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WATER AND FOOD QUALITY

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Abstract: Despite recent advances in food product development (e.g. nutraceuticals and functional foods) our understanding of the role of water in foods is still in its infancy. Monitoring of food quality via optical methods such as near infrared (NIR) and terahertz spectroscopy is made possible due to the interaction of electromagnetic energy and the water matrix. Aquaphotomics provides a framework for understanding the role of water in food systems and processes. This paper highlights the importance of water in food quality and presents a number of case studies that demonstrate the potential of NIR hyperspectral imaging for monitoring food quality through observation of water absorbance bands.

Keywords: water, food, near infrared, quality, hyperspectral, imaging.

1. INTRODUCTION

Food quality is essentially a multivariate concept, encompassing a number of quantifiable properties, such as color, moisture content, texture, and other, more elusive, properties such as aroma and taste. Most fresh foods contain more than 70% water, while fresh fruits and vegetables can contain up to 95% water. Thus water status of foods is deeply related to their quality. The water contained in foods is broadly categorized into two classes: free and bound water. Free water is defined as the water that can be easily extracted from foods by squeezing, cutting or pressing, while bound water is not as easy to extract. Bound water molecules cannot be easily extracted and thus, even upon dehydration, foods contain bound water. This type of water is bound to food constituents such as proteins and is therefore not free to act as a solvent for salts and sugars. It exhibits a very low vapor pressure and can therefore only be frozen at very low temperatures [1,2].

Drying prolongs the shelf life of foods by reducing the amount of water available for undesirable chemical reactions and microbial proliferation. In order to maximize consumer acceptability, it is generally accepted that the dry product should resemble the fresh one as much as possible. However, the removal of water during drying inevitably alters food structure and composition, and can result in quality deterioration, the extent of which depends both on the drying method and processing conditions. Therefore, in order to optimize any drying method it is necessary to quantify the extent of quality change that occurs during the drying process. Multiple parameters are typically measured to quantify these changes, such as colour, texture, moisture content and water activity [3].

The concept of water activity was introduced by W.J. Scott in 1952, when it was demonstrated that it was not water content that correlated with bacterial growth in foods, but water activity, defined as the ratio of the water vapor pressure of the food to the water vapor pressure of pure water under the same conditions. Water activity is a dimensionless measure of the free water in a food system, available to support biological, physical and chemical reactions. It is related to the concept of vapor pressure, i.e. the pressure exerted by a vapor held in equilibrium with its solid or liquid state. During dehydration, the majority of free water contained in a food is removed and a_w subsequently decreases, inhibiting the onset of undesirable reactions such as lipid oxidation and microbial growth. Growth of bacteria is inhibited at specific water activity values, and U.S. Food and Drug Administration (FDA) regulations for intermediate moisture foods are based on these values. Water activity is now regarded as one of the most important indicators of food quality

Near infrared spectroscopy (NIRS), based on the 780 – 2,500 nm wavelength region of the electromagnetic spectrum has been developed as a non-destructive tool for food quality monitoring. It has been observed that in many foods the NIR signal is dominated by the absorbance of water and multivariate analysis of NIRS frequently demonstrates that the water absorbance band, located around 1300-

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1500 nm, is the main contributor to quality prediction [4]. This confirms that water status is a key indicator of food quality. Indeed, the concept of water activity is intimately related to NIRS: as the amount of free water in a system is increased, spectral features around 1400 nm increase in intensity [5]. Imaging spectroscopy combines imaging and spectroscopy to extract intrinsic chemical information from a sample. It extends the capability of conventional spectroscopy through rapid collection of thousands of spectra and has shown much promise for quality evaluation and contaminant detection in food products [6].

More recently, NIRS has been applied for the evaluation of water status in food systems. This can be understood within the framework of Aquaphotomics, a new scientific discipline that investigates the structure of water in biological systems through the prism of NIRS [4]. Aquaphotomics has been applied to understanding the role of water in food quality, for instance in the detection of surface damage in mushrooms [5] or for the quality monitoring of milk [7].

