Dvash, L. (2006). Monitoring nutrition in small ruminants with the aid of near infrared reflectance spectroscopy (NIRS) technology: A review. *Small Ruminant Research*. **61(1)**: 1-11.

Lin, M., Al-Holy, M., Mousavi-Hesary, M., Al-Qadiri, H., Cavinato, A.G., and Rasco, B.A. (2004). Rapid and quantitative detection of the microbial spoilage in chicken meat by diffuse reflectance spectroscopy (600–1100 nm). *Letters in Applied Microbiology*. **39**: 148-155.

Liu, L., Cozzolino, D., Cynkar, W.U., Dambergs, R. G., Janik, L., O'Neill, B. K., Colby, C. B., Gishen, M. (2008). Preliminary study on the application of visible–near infrared spectroscopy and chemometrics to classify Riesling wines from different countries. *Food Chemistry*. **106**: 781-786.

Liu, L., Cozzolino, D., Cynkar, W.U., Gishen, M., and Colby, C. B. (2006). Geographic Classification of Spanish and Australian Tempranillo Red Wines by Visible and Near-Infrared

Spectroscopy Combined with Multivariate Analysis. *Journal of Agricultural and Food Chemistry*. **54**: 6754-6759.

Liu, S. L., Tsai, Y. S., Ou, A. S. (2010). Classifying the Variety, Production Area and Season of Taiwan Partially Fermented Tea by Near Infrared Spectroscopy. *Journal of Food Drug Analysis*. **18(1):** 34-43.

Liu, Y. L., Chen, Y. R., Kim, M. S., Chan, D.E., and Lefcourt, A. M. (2007). Development of simple algorithms for the detection of fecal contaminants on apples from visible/near infrared hyperspectral reflectance imaging. *Journal of Food Engineering*. **81**: 412-418.

Lu, C., Xiang, B., Hao, G., Xu, J., Wang, Z., and Chen, C. (2009). Rapid detection of melamine in milk powder by near infrared spectroscopy. *Journal of near infrared spectroscopy*. **17**: 59-67.

Luypaert, J., Massart, D.L., and Heyden, Y. V. (2007). Near-infrared spectroscopy applications in pharmaceutical analysis. *Talanta*. **72**: 865-883.

Mauer, L.J., Chernyshova, A.A., Hiatt, A., Deering, A., and Davis, R. (2009). Melamine detection in infant formula powder using near- and mid-infrared spectroscopy. *Journal of Agricultural and Food Chemistry*. **57**: 3974-3980.

McGraw, L. C. (1998). NIR Detects, Destroys Insect Pests. *Agricultural Research*. pp14.

ACCEPTED MANUSCRIPT

Munck, L., Møler, B., Jacobsen, S., Sødergaard, S. (2004). Near infrared spectra indicate specific mutant endosperm genes and reveal a new mechanism for substituting starch with (1/3, 1/4)-b-glucan in barley. *Journal of Cereal Science*. **40**: 213-222.

Naes, T., Isaksson, T., Fearn, T., and Davies, T. (2002). A user-friendly guide to multivariate calibration and classification. Chichester, UK: NIR Publications.

Nakariyakul, S., and Casasent, D. P. (2007). Improved forward floating selection algorithm for chicken contaminant detection in hyperspectral imagery. Algorithms and Technologies for Multispectral, Hyperspectral, and Ultraspectral Imagery XIII, *Proceedings of SPIE*. **6565**: 65651.

Neethirajan, S., Karunakaran, C., Jayas, D.S., and White, N.D.G. (2007). Detection techniques for stored-product insects in grain. *Food Control*. **18**: 157-162.

Nicolaï, B. M., Beullens, K., Bobelyn, E., Peirs, A., Saeys, W., Theron, K. I., and Lammertyn, J. (2007). Nondestructive measurement of fruit and vegetable quality by means of NIR spectroscopy: A review. *Postharvest Biology and Technology*. **46**: 99-118.

NY/T 1372-2007. Determination of melamine in feedstuffs. Chinese Ministry of Agriculture Standard.

