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Simon Goisser

Suitability of portable NIR sensors (food-scanners) for the determination of fruit quality along the supply chain using the example of tomatoes

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Lebenswissenschaftliche Fakultät,

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Suitability of portable NIR sensors (food-scanners) for the determination of fruit quality along the supply chain using the example of tomatoes

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Preface

The content of this thesis is based on reformatted work, which has been published as follows:

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2. Goisser, S.; Krause, J.; Fernandes, M.; Mempel, H. (2019): Determination of tomato quality attributes using portable NIR-sensors. In: Jürgen Beyerer, Fernando Puente León und Thomas Längle (Hg.): OCM 2019 - 4th International Conference on Optical Characterization of Materials. March 13th - 14th, 2019. Karlsruhe: Scientific Publishing, p. 1–12. DOI: https://doi.org/10.5445/KSP/1000087509.

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Summary

The quality of fruit and vegetables is subject to continuous postharvest change due to ongoing metabolic and post-ripening processes. In the course of the supply chain from production to the end-consumer various factors, e.g., storage and transport conditions, mechanical stress and packaging, determine the degree and speed of further degeneration of product quality. The task of postharvest quality assurance is to monitor the quality of fresh produce and to counteract processes that reduce quality in order to keep losses along the value chain as low as possible. Optical measuring methods, such as visual and near-infrared spectroscopy (VIS/NIRS), offer numerous advantages over conventional measuring methods for determining important quality parameters of fruit and vegetables, such as fast and non-destructive measurements and simple sample preparation. The need for a more cost-effective and compact application of NIR spectroscopy in contrast to conventional laboratory instruments has led to the development of a wide range of portable handheld devices and miniaturized sensors in recent years. In contrast to laboratory instruments, these devices allow on-site and in-field measurements. In the case of fruit and vegetables, quality measurements can be carried out at various points along the entire supply chain, therefore the actual quality can be determined non-destructively. Some commercial portable and miniaturized instruments have been developed specifically for fresh produce and are designed to help the user to determine key quality parameters in the orchard, in the incoming goods control or at the point of sale in retail outlets.

The present study evaluated the suitability of these portable and partly miniaturized NIR sensors, so-called food-scanners, for determining fruit quality along the supply chain of fruit and vegetables. Using the approach of qualitative research, the first step comprised interviews of experts at different positions of the fruit and vegetable value chain. In this way preferences and concerns regarding the implementation of this technology for fresh produce were investigated. Based on the findings, non-destructive prediction models for a number of important quality characteristics and secondary plant constituents were developed on the model fruit tomato. In addition, the suitability of the practical use of these devices was evaluated and a first trial for use in daily incoming goods control was carried out.

The results of the qualitative study showed a wide variation in the practices currently used in quality control to determine product quality, particularly between production companies and wholesale and retail businesses. In general, the determination of quality often depends to a large extent on trained and experienced personnel who test the products subjectively and oftentimes use haptical and visual inspections. In addition, wholesalers often follow established protocols to ensure quality and conformity with the given statuatory standards. The results show that food-scanners can facilitate quality control at different levels of the fresh produce value chain by providing fast, non-destructive and objective measurements, while helping to overcome existing discrepancies in quality assessment along the supply chain by introducing a common measurement method. Concerns about the use of food-scanners have been identified with regard to possible additional requirements within the fruit trade, which could lead to more pressure and additional obligations for producers.

Subsequent studies evaluated the performance of three commercially available portable and miniaturized VIS/NIR spectrometers. The studies focused on the non-destructive prediction of various important quality characteristics of the model fruit tomato. The evaluation of the food-scanner spectra led to prediction models with high correlations ($r^2 > 0.90$) for the quality traits firmness, dry matter, sugar content and the colour values L*, a* and h°. In the course of further investigations, prediction models with high prediction capabilities ($r^2 > 0.92$) were obtained for the non-destructive determination of the secondary plant metabolite lycopene in intact tomatoes. In addition, the software provided by the sensors manufacturers to create prediction models was evaluated by comparing the results derived from these software tools with state-of-the-art software for multivariate analysis. The direct comparison of the evaluation software showed very similar accuracies for the calculated prediction models. In a further experiment, the decrease in firmness, which is considered an important indicator for the shelf life of tomatoes, could be modelled over the storage period in connection with the respective storage temperature. By combining these firmness models with non-destructive NIR predictions of the current firmness, a first approach for a shelf life model of tomatoes could be developed. Investigations comparing the performance of a food-scanner with a conventional laboratory spectrometer for the prediction of the tomato quality parameters sugar content and firmness underlined the high accuracy of the food-scanner predictions and the comparability to laboratory instruments.