The Terahertz (THz) region of the electromagnetic spectrum, spanning the range between 100 GHz and 30 THz, has recently enjoyed a renaissance due to technological developments in source and detector components. Terahertz radiation has sufficient energy (1-10 meV) to promote rotations and vibrations of molecules and can thus be used for their identification. It is non-ionising and sensitive to polar molecules such as water. Due to the high absorbance of THz radiation by water, the most obvious application of THz spectroscopy would seem to be for quantification of moisture content in foods. This is especially important in controlling drying processes where low moisture content can alter the sensory qualities and shelf life of products. Although there has been very little research carried out in this area to date, the possibility of characterising the molecular nature of water in low moisture content products (e.g. free versus bound water) could be used for more accurate determination of shelf life [8].

Aquaphotomics requires the perturbation of a system and observation of resultant changes in spectra. The remainder of this paper focuses on the application of NIR hyperspectral imaging for quality monitoring of food products via observation of water absorbance patterns. Three case studies related to different aspects of food quality are presented.

2. MATERIALS AND METHODS

2.1.1. Physical damage of mushrooms

The perturbation examined in this study was vibration of mushrooms to induce physical damage on the mushroom surface. A vibration speed of 400 revolutions per minute (rpm) was applied, using a reciprocating vibration table, for five different time periods: 0, 60, 120, 300 and 600s. The vibration of mushrooms in this manner and the resulting mushroom-to-mushroom impacts induces development of browning on the mushroom surface. Extended multiplicative scatter correction was applied to the spectra in order to reduce effects due to the curvature of the mushroom surface [5].

2.1.2.Dehydration of various foods

Three different types of food (bread, cheese and banana, see Fig. 3) were allowed to dry at room temperature over a 27 hour period. In this case the perturbation applied was drying of the sample by exposure to room temperature and humidity conditions. Slices of each sample were obtained and left at room temperature; images were obtained after 0, 1, 2, 3, 4, 21, 24, 25, 27 h. Standard normal variate (SNV) preprocessing was applied to the spectra and principal components analysis was applied to the data to investigate changes occurring in the samples during dehydration [9].

2.1.3. Hydration of chickpeas

This dataset consisted of chickpeas (*Cicer arietinum L.*), hydrated to different moisture contents by immersion in tap water at 40 ± 1 ^{o}C. Ten chickpeas were removed from the water after the following soaking times: 30 min, 1, 2, 3, 4, 5, 6 hours. Their surface was lightly dried using tissue paper and the samples were allowed to equilibrate with room temperature for 20 min. Each chickpea was subsequently sectioned along its central axis, and the inner surface of the chickpea was imaged using the hyperspectral imaging equipment described in 2.2. Moisture content was determined by oven drying, as described in [3]. Partial least square regression (PLSR) models were constructed from the mean spectra of each image, to predict moisture content [10].

2.1.4. Hyperspectral imaging equipment

Hyperspectral images were obtained using a pushbroom line-scanning HSI instrument (DV Optics Ltd., Padua, Italy), operating in the NIR (950 – 1700 nm) wavelength range. The main components of these instruments are as follows [4]: translation stage, illumination source (150 W halogen lamp) attached to a fibre optic line light positioned at an angle of 45º to the translation stage, mirror, objective lens (16 mm focal length), spectrograph (Specim N17E (Spectral Imaging Ltd., Oulu, Finland)), detector (InGaS camera (Sensors Unlimited, effective resolution of 320 x 240 pixels by 12 bits)), acquisition software (SpectralScanner, DV Optics, Padua, Italy) and PC. Due to the noise characteristics of the detector, subsequent analysis was performed in the attenuated wavelength range of 950 – 1650 nm.

3. RESULTS

3.1. Physical damage of mushrooms

Mean spectra of the mushrooms subjected to different durations of vibration (and consequently different damage levels) are shown in Fig 1 (a). It is evident that the mean spectra at different damage levels are very similar to each other in profile. However, when the mean spectrum of undamaged mushrooms is subtracted from that of mushrooms subjected to different damage treatments, we can see that the main change in the spectra arising due to physical damage of the surface occurs at 1398 nm. This wavelength is related to the development of free water on the mushroom surface due to disruption of cells on the mushroom surface and the subsequent releases of intra-cellular water. Thus the emergence of free water from the mushroom surface can be used as an indicator of physical damage.

