Programme and Book of Abstracts

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sensor FINT

Córdoba, Spain

FINAL
CONFERENCE

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Preface by Dolores Pérez Marín

On behalf of the Organising Committee and Cost Action 19145 **SensorFINT** — *European Network for assuring food integrity using non-destructive spectral sensors* — is proud to present the Book of Abstracts of our **Final International Conference** "*Nondestructive Spectral Sensors & Food Integrity: Advances, Challenges and Future Trends*" (29th-31st May, Cordoba, Spain).

This is the last Conference of the Action in which all the participants will have the opportunity to share ideas, knowledge, challenges, and reflexions about the present and future of the key role of nondestructive spectral sensors for the innovation of control and monitoring systems for food quality and authenticity.

Since the start of the Action in 2020, in a very difficult international situation, the SensorFINT community has worked hard to expand the network, spread the importance of nondestructive spectral sensors in the food industry and train new young researchers in this emerging field. I must proudly say that it has been an honour for me to coordinate SensorFINT, giving me the opportunity to share experiences with colleagues I already know and above all to meet new colleagues and friends in this scientific field.

I would like to take this opportunity to thank the keynote speakers, industry speakers, presenters and authors for their contribution and Cost for providing funds for this event and this Action, and to wish you all a satisfactory experience and a very pleasant stay in our town and in our country.

I would also like to express my sincere personal thanks to Prof. Tom Fearn, Vice President of this Action, for his continued support and reassurance throughout. In addition, I would like to thank the Core Group, the MC members and all SensorFINT participants for their support and implications. Finally, a special thanks to all the members of my group: Ana, Irina, Paco, José, Gema, Mar, Jesús, Eseró, Manuel, Miguel, Antonio, Mª Carmen y Pilar.

I hope everyone enjoys this conference, the ideas and knowledge shared and, of course, the networking opportunities it will provide. I hope this is not the end but the beginning of new projects and collaborations together in the near future.

Signed: Prof. Dr. Dolores Pérez Marín
Chair of SensorFINT
(Cost Action 19145)

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3nd SENSORFINT FINAL International Conference
29-31 May 2024, Cordoba, Spain

CONFERENCE PROGRAM

Day 1: Wednesday 29.05.2024

08:30	**Registration /Attendance list**	
09:00	**Welcome: Prof. Mª José Polo (Scientific Policies Vice-chancellor, UCO) & Prof. Lola Pérez Marín (SensorFINT Chair)**	
Session 1: NDSS for food quality control and authentication along the entire supply chain Chairs: Prof. Marena Manley (Stellenbosch University, South Africa) & Dr. Jens P. Wold (Nofima, Norway)		
09:15	**Daniel Cozzolino #Keynote 1**	**NIR in the agri-food industries: what have we learned and where are we going?**
10:00	Vilde Vraalstad	Get to know your spectrometer, and how it compares to other spectrometers on the market
10:15	Christian Huck	Celebrating the 25th Anniversary of NIR Spectroscopy at the University of Innsbruck, Austria: Contributions to material-, bio-, medicinal plant and food analysis
10:30	Maria Tarapoulouzi	The Development of Determining Milk Species' Origin in Halloumi Cheese: A Journey from MIR to NIR Measurements.
10:45	Mar Garrido	Enhancing olive oil quality assurance using portable NIRS instruments
11:00 11:30	**Coffee break**	
11:30	Ana Soldado	The effect of sampling on Miniaturized Near-Infrared Spectroscopy: forage analysis
11:45	*Gold Sponsor Time: SafetySpect*	
12:00	Myrsini Chroni	Exploring alternative test methods for the classification of saffron (Crocus sativus L.) according to ISO 3632: preliminary results with a miniaturized Near-Infrared (NIR) spectroscopic sensor
12:15	*Silver Sponsors Time: Bruker, Si-Ware, Viavi*	

12:35	Antoine Deryck	Individual authentication of cocoa beans using Vis-NIR spectroscopy
12:50	Sebahattin Serhat Turgut	Spectral Assessment of Adulteration in Ground Pistachio
13:05 14:30	**Lunch & Visit to Poster Exhibition**	
Session 2: Sensor fusion for reaching complex issues in food integrity **Chairs: Prof. Mecit Oztop (Middle East Technical University, Turkey) &** **Prof. Radmila Pajovic (University of Montenegro, Montenegro)**		
14:30	**Byoung-Kwan CHO #Keynote 2**	**Spectral imaging application for quality and safety measurement for agricultural materials**
15:15	Miguel Vega-Castellote	Detection of peanut fragments in chopped almonds using hyperspectral imaging technology
15:30	Esteban Roca Nasser	Grain-based authentication of bread with hyperspectral imaging for quality control
15:45	Saeys Wouter	Laser spectroscopy for monitoring pome fruit respiration
16:00 16:15	 **Coffee break**	
16:15	Elena Fulladosa	Hyperspectral imaging as a non-invasive tool to evaluate pathogen's growth behaviour: effect of image pre-processing.
16:30	Belmin Lisicic	Optical detection of mold growth on apples
16:45	Áine Ní Fhuaráin	Preliminary comparison between using Mid-Infrared (MIR) and Raman spectroscopy with chemometrics to predict the gel onset of raw bovine milk samples.
17:00 19:00	**MC meeting** (only for MC members)	**VISIT TO THE SENSOR LAB UCO (CAMPUS RABANALES)**
20:15	**ICE-BREAKER**	

Day 2: Thursday 30.05.2024

08:45	 **Attendance list**	
Session 3: Data management tools for processing and modelling nondestructive spectral sensor signals **Chairs: Prof. Marina Cocchi (UNIMORE, Italy) & Dr. Jean-Michel Roger (INRAE, France)**		
09:00	**Federico Marini #Keynote 3**	**Present and future trends in chemometrics for spectral data**
9:45	Krzysztof Bec	A multispectral NIR/UV-Vis approach to discrimination between subvarieties of arabica coffee: variable selection, non-linear classifiers, artificial neural networks and data fusion
10:00	Tassos Koidis	AI-boosted artificial spectral pipeline augments chemometric models and improves performance in real world applications
10:15	Hilmi Eriklioğlu	Beet & Cane Sugar Classification by Using NIR Spectroscopy and Chemometrics
10:30	Uladzislau Blazhko	Breaking Spurious and Systematic Correlations by Augmenting Datasets
10:45 11:30	 **Coffee break & Poster session**	
11:30	Lorenzo Strani	Exploring Apple Diversity: Non-destructive Spectroscopic Analysis and Chemometric Insights
11:45	Dário Passos	Exploring CNN architectures for dry matter prediction on a multi fruit NIR data set
12:00	Puneet Mishra	Implementing pre-trained open AI models for near-infrared spectroscopy applications
12:15	Arnaud Molle	Targeted iPLS for the prediction of cheese-making traits from individual milk FTIR spectra
12:30	Salvador Castillo Gironés	Detection of invisible damages in plums with deep learning
12:50 14:00	**Lunch & Visit to Poster Exhibition**	

Session 4: STSM results Chairs: Dr. Elena Fulladosa (IRTA, Spain) & Dr. Ana Mª Jiménez (University of Granada)		
14:00	C. Pretorius	Investigating the Effect of Refining Time on Dark Chocolate Particle Size using NIR Spectroscopy
14:10	Gonçalo Guedes	A Hyperspectral Inspection System to Classify Corks Surface Treatments Homogeneity
14:20	Yangyue Chen	Can Near-Infrared Spectroscopy (NIRS) Be Used for Rapid Discrimination of Fresh Eggs with Different Infection Statuses?
14:30	Zaqlul Iqbal	Comparative study of Raman and Near Infrared (NIR) spectroscopy to detect Pork Adulteration in Meatballs
14:40	Candela Melendreras	Development of Chemometric strategies for quality Control in Breast Milk
14:50	Miriam Muñoz Lapeira	Discrimination of Normal and Wooden Breast Chicken Fillets Using NIR, fluorescence, and Raman Spectroscopy
15:00	Ahmed Menevseoglu	Non-destructive and rapid discrimination of carob adulteration in cocoa powders using NIR and MIR spectroscopy
15:10	N. Douglas	Effect of different Temper Regimes on the Polymorphic Behaviour of Dark Chocolate using Near-infrared (NIR) spectral data
15:20	Claudia Beleites	Adjustable Lab Sample Divider
15:30 15:50		**Coffee break**
15:50 **17:30**	**INDUSTRIAL ROUND TABLE** Moderators: Prof. Lola Pérez Marín (SensorFINT Chair) & Prof. Tom Fearn (SensorFINT Vice-Chair). Participants: • Fartash Vasefi, SafetySpect • André Kok, Bruker Optics • Javier Echevarría, Kaura Coproducts • José María Penco, AEMO (Olive Municipalites Spanish Association) • Sergio Martín, ANICE (Spanish National Association of Meat Industries) • Andrés Martín, COVAP (Food Cooperative in Pedroches Valley, Cordoba) • Luis Serrano, Olimarker Company	
20:00	**SENSORFINT GALA DINNER** **Place: Círculo de la Amistad Social Club** Dress code: long trousers for men is required	

Day 3: Friday 31.05.2024

09:00		**Attendance list**
Session 5: Innovation and future trends in the use of NDSS and its industrial implementation: AI, sampling, non-targeted approaches, decision support system, digital labelling, interoperability **Chairs: Prof. Wouter Saeys (KU Leuven, Belgium)** **& Prof. Christian Huck (Leopold-Franzens University, Austria)**		
09:15	**Vincent Baeten #Keynote 4**	**Advances and challenges for NDSS in food and agriculture: this is just the beginning!**
10:00	Dario Benedini	Multiway approach to milk coagulation using MicroNIR
10:15	Cristina Alamprese	FT-NIR spectroscopy for fermentation monitoring of purslane-fortified yogurt
10:30	Tomasz Czaja	NIR Spectroscopy: Searching for optimal crops for the green food transition
10:45	Jens Petter Wold	Rapid and non-destructive quantification of meat content in the legs of live red king crab (Camtschaticus paralithodes) by near-infrared spectroscopy
11:00 11:30		**Coffee break**
11:30	Nikos Chorianopoulos	Non-destructive spectroscopic-based instruments; their implementation in food sector in tandem with artificial intelligent tools and Blockchain technologies
11:45	José Antonio Entrenas	Improving NIR models performance in the Rendering industry through database enhancement
12:00	Krzysztof Rutkowski	The usefulness of VIS/NIR techniques for maturity and quality assessment of selected fruit species – resume of 18 years experiments and future perspective
12:15	Justyna Grabska	Comparison and evaluation of miniaturized NIR sensors for on-site discrimination of microplastics in soil
12:30	Glen Fox	Improving quality in breweries with real-time Raman NIR technology

12:45	Søren Balling Engelsen	Process Analytical Technology with NIRS as a Key Ingredient Helps Facilitate a Sustainable Food Production
13:00 13:30	**Closing**	
13:30 14:30	**Lunch**	
15:30	**Visit to the Mezquita & Cordoba Tour**	

POSTER COMMUNICATIONS

P01	Katarzyna Pawlak-Lemańska	Apple quality assessment using benchtop NIR and portable VIS-NIR instruments - comparative study
P02	Krzysztof Wójcicki	Application of NIR spectroscopy for quality assessment of Yerba mate
P03	Katarzyna Włodarska	Application of visible and near infrared spectroscopy for non-destructive food quality analysis – a study of berry fruit beverages
P04	Katarzyna Pawlak-Lemańska	Benchtop and portable NIR spectroscopy equipment for detection of apple quality
P05	Radmila Pajovic Scepanovic	Characterization of Cabernet Sauvignon wines from Western Balkan countries using spectrophotometrically methods
P06	Fatih KAHRIMAN	Discrimination of Haploid and Diploid Maize Seed Samples Using Vis-NIR Imaging Technique
P07	Puneet Mishra	fCovSel: A new faster covariates selection algorithm for NIR spectral data
P08	Federica Amato	Hybrid modelling applied to spectroscopic data in bioreactors
P09	Ewa Sikorska	Managing control of food authenticity using spectroscopy – the example of apple juice
P10	Nikos Chorianopoulos	Microbiological quality assessment of aerobically stored Feta cheese using spectroscopy-based sensors
P11	Miguel Vega	Monitoring almonds sun-drying process using handheld portable NIR sensors
P12	Stella Ordoudi	Novel diagnostic markers for the quality of traded saffron based on Fourier Transform Infrared (FT-IR) spectroscopy and chemometrics: what is still underexplored?
P13	Andrea Fernández Veloso	Nuclear Magnetic Resonance-based Metabolomics in conjunction with Machine Learning Algorithms for Food Analysis
P14	Irina Torres	Optimization of a fiber optic probe for the *in situ* quality evaluation of virgin olive oil

P15	Jesús Galán-Romero	Optimizing spectral analysis for improved precision in Iberian ham quality control with portable NIRS devices
P16	Lorenzo Serva	Predicting Italian polyflora honey geographical origin by visible and NIR spectroscopy
P17	Lorenzo Serva	Predicting milk quality using portable NIR instruments
P18	Giorgia Stocco	Use of NDSS to authenticate Parmigiano Reggiano and Grana Padano PDO grated cheese
P19	Pablo Roig	Use of vine shoots as biomass energy. In-situ quality evaluation by near infrared spectroscopy
P20	Mónica Sánchez-Parra	Screening of tuna samples for evaluation of histamine content using Fourier-transform mid-infrared (FT-MIR) and chemometrics
P21	Puneet Mishra	Near-infrared, Raman and ultrasound sensing fusion for mango properties prediction
P22	Louis Paternostre	Evaluation of handheld spectrometers and development of robust models
P23	Alejandra Arroyo-Cerezo	The potential of a benchtop LF-NMR equipment for food authentication assessment by a non-targeted approach
P24	Ricardo dos Santos	Alternative plant-based protein analysis using NIR and MIR spectroscopy
P25	C. Barnés-Calle	Exploring protein secondary structure changes of high moisture extrudates using FT-IR Amide I band deconvolution
P26	Ana M. Jiménez Carvelo	Quantification based on pixel counting by classification (QPC) methodology and its application in hyperspectral imaging
P27	Svetoslava Terzieva	Differentiation of Amaranthus Species Using Near-Infrared Spectroscopy
P28	Miriam Medina García	Microplastics analysis in marine salt by hyperspectral imaging
P29	Ben Aernouts	On-farm real-time near-infrared spectroscopic sensor system for milk composition analysis

P30	Marta Rodríguez-Fernández	Use of a portable NIR spectrometer for the classification of fresh pork meat according to diet
P31	Miriam Hernández-Jiménez	Feasibility of using a portable spectrometer (vis-NIR) during the production and ripening of Protected Designation of Origin Casín cheese.
P32	Julio Nogales-Bueno	Non-destructive, in-situ varietal discrimination of walnut tree by portable near infrared spectroscopy
P33	Tom Fearn	Testing differences in predictive ability
P34	Yuanyuan Pu	Evaluating potential fouling of a Near Infrared (NIR) process sensor during protein measurements in dairy concentrate processing
P35	Cecilia Riccioli	Towards the automated quality control of olives in the reception yard of the olive mill.
P36	Marina De Géa Neves	Investigation the proteolysis reaction in dry-cured ham using NIR spectroscopy and evolving difference calculations
P37	Begonya Marcos	NIR spectral imaging for non-destructive detection of microplastics in sea salt
P38	Miriam Hernández-Jiménez	NIR Spectroscopy and Artificial Neural Networks for predicting sensory parameters in Iberian ham
P39	C. Ricci	Rapid, high-throughput screening of traded saffron using a portable multimodal spectroscopic sensor and data fusion analysis
P40	Macarena Rojas Rioseco	Precise and Efficient Brixº Determination in Molasses Using Combined NIR/MIR Spectroscopy and Chemometrics
P41	J.M. Cáceres-Nevado	Prediction of the fatty acid profile using NIRS technology to optimize the curing process of Iberian ham
P42	Rukiye Şengün	Determination Galactomannan and Fat Content of Guar (Cyamopsis tetragonoloba) using NIR Spectroscopy
P43	Lidia Zaharieva	BG Wine - a database of spectral and chromatographic characteristics of traditional Bulgarian wines
P44	D. Antonova	Fast estimation of Citronellol, Nerol and Geraniol content in Bulgarian rose oil by NIR spectroscopy

P45	Y. Medarska-Georgieva	Volatile organic compounds in traditional Bulgarian red wines - optimization of analytical method using solid phase microextraction and head space gas chromatography
P46	Volkan Göçebe	Classification of Moisture Content of Milk Powder by Using NIR Spectroscopy and Chemometrics
P47	Nazan Altun	Classification of Surface Contamination as Biofilms of Foodborne Bacteria with Visible and Short Wave Infrared Spectral Data Fusion
P48	F. Hoxha	Hyperspectral imaging: a new frontier in honey authenticity
P49	Mădălina Belous	Food waste and safety food
P50	Víctor Fernández-Cabanás	Discrimination of goat dairy products according to feeding regimes by NIR spectroscopy
P51	Jasenka Gajdoš Kljusurić	Application of Near Infrared Spectroscopy in detecting adulteration - case of honey

SESSION 1: NDSS for food quality control and authentication along the entire supply chain

Keynote #1: DANIEL COZZOLINO

NIR in the agri-food industries: what have we learned and where are we going?

The University of Queensland, Centre for Nutrition and Food Sciences (CNAFS), Queensland Alliance for Agriculture and Food Innovation (QAAFI), Brisbane, Queensland 4072, Australia.
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Since the first application of near infrared (NIR) spectroscopy in the agri-food industry, the utilization of this technique has evolved from the development of calibrations used to predict proximate composition (e.g. protein, dry matter) to a versatile tool that is able to monitor all the steps of the agri-food production, supply and value chains. Food safety and security, climate change, sustainability, circular economy, and food waste have become contemporary issues for primary producers and consumers (Cozzolino, 2023). Monitoring and trace food fraud, composition, nutritional value, shelf life and waste have become of interest to consumer where these issues are prevalent disruptors of the food supply and value chains. The incorporation of technology (e.g. sensing technologies, Internet of Things) has been considered of great benefit to address the different issues that disturb the modern agri-food systems (Cozzolino and Chapman, 2024). The advantages and drawbacks of implementing NIR spectroscopy in the agri-food sector and future applications of this technology will be discussed.

Keywords: NIR, food, agriculture, chemometrics, sensors.

References

Cozzolino, D., Chapman, J. 2024. Advances, limitations, and considerations on the use of vibrational spectroscopy towards the development of management decision tools in food safety. Anal. Bioanal. Chem., 416, 611-620.

Cozzolino, D. 2023. Advances in spectrometric techniques in food analysis and authentication. Foods, 12, 438.

Get to know your spectrometer, and how it compares to other spectrometers on the market

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In our talk, we will present a first principles method for characterising and comparing spectrometers, that is intended to be used by spectroscopists and chemometricians wanting to improve or develop new spectroscopic measurement solutions.

The already large spectrometer market is rapidly growing, with new additions promising to be smaller, cheaper, faster, with higher performance, and more suitable for a large variety of applications. It can however be challenging to assess whether new instruments are better for your application than those you already have in your lab, and if the cheap and small instruments will provide you sufficient data quality. Unfortunately, data sheets are inadequate for proper assessment and comparison of spectrometer performances, with differences in terminology, levels of detail, and parameters that do not characterise the application-specific performance. For example, the signal-to-noise ratio (SNR) is often specified by the signal at optimal reflectance conditions. This makes it challenging to evaluate a spectrometer using first principles, to understand how the spectrometer design could be further optimised to improve performance, and to understand how it compares to other spectrometers on the market.

We have developed a tool for characterising a spectrometer in a robust manner, that allows a user to objectively characterise spectrometers before going straight to testing on the intended application. It also allows you to compare instruments without needing to extract information from datasheets, which can be inconsistent and hard to interpret. By employing a user-friendly, reasonably priced, and reproducible experimental set-up, a set of performance characteristics is measured. In our talk, we will use examples for NIR absorbance spectroscopy, and show how these characteristics can be used to understand data quality, discover possible improvements to the instrument design, and understand the effect of data processing. The goal is to help the realisation of more commercial spectroscopic measurement solutions.

Keywords: NIRS, instrumentation, spectrometer design, performance, data quality.

Acknowledgements: This work was a part of the project SFI Digital Food Quality (project number 309259), partially funded by the Norwegian Research Council.

Celebrating the 25th Anniversary of NIR Spectroscopy at the University of Innsbruck, Austria: Contributions to material-, bio-, medicinal plant and food analysis

Christian W. Huck*

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Near-Infrared (NIR) spectroscopy has profoundly impacted material, bio, medicinal plant, and food analysis during its 25-year tenure at the University of Innsbruck, Austria. Huck's seminal contributions have significantly advanced this field, shaping its evolution and application across diverse scientific disciplines. In material analysis, NIR spectroscopy has enabled rapid and non-destructive characterization of substances, fostering innovations in polymer science, pharmaceuticals, and geological studies. In bioanalysis, NIR spectroscopy has revolutionized biomedical research by providing valuable insights into biochemical processes. Moreover, in medicinal plant analysis, NIR spectroscopy has facilitated authentication and quality assessment of herbal medicines. Additionally, NIR spectroscopy has emerged as a vital tool in food analysis, ensuring food safety and quality.

As NIR spectroscopy celebrates its 25th anniversary at the University of Innsbruck, Huck's pioneering research underscores its pivotal role in driving advancements and fostering interdisciplinary collaborations in analytical chemistry.

Keywords: NIR spectroscopy, University of Innsbruck, material analysis, bioanalysis, medicinal plants, food analysis, interdisciplinary collaboration, analytical chemistry.