Based on the results derived from tomatoes, further studies were carried out to predict important quality parameters in a wide range of fruit and vegetables (apple, avocado, blueberry, ginger, persimmon, kaki, kiwi, mandarin, mango, table grapes). The evaluations showed that in particular the quality traits sugar content, dry matter as well as the relative water content of fruit can be predicted non-destructively with high accuracy. In a concrete practical example, a food-scanner was also used for non-destructive quality assessment in the course of incoming goods control of a fruit and vegetable wholesaler. The evaluation showed a high degree of agreement between the food-scanner predictions and conventional destructive measurements using refractometers and furthermore illustrated the possibility of saving working time by using these measuring devices.

The results of this doctoral thesis illustrate the great potential of food-scanners for the non-destructive quality measurement of fruit and vegetables along the fresh produce supply chain. Some of the commercially available devices investigated in these studies already showed a high degree of compatibility with the requirements of the fruit and vegetable industry, such as a robust design, long battery life and the possibility of personalized modelling and data evaluation by users. In addition to the possibility of integrating the generated data into existing information technology systems, confidence in the accuracy of the food-scanner predictions was identified as an important prerequisite for implementation in practice. Targeted cooperation between food-scanner manufacturers and companies in the fruit and vegetable sector, the publication of new findings in specialized journals for producers and trading companies and the provision of targeted training programmes could lead to a better adaption of food-scanner to the requirements of the fresh produce supply chain in the future. Ultimately, this could allow the implementation of these novel devices in everyday practice of fruit quality control.

Zusammenfassung

Die Qualität von Obst und Gemüse unterliegt nach der Ernte einer kontinuierlichen Veränderung auf Grund anhaltender Stoffwechsel- und Nachreifeprozesse. Im Verlauf der Wertschöpfungskette von der Produktion bis zum Endkunden bestimmen zudem verschiedene Einflussfaktoren, wie beispielswiese Lager- und Transportbedingungen, mechanische Belastung sowie Verpackung, den Grad sowie die Geschwindigkeit der weiteren Degeneration der Produktqualität. Die Aufgabe der Qualitätssicherung nach der Ernte ist dabei, die Qualität der Frischeprodukte zu überwachen und qualitätsmindernden Prozessen entgegenzuwirken, um Verluste entlang der Wertschöpfungskette so gering wie möglch zu halten. Optische Messmethoden, wie beispielsweise die Visuelle- und Nahinfrarot-Spektroskopie (VIS/NIRS), bieten gegenüber herkömmlichen Messverfahren zur Bestimmung wichtiger Qualitätsparameter an Obst und Gemüse zahlreiche Vorteile, wie beispielsweise eine schnelle und zerstörungsfreie Messung sowie eine einfache Probenvorbereitung. Der Bedarf nach einer kostengünstigeren und kompakteren Anwendung der NIR-Spektroskopie im Gegensatz zu den herkömmlichen Laborinstrumenten führte in den vergangenen Jahren zur Entwicklung verschiedenster tragbarer Handgeräte sowie miniaturisierter Sensoren. Im Gegensatz zu Laborinstrumenten ermöglichen diese Geräte eine Messung vor Ort. Im Fall von Obst und Gemüse können Qualitätsmessungen an verschiedenen Stellen der gesamten Wertschöpfungskette durchgeführt und so tatsächliche Produktqualitäten zerstörungsfrei ermittelt werden. Einige kommerzielle portable und miniaturisierte Geräte wurden speziell für Frischeprodukte entwickelt und sollen dem Anwender dabei helfen, wichtige Qualitätsparameter in der Obstplantage, der Warenkontrolle oder am Verkaufsort im Einzelhandel zu bestimmen.