Oliveri, P., Egidio, V. D., Woodcock, T., and Downey, G. (2010). Application of class-modelling techniques to near infrared data for food authentication purposes. *Food Chemistry*. **125**: 1450-1456.

Ortelli, D., Edder, P., and Corvi, C. (2006). Multiresidue analysis of 74 pesticides in fruit and vegetables by liquid chromatography-electrospraytandem mass spectrometry. *Analytica Chimica Acta*. **520**: 33-45.

Perez-Mendoza, J., Throne, J. E., Maghirang, E. B., Dowell, F. E., and Baker, J. E. (2005). Insect Fragments in Flour: Relationship to Lesser Grain Borer (*Coleoptera: Bostrichidae*) Infestation Level in Wheat and Rapid Detection Using Near-Infrared Spectroscopy. *Journal of Economic Entomology*. **98(6)**: 2282-2291.

Petya, V., Tsvetelina, D., Stefka, A., and Roumiana, T. (2010). Detection of bacterial contamination in milk using NIR spectroscopy and two classification methods-SIMCA and neuro-fuzzy classifier. Third IFAC International Conference Agricontrol. 3(1), 10.3182/20101206-3-JP-3009.00039.

Prevolnik, M., Candek-Potokar, M., and Skorjanc, D. (2004). Ability of NIR spectroscopy to predict meat chemical composition and quality - a review. *Czech Journal of Animal Science*. **49(11):** 500-510.

Prieto, N., Roehe, R., Lavin, P., Batten, G., and Andres, S. (2009). Application of near infrared reflectance spectroscopy to predict meat and meat products quality: A review. *Meat Science*. **83**: 175-186.

Reich, G. (2005). Near-infrared spectroscopy and imaging: basic principles and pharmaceutical application. *Advanced Drug Delivery Reviews*. **57**: 1109-1143.

Rinnan, A., Berg, F.V.D., and Engelsen, S.B. (2009). Review of the most common pre-processing techniques for near-infrared spectra. *Trends in Analytical Chemistry*. **28(10)**: 1201-1222.

Riovanto, R., Cynkar, W.U., Berzaghi, P., and Cozzolino, D. (2011). Discrimination between Shiraz Wines from Different Australian Regions: The Role of Spectroscopy and Chemometrics. *Journal of Agricultural and Food Chemistry*. **59**: 10356-10360.

Roberts C. A. (2001). The food safety information handbook. ORYX press, USA.

Rodriguez-Saona, L. E., Khambaty, F. M., Fry, F. S., and Calvey, E. M. (2001). Rapid Detection and Identification of Bacterial Strains By Fourier Transform Near-Infrared Spectroscopy. *Journal of Agricultural and Food Chemistry*. **49**: 574-579.

ACCEPTED MANUSCRIPT

Roggo, Y., Chalus, P., Maurer, L., Lema-Martinez, C., Edmond, A., and Jent, N. (2007). A review of near infrared spectroscopy and chemometrics in pharmaceutical technologies. *Journal of Pharmaceutical and Biomedical Analysis*. **44**: 683-700.

Roussel, S. A., Hardy, C. L., Hurburgh, C. R., and Rippke, G. R. (2001). Detection of Roundup Ready™ soybeans by near-infrared spectroscopy. *Applied Spectroscopy*. **55(10)**:1425-1430.

Rui,Y., Luo, Y., Huang, K., Wang, W., Zhang, L. (2005). Application of near-infrared diffuse reflectance spectroscopy to the detection and identification of transgenic corn. Spectroscopy and Spectral Analysis. 25: 1581.

Sánchez, M., Flores-Rojas, K., Guerrero, J. E., Garrido-Varo, A., and Pérez-Marín, D. (2010). Measurement of pesticide residues in peppers by near-infrared reflectance spectroscopy. *Pest Management Science*. **66**: 580-586.

Saranwong, S., and Kawano, S. (2008a). System design for non-destructive near infrared analyses of chemical components and total aerobic bacteria count of raw milk. *Journal of Near Infrared Spectroscopy*. **16(4)**: 389-398.

