sensor FINT

1th sensorFINT International Conference

Non-Destructive Spectral Sensors
advances and future trends

10-12.05.2022 Izola, Slovenia

Book of abstracts

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1st SensorFINT International Conference
COST chair welcome

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 First International Conference “Non Destructive Sensors; Advances and Future Trends” (10-12 May, Izola, Slovenia).

I live with high enthusiasm the opportunity to be together again in this First SensorFINT International Conference sharing ideas, knowledge, challenges, and reflections on the advances and trend in the use of non-destructive spectral sensors for the food control, monitoring and authenticity issues, and I hope this enthusiasm be also mutual for all of you . I am convinced that SensorFINT Action gives us a great opportunity to spread the innovation of spectral technologies, improve the integrity of food chain, introduce and train the new professionals in this field and match industrial and business needs to the knowledge generated at the research level, reinforcing the European food industry competitiveness.

I would like to express my sincere personal thanks to Anna Sandak and InnoRenew CoE for providing the local organization and the Vice-Chair of this Action (Tom Fearn). Thanks to all of them for all the support, ideas and time dedicated to this event. Moreover, I would like to thank the keynote and the industry speakers for their kind availability to participate, the SENSORFINT MC and Core Group members, and all SensorFINT participants for making this possible. Finally, thanks of course to Cost for providing funds for this event.

I wish you all enjoy this Conference, the ideas and knowledge shared and the networking opportunities it will open up for us.

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

1st SensorFINT International Conference host welcome

We are very pleased to welcome you to the 1st SensorFINT International Conference of the COST Action 19145 “European Network for Assuring Food Integrity using Non-destructive Spectral Sensors”, dedicated to “Non-Destructive Spectral Sensors Advances and Future Trends”. Organising the conference has been a point of pride for us at the University of Primorska and InnoRenew CoE. We are particularly pleased to organise this event in our new building, which we hope you will have an opportunity to see and will inspire you to visit us again in the near future.

The programme is filled with novel research and we are looking forward to hearing all about it. We are sure the conference will foster open discussion and knowledge-sharing of past experiences and encourage you to reach out to your peers and continue with the discussions after the conference.

Non-destructive spectral sensors are widely applicable in various disciplines. This sort of interdisciplinary science is exciting for us, and this is why the University of Primorska and InnoRenew CoE have invested in personnel and spectroscopic equipment to help shape the future of spectroscopy in science and industry.

On behalf of both the University of Primorska and InnoRenew CoE, we would like to thank

Michael Burnard, PhD
Deputy Director InnoRenew CoE

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Programme Coordinator, Data Science
Master’s Degree Programme
University of Primorska

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PhD Programme
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1st SensorFINT International Conference organising committee welcome

Despite the pandemic that continues to affect Europe and the whole world, and the difficult political situation in Europe related to the ongoing war in Ukraine, we are very pleased to be able to organise the 1st SensorFINT International Conference in Izola, Slovenia. We do believe it is a great opportunity to meet each other face to face, to present our work, as well as exchange ideas, opinions, and future research topics.

We are especially pleased to present our four distinguished keynote speakers and dear friends, Dr. Jean-Michel Roger, Dr. Jens Petter Wold, Dr. Marena Manley, and Dr. Wouter Saeys who will share with us their years of experience in spectroscopy and present cutting-edge research in this field. We are also happy to organise a round table session to connect science and industry and facilitate discussions on how to meet and implement the needs of the industry We are thankful to our sponsors VIAVI Solutions, Optic Instruments, GranIT, and Q-interline for their generous support.

Wishing you a fruitful and inspirational time,

Associate Prof. Anna Sandak MC and CG member on behalf of the 1st SensorFINT International Conference organising committee

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- Anna Sandak, InnoRenew CoE, University of Primorska, FAMNIT

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Conference program

Tuesday, 10. 5. 2022

08:30	Registration	
09:00	Welcome	
	Session #1: Innovation in process control by means of NDSS *Session chairs: Tiziana Cattaneo and Christian Huck*	
09:15	**Keynote #1:** **Jens Petter Wold**	**In-line NIR spectroscopy for quality assessment of heterogeneous foods**
09:45	Coffee break	
10:15	Krzysztof Rutkowski	The usefulness of VIS/NIR techniques for maturity and quality assessment of plums at harvest and after storage
10:30	Alejandra Arroyo Cerezo	Raman through original food packaging – Authentication of the milk origin by animal species of sliced cheeses
10:45	Miguel Vega-Castellote	Optimization of the spectral acquisition process of watermelons using new generation portable and online instruments and study of the quality of the spectral data
11:00	Sílvia de Lamo Castellví	Authentication and quality control of edible insects using portable infrared spectroscopic devices
11:15	Jose Luis Aleixandre-Tudo	Non-invasive quantification of phenolic content in red and white wines using a portable fluorescence spectrometer
11:30	Eleonora Mustorgi	Multivariate online monitoring of a powder blending process using a miniaturized near infrared sensor
11:45	**Virtual poster session :** **Innovation in process control by means of NDSS** *Session chairs: Matija Milanič and Anna Sandak*	
3 min /poster	Clara Barnés i Calle	Determination of hydroperoxides by near infrared spectrometry as a rapid procedure to evaluate oxidation susceptibility in fish
	Cristina Zomeño	Predicting pork belly firmness with a portable NIR device
	Elena Fulladosa	In search to robust predictive models to determine the texture and ripening level of dry-cured ham

3 min /poster	Jakub Sandak	Using infrared spectra and molecular dynamic modelling for identification of valuable molecules in olive leaves
	Maria del Mar Giró Candanedo	Low-cost portable NIR spectrometers for fraud detection in fish
	María del Mar Garrido Cuevas	Suitability of a portable Near Infrared Spectroscopy sensor for its applicability to the on-site analysis of Extra Virgin Olive Oil
	Mecit Oztop	Predicting the Crystallinity of MW-Vacuum Crystallized Sucrose by Time Doman NMR
	Tiril Aurora Lintvedt	Raman Spectroscopy for In-line Estimation of Fatty Acid Features in Salmon Fillets
	Víctor Manuel Fernández Cabanás	Authentication of green asparagus of the Huétor-Tájar population variety by NIRS spectroscopy
	Giorgia Stocco	Rapid and non-destructive determination of Ca and P in milk using WDXRF
12:15 13:30	Lunch	
Session #2: Novel approaches for NDSS signal integration ***Session chairs: Jasenka Gajdoš Kljusurić and Vincent Baeten***		
13:30	Keynote #2: Marena Manley	**The road less travelled: NIR (hyper)-spectral imaging in cereal quality and safety**
14:00	Benoit Jaillais	Extraction of phenotypic traits from multispectral images by Deep Learning
14:15	Salvador Castillo Gironés	Use of hyperspectral imaging to classify 'Rojo Brillante' persimmon in three texture classes before and after storage
14:30	Luca Fiorani	DIALPAS, a New Non-destructive Spectral Sensor for Easy Real-time Sensitive Detection of Food Fraud
14:45	Krzysztof Bec	Sensor Fusion and Interpretation of Chemical Information in the Performance Profiles of Miniaturized NIR Sensors in Food Analytical Framework
15:00	Zakarya Al-Shaebi -online	Synergetic of Surface-Enhanced Raman Spectroscopy and Deep Learning in Antimicrobial Resistance Identification
15:15	Iztok Prislan	Hyperspectral imaging of gluten-free dough and bread
15:30	Coffee break	

	STSM Session *Session chairs: Cecilia Riccioli and Radu Ionescu*	
16:00	Sebahattin Serhat Turgut	An approach towards the evaluation of quality attributes of black tea samples: Implementation of a NIR-Spectroscopy based technique
16:10	Gonçalo Guedes	Toward a NIR smart sensor: digital filters for data curation
16:20	Irina Torres Rodríguez	Selection of the optimal region of interest for the quality prediction in oranges analysed using hyperspectral imaging technology
16:30	José Antonio Entrenas de León	Optimization and development of NIRS prediction models for their implementation in food process control
16:40	María del Mar Garrido Cuevas	Non-targeted multivariate methods using NIR sensors for increasing sampling during on-site official inspections of virgin olive oils
16:50	Stella Ordoudi	Methodological challenges in the assessment of virgin olive oil (VOO) adulteration using FTIR spectroscopy and chemometrics
17:00	Ice breaker	

Wednesday, 11. 5. 2022

08:30	Registration	
	Session #3: Real-time methodologies for processing NDSS data *Session chairs: Marina Cocchi and Soren Engelsen*	
09:00	**Keynote #3: Jean-Michel Roger**	**Increasing the robustness of chemometric models by calibration transfer, orthogonal projections, domain adaptation**
09:30	Sebastian Orth	Spectral sensors and a novel multiblock data fusion approach for barley pre-harvest germination discriminant analysis
09:45	Marina De Gea Neves	Investigation of bread staling by handheld NIR spectroscopy in tandem with 2DCOS and MCR-ALS analysis.
10:00	Candela Melendre-ras García	On-site sensors for quality control of Breast Milk
10:15	Sergio Forcada	In-situ quantification of sugar content in intact green bean pods by Near Infrared Spectroscopy
10:30	Coffee break	