References

Beć, K.B.; Grabska, J.; Huck, C.W.; In silico NIR spectroscopy – A review. Molecular fingerprint, interpretation of calibration models, understanding of matrix effects and instrumental difference. Spetrochim. Acta A 2022, 279, 121438; DOI: 10.1016/j.saa.2022.121438

Moll, V. Beć, K.B.; Grabska, J. Huck, C.W. Investigation of water interaction with polymer matrices by near-infrared (NIR) spectroscopy. Molecules 2022, 27, 5882; DOI: 10.3390/molecules27185882

Losso, K.; Beć, K.B.; Mayr, S.; Grabska, J.; Stuppner, S; Jones, M.; Jakschitz, T.; Rainer, M.; Bonn, G.K.; Huck, C.W. Rapid discrimination of Curcuma longa and Curcuma xanthorrhiza using direct analysis in real time mass spectrometry and near infrared spectroscopy. Spetrochim. Acta A 2022, 265, 120347; DOI: 10.1016/j.saa.2021.120347

The Development of Determining Milk Species' Origin in Halloumi Cheese: A Journey from MIR to NIR Measurements

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Halloumi cheese has recently gained a Protected Designation of Origin (PDO) indicator, which is related to the place (Cyprus) in which halloumi cheese is made. The PDO label is linked with several requirements, e.g., milk species, quantities, etc.; thus, it is important to study this product regarding quality and authenticity (Tarapoulouzi et al., 2024). Near-Infrared (NIR) as well as Middle-Infrared (MIR) are fast and easy techniques in application, both of which provide significant information in food analysis (Silva et al., 2022).

The aim of this presentation is to show the differences and similarities of a halloumi cheese sample set measured by using NIR (Tarapoulouzi et al., 2024) as a comparison to a previously acquired MIR spectroscopy dataset (Tarapoulouzi et al., 2020). Chemometric analysis was crucial for interpreting the spectroscopic data by applying both supervised and unsupervised methods. To the best of our knowledge, literature related to halloumi cheese using these spectroscopy-based measurements is scarce.

The NIR model revealed that the grouping of samples was determined to be based on composition, mainly fat, protein and lactose content of the cheese samples. The MIR model showed that the subregion 1150-720 cm−1 was only important for discrimination regarding species' origin, which contains absorptions due to –NH2 deformation, C–OH bending, and C–C stretching with the contribution from O–H bending and O=P–O (phosphate groups stretch) covalently bound to casein proteins and -C=O from polysaccharides and C=C stretching of acids (Tarapoulouzi et al., 2020). Both models returned distinct clusters of the two halloumi cheese types, cow and goat-sheep origin.

Keywords: FTIR, NIR, halloumi cheese, milk species.

References

Silva, L.K., Santos, L.S. and Ferrão, S.P., 2022. Application of infrared spectroscopic techniques to cheese authentication: A review. International Journal of Dairy Technology, 75(3), 490-512.

Tarapoulouzi, M., Kokkinofta, R. and Theocharis, C.R., 2020. Chemometric analysis combined with FTIR spectroscopy of milk and Halloumi cheese samples according to species' origin. Food science & nutrition, 8(7), 3262-3273.

Tarapoulouzi, M., Logan, N., Hardy, M., Montgomery, H., Haughey, S.A., Elliott, C.T. and Theocharis, C.R., 2024. A Pre-Trial Study to Identify Species of Origin in Halloumi Cheese Utilising Chemometrics with Near-Infrared and Hyperspectral Imaging Technologies. Analytica, 5(1), 17-27.

Enhancing olive oil quality assurance using portable NIRS instruments

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Given the increasing rise in olive oil (OO) prices, consumers demand detailed information to strengthen their confidence in the quality and authenticity of the product they are paying for. The European Commission's stringent standards governing olive oils in international trade require rigorous conformity checks to assess their physicochemical and sensory properties, which are crucial for labelling and categorization. However, most of these evaluation methods are economically prohibitive for many producers and retailers. Moreover, the considerable expense and time needed to collect this data result in only a small fraction of OOs is inspected annually in relation to total production. For these reasons, there is a growing and pressing need for innovative, rapid, and cost-effective analytical techniques to ensure the quality and authenticity of OOs, and to increase consumer confidence within the global olive oil market. This study aims to provide scientific evidence of the potential of two portable NIRS instruments - MicroNIR Pro 1700 (908-1676 nm) and AlbaNIT (950-1650 nm) - for the *in situ* analysis of olive oils. For this purpose, a total of 300 OO samples were analysed in transmission. MPLS regression was used to predict the main physicochemical and sensory parameters related to olive oil quality, according to the current regulations. The results show that both MicroNIR Pro 1700 and AlbaNIT instruments exhibited promising performance in predicting the main quality parameters of olive oils. It is also shown that the predictive capability of portable NIRS instruments, even when using a very low-cost sensor, is comparable to that obtained with high-performance laboratory NIRS instruments. This is of great relevance to OO producers, laboratories and official inspectors that can benefit from this affordable and fast technology, helping them to increase the volume of marketed OOs already analysed according to the EU standards.

Keywords: Olive Oil quality, portable NIRS sensors, cost-effective analysis, authentication, consumer confidence.

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The effect of sampling on Miniaturized Near-Infrared Spectroscopy: forage analysis

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The demand for fast, non-invasive, and user-friendly tools to assess the physical and chemical properties of agricultural samples is steadily rising, particularly in precision farming. In this agricultural approach, reducing delay time and enhancing data accuracy are key factors to optimize the farming process. These precision farming techniques significantly enhance production outputs, influencing quality, quantity, economic performance, and environmental impact. To acquire valuable and accuracy information on-site and in real time is essential to asses the quality of the results and to implement necessary actions. In terms of evaluating the nutritive value of forage productions, near-infrared spectroscopy (NIRS) stands out as one of the most effective options for real-time analysis (Beć et al., 2021; Pasquini, 2018). Additionally, the feasibility of NIRS analysis is linked to the use of low cost and easy to use portable/miniaturized sensors. However, when using miniaturized NIR instrumentation, the sampling strategy needs to be evaluated in order to improve the quality of the calibration model.

In this work, a comparative analysis was conducted between a commercial spectrometer (VIAVI MicroNIR 1700) and a prototype nanoNIRscan Nano spectrometer (Texas Instruments), using alfalfa samples. The study emphasizes the crucial role of the sampling procedure in ensuring accurate results when assessing the nutritive value of forage feed samples. Notably, when developing calibration models with spectra collected using the NIRscan Nano instrument, with either a fiber optic or cuvette, different calibration statistics were obtained. The fiber-optic probe yielded the most favourable values, characterized by minimal error and with correlation coefficients of calibration (R2) values exceeding 0.9. Moreover, when comparing the commercial device with the prototype, higher R2 values were achieved with the fiber-optic system, while calibration errors were 50% lower when using the proposed prototype.

Keywords: forage, sampling, fiber optic, nanoNIR.

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Exploring alternative test methods for the classification of saffron (Crocus sativus L.) according to ISO 3632: preliminary results with a miniaturized Near-Infrared (NIR) spectroscopic sensor

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So far, the classification of saffron, the most expensive spice in the world, relies on the ISO 3632 trade standard specifications and test methods. Above all, the coloring (CS), aroma (AS) and flavor strength (FS), associated with the total content in major metabolites (crocins, safranal, and picrocrocin, respectively), are used to classify the product into three quality grades. These values are determined by UV-Vis spectrophotometry using a considerable amount of the product, a one-hour extraction protocol, and absorption coefficient values at three specific wavelengths, which are 440, 330, and 257 nm, respectively (ISO 3632-2, 2010). The interest in developing alternative test methods for the quality classification of saffron was initiated many years ago aiming either at increasing the accuracy of the determinations (Li et al., 2018) or speeding up the analyses with the aid of non-destructive techniques (Zalacain et al., 2005, Kiani et al., 2023). In this work, a portable miniaturized NIR sensor combined with chemometrics was employed for the first time to comparatively evaluate its prediction performance against the traditional ISO-based method. The reflectance spectra of a set of 123 reference saffron samples (same origin and harvest year, different producers, different storage periods) were acquired with a NANQQ-2.5, Ocean Insight (Orlando, FL) NIR sensor and chemometrically evaluated. For the chemometrics, multivariate analysis data analysis was conducted with principal component analysis (PCA), partial least square(PLS) and Response-Oriented Sequential Alternation (ROSA). Reference measurements were carried out according to ISO 3632-2. The results of this preliminary work underline the great potential of implementing the miniaturized NIR sensor technology for the rapid, cost-effective quality control of saffron.

Keywords: Non-Destructive Spectroscopic Sensors (NDSS), miniaturized NIR sensor, chemometrics, ISO 3632-2:2010.

Acknowledgments: The authors thank Krokos Kozanis Producers Cooperative (Kozani, Greece) for kindly providing saffron samples and the SensorFINT COST Action CA19145 "European Network for assuring food integrity using non-destructive spectral sensors" for strengthening the collaboration among our teams.

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Individual authentication of cocoa beans using Vis-NIR spectroscopy

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Cocoa (*Theobroma cacao* L.) and its derived products are appreciated worldwide for their distinctive flavors and health benefits. The quality of cocoa beans is determined by post-harvest processing—mainly fermentation and drying—as well as by the cocoa genotype, which significantly impacts the economic value of the products. Fermentation is vital for high-quality cocoa derivatives. However, common adulteration practices include mixing unfermented beans with fermented ones, driven by cost-saving pressures. Additionally, co-planting of genotypes and seed mixing complicate the identification of genotypes with higher economic value and quality assurance of derived products (Cruz-Tirado et al., 2020). Therefore, robust authentication methods are required to ensure food and economic security for both the industry and consumers. Conventional authentication methods are costly, destructive, labor-intensive, and environmentally harmful. In contrast, Vis-NIR spectroscopy presents a promising non-destructive, rapid, and simple alternative capable of analyzing individual beans in their natural state. This study investigates the efficacy of Vis-NIR in the analysis of individual cocoa beans within a batch, evaluating 400 beans from 19 genotypes, each represented by both fermented and unfermented beans. Vis-NIR successfully discriminated between fermented and unfermented beans. Partial Least Squares Discriminant Analysis (PLS-DA) models targeting specific spectral regions within the visible and NIR spectra facilitated discrimination. Linear Discriminant Analysis (LDA) demonstrated that absorbances at specific wavelengths in both the visible and NIR spectra are adequate for distinguishing between fermented and unfermented beans. Preliminary genotype discrimination results showed promising accuracy. Hence, Vis-NIR spectroscopy could enhance cocoa authentication, providing a scalable and efficient solution to increase industry standards and consumer confidence.

Keywords: *Theobroma cacao*, fermentation, genotypes, authentication, Vis-NIR spectroscopy.

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Spectral Assessment of Adulteration in Ground Pistachio

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Ground pistachio is one of the most common products used in the production of a multitude of desserts in Türkiye. However, the ground pistachio is frequently subjected to adulteration due to high demand and high cost. This is done by mixing ground pistachio with dried green peas and/or spinach, which has unrecognisable organoleptic and colour properties and is cheaper. Furthermore, rapid and on-site detection of the adulteration is not possible using old school techniques such as visual examination. Therefore, chemometric techniques and a low-cost custom-built spectral sensor were used in this study to identify adulteration of spinach and green peas (up to 50% (w/w) adulteration) in ground pistachios. Reflectance spectra of the samples were collected by the spectral sensor with a wavelength range between 410 and 940 nm. A deep sequential neural network model was trained using preprocessed spectra to predict the ratio of adulterations in the adulterated ground pistachios. The results demonstrated that the sensor with the developed model achieved an accuracy of over 80% in predicting the ratio of adulterations in the ground pistachios. The preliminary findings of the sensor under development indicated encouraging results, suggesting that it is feasible and promising to rapidly, non-destructively, and on-site detect potential adulterations in ground pistachios using the low-cost spectral equipment.

Keywords: PCA, ANN, food fraud, chemometrics.

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SESSION 2: Sensor fusion for reaching complex issues in food integrity

Keynote #2: BYOUNG-KWAN CHO

NIR in the agri-food industries: what have we learned and where are we going?

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Food quality and safety, commonplace throughout human history, remains a concern today, with several notable instances involving the agro-food industry. Recent food safety incidents and public health concern related to detrimental food additive issues have driven the need to develop fast, sensitive, and reliable methods to detect food hazards, adulteration and degradation. Here, we assess the applicability of line-scan spectral imaging technique for quality and safety measurement of various food and agricultural materials. In this presentation, the characteristics and applications of spectral imaging techniques, along with the major barriers and limitations, are discussed, with an emphasis on the treatment of spectral data. Spectral imaging techniques have potential to fulfill the industrial need for quality and safety analysis of food and agricultural materials, however, still requires measurement accessories and dynamic chemomatric analytical methods for modern inspection. We believe this discussion will be an effective guide for food and agricultural industry researchers and engineers to aid in the selection of spectral imaging methods to measure quality and safety parameters of food and agricultural products.

Keywords: spectral image, hyperspectral image, food quality, food safety

Detection of peanut fragments in chopped almonds using hyperspectral imaging technology

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Cross-contamination or the presence of unintentional allergens in food products can occur during the production process in the industry. The presence of peanuts in other nuts products takes place in those cases in which different nuts are handled in the same food manufacturing line. This is a major food safety issue to be addressed, given the potential health risk it can have on consumers with allergy to peanuts. In those cases, in which the nuts are chopped and commercialized in small fragments, it is not possible to visually identify whether the fragment corresponds to peanuts or to other nuts. Consequently, there is a need for high throughput techniques to be implemented in the processing lines that enable to discriminate fragments of peanuts from small pieces of other nuts in a fast and non-destructive way. Hyperspectral imaging technology combines conventional imaging and spectroscopy techniques offering both spatial and spectral information from the analysed product which is extremely useful for evaluating individual food items. The aim of this study was to evaluate a hyperspectral imaging system working in the 842-2532 nm range to identify small fragments peanuts in chopped almonds. Partial Least Squares Discriminant Analysis (PLS-DA) was used to develop discriminant models and different approaches were followed: firstly, the mean spectrum per nut piece was calculated to be included in the calibration and validation sets and secondly individual pixels (i.e., spectra) were selected from Regions of Interest (ROI) to carry out the prediction equations. Finally, the calculated models were externally validated using an independent set of samples. Promising results were obtained showing that hyperspectral imaging technology could be a very useful tool to address food safety issues in the nut industry.

Keywords: food safety, allergy, peanut, almond, hyperspectral image.

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Grain-based authentication of bread with hyperspectral imaging for quality control

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As people become increasingly conscious on how food affects their health, misleading consumers with deceptive product labelling could find its way into the market. Bread, for example, is a type of food that can be made from a variety of flours (e.g. wheat, oats, spelt, rye), and there is currently no method for its authentication based on the type of grain used. So, even though some legislation is directed towards bread labelling both in Spain and Europe, there is no way to determine if products are true to their label. Therefore, to combat this problem, this study proposes the use of an environmentally friendly method based on hyperspectral imaging (HSI) to classify bread samples from different grain compositions.

For this study, three types of flours were used to make the 78 bread samples: wheat, spelt and oat. These were analysed using two hyperspectral imaging cameras: one with a spectral range from 400 to 1000 nm (VNIR) and a second camera ranging from 900 to 1700 nm (SWIR). The samples prepared were made with both white and wholemeal versions of each type of flour. After the bread making process, and before analysing the samples, treatment had to be performed, which was done by drying and grinding the samples into small particles. Hyperspectral images were captured, pre-processed and examined via exploratory analysis applying principal component analysis (PCA) and partial least-squares regression (PLS). These were applied to the average spectra from the selected region of interest (ROI) of each sample. Data from the SWIR camera demonstrated a natural clustering of the samples into "wheat" and "not wheat". Lastly, supervised analysis methods such as partial least square-discriminant analysis (PLS-DA) and support vector machine (SVM) were employed to classify samples into classes composed of grain variety (wheat, spelt, and oat).

Keywords: hyperspectral imaging, chemometrics, bread authentication, quality control.

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Laser spectroscopy for monitoring pome fruit respiration

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The postharvest evolution of fruit quality is strongly related to the respiration activity, which depends on the intercellular O_2 concentration. To limit the respiration related quality loss, fruit are stored under controlled atmosphere conditions. However, too low internal O_2 concentrations result in internal browning and the formation of cavities. Therefore, there is a strong interest in postharvest research to monitor the intercellular O_2 concentration in pome fruit. Conventional sensing approaches for O_2 in fruit are invasive and prone to measurement artefacts, limiting their application for pre- and post-harvest monitoring of the oxygen dynamics. Therefore, the aim of this study was to investigate the potential of pathlength calibrated gas in scattering media absorption spectroscopy (GASMAS) in diffuse transmittance mode for non-destructive and quantitative determination of the O_2 concentration in intact pome fruit. Furthermore, we explored the application of GASMAS to determine the gas exchange and respiration dynamics properties of pome fruit.

A custom built pathlength-calibrated GASMAS O_2 sensor was used to quantify the intercellular O_2 concentration in an intact apple and pear fruit during dynamic experiments. Next, the measured O_2 profiles were fitted with a lumped respiration-diffusion model to estimate the effective mass transfer coefficient, maximum respiration rate and Michaelis Menten constant of intact fruit.

The average O_2 level in intact apples and pears under ambient conditions at room temperature was found to be considerably lower than the ambient O_2 concentration with clear differences among the studied cultivars. After optimization of the model parameters the simulated O_2 profiles matched well with the measured O_2 profiles and the uncertainty on the estimates for the gas exchange and respiration parameters was low. This demonstrates the potential of GASMAS in transmission mode for non-destructive monitoring of the intercellular O_2 concentration in intact fruit and estimating the gas exchange and respiration properties of porous fruit.

Keywords: tunable diode laser absorption spectroscopy, pathlength calibration, oxygen, pome fruit, respiration, diffusion.

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Hyperspectral imaging as a non-invasive tool to evaluate pathogen's growth behaviour: effect of image pre-processing

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Safety of dry-cured ham might be compromised by the salt content variability of the production. The combination of predictive microbiology models, which uses as input the food product temperature, the a_w (measured using hyperspectral imaging (HSI) systems) and the pH, could help to non-invasively evaluate its safety. The aim of this work was to evaluate feasibility of HSI to predict a_w as well as the effect of image pre-processing (using image segmentation at different thresholding values) on the prediction of the *S. aureus* growth probability at room temperature in sliced dry-cured ham. The calibration model for the prediction of a_w was developed using Partial Least Square Regression after scanning the samples (n=411) using a HSI system (wavelength range of 400-1000 nm) and analysing them using Aqualab. Dry-cured ham slices manufactured using standard and reduced salting procedures (n=66) were scanned using the same HSI system. Different thresholding values for image segmentation were applied to remove the fat areas and streaks of the image. Chemical images and histograms of predicted a_w were calculated and the a_w values at different percentiles determined. Finally, the growth/no growth boundary model for *S. aureus* at room temperature (21ºC) developed by Borneman et al., (2009) was applied. The developed model can predict the a_w with a predictive error of 0.013 and R^2 of 0.933. The image segmentation applied was able to identify and remove those pixels corresponding to fat streaks and specular highlights artifacts. However, the different thresholding values did not significantly affect the distribution of the a_w values obtained ($p>0.05$). Only when segmenting resulted in the removal of a high number of pixels, a_w at different percentiles were slightly higher than for other segmentation levels. Therefore, the more intense cleaning of the image the more conservative a_w values, although these differences on a_w did not affect pathogen growth probability and thus, they are not relevant from a food safety perspective. In conclusion, HSI in combination with predictive microbiology is a useful tool to non-destructively evaluate microbiological safety of sliced dry-cured ham.

Keywords: dry-cured ham, predictive microbiology, food safety, *S. aureus*, chemical images.

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Optical detection of mold growth on apples

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This work investigated the suitability of optical non-destructive methods such as hyperspectral imaging (HSI) and optical coherence tomography (OCT) for detecting P. expansum growth on apples. Treated and control apple samples of 'Golden Delicious' and 'Evelina' cultivars were monitored with HSI and OCT during incubation until the occurrence of the mould. After image processing, we classified mould in an image using a support vector machine (SVM) algorithm.

Analysis of the hyperspectral images provided different spectra of the infected and control samples. Using a support vector machine (SVM) algorithm, we successfully classified moulds in images of Golden Delicious from day three onwards (using a wavelength of 495,9 nm). The application of SVM to Evelina cultivar was less successful (using 403,09 nm and 847,25 nm).

We observed distinct changes in the apple's microstructure using OCT images during mould growth. Mold activity affected the necrotic area's expansion and the apple's microstructure through invasion, which affected the sample's light-scattering properties. OCT proved to be more effective for the early detection of mould, detecting mould growth on both cultivars on the first day of incubation. We found that mould growth was slower on the 'Evelina' cultivar, although the characteristics were similar for both cultivars.

Optical imaging techniques in this study yield complementary information about mould growth: HSI, the chemical, and OCT, the structural information. By combining both of them more complete information about the growth is obtained. The same approach can also be applied to other food samples where mould growth is present.

Keywords: apples, mold, decay detection, hyperspectral imaging, image processing, optical coherence tomography.