Saranwong, S., and Kawano, S. (2008b). Interpretation of near infrared calibration structure for determining the total aerobic bacteria count in raw milk: interaction between bacterial metabolites and water absorptions. *Journal of Near Infrared Spectroscopy*. **16(6)**: 497-504.

Saranwong, S., Sornsrivichai, J., and Kawano, S. (2001). Improvement of PLS calibration for Brix value and dry matter of mango using information from MLR calibration. *Journal of Near Infrared Spectroscopy*. **9**: 287−295.

Shen, F., Yan, Z. K., Ye, Z. Z., and Ying, Y. B. (2009). Application of Near-Infrared Spectroscopy to Detection of Pesticide Phoxim Residues. *Spectroscopy and Spectral Analysis*. **29(9)**: 2421-2424.

Shen, F., Yang, D., Ying, Y., Li, B., Zheng, Y., and Jiang, T. (2012). Discrimination Between Shaoxing Wines and Other Chinese RiceWines by Near-Infrared Spectroscopy and Chemometrics. *Food Bioprocess Technology*. **5**:786-795.

Siesler, H. W., Ozaki, Y., Kawata, S., and Heise, H. M. (2007). Near-infrared spectroscopy: principles, instruments, applications. Publisherz: Willey-VCH Verlag GmbH.

Sivakesava, S., Irudayaraj, J., and DebRoy, C. (2004). Differentiation of microorganisms by FTIR-ATR and NIR spectroscopy. *Transactions of the ASAE*. **7(3)**: 951-957.

Sun, S., Guo, B., Wei, Y., and Fan, M. (2011). Application of near infrared spectral fingerprint technique in lamb meat origin traceability. *Spectroscopy and Spectral Analysis*. **31(4)**: 937-941.

Suthiluk, P., Saranwong, S., Kawano, S., Numthuam, S., and Satake, T. (2008). Possibility of using near infrared spectroscopy for evaluation of bacterial contamination in shredded cabbage. *International Journal of Food Science and Technology*. **43**: 160-165.

Tateo, F., and Bononi, M. (2007). Identification of organic contaminants in disposable aluminium foil containers. *Food Additives and Contaminants*. **23(10)**: 1030-1037.

Tewari, J. C., Dixit, V., Chob, B., and Malikc, K. A. (2008). Determination of origin and sugars of citrus fruits using genetic algorithm, correspondence analysis and partial least square combined with fiber optic NIR spectroscopy. *Spectrochimica Acta Part A*. **71**: 1119-1127.

Tsenkova, R., Atanassova, S., Morita, H., Ikuta, K., Toyoda, K., Iordanova, I. K., and Hakogi, E. (2006). Near infrared spectra of cow's milk for milk quality evaluation: disease diagnosis and pathogen identification. *Journal of Near Infrared Spectroscopy*. 14(6): 363-370.

Tsuchikawa, S. (2007). A review of recent near infrared research for wood and paper. *Applied Spectroscopy Reviews*. **42(1)**: 43-71.

Tyan, Y. C., Yang, M. H., Jong, S. B., Wang, C. K., and Shiea, J. (2009). Melamine contamination. *Analytical and Bioanalytical Chemistry*. **395(3)**: 729-735.

USDA. (1994). Enhanced poultry inspection. Proposed rule. Fed. Reg. 59: 35659. Washington D.C.

Wang, S., Xiang, B., Su, Y., Tang, Q. (2012). Direct determination of dichlorvos in water by partial least square-discriminant analysis. *Environmental Chemistry Letters*. DOI 10.1007/s10311-012-0363-5.

Williams, P. C., Norris, K. H., and Zarowski, W. S. (1982). Influence of Temperature on Estimation of Protein and Moisture in Wheat by Near-Infrared Reflectance. Cereal Chemistry. **59**: 473- 476.

Windham, W. R., Lawrence, K. C., Park, B., and Buhr, R. J. (2003b). Visible/NIR spectroscopy for characterizing fecal contamination of chicken carcasses. Transactions of the ASAE. 46(3): 747-751.