In der vorliegenden Studie wurde die Eignung dieser tragbaren und zum Teil miniaturisierten NIR-Sensoren, sogenannten Food-Scannern, für die Bestimmung der Fruchtqualität entlang der Wertschöpfungskette von Obst und Gemüse evaluiert. Mittels Methoden der qualitativen Sozialforschung wurden in einem ersten Schritt Experten an verschiedenen Positionen der Obst und Gemüse Wertschöpfungskette befragt und Präferenzen und Bedenken hinsichtlich der Implementierung dieser Technologie für Frischeprodukte untersucht. Aufbauend auf den gewonnenen Erkenntnissen wurde an der Modellfrucht Tomate zerstörungsfreie Vorhersagemodelle für eine Vielzahl wichtiger Qualitätsmerkmale sowie sekundärer Pflanzeninhaltsstoffe entwickelt. Darüber hinaus wurde die Eignung des praktischen Einsatzes dieser Geräte evaluiert und ein erster Versuch zur Verwendung in der täglichen Wareneingangskontrolle durchgeführt.

Die Ergebnisse der qualitativen Befragung zeigten eine große Variation der aktuell in der Qualitätskontrolle durchgeführten Praktiken zur Ermittlung der Produktqualität, insbesondere zwischen den Unternehmen der Produktion und des Groß- und Einzelhandels. Generell hängt die Qualitätsbestimmung oft in hohem Maße von geschultem und erfahrenem Personal ab, welches die Produkte subjektiv und meist haptisch und visuell prüft. Darüber hinaus halten sich Großhändler oft an etablierte Protokolle, um Qualität und Konformität mit den gegebenen rechtlichen Standards zu gewährleisten. Die Ergebnisse verdeutlichen, dass Food-Scanner die Qualitätskontrolle auf den verschiedene Ebenen der Wertschöpfungskette von Frischeprodukten durch schnelle, zerstörungsfreie und objektive Messungen erleichtern und gleichzeitig dabei helfen können, bestehede Diskrepanzen bei der Qualitätsbeurteilung entlang der Lieferkette durch die Einführung einer einheitlichen Messmethode zu überwinden. Bedenken über den Einsatz von Food-Scannern konnten im Hinblick auf mögliche zusätzliche Anforderungen des Fruchthandels identifiziert werden, die zu mehr Druck und zusätzlichen Auflagen für die Produzenten führen könnten.

In den anschließenden Untersuchungen wurde die Leistungsfähigkeit von drei kommerziell erhältlichen portablen und miniaturisierten VIS/NIR-Spektrometern bewertet. Im Fokus der Studien stand die zerstörungsfreie Vorhersage verschiedener wichtiger Qualitätsmerkmale der Modellfrucht Tomate. Die Auswertung der Food-Scanner Spektren führte zu Vorhersagemodellen mit hohen Korrelationen ($r^2 > 0,90$) für die Merkmale Festigkeit, Trockenmasse, Zuckergehalt sowie die Farbwerte L*, a* und h°. Im Zuge weiterer Untersuchungen konnten zudem Vorhersagemodelle mit hohen Vorhersagegüten ($r^2 > 0,92$) für die zerstörungsfreie Bestimmung des sekundären Pflanzeninhaltsstoffs Lycopin in Tomaten erzielt werden. Zusätzlich wurde die von den Herstellern der Sensoren zur Verfügung gestellte Software zur Erstellung von Vorhersagemodellen evaluiert, indem die von diesen Software-Tools abgeleiteten Ergebnisse mit modernster Software für multivariate Analysen verglichen wurden. Der direkte Vergleich der Auswertungs-Software ergab sehr ähnliche Genauigkeiten für die berechneten Vorhersagemodelle. In einem weiteren Versuch konnte die Abnahme der Festigkeit, welche als wichtiger Indikator für die Haltbarkeit von Tomaten gilt, über die Lagerzeit in Zusammenhang mit der jeweiligen Lagertemperatur modelliert werden. Durch die Kombination dieser Festigkeitsverlaufsmodelle mit zerstörungsfreien NIR-Vorhersagen zur aktuellen Festigkeit konnte ein erster Ansatz für ein Haltbarkeitsmodell von Tomaten entwickelt werden. Untersuchungen, welche die Leistungsfähigkeit eines Food-Scanners mit einem herkömmlichen Labor-Spektrometer für die Vorhersage der Tomatenqualtätsparameter Zuckergehalt und Festigkeit verglichen, verdeutlichten die hohe Genauigkeit der Food-Scanner Vorhersagen und die Vergleichbarkeit zu Labormessungen.