11:00	Arnaud Molle	The use of milk Fourier-Transform Infrared spectra for predicting cheese making traits in Grana Padano PDO
11:15	Lorenzo Strani	Different chemometric approaches to monitoring pesto sauce quality in an industrial process
11:30	Justyna Grabska	NIR Spectra Simulation in Aid of Food Analytical Framework. Understanding of Matrix Effects and Improved Detection of Adulterants
11:45	Fatih Kahrıman	Comparison of Different NIR Instruments for the Determination of Oil Content in Single Maize Kernel
12:00 13:00		Lunch
	**Virtual poster session:** **Real-time methodologies for processing NDSS data** ***Session chairs: Matija Milanič and Anna Sandak***	
3 min /poster	Jana van Rooyen	Application of ASCA to characterise effects of roasting temperature, -time and milling method on SWIR spectral data of whole and milled wheat
Advances in decision support systems for efficient control in the food supply chain		
3 min /poster	Irina Torres Rodríguez	In situ authentication of Iberian pork meat using Near infrared spectroscopy
	Jasenka Gajdoš Kljusurić	Near infrared spectroscopy as authentication tool of protect design of origin for Dalmatian wine produced from grape Maraština
	José Antonio Entrenas de León	Ready to use vs specific NIRS calibrations for determination of chemical parameters of Processed Animal Proteins (PAPs) meals
	Liudmil Antonov	Near Infrared Diffuse Reflectance Spectroscopy with Partial Robust M- Regression(PRM) as Sensory Tool for on-line Control of Biscuit Dough Production
	Madalina Belous	Evaluation of Plant Bioactive Compounds Activity and Stability by Spectroscopic Methods
	Sebahattin Serhat Turgut	Use of chemometrics for decision support in food quality assurance: an example study for tea blending
	Tassos Koidis	Detection of offal adulteration in minced beef products using Near-Infrared (NIR) spectroscopy
Matching scientific progress to industrial needs – alternative strategies for knowledge transfer		
3 min /poster	José Blasco	A non-destructive method to measure the light penetration depth and optical properties of “Rojo Brillante” persimmons

3 min /poster	Dijana Blazhekovikj Dimovska	Determination of polycyclic aromatic hydrocarbons (PAHs) in commonly consumed smoked fish
	Dilip Sing -online	Rapid quality assessment of Andrographis paniculata using a developed portable infrared spectroscopy instrument
	Maria Tarapoulouzi -online	Discrimination of Halloumi cheese samples regarding species' origin
	Sara Chumillas Lidón	A collaborative platform economy to accelerate the democratization of NIR-based quality control in the food industry
	Tiziana Cattaneo	Evaluation of the effect of different soil fertilizers on rice plants using a hyperspectral imaging system
	Tiziana Cattaneo	NIR calibrations to predict stress related parameters in rice plants fertilised with sewage sludge
	Nežka Sajinčič	Learning about NDSS through video – Evidence-based guidelines for effective instructional videos for a smooth transition into industry
14:00	**Sponsors session** ***Session chairs: Anna Sandak and Matija Milanič***	
14:30	 Coffee break	
15:00 16:30	 **Industry round table** ***Session chairs: Lola Pérez-Marín and Tom Fearn***	
16:30- 19:00	 Free time	
19:00 21:30	 Gala dinner	

Thursday, 12. 5. 2022

08:30		Registration
	Session #4: Advances in decision support systems for efficient control in the food supply chain & 5 Matching scientific progress to industrial needs – alternative strategies for knowledge transfer *Session chairs: Elena Fulladosa and S. Serhat Turgut*	
09:00	**Keynote #4: Wouter Saeys**	**Harvest planning in apple and pear with spectral sensors in the orchard**
09:30	Evgeni Eltzov	Reduce food losses by developing non-destructive biosensors for real-time rots detection in the stored agriculture produce
09:45	Stefka Atanassova	Dairy products quality assessment by use of near-infrared spectroscopy
10:00	Christian Huck	Current Status and Future Trends of NIR Spectroscopic Analysis of Foods
10:15	Szilveszter Gergely	Monitoring the change in particle size of dried egg-pasta due to different grinding parameters by diffuse reflection near-infrared spectroscopic techniques
10:30	Claudia Beleites	Open-Source Development of Portable NIR-Sensor Measurement Setups for Plant Leaves
10:45	Marcello Vanzulli	QualiControl: Smart Cloud based NIR solutions for industry
11:00		Closing of the conference
11:10		Coffee break
11:30-12:45		MC meeting
12:45 13:45		Lunch
14:00-17:00		Post-conference tour

Session #1:
Innovation in process control by means of NDSS

Keynote #1: Jens Petter Wold
In-line NIR spectroscopy for quality assessment of heterogeneous foods

Dr. Jens Petter Wold is a senior research scientist at Nofima AS, Norwegian Food and Fisheries Research Institute, Norway. He has a PhD in Food science and bio-spectroscopy from The Norwegian University of Life Sciences in Ås, Norway. In 2001-2002 he spent one year at Centre for process analytical chemistry (CPAC) in Seattle, WA. He has published more than 100 scientific papers within the field of rapid and non-destructive quality assessment of foods and is specialized within fluorescence, near-infrared and Raman spectroscopy, including hyperspectral imaging. He has contributed to a successful in-line NIR hyperspectral imaging system (QVision 500, TOMRA) which is used worldwide for in-line food quality control. Jens Petter is now director of SFI Digital Food Quality (www.digifoods.no), a centre for research driven innovation with the aim of developing smart sensor-driven solutions that deliver the essential food quality information required for successful process optimization and digitalization of the food industry.

Lecture: In-line NIR spectroscopy for quality assessment of heterogeneous foods

Near-infrared spectroscopy (NIRS) is a potent method for true-time quality control and process monitoring in the food industry, and the potential for process optimization is large. NIRS is an excellent tool for rapid and nondestructive determination of typically fat, water, protein and carbohydrates in various foods and different applications are established for both at-line and in-line monitoring, and different types of commercial near-infrared (NIR) instruments are used for this.

Representative sampling is often a limitation with spectroscopic methods regarding heterogeneous foods. NIR reflection works very well on continuous streams and for determination of bulk composition of e.g. ground meat. But when single products need to be characterized, such as chicken fillets, fish fillets or crabs, we meet challenges due to heterogeneity of the products. The surface is usually not representative for the interior of the sample. And maybe the chemical composition varies also around at the surface. Near-infrared radiation in the wavelength region 760-1100 nm is relatively weakly absorbed by water and has therefore a good penetration depth in most foods. This enables transmission and interactance measurements so that larger volumes of the samples can be probed. NIRS also lends itself very well to hyperspectral imaging, which is a powerful tool for effective sampling of heterogeneous foods. In this talk I will present and discuss the challenges of heterogeneity and how they can be solved by novel and tailor-made instrumentation. Many of the presented examples are now well working smart sensors in the food industry.

Krzysztof Rutkowski

The usefulness of VIS/NIR techniques for maturity and quality assessment of plums at harvest and after storage

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The usefulness of methods based on VIS/NIR for nondestructive assessment of maturity and quality of plums ('Presenta', 'President' and 'Tophit' cvs) at harvest and after storage was evaluated. Nondestructive measurements were performed using DA meter (Sintéleia, Italy) and CP Pigment Analyzer PA110[1] (Control in Applied Physiology GbR., Germany). The DA index (DA meter) was calculated as DA=A670-A720 (A670 and A720 are absorbances at 670 and 720 nm). In the case of CP Pigment Analyzer signal at wavelengths in the range from 400 nm to 1100 nm was gathered. Two standard indices were computed: Normalized Difference Vegetation Index NDVI calculated as (I780-I660)/(I780+I660) and Normalized Anthocyanin Index NAI (I780-I570)/(I780+I570) where I570, I660, and I780 are reemittances at 570, 660 and 780 nm.

Besides the nondestructive measurements, the following quality parameters were measured: fruit weight, skin colour (with and without epicuticular wax), fruit firmness, soluble solids content, and titratable acidity.

During fruit storage, DA, NDVI, and NAI indices steadily changed. The rate of changes depended on storage conditions and cultivar.

On the raw spectra collected from CP Pigment Analyzer we found changes in signals reemission in the case of plums with internal browning in comparison to sound plums. However, further detailed research is required to fully utilize non-destructive methods based on VIS/NIR to assess internal damage to plums as well as estimation of soluble solids content, acidity, and firmness.

The results of the conducted research indicate the possibility of limiting the naturally occurring variability in the quality and maturity of plums intended for storage. By using VIS/NIR spectroscopy, plums can be sorted into "ripeness" classes. Because the fruits from individual classes kept their "distinctiveness" until the end of the storage period, it should be stated that VIS/NIR is a very useful tool for qualitative equalization of the plums offered on the market.