Windham, W. R., Lawrence, K. C., Park, B., Smith, D. P., and Poole, G. (2002). Analysis of reflectance spectra from hyperspectral images of poultry carcasses for fecal and ingesta detection. Imaging Spectrometry, *Proceedings of SPIE*. **4816**: 317-324.

Windham, W. R., Smith, D. P., Park, B., Lawrence, K. C., and Feldner, P. W. (2003a). Algorithm development with visible/near-infrared spectra for detection of poultry feces and ingesta. *Transactions of the ASAE*. **46(6)**: 1733-1738.

Woodcock, T., Downey, G., and O'Donnell, C. (2008). Confirmation of Declared Provenance of European Extra Virgin Olive Oil Samples by NIR Spectroscopy. *Journal of Agricultural and Food Chemistry*. **56**: 11520-11525.

World Health Organization. (2002). WHO global strategy for food safety: safer food for better health. ISBN 92 4 154574 7.

Xiccato, G., Trocino, A., Tulli, F., and Tibaldi, E. (2004). Prediction of chemical composition and origin identification of European sea bass (Dicentrarchus labrax L.) by near infrared reflectance spectroscopy (NIRS). *Food Chemistry*. **86**: 275-281.

Xie, L., Ying, Y., and Ying, T. (2007b). Combination and comparison of chemometrics methods for identification of transgenic tomatoes using visible and near-infrared diffuse transmittance technique. *Journal of Food Engineering*. **82(3):** 395-401.

Xie, L., Ying, Y., and Ying, T. (2009). Classification of tomatoes with different genotypes by visible and short-wave near-infrared spectroscopy with least-squares support vector machines and other chemometrics. *Journal of Food Engineering*. **94(1):** 34-39.

Xie, L., Ying, Y., Chen, M., and Ying, T. (2010). Detection of Transgenic Tomato Leaf with LeETR 1 Antisense Gene by Near-Infrared Spectroscopy. *Transactions of the ASABE*. **53(1)**: 313-318.

Xie, L., Ying, Y., Ying, T., Yu, H., and Fu, X. (2007a). Discrimination of transgenic tomatoes based on visible/near-infrared spectra. *Analytica Chimica Acta*. **584**: 379-384.

Xu, X. M., Ren, Y. P., Zhu, Y., Cai, Z. X., Han, J. I., Huang, B. F., and Zhu, Y. (2009). Direct determination of melamine in dairy products by gas chromatography/mass spectrometry with coupled column separation. *Analytica Chimica Acta*. **650**: 39-43.

Yan, Y. (2005). Analytical basics and applications of near infrared spectroscopy. Bejing. China Light industry Press.

Yang, R., Liu, R., Xu, K. (2012). Discriminant Analysis of Urea in Milk Based on Near Infrared Spectroscopy. *Food Science online*, 2012-04-17.

Yu, H., Zhou, Y., Fu, X., Xie, L., and Ying, Y. (2007). Discrimination between Chinese rice wines of different geographical origins by NIRS and AAS. *European Food Research Technology*. **225**: 313-320.

Zhou, Y. J., Xiang, B. R., Wang, Z. W., and Chen, C. Y. (2009). Determination of Chlorpyrifos Residue by Near-Infrared Spectroscopy in White Radish Based on Interval Partial Least Square (iPLS) Model. *Analytical Letters*. **42(10)**: 1518-1526.

Zhou, Z. (1994). Agricultural materials. Bejing, Agriculture Press.

Figure 1 Light propagation in a biological object (fruit for example)

Body
reflectance
$(0.01-0.8I_0)$

Absorption

Transmitance
$(10^{-8}-10^{-3}I_0)$

Incident light
(I_0)