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Preliminary comparison between using Mid-Infrared (MIR) and Raman spectroscopy with chemometrics to predict the gel onset of raw bovine milk samples

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Gelation represents one of the fundamental functional properties of milk, under-pinning a variety of commodity products. The robust prediction of the gel onset of bovine milk would facilitate more sustainable and cost-efficient cheese manufacture for dairy processors, as milk suitable for various products could be identified earlier in the production process (Visentin et al., 2015). At present, MIR spectroscopy is being used to predict compositional properties of milk in industry. However, predicting functional properties such as gel onset would contribute to increased adoption of an agile manufacturing approach in milk processing. This study presents a comparison between MIR and Raman spectroscopy to predict gel onset. Raw milk samples were supplied by 7 dairy processors in Ireland over the period January 2021 to May 2023. This research used 830 samples with gel onset reference measurements obtained using a Discovery HR-S rheometer. The rennet used was Chy Max-Extra (Novonesis). The spectroscopic data was taken with a DairySpec FT (Bentley) milk analyser and an i-Raman Plus 785S Portable Raman (Metrohm) spectrometer. Removal of spectral noise, Principal Component Analysis (PCA) and Partial Least Squares (PLS) regression were used to create predictive models. The best prediction using MIR gave an RMSEcv of approx. 125 s using 6 Latent Variables (LV) and 1st derivative preprocessing. The best prediction using Raman spectroscopy gave an RMSEcv of approx. 132 s using 8 LV and 1st derivative and Standard Normal Variate (SNV) preprocessing. These preliminary results show that MIR spectroscopy gives a lower error for the prediction. Further analysis will include various validation studies.

Keywords: Spectroscopy, dairy, predictive modelling, PCA, PLS

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SESSION 3: Data management tools for processing and modelling

Keynote #3: FEDERICO MARINI

Present and future trends in chemometrics for spectral data

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The communication aims at providing an overview of chemometric strategies and tools that can be relevant for the analysis of spectral data and to identify what the main lines of development could be for the foregoing years. Some of the topics that will be covered are: the use of high dimensional ANOVA models such as ANOVA simultaneous component analysis (ASCA) (Smilde et al, 2005), or ANOVA target projection (ANOVA-TP) (Marini & Walczak, 2020) for identifying and interpreting the effect of controlled factors on the multivariate spectroscopic profile; how to implement non-linear models that, at the same time can be straightforwardly interpretable and robust; how to integrate the data from different spectroscopic platforms through data fusion approaches (Mishra et al., 2021) and possibly how to implement non-linear strategies in that context; how to more effectively deal with the need for data preprocessing (Mishra et al., 2020).

Examples taken from the authors' own experience and from the literature will be used to illustrate the above-mentioned topics and possible future scenarios will be sketched.

Keywords: chemometrics, non-linear modeling, data fusion, analysis of variance, variable selection, calibration transfer.

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A multispectral NIR/UV-Vis approach to discrimination between subvarieties of arabica coffee: variable selection, non-linear classifiers,artificial neural networks and data fusion

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Coffee has emerged as one of the most widely consumed beverages globally, valued for its flavor and cultural significance. Given the intricate market dynamics, substantial demand, and complex supply chains inherent in the coffee industry, the sector is particularly susceptible to fraudulent practices, including mislabelling and adulteration. This susceptibility is further exacerbated by the differential valuation among coffee varieties, with high-quality beans often fetching premium prices due to their scarcity and unique flavor.

Coffea Arabica is a highly valued commodity in particular, and is therefore prone for mislabelling and counterfeit. In this context, the present study aimed to assess the utility of NIR and UV-Vis spectroscopy for discriminating between the primary Arabica coffee varieties, Typica and Bourbon, their natural crossing, Mundo Novo, and several of their prominent sub-varieties. The investigation encompassed an array of specialty coffees sourced from diverse origins, providers, processing methods, and roasting levels.

NIR measurements were conducted using both benchtop FT-NIR (10,000–4,000 cm^{-1}; 1,000–2,500 nm) and portable Vis-NIR (28,570-4,000 cm^{-1}; 350–2,500 nm) spectrometers, while UV-Vis spectroscopy involved the preparation of aqueous coffee extracts for transmission measurements. Spectral data were subjected to comprehensive analysis and interpretation, employing various chemometric techniques such as Median Linkage Clustering, Linear Discriminant Analysis, SVM, K-Nearest Neighbour, and Subspace KNN Ensemble classification methods.

Furthermore, the study explored the potential of ANN models for precise differentiation between Arabica coffee varieties. Additionally, advanced data fusion techniques, including Low-Level Data Fusion (LLDF), Mid-Level Data Fusion (MLDF), and Variable Selection (VS), were employed to enhance feature representation and improve the discriminatory power of the analysis.

Keywords: NIR, UV-Vis, multispectral, coffee arabica, authentication, data fusion, artificial neural networks (ANN), variable selection

AI-boosted artificial spectral pipeline augments chemometric models and improves performance in real world applications

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Studies based in vibrational spectroscopy involve rapid determination of a food property and rely on chemometric data analysis. Original food samples are therefore required to build calibration models. The number of calibration samples used is relatively low because of availability, cost, and hardship to obtain truly authentic samples. This is in contrast with the chemometric techniques which perform better with larger sample-sets. As a result, there are many studies featuring only 10-50 original samples and yet claiming to produce general models. With the help of modern AI-driven approaches, our aim is to enhance the prediction power of a calibration model, starting from a limited number of original samples, by adding artificially generated spectra from a data augmentation pipeline, firstly developed in our previous work (Georgouli et al., 2018). This involves 4 modules: spectral intensifier, x and y shifter, and a gaussian noise generator. The open source dataset was composed of FT-IR spectra from cow's milk divided into 3 classes depending on the diet of the animals. The real dataset (3200 samples) was used as a benchmark. From there, a randomly selected reduced sample set (240) was created and formed the baseline of the prediction. The AI boosted sample-set consisted of these 240 samples and another 2160 artificial spectra generated from the augmentation pipeline with careful tuning. After calibration, the models were validated with their respective independent sets consisting of only true samples. Results show that the AI boosted model significantly improved the accuracy of the reduced samples model, consistently improving performance in all classes involved and in both cross validation (30% better) and external validation exercises (9% better). As the augmentation procedure involves recycling of information included in the samples, its value cannot outperform the value of having more original real samples yet achieving 96% of the real full sample model's accuracy.

Keywords: augmentation, artificial intelligence, chemometrics, multivariate analysis, food analysis, prediction.

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Beet & Cane Sugar Classification by Using NIR Spectroscopy and Chemometrics

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Sucrose is one of the main ingredients used in sugar industry. Worldwide sucrose is produced from two different sources, sugar beet and sugar cane. However, different sources have been dominating the market due to governmental policies. So, it is important to understand the source of the sugar in the market. Since molecular structure of sucrose is same, it is difficult to differentiate sources by using chemical methods. Therefore, developing more practical and affordable methods would be valuable for food industry. NIR spectroscopy is a promising technique that can detect the differences in the plant base and production steps in a non-destructive manner (Morellos *et al.*, 2016). In this research, sucrose samples from different plant sources (cane, beet) were collected from 12 countries to prepare crystal sucrose samples and their absorbances were recorded between 1000-2500 nm. Measurements were directly taken from sucrose crystals as they were collected from local markets. Results showed that in all regions spectral signature differences were observable. First a PCA with 2 components was conducted to have an exploratory analysis then prediction algorithms were used. It is known that improving the prediction accuracy requires chemometric approaches such as spectral preprocessing and k-Nearest-Neighbor (kNN) (Fetitah et al., 2021). The results indicate that several methods showed high performance, but kNN gave 97% correct classification with 10 fold cross-validation. The obtained results seemed promising that the plant source of sucrose can be detected by using NIR region and chemometric methods.

Keywords: sucrose, sugar cane, sugar beet, NIR spectroscopy, chemometrics.

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Breaking Spurious and Systematic Correlations by Augmenting Datasets

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Recent advances in infrared spectroscopy have significantly enhanced food quality assessment and safety monitoring, which are vital in the food industry. Predictive models, however, often perform poorly across different operational conditions (e.g. in varied research groups) due to biases introduced by environmental and instrumental variations. These biases can lead models to establish spurious and/or systematic correlations that compromise their utility across different experimental conditions. Traditional preprocessing techniques are typically limited to correcting known, quantifiable variations and may not adequately address more complex or unrecognized discrepancies. Moreover, designing preprocessing methods to handle numerous variations can become overly complex, risking the loss of useful information when attempting to eliminate unwanted variation. This presentation discusses the application of data augmentation techniques, such as Extended Multiplicative Signal Augmentation (EMSA) (Blazhko et al., 2021), to enhance the robustness and generalizability of spectroscopic models. These techniques, including EMSA, broaden the range of conditions represented in training datasets, thus enhancing the predictive accuracy and reliability of models in practical applications like dairy farming. Notably, deep learning methods usually benefit more from these augmentation techniques than classical machine learning models, given their capacity to learn complex patterns from larger and more varied datasets. By applying these methods, we aim to enhance the robustness of models in uncontrolled environments, thereby broadening their application across varied research groups and conditions, and increasing their overall practical utility.

Keywords: infrared spectroscopy, data augmentation, model robustness, generalization, dairy farming.

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Exploring Apple Diversity: Non-destructive Spectroscopic Analysis and Chemometric Insights

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This study centers on analysing apple samples from two different varieties and origins. The objective was to devise an analytical method capable of distinguishing between variety and origin using non-destructive spectra sensors. The samples underwent analysis utilizing a UV-Vis-NIR benchtop spectrometer, a portable NIR device, and a confocal micro-Raman instrument. Initially, optimal spectral pre-processing methods were determined for each technique to eliminate instrumental noise, fluorescence background, scattering, and baseline drift. The collected spectra were utilized to construct exploratory models employing PCA and ASCA methodologies. PCA facilitated the identification of differences among samples of various varieties and origins, emphasizing distinctions in coloration (attributed to sun exposure) and preservation levels. ASCA was employed to evaluate the significance of variety and origin factors, confirming their influence for both NIR and UV-Vis techniques, while Raman analysis demonstrated significance only for variety. Subsequently, the PLS-DA classification method was employed to predict the variety and origin of apple samples, yielding promising outcomes for Raman-based variety prediction and satisfactory performances for NIR- and UV-Vis-based variety and origin prediction. The spectral data obtained from different techniques were further evaluated collectively using a low-level data fusion approach, incorporating exploratory PCA and PLS-DA classification to assess variety and origin separation and classification. Fusion models yielded the most favorable classification results, achieving 100% sensitivity and specificity for both variety and origin classification. UV-Vis and NIR techniques exhibited promising results for distinguishing variety and origin, whereas Raman's effectiveness was limited, potentially due to suboptimal instrumentation for this particular application. The utilization of a portable NIR instrument for analysis shows promise in monitoring quality and ensuring geographical traceability throughout the production process. Furthermore, the study demonstrates how a data fusion approach can enhance the performance of classification models.

Keywords: apples, traceability, portable instruments, data fusion

Exploring CNN architectures for dry matter prediction on a multi fruit NIR data set

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A recent review about deep learning algorithms applied to NIR spectra to predict fruit internal quality parameters (Walsh et al., 2023) highlights Convolutional Neural Networks (CNN) as one of the most promising algorithms to build chemometric models for this type of task.

In this work we present a pipeline aimed at optimizing CNN architecture design to produce global chemometric models for fruit dry matter (DM) estimation. This pipeline involves testing various designs and optimization strategies to achieve generic CNN models that are robust against data fluctuations. The CNNs global models (trained on a multifruit dataset of NIR spectra of apples, kiwis, mangoes and pears) are compared with other chemometric techniques such as PLS and Locally Weighted PLS. The optimized CNN models perform better than global PLS and LW-PLS and even surpass individual fruit PLS models. CNNs show strong performance and generalization for NIR-based dry matter estimation across diverse fruits (Passos & Mishra 2023).

Keywords: Fruit dry matter, Chemometrics, Deep learning, NIR spectroscopy

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Implementing pre-trained open AI models for near-infrared spectroscopy applications

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Artificial intelligence (AI) methods such as deep learning are becoming popular in different domains of sciences. Several models such as convolutional, generative, time series etc. are now available open source to adapt and develop new applications. Near-infrared spectroscopy is also an area which can benefit from open AI models, for example to simplify tasks such as object detection, generative predictive modelling, and feature extraction. This presentation will cover different successful implementation of open AI models for dealing with NIR data. Focus will be NIR imaging data. Cases such as object detection in complex scenarios, generative modelling for predictive modelling, fusion of spatial and spectral information will be demonstrated.

Keywords: GAN, resnet, chemometrics, fusion

Targeted iPLS for the prediction of cheese-making traits from individual milk FTIR spectra

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Cheese yield and nutrients recovery in the curd are crucial metrics for cheesemaking efficiency. Traditionally, predictions of cheese-making traits rely on time-consuming compositional analysis (Emmons & Modler, 2010). This work explores a faster and non-destructive method to predict these traits using Fourier-Transform Infrared (FTIR) spectroscopy. Milk samples from 1,080 cows were collected between February 2021 and April 2022, used for composition and spectra collection using a FTIR spectrophotometer (Milkoscan FT3, FOSS), then for cheese production using a cheese-making lab procedure (Cipolat-Gotet et al., 2013). Models were developed using 10-fold cross-validation to correlate FTIR spectral data with cheese-making traits. Targeted iPLS selected the spectral regions associated with milk components: 3700-3052 cm^{-1} and 1700-1586 cm^{-1} to water, 2970-2800 cm^{-1} and 1770-1720 cm^{-1} to fat, 1600-1420 cm^{-1} to protein and 1300-1000 cm^{-1} to lactose, respectively. Targeted iPLS also selected the optimal pre-treatments (SNV, MSC, centering, scaling) and derivatives (1^{st} or 2^{nd}). Moreover, residuals from a mixed model including herd and cow-related factors were used as corrected cheese-making traits to be predicted. The best combination (spectral region + pre-treatments) for each trait was identified based on the coefficient of determination in validation and residual predictive deviation (R^2_{VAL} and RPD). The targeted iPLS yielded promising results, with good R^2_{VAL} (from 0.50 to 0.90) and RPD (from 1.72 to 3.23 for cheese yield, and from 1.42 to 2.15 for nutrients recovery in the curd). The use of corrected cheese-making traits resulted in a slight decrease in the prediction error, but also in the R^2_{VAL}. Importantly, targeted iPLS reduced overall computation time and offered trait-specific calibrations. This technique could be used to study the contribution of the selective spectral range on the prediction of a wide variety of phenotypes, validating or refuting earlier studies on the removal of the water region for the prediction.

Keywords: FTIR, cheese-making, wavelength selection, spectral treatment, multivariate analysis.

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Detection of invisible damages in plums with deep learning

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Plums, such as the 'Presenta' cultivar with yellow flesh and dark purple skin, can sustain hidden damages during harvest and transportation, potentially leading to decay and significant losses in the supply chain. Detecting these damages early is crucial, as they are internal and hence invisible to the human eye. For this study, 375 'Presenta' plums were sourced from a local Belgian producer and split into two lots corresponding to different weeks. The fruit was stored at 6 °C and 80 % relative humidity until 24 hours before each experiment when it was moved to room temperature (20 °C). Bruising was induced using a pendulum. The impact energies varied with three different angles: soft (20°), medium (30°), and hard (40°). Hyperspectral images were then acquired at 0, 24, and 48 hours after bruising, using a hyperspectral line-scan camera (400 to 1,000 nm). Wavelength selection identified ten key wavelengths. Three different Deep Learning models were used: an HSCNN proposed by Varga et al. (2021), ResNet and a custom 3D-CNN. Models were trained using all wavelengths, ten selected wavelengths (621, 661, 680, 686, 694, 705, 735, 822, 884, and 985 nm), 3 wavelengths (985, 822, and 705 nm) and one wavelength (985 nm). HSCNN excelled, achieving a 90 % F1 score using full spectral images. Notably, models using the most important three wavelengths demonstrated comparable performance with F1-scores exceeding 86 % in all cases, highlighting HSCNN with 89 %, with shorter training times.

Keywords: bruise, invisible, hyperspectral, deep learning

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Investigating the Effect of Refining Time on Dark Chocolate Particle Size Using NIR Spectroscopy

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The refining process in chocolate manufacturing plays a critical role in reducing particle size (Rohm et al., 2018), with shear stress and pressure from the machinery contributing significantly to particle breakage (Khajehesamedini et al., 2021). This study investigated dark chocolate refining using near-infrared (NIR) spectroscopy to assess how different refining durations influence the particle size. During an eight-hour refining period, spectral data was collected every 15 minutes using both handheld and benchtop NIR devices. Spectral data for both devices showed the presence of two principal components (PC1 and PC2) indicating distinct trends in refining time that correspond to variations in particle size, with PC1 and PC2 representing different dimensions of variation in the spectral data. Partial least squares (PLS) regression models, incorporating a combined principal component analysis (PCA) approach, were developed to predict refining times based on standard normal variate (SNV) and mean-centered pre-treated spectra from both devices, employing Venetian blinds cross-validation with 14 splits. The two models generated were compared based on the root mean square error of prediction (RMSEP), coefficient of determination in prediction (R^2_{Pred}), and a ratio of performance to deviation (RPD). The benchtop device had a lower RMSEP (6.2 µm) and higher R^2_{Pred} (0.97) and RPD (4.89) when compared to the RMSEP (6.44 µm), R^2_{Pred} (0.96) and RPD (4.68) of the handheld device. Although these results indicated higher accuracy for the benchtop device, it obtained a larger prediction bias of 2.38, compared to 1.83 for the handheld device. This work illustrates the potential of using NIR spectroscopy as a process analytical technique for monitoring refining during chocolate manufacturing.

Keywords: Refining, Dark Chocolate, Particle Size, Chemometrics.

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A Hyperspectral Inspection System to Classify Corks Surface Treatments Homogeneity

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Oxidation variability, which may occur during bottle aging of white wines, impacts the perceived sensory quality of the product. The primary factors driving oxidation in bottled wine can be categorized into five classes: (i) wine matrix, antioxidant fraction; (ii) wine bottling process; (iii) bottleneck variability; (iv) surface treatments at the cork-glass interface; and (v) Oxygen Transmission Rate (OTR) through the natural cork (Ferreira et al., 2023). These factors are greatly amplified by time, temperature, pH, and bottle position during storage.

To address the inherent variability in natural cork stoppers, the selection and application of the coating are critical steps in cork production. The homogeneity of the polymer distribution on the body of the stopper is crucial for the proper sealing of the bottle neck-cork interface, namely between the glass and the cork (González-Gaitano & Ferrer, 2013). Therefore, tools are needed to monitor the proper distribution as well as the thickness of the coating.

In this study, cork stopper samples are classified based on whether they are coated with a treatment (Bopsil or CAF) or not coated using hyperspectral imaging. The cork coating heterogeneity is evaluated using hyperspectral imaging to investigate which coating application method, a stationary or a movable pneumatic pistol, allows for lower coating heterogeneity on the cork surface. PLS-DA on hyperspectral images of the corks showed that there is more coating heterogeneity when applied with a movable pneumatic pistol method than with the fixed pistol. There is also greater heterogeneity achieved using the CAF treatment than the Bopsil treatment. This is advantageous for the industry as they can potentially alter their coating material and application method to achieve greater coating homogeneity on their cork samples.

Keywords: Hyperspectral Imaging, Oxygen transmission rate (OTR), Cork stoppers, Coating

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Can Near-Infrared Spectroscopy (NIRS) Be Used for Rapid Discrimination of Fresh Eggs with Different Infection Statuses?

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Helminth infection is one of the most prevalent and important diseases of laying hens in free-range systems, which is associated with reduced nutrient supply, immunity, and egg production. It can further affect egg quality according to the different resistances of breeds (Stehr et al., 2019). This study aimed at evaluating the capability of near-infrared spectroscopy (NIRS) to discriminate eggs from German local chicken breeds in different infection statuses (three breeds × two infection statuses). Hens at 59 weeks of age (Altsteirer n = 56, Bielefelder n = 42, and Ramelsloher n = 61) were divided equally into two groups: control and treatment. A total of 125 eggs were collected from six groups on experiment weeks 0, 2, 4, 6, and 8, respectively (3-5 eggs/group/day). Hens from the treatment group were infected with *Ascaridia galli* artificially after the first collection, while the control group did not receive any treatment. The NIR spectra of fresh egg albumen and egg yolk were recorded in transflection mode using a FT-NIR benchtop with a wavenumber range from 11536 to 3952 cm^{-1}. The classification model was developed using the partial least squares discriminant analysis (PLS-DA) and assessed by confusion matrices in stratified k-fold cross-validation. It was revealed that the Matthew´s correlation coefficients (MCC) value of infection discrimination models is only 0.2 on both egg albumen and egg yolk samples. On the other hand, the breed discrimination accuracy using egg yolk (0.8) is higher than that using egg albumen (0.4). The specificity of yolk models for three breeds is 0.89, 0.90, and 0.90, respectively. The results of this pilot study indicate that eggs with different infection statuses can be poorly discriminated using NIRS combined with PLS-DA. By contrast, eggs from different breeds can be well classified based on fresh egg yolk spectra.

Keywords: layers, egg yolk, egg albumen, traditional breeds, discrimination model

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Comparative study of Raman and Near Infrared (NIR) spectroscopy to detect Pork Adulteration in Meatballs

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Halal assurance has been extended into food quality standards, especially in Indonesia. However, some food producers replace the food composition with cheaper and non-halal ingredients to reduce the production cost or gain the taste of food without considering food safety and prohibition to consumers. Pork adulteration in meatballs has become a halal issue in the Indonesian food industry. The detection of this adulteration mainly relies on Real-Time PCR (RT-PCR) as a standard technique for halal certification to check the presence of pork and its derivatives on food products. The method is accurate but expensive and requires complex procedures, which makes it unsuitable as a screening method. Vibrational spectroscopy methods including Raman and Near Infrared (NIR) spectroscopy are widely studied as fast screening methods in the food industry assessment. Therefore, the aim of this study was to investigate the potential of Raman and NIR Spectroscopy to detect adulteration of meatballs with pork meat. Two sample groups were prepared comprising adulterated (beef meatballs with 3, 5, 10, 50, and 100% pork adulteration) samples in triplicate and non-adulterated (100% beef meatballs) samples in 10 replications, resulting in 125 total samples. Intact and cross-section samples were measured in reflectance mode. Partial least squares discriminant analysis (PLS-DA) was used to classify between adulterated and non-adulterated meatballs. Around 2/3 of the total samples were allocated for calibration with the remaining 1/3 for an independent test set. Raman spectra showed pronounced peaks around 1657 cm^{-1}, 1443 cm^{-1}, and 1299 cm^{-1} which correspond to the fat and fatty acid. As for NIR spectra, detectable peaks of fat and lipids appeared at 1732 nm and 2312 nm. It was found that the accuracy in pork meat adulteration detection was higher for Raman spectroscopy (82.5%) than for NIR spectroscopy (75.0%). Most misclassifications were found on adulteration below 50%.