If we examine the NIR hyperspectral images of the mushrooms at a single wavelength, more precisely, the wavelength related to the emergence of free water, located at 1398 nm, it is possible to observe directly the emergence of free water on the mushroom surface as the vibration time increases (Fig. 2). As the vibration time (i.e. physical damage level) increases, absorbance of light at 1398 nm increases due to the increased concentration of free water, and the mushrooms appear brighter. Thus, information of the water status of mushrooms can be used to evaluate their quality.

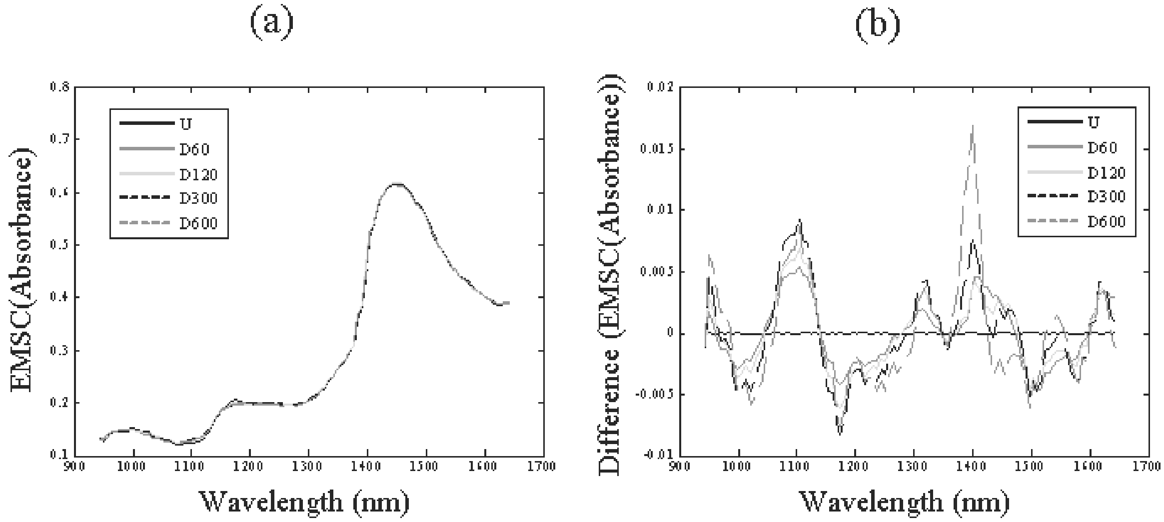

Figure 1. (a) Mean EMSC Absorbance spectra from mushrooms at different damage levels (U = undamaged, Dn= damaged by vibration for n seconds). (b) Difference spectra obtained by subtracting mean spectrum of undamaged (“U”) mushrooms from that of mushrooms damaged by vibration for different times periods (“Dn, n = 0-600s”) [5].