Regular
reflectance
$(0.04 I_0)$
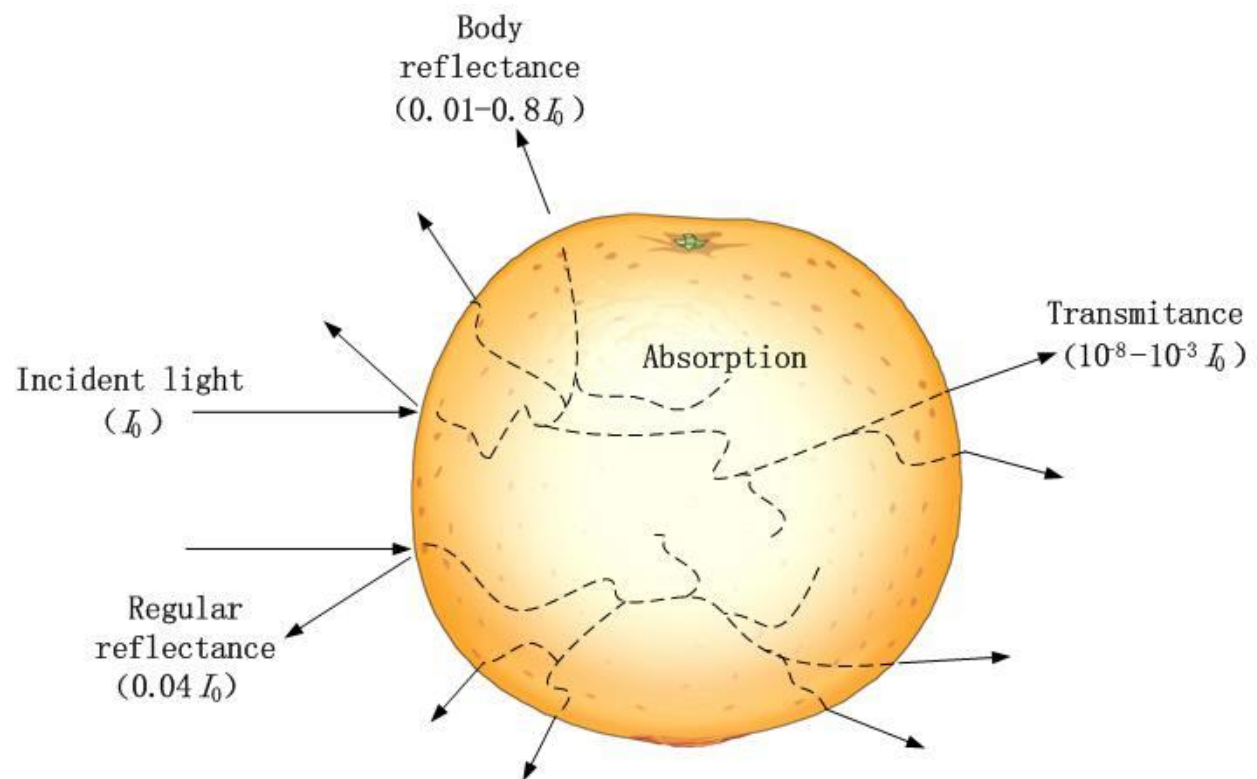
*Contribution of each phenomenon (relative intensity to the incident light) refers to Zhou Z. (1994)