Keywords: Pork adulteration, Meatballs, Raman spectroscopy, NIR spectroscopy, PLS-DA

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Development of Chemometric strategies for quality Control in Breast Milk

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Breast milk is the main source of nourishment for humans, containing essential nutrients and bioactive compounds crucial for the growth of newborns. Although it's commonly understood that a mother's milk provides the best nutrition, there are situations where this is not feasible. Hence, the establishment of milk banks within hospital neonatology departments is advocated to address such situations. However, a significant challenge lies in ensuring that the breast milk provided from these banks meets the nutritional requirements of neonates. Currently, laboratories utilize costly, specialized milk analyzers manned by skilled technicians to assess milk quality. An emerging solution involves the adoption of portable Near Infrared devices for real-time monitoring of milk quality, offering on-site efficiency and timely quality control (Fusch, 2017).

Previous research has shown that portable Near Infrared Spectroscopy (NIRS) systems are effective in quantifying nutrients in pasteurized donated human milk (Melendreras et al.,2022). However, these milk samples, typically stored frozen, need to be thawed before analysis. This study aims to evaluate the effect of sampling on the development of calibration models. To achieve this, samples of pasteurized donated human milk were analyzed in both liquid form at 37°C (optimal temperature) and frozen states, stored in their original containers or in alternative storage methods such as plastic bags. The collected data are incorporated into a multi-block dataset, forming the foundation for chemometric analysis.

Keywords: breast milk, sampling, multiblock analysis

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Discrimination of Normal and Wooden Breast Chicken Fillets Using NIR, fluorescence, and Raman Spectroscopy

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Wooden breast (WB) syndrome adversely affects commercial meat-type chickens, and result in hardened and pale fillets, with lowered meat quality and unpleasant sensorial characteristics. This issue is caused by a replacement of the muscle fibres with water, adipose and connective tissue, affecting the welfare of the bird (Petracci et al., 2019). Spectroscopic methods, including near-infrared spectroscopy (NIRS), have previously shown capacity for discriminating WB from normal breasts (NO) (Wold et al., 2019). In this study, the differences between NO and WB are explored by fluorescence and Raman spectroscopy and results are compared with NIR.

In total, 80 skinless and boneless breasts (40 NO, 40 WB) were randomly chosen from a commercial slaughterhouse by an experienced veterinarian. Measurements included NIRS (780 – 1080 nm), fluorescence emission (350-580 nm) after excitation at 330 nm, and Raman (100–3250 cm−1, 50s of exposure moving the sample).

WB measured by NIR showed a shift on the 980 nm absorption peak toward shorter wavelengths, indicating lower protein-bound water relative to normal samples (Wold et al., 2019). Fluorescence and Raman spectra reflected other known characteristics of WB, including lower protein content and higher collagen and lipid content. Specifically, fluorescence peaks aligned with known collagen and adipose tissue emission wavelengths and were registered higher for WB compared to normal. This aligns with the presence of a thickened connective tissue and infiltrated adipose tissue in the muscle of WB. Raman provided general lower signals in protein-associated bands and higher in lipid-associated bands in WB. Additionally, signals related to collagen could be observed in the spectra. Overall, fluorescence and Raman provide additional biochemical information compared to NIRS, that can be used to characterize and better understand WB myopathy, as well as potentially assess WB non-invasively in chicken fillets in an industrial environment.

Keywords: Woody breast, poultry, collagen, NIRS, Raman, fluorescence

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Non-destructive and rapid discrimination of carob adulteration in cocoa powders using NIR and MIR spectroscopy

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The adulteration of cocoa products with carob represents a significant challenge in the chocolate industry due to its economic impact and implications for product quality and consumer health. Carob, a leguminous plant native to the Mediterranean region, shares similarities in appearance and chemical composition with cocoa, making it an attractive adulterant. Economic factors, including fluctuating cocoa prices and the increasing demand for chocolate, contribute to the incentive for adulteration. Various analytical techniques, including chromatography, spectroscopy, and DNA analysis, have been employed to identify carob adulteration accurately. Vibrational spectroscopy techniques, including NIR and MIR, can be a suitable method to detect carob adulteration in cocoa powders. A total of 105 samples were collected. Carob was grounded by using a coffee grinder after removing its shells and seeds. Cocoa and carob powder mixtures were prepared as binary mixtures with a carob percentage of 0-60% (1% intervals) by weight. The spectra of the samples were collected by a benchtop and a portable NIR, and benchtop FT-IR spectrometers. Partial Least Squares-Discriminant Analysis (PLS-DA), and Soft Independent Modelling of Class Analogy were used to classify pure and adulterated samples. Moreover, the Partial Least Squares Regression method was used to determine the adulteration level of cocoa powders in binary mixtures. PLS-DA, and SIMCA provided 100% accuracy for classification of pure samples with inter-class distance (ICD) over 3. The spectroscopic units also showed superior performance in predicting adulterant levels with r_{Val}>0.99, standard error of prediction (SEP) < 2.5%. FT-IR and NIR units can be used as alternative methods to traditional methods and showed great potential for real-time surveillance to detect carob adulteration in cocoa powders.

Keywords: cocoa, carob adulteration, NIR, FT-IR, chemometrics

Effect of different Temper Regimes on the Polymorphic Behaviour of Dark Chocolate using Near-infrared (NIR) spectral data

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Dark chocolate, consumed worldwide, comprises sugar and cocoa particles embedded within cocoa butter (Peyronel & Pink, 2021). Achieving a high-quality product necessitates precise manufacturing practices, particularly tempering. This process involves controlled melting and cooling of chocolate, to acquire the appropriate crystalline form of cocoa butter (Peyronel & Pink, 2021). The βV polymorphic form of cocoa butter is desired and promotes favourable sensory characteristics in chocolate such as a pleasing mouthfeel, good snap, glossiness, stability and resistance to fat bloom (Häupler et al., 2014; Peyronel & Pink, 2021). This research investigates how different temper regimes influence the polymorphic form of cocoa butter in dark chocolate, using near-infrared (NIR) spectroscopy for analysis. Experiments involved producing dark chocolate samples under various temper conditions (under-tempered, well-tempered, over-tempered and untempered). Using a Viavi handheld MicroNIR device, spectra from molten chocolate samples were collected post-tempering. Partial least squares discriminant analysis (PLS-DA) models were then developed for classifying samples based on tempering status. The most accurate model used six latent variables (LVs) and spectral pre-treatment with external parameter orthogonalisation (EPO) and mean-centering. Validated through full-cross validation a minimum root mean square error of cross-validation (RMSECV) of 0.146 was achieved. The model demonstrated high sensitivity and specificity values, with 100% accuracy for untempered classes, indicating near-perfect classification. Sensitivity for over-tempered samples showed 85% accuracy, due to some misclassified samples. NIR spectroscopy, in conjunction with chemometrics, could be a valuable analytical tool for monitoring the tempering process during chocolate manufacturing, contributing to the enhancement of chocolate quality.

Keywords: chemometrics, chocolate, classification, NIR, PLS-DA, tempering

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Adjustable Lab Sample Divider

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Sample dividers split particulate bulk material into representative subsamples. Field sampling or harvesting experimental plots in agricultural studies often produces samples that are much larger than the sample volume that can actually be measured in lab analyses. The feasible total number of measurements is typically limited. Field samples may also need to be split into several representative subsamples for different chemical analyses. With respect to Non-Destructive Spectroscopic Sensor (NDSS) calibration, the actually measured volume for the NDSS may differ about an order of magnitude from the actually measured volume of reference analyses. Being able to prepare small, but still representative, subsamples is required in all these situations. The Theory of Sampling (Gy, 1992) guides representative (sub)sampling. Some recommendations, such as reducing particle size e.g. by grinding, however, are not possible in applications that require non-destructive treatment of the sample. Commercially available sample dividers can help; but they work most efficiently with spherical particles of the maximum diameter the divider is constructed for. For materials such as caraway or aniseed with elongated shape and stem, the commercially available sample dividers are considerably less efficient. In addition, they can be adapted to particle size only in a limited way (if at all).

We present a sample divider that is adjustable to different particle sizes, works with elongated shapes or seeds with stem and provides small increment sizes without compromising the correctness of the splitting procedure. Our sample divider uses a mini-conveyor belt to form a material stream of small cross section from the bulk sample and splits a given fraction of material off the bulk. The design can easily be extended to split off multiple samples (providing replicate portions). Another minor modification allows preserving increments and thus facilitating variographic analysis to obtain more detailed insight about segregation in the bulk.

Keywords: sampling, sample division, Theory of Sampling.

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SESSION 5: Innovation and future trends in the use of NDSS and its industrial implementation: AI, sampling, non-targeted approaches, decision support system, digital labelling, interoperability

Keynote #4: Vincent Baeten[1]

Advances and challenges for NDSS in food and agriculture: this is just the beginning!

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With the implementation of the 4th industrial revolution and the onset of the 5th industrial revolution, the utilisation of Non-destructive Spectroscopic Sensors (NDSS) has become a reality and is expected to play a pivotal role in our future enterprises and industries. This trend is further reinforced by our society's shift towards more environmentally friendly solutions, with increasing interest in Green Analytical Technology (GAT).

NDSS have demonstrated promising results in determining and monitoring quality parameters for complex matrices and ensuring product integrity. They facilitate the simultaneous acquisition of in-situ, spatial, temporal, and spectral (and therefore chemical) information characterizing the samples or process under investigation.

The achievements of Non-destructive Spectroscopic Sensors (NDSS) in assessing the integrity of the food chain are noteworthy. NDSS has revolutionized the food industry by offering rapid and non-invasive methods for quality assessment, allowing for real-time monitoring from farm to fork. NDSS can analyse the nutritional content of food items but also detect contaminants and adulterants. This is crucial in our effort to ensure the quality, safety and authenticity of food products.

What are the current trends, advances, and challenges for NDSS in food and feed chains, particularly regarding on-field and industrial adoption? Progress from industrial players, equipment manufacturers, and the scientific community has yet led to significant advancements. However, the work is not complete, and numerous challenges remain to be addressed.

Keywords: NDSS, quality, safety, authentication, challenges, food integrity

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Multiway approach to milk coagulation using MicroNIR

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Grana-type cheese production is an artisanal process influenced by cheesemaker's skills. In this process, poor standardization of stages occurring in the coagulation vat can lead to decreased cheese yield and lower final product quality. This work proposes a method based on near-infrared (NIR) spectroscopy that can be used for on-line milk renneting monitoring to support cheesemakers reducing non-conformities in Grana-type cheese production. Twenty-nine renneting batches were set up according to a full factorial design using milk skimmed by natural creaming at different acidification levels (obtained adding different volumes of natural whey starter), different coagulant concentrations, and different kinds of coagulant (1 calf rennet and 2 microbial coagulants). Temperature was maintained at 35°C and coagulation was monitored with both mechanical lactodynamograph (LDG), as reference method, and portable NIR spectrometer (MicroNIR, Viavi Solutions) mounted on a food-grade probe suitable for immersion in coagulation vat. Full NIR spectra (125 wavelengths ranging from 908 to 1676 nm) were recorded continuously with 13.5 seconds interval for more than 30 minutes after coagulant addition obtaining 139 spectra for each batch. The observed spectral variations are mainly related to backscattering variations during the casein micelle aggregation process and the subsequent curd formation. As well known, monitoring a single wavelength (1304 nm), good correlation with the coagulation time estimated using lactodynamograph (LDG r parameter) were obtained, R^2 ranging from 0.885 to 0.987 depending on kind of coagulant. Furthermore, this study evaluated the feasibility of monitoring the full spectra and applying a tensorial multiway approach (NPLS) obtaining good correlations with the others two coagulation parameters estimated using lactodynamograph, namely, curd firming-rate (LDG, k20) and curd firmness (LDG, a30); the values of R^2_{CV} obtained were ranging from 0.836 to 0.906 for k20 and from 0.71 to 0.823 for a30, depending on kind of coagulants.

Keywords: milk coagulation, Grana-type cheese, on-line monitoring, near infrared spectroscopy, multi-way data, NPLS.

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FT-NIR spectroscopy for fermentation monitoring of purslane-fortified yogurt

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Stems and leaves of *Portulaca oleracea* L., also known as purslane, contain nutrients such as omega-3 fatty acids, vitamins A, C, and E, electrolytes like potassium and sodium, minerals like calcium, magnesium, and phosphorus, as well as a variety of phenolic compounds. Fortification of yogurt with lyophilized purslane can help in spreading its consumption, taking advantages of its nutritional, therapeutic, pharmaceutical, and phytoremediation benefits. However, changes in yogurt formulation can affect the final product structure and consumer acceptance. The aim of this study was therefore the evaluation of FT-NIR spectroscopy, combined with chemometrics, as a tool for monitoring lactic acid fermentation of lyophilised purslane-fortified yogurt. Two production replicates of set-style yoghurt with and without lyophilised purslane addition (0.55%) were performed, monitoring in continuous the fermentation step by FT-NIR spectroscopy with a transflectance adapter (0.2 cm total effective pathlength) and fundamental rheology (time sweep test, followed by strain and frequency sweep tests). Moreover, lactic acid bacteria count was determined at the beginning and the end of the fermentation. Results showed that the addition of lyophilised purslane had a beneficial effect on yogurt setting, increasing the firmness of the final gel and shortening the gelation time, despite the similar development of lactic acid bacteria. FT-NIR spectroscopy proved to be a valuable tool for monitoring the fermentation step, being able to detect the anticipated gelation of the fortified yogurt. Thus, in conclusion the work demonstrated that the purslane-fortification in yogurt can have beneficial effects in product structuring, enabling a shortening of the fermentation step. A processing monitoring method based on FT-NIR spectroscopy can be successfully developed following the principles of the Process Analytical Technology, thus boosting the application of smart manufacturing solutions under the frame of the Industry 4.0 plan.

Keywords: e-sensors, process analytical technology, yogurt fortification.

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NIR Spectroscopy: Searching for optimal crops for the green food transition

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The shift towards sustainable food production is rapidly becoming more than just a trend. The green transition places the food industry at a pivotal and transformative stage, as consumers increasingly seek control over their dietary choices. In response to the growing popularity of flexitarian and vegetarian lifestyles, food manufacturers have begun adapting to these shifts. This heightened focus on sustainability necessitates a significant increase in the utilization of plant-based raw materials and ingredients.

Plant proteins, requiring less energy and emitting less greenhouse gases for their production and serve not only as essential nutritional components, but also as food structuring agents. Their effectiveness in this regard is dependent upon their functional properties, influenced by factors such as composition, pH, salt concentration, temperature, and processing methods.

Faba beans, peas, and oats stand out as prime sources of protein, fiber, and essential nutrients, making them optimal for plant-based products. Their versatility allows for the creation of a wide range of nutritious options that support both health and environmental sustainability. It is therefore becoming most interesting to investigate how different varieties and cultivation methods, conventional or organic, may influence the bulk composition of these ingredients and thus expand possibilities for their use as plant-based protein sources.

This research investigates the use of NIR spectroscopy for screening different cultivars and varieties for future use as sustainable protein source for plant-based food. Ten different varieties across three distinct crops (faba bean, pea and oat), were cultivated in three different locations: two under conventional and one under organic farming. NIR spectra were obtained for raw materials and derived extracts, concentrates, isolates and extrudates of oat, pea and faba bean and the results are correlated to protein content and dietary fiber analysis as well as other critical parameters such as saponin and lectin content.

Keywords: NIR, plant-based food, plant proteins

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Rapid and non-destructive quantification of meat content in the legs of live red king crab by near-infrared spectroscopy

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Red king crab is one of the most widely distributed and well-known of all king crabs, and extensive fishing occurs in the northern ocean expanses. The edible meat of the king crabs is in the legs and claws and is considered a delicacy and, therefore, highly priced. Occasionally, the content of meat is low, and this is regarded as the single most negative quality attribute. In this study, we elucidated how rapid and non-destructive near-infrared spectroscopy (NIRS) on live crabs can be used to predict the meat content in the cooked legs.

A NIRS prototype, based on interactance in the wavelength range 760-1080 nm, was used to obtain spectra from the interior tissue of the live crab legs. Three different measurement campaigns, including a total of 99 crabs (380 legs), were conducted over a 10-month period. Calibration models were developed based on the data, with a prediction error (REMSEP) for meat content of 6.4 %-points, which is accurate enough to classify the crabs into low (< 80 %) and high meat content. The meat content, which is the proportion of meat relative to the total cross section of the leg, typically varies in the range 30 - 100%. The amount of cooked meat is inversely proportional to the amount of free water in the leg and proportional the amount of protein in the muscle, both of which can be measured by NIRS. A limitation with the method is that it may overestimate the meat content if the legs have lost free water due to e.g. injuries in the exoskeleton. The technology described here can facilitate a more selective and sustainable king crab fishery, and significantly improve the subsequent trade negotiations and processing.

Keywords: Near-infrared spectroscopy; red king crab; meat content; quality control; sustainable fishery

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Non-destructive spectroscopic-based instruments; their implementation in food sector in tandem with artificial intelligent tools and Blockchain technologies

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The food system is a complex concept that involves various stages and processes from farm to fork, while assessment of quality and safety at every stage is of great importance. The current safety and quality controls relying on chemical and microbiological analyses, which are time-consuming, laborious and provide retrospective results. In this context, spectroscopy-based sensors in tandem with Artificial Intelligence tools and Information Technologies, such as cloud computing, Internet of Things, big data and Blockchain to assure food quality and safety is a very challenging topic for the food industry. This study focuses on the investigation and the current implementations of spectroscopy-based sensors coupled with Artificial Intelligence tools and Blockchain Technologies, for assuring food integrity from farm to fork.

Keywords: Artificial Intelligence, Spectroscopy-based Sensors, Big Data Analyses, Blockchain Technologies

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Improving NIR models performance in the Rendering industry through database enhancement

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Rendering industries convert animal by-products into high quality feed ingredients of animal origin, traditionally referred to as processed animal proteins (PAPs). Since the emergence of the Bovine Spongiform Encephalopathy (BSE), Europe has the most effective regulatory framework for animal by-products to ensure the safety and quality of finished products. The most innovative PAPs producers have chosen to implement new process control technologies, enabling them to provide their customers with more information on the quality of the PAPs produced. The authors' Research Group has maintained a close collaboration with the largest Spanish rendering plant since 2001. Through several research projects and publications (Garrido et al., 2006, 2018), the feasibility of Near Infrared Spectroscopy for chemical and nutritional NIR analysis of animal by-products was clearly demonstrated. However, industries undergo changes over the years, not only at the production level, but also at the supplier level, even moving to more modern NIR instrumentation. This means that the predictive models used on a daily basis become less efficient and accurate over time, resulting in the need to transfer database, extend them and ultimately recalibrate the models if needed. The main objective of this work is to show the need to extend the current NIR databases used in a real industrial environment, thus improving calibrations and therefore the quality of the final product. For this purpose, it was used 170 samples, detected as anomalous on the at-line instrument DS2500 (FOSS, Hillerød, Denmark) from 2023-2024,), which was running models developed from a database transferred from an F5000 (FOSS, Hillerød, Denmark). For database expansion, 4/5 of the samples were used, leaving the remaining 1/5 for validation of the models, which were developed through MPLS regression. The results highlight the importance of updating databases in real, live, and changing industrial environments.

Keywords: At-line NIR analysis, rendering process, protein animal by products

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The usefulness of VIS/NIR techniques for maturity and quality assessment of selected fruit species – resume of 18 years experiments and future perspective

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Since 2006 at the Fruit and Vegetables Storage and Processing Department of the National Institute of Horticultural Research, the usefulness of methods based on VIS/NIR for nondestructive assessment of maturity and quality of apples, apricots, nectarines, peaches, pears, and plums was evaluated. The equipment used was: CP Pigment Analyzer PA1101 (Control in Applied Physiology GbR., Germany), DA meter (Sintéleia, Italy), Quality Station QS 120 (UNITEC, Italy), and F-750 Produce Quality Meter (Felix Instruments, USA). Besides the nondestructive measurements, the following maturity/quality parameters were measured: ethylene and CO_2 production, internal ethylene concentration (apples), starch index (apples and pears), fruit weight, skin colour (for plums with and without epicuticular wax), fruit firmness (FF), soluble solids content (TSS), and titratable acidity (TA). The experiments with the UNITEC spectrophotometer were also focused on the creation and verification of calibration models.

For CP and F-750, signals at wavelengths in the range 400 - 1100 nm were gathered Standard indices were computed: for CP - Normalized Difference Vegetation Index NDVI and Normalized Anthocyanin Index NAI, for DA - the DA index.

The VIS/NIR methods allowed to estimate fruit maturation/ripening and quality (TSS, TA, and FF). The precision of the estimation depended on species, cultivars, and ripening conditions (storage). The results indicated the possibility of limiting the naturally occurring variability in the quality and maturity of fruits intended for storage (the possibility of distinguishing the "ripeness" classes).

