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Abstract

Visible-Near-Infrared Scanners enable a noninvasive prediction of quality properties of fruit and vegetable based on previously created models. A combination of NIR scanners and machine learning methods can lead to economic improvements and reduction of food waste by strategies like "first expired, first out" and dynamic pricing. In order to identify parameters capable of showing dynamic postharvest development, three horticultural products with different postharvest behavior (e. g. strawberry, table grape and mango) were chosen for morphological and statictical analysis. According to the results, a graduation of spectra in correspondence to the day of measurement was noticeable for strawberry regarding the a-value as well as presumingly mass loss for both mango and table grape. Furthermore, a PLS model for the a-values r^2_{cv} = 0.80 was developed for strawberries.

1. Introduction, Knowledge, Objectives

Visible-Near-infrared (Vis-NIR) scanners are applied in different stages of the horticultural supply chain. These NIR scanners are available in a variety of price and wavelength ranges as well as different sizes to cover a wide spectrum of applications (Goisser et al., 2020; Walsh et al., 2020). The devices enable a noninvasive prediction of properties of fruit and vegetable based on previously created models. This information supports decision making of producers and wholesalers regarding date of harvest, storage and compliance with standards. Due to a high biological variability, fruit quality can vary greatly in their properties. Nevertheless, quality parameters of many fruit and vegetable such as Brix, firmness and dry matter can be successfully predicted by those scanners at a certain point in time (Goisser et al., 2021). The use of this approach is one main target in the project FreshAnalytics (FreshAnalytics, 2021), which aims to develop a tool for shelf life predictions. If successful, the tool, which consists of Vis-NIR scanner, statistical models and machine learning, contributes to methods like “first expired, first out” and dynamic pricing. Methods like this can lead to economic improvements and reduction of food waste.

In order to evaluate parameters which can be predicted by handheld Vis-NIR scanners while showing a relevant postharvest development, the aim of the very first experiments was to examine, whether significant changes in the Vis-NIR absorbance spectra can depict the course of storage over time for strawberry, table grape and mango using a qualitative approach. For strawberries, a complementary statistical approach was taken to identify post-harvest quality changes and shelf-life prediction possibilities.

2. Data, Methods and Approach

2.1 Materials

Three horticultural products representing different postharvest behavior were chosen. The strawberries (variety not displayed, cultivated in Greece), mangoes (variety 'Kent', cultivated in Peru) and table grapes (variety 'Prime Seedless', cultivated in South Africa) were purchased at a local supermarket (Munich/Germany) in February 2021. The quantity of each fruit differed because of organizational considerations and reached from 40 strawberries over five single table grapes berries (randomly chosen from one package) to three mangoes. The number of strawberries decreased over the storage period due to the invasive inspections. All chosen fruits were numbered using a waterproof marker. A point of measurement was determined and marked at each fruit, in case of the strawberries (one point in the convex arched part of the fruit) and the mangoes (two points in total, one at a green part and one at a red part of the fruit). The strawberries and mangoes were placed on a metal grid to allow free convection and stored in a room without climate control. The single table grapes berries were numbered, measured and then stored with the rest of the bunch in their plastic clamshell container, which was placed in the same room. The temperatures during the storage period ranged from 14.0 – 18.4 °C and the relative humidity ranged from 39 % to 52 %. The storage period for the strawberries lasted 5 days. Table grapes and mangoes were stored for 9 and 10 days, respectively. Spectra and reference values such as mass and color were collected every day except on the weekend. The experiment was conducted at the facilities of the University of Applied Sciences Weihenstephan-Triesdorf in Freising/Germany.

2.2 Recording of spectra

The collection of spectral data was performed by the F-750 Produce Quality Meter (Felix Instruments, Portland, USA). This commercially available NIR spectrometer is built as a hand-held device and covers a wide variety of use cases in horticultural production and commerce (Felix Instruments, 2021). For each new measurement recording, the F-750 uses a reference shutter for normalization output as well as dark scans to account for dark current and ambient light automatically. The measurement of the strawberries and the mango was taken at predefined points. In case of the table grapes, the fruit was placed on top of the device with the bottom part pointing towards the device. One spectrum was acquired per fruit and per day (in case of mango: two spectra per fruit per day, because of two measurement points on each mango).

2.3 Determination of reference values

After recording the spectra, the fresh mass of each fruit was taken applying the KERN KB 3600-2N scale (KERN & SOHN GmbH, Balingen-Frommern, Germany). The next step was the determination of color by using the colorimeter PCE-CSM 2 (PCE Instruments, Meschede, Germany) which recorded L*-, a*-, b*-values of the CIELAB color space. The procedure of acquiring the color data was corresponding to the procedure of taking spectra. Due to technical problems, 129 color measurements of strawberries were captured during the storage period instead of 140 planned measurements.