Keywords: plums, nondestructive, VIS/NIR, ripening, quality, storability, disorders

Acknowledgements: The research was carried out within the statutory programme of the National Institute of Horticulture Research (ZPiPOiW/5/2016 - P 6.1.3).

Alejandra Arroyo Cerezo

Raman through original food packaging – Authentication of the milk origin by animal species of sliced cheeses

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The animal origin from which some types of foodstuffs are produced is a determining factor leading to a higher or lower quality of the product. As a consequence, these foods can be subject to fraud and require adequate authentication. In this sense, dairy products such as cheese are susceptible to fraud. The main ingredient is milk, which can be obtained from cows, goats, sheep or buffalo, among other animals. The mammal from which the milk used to produce cheese is obtained gives this product different characteristics and qualities. One of the reported frauds in this type of food is, for example, the substitution of milk with cheaper lower quality milk or misleading labeling statements. The methodologies used for the milk/cheese authentication are complex, especially as they require pre-treatment of the sample. Moreover, they are based on the study of specific compounds (chemical markers), without taking into account that the final composition can be affected by many factors. Therefore, it would be advisable to develop new analytical methods for assessing the authenticity according to the animal species from which it was produced. This research presents the application of a portable device with the ability to perform non-invasive measurements through the original food packaging. The spatially offset Raman spectroscopy (SORS) technique was used to acquire rapidly and easily the instrumental fingerprint of 105 sliced cheese samples measured through their original packaging. The application of chemometrics to the Raman data allowed the development of a machine learning model to differentiate the animal species providing the milk used in production of cheese samples studied and thus reliably verify the labeling conformity of these products.

Keywords: Spatially offset Raman spectroscopy (SORS), cheese authentication, milk origin by animal species, machine learning methods.

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This work was partially supported by University of Granada (Spain), program 'Pre-competitive Research Projects for Young Researchers' (PPJIA2021.09). REFERENCES

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Miguel Vega-Castellote

Optimization of the spectral acquisition process of watermelons using new generation portable and online instruments and study of the quality of the spectral data

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The acquisition of high quality spectra and the optimization of the spectra taking process are crucial for the success of the non-destructive quality characterization of horticultural products by near infrared spectroscopy (NIRS), during their growing period in the field and in the industrial processing lines. The aim of this research was to assess various alternatives related to the mode of analysis and the configuration of two new generation NIRS instruments, which were suitable for the in situ and online analysis of the watermelons respectively, in order to optimise the quality of the NIRS fingerprint of fruits acquired. Once the alternatives were evaluated, the most suitable option was identified for each instrument. In addition, given the importance of obtaining representative spectral libraries of the watermelons analysed in order to develop robust quality prediction equations, the RMS statistic was calculated, and the spectral repeatability results were evaluated for the all the fruits analysed in the assays.

Keywords: watermelon, optimization, spectral repeatability, portable device, online NIRS instrument

Sílvia de Lamo Castellví

Authentication and quality control of edible insects using portable infrared spectroscopic devices

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Analytical chemistry is moving towards simpler, and less time-consuming methods. Progress in miniaturization of vibrational spectroscopy components (micro-electro-mechanical systems (MEMS), solid-state lasers, optical components, wavelength selectors, and detectors) has allowed the development of portable or hand-held systems. These devices are simple to use, require minimal or no sample preparation with higher operational speed. Moreover, these spectrometers perform similar than laboratory benchtop instruments without compromising spectra sensitivity and quality (Rodriguez-Saona et al., 2020; Yan and Siesler, 2018).

By miniaturizing vibrational spectroscopy equipment, the food industry can monitor food products and production processes in-situ and in real-time to ensure product safety, quality assurance, authentication, and detection of adulteration, and contaminants in foods (Rodriguez-Saona et al., 2020; Shiroma and Rodriguez-Saona, 2009).

This technology can be easily applied to the emerging insect sector. As an alternative to ensuring food and feed security, edible insects are being considered, are good source of nutrients such as proteins, lipids, minerals, and chitin. Additionally, insects are considered an innovative technology for waste management (Gkinali et al., 2022).

The present study evaluates a new approach to predict the amount of lipids present in commercial edible Tenebrio molitor using near infrared mini spectrometer. Insect powders were placed inside a polyethylene bag of 7 x 11 cm (30 g, 1 cm of height). The spectra were collected by direct contact between the detector and the plastic bag from 7750 to 3750 cm-1. Principal Components Analysis (PCA) model was to build up to identify the differences among the samples tested and Partial least squares regression (PLSR) model was used to quantify the amount of lipids present in the insect powder.

Keywords: miniaturization, chemometrics, NIR, food safety, edible insects

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Jose Luis Aleixandre-Tudo

Non-invasive quantification of phenolic content in red and white wines using a portable fluorescence spectrometer

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Phenolic compounds contribute to some of the most important red and white wine quality attributes. These compounds are mainly involved in the colour and mouthfeel properties of wines. In red wines, phenolic compounds are extracted during maceration as the goal is to optimise the phenolic extraction and ensure optimal colour and mouthfeel properties. In white wines, the objective is to minimize and control phenolic extraction during early stages of winemaking to ensure that the mouthfeel properties are not compromised. In a previous study, we first assessed the suitability of fluorescence spectroscopy to quantify phenolic content from undiluted and untreated samples (dos Santos et al., 2022). Accurate regression calibrations were obtained making use of XGBoost regression. After the identification of the fluorescence parameters that allowed for the accurate quantification of phenolic compounds, a simplified portable fluorescence spectrometer was built making use of single excitation (280 nm) and multiple emission. The fluorescence properties of red wine fermenting samples were measured together with the phenolic content. PLS calibrations were then attempted, and accurate models were obtained. For white wines, the spectral properties of samples at different times during the pressing operation were obtained. In this case, the total phenol content of the samples was measured. The results showed that it was also possible to quantify the total phenol content in white wine juice samples. In addition, a measuring chamber was constructed allowing for front-face and direct reflection measurements. The chamber can be incorporated in a fermenting tank or in a pipe at the outlet of the press. The nature of fluorescence technology and the set up of the instrument also allows for direct reflexion ultraviolet measurements. The simplicity of this portable spectrometer and the fact that relies on ultraviolet visible technology provides a valid and cost-effective alternative to other available technologies.

Keywords: fluorescence spectroscopy, unaltered samples, direct measurements, phenolic compounds, chemometrics

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Eleonora Mustorgi

Multivariate online monitoring of a powder blending process using a miniaturized near infrared sensor

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In the present work, the blending process of the solid fraction of a commercial energy drink has been monitored thorough the implementation of a miniaturized near infrared (NIR) device coupled with multivariate process monitoring. A critical step in energy drink production is the blending phase, in which the ingredients are mixed together until the endpoint of the process is reached, so when the product can be considered as homogeneous as possible. The definition of the process endpoint is, usually, done according to a specific blending duration, decided on experience bases – an approach that is totally blind to any modification occurring during the process itself. The main goal of the present work was the development of a multivariate strategy for the real-time monitoring and verification of the blending phase in a continuous and non-destructive way, determining a specific process endpoint for every single batch, in a quality by design (QbD) view.

In order to reach the aim, a MicroNIR PAT-W sensor (Viavi Solutions), working in the spectral range between 900 and 1700 nm, has been directly setup on a laboratory-scale blender, enabling the acquisition of a spectrum every 4 s, through a sapphire window during the whole process. The spectral information provided by a portable device has been modelled with three different chemometric strategies for the qualitative blend endpoint determination: Principal Component Analysis (PCA), Moving Block Methods (MBM) and Multivariate Curve Resolution (MCR). The outcomes obtained for seven independent batches have been critically commented highlighting the pros and cons of each strategy.

Keywords: Process monitoring, PAT tool, NIR portable device, Chemometrics

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Session #2:
Novel approaches for NDSS signal integration

Keynote #2: Marena Manley

The road less travelled: NIR (hyper)-spectral imaging in cereal quality and safety

Marena Manley initiated and implemented research using and applying near-infrared (NIR) spectroscopy research at the University in the late 1990s. This was followed by the introduction of NIR hyperspectral imaging research in the mid-2000s. Her research group was one of the first to perform such work in South Africa and Africa and to publish cereal NIR hyperspectral imaging investigations. After completing her PhD and 18 months at an NIR spectroscopy instrument manufacturing company in the United Kingdom, Marena joined Stellenbosch University in 1997. She has been a professor at the Department of Food Science since 2010 where she has supervised more than 70 postgraduate students and published more than 110 papers. In addition to NIR spectroscopy and hyperspectral imaging research, which focuses mainly on grain (wheat, maize, barley), Marena and her postgraduate students also investigate X-ray microcomputed tomography as an analysis technique. This is mostly applied to study and characterise cereal grains and baked products. Marena also supervises cereal technology and chemistry research projects.