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Figure 2 Typical NIR reflectance spectra of some kinds of food
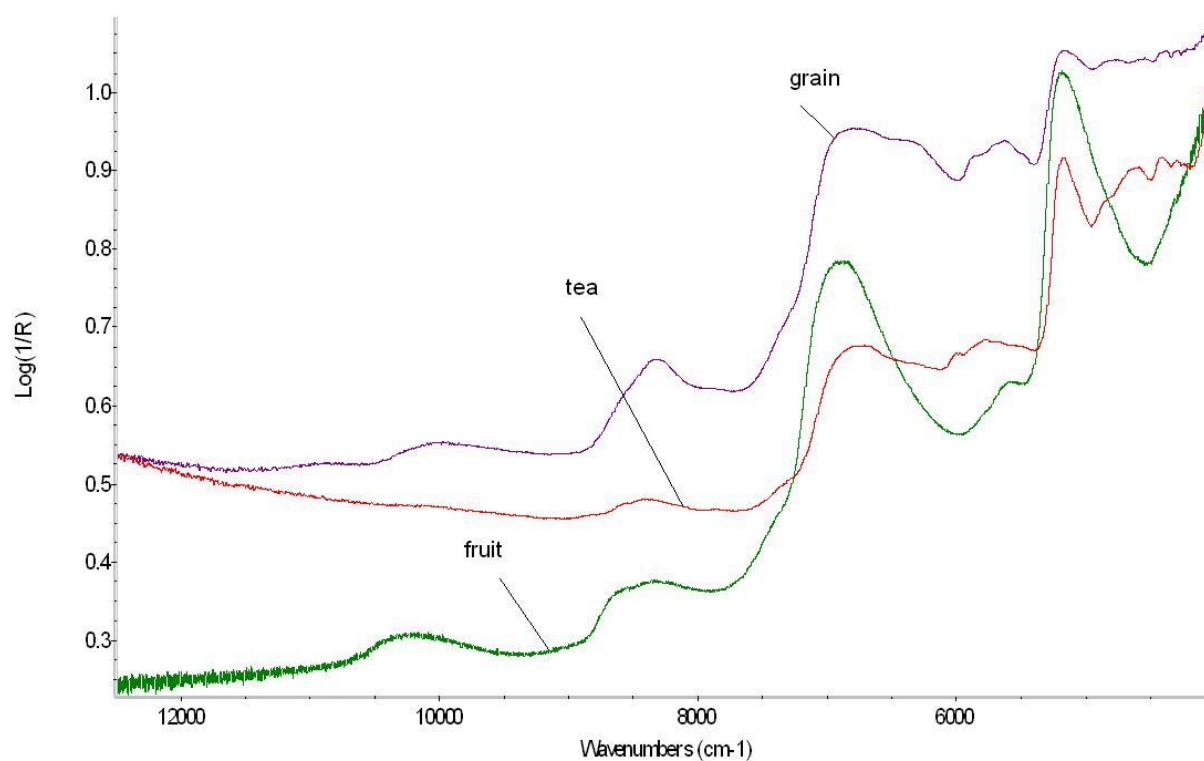
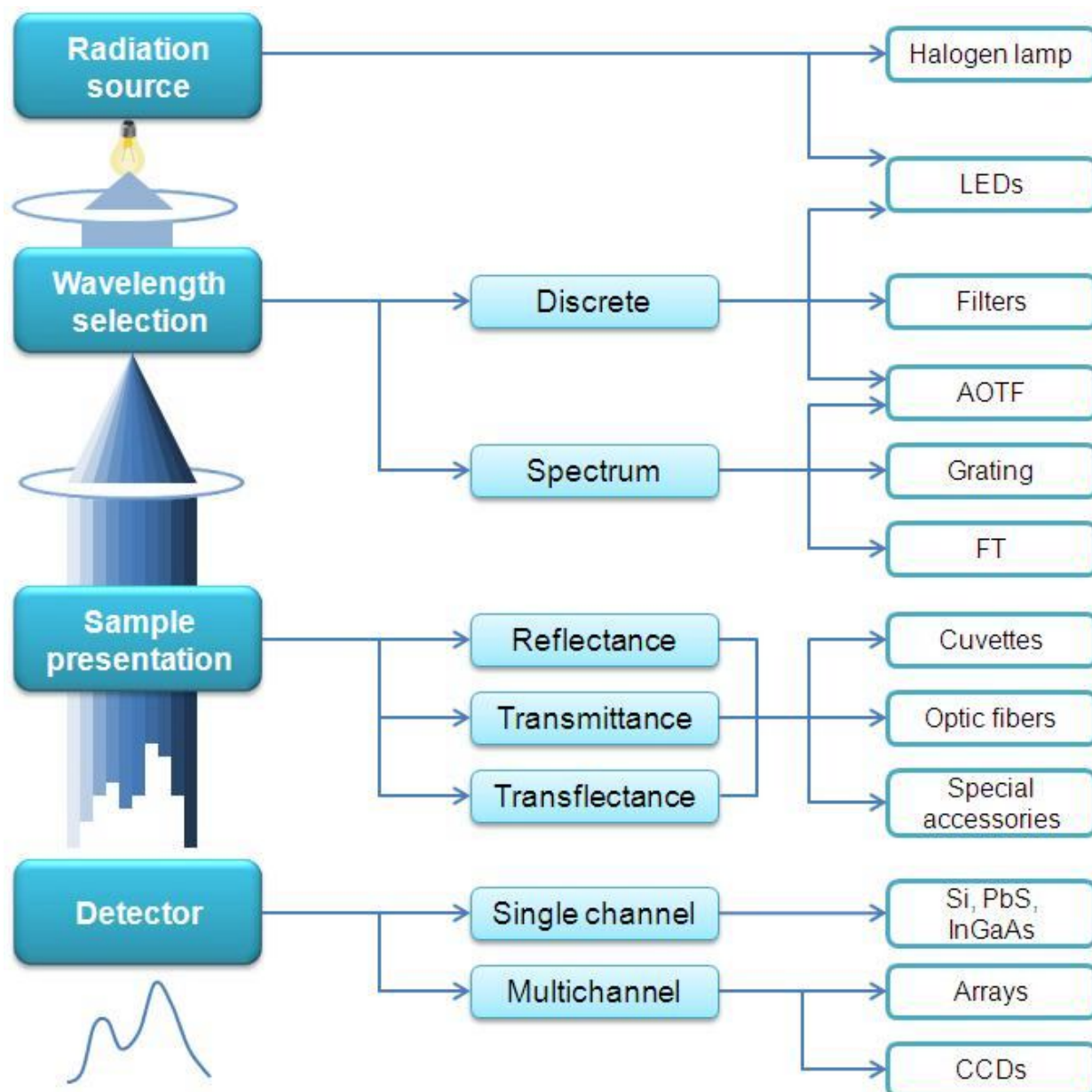Figure 3 Principal features of NIR spectroscopy equipment (Blanco and Villarroya, 2002)