2.4 Morphological analysis and statistical analysis

The first step was to determine whether differences in the spectra were evident during the storage test of the different fruits. Therefore, a qualitative approach was chosen in which the spectra of the fruits were recorded daily. For this purpose, the default Model Builder (version 1.3.0.192, Felix Instruments, Portland, USA) was used to visualize the second

derivative of the absorbance spectra in a wavelength range of 366 – 1083 nm. For analysis of morphological properties as well as the model building, the same wavelength range was utilized. The goal was to identify an order of spectra in a certain range of wavelength which corresponds with the date of measurement.
The second part of analysis was a statistical approach, which was only applied in case of strawberries due to the acceptable sample size of 140 absorbance spectra from 366 –1083 nm. In this case no derivative was used. Partial least square regression (PLS) as supervised machine learning algorithm was chosen as a commonly used method to evaluating the relationship between spectral values and measured parameters of interest (Wang et al., 2015). Calculations were performed using Python (version 3.8) and sklearn (version 1.0.1) library without any preprocessing of spectra. The code was executed in Jupyter notebook. A PLS model was built in order to correlate the CIE-Lab color e.g. a-values with the spectra. Therefore the selection of PLS components was supported by calculating and finding the minimum of root mean squared error of cross validation (RMSECV) as function of PLS components. A 5-fold cross validation was used. In addition, a principal component analysis was performed in order to understand which spectral region varied the most. The first principal component (PC) describes the most frequent variance.

3. Results

3.1 Results of morphological analysis

Five spectra of the same strawberry taken on five consecutive days showed a change in absorbance in the range between approximately 649 nm and 680 nm, a wavelength range which is typical for the absorption of chlorophyll a and chlorophyll b (Scheer, 1991; Mu et al., 2021) (Figure 1-A). A similar but more complex change of spectra (between approx. 700 nm and 770 nm) was recognizable in case of the mango (10 days storage, 8 measurements). Beside a change in absorbance also a shift of wavelength was observed. This effect will not be discussed further because of its complexity. This wavelength range typically contains superpositions of absorptions based on the vibration (3rd overtone) of e.g. R-OH but also H_2O (Xiaobo et al., 2010). A gap between the spectra can be seen by two missing spectra due to the weekend (see Figure 1-B). On the example of a single grape, a change in the wavelength range between approximately 930 nm and 940 nm was observed for seven consecutive spectra (9 days storage, seven measurements, Figure 1-C).

The results regarding reference color measurements of strawberry showed a decrease in the a-value (a-coordinate) from 37.67 to 24.27 and the b-coordinate decreased from 27.96 to 15.20 in 5 days. In case of our measurements on mango the a-coordinate increased from -3.2 to 11.01 during the storage time of 10 days.