Lecture: The road less travelled: NIR (hyper)-spectral imaging in cereal quality and safety

Near infrared (NIR) hyperspectral imaging has increasingly been investigated for the quantification of cereal grain composition and detection of quality and safety characteristics, since the first publication in the mid-2000s. It advances on conventional NIR spectroscopy by offering, in addition to compositional, spatial information. This enables more detailed characterisation of heterogenous cereal samples. Early studies on whole grain cereals used the advantage of pixel-wise information. However, when objects from different classes have many similar pixels, the object-wise approach may provide more accurate predictions. The object-wise approach is increasingly used in recent NIR hyperspectral imaging (or in this case rather spectral imaging) investigations. Object-wise refers to the average or median spectrum of all pixels in an image (or part thereof) for development of prediction or classification models. Although there is merit in the use of the object-wise approach, the value of the information provided in the spatial dimension of a hyperspectral image with the pixel-wise approach should not be underestimated or neglected. These and other trends/advances in cereal quality and safety applications with NIR (hyper)-spectral imaging will be presented and discussed.

Benoit Jaillais

Extraction of phenotypic traits from multispectral images by Deep Learning

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Plant phenotyping corresponds to the identification of effects resulting from interactions between genotype and environmental conditions. Among fast and non-destructive technologies, multispectral imaging, combining image and spectrum, increases the understanding of biology by allowing the measurement and quantification of a large amount of phenotypic information in a single analysis.
A phenotyping robot "Phenotim" has been specially designed and developed, with a multispectral LED imaging system as detector. The high throughput of the robot (about 500 images per 24-hour period) requires a paradigm shift in data processing to deep learning, based on the use of UNet.
From the obtained multispectral images, phenotypic traits were estimated on 80 sample lots, constituted by 20 accessions × 2 locations × 2 years. The number of grains per lot was 500 minimum. The traits were the following ones for each grain and for each batch of samples: dimensions of the cut grain as length and width, the depth of the crease, the thickness of the peripheral layers and the vitreousness.
Two UNet models were built to transform a multispectral image of cut grain into a segmented image: one corresponding to the whole grain and the second to the grain without the peripheral layers. These models were trained with a random selection of images coming from various lots. All multispectral images were projected onto both models leading to segmented images on which phenotypic traits were estimated.
The design and realization of the robot has thus solved the bottleneck problem of phenotyping. The optimized image processing procedure based on deep learning on the one hand and GPU computing on the other hand allowed to process a collection of 32,000 multispectral images in two hours.

Keywords: deep learning, high-throughput phenotyping, multispectral image, wheat.

Acknowledgements: This study was supported by the Agence Nationale de la Recherche of the French government through the programmme “Investissements d’Avenir” (16-IDEX-0001 CAP20-25) and by the Infrastructure Biologie Santé “Phenome-Emphasis” (PIA) (ANR-11-INBS0012).

Salvador Castillo Gironés

Use of hyperspectral imaging to classify 'Rojo Brillante' persimmon in three texture classes before and after storage

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Fruit preservation can cause texture alterations which may affect consumers acceptance if conditions are not appropriate. Hence, fruit classification based on texture alterations can be of interest for food industries. Whereas artificial vision systems have been used in fruit to detect external quality of fruit, detection and classification based on texture cannot be done accurately using external information. Hyperspectral visible (VIS) and near-infrared (NIR) imaging has already been used to assess internal and external quality of the fruits, and thus, it can be a tool to obtain texture classification. The objective of this work was to predict three types of changes in the texture of persimmon fruits under different types of storage conditions using Vis/NIR hyperspectral imaging.

A total of 3,340 persimmon cv 'Rojo Brillante' were stored for three months at different conditions of temperature, and part of the fruits were treated with 1-MCP before storage with the aim to produce different texture alterations. At the beginning of the experiment, and every month, the texture of a random set of fruits was measured with a texturometer, recording the force curve until fracture. In addition, Hyperspectral images of these fruits were acquired with a Vis-/NIR hyperspectral imaging system (420-1010 nm), and mean of each persimmon was extracted. Samples were randomly divided into training set (70%), used used 10-fold cross-validation, and independent test set (30%). Then, spectra was were pre-treated with standard normal variate (SNV). Models based on partial least squares discriminant analysis (PLS-DA), support vector machine (SVM) and random forest (RF) were used to separate the fruit with different textures. Preliminary results obtained from the test set showed a prediction accuracy higher than 90%.

Keywords: Diospyros kaki, hyperspectral imaging, VIS-NIR, prediction, texture

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Luca Fiorani

DIALPAS, a New Non-destructive Spectral Sensor for Easy Real-time Sensitive Detection of Food Fraud

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The increasing globalization of world trade, without mutual recognition of international standards, urgently requires new technologies for reliable assessment of food integrity. The DIM Laboratory of FSN Department – ENEA applies spectroscopic techniques to fraud detection in fruit juice, oil, oregano, milk, pollens, rice, saffron, and sea food. Although a wide range of cutting-edge methods are in the DIM Laboratory armoury – LIBS (laser induced breakdown spectroscopy), FTIR (Fourier-transform infrared spectroscopy), Raman spectroscopy, spectro fluorometry, remote sensing – its flagship technology is LPAS (laser photoacoustic spectroscopy). In a typical LPAS system (Fiorani L. et al., 2021), a laser beam is modulated at an audio frequency and injected into a resonant cell where it hits the investigated sample that absorbs the incident radiation. The sample therefore experiences a rise in temperature and volume, thus producing a pressure wave. In general, the sound detection subsystem is made of a microphone connected with a lock-in amplifier synchronized with the modulator. The output signal is proportional to the sample absorption and typical experiments are conducted in the “fingerprint region”, a large band of the infrared (IR) spectrum where many organic compounds can be identified. The studies carried out at the DIM Laboratory showed that LPAS has the following advantages: rapidity, sensitivity, specificity, simplicity, repeatability, in situ measurement, uncomplicated sampling, ease of use and cost-effectiveness. Current systems are based on quantum cascade laser (QCL) that can be continuously tuned in a large spectral range. This latter characteristic is very important for non-targeted approaches. Moreover, QCLs are robust and small, allowing one to develop a portable system for rapid detection of food fraud in industrial settings. Recently, DIALPAS – an improved approach of LPAS (patented) – spotted within seconds a significant economically motivated adulteration (EMA) on untreated samples with a limit of detection of a few percent.

Keywords: quantum cascade laser application, laser spectroscopy, photoacoustic technique, differential absorption, food fraud

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Krzysztof Bec

Sensor Fusion and Interpretation of Chemical Information in the Performance Profiles of Miniaturized NIR Sensors in Food Analytical Framework

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Handheld NIR spectrometers are becoming essential in food analytical framework (Bec, Grabska and Huck, 2020). However, sensor miniaturization requires implementing a number of distinct engineering solutions, and these sensors differ by the key elements used for their construction, performance and applicability. Recent advancements have brought feasibility of theoretical in silico simulation of NIR spectra (Bec and Huck, 2019; Ozaki et al., 2021). Narrow spectral working regions of miniaturized instruments limit their ability to measure meaningful vibrational bands, making them selective towards specific chemical constituents in food matrices. Through in silico approach, the location of meaningful variables can be associated with specific molecular vibrations. The sensitivity and specificity of a sensor to chemical information from a given ingredient in a complex NIR lineshape of a food sample can be determined enabling smart design of NIRS application (Grabska et al., 2021).

Detailed comprehension of the analysed spectral signal opens the pathway to knowledge-based design of the food analytical framework by NIRS towards better performance. A direct improvement of performance of sensors with mutually exclusive operational spectral regions may be accomplished by data fusion. Several cost-effective miniaturized NIR sensors appeared at the market, specifically intended for food analysis. Sensor fusion offers convenient uplift in performance by combining spectra measured in different wavenumber regions enabling an extended access to chemical information for more reliable calibration.

Keywords: sensor fusion, chemical interpretation of calibration models, in silico NIR spectroscopy

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Zakarya Al-Shaebi

Synergetic of Surface-Enhanced Raman Spectroscopy and Deep Learning in Antimicrobial Resistance Identification

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Antimicrobial Resistance (AMR) has become one of the global threats causing ten million deaths each year when reaching 2050 (WHO, 2019). To tackle this pandemic, increasing people's awareness of the risk and consequences of the misuse of antimicrobial drugs is a priority. Secondly, to decrease the number of cases, rapid, reliable, and easy-to-use technology should exist to enable identifying the type of bacterial infection properly and recommending the appropriate drug. In this study, Surface-Enhanced Raman Spectroscopy (SERS) combined with deep learning was used to detect and identify antimicrobial resistance with a high-accurate rate. Methicillin-resistant Staphylococcus aureus (MRSA) and methicillin-sensitive Staphylococcus aureus (MSSA), which are common AMR causing several health concerns, were studied and large data were collected for both AMR by SERS and then two deep learning models, U-Net and VGG-16, were employed to classify them. Before classifying our dataset (Uysal et al., 2020), we carried out the U-Net architecture to classify data for MRSA and MSSA collected by (Ho et al., 2019). With an accuracy of 95%, the model had the lead over different models that used the same data. For our data which consists of 9000 spectra for MRSA and 4500 spectra for MSSA, we used 5-fold cross-validation to ensure the efficiency of the models. The U-Net architecture was successfully able to extract the feature map and then classify AMR astonishingly with an accuracy of 98.83 ± 0.13%. The VGG-16 has shown brilliant performance as well with an accuracy of 99.87 ± 0.014%. In brief, this study has demonstrated the important role of the synergy between SERS and deep learning in the identification of bacterial infection and we believe it can be used and extended for several biomedical and food security applications.