Basierend auf den an Tomaten gewonnenen Erkenntnissen wurden weitere Untersuchungen zur Vorhersage wichtiger Qualitätsparameter an zahlreichen Obst- und Gemüsearten (Apfel, Avocado, Blaubeere, Ingwer, Kaki, Kiwi, Mandarinen, Mango, Tafeltrauben) durchgeführt. Die Auswertungen zeigten, dass insbesondere die Merkmale Zuckergehalt, Trockenmasse sowie der relative Wassergehalt der Früchte mit hoher Genauigkeit zerstörungsfrei vorhergesagt werden können. In einem konkreten Praxisbeispiel wurde zudem ein Food-Scanner im Zuge von Wareneingangskontrollen des Obst- und Gemüsegroßhandels zur zerstörungsfreien Qualitätsbewertung eingesetzt. Die Evaluierung ergab eine hohe Übereinstimmung der Food-Scanner Vorhersagen mit herkömmlichen zerstörerischen Messungen mittels Refraktometer und veranschaulichte zudem die Möglichkeit der Einsparung von Arbeitszeit durch den Einsatz dieser Messgeräte.

Die Ergebnisse dieser Doktorarbeit veranschaulichen das große Potential von Food-Scannern für die zerstörungsfreie Qualitätsmessung von Obst und Gemüse entlang der Wertschöpfungskette. Einige der untersuchten kommerziellen Geräte zeigten bereits eine hohe Kompatibilität mit den Anforderungen der Obst- und Gemüsebranche, wie beispielsweise eine robuste Bauweise, lange Batterielaufzeit sowie die Möglichkeit der personalisierten Modellbildung und Datenauswertung durch die Anwender. Als wichtige Voraussetzungen für die Implementierung in der Praxis wurden neben der Möglichkeit der Integrierung der generierten Daten in bestehende Systeme der Informationstechnologie auch das Vertrauen in die Genauigkeit der Food-Scanner-Vorhersagen ermittelt. Eine gezielte Zusammenarbeit der Food-Scanner Produzenten mit den Unternehmen der Obst- und Gemüsebranche, die Publikation von neuen Erkenntnissen in Fachzeitschriften für Produzenten und Handelsunternehmen sowie die Bereitstellung von gezielten Weiterbildungsprogrammen könnte dazu führen, dass Food-Scanner in Zukunft noch besser auf die Anforderungen der Wertschöpfungskette von Frischeprodukten abgestimmt werden und letztendlich die Implementierung in den praktischen Alltag der Qualitätskontrolle finden.

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Index

Alphabetical list of abbreviations and symbols

Abbreviation / symbol	Description
a*	Color value indicating the red/green coordinate
b*	Color value indicating the yellow/blue coordinate
C*	Color value indicating the chroma
CA	Cluster analysis
DA	Discriminant analysis
FEFO	First-expired-first-out
FIFO	First-in-first-out
FSC	Fresh produce supply chain
h°	Color value indicating the hue
KNN	K-nearest neighbor
L*	Color value indicating the lightness
LDA	Linear discriminant analysis
LED	Light-emitting diode
MAA	Multi-Actor Approach
MNPLS	Mixed-norm partial least squares
NIPALS	Nonlinear iterative partial least squares
NIRS	Near infrared spectroscopy
PCA	Principal component analysis
PLSR	Partial least squares regression
r^2_C	Coefficient of determination in calibration
r^2_{CV}	Coefficient of determination in cross validation
$RMSE_C$	Root mean square error of calibration
$RMSE_{CV}$	Root mean square error of cross validation
SIMCA	Soft independent modeling of class analogy
SPLS	Sparse partial least squares
SSC	Soluble sugar content
SVM	Support vector machine
VIS	Visual spectrum