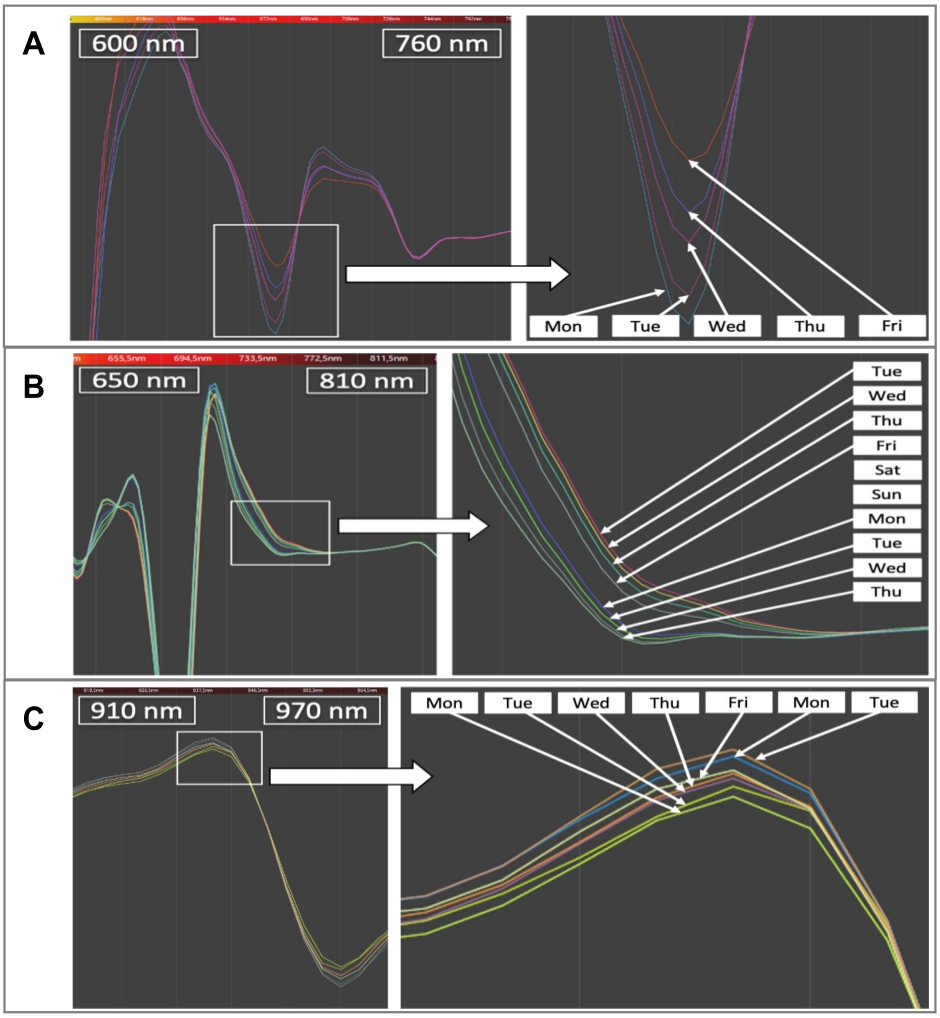

Figure 1: Spectra of a (A) single strawberry, (B) single mango (and single point of measurement), and (C) single table grape graduated by day of measurement

3.2 Results of statistical analysis

The PLS model for strawberries consisted of 9 PLS components using the 140 absorbance spectra and corresponding a-values as reference. The model showed a high linear correlation of $r^2_c = 0.87$ for calibration data (plotted values in Figure 2-A). The corresponding cross validation delivered linearity of $r^2_{cv} = 0.80$ and a RMSECV = 5.99. The score plot of the first and second principal component indicated by using color labeled scores that no groups or gradients are formed according to the nominal age of samples (Figure 2-B). This is also the case for the other score plots (not shown). A closer look at the first PCA loading showed that the main source of variation arised from spectral changes between 500 – 700 nm (see plot in Figure 2-C). The same 140 absorbance spectra were investigatet by sorting spectra according to date of measurement and calculating the variances at each wavelength (see plot in Figure 2-D). As can be seen two main ranges of absorbances appear. The absorbance at around 585 nm is in correspense with those of anthocyanines. As mentioned for a single strawberry in section 3.1 also time related changes in the region of absorbance of chlorphyll as well as anthocyane can be observed for all 40 strawberries in a statistical sense. The plot of the entire wavelength range clearly shows that main variance arised in the range from 500 – 700 nm.