Keywords: antimicrobial resistance, surface-enhanced Raman spectroscopy, Staphylococcus aureus, deep learning, MRSA, MSSA

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Iztok Prislan

Hyperspectral imaging of gluten-free dough and bread

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Production of a high quality gluten free bread is a big challenge due to the absence of gluten, which confers unique viscoelastic properties to dough (Houben et al., 2012). To overcome this challenge, different approaches are used in preparing gluten-free products, such as the use of different gluten-free flours (rice, maize), starches (corn, potato, cassava) and ingredients such as hydrocolloids

Food is a complex system that contains a lot of different compounds. These compounds can interact with each other and with food additives, such as hydrocolloids and may change the quality of the baked gluten-free product. Sensory analysis is usually a method of choice in food product development and quality control but tests must be set up in a specific way to minimize errors and biases during testing. To ensure both high food quality and requisite safety standards new analytical procedures using cameras and spectral imaging devices are being developed. In recent years HSI has become an important imaging modality in the food science and agriculture, especially in the food safety inspection and food quality control (Liu et al., 2017). The objective of this study is to explore sensory and spectral properties of gluten-free bread. We have used sensory analysis and HSI to evaluate baked gluten-free bread. The obtained data were compared to try to find correlation between physico-chemical properties of different model doughs and sensory properties of gluten-free breads with a final goal to identify the crucial factors that yield better gluten-free bread.

Keywords: gluten-free bread, hydrocolloids, hyperspectral imaging, dough, sensory analysis

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STSM Session

Sebahattin Serhat Turgut

An approach towards the evaluation of quality attributes of black tea samples: Implementation of a NIR-Spectroscopy based technique

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To assure the quality and economy of black tea, its quality attributes are frequently checked before it is bought, blended, and marketed. Although some of these quality attributes may be measured analytically, others must be evaluated as sensory scores as a result of cupping tests undertaken by tea professionals. However, most of these assessments (particularly sensory ones) need experience and training, require time, and are open to human mistakes. Addressing these reasons, non-destructive spectral sensors were combined with chemometric methods in this study to examine the feasibility of rapid measurement of the cupping test scores for appearance, body, colour, and overall quality, as well as some other important sensory-related quality attributes (bulk density, cellulose, water extract, and moisture) of black tea samples. As regression techniques, Partial Least Squares Regression and Principal Components Regression with stepwise variable elimination were utilised, and three separate spectrum instruments were used. The findings show that Partial Least Squares Regression combined with FT-NIR technology may be promising for the quick and cost-effective evaluation of sensory scores and associated attributes for usage in the tea industry.

Keywords: black tea, cupping, sensory, blend

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Gonçalo Guedes

Toward a NIR smart sensor: digital filters for data curation

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Handheld NIR spectrometers can be used for on-site and in-the-field analysis, have a high acquisition rate and, in most of the cases, do not require sample preparation. However, some shortcomings are also noteworthy in industrial settings such as variability on signal-to-noise ratio, low reproducibility induced by movement, changes in luminosity and temperature, to mention just a few. Hence such “faulty spectra” generated during on-line data acquisition require a data curation step later in the data evaluation process, otherwise they will impact calibration performance.

The main objective of this work is to develop a set of digital filters for data curation enabling real-time database loading and data visualization as steps towards a “smart sensor” superseding operation supervision.

Port wine was chosen as a model system, since it represents a complex matrix due mainly to changes on chemical profile occurring with time. Firstly, spectra selected for the present investigations were collected using a benchtop FT-IR spectrometer. The consistency offered by the benchtop FT-IR spectrometer was essential for the comparison of the behavior of the digital filters. For this purpose, the samples were divided according to the color of the wine (White, Red, Rose). A PCA model was created for white wines and the distance between new samples and the center of the PCA (T2 Hotelling), as well as the distance between the plane of the PCA and the new samples (Q Residual) were used with digital filters. Thus, when a sample presents values of Q residual and T2 Hotelling that are outside the model, it is considered an outlier and discarded.

Secondly, model transfer between the benchtop spectrometer and a handheld instrument were attempted in order to make this approach available for on-site measurements suitable for authentication process with promising preliminary results.

Keywords: NIR, Smart Sensor, Digital Filter, Data Curation

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Irina Torres Rodríguez

Selection of the optimal region of interest for the quality prediction in oranges analysed using hyperspectral imaging technology

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The use of Hyperspectral Imaging (HSI) for the determination of quality in oranges has been previously assessed in different research works. However, since this technology provides both spectral and spatial information, it is essential the reduction of data for the implementation of this technology at industrial level. Nevertheless, an excessive reduction can cause a loss of important data, being crucial to select the most representative information of the sample, which is especially challenging in the case of products of great heterogeneity. It is in this context that the importance of this work, carried out in the framework of a SensorFINT Short-Term Scientific Mission (STSM) at the University of Modena and Reggio Emilia, lies. The aim of this work was the optimization of the selection of the region of interest (ROI) in oranges hyperspectral data to determine internal quality parameters related to the consumer acceptance, such as soluble solid content (SSC), titratable acidity (TA), maturity index and BrimA. For this purpose, a total of 250 oranges were analysed using a hyperspectral camera working in the spectral range 946.6-1648.0 nm. Partial least squares regression (PLS) and its multilinear version (NPLS) were compared. VIP scores obtained from the NPLS model were used to select the most relevant pixels to predict the studied parameters, reducing the data redundancy. The results obtained demonstrated the viability of using HSI for predicting internal quality in oranges. Furthermore, the selection of the most representative pixels by means of the VIP scores confirms its adequacy for data selection, enabling to reduce the computational time without a reduction of the robustness, when applied to a hyperspectral data set of oranges as complex and large as the one used in this work.

Keywords: Hyperspectral imaging, oranges maturity, pixel selection, multilinear models

Type of presentation: STSM Presentation

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values of Q residual and T^2 Hotelling that are outside the model, it is considered an outlier and discarded.

José Antonio Entrenas de León

Optimization and development of NIRS prediction models for their implementation in food process control

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Due to the complexity involved in obtaining robust NIR agri-food applications, it is crucial to reinforce the links between the academia and instruments and software developers, in order to exchange knowledge and practice about the opportunities offered by the different instruments and accessories available in the market for each food and feed application as well as optimize sample analysis and data treatment adapting them to the requirements of a given food/feed industry. For this purpose, a SensorFINT Short-Term Scientific Mission (STSM) was carried out from July 26th, 2021, to August 6th, 2021, by the first author and under the supervision of Dr. Andreas Niemöller.

First, the equipment assembly plant of Bruker Optik GmbH was visited to obtain knowledge about the design and technologies in which the instruments offered by Bruker are based. Then, a training was completed on the OPUS and CMET software for the development and optimization of quantitative models for the prediction of parameters related to food quality, with special emphasis on the real implementation of these models. Finally, thirty-one different types of vegan spreads were analysed in the MPAII and Tango instruments which are based on FT-NIR technology. All samples were analysed both in glass and polystyrene petri dishes (GLPD and PSPD respectively), in all cases in duplicate. Prediction models of Fat (%) and Protein (%) parameters were developed, for which the commercial reference values were used. Four Hummus samples ,from the total of 31 vegan spread samples available were used to make the validation set. The results obtained showed that this type of samples can be analysed using both GLPD and PSPD dishes, obtaining prediction models of high quality.
Keywords: food process control, FT-NIR analysis, vegan spreads, sample presentation

Acknowledgements: J. Entrenas deeply thank to the “European Network for assuring food integrity using non-destructive spectral sensors” (SensorFINT) for providing funding that enabled him to conduct this fruitful training.