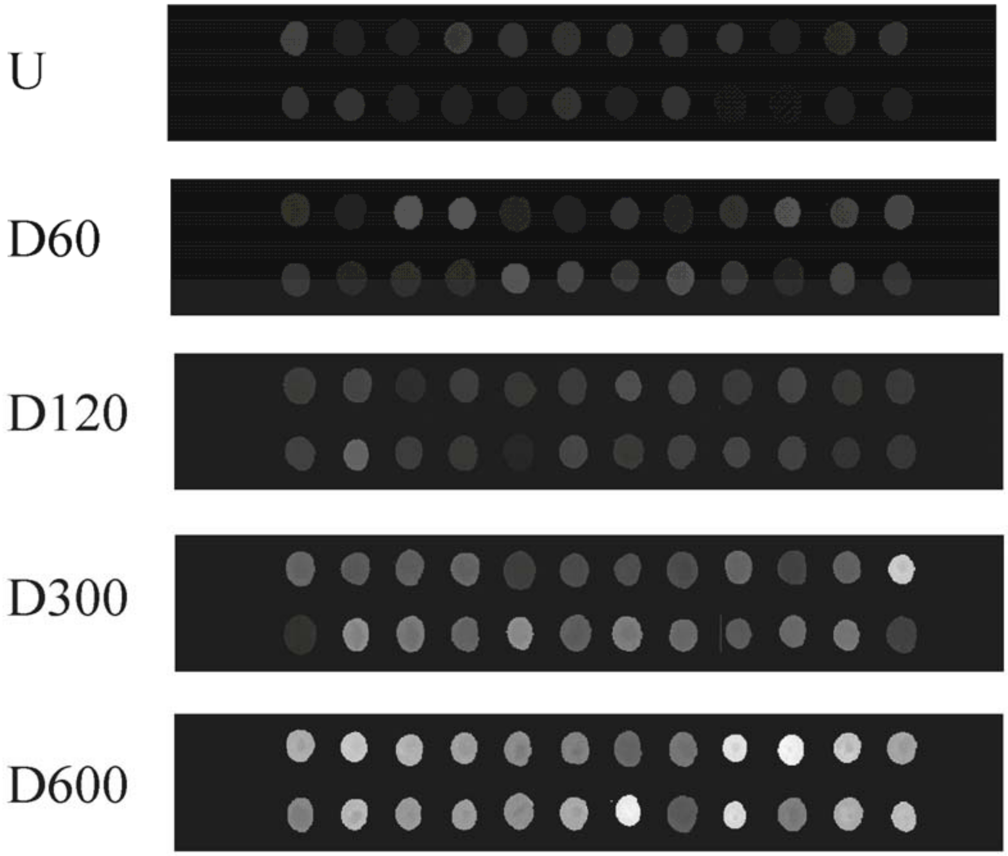

Figure 2. EMSC Absorbance images of mushrooms for different vibration time (U = undamaged, Dn= damaged by vibration for n seconds) [5].

3.2. Dehydration of various foods

The mean spectra for the bread, cheese and banana samples are shown in Figure 3. Although major compositional differences exist between the different samples examined, their NIR spectra appear strikingly similar, with the main feature being a large absorption band around 1450 nm, related to the presence of water in the samples. As the samples are subjected to perturbation (i.e. drying) their water structure changes and these changes can be monitored using NIR hyperspectral imaging. For instance, after applying principal component analysis to the images, it is evident that the first PC loading, which represents the main variation occurring in each sample during perturbation, shows a different pattern for each sample studied. Similar to the mushroom example above, the major feature of each PC1 loading is located around the water band at 1398-1400nm. However, in this case, we can expect a reduction in the amount of free water in the samples as the perturbation (drying) proceeds.

However, it must be noted that, apart from moisture loss, numerous other biochemical changes occur in the different food systems studied during the period of the perturbation (e.g. lipid oxidation in the cheese sample and enzymatic browning in the banana sample). These changes are also represented in the PC1 loading of the samples shown in Figure 3. However, the water band is the dominant feature in each, which exhibits the importance of water in the NIR spectra of foods. NIRS can be used to detect the multivariate changes that occur in such systems via changes in the water matrix. The PC1 score images of the different samples during drying are also shown in Figure 3. It can be seen that the PC 1 scores become darker as the drying proceeds: this is also a sign that the free water is decreasing. The spatial features on the cheese and bread samples are not very remarkable, due to the relative homogeneity of these samples. However, the spatial features on the banana are more interesting – the central region of the banana becomes smaller on drying, due to shrinking. This shows the benefit of NIR hyperspectral imaging over conventional spectroscopy – the ability to visualize spatial and spectral changes simultaneously.