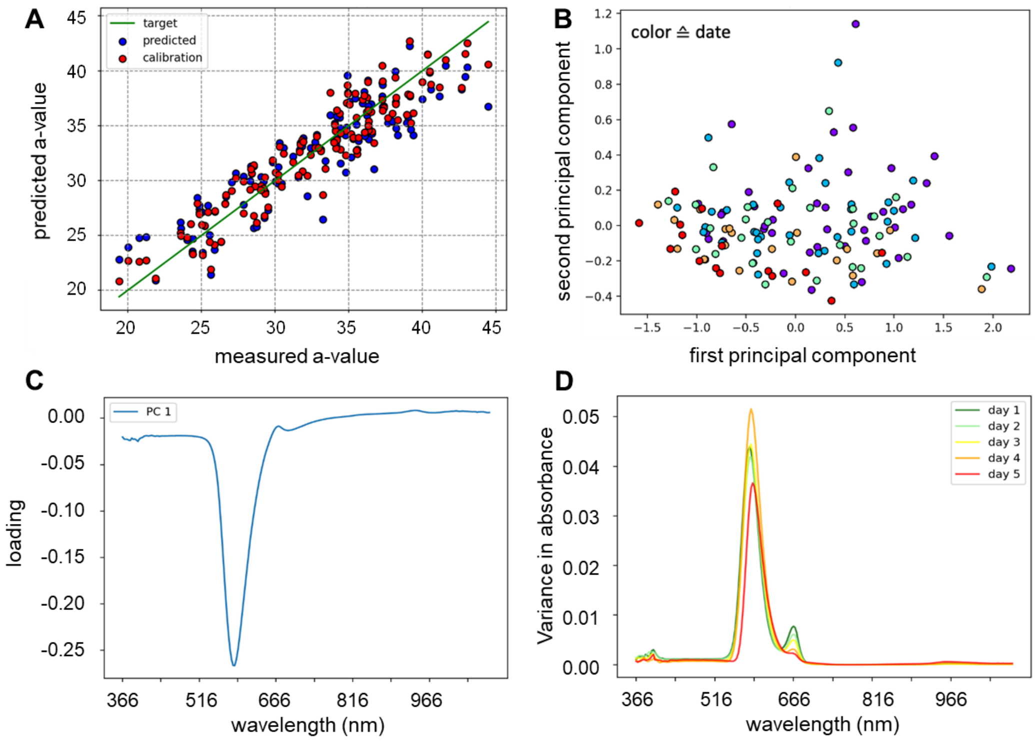

Figure 2: (A) Graphical output of the PLS model showing calibration (red dots) and prediction (blue dots) and the best fit (green line), (B) Graphical Analysis of the first PC with colored labels corresponding to the date of measurement, (C) Loading of first principal component depending on the wavelength, (D) Variances of absorbance spectra from strawberries at four different days

4. Discussion

Three different kinds of fruit were used for the investigation, which differed significantly in their relevant parameters for describing shelf life. For strawberries, which are very persihable, a strong reduction in firmness as well as color loss and pathogens has been cited (Chiabrando et al., 2019). Similar parameters (e.g. water loss, color loss, reduction in firmness) were described for table grapes (Palou et al., 2010). The degree of ripeness of mangoes as a climacteric fruit, on the other hand, has been primarily described on the basis of dry matter, flesh color and fruit firmness (Saranwong et al., 2004). The morphological analysis showed that graduation of spectra in correspondence to the day of measurement was noticeable even without any further processing of spectra. The identified spectral ranges which were able to depict the course of storage over time for strawberry (approx. 650 nm – 680 nm) and mango (approx. 700 nm – 770 nm) were both in the range of the VIS, even though regarding mango at the edge of the visible range. In case of strawberry fruit, the changes of the spectra over time could be explained by a decrease of chlorophyll content during the aging process of the fruit (Nunes et al., 2006). In the CIELAB color space, this means that the a-value increases and the b-value decreases. A decrease of both values, as it was the case in our measurements, could indicate a potential brake down of dyes e.g. anthocyanines, which are responsible for red colors. The measured a-value of mango increased over a storage time of 10 days. Especially for mango the absorption in the red spectral range from 625-740 nm might be explained by the presence of reddish pigments, which have been described in more ripe mangoes in some varieties (dos Santos Neto et al., 2017). Among others, fruit color has been described as one of the most common and widely used methodes to determine the ripening stage as well as the monitoring of shelf life of fruit and vegetable (Kasampalis et al., 2021). Therefore, the color values might serve as an indication for strawberry and also mango to depict storage days. Nevertheless, in case of mango a measurement on the fruit skin must be viewed critically, as it can show significant differences both within the variety as well as within one fruit. For example, the wavelength range has also been listed for the measurement of Brix and dry matter in mango using VIS-NIR (Guthrie and Walsh, 1997). For the identified spectra of table grape of approx. 930 nm and 940 nm, which was beyond the visible light a different quality parameter must be assumed. Harris and Altaner (2013) describe the absorption caused by OH groups in this section of the wavelength. A correlation between the mass loss of the table grapes (in average 5.4 %) which is caused i. a. by loss of water and the change of OH groups seems possible.

The PLS model of the a-values showed, that a property of the fruit (color) can be correlated and predicted in a reliable way. Because the property color contained some information about the stage of development and age of the fruit (Nunes et al., 2006), a prediction of the age seems likely. However, a model must be built by using fruit with defined properties and age, which was successfully done by Weng et al. (2020). If the starting point of the fruit development is known, a valid classification of further development stages might be possible. The unsupervised approach seemed to work because of the property color, too. The first PCA component reflected variation in spectral section from approx. 500 – 700 nm. This region is typical for absorption of anthocyanins and chlorophyll (Da-Silva et al., 2007). The results obtained by the three different approaches showed, that it was possible to measure and understand some changes on an individual bases, but the lack of information about the starting point of the postharvest development leads to difficulties in the interpretation. Further research should use fruit and vegetable with a known and uniform development stage for the creation of models under ideal conditions. If successful, experiments with known disturbance variable can be conducted. The sample size will be significantly increased in following studies.

5. Conclusions

The very first experiments showed that changes during a storage period are visible in spectra of mango, strawberry and table grape taken by Vis-NIR scanners. Based on the exemplary parameter color, the measurement and prediction by Vis-NIR scanner and PLS model was successfully demonstrated. Due to the low number of iterations, it is difficult to draw a general conclusion. Therefore, further experiments will be carried out in this regard.

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