Type of presentation: STSM Presentation

María del Mar Garrido Cuevas

Non-targeted multivariate methods using NIR sensors for increasing sampling during on-site official inspections of virgin olive oils

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Despite the huge amount of efforts invested in research into physic-chemical and sensory methods for determining the quality, purity and authenticity of virgin olive oils (VOOs), the adulteration of VOO with low-quality oil remains a major international problem. One of the main reasons for the recurrent frauds episodes is that the volume of VOOs officially inspected is low, due to reduced national budget for the analysis of the inspected samples by the International Olive Council (IOC) and European standardised wet chemistry methods. Near Infrared Spectroscopy (NIRS) technology has shown its potential both for the prediction of quality and purity parameters in olive oil and for its classification into commercial categories. Portable NIRS sensors, machine learning methods and ICT could offer a radical new approach for on site official inspections. However, there is still a wide field of research before offering olive oil Official Inspectors a ready-to-use portable NIRS instrument and on-site applications. The first author is in the first year of her PhD studies and her research is in the framework of a large national R & D project entitled “NIRS technology and IoT platforms for ensuring the integrity of high added value Spanish products: Iberian cured ham and Extra-virgin olive oil”

A short-term scientific mission (CA19145) has been approved to be carried out during July 2022, under the supervision of Prof. Paolo Oliveri. The main goal of the STSM is to improve the chemometric skills, on novel mathematical pattern recognition algorithms for the development of non-targeted applications, to undertake real-time on-site analysis of a large volume of VOO samples. To accomplish that goal, it will be used a database of about 500 olive oil samples already analysed in several NIRS instruments of different optical configurations.

Keywords: Portable Near infrared spectroscopy, pattern recognition methods, non-targeted spectral methods, Virgin Olive Oil integrity.

Acknowledgements: Mar Garrido-Cuevas would like to thank to the Chair, the Vice Chair and the STSM coordinator of CA19145, for providing her this great learning and networking opportunity. The STSM is expected to provide many learning opportunities and perhaps to publish a relevant paper of interest, not only for scientists, but also to VOO industrialists, instrument developers and regulatory agencies.

Stella Ordoudi

Methodological challenges in the assessment of virgin olive oil (VOO) adulteration using FTIR spectroscopy and chemometrics

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Literature survey indicates a plethora of published research efforts over the decades to address VOO adulteration, an ever existing problem in the market (Casadei et al., 2021). Since early 90's when FTIR spectroscopy was first applied to this field, its proof-of-concept was explored in many studies on substitution of VOO by cheap seed oils (e.g. sunflower, corn, soybean and canola oil) or nut oils, such as peanut and hazelnut (Nenadis & Tsimidou, 2017). The studies employ FTIR spectroscopy alone or in combination with other spectroscopic techniques to assess VOO adulteration using either targeted or non-targeted methods of data analysis. This work critically analyses literature findings regarding the methodological strategy from sampling design, spectra acquisition to data modelling, after searching the Web of Science and Scopus databases.The need to develop guidelines covering the criteria for the selection of the "reference" oil samples and the preparation of admixtures, measurement conditions (type of Attenuated Total Reflectance cell, resolution, number of scans, replicates) and steps for the development and validation of models was revealed. Existing issues of sensitivity, specificity or reliability are challenging and discussed in depth.
Keywords: virgin olive oil, adulteration, seed oils, FTIR spectroscopy, PCA, PLS, SIMCA

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Session #3:
Real-time methodologies for processing NDSS data

Keynote #3: Jean-Michel Roger

Increasing the robustness of chemometric models by calibration transfer, orthogonal projections, domain adaptation

Jean-Michel Roger focused his research on the robustness problem. In 200[3], simultaneously with Prof. Tom Fearn, he proposed a new generic method called External Parameter Orthogonalization (EPO) which permits to eliminate specific spectral effects from the NIRS calibration and thus to solve certain problems of robustness. He is also involved in the design of portable or online spectrometers using filters technology. In this aim, he developed a method (CovSel) that allows to select wavelengths with regard to multiple responses. He has created ChemHouse, a chemometrics research group, forge of the ChemFlow software (see https://chemproject.org).

Lecture: Increasing the robustness of chemometric models by calibration transfer, orthogonal projections, domain adaptation

Because they rely on indirect measurements, spectrometry-based sensors require the use of a calibration model. Typically, this model is performed on a sample basis that is representative of variations in the variable of interest. However, the use of these sensors can subject this model to robustness problems. These robustness problems are due to the variation of external factors, such as temperature, chemical composition or changes on the spectrometer. A strategy for dealing with robustness problems will be presented, depending on the availability of knowledge about the influencing factors. An overview of correction methods will be presented. A focus will then be made on robust modeling methods, in particular on methods using orthogonal projections and domain adaptation.

Sebastian Orth

Spectral sensors and a novel multiblock data fusion approach for barley pre-harvest germination discriminant analysis

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During every growing season, pre-harvest germination of malting barley (Hordeum vulgare L.), leads to major economic losses globally. Culminating toward a breaking point, where a new, unbiased and rapid detection method, capable of early stage germination is required to fill a gap in industry. Indeed, malting barley is cultivated for the purpose of controlled malting, where barley grain undergoes a series of steeping phases followed by controlled germination. Thus, barley damage through pre-harvest germination, a process triggered by untimely germination due to adverse environmental factors, is a major role player in detrimental and non-uniform malting. In addition to the detrimental nature, early-stage detection of pre-harvest germinated grain, using conventional rheological methods is not easy and mostly not possible, whilst also not including sample variation to justify grading decisions. The use of spectral imaging, to solve this specific industry problem, was investigated. Spectral information was obtained from two independent hyperspectral camera systems in the visible near-infrared and shortwave infrared waveband regions. Bringing about the necessity to maximise the spectral information available, a multiblock method was deemed viable. Thus, novel orthogonalised multiblock and multiblock variable selection classification methodologies, sequential and orthogonalised partial least squares linear discriminant analysis (SO-PLS-LDA) and sequential and orthogonalized covariance selection-linear discriminant analysis (SO-CovSel-LDA), were used. The aim, to ultimately classify between early stage, germinated and non-germinated single barley kernels, to capture intra- and inter sample variation. Classification accuracy of SO-PLS-LDA was 99.76% and when selecting and limiting the number of variables to 8, using SO-CovSel-LDA, an accuracy of 97% was obtained. This truly novel approach showed how VNIR and SWIR spectral information and a multiblock method is viable for industry and research applications. Further, orthogonalised data fusion allowed for modelling with a high degree of precision and sensitivity, without introducing redundant spectral variables commonly found in conventional low-and-mid-level approaches.

Keywords: Spectral imaging, SO-PLS-LDA, SO-CovSel-LDA, Single kernel analysis, Data fusion

Acknowledgements: The authors gratefully acknowledge receiving funding from ABInBev Pty Ltd.

Marina De Gea Neves

Investigation of bread staling by handheld NIR spectroscopy in tandem with 2DCOS and MCR-ALS analysis.

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During the process of staling (aging) bread not only loses its texture, flavor, and freshness but also increases its hardness (Fadda et al., 2014). As a result of these palatable changes, consumer disapproval of bread grows quickly. It is known, that one of the critical factors in the staling process is the retrogradation (recrystallization) of amylopectin in starch. The decrease of water content by evaporation and diffusion from core to crust also contributes to aging. The present investigation was carried out using the technique of handheld near-infrared (NIR) spectroscopy. Apart from a considerable reduction of hardware price, this technique has recently become a powerful tool for in-the-field and on-site investigations of a broad range of materials. Time-resolved measurements were made in diffuse reflection of a fresh bread surface, thereby allowing the interpretation of the structural changes in bread as a function of the observed spectroscopic changes.

To quantitatively compare the patterns of spectral intensity variation over time, two-dimensional correlation spectroscopy (2DCOS) (Noda and Ozaki, 2004) was applied and the synchronicity and sequence of structural changes were proposed. Due to the variation of spectral changes, especially at the beginning of the aging process, the data was split into time-segmented sets. For the first six hours of staling white bread, the sequence of events is: crystallization of amylopectin (4703, 4346 cm-1) < evaporation of weakly hydrogen bonded water (5311 cm-1) < reorganization of starch OH-functionalities (5158 cm-1) < diffusion and evaporation of strongly hydrogen bonded water (4964 cm-1) and final crystallization of starch CH-functionalities (5851 cm-1). From 6 to 48 hours on the other hand, the sequence of events was: 4964, 5311 (OH water) < 5158 (OH starch) < 5851 (CH starch) < 4703, 4346 cm-1 (CH starch).

In addition, Multivariate Curve Resolution-Alternating Least Squares (MCR-ALS) (Piqueras et al., 2012) was used to investigate the changes in the spectra profile as a function of aging time. The cross-over points of the concentration profiles provide information regarding the progress of the above mentioned water evaporation/diffusion and the amylopectin crystallization processes.