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1 Introduction

1.1 Problem statement and research questions

For the field of quality assurance, a comprehensive and holistic approach from production to marketing is of high importance. Within the fruit and vegetable sector, this is particularly important, as various factors during the production of fresh produce, such as mineral nutrition, climatic conditions, selection of variety, or maturity at harvest have a significant influence on the subsequent quality along the supply chain (Hewett 2006). Furthermore, the quality of fruit and vegetables changes immediately after harvest due to ongoing metabolic processes (Martínez-Romero et al. 2007). The quality of produce deteriorates at a different pace (Kong and Singh 2016) depending on various influencing factors during the further course along the supply chain (e.g., storage and transport conditions, packaging, mechanical handling, post-ripening processes). Postharvest quality assurance has to monitor the quality of fresh produce and counteract quality-reducing processes in order to keep potential losses along the supply chain as low as possible. Depending on the respective product, specific standards concerning the commercial quality of some fruit parameters must be met to allow the distribution via retail chains (UNECE 2019). In addition to these standards required by law, retail companies oftentimes impose requirements, which exceed statutory provisions.

The verification and assessment of quality of intact fruit can be made based on human senses, such as visual inspection of colors, smelling of volatile organic compounds or touching to control fruit firmness (Walsh 2006). However, these judgements are often subjective, therefore the quality of these evaluations highly depends on personal experience. The utilization of instrumental measurement methods for commercially important quality traits is often preferred over sensory evaluations and help to reduce the variation between individuals, provide high precision and offer a common language between consumers, researchers and industry (Abbott 1999). Furthermore, the determination of internal quality standards is often simply not possible using solely sensory assessments. In order to measure and verify these internal quality parameters, destructive measurements have to be conducted, e.g. the determination of sugar content using pressed fruit juice and a refractometer or measurement of firmness via penetrometer. Other measurements, such as the determination of dry matter, are extremely time-consuming, and in the case of acidity measurement, elaborate sample preparation and handling of chemicals is necessary for titration (OECD 2018).

In the past, various studies investigated the feasibility of optical measurement methods like visible and near-infrared (VIS/NIR) spectroscopy for the determination of important quality parameters of various agricultural and horticultural products (Nicolaï et al. 2007; Cortés et al. 2019). NIR spectroscopy, as a type of vibrational spectroscopy, employs the stimulation of molecular vibration using infrared light in the wavelength range 750 to 2500 nm. NIR electromagnetic waves interact with various molecular bonds (especially C-H, O-H, N-H or S-H bonds) of the respective sample constituents and result in a spectra, which is recorded by an optical sensor (Pasquini 2003). This NIR spectral data can be evaluated using various algorithms and multivariate statistical analysis and allows the development of qualitative and quantitative prediction models (Cozzolino 2009; Pasquini 2018). Whereas qualitative models are designed to enable classification, identification and authenticity verification of products (e.g., origin, variety, grade), quantitative models aim to determine the concentration of known constituents in samples, such as sugar concentration or dry matter content of fruit and vegetables (Figure 1). NIR spectroscopy offers various advantages compared to traditional measurement methods of fruit and vegetables, such as a fast and non-destructive operating principle, simple sample preparation as well as the possibility of using one spectrum for multidimensional evaluation of various parameters in one work step (McClure 1994; OECD 2018).