On the raw spectra collected from the instruments, some changes were observed when the internal disorders were found. However, detection is still not satisfactory. Since 2023 we use the SkyScan 1273 (Bruker, Belgium) for a nondestructive 3D imaging technology based on X-ray, µCT tomography. Within the running and future experiments, the joint VIS/NIR and X-ray methods for the detection of internal disorders will be used.

Keywords: VIS/NIR, µCT, fruit maturity, quality, disorders

Acknowledgements: The experiments were carried out within the statutory programme of the National Institute of Horticulture Research (P 6.1.2.; P 6.1.3.; P 12.26; 12.27); Multiannual programme 2015-2020, financed by the Polish Ministry of Agriculture and Rural Development; The ISAFRUIT project (Contract no. FP6-FOOD–CT-2006-016279); framework of COST Action 924 activity and partially financed by Polish Ministry

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Comparison and Evaluation of Miniaturized NIR Sensors for On-site Discrimination of Microplastics in Soil

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Microplastics present a growing environmental concern, endangering diverse ecosystems including soil, with potential implications for food safety and human health. Advanced analytical methods are essential for effective monitoring and mitigation of this pollution. Current focus analytical methods face practical limitations hinder comprehensive assessment, particularly in agricultural settings where soil quality directly impacts food production.

This study investigates the application of handheld near-infrared (NIR) spectroscopy for rapid screening of microplastics in soil. We evaluated six handheld instruments alongside a reference benchtop NIR spectrometer for their ability to detect and discriminate various polymer types directly in soil samples, including ASA, EVAC, HDPE, LDPE, PA6, PET, PMMA, POM, PS, and SBR, at concentrations as low as 0.75% (w/w), without the need for sample preparation.

Through covariance analysis, Principal Component Analysis (PCA), and mid-level data fusion techniques, we elucidated the instrumental disparities in polymer discrimination within soil samples. Our findings reveal significant differences among instruments, with FT-NIR spectrometers (benchtop and handheld) demonstrating superior discrimination performance accuracy compared to other handheld devices. Miniaturized NIR spectrometers, despite facing limitations related to instrumental design, show promise for rapid, practical, and on-site screening, particularly in agricultural landscapes where rapid assessment of soil quality is paramount for food production. Our results demonstrate the potential of handheld NIR spectroscopy for rapid, on-site assessment of microplastic contamination in soil.

Keywords: NIR spectroscopy, miniaturized/handheld spectrometers, sensor comparison, on-site application, microplastic, soil analysis.

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Improving quality in breweries with real-time Raman NIR technology

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The brewing process may well be the oldest human process, with historical evidence suggesting it is more than 10,000 years old. The transformation of water and malted grain into a tasty (and safe) beverage resulted in people believing fermentation was an act of the gods. Jumping forward to the 1700s, science started to shine light on the biochemical processes responsible for the transformation of water, malt, hops and yeast into beer. Infrared has been used to measuring the quality of the malted grains and hop quality for decades and recent publication have identified opportunities in brewing for at-line and in-line testing in breweries (Grassi et al., 2014, Fox, 2020). To simplify the need to have a PC with software for calibration development and carrying out predictions, a novel approach is to use cloud-based algorithms and requiring only a portable near infrared device with a PC. In addition, no staff is required for calibration development and maintenance. For this experiment, calibrations were developed for beer gravity (°Plato) and alcohol content (%) using the portable Raman NIR device. Further calibrations for color and free amino nitrogen content are being developed. This portable device using cloud-based data analysis will provide breweries with real-time data for improved quality control.

Keywords: Alcohol, At-line, Beer, Raman NIR, Real-time analysis

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Process Analytical Technology with NIRS as a Key Ingredient Helps Facilitate a Sustainable Food Production

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In 2004 the US FDA introduced process analytical technology (PAT). The idea was to let the industry lift the quality control by developing "a system for a system for designing, analyzing, and controlling manufacturing through timely measurements (i.e., during processing) of critical quality and performance attributes of raw and in-process materials and processes, with the goal of ensuring final product quality". The main ingredients in this industrial revolution was spectroscopy (vibrational spectroscopy and in particular NIRS), multivariate data analysis and process control. The use of rapid and timely spectroscopic measurements and multivariate data analysis are key technologies for the successful implementation of PAT in the food industry.

The aim of implementing PAT in the AgriFood industries (van den Berg et al., 2013) was primarily to improve process efficiency and product quality, but as a side effect, significant sustainability benefits are obtained such as minimizing energy, water, waste and material expenditure. Also the introduction of PAT facilitates the digitalization of the food production. These side-effects may turn out to be future main benefits for the food industry in order to minimize its environmental footprint. Examples of PAT implementations will be given in different areas of food production.

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POSTER SESSION

P01. Apple quality assessment using benchtop NIR and portable VIS-NIR instruments - comparative study

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Technologies based on nondestructive measurements and prediction AI-based systems are extensively applied in food industry. It enables to efficiently optimize the production problems and transfigure food industry products, as well facilitate solving problems at the consumer and global level. Quality of food product can be defined through various characteristics, including nutritional value, physicochemical properties, microbiological safety, sensory attributes, and shelf-life stability. Near-infrared spectroscopy (NIR) enable to carry out fast, reliable in situ measurements of the fruits, however the prediction results of food quality parameters often need to be improved due to inherent variability of their composition.

The aim of the study was to compere the methodology of prediction of total soluble solid content (TSS) parameter in apples using benchtop NIR and portable VIS-NIR spectrophometers. Fruits from Empire apple cultivar were studied. The spectra of intact apple fruits were measured using diffuse reflectance techniques by benchtop spectrophotometer (MPA, Bruker Optics, Ettlingen, Germany) and portable (F-750 Produce Quality Matter, CID Bio Science, Inc., Camas, USA). The TSS was determined as °Brix [%] of the juice pressed from each measurement point on the apple fruit. Partial least squares (PLS) regression and artificial neural network (ANN) models were used to predict quality parameters based on NIR and VIS-NIR spectra. The performance of the calibration models depended on the spectral range and data pre-processing and was similar for data acquired using both benchtop and portable instruments. This preliminary study indicates that both systems portable and benchtop performed well during calibration for TSS. Among the esquired models the best parameters had ANN model (R^2 =0.81, RMSE= 0.53) for data from portable quality matter and PLS model for not pre-treatment data (R^2 = 0.82, RMSE = 0.51) from all spectra range gain from VIS-NIR benchtop spectrophotometer.

This information can be used to develop more advanced systems inclusive of portable tools and advanced technologies for fast evaluation to support operators and ensure better pre- and postharvest management of apple quality.

Keywords: fruit quality, sustainable production, non-destructive evaluation, Industry 4.0.

P02. Application of NIR spectroscopy for quality assessment of Yerba mate

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Sustainability, as a fundamental pillar of Society 5.0, plays a key role in shaping practices that are not only environmentally friendly, but also economically viable in the long run. To achieve economic growth and sustainable development, both production and consumption must be carried out responsibly (Ramirez et al. 2024). Modern technologies such as spectroscopy can monitor production and product quality, providing data that can support sustainable and efficient production (Kharbach et al. 2023).

The aim of this study was to test NIR spectroscopy coupled with multivariate data analysis as a non-destructive tool to evaluate the quality of yerba mate. A total of 55 dried samples and 13 infusions made from selected products were tested. The samples differed in country of origin, texture, and characteristics of the dries due to varying processing methods during production. Principal component analysis (PCA) was used to group the samples by country of origin. The total content of phenolic compounds (TPC) in the infusions was measured using Folin-Ciocalteu reagent and then used in partial least squares (PLS) regression analysis to build the prediction model.

Based on the obtained spectra, it was possible to characterise the bands derived from various compounds. PCA analysis made it possible to group the samples according to the region of origin. The obtained regression results confirmed that it was possible to apply NIR spectra to predict the phenolic compounds of tea infusion samples. The good correlation between spectra and TPC was evidenced by the high values of the R2 and the relatively low values of the mean squared errors.

The results indicate that NIR offer a great solution for food composition analysis, presenting a non-destructive, rapid, cost-effective, and eco-friendly alternative to traditional methods. This solution aligns with the trend of Economy 5.0.

Keywords: NIR, PCA, PLS, spectroscopy, sustainability, quality, Economy 5.0.

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P03. Application of visible and near infrared spectroscopy for non-destructive food quality analysis – a study of berry fruit beverages

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Berry fruit beverages are product with attractive sensory and health promoting properties. They are rich source of nutrients, vitamins, and bioactive compounds, in particular the polyphenols, which determine high bioactivity. Non-targeted fingerprinting methods that enable the acquisition of information about several parameters simultaneously are more appropriate for food analysis than standard physicochemical methods. The use of these methods at different stages of the food production chain reduces the consumption of reagents and energy and enhances digitalization and automation. Recent advances have shown good potential of near infrared (NIR) or NIR combined with visible (VIS) spectroscopy for non-destructive determination of characteristics of berry fruit (Li et al., 2019).

The aim of this study was to test the feasibility of VIS and NIR spectroscopy coupled with multivariate analysis for prediction sensory-related and health promoting properties: soluble solid content (SSC), titratable acidity (TA) and total phenolic compounds (TPC) in commercial chokeberry and black currant beverages including juices, nectars, drinks and syrups. Spectra of studied samples were measured in transmission mode using two types of instruments: Fourier transform and dispersive spectrophotometers. Partial least squares (PLS) regression was used for development the calibration models. The models were optimized using various spectral pre-processing methods. The Variable in Projection (VIP) and selectivity ratio (SR) were used for selection of the optimal spectral ranges. The best model for the prediction of SSC (R^2_P=0.999, RMSEP=0.598) was obtained for the pre-processed NIR (dispersive) spectra and for TA (R^2_P=0.960, RMSEP=1.870) for the pre-processed FT-NIR spectra. The optimal model for prediction of TPC (R^2_P=0.850, RMSEP=717.93) was obtained for the VIS-NIR spectra without any pre-processing.

The results indicate that VIS and NIR spectroscopy combined with multivariate analysis represents a valid tool for high-throughput quality screening of commercial berry beverages in a non-destructive, rapid way and should be promoted to support responsible production.

Keywords: food quality, berry fruit, non-destructive testing, sustainable food system, responsible production

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P04. Benchtop and portable NIR spectroscopy equipment for detection of apple quality

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Technologies based on nondestructive measurements and prediction AI-based systems are extensively applied in food industry. It enables to efficiently optimize the production problems and transfigure food industry products, as well facilitate solving problems at the consumer and global level. Quality of food product can be defined through various characteristics, including nutritional value, physicochemical properties, microbiological safety, sensory attributes, and shelf-life stability. Near-infrared spectroscopy (NIR) enable to carry out fast, reliable in situ measurements of the fruits, however the prediction results of food quality parameters often need to be improved due to inherent variability of their composition.

The aim of the study was to compere the methodology of prediction of total soluble solid content (TSS) parameter using benchtop and portable NIR spectrometer and multivariate analysis. Samples (45) from Empire apple cultivar were studied. The spectra of intact apple fruits were measured using diffuse reflectance techniques by benchtop spectrophotometer (MPA, Bruker Optics, Ettlingen, Germany) and portable (F-750 Produce Quality Matter, CID Bio Science, Inc., Camas, USA). The TSS was determined as °Brix [%] of the juice pressed from each measurement point on the apple fruit. Partial least squares (PLS) regression and artificial neural network (ANN) models were used to evaluate the models. Different methods of pre-processing were tested for model optimization. This preliminary study indicates that both systems portable and benchtop performed well during calibration for TSS. Among the esquired models the best parameters had ANN model (RMSE= 0,53 and R^2 =0.81) for data from portable quality matter and PLS model for not pre-treatment data (RMSE = 0,51, R^2 = 0,82) from all spectra range gain from FTNIR benchtop spectrophotometer.

This information can be used to develop more advanced systems inclusive of portable tools and advanced technologies for fast evaluation to support operators and ensure better pre- and postharvest fruits (apples) managements.

Keywords: fruit quality, sustainable production, non-destructive evaluation, Industry 4.0.

P05. Characterization of Cabernet Sauvignon Wines from Western Balkan Countries using Spectrophotometrically Methods

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Viticulture and winemaking have a long tradition in the Western Balkan countries. This important agricultural activity is based on autochthonous and international varieties. One of the most important international varieties in Western Balkans countries is Cabernet Sauvignon, whose wine production has recently increased. To characterize the wines of this variety from different Balkan countries (Montenegro, Serbia, Macedonia, and Croatia), we studied the chemical parameters, polyphenolic composition, and sensory evaluation of commercial wines from vintage 2019. The chemical analyses were performed based on classic OIV methods. Phenolic composition, including total phenols, the total phenols index (TPI), total anthocyanins, and low and high molecular weight proanthocyanidins (LMPs and HMPs, respectively), were determined spectrophotometrically according to the methodologies of Di Stefano and Guidoni (1989) and Di Stefano et al. (1989). Sensory evaluation was performed according to the OIV method, using a scale of 100 points. Cabernet Sauvignon commercial wines reported a similar chemical composition, independently of geographical origin. Wines were characterized by a high alcohol content (>13.5 vol%), high extract (30 g/L), low residual sugars content, total acidity between 4.5–6.8 g/L, and pH values higher than 3.50.

Phenolic composition also reported similarities among the commercial wines studied. However, some specificities were observed, related to the geographical origin. Total phenols content was lower than 2000 mg/L, reporting Montenegrin wines the highest content. TPI showed a similar trend. Total anthocyanins varied between 183–426 mg/L. HMPs reported the highest contents in Macedonian and Croatian wines (>2000 mg/L). LMPs were found to have high contents in Montenegrin wines (2000 mg/L).

Sensory evaluation showed that the majority of wines assessed were of high quality, reporting a score >85 in a scale of 100 points. Principal component analyses showed that Cabernet Sauvignon wines chemical and phenolic composition could differentiate wines according to their geographical origin.

Keywords: chemical composition, phenols content, sensory evaluation, geographical origin, principal component analyses.

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P06. Discrimination of Haploid and Diploid Maize Seed Samples Using Vis-NIR Imaging Technique

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The success of classification of haploid and diploid maize samples has a critical importance in the in vivo doubled haploid technique which is a hot topic in maize breeding studies. There are various techniques using different spectral devices to discriminate the seed samples obtained from induction crossing. Vis-NIR imaging is one of them and has a potential use for discriminating haploid from the other samples. This study was conducted to evaluate the effectiveness of low-resolution vis-NIR imaging, coupled with machine learning techniques, in discriminating between haploid and diploid seed samples of maize. Ten donors and three inducers were used to obtain the haploid and diploid seed samples. A custom spectral setup was created and a low-resolution (3.2 MP) vis-NIR camera was used to obtain digital images. For training, 400 haploid seed images (102 for testing) and 1328 diploid seed images (333 for testing) were captured in batches of 100. Images of single seeds were then extracted from these batches of 100 images. 20% of the data set is reserved for testing. Custom CNN architecture was used to develop classification models and evaluate them according to robustness statistics. The results showed that both RGB (Sensitivity=0.80, Specificity=0.95, Accuracy=0.91) and NIR (Sensitivity=0.79, Specificity=0.96, Accuracy=0.92) models obtained by low-resolution Vis-NIR imaging successfully discriminated between haploid and diploid seed samples. Our investigations revealed that the results obtained with NIR-based images achieved model evaluation criteria similar to those of RGB-based images (F1 score macro avg, NIR=0.89, RGB=0.88). In the developed models, the discrimination of diploid samples was found to be more successful than that of haploid samples. In conclusion, this study demonstrates the potential of low-resolution Vis-NIR imaging coupled with machine learning techniques for effectively discriminating between haploid and diploid maize seed samples.

Keywords: maize breeding, doubled haploid, ploidy, *Zea mays*

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P07. fCovSel: A new faster covariates selection algorithm for NIR spectral data

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Covariate's selection (CovSel) (Roger et al., 2011) is a variable selection technique in the domain of near-infrared spectroscopy and is commonly used for extracting variables carrying high covariance with response variables. CovSel is a special case of partial least square analysis, where at each weight estimation step, the weight vector is of the binary form to select the variables. In the earlier algorithm of the CovSel which is identical to the nonlinear iterative partial least square (NIPALS), there is a key step of predictor matrix deflation which makes it a time-consuming approach leading to longer time consumption during tasks such as cross-validation or in multiblock multiway CovSel scenarios where a wide number of variables combinations are usually explored for model optimization. In this presentation, a new CovSel algorithm called faster CovSel (fCovSel) (Mishra 2022) which drops the need for predictor matrix deflation. By dropping the predictor matrix deflation step, the method naturally becomes faster than the CovSel based on NIPALS. Mathematical and analytical comparisons of the CovSel and the fCovSel in terms of achieving the same solution and time requirements will be presented.

Keywords: feature selection, sparse modelling, dimensionality reduction.

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P08. Hybrid modelling applied to spectroscopic data in bioreactors

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Monitoring and controlling growth media and microbial biomass are critical for developing cost-effective bioprocesses. Traditionally, process monitoring relies on standard parameters such as pH, temperature, and gases. However, today, advanced techniques such as Raman and infrared spectroscopy enable precise control of critical process parameters including biomass, product, and substrate concentrations, benefitting from advanced sensors. Multivariate calibration models are extensively used to correlate spectral data with biomass, product, and substrate concentrations, including lipid profiles (Dzurendova, et al., 2023).

The production of cellular and extracellular products and the consumption of media can be effectively described using first-principle models, which provide a stable foundation for modelling. It is important to note that first-principle models, while robust, may exhibit errors and should not be overfitted to measured data due to inherent sources of variability. Therefore, a hybrid modelling approach combining first-principle models of media consumption and biomass production with data-driven models is recommended.

To demonstrate this approach, we utilised spectroscopic data collected during submerged fermentation involving two different oleaginous and carotenogenic microorganisms grown on distinct carbon substrates: glucose fermentation by the yeast *Rhodotorula toruloides* and glycerol fermentation by the marine thraustochytrid *Schizochytrium sp*. We are developing a hybrid modelling approach to investigate how spectral data can refine first-principle models by reducing assumptions. Additionally, we are exploring how these first-principle models can enhance predictive models by constraining the solution space. This model will be further used to predict component consumption and optimise biomass production in bioreactor systems.

Keywords: hybrid modelling, Raman spectroscopy, fermentation, microbial biomass.

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P09. Managing control of food authenticity using spectroscopy – the example of apple juice

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Controlling the authenticity of products in the food value chain is of great importance for safety, quality, and economic reasons and is a necessary function of regulatory authorities. However, due to the natural variability of food and the large variety of fraudelant practices, developing methods for detecting fraud in the food sector is a difficult task. As an alternative to traditional chemical methods, innovative methods of detecting counterfeit products are being developed based on the use of spectral fingerprints combined with advanced data analysis methods (Ellis et al., 2012).

One of the products that are the target of fraudulent practices are fruit juices. An example of illegal practices is the replacement of juice, obtained directly from fruit (not from concentrate, NFC) with juice reconstituted from concentrate (FC) by adding water. The direct juices preserve more of the the health-promoting properties of fresh fruit, have more attractive sensory properties and are valued higher by the consumers than FC juices.

Previously, we have demonstrated the utility of synchronous fluorescence (SF) spectroscopy for distinguishing NFC and FC commercial apple juices (Włodarska et al., 2018). The aim of presented studies was to compare the feasibility of near infrared (NIR) spectroscopy and diffrent fluorescence techniques and for discrimination between those two juice categories. Partial least squares discriminant analysis (PLS-DA) was used to develop the classification models based on NIR spectra and various types of fluorescence spectra, including excitation-emission matrices (EEM) and SF spectra. The best discrimination between studied juice categories was obtained using fluorescence spectra, which are related to the fluorescence of non-enzymatic browning products and polyphenols. The models based on NIR spectra had lower discrimination performance. The presented results may be important for the potential practical applications, enabling development of innovative, rapid, high-throughput screening tools for managing juice authenticity in the entire food chain.

Keywords: food fraud, quality management, NIR, fluorescence, nontargeted analysis

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P10. Microbiological quality assessment of aerobically stored Feta cheese using spectroscopy-based sensors

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Rapid and non-destructive detection of food spoilage is of major interest to food industries and authorities. Therefore, developing novel detection techniques for food quality assessment is of great importance. Such methods involve spectroscopy-based sensors. The purpose of this study was to predict the microbiological quality (total viable count-TVC) of aerobically stored Feta cheese using Fourier-transform infrared spectroscopy (FTIR) and two Multispectral imaging (MSI) instruments in conjunction with chemometric models. Partial least squares regression (PLS-R) was applied with a stratified sampling of the data, 70% of each dataset was used for training and 30% for testing the models, with no further preprocessing of the spectral data. RMSE and R^2 scores were used to assess the accuracy of the models. The R^2 and RMSE scores for external validation were 0.657 και 0.154 for FTIR, 0.676 and 0.177 for MSI_1 (benchtop), 0.458 and 0.210 for MSI_2 (portable), respectively. The findings of this study were promising and showed that the sensors used could be useful for predicting the microbiological quality of various food commodities.

Keywords: spectroscopy-based sensors, chemometrics, feta cheese, microbiological quality.

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Ethical committee

"Not applicable due to there is no relevant research connected with Ethics committee".