Keywords: handheld NIR spectroscopy, bread staling, 2DCOS, MCR-ALS

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Candela Melendreras García

On-site sensors for quality control of Breast Milk

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Breast milk is the first source of human nutrition. It contains a lot of bioactive components and nutrients for infants' growth. It is extremely important for immune systems, affecting a child's health for life. It is well established that the ideal nutrition is a mother's own milk, however, sometimes it is not possible. These reasons justify that milk banks as a specialized service integrated into the neonatology units of hospitals. When feeding neonates with breast milk from hospital banks, one key problem is the milk's nutrients, which should be adequate for neonates' nutritional needs. Milk quality is now monitored in laboratories with fully verified chemical reference procedures or milk analyzers with pre-calibrated medium or near-infrared (IR) devices, but an alternative for on-site and real-time monitoring milk quality control is the best option for adequate nutrition of neonates. [1].
Near-infrared spectroscopy (NIRS) is a real-time, non-contaminating, and versatile technique that provides information on food nutritive value. It allows the analysis of intact samples and it is a waste-free technique.
In this research work, we have worked in the development of quantitative calibration models to determine nutritive value in breast milk (energy, fat, carbohydrate and protein). A total of 68 samples were involved in this study. After trying different chemometric strategies with Unscrambler X software, we obtained the best coefficients of determination for calibration (R2) for fat developing models with intact spectra (R2= 0.910) and for energy, carbohydrates and total solids after standard normal variate and first derivative (R2Energy= 0.927; R2carbohydrates= 0.894; R2Total Solids= 0.929).

Keywords: breast milk, nutrients; chemometrics; handheld; near infrared spectroscopy

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Sergio Forcada

In-situ quantification of sugar content in intact green bean pods by Near Infrared Spectroscopy

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A non-destructive methodology based on portable Near Infrared Reflectance Spectroscopy (NIRS) has been evaluated for pre-harvest and on-site quantify moisture, fructose and soluble sugars in bean pods, with the objective of helping agro-food producers to evaluate the optimal harvest strategy to obtain the best quality product. 144 green pod samples were scanned on intact mode using a Handheld NIRS PhazirTM (Polycromix, wavelength range 1595-2395nm). The potential of the proposed methodology combined with chemometric strategies was validated by comparison with the laboratory traditional methods. Chemometric analysis was performed using Partial Least Squares (PLS) regression with internal cross-validation for several combinations of pre-treatments: 1st and 2nd derivatives and Standard Normal Variate (SNV) or Multiplicative Scatter Correction (MSC) to minimize scatter effects (Unscrambler v. 10.[1] software). Good prediction statistics were achieved for the moisture content of bean pods (R2v = 0.70; SEP = 1.51 %), fructose (R2v = 0.79; SEP = 18.02 mg g-1) and soluble sugars (R2v = 0.71; SEP = 30.98 mg g-1). In addition, no significate differences ($p > 0.05$) were found when comparing reference with predicted mean values in each parameter. Those results demonstrate that NIRS is a suitable alternative technology which can be on-vine implemented by producers and food processers to optimal harvest bean pods attending their moisture and sugar content.

Keywords: on-site analysis, portable sensor, NIRS, green bean

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Arnaud Molle

The use of milk Fourier-Transform Infrared spectra for predicting cheese making traits in Grana Padano PDO

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This study investigates the prediction reliability of cheese making traits [3 measures of cheese yield (%CY): fresh, solids and retained water (%CYCURD, %CYSOLIDS, %CYWATER); 4 recovery traits (%REC): milk fat, protein, solids and energy in the curd (%RECFAT, %RECPROTEIN, %RECSOLIDS and %RECENERGY)] (Ferragina et al., 2013) applying Bayesian models on the Fourier-transform infrared spectroscopy (FTIR) spectra of vat milk samples used for Grana Padano PDO production. Information from 50 cheese-making days (in total 139 vats) from two dairy industries were collected. For each vat, the milk, and the cheese after 48h from cheese making, were weighted while milk and whey composition (total solids, lactose, protein and fat) was analyzed. Two spectra from each milk sample were collected in the range between 5,011 and 925 cm-1 and averaged prior the data analysis. The calibration models were developed with a Bayesian approach (Ferragina et al., 2015) by using the BGLR (Bayesian Generalized Linear Regression) package of R software (R Core Team, 2013). Performance of models was assessed by coefficient of determination (R2VAL) and the root mean squared error of validation (RMSEVAL). A random cross-validation (CV) was applied [80% calibration (CAL) and 20% validation (VAL) set] with 10 replicates. The most accurate predictions after CV were obtained for %CYCURD and %CYSOLIDS, which exhibited R2VAL and RMSEVAL values of 0.55 and 0.27, and of 0.65 and 0.18, respectively. The %CYWATER showed the lowest R2VAL (0.53), being the least repeatable among cheese making traits. Considering %REC traits, promising results were obtained for the recovery of protein (RMSEVAL = 0.31%). In opposite, the recovery of energy (RMSEVAL = 0.81%) and fat (RMSEVAL= 1.83%) showed a less favorable result. These results demonstrate FTIR spectroscopy could be a valid method to indirect monitor cheese

Lorenzo Strani

Different chemometric approaches to monitoring pesto sauce quality in an industrial process

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Nowadays, companies are increasingly required to improve the control of industrial processes, in order to ensure a product of high and uniform quality and to reduce wastes for more environmentally friendly products. To this aim, thanks to the modern technological progresses, companies can install an increasing number of different type of sensors along the industrial plant. The huge amount of data generated can be analysed with chemometric tools to improve the efficiency of process monitoring and to predict the final product quality.

Pesto Barilla, a sauce obtained by a mixture of basil, garlic, parmesan cheese, extra-virgin olive oil and other ingredients, is one of the most important food products of the company. The main ingredient of pesto sauce is basil, which has an important impact on the features of the pesto sauce (Nicoletto et al., 2013; Strani et al., 2022). For this reason, an accurate monitoring on the early stage of the process, where the basil plants enter in the production line.
Basil plants were analysed with an RGB camera that has been installed on the conveyor belt, able to extrapolate in real-time information about the colour of plants and detect if there are some defects, such as dark spots on the leaves. In addition, spectra of an intermediate product, i.e. grinded plants mixed with oil and garlic, were collected by an on-line NIR probe. The final product quality was assessed by off-line laboratory analysis.

In this work, the focus has been on the real-time prediction of final pesto quality, using NIR and Imaging data for the computation of regression and classification models. In this context, were evaluated different data fusion strategies as well as different multiblock methods.

Keywords: NIR, Basil, RGB imaging, Data Fusion, Process Monitoring.

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Justyna Grabska

NIR Spectra Simulation in Aid of Food Analytical Framework. Understanding of Matrix Effects and Improved Detection of Adulterants

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Multi-variate analysis forms the backbone of analytical framework of NIR spectroscopy, but it lacks in providing answers on the origins of the spectral variability nor its relationships with the molecular background. In recent few years, advancement of in silico NIR spectroscopy, where spectra can be simulated ab initio, created an opportunity to make a decisive step beyond this barrier (Bec and Huck, 2019; Ozaki et al., 2021). This improves the comprehension of the spectral information enabling access to rich and detail molecular footprint, essential for fundamental research and providing innovative advances to analytical framework of NIR spectroscopy combined with chemometrics.
In addition to detailed NIR band assignments, accurately simulated NIR spectra enable new discoveries in physicochemical studies, e.g. the matrix effects. Intricate NIR spectral effects result from the interaction between the analyte and its chemical neighbourhood. Examples here include carbohydrates in aqueous solution, which are model system for numerous food products. On the other hand, detailed interpretation of NIR spectra of food adulterants, such as melamine, provides understanding of the differences that vibrational spectroscopic techniques (i.e. NIR vs. mid-IR) exemplify in food quality control framework.

Keywords: NIR interpretation, matrix effects, food adulterants, melamine, carbohydrates

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Fatih Kahrıman

Comparison of Different NIR Instruments for the Determination of Oil Content in Single Maize Kernel

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Near Infrared Reflectance (NIR) spectroscopy is a user-friendly tool for analysing agricultural products. This tool is currently used to serve a wide variety of purposes, including single seed analysis. Single seed analysis is an important issue especially for plant breeders. Oil content determination is one of the most tedious analyses at the single seed level. NIR spectroscopy has a potential for this purpose, however there is a need for investigation of the best instrument and chemometric technique. In this study, two different NIR devices (a bench-top and portable instrument) were used to develop prediction models.Totaly, five hundred kernels were used as experimental material which have a wide range of oil content (2.54%-8.88%). Spectral models were developed and evaluated using the SelectWave application based on the support vector machine regression method. Results showed that there are important differences for prediction success between NIR instruments tested here. Bench-top NIR instrument gave more reliable results according to model evaluation parameters. This is due to differences between measurement specialties of the instruments used here. Overall, NIR spectroscopy had a considerable potential for analysis of oil content in a single maize kernel.