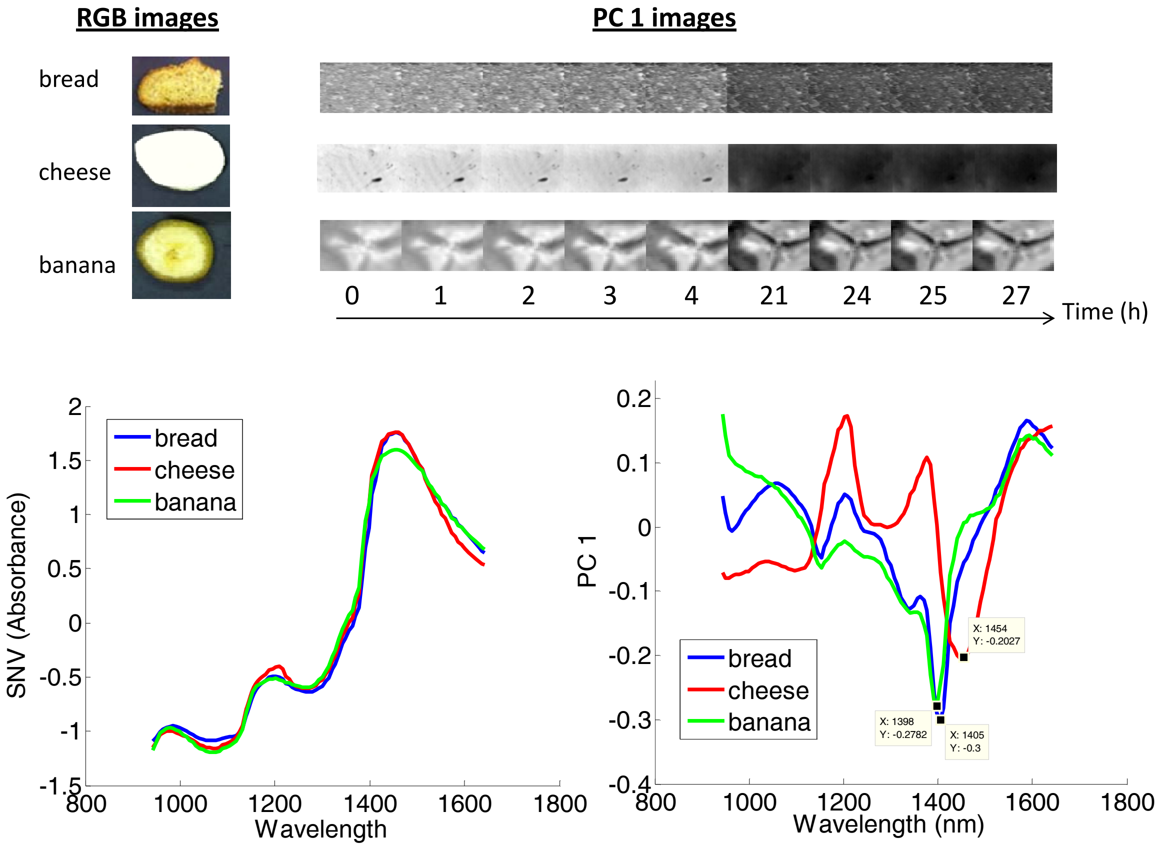

Figure 3. Color (Red ,Green , Blue (RGB)) images of the different food samples imaged during dehydration. First principal component (PC 1) images are also shown for the different drying times examined. Mean SNV absorbance spectra for the different samples are shown on the lower left hand side, while the 1st PC loading for each sample imaged over time is shown on the lower right hand side.

3.3. Hydration of chickpeas

Difference spectra for the chickpea samples, obtained by subtracting the spectra of dry chickpeas from those of hydrated ones, are shown in Figure 4. As for the previous examples considered, it can be seen that the main feature is at 1405 nm. In this case, absorbance at this wavelength increases as the soaking time increases. During hydration, the water in the chickpeas goes from being tightly bound to being free to participate in biochemical reactions [11]. After 3-4 h soaking, changes in the mean spectra became minimal. This can be related to previous work on the hydration of chickpeas, where it was reported that changes in texture became minimal after 4 hours soaking [12].

On consideration of the prediction of moisture content over the chickpea surface, obtained by application of partial least squares regression to the data, it is possible to appreciate the advantage of NIR hyperspectral imaging. In the case where moisture content is low (during the 1st 2 hours of soaking) the distribution of moisture content is not constant, being lowest at the centre of the chickpea. As soaking proceeds, the distribution becomes more homogenous. This can explain why differences in texture become minimal after 4 hours soaking at this temperature.

4. CONCLUSIONS

NIRS and Aquaphotomics facilitate an understanding of the water status in foods. NIR hyperspectral Imaging enables spatial distribution of water status to be evaluated. However, despite these recent advances, our understanding of the role of water in foods is still in its infancy. The role of water in food flavor is one area that remains relatively unexplored. The development of new food products with increased functionality and health promoting properties (e.g. reduced salt and fat) all require knowledge of the function of water in food systems. Future research paths will look at the potential of HSI NIR to understand the concept of water activity in foods. It is envisaged that the development of novel techniques for understanding the role of water in biological systems, such as Terahertz spectroscopy and imaging, will open up new avenues of research on this important subject.