Sources of funding

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P11. Monitoring almonds sun-drying process using handheld portable NIR sensors

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The traditional drying process to reduce water content in raw in-shell almonds, until at around 10 % to meet the market specifications, entails the outdoor spreading of the fruits over a flat surface during a certain number of days. This drying method present some advantages, mainly the low cost of the processing. However, it is highly dependent on the climatologic conditions of the area during that specific time in which the almonds are sun-drying. Consequently, it is of paramount importance to monitor the moisture content of the almonds during that process to obtain a product with the desired characteristics. Hitherto, the techniques applied by the almonds industry to measure the moisture content of the fruits are based on destructive methods that require a long sample preparation and analysis time. Among the new analytical techniques available, near infrared spectroscopy (NIRS) arises as a suitable alternative to be incorporated in the monitoring of almond sun-drying process given the fast-response of this technique along with its non-destructive nature and the availability of handheld portable sensors to perform the *in situ* measurements in the drying areas. In this study, two handheld portable NIRS sensors were used, and the static (punctual readings) and dynamic (moving the sensor along the drying surface) analysis modes were evaluated for the quantification of the moisture content (% fw) and water activity parameters. Partial Least Squares (PLS) regression was used to develop the prediction models. Excellent prediction results were obtained which highlighted the possibility of incorporating NIRS technology to monitor *in situ* the evolution of aforementioned parameters throughout the sun-drying process of the almonds.

Keywords: almonds sun-drying process, handheld portable sensors, NIRS spectroscopy, moisture content monitoring, water activity

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P12. Novel diagnostic markers for the quality of traded saffron based on Fourier Transform Infrared (FT-IR) spectroscopy and chemometrics: what is still underexplored?

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In recent years, saffron (*Crocus sativus* L.), an ancient spice with medicinal properties and high socio-economic value in certain rural areas of the Mediterranean and Middle-East Asia, has attracted increasing research interest. While the development of new food, nutraceutical, and pharmaceutical products from saffron extracts and constituents is on the rise, the shortage of authentic high-quality raw material limits commercial growth. There is a pressing demand for precision farming, controlled production processes, and fair trade, all to be supported by on-site monitoring and quality control systems. In this context, novel non-invasive diagnostic tests for the purity and quality of the traded product have been intensively explored in the last decade (Kiani et al., 2018; Ordoudi et al., 2014). So far, most application studies focus on identifying new authenticity markers after chemometric assessment of Fourier Transform mid-infrared (FTIR), Near-Infrared (NIR), or Visible-Near Infrared (Vis-NIR) spectra. This work compiles the results from different FTIR-based methods that were developed through past and ongoing collaborative research in LFCT and discusses the outcomes within different contexts (e.g. authentication, quality grading), and characteristics of the reference samples (e.g. origin, age, production process, grade, composition). The main objective is to highlight intrinsic product features and spectral acquisition aspects that may critically influence the extraction of novel quality diagnostic markers from the datasets. Recent progress made in the frame of the "SensorFint" COST Action is also highlighted. The raised points strengthen the view that non-destructive mid-infrared spectroscopic sensors could greatly benefit the saffron industry. This requires a multi-disciplinary framework of experts that will jointly design, collect, and analyze comprehensive spectral data from well-defined reference samples.

Keywords: FT-IR spectroscopy, saffron, quality control, authenticity

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P13. Nuclear Magnetic Resonance-based Metabolomics in conjunction with Machine Learning Algorithms for Food Analysis

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The agri-food industry is nowadays one of the most relevant industry sectors on different levels, including economic, healthcare, or sustainability (Pattara et al., 2017). As such, there has been an increasing interest in product traceability, with the subsequent need for fast and economical methods for analysis, capable of highlighting the peculiarities that characterize and identify different products, therefore reducing frauds (Yamada et al., 2020). Such has been the relevance that, in 2009, the term foodomics arose as the discipline that studies the domains of Food and Nutrition through the application and integration of omic technologies. Foodomics can be applied in every step of production/consumption chain, thus being able to guarantee that products adjust to corresponding regulations throughout all their life cycle (Vignoli et al., 2019).

On this matter, the application of Nuclear Magnetic Resonance (NMR) for metabolomic analyses emerges as a valuable tool, since it is a non-destructive, non-invasive, highly reproducible, and quantitative technique that permits the analysis of the whole composition of a sample (Crook and Powers, 2020). Nonetheless, the analysis of complex samples by NMR entails some issues. Typically, samples are composed of more than 1000 overlapping peaks whose position, intensity and width are dependent on numerous factors, e.g. sample pH, salt concentrations, the solvent used, or temperature. Furthermore, at present, processing, and analysis of a batch of NMR spectra are time-consuming, since they are performed in a manual and individual manner, thus standing in the way of the standardization of this technique in the agrifood industry (Emwas et al., 2018).

In this oral communication, some light will be shed on the cited difficulties found for the standardization of NMR in the food industry. In particular, a workflow that combines NMR data preprocessing with machine learning algorithms for the automated analysis of agri-food products is presented.

Keywords: nuclear magnetic resonance, machine learning, metabolomics, agri-food, food.

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P14. Optimization of a fiber optic probe for the *in situ* quality evaluation of virgin olive oil

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Commission Delegated Regulation (EU) 2015/18304 establishes the physicochemical and sensory characteristics related to the characterisation of olive oil, with acidity being the main quality parameter. Therefore, the control of this parameter at the reception of bulk olive oil before packaging is essential for producers and packagers, allowing them to detect possible irregularities or fraud in the primary stages of the production chain. In this context, accurate analytical technology capable of analysing large quantities of the traded olive oil is required. Near Infrared Spectroscopy (NIRS) has proven to be suitable for its implementation at any point in the industrial process to analyse thousands of samples per day, at a low cost per sample and without the need for sample preparation. The main objective of this work is to fine-tune and evaluate a fiber-optic probe design for product analysis in trucks. To this end, a total of 750 olive oil samples from different commercial categories were analysed using two transmission probes, one commercial laboratory-scale probe and one probe designed *ad hoc* for industrial scale use. Both probes were connected to the same FT-NIR instrument, the Matrix-F (Bruker Optics), and spectra were acquired in the spectral range 834 – 2502 nm. After the optimization procedure, calibration models for the prediction of acidity were developed using PLS regression. The results indicated that the use of a fiber-optic probe connected to the FT-NIRS instrument is suitable for the *in-situ* quality control of the olive oil analysed in bulk.

Keywords: olive oil, quality determination, in bulk NIR analysis, fiber-optic probe

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P15. Optimizing spectral analysis for improved precision in Iberian ham quality control with portable NIRS devices

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Near-Infrared Reflectance Spectroscopy (NIRS) has become an extremely useful tool for quality control and traceability in the agri-food industry, thanks in part, to the development of portable sensors, apt for the *in-situ* analysis. The incorporation of these sensors is particularly valuable for high-value products like 100% Iberian cured ham with black seal, because the perishable nature and high cost of samples make necessary the implementation of an analysis methodology that optimizes both efficiency and cost-effectiveness. The aim of this research was to assess various alternatives for the *in situ* NIRS implementation of Iberian cured ham, analysed packaged and unpackaged, related to the configuration of two new generation portable NIRS devices, a Linear Variable Filter (LVF) sensor, the MicroNIR™ Pro 1700 and the Fourier Transform (FT)-NIR device, the NeoSpectra, whose uses must be evaluated and optimized, previously to their incorporation at industrial level. These parameters were the number of scans, the integration time, and the use of 'autozero' for the LVF instrument, and the optical gain configuration, the linear interpolation, the apodization function, the number of Fast Fourier Transform (FFT) points, and the scan time for the FT-NIR device. Once the different alternatives were evaluated, the most suitable option was identified for each instrument. To evaluate the results, the RMS statistic, that enables to compare the similarities between spectra, was calculated. In conclusion, the proper setup and optimization of portable NIRS devices mark a significant step towards establishing efficient and reliable analysis methodologies in the agri-food industry, highlighting a commitment to quality and precision in the control of premium products.

Keywords: NIRS (Near-Infrared Reflectance Spectroscopy), quality control, Iberian cured ham, portable devices, measurement optimisation

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P16. Predicting Italian polyflora honey geographical origin by visible and NIR spectroscopy

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The feasibility of the application of an instrumental spectrophotometer (400-700 nm) and two portable near-infrared (NIR) instruments operating in the range of 700-1080 nm (NIR#1) and 902-1680 nm (NIR#2) was assessed coupled with chemometric as a rapid tool for honey geographical authentication. A total of 215 polyflora samples were collected from all Italian regions. Geographical features were also used to categorize honey samples in three ecological macro-area. Samples underwent heat treatment at 40 ± 2 °C for 30 min, before spectroscopy data collection, which was performed in triplicate in approximately 1 hour. Outcomes from the three spectroscopic instruments were standardized and used as fused datasets. Four supervised or unsupervised classification algorithms (support vector machine SVM linear kernel, SVM radial kernel, k-nearest neighbours KNN, and conditional random forest cforest) were tested after randomly splitting the dataset in training (70%) and testing set (30%). The random splitting process was repeated 100-500 times for regional or Italian macro-areas classification, respectively. Results from fused data showed overall accuracy ranging from 0.51 to 0.58 (KNN the lower, cforest and SVM-linear the higher) for Italian macro-areas and 0.11 to 0.49 (KNN the lower, cforest and SVM-radial the higher). Results from single spectroscopy instruments showed similar performances for NIR#1 (overall accuracy = 0.60 for all tested algorithms) or NIR#2 (overall accuracy = 0.6 for cforest and SVM-radial), predicting the three macro-areas and better results with SVM-linear for NIR predicting regions origin. An ANOVA showed significant ($P < 0.001$) differences among LSmenas of the visible coordinates (L*, a* and b*) according to both geographically tested factors. Summarising, results demonstrated that both visible and NIR spectroscopies are rapid and low-cost but effective techniques to identify the geographical origin of polyflora honey, even though a better discriminant capacity was observed when grouping the samples in specific ecological macro-areas.

Keywords: honey, authentication, spectroscopy, classification

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P17. Predicting milk quality using portable NIR instruments

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The suitability of employing two portable near-infrared (NIR) instruments operating within the ranges of 950-1550 nm (NIR#1) and 1350-2150 nm (NIR#2) was evaluated alongside chemometric techniques as a rapid method for determining milk quality. A total of 205 samples were sonicated and subsequently pre-heated to 40°C before being scanned twice in transmission mode using a cuvette with a path length of 1 mm. Spectra from 22 samples with Mahalanobis distance exceeding the third quartile were excluded. After averaging the replicate scans, spectra preprocessing was conducted to mitigate multiplicative effects caused by light scattering (Roger et al., 2022). The data sets were randomly divided into training (tr, 70%) and testing (ts, 30%) sets, and partial least squares (PLS) regression was performed on tr and validated on ts. The optimal number of principal components (PCs) for PLS was determined by minimising Root Mean Square Errors (RMSE) in cross-validation (cv) with a maximum of 5 PCs to prevent overfitting. The splitting of the data set and PLS algorithm was repeated 100 times, and average metrics, including coefficient of determination (R^2), RMSE, and the ratio of performance to deviation (RPD), were reported for cv and validation (v). Milk samples were analysed for various parameters, including casein (%m/m), crude fat (%m/m), lactose (%m/m), crude protein (%m/m), and true protein (%m/m). The results indicated poor performance of both instruments, with RPDcv < 1.2 and RPDv < 1. The suboptimal performance is likely attributed to high absorbances (log 1/R), reaching values of 4 within the water bands, recorded with a noisy signal. Therefore, it can be hypothesised that the scanning method (cuvette path length, light intensity, integration time, or sample preparation) must be further optimized in order to be suitable for this specific application.

Keywords: raw milk, NIR, transmission, scattering

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P18. Use of NDSS to authenticate Parmigiano Reggiano and Grana Padano PDO grated cheese

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Parmigiano Reggiano (PR) and Grana Padano (GP) are the most produced and exported PDO Italian cheeses (CLAL, 2022). They are both artisanal, cooked, extra-hard, long-ripened cheese from partially skimmed raw milk. Due to its versatility, the grated product from these two PDO is frequently preferred by consumers and largely used in the food service sector. However, grated cheese is more easily subjected to fraud, by adding low quality ingredients, or by mixing it with non-PDO or foreign cheeses. This compromises the product's authenticity and affect its quality. It is therefore important to ensure the traceability and authenticity of this product. Hence, this study investigated the potential of near-infrared (NIR) spectroscopy to discriminate between grated PR and GP PDO cheeses. A total of 18 cheese samples were collected from 6 dairy plants, 3 belonged to GP and 3 to PR. For each dairy plant, samples were selected from 3 seasoning times (12, 22, 36 months, respectively) and grated according to each PDO regulation. The 3 ripening times were also blended within cheese, for a total of 36 samples. Spectra were collected with a benchtop (Perten DA7250, PerkinElmer Inc., Waltham, MA) and a portable (LabSpec2500, ASD Inc., Boulder, CO) NIR instrument. After spectral pre-treatment (e.g., SNV, scaling), PLS-DA models were built to differentiate the PDO (PR, GP) and their ripening times (12, 22, 36 months, and blended product). The results showed >0.97 and 0.83 F1 score for the PDO, and the ripening time was discriminated with 0.86 and 0.62 F1 score for benchtop and portable instruments, respectively. These results demonstrate the feasibility of using NIR spectroscopy coupled with chemometrics to accurately authenticate the 2 PDO and distinguish their ripening times.

Keywords: PDO cheese, grated, ripening, NIR, classification, PLS-DA

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P19. Use of vine shoots as biomass energy. In-situ quality evaluation by near infrared spectroscopy

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One of the main concerns of today's society is the impact of its activities on the environment. Among these impacts is that of fossil fuel consumption. In recent decades, much effort has been devoted to the search for new alternative energy sources (Patel et al., 2020). In this context, special attention to forestry and agro-industrial wastes for heat and electricity production has been paid (Pachón et al., 2020). Among these wastes, lignocellulosic biomass is a sustainable resource that can replace fuels, chemicals and fossil materials (Dávila et al., 2016). In the present study, vine shoot, as a promising alternative raw material for energy applications, has been tested. Biomass quality parameters, such as moisture, ash, volatile content, fixed carbon and calorific value, are key for determining the suitability for energy production (Sirisomboon et al., 2020). However, the use of traditional laboratory analytical techniques constitutes a slow and costly process. For this reason, non-destructive spectroscopic technologies have been gaining interest among the scientific community. This methodology is economical, fast, non-invasive and non-polluting, in contrast to traditional chemical analysis. In the present work, 150 intact samples were selected, showing a moisture content range from 5.00 to 42.33%, ash content from 1.43 to 49.14% and higher calorific value (HCV) from 12935 to 18208 J/g. Spectra were obtained with a portable ASD QualitySpecVR Trek NIRS instrument (Malvern Panalytical, Longmont, US) and corrected with various signal pretreatments. To design prediction models, PLSR was used as regression method, showing R^2 values of 0.91 for moisture, 0.75 for ash content and 0.62 for HCV. It can be concluded, from this field trial, that the use of portable NIRS technology may significantly improve waste management, thus increasing farm efficiency.

Keywords: Alternative energy sources, lignocellulosic biomass, energy production, NIRS

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P20. Screening of tuna samples for evaluation of histamine content using Fourier-transform mid-infrared (FT-MIR) and chemometrics

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Yellowfin tuna (*Thunnus albacares*) is one of the most important fish species belonging to the *Scombridae* family, constituting approximately 30% of the global tuna harvest (FAO, 2011). With regard to food safety, fish and its derived products are considered one of the most perishable products. Their most widely known hazard associated is the presence of high levels of histamine, which constitutes an issue for the food industry (Feng et al., 2016). Histamine is a biogenic amine produced in the flesh from histidine due to the activity of the bacterial enzyme histidine-decarboxylase (Ordóñez & Callejón, 2019). Although histamine is essential to many key functions in humans and animals, consumed in high concentrations may cause adverse toxicological effects. In this context, the purpose of this research was to evaluate the use of FT-MIR spectroscopy in combination with chemometric methods for two main objectives: firstly, the quantitative measurement of different histamine levels in raw tuna fillets; secondly, consisted on the integration of discrimination algorithms (PLS-DA, SVM, and KNN) to distinguish tuna samples according to their histamine concentration, in accordance with European Commission and FDA regulations (100 mg/kg and 50 mg/kg, respectively). The results obtained underscore the feasibility of using FT-MIR spectroscopy combined with multivariate analysis for rapid and non-destructive safety inspections and to support the internal safety procedures of the industry. This technology serves as a vital and expeditious complement to the reference HPLC-DAD method in the industry.

Keywords: Food safety, Histamine, Tuna, FT-MIR, HPLC, Machine learning

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P21. Near-infrared, Raman and ultrasound sensing fusion for mango properties prediction

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Prediction of fruit properties such as soluble solids, moisture, and firmness is an important task in pre- and post-harvest fruit quality management (Walsh et al., 2020). The traditional approach to assessing such properties is destructive and requires cutting and sampling the fruit, followed by analysis of the fruit flesh and juice. This approach is time-consuming, labour-intensive, and leads to fruit waste. In pre-harvest scenarios, such destructive approaches are impossible to implement as the fruit is still on the tree. To solve this challenge, sensors are being implemented to predict such properties. The most popular spectral sensor currently being implemented is the near-infrared (NIR) sensor, which allows the prediction of moisture and other related properties. A main challenge with NIR spectroscopy is that it is highly attenuated by the water signal, and fresh fruit typically contains 80-90% moisture. Therefore, most of the other properties predicted with NIR spectroscopy are somehow correlated with the moisture signal. On the other hand, Raman spectroscopy is minimally attenuated by moisture and captures specific information about different macromolecules in fresh fruit. The challenge with Raman spectroscopy is that it minimally penetrates the fruit skin. This study explores the fusion of complementary sensing technologies, i.e., NIR, Raman, and Ultrasound, to predict mango properties, i.e., Fmax and soluble solids content. The findings suggest that the fusion of NIR, Raman, and Ultrasound improved the prediction of soluble solids content, but the improvement in Fmax prediction did not benefit from information fusion.

Keywords: fusion, multivariate, fruit

Acknowledgements: KB-sensing potential project.

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P22. Evaluation of handheld spectrometers and development of robust models

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In recent years, an increasing number of handheld spectrometers have become available in the market. These spectrometers, with variable spectral ranges, offer an alternative to traditional benchtop spectrometers due to their portability, ease of use, and affordability. However, concerns often arise regarding their utility due to lower performance and stability.

As part of the Walloon Walopea project, which aims to enhance Europe's self-reliance on plant proteins, the handheld spectrometer "Neospectra" (Si-Ware) has been acquired. The aim was to develop rapid analysis methods on this device to predict the protein content of peas at the field and industrial levels.

First, a robust evaluation protocol was created and applied on the spectrometer. This protocol aims, among other things, to assess precision, short- and medium-term repeatability, and long-term stability. For this purpose, samples of various composition were measured according to different modalities. Subsequently, a predictive model was built. Two mains strategies were explored; building a model from scratch or transferring database from our reference benchtop spectrometer.

Keywords: handheld spectrometer, evaluation, models, peas.

Acknowledgements: We gratefully acknowledge the technicians of CRA-W (Gembloux, Belgium) for their assistance and support.

P23. The potential of a benchtop LF-NMR equipment for food authentication assessment by a non-targeted approach

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Nowadays, conventional analytical techniques recognised for routine use and implementation in the field of analytical food control have several disadvantages. The gap in this field with new emerging technologies is becoming noticeable. One such technology is nuclear magnetic resonance (NMR) spectrometry, which offers significant advantages for the determination of substances in low concentrations.

The commonly used NMR instruments operate at high-field-frequency (HF-NMR) above 250 MHz. However, these instruments pose challenges for routine control laboratories due to their high cost, space requirements, and maintenance needs. These disadvantages are addressed by low-field-frequency, high-resolution (LF-NMR) benchtop instruments operating in the 20-100 MHz range. In addition to overcoming the aforementioned drawbacks, LF-NMR instruments provide the possibility of performing non-destructive measurements, allowing samples to be measured even in the absence of solvent. With sample volumes of less than 1 mL required, the amount of sample waste is negligible when solvent is necessary (Yu et al., 2021).

The acquired NMR spectra can be considered as an instrumental fingerprint characteristic of the measured sample. The information provided by the spectra can be analysed by a non-targeted approach for both qualitative and quantitative applications. In food analysis, numerous applications using NMR have been described, and with the availability of LF-NMR equipment, non-targeted methods can be now developed for use in control laboratories (Hatzakis, 2019; Cao et al., 2021).

This communication presents the results of a preliminary study aimed at developing qualitative and quantitative (non-targeted) analytical applications in food using a benchtop LF-NMR equipment to generate rapid and non-destructive analytical methods. For this purpose, NMR spectra of a set of vegetable oils were acquired. Currently, there is an ongoing project funded by the Ministry of Science and Innovation of the Spanish Government aimed at implementing non-targeted analytical methods based on the use of an LF-NMR instrument in control laboratories.

Keywords: low-field-frequency NMR, food control, non-destructive measurements, fingerprinting, rapid analytical method.

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P24. Alternative plant-based protein analysis using NIR and MIR spectroscopy

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Non-invasive spectrometric sensors (NDSS) have great potential to optimize the extrusion process for meat analogues production. The control of alternative protein powder composition (e.g. insect, barley, buckwheat, fava bean, and lupin) used as raw materials, is essential to ensure the appropriate texture of the extrudates (van der Sman and van der Goot, 2023). This study aims to determine the proximate composition of alternative, plant-based protein powder blends from different sources using two near-infrared (NIR) (a low-cost and a benchtop) and a mid-infrared (MIR) spectrometers. The detection of gluten in these protein powder blends was also investigated. A design of experiments using The Design-Expert ® (Stat-Ease Inc., USA) was defined and 100 different blends using the five protein powders (barley flour, wheat vital gluten isolate, fava bean protein concentrate, lupin protein isolate, and buckwheat flour) were created. Firstly, a qualitative analysis of the spectra was performed. Partial least square regressions (PLSR), partial least square discriminant analyses (PLS-DA) and Convolutional Neural Networks (CNN) were performed using PLS toolbox 9.2 (Eigenvector Inc., Manson, WA, USA) and Python 3.12 to determine proximate composition and discriminate samples containing gluten, respectively. The best PLSR models for protein, moisture, carbohydrates, and fat had predictive errors of 1.59 %, 0.18 %, 1.41 %, and 0.19 % respectively when using benchtop NIR spectrometer data. The models developed using the data from the other two spectrometers also had successful results. The approach to gluten detection was promising with sensitivities (a measure of prediction's false negatives) of 0.611, 0.842, and 0.778 using PLSDA and 0.920, 1.000, and 0.909 using CNN for the low-cost NIR, benchtop NIR, and MIR spectrometers respectively. It can be concluded that these sensors are useful to control the quality of the raw materials before extrusion.