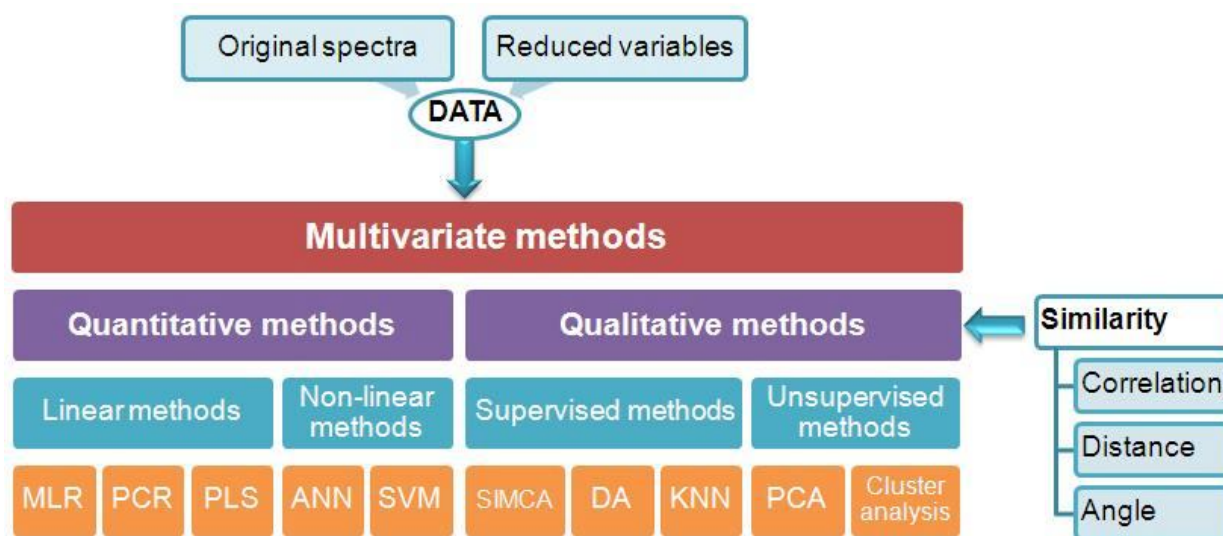Figure 4 Commonly used multivariate methods in NIR spectroscopy