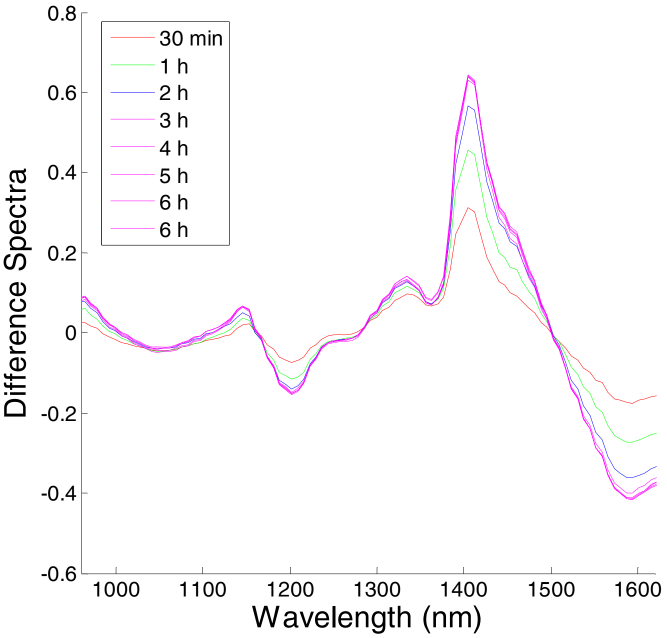

Figure 4. Difference spectra of chickpeas hydrated by soaking for different times (shown in inset). After 3 hours soaking differences in mean spectra are minimal.

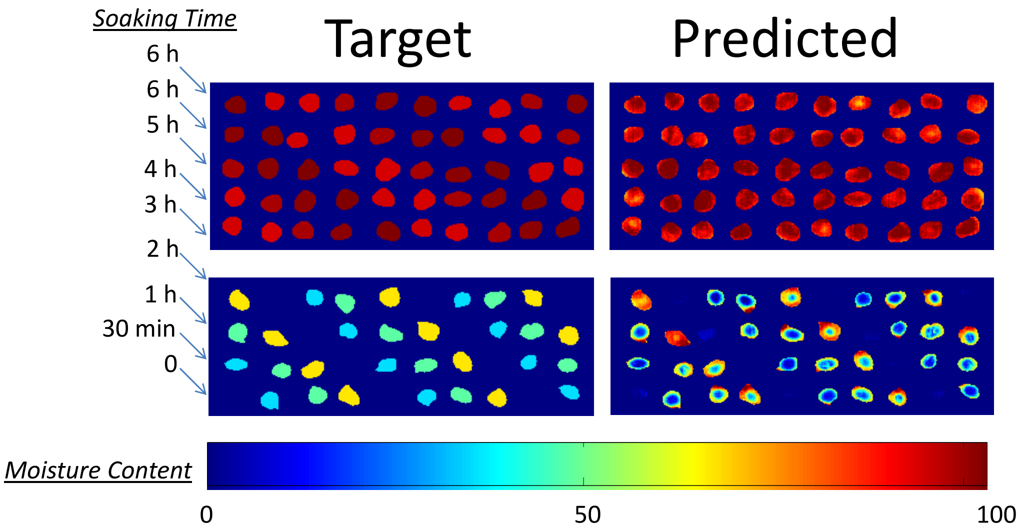

Figure 5. Prediction images for moisture content in chickpeas during soaking. Target moisture contents are shown on left hand side and predicted moisture content is shown on the right hand side. Samples were arranged in a diagonal lattice according to soaking time, as shown in the target images.

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ВОДА И КВАЛИТЕТ ХРАНЕ

Сажетак: Без обзира на најновија постигнућа у развоју прехрамбених производа (нпр. нутрацеутикали и функционална храна), наше разумијевање улоге коју вода има у храни још је увијек на почетку. Праћење квалитета хране уз помоћ оптичких метода као што су блиска инфрацрвена (NIR) и терахерц спектроскопија омогућено је интеракцијом електромагнетне енергије и воденог матрикса. Аквафотомика обезбјеђује оквир за разумијевање улоге воде у системима и процесима који укључују храну. У овом раду наглашен је значај воде за квалитет хране и представљено је неколико студија случаја које приказују потенцијал NIR хиперспектралног снимања у праћењу квалитета хране посматрањем опсега апсорпције воде.

Кључне ријечи: вода, храна, блиско инфрацрвено, хиперспектрално, снимање.

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