Keywords: meat analogues, gluten detection, proximate composition, process monitoring, high moisture extrusion

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P25. Exploring protein secondary structure changes of high moisture extrudates using FT-IR Amide I band deconvolution

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High-moisture extrusion processing (HMEP) is gaining interest for the obtention of meat analogues with fibre-like structures from alternative protein sources. However, protein texturisation is often described as a "blackbox" system. Further knowledge on protein structure changes caused by HMEP could help understand the role of protein structure during texturization, as well as giving information on nutritional aspects related to altered digestibility on the final product (Carbonaro et al., 2012). The aim of this work was to explore possible changes on fava bean protein secondary structure caused by high temperatures, pressure, and shear stress occurring during HMEP using Fourier Transform Infrared (FT-IR) spectroscopy. To do so, fava bean protein concentrate (FBPC) was thermally treated at different temperatures (110 to 165 °C). High moisture extrudates (HME) were elaborated from the same FBPC using a twin-screw extruder at different barrel temperatures (110 to 165 °C). FT-IR spectra of the thermally treated FBPC and HME were acquired in the mid-infrared region (400–4000 cm^{-1}) with 4 cm^{-1} resolution using an ATR interface. Protein secondary structure peaks comprised in the Amide I band (1600-1700 cm^{-1}) were identified and fitted using ORIGIN (v2020, OriginLab Corporation, USA) following different numerical analytical procedures: literature-based, second derivative, and Fourier self-deconvolution analysis. Results obtained by the different procedures were not consistent, evidencing the effect of band narrowing on secondary protein structure associations. Still, a decreasing tendency of ordered structures and increasing simpler and unordered structures was observed with temperature and HMEP, suggesting that these treatments could be increasing protein digestibility. It can be concluded that FT-IR spectroscopy can be useful to investigate protein structural changes, but the procedure of analysis should be optimized to obtain consistent results.

Keywords: FT-IR spectroscopy, protein structure, high-moisture extrusion processing, Amide I band deconvolution

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P26. Quantification based on pixel counting by classification (QPC) methodology and its application in hyperspectral imaging

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Hyperspectral imaging (HSI) is a rapid, non-destructive, non-invasive technique widely applied in food research field. It can provide simultaneously spectral and spatial information about food samples being a promising analytical platform for quality and safety food assessment. This technique in combination with multivariate analysis methods are especially useful to detect and identify discernible particles dispersed in a homogeneous sample matrix. The data analysis methodology presented in this study uses this powerful tool under an innovative approach to quantify discernible particles in samples. This methodology is called "Quantification based on pixel counting by classification" (QPC). It stemmed from the hypothesis that images captured from samples, which present homogenous matrix with discernible particles dispersed therein, are constituted by spectral heterogeneous pixels. Spectral pixels can be divided in two main groups: matrix spectral-pixels and dispersed particle spectral-pixels. The last ones identify and characterise dispersed particles which could be captured using HSI and quantified by QPC methodology. QPC consists of four stages: (i) a prior spectral homogeneity study of sample pixels; (ii) exploratory analysis of sample spectral-pixels; (iii) classification model building to discriminate between dispersed particle spectral-pixels and matrix spectral-pixels; (iv) quantification by pixel counting. QPC methodology has demonstrated high potential to estimate the content of discernible particles in food quality control fields. In this regard it has been applied to carry out the authentication of wholemeal flour content in bread. Wholemeal bread is one of the most widely consumed wholemeal products, there is currently lack of an official method to authenticate its composition rendering it vulnerable to fraud. This study offers not only an innovative solution to authentication problem of wholemeal bread but also a potent methodology to authenticate the composition of materials with similar characteristics to those described.

Keywords: data analysis method, HSI, quantification, bread.

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P27. Differentiation of Amaranthus Species Using Near-Infrared Spectroscopy

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Interest in the research about underexploited foods has increased recently. In many countries, Amaranthus species are cultivated for use as pseudo cereals, vegetables, or ornamentals. Some of them were used as fodder, a few species are considered weeds. The plants are rich in protein, fiber, minerals, and other nutrients and have various health benefits. The seeds are gluten-free. The genus is taxonomically difficult due to the high phenotypic plasticity of its species and the spontaneous introgression and hybridization between them. The purpose of the study is to evaluate the possibilities of NIRS for the taxonomic differentiation of some of the Amaranthus species common in Bulgaria.

The tested samples were collected from the territory of 6 Bulgarian floristic regions - Thracian plane, Stara Planina (Central), West Frontier Mountains, the Tundzha Hilly Plane, Rhodopes (West), and the Strandja Mountain. Five species (*Amaranthus albus* L., *A. blitum* L., *A. deflexus* L., *A. hybridus* L., *A. retroflexus* L.) of the genus Amaranthus from 31 local populations were studied. The NIR spectra of dried and ground leaf and stem samples were by NIR Quest 512 spectrometer (Ocean Optics, Inc.) in the region 900-1700 nm using a reflection fiber-optics probe. A Pirouette 4.5 (Infometrix, Inc.) was used for performing spectral data processing. Soft Independent Modeling of Class Analogy (SIMCA) was used to develop the classification models.

The performance of developed SIMCA models was very high. The precision varied from 88.46 to 100% and the total accuracy was 96.15%. The results show successful differentiation of the plant materials by taxonomic species.

Keywords: Amaranthus species, NIR Spectroscopy, differentiation, SIMCA.

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P28. Microplastics analysis in marine salt by hyperspectral imaging

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The latest researches point up that 8 million tons of plastic was enter the marine system annually becoming one of the main problems worldwide today [1]. Marine plastics undergo a degradation process which produces their fragmentation due to the exposure to UV light and ambient temperature. These plastic fragments of tiny sizes are called microplastics and they present more than 70% of the waste present in the seas. To meet this challenge, several international organizations have developed action plans to monitoring, mitigating and preventing these pollutants. Under this scenario, the present study aims to develop an analytical method based on hyperspectral imaging, an environmental friendly technique, to monitoring microplastics along the Andalusian Mediterranean coast.

Salt works act as a high-scale natural "pre-concentrators" of microplastics in seawater during the process of salt extraction. For this reason, marine salt for human consumption were selected in this study as indicator of microplastic presence in sea water. Microplastics present in sea salt samples were monitored using hyperspectral camera which measured in two spectral ranges: from 400 to 1000 nm (VNIR) and from 900 to 1700 nm (SWIR). To achieve this, five of the plastics most commonly used in the industry (PP, PE, PS, PVC and PET) were acquired from chemical manufacturers and from industrial products composed of them as microplastic standards. They were crushed to reach microplastics size. Salt from inland salt works was selected as a 'salt blank' (microplastics-free). An image of sea salt, microplastic-free salt and standard samples was captured in both spectral ranges. Then, the region of interest (ROI) of each sample was selected. As exploratory analysis, principal component analysis (PCA) was performed using the pixel-spectra information of ROIs. In addition, support vector machine (SVM) was applied to build a classification model capable of discriminate between sample pixel-spectral which contain salt or any kind of microplastic.

Keywords: HSI, environmental analysis, food analysis, microplastics.

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P29. On-farm real-time near-infrared spectroscopic sensor system for milk composition analysis

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Near-infrared (NIR) spectroscopy has shown useful for characterizing the main milk. These components contain valuable information on the udder health and energy balance of individual dairy cows, as milk plays a critical role in their metabolism. In current practices, milk composition is monitored with a low frequency, or on-farm with poor prediction performance. We developed an accurate analyzer for the on-farm, real-time monitoring of milk composition.

For every milking performed by an automatic milking system, the milk analyzer extracts milk and stabilizes its temperature before the NIR (960 to 1690 nm) reflectance and transmittance spectra are measured. Dark and white reference spectra were acquired autonomously using the same settings. During a test period of 2 years, the system measured reflectance and transmittance spectra from over 100.000 raw milk samples. For about 7% of these samples, laboratory reference values were obtained for fat, protein and lactose (Díaz Olivares et al., 2023). This dataset allowed us to develop, test, update and maintain models to predict the main milk components under different strategies (Fonseca Diaz et al., 2023).

Randomly selecting samples for calibration over the 2-year period resulted in a root-mean-square error of prediction (RMSEP) for the remaining samples of less than 0.1% for all three milk components. Taking samples of the first 3 months for calibration and applying the models on samples of the following 21 months almost doubled the RMSEP. Studying the prediction versus measured plots at week-level revealed that the error was mainly coming from a variable bias. Our unsupervised bias correction method helped to lower the RMSEP back below 0.12%.

Keywords: on-farm, raw milk, quality, NIR sensor, PAT, bias correction

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P30. Use of a portable NIR spectrometer for the classification of fresh pork meat according to diet

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Near Infrared Spectroscopy has emerged as a promising tool in the meat industry, as it allows improving efficiency in the production chain, guaranteeing the authenticity and traceability of meat products. Most research in the pig sector has focused on authenticity in the Iberian pork meat sector. Thus, it has been successfully used to differentiate the 100% Iberian breed vs Duroc crosses or feed vs montanera diets (Horcada et al., 2020). However, work on white pigs is scarcer and focuses on classifying according to breed and predicting compositional parameters related to meat quality.

The present study aims to classify white pig meat according to the inclusion of vegetable by-products in the diet. For this purpose, a total of 100 white pork loins from two trials were analysed. In both trials, the controls were fed with conventional feed, while in the first trial the second batch was fed with citrus by-products and in the second trial with carob by-products. The portable equipment used was the MicroNIR 1700, in reflectance mode with measurement in the spectral range of 908-1676 nm. The spectrum was recorded by direct application of the probe on minced meat of the *Longissimus dorsi* muscle (T7-T9). The OPLS-DA discriminant method was applied using both raw spectra and those treated with scatter treatments (SNV, Detrend and both) combined with the first and second derivative and smoothing. The goodness-of-fit of the model was determined as a function of the % success in classification according to diet. The model that provided the best classification results was SNV+Detrend with the second derivative with 90% success in calibration and 55% in validation. The results obtained suggest that portable equipment could be a viable alternative for classification, but the sample set needs to be expanded to improve the results.

Keywords: pork meat, classification, SIMCA software, NIRS, portable spectrometer

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P31. Feasibility of using a portable spectrometer (vis-NIR) during the production and ripening of Protected Designation of Origin Casín cheese.

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Near infrared spectroscopy (NIRS) is a widely used technology in the food industry. Technological advances have allowed the development of portable equipment that is increasingly demanded by the industry. This has extended the field of application of both visible and NIR (vis-NIR) spectroscopy in the dairy sector (Pu et al., 2021). The application of portable equipment is an important novelty that can be easily implemented in the cheese sector as it is very powerful and has several advantages such as low cost and portability. The aim of this research was to assess the feasibility of using portable equipment in the artisanal production of Casín Protected Designation of Origin cheese. A portable VNIR-SWIR equipment with a measuring range of 350-2500 nm was used. A total of 90 samples were analysed, including curds, fresh and ripened cheeses, from all the cheese dairies currently covered by the PDO 'Queso Casín'. The OPLS-DA method was applied to the spectral data, both raw and pre-treated with scatter and smoothing treatments. In order to establish the goodness of fit of the models, the overall % correctness was taken into account for each one of the groups established. The generated model obtained percentages of correct classification of the samples of 100% in the discrimination of the products within the manufacturing process. It was also possible to discriminate the producer dairy in the 100% of the case. The results obtained with the portable equipment are comparable to those obtained with desktop equipment, making the use of low-cost, easy-to-use portable equipment a viable alternative in the cheese industry.

Keywords: Cheese, Classification, NIRS, Portable spectrometers

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P32. Non-destructive, *in-situ* varietal discrimination of walnut tree by portable near infrared spectroscopy

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The possibility of mixing fruits of different varieties is a major problem in the walnut market, among others, because it leads to heterogeneous batches with no guarantee of the desired quality. Traditionally, walnut varietal discrimination has been carried out using some physical and chemical parameters, such as the viscosity or fatty acid profile of the walnut oil, color or shape of the walnut or leaf, or even genetic analysis (Guerrero et al. 2000). The aim of this study is to develop and optimize methodologies for the discrimination of walnut tree varieties by the use of a portable near infrared (NIR) device (MicroNIR Pro Lite 1700, VIAVI).

A total of 768 different walnut leaf spectra were acquired *in-situ* in two different orchards located in the Alentejo region (Portugal). In each orchard, 4 different varieties are cultivated: 'Lara', 'Howard', 'Chandler', and 'Tulare'. A total of 96 leaves were measured in each orchard (24 per variety). For each leaf, two spectra were acquired on the lower surface and two on the upper surface. The spectral matrix was randomly divided into a training set (75% of the samples) and a test set. A principal component analysis was used to study the whole spectral matrix and identify spectral outliers. Then, linear discriminant analysis (LDA) and support vector machine classification (SVM) were applied to the training matrix to obtain different walnut tree classification methods. Different conditions were tested, obtaining the best results by the application of a standard normal variate pretreatment to the whole training matrix and applying the SVM procedure. Thus, a 100% of the samples were correctly classified at internal validation (train), 91.56% in cross validation, and 91.58% in external validation (test). These results suggest that portable NIR spectroscopy is a suitable tool for rapid *in-situ* identification of the walnut variety in the field.

Keywords: walnut, near infrared, varietal discrimination, non-destructive, *in-situ*

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P33. Testing differences in predictive ability

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It is common in the chemometric and spectroscopic literature to see small differences in the predictive ability of competing multivariate calibrations being interpreted as meaningful when they are probably due to chance. With the aim of encouraging researchers to check before over-interpreting their results, we present some simple statistical tests for comparing two or more sets of predictions. Tests for both quantitative and qualitative prediction rules are included.

Keywords: model comparison, prediction, qualitative, quantitative, statistical tests

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P34. Evaluating potential fouling of a Near Infrared (NIR) process sensor during protein measurements in dairy concentrate processing.

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Near Infrared (NIR) spectroscopy is a common process analytical technology tool used for in-line real-time compositional measurements (Wu et al., 2012). However, it is crucial to evaluate installation parameters before integrating it into a process. In particular, fouling of the sensor (i.e. a layer of material potentially adhering to the surface of the sensor face overtime) could occur potentially impacting the quality of the acquired signal.

During the production of milk protein concentrate (MPC), a full production cycle takes 18~20 hours. In a laboratory experimental setup, one litre of liquid MPC samples (~17% protein content, ~22% total solids, was collected from a local dairy company) was mixed using an overhead mixer at a speed of 500 rpm to mimic dynamic conditions. A NIR transflectance process probe (Bruker Optics, Germany) connected to a FT-NIR spectrometer (Matrix-F, Bruker Optics, Germany) via a 15-meter fibre optic cable, was used to collect spectral signal of MPC samples every 20 min for a duration of 26 hours. The viscosity of MPC samples was also measured at selected time points (0 h, 3 h, 6 h, 9 h, and 26 h) using a rheometer (Anton Paar, Austria). Results showed that the viscosity of MPC samples decreased from 50 mPa.s to 28 mPa.s due to the shear-thinning property of MPC. However, the predicted protein content from all collected NIR spectra was maintained within the range of 16.8~16.9%, indicating that there was a negligible impact of fouling on the NIR spectral signal and model performance.

Using the current experimental settings it can be concluded that no obvious fouling on the surface of the NIR process probe was observed during a full MPC production run. However, it should be evaluated for potential fouling when the process sensor is installed in a commercial scale process to validate sensor performance.

Keywords: Fouling, Dairy Concentrate, Process Sensor, NIR.

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P35. Towards the automated quality control of olives in the reception yard of the olive mill.

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The mature phase of the olive fruits is typically assessed through hands-on sampling and offline laboratory examination, a process that demands significant labor, time, and may be susceptible to sampling prejudices. With the growth of olive oil mills, automation opportunities are on the rise; for instance, modern large mills boast multiple distinct processing lines that are entirely automated. Ensuring conformity during the olive reception phase is crucial for securing top-notch virgin olive oils, adhering to quality benchmarks, and fairly compensating producers. Near Infrared Spectroscopy (NIRS) emerges as a promising technology to elevate efficiency and streamline decision-making protocols.

This research investigates the feasibility of transferring calibrations from a NIR benchtop instrument to an online sensor utilizing the Honigs Regression (HR) approach to facilitate instant determination of moisture and fat content in intact olives. NIR spectra from around 2000 intact olive samples, sourced from diverse geographical locations and gathered over multiple harvest seasons, were captured using different benchtop Perten diode array sensors (DA 7250) positioned at various sites (olive mills, laboratories). Models were then migrated to an online sensor (DA 7440, Perten). Subsequent evaluations focused on comparing the performance or accuracy of the online NIR instrument against the benchtop NIR instrument. This evaluation was conducted via a fitting procedure that juxtaposed the calibration parameters of the benchtop and process instruments, along with the sample.

Fifty samples underwent analysis using a DA 7250 instrument and a DA 7440, and models were subsequently applied to the respective spectra. The fitting process unveiled a strong correlation (R^2>0.70 for oil content and 0.90 for moisture) between the two instruments, showcasing the potential of the HR method in transferring calibration models from at-line to on-line diode array instruments. This underscores its utility in quality control and automation at the olive oil mill reception point, enabling the grading of olives based on quality for subsequent processing into distinct lines.

Keywords: quality control, olive, Honigs Regression

P36. Investigation the proteolysis reaction in dry-cured ham using NIR spectroscopy and evolving difference calculations

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Pastiness is a texture defect that appears in dry-cured ham when there is an excessive breakdown of the protein structure of the muscle due to the action of a series of autochthonous enzymes and therefore related to an excessive proteolysis (Pérez-Santaescolástica et al., 2018). Pastiness is sometimes difficult to determine non-invasively because of the variation of many factors such as salt, fat or water contents. The aim of this study was to identify the NIR spectral bands linked to the amide groups found in meat, as well as the newly generated amine groups formed during proteolysis reactions as a way to improve prediction of dry-cured ham texture and pastiness defect. To do so, 125 dry-cured ham samples with proteolysis index (PI) ranging from 22.91 to 36.73 were examined using a high-performance Fourier Transform NIR spectrometer. Due to the significant variability in nutritional composition, maturation time and other process factors across these samples, the approach of analysing evolving difference calculation was chosen. The samples were arranged in ascending order based on their PI values. Due to the significant variability among the samples, the data were divided into four blocks with different PI level, obtaining mean PI of 24.43%, 27.8%, 30.78% and 34.57% for block 1, 2, 3 and 4, respectively. Average spectra were compared calculating the spectral differences. Results indicate that evolving plots are able to show how the amide group of native proteins undergoes transformation into a carboxylic acid and amine through the different blocks. In block 4, characterized to have samples with high PI values, the primary species are amines (resulting from the proteolysis reaction) and water, specifically with strong O-H bonds. These dominant species are indicated by bands at 7160 cm^{-1} and 5300 cm^{-1} representing O-H bonds, and at 4720 cm^{-1} representing N-H bonds of amines. The reduction in the amide group (native protein) is observed at 6330 cm^{-1} in the other blocks (characterized to have lower PI than block 4) supporting the explanation for the observed proteolysis reaction investigated in this study. It can be concluded that using NIR spectroscopy in tandem with evolving difference plots provides valuable insights into reaction kinetics stablishing knowledge on the proteolysis mechanism. The use of this information to improve prediction of texture related to proteolysis reactions needs to be further studied.

Keywords: proteolysis, NIR spectroscopy, dry-cured ham, evolving difference

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P37. NIR spectral imaging for non-destructive detection of microplastics in sea salt

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Microplastics (MP) are emerging environmental and health risks, but understanding their occurrence and sources remains limited due to the absence of a standardized and cost-effective analytical methodology. The use of optical non-destructive technologies, particularly Near-Infrared (NIR) and spectral imaging, show great potential as a non-destructive technology for detecting MP in complex matrices such as food (Zhang et al., 2019; Faltynkova et al., 2021). This study seeks to assess the viability of analysing polyethylene terephthalate (PET), polyethylene (PE), polypropylene (PP) and polystyrene (PS) microparticles in sea salt without the need for sample pretreatment. With this purpose, PET, PE, PP, and PS microparticles (2.5, 1, and 0.3 mm) were obtained by grinding and sieving virgin pellets. Fine and coarse salt samples were artificially contaminated with the obtained MPs. A push-broom Specim FX17 camera (935-1720 nm) equipped with a FOV38 lens was used to acquire spectral images. SpecimINSIGHT was used for analysis. The best combination of spectra preprocessing strategies were used to develop models (partial least square discriminant analysis, PLS-DA) for MP classification.

PLS-DA classification models able to identify PET, PE, PP, and PS microparticles in fine and coarse salt samples were developed with CV accuracies of 95.67, 78.33, 97, and 99%, respectively. Particles of similar dimensions to the pixel size of the HSI equipment (0.21 mm) were detected for PS, while particles in the range of 1- 2.5 mm were detected for PET, PE, and PP. Further chemometric techniques and experimentation with macro lenses will be investigated to enhance the size detection threshold across all studied polymer types.