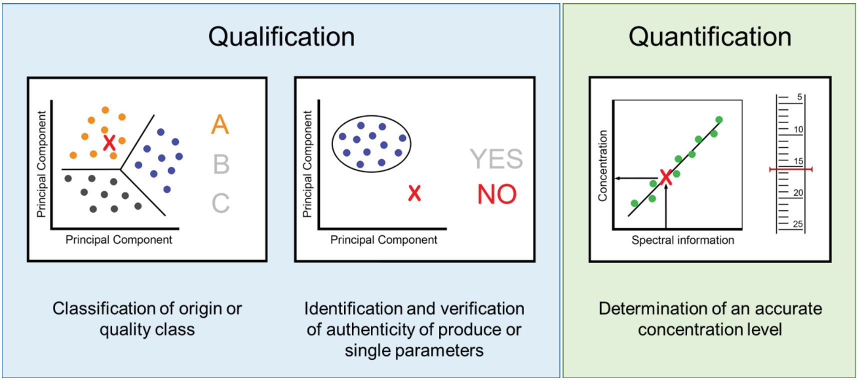

Figure 1: Application types of NIR spectroscopy (adapted and redesigned according to Langer (2019))

Next to laboratory applications, which employ benchtop instruments, the technique of NIR spectroscopy found its way into automated sorting and grading machines for fruit and vegetables. These on-line NIR applications are designed for real-time determination of important quality attributes (e.g., sugar content, acidity) and the detection of internal fruit disorders such as internal browning of fruit (Huang et al. 2008). The need for a more cost-effective and compact application of NIR spectroscopy led to the development of portable handheld devices (dos Santos et al. 2013). These sensors allow the transfer of traditional laboratory work to in-field applications, which can be implemented along the whole supply chain of fresh produce. Some companies are already marketing devices specifically designed for horticultural applications, such as the determination of fruit quality parameters in the orchard (Felix Instruments 2020b) as well as measurements along the supply chain to the point of sale (Sunforest 2020).

Subsequent technological developments led to an increasing miniaturization of NIR sensors. Some of these devices, so called food-scanners, were initially designed for end-consumers and were commercially distributed by various start-up companies (Consumer Physcis 2020; Tellspec Inc. 2020a; Spectral Engines Oy 2020). Oftentimes, these food-scanners work in combination with a mobile app on a smartphone or tablet and make use of cloud-based platforms, which hold vast material libraries and employ advanced algorithms. These applications aim to identify various food-related parameters (e.g. protein, fat, calories, allergens, contaminants, macronutrients) as well as the total energy content and provide important information such as food adulteration, food fraud, and food quality (Rateni et al. 2017). Currently, some of these start-up companies collaborate with industrial partners and target real-time in-field solutions for specific industries, e.g., monitoring of corn, grains and animal feed quality (Consumer Physcis 2020) as well as the analysis of fish, fruit and liquids (Tellspec Inc. 2020a).

Due to the novelty of portable and miniaturized devices, scientific research about the performance and suitability of food-scanners for a reliable determination of the quality of fruit and vegetables is currently still sparse. Initial studies compared various commercially available instruments for their prediction accuracy of specific fruit quality traits such as dry matter (Kaur et al. 2017) or examined the performance of individual devices (Ncama et al. 2018; Li et al. 2018; Choi et al. 2017) . Most of these studies regarding the performance of food-scanners evaluated selected fruit within a laboratory setup without reference to the practical use of these devices in daily processes of quality control along the fresh produce supply chain (FSC). At the beginning of this work, the use of miniaturized sensors for the concrete determination of fruit quality and their application along the FSC had not yet been investigated. In this context, the overall aim of this study was to evaluate the suitability of portable NIR sensors (food-scanners) for the determination of fruit quality along the supply chain of fruit and vegetables. This thesis focused on tomato as model fruit for the development of non-destructive prediction models of a variety of important quality attributes and evaluated the practicability of already existing and commercially available portable and miniaturized food-scanners.

Given this background information, the research questions for this doctoral thesis were formulated as follows:

- Miniaturized NIR instruments (food-scanners) are relatively new to the scientific literature. Is their performance comparable to traditional laboratory benchtop NIR instruments for the prediction of fruit quality traits?
- Currently there are various different food-scanners commercially available. Are there major differences with respect to the predictability of fruit quality parameters?