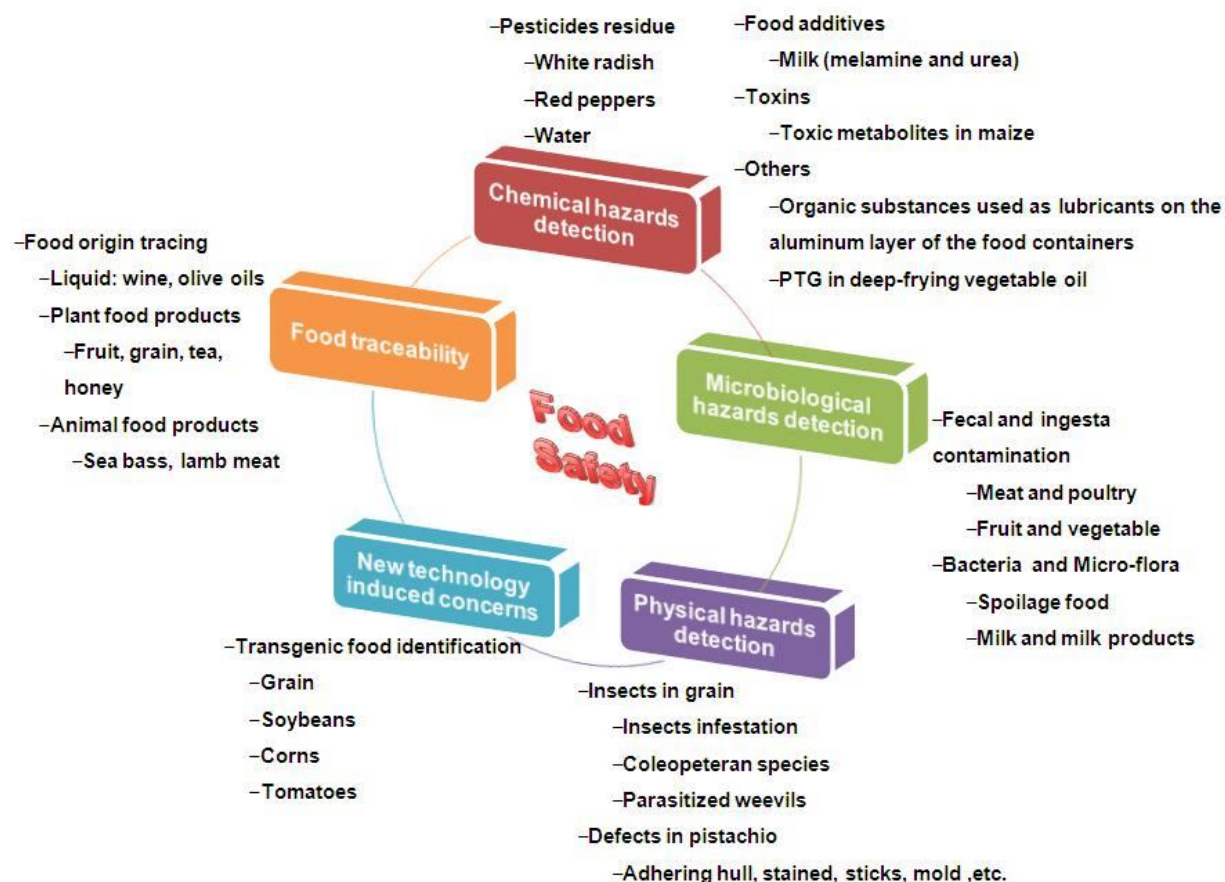Figure 5 Schematic view of NIR spectroscopy and imaging applications in food safety evaluation

Table 1 Approximate positions of overtones and combination bands of main functional groups

and water (Yan et al., 2005)

Functional group	Combination	1st overtone	2nd overtone	3rd overtone
C-H	2350 nm	1720 nm	1180 nm	900 nm
N-H	2150 nm	1500 nm	1050 nm	800 nm
O-H	2000 nm	1430 nm	950 nm	740 nm
H_2O	1940 nm	1440 nm	960 nm	750 nm