Keywords: microplastics, polymer microparticles, sea salt, NIR spectral imaging.

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P38. NIR Spectroscopy and Artificial Neural Networks for predicting sensory parameters in Iberian ham

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Iberian ham is characterised by its intense aroma, its unique texture and its characteristic visual appearance due to the infiltration of fat in the muscle. The evaluation of these quality characteristics is carried out by sensory analysis, but this methodology is costly and for this reason, the sector is looking for other alternatives to determine quality in a simple way that can be implemented in the industry.

This study explores the feasibility of predicting sensory parameters from NIRS recording of central ham slices. The spectra were obtained by Büchi NIRFlex N-500; SCiO Sensor and MicroNIR 1700 ES devices. The objective was to compare the predictive potential of the three spectrometers, using their entire measurement range, for 8 texture parameters (hardness, juiciness, fatness, fibrosity, chewiness, gumminess, heterogeneity and chewing residue). The sensory analysis was carried out by a panel of 10 expert tasters with experience in QDA analysis, using a 9-point structured scoring scale. A total of 60 hams were analysed.

A Multi-Layer Perceptron (MLP) Feedforward Artificial Neural Network (ANN) with a Levenberg-Marquardt Backpropagation training algorithm was used. The input-output data pair sets were divided into 70%, 15% and 15% for training, validation and test sets, respectively. Each ANN was trained using a different number of neurons (1-25) in the hidden layer and 100 different known seed values.

Correlation coefficient (RSQ) results for calibration ranged between 0.64 for fatness and 0.96 for juiciness, between 0.72 for gumminess and 0.91 for fibrosity and between 0.56 for fatness and 0.82 for juiciness for NIRFlex, MicroNIR and SCiO respectively. The RSQ values of the test set ranged from 0.55 (fatness) to 0.88 (juiciness). The Büchi NIRFlex N-500 generally obtained the best results, but the handheld devices showed good potential, which points to the possibility of predicting sensory parameters from handheld NIR technology.

Keywords: Iberian ham, sensory parameters, Artificial Neural Networks, portable devices, NIRS

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P39. Rapid, high-throughput screening of traded saffron using a portable multimodal spectroscopic sensor and data fusion analysis

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Integrating non-destructive spectroscopic techniques into routine quality control of saffron has recently attracted the interest of many researchers. Along with the development of reference spectral databases, various chemometric tools are investigated to maximize this potential and unravel spurious spectral features owed to unauthorized additives, contaminants, oxidation products or possibly masked origin. Bulky laboratory benchtop instruments are quite common while spectroscopic sensors that may facilitate on-site, high-throughput testing and help enforce high-quality standards in the saffron industry are rarely exploited (Kiani et al., 2018). In the present work, we evaluated a cheap multimodal optical sensor that sequentially acquires visible, fluorescence, and near-infrared spectra of powdered saffron, in the same acquisition routine. First developed in the frame of the 'PhasmaFood' EU-funded project, the device aimed at non-invasively collecting different optical properties from the same area of the sample using miniaturized diffuse reflectance visible (400-800 nm), fluorescence (365 nm) and near-infrared (950−1900 nm) spectrometers. UV-Vis absorption and front-face fluorescence measurements were also performed on benchtop instruments. Certified samples of authentic, top-quality saffron and adulterant species (either low-quality saffron or dried flowers of buddleja, calendula, safflower) were used as References. Binary mixtures of the ground plant materials containing 50 to 95% authentic saffron (w/w) were prepared for calibration. The most relevant results were obtained from visible and fluorescence spectra. Weak emission bands between 500 and 670 nm helped to discriminate top-quality saffron and proved most useful for the development of a sensitive PLS-regression model. Our findings underscore that sensing autofluorescence of traded saffron presents an innovative quality diagnostic approach to rapidly sort out low-quality or adulterated products across the supply chain.

Keywords: Fluorescence, Visible spectroscopy, portable sensor, saffron, quality control, adulteration

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P40. Precise and Efficient Brixº Determination in Molasses Using Combined NIR/MIR Spectroscopy and Chemometrics

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Brixº determination in sugar beet and sugarcane molasses presents a challenge due to their complex composition of sugars (sucrose, glucose, fructose) and non-sugar organic materials. While refractometers are commonly used, this study explores a more precise approach using different spectroscopic methods using near-infrared (NIR) and mid-infrared (MIR) coupled with chemometric analysis. For that, molasses samples from various origins were collected and their Brixº values referenced using a refractometer. Three spectroscopic instruments were employed: a portable FT-NIR (1300-2600 nm); a benchtop FT-NIR MPA (800-2500 nm); and a benchtop FTIR (4000-400 cm^{-1}). Principal component analysis (PCA) and partial least squares (PLS) regression with PLS-Toolbox software (Eigenvector Research Inc., Manson, WA USA) were utilized to correlate spectroscopic data with Brixº values. The results showed that the FT-NIR MPA instrument achieved the most robust model with a 5-points first derivative pre-processing step. This model yielded impressive performance, with R^2 values of 0.92 and 0.70 for training and cross-validation, respectively, and a low prediction error of 14.5%. Conversely, FT-NIR portable and FTIR models demonstrated lower efficacy. While the FT-NIR portable model achieved R^2 value around 0.79 for training, and the FTIR model reached a calibration R^2 of 0.78, their cross-validation R^2 values dropped significantly (0.62 and 0.39, respectively). Both models exhibited prediction errors close to 25%. In conclusion, this study demonstrates the effectiveness of combined NIR/MIR spectroscopy and chemometrics in achieving superior Brixº measurement accuracy in molasses compared to traditional refractometry. The NIR-based model eliminates human error inherent in refractometry and offers significant improvement in prediction precision. This innovative approach presents a valuable tool, ensuring consistency and efficiency in Brixº determination.

Keywords: molasses, Brixº, near infrared (NIR), spectroscopy, chemometrics

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P41. Prediction of the fatty acid profile using NIRS technology to optimize the curing process of Iberian ham

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The first step of the Iberian ham curing is salting the pieces. Currently, salting days are stablishes based on the weight and pH of the pieces, without takin into consideration any other parameter. However, the composition of the fat (fatty acid profile) would be a key parameter to be able to stablish with greater rigor and accuracy the duration of this step (Ventanas et al., 1999; Domínguez, 2021). Given that traditional analysis methods require a lot of time and high financial investment, this parameter is neglected for decision making. As a consequence of this, CICAP technology centre has developed chemometric models for the prediction of fatty acid profile in liquid adipose subcutaneous tissue, allowing us to know this parameter for each piece and to include it as a key parameter to establish the days in salt, which generates added value for the industry. For this, NIRS technology has been implemented as a fast, non-destructive, multiparametric and low-cost technique.

The objective of this work was to develop and optimize chemometric models using a multipurpose FT-NIR analyser (MPA I, Bruker Optics, Ettlingen, Germany) for the prediction of the fatty acid profile in subcutaneous adipose tissue of Iberian pork. To carry out this study, the sample set used was composed of three hundred and five samples (N=305) of subcutaneous adipose tissue from Iberian pigs (100% Iberian pigs and crossed with Duroc) belonging to different batches.

The statistics related to calibration, cross validation and external validation showed the high prediction accuracy of models developed for each of the acids that compose the profile, highlighting that lauric acid is the acid that shows the lowest accuracy (R^2_p=70.18%).

Keywords: Fatty acid profile, Iberian pigs, NIRS technology, salting, added value, product homogenization.

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P42. Determination Galactomannan and Fat Content of Guar (*Cyamopsis tetragonoloba*) using NIR Spectroscopy

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Guar (*Cyamopsis tetragonoloba*) is an important plant with versatile uses as human food, animal feed and industrial. Guar gum obtained from the seeds of the plant is used as a thickener, emulsifier and stabilizer as a raw material in many industries such as food, paper, cosmetics, pharmaceuticals, petroleum and mining, textiles. Galactomannan and fat content are important components in guar seeds. There is a need to alternative methods to detection of the fat and galactomannan content. One of these alternatives is NIR (Near Infrared Reflectance) Spectroscopy, which is widely used in the analysis of other agricultural products. The aim of the study was to develop the NIR calibration models for the determination of galactomannan and fat content in milled guar seed samples. In the present study, 149 guar samples were used for galactomannan content and 202 guar samples for fat content. Partial Least Squares Regression (PLSR) was used to model development. The developed models were compared based on common statistics for model evaluation. The results of study showed that the galactomannan content can be accurately predicted in guar samples. The prediction model for fat content had lower accuracy (R^2=0.75 for calibration and R^2=0.73 for validation set) than model for galactomannan content (R^2=0.95 for calibration and R^2=0.88 for validation set). Nevertheless, it was found that the fat content of guar samples can also be determined with acceptable accuracy using NIR spectroscopy.

Keywords: guar, galactomannan content, fat content

P43. BG Wine - a database of spectral and chromatographic characteristics of traditional Bulgarian wines

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Mavrud, Shiroka Melnishka Loza, Gamza, Misket Cherven and Dimyat are indigenous grape varieties grown in the local regions of Bulgaria for thousands of years. In the recent past they used to occupy a large part of the fruit bearing wines area in the country. These varieties belong to the Black Sea bio-geographical group with typical characteristics: lusty growth, high fertility and yield, late ripening and moderate to poor frost resistance. Their late ripening and high yield are a prerequisite, in some less favourable harvests, for the grapes to fail to reach optimal technological, phenolic and aromatic maturity, which compromises the quality of the produced wines. The white wine variety Sandanski Misket and the red wine varieties Melnik 55 and Rubin have been created in Bulgaria via hybridization of old local grape varieties with varieties from the Western European bio-geographical group. The newly created hybrid varieties are characterized by a shorter vegetation period, earlier ripening and are suitable for distribution in a wider range of soil and climatic conditions.

The traditional Bulgarian wines, produced from the above-mentioned varieties, have never been systematically studied. At the same time, the industry and the society need a tool for fast and low-cost control. We have used the opportunity to collect more than 100 commercial wine samples of traditional Bulgarian wines and to measure their Raman, UV-VIS-NIR absorption and emission spectra (using both benchtop and portable instruments). The created database BG Wine contains information about the production details of each sample, general chemical parameters and phenolic content. The content of the volatile compounds has been determined by using GC/MS/FID. The created database gives opportunity for development of calibration or classification models to serve the industry.

Keywords: wine, NIRS, Raman, optical spectroscopy, gas chromatography

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P44. Fast estimation of Citronellol, Nerol and Geraniol content in Bulgarian rose oil by NIR spectroscopy

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Near-infrared (NIR) spectra of over one hundred Bulgarian rose oil samples were measured in parallel with gas-chromatographic analysis by mass-selective and flame ionization detection (GC/MS/FID). Chemometric analysis was applied to the spectra and chromatographic data in order to build regression models for determination of the three main terpene alcohols in the rose oil – citronellol, geraniol and nerol. As a first step principal component analysis (PCA) was carried out on the spectra in order to detect outliers. Cross-correlation statistic between the NIR data and the GC/FID determined components allowed to find the spectral ranges strongly related to content of the analytes of interest. Twenty two samples were chosen for creating the models. Partial least squares regressions (PLS) were carried out for each of the 3 components and correlations > 0.91 for all of them was achieved, along with root mean square error (RMSE) values <1.2.

The test of the model prediction of all samples (except the outliers) has shown less than 10% deviation from experimentally estimated values. These preliminary results indicate the capability of the NIR spectroscopy for fast and nondestructive analysis of the essential components in the rose oil, responsible for the rose oil quality and authenticity.

Keywords: rose oil, NIRS, gas chromatography

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P45. Volatile organic compounds in traditional Bulgarian red wines - optimization of analytical method using solid phase microextraction and head space gas chromatography

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The content of volatile aroma compounds in wine depends on the varietal characteristics, viticulturally practices and wine-making technology. The aim of this study was to develop sensitive and reproducible procedure using headspace solid-phase micro extraction (HS-SPME) combined with gas chromatography/mass spectrometry (GC/MS) for fast profiling of the free volatile organic compounds (VOCs) in Bulgarian red wines. A semi-quantitative HS-SPME-GC/MS method has been developed for the red wine aroma profile analysis. Semi-polar divinylbenzene/carboxen/polydimethylsiloxane (DVB/CAR/PDMS) fibres were used for extracting the free wine VOCs. An optimization of the experimental conditions (conditioning temperature, conditioning and extraction time) was performed, in order to study their influence on the qualitative and quantitative composition of the wine samples. The effect of addition of NaCl was also studied.

More than 50 individual free volatile and semi-volatile compounds were identified, with the representatives of terpenes, esters, alcohols, fatty acids, sulphur compounds, etc. The study revealed that 3-methyl, 1-butanol was the most abundant component, ranging from 55.23% - 28.76%, followed by octanoic acid, ethyl ester (26.34% -7.52%), phenylethyl alcohol (18,61% - 8,04%) and butanedioic acid, diethyl ester (7.34% - 4.71%). The best HS-SPME conditions were as follows: conditioning time 45 min, conditioning temperature 45oC and extraction time 60 min, with addition of 4 grams NaCl. All the samples were analysed in triplicates, with St Dev <5%.

The developed easy and solvent-less HS-SPME-GC/MS method is suitable for fast, sensitive and reproducible analysis of VOCs and can be used for comparative aroma profiling of Bulgarian red wines as a part of the BG Wine database.

Keywords: wine**,** volatile organic compounds, gas chromatography

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P46. Classification of Moisture Content of Milk Powder by Using NIR Spectroscopy and Chemometrics

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Ensuring the quality of milk powder is crucial due to its nutritional importance. This study investigates the use of Near-Infrared (NIR) spectroscopy as a nondestructive, rapid alternative for the classification of milk powders under various relative humidity conditions. Samples, including whole, skim milk, and lactose-free milk powders, were analyzed using both a desktop (NIRFlex N-500) and a portable (NIR-S-G1) NIR spectrometer. Advanced chemometric methods, such as mean centering, baseline correction, Gaussian smoothing, and derivative processing, were applied to the raw NIR spectra using Orange data analysis software (Demšar et al., 2013). The study revealed that whole milk powder samples with different relative humidity rates showed distinct NIR spectra at 1455 nm and 1927 nm, corresponding to water absorption. High relative humidity samples exhibited higher absorbance values. Principal Component Analysis (PCA) was employed to explore sample differences, with k-Nearest Neighbors (kNN) and Support Vector Machine (SVM) models achieving 100% classification accuracy based on relative humidity. The portable NIR device demonstrated high efficiency for the project due to its fast data collection, ease of transportation, cost-effectiveness, and robust classification ability. Our findings affirm that NIR spectroscopy combined with robust chemometric techniques provides a reliable, efficient method for nondestructive moisture content determination and classification in milk powder, enhancing real-time quality control and product standardization.

Keywords: milk powder, moisture, NIR spectroscopy, chemometrics.

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P47. Classification of Surface Contamination as Biofilms of Foodborne Bacteria with Visible and Short Wave Infrared Spectral Data Fusion

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Bacterial contamination in food products is a global health concern, leading to foodborne diseases. One of the main potential contamination sources in these cases is food contact surfaces, which may be associated with biofilm formation by pathogenic bacteria (Xu et al. 2022; Altun et al., 2023). Biofilms are organized communities of mono- or multi-species bacteria, embedded in a protective and self-produced extracellular polymeric substances matrix (overall composed of carbohydrates, lipids, and proteins) with an increased resistance to environmental factors, drugs and disinfectants.

The objective of this work was to evaluate the combination of visible and near infrared hyperspectral imaging to detect the presence of pathogenic biofilms on food related surfaces. Biofilms of *Escherichia coli* and *Salmonella enterica* were prepared on aluminum substrates, in 3 independent experimental batches. They were imaged with two spectral cameras of VNIR (400-1000 nm) and SWIR (950-2500 nm). The mean spectra of each sample were used at a low level data fusion application by merging these two types of spectra. The presence and type of contamination were predicted with PLS-DA classification in a single model. 0.85 accuracy in the external test predictions was achieved, while 21% of the data were not assigned and left aside the model by the algorithm. It was concluded that the data fusion approach showed an increased performance in detection and identification of biofilms, simultaneously.

Keywords: classification, detection, microorganism, hyperspectral.

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P48. Hyperspectral imaging: a new frontier in honey authenticity

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Honey is considered one of the most adulterated products, and has been a target by fraudsters to make profit (EMA - *Economically Motivated Adulteration*). This is mostly related to the composition of honey, which represents a large variance, because of the fact that honey is produced by bees collecting the nectar (or honeydew produced by insects) visiting different flowers, and transforming it in a sugar solution - called *natural honey*. Since the flora in different parts of the World is different and represents a large biodiversity (*in some cases the composition of honey is influenced by the bee species*), the authenticity of honey is challenging and requires a lot of data based on genuine honey samples and a high level of expertise; that not all countries can afford to have it.

Hyperspectral imaging, also known as spectral imaging or chemical imaging, is a cutting-edge method that simultaneously combines imaging and spectroscopy from a tested object. By using hyperspectral imaging, it is possible to analyse and visualize the composition of honey samples at the pixel level. The chemical composition of individual pixels in a honey image can be identified by using their spectrum as a *fingerprint*.

Keywords: *spectral images*, *honey*, *authenticity*.

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P49. Food waste and safety food

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According some global studies a 40 percent of our food is wasted. Food is wasted at every point along the food chain: on farms and fishing boats; during processing and distribution; in retail stores and restaurants; at home; and after it enters our trash cans (USDA, 2013).

It's a general preoccupation among the management of waste – how can it be reduced. For example, some supermarkets came out with the idea to scrap potentially confusing "best before" dates from dozens more of its fresh fruit and vegetable lines after research found ditching the labels helped customers reduce their food waste at home (Smithers, R., 2018).

The market initiated the idea of taking off the expiry date from some fruits and vegetables to prevent food from being thrown away while still edible. This practice may be applicable also for some animal origin food products like maturated cheese or salami with a real validity in real life longer that is marked on the label. Also a mature product from this category could have a better taste. The question issue on this practice is: Are these specific aged foods safe for consumers?

The topic of research will be to investigate if sensors applied to packaging may detect alterations in foods?

The paper will try to identify a new opportunity for food industry producers regarding the extended shelf life foods.

Keywords: food waste, extended validity, aged foods, safety food

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P50. Discrimination of goat dairy products according to feeding regimes by NIR spectroscopy

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There are many aspects of the current agricultural and livestock production model that need to be changed in order to make it more sustainable, more respectful of the environment and animal welfare, and to reduce its impact on the environment. A key factor to be addressed is the feeding of livestock through a grazing system, which results in a better use of natural resources and an increase in the biodiversity of the ecosystem.

This study evaluates the feasibility of discriminating milk, cheese and yoghurt from Murciano-Granadina goats using near infrared spectroscopy (NIR) as a function of the feeding system (grazing or permanent housing). Samples of milk and dairy products were collected from May to June 2021 from 8 different farms, 5 grazing and 3 intensive. In total, 12 samples of each product were available for intensively housed animals and 20 for grazing.

PLS2 discriminant models were developed using Winisi software, with classification errors of 9.4, 12.5 and 25% for milk, cheese and yoghurt respectively. In the case of the yoghurt samples, textural heterogeneity (presence of lumps of irregular size) was observed, which may have led to poorer results in the discriminant models developed.

P51. Application of Near Infrared Spectroscopy in detecting adulteration - case of honey

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Near Infrared Spectroscopy (NIRS) has emerged as a valuable tool for detecting adulteration in various food products. This technique offers advantages such as real-time response, non-destructive analysis, and the ability to detect a wide range of adulterants (Raypah et al., 2022; Liu et al., 2021; Couto et al., 2021). Studies have shown that honey adulteration can be direct, involving the addition of various syrups to natural honey, or indirect, through feeding honey bees with sugar syrups (Al-Mahasneh et al., 2021). Detection methods combined with machine learning algorithms have demonstrated high accuracy in detecting honey adulteration, showcasing the potential of advanced spectroscopic techniques in ensuring honey authenticity (Phillips & Abdulla, 2022). Additionally, NIRS combined with chemometric methods has been successfully utilized to detect adulteration in honey samples, providing a rapid and non-destructive approach to identifying adulterants (Venecia et al., 2022).

The aim of this study was to apply NIRS in order to investigate if its application is effective in detecting inverted sugar adulteration in honey sugars. Three samples of acacia honey from the Northwest part of Croatia. Samples were harvested in 2018. Adulterated samples were prepared by mixing pure honeys with agave and maple syrups in the range from 10% to 90% by weight. For all samples, NIR spectra were recorded with three different instruments: (i) NIR spectrometer (NIR-128-1.7-USB/6.25/50 µm, Control Development Inc.; λ = 904 - 1699 nm); (ii) NIR spectrometer (AvaSpec-NIR256-2.5-HSC-EVO, Avantes; λ = 1000 - 2500 nm) and (iii) portable NIR spectrometer (NIR-M-R2, InnoSpectra; λ = 900 - 1700 nm). Qualitative and quantitative ability of adulterant prediction was investigated by use of chemometrics. Multivariate tools were used (i) for identification of similarities and differences between pure honey samples and prepared adulterations based on continuous raw NIR spectra and (ii) evaluating the accuracy of determining the level of adulteration for three different NIR devices was also compared.

The obtained results indicate the qualitative efficiency in separation of adulterated honey samples (average (93%), based on the type and the content of added adulterants. In conclusion, by leveraging the capabilities of NIR spectroscopy, food safety and quality control measures can be significantly enhanced, ensuring the authenticity and integrity of honey in the market, ensuring consumers receive authentic and high-quality honey products.

Keywords: NIRS, Honey, Adulteration Maple & Agave syrups, detection accuracy

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