Keywords: spectrum, support vector machines, oil

Session #4:
Advances in decision support systems for efficient control in the food supply chain & 5 Matching scientific progress to industrial needs – alternative strategies for knowledge transfer

Keynote #4: Wouter Saeys

Harvest planning in apple and pear with spectral sensors in the orchard

Wouter Saeys obtained his Master's degree in Bioscience Engineering: option Agricultural Engineering from KU Leuven, in 2002. On the basis of his Master's thesis on plant distance control for precision agriculture applications, he was awarded the engineering prize by the Royal Flemish Society of Engineers (KVIV). In 2006, he obtained a PhD in Bioscience Engineering from KU Leuven under the supervision of Professors Herman Ramon and Josse De Baerdemaeker for his research on precision fertilization with animal manure using NIRS for on-line manure composition measurement. As a postdoctoral fellow of the Flemish Research Foundation (FWO-Vlaanderen), he specialised in light transport modelling during a six month stay at the School for Chemical Engineering and Advanced Materials of the University of Newcastle upon Tyne, UK, under the supervision of Dr. Suresh Thennadil, and in Chemometrics during a six month stay at the Norwegian Food Research Institute – Matforsk, Norway, under the supervision of Dr. Tormod Naes. In 2010, he was appointed as assistant research professor at the KU Leuven Department of Biosystems, where he leads the Biophotonics group (www.biophotonics.be) with a focus on applications in the AgroFood chain and is responsible for the Master in Biosystems Engineering. His main research interests include light transport modelling and optical characterisation of biological materials, chemometrics and digital agriculture. In 2013, he was awarded by the European Network of Business and Industrial Statistics (ENBIS) with the 'Young Statistician Award' for his work on multivariate calibration of spectroscopic sensors in the agrofood industry. Since 2019, he is professor in the KU Leuven Department of Biosystems and in 2022 he has been rewarded by the Special Research Fund (BOF) with a 3rd term of 5 years as Research Professor. He is member of the editorial boards of the Journal of Near Infrared Spectroscopy and Biosystems Engineering and of the Chairman Advisory Committee and the Education Committee of the International Council of Near Infrared Spectroscopy (ICNIRS).

Lecture: Harvest planning in apple and pear with spectral sensors in the orchard

Although pome fruit such as apples and pears are only harvested once per year, they can be consumed year-round thanks to controlled atmosphere storage. However, as the biochemical processes in the fruit continue during storage, the harvest time determines the storage potential and the final consumption quality. If fruit are harvested too early, they may not mature fully,

resulting in poor consumption quality. On the other hand, if the fruit are harvested too late, the enzymatic maturation processes are already too far advanced to allow long term storage. Therefore, it is crucial to harvest the fruit at the optimal state for the intended storage period. As the harvest of pome fruit for fresh consumption is still done manually, most growers have to rely on seasonal workers to pick the fruit. To hire these seasonal workers for the right period, fruit growers should thus have information on the optimal harvest window well in advance. To this end, the Flanders Centre of Postharvest Technology combines spectral measurements on the fruits throughout the season to quantify their maturity state with fruit growth models. In the past, the fruit measurements were performed destructively in the laboratory which involved considerable sample logistics and limited the number of samples that could be analyzed. Recently, these sample logistics have been reduced considerably thanks to the use of portable spectral sensors which allow to measure the fruit non-destructively on the tree. As the spectral sensors are equipped with a GPS, the maturity indicators (SSC, firmness) are automatically linked to the location in the orchard. This supports the growers in planning their harvest logistics and deciding on the order in which their orchards and even the zones within their orchard are harvested.

Evgeni Eltzov

Reduce food losses by developing non-destructive biosensors for real-time rots detection in the stored agriculture produce

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Worldwide, postharvest losses have been estimated to be 40%-50% of the harvested crop, mostly due to rots caused by microorganisms (Okawa, 2015). Plants emit various volatile organic compounds (VOCs) into their surrounding environment, and the VOC profiles of healthy crops are altered upon infection. Therefore, monitoring these changes will allow the identification of infected crops at an early stage. The traditional approaches, which are based on gas chromatography, are complicated, not portable, and unable to conduct continuous monitoring of VOCs in the air. Therefore, there is a need for alternative monitoring techniques that are sensitive and able to monitor full VOCs profile in real and continuous time in the storage room or during shipment. Biosensors may be a preferable choice for VOC profiling in agriculture. A whole-cell-based biosensor is a self-contained bionic integrated device that includes microorganisms, which can respond in a concentration-dependent pattern to monitor a biochemical species (Rodriguez-Mozaz et al., 2005). Concerning the analysis of VOC profiles, biosensors provide various benefits, including low-cost, ease of operation, portability that allows utilization in the field, and continuous monitoring of VOCs presence without requiring sample preparation. The bioluminescent bacteria will monitor the VOC's profile in the air, and a signal change will be generated reflecting the status of the crop's health or disease prior to visible disease symptoms. Coupled with the optical sensors, these signals are transmitted and translated to a smartphone application for the end-user ease of usage. The developed whole-cell biosensor system based on bacterial detection will allow more efficient crop management during postharvest treatment, storage, and transport phases and reduce food losses.

Keywords: optical sensors, genetically modified organisms, VOCs, food loses, real-time monitoring

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Stefka Atanassova

Dairy products quality assessment by use of near-infrared spectroscopy

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Dairy products are worldwide spread and have great commercial importance within the food industry. Rapid and reliable analysis of these products would be highly desirable both for the manufacturers and consumers. Near-infrared spectroscopy has been used as a method to predict the quality of different foods due to the speed of analysis and minimal sample preparation.
The results of several experiments, related to the application of near-infrared spectroscopy to study the degree of ripeness of white brined cheese and yellow cheese and the discrimination of natural and imitation cheese and yogurt, will be presented.

- Investigation of the ripening process of Bulgarian white brine cheese and Bulgarian yellow cheese from cow milk, coagulated with cheese rennet and went through a process of ripening. Samples for spectral analysis were taken from the first up to 74 days.
- Yogurt from cow milk (natural or mixed with 5, 10, 15, and 20% dry skim milk), prepared in laboratory conditions.
- Bulgarian white brine cheese - natural from cow milk, produced from a mixture of cow milk and dry skim milk, imitation products with vegetable oil.

Spectra of all tested samples were obtained with a scanning NIRQuest 512 (Ocean Optics, Inc.) instrument in the range of 900-1700 nm using a reflection fiber-optics probe. PLS models were developed for quantitative determination and SIMCA for classification.

Results showed the potential of near-infrared spectroscopy as a non-destructive and rapid screening tool for assessing cheese ripening and detecting the adulteration of dairy products.

Keywords: cheese, natural, imitation products, near-infrared spectroscopy

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Christian Huck

Current Status and Future Trends of NIR Spectroscopic Analysis of Foods

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The ability of straightforward on-site usage, non-destructive analysis of samples featuring wide variety in chemical composition and physical form, while remaining sensitive to the chemical fingerprint is the hallmark of NIR spectroscopy (Bec and Huck, 2020). High performance, sensitivity, reproducibility with low methodological development costs, accompanied by the capacity to perform through-package analysis, makes NIR technique particularly valued in food quality control. In the near future, the problem of food quality control will be one of the most important and focused topics in the public debate, where the food risk is seen two-fold, intentional or accidental; to address both, new, powerful and efficient analytical methods need to be established (Charlebois et al., 2016). NIR spectroscopy appears as one of the most promising analytical frameworks for fulfilling this urgent demand.

In general, the design principles of the NIR instrumentation (spectrometers, optics, cells, sample handling) guarantee a wide area of expansion in the currently rapidly diversifying food production and supply chain. The possibility of high sample volume and fiber probe instrumentation enables a fundamental reduction of the necessity of sample preparation. One of the most up-to-date breakthroughs is the sensor miniaturization. Low-cost, portable NIR spectrometers have become reality, and in the next few years, with ultra-miniaturized spectrometers directly integrated smartphone devices being developed nowadays (Bec, Grabska and Huck, 2021). Currently, there are two major trends in advancing NIR spectroscopy in food analysis which are followed in our working group. The first is the development and employment of miniaturized NIR sensors for approaches in the discussed fields. The second trend is the implementation of innovative frameworks for spectra interpretation and calibration, where quantum chemistry provides deeper understanding about the performance of individual spectrometers and chemometric models, respectively.

Keywords: sensor fusion, chemical interpretation of calibration models, in silico NIR spectroscopy

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Szilveszter Gergely

Monitoring the change in particle size of dried egg-pasta due to different grinding parameters by diffuse reflection near-infrared spectroscopic techniques

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The pandemic has boosted demand for durable foods such as dried egg-pasta. Due to the increased production capacity, continuous QA/QC is an important task, in which near-infrared (NIR) spectroscopy, as a rapid test methods, plays an important role. Because the shape of dried egg-pasta (e.g., penne, farfalle, fusilli, etc.) has a significant influence on egg content calibrations developed for NIR spectra, it is necessary to prepare the sample by grinding (De Girolamo et al., 2020). Because different grinders (e.g., hammer mills, disc mills) are used in different laboratories, the question rightly arises as to how differences in particle size profile due to different milling techniques and settings affect the proprtion of light scattering (Dahm and Dahm, 2004), and as a result, predicted constituent values based on NIR spectra.

During our work, commercially available 1, 4 and 8 eggs per kg dry pasta samples were ground with two hammer mills (Konzum Trade KT100 and Perten LM 120) and one disc mill (Perten LM 3610). The ground samples were scanned using three different instruments parallel to collecting the reflection spectra: the dispersive NIRSystems 6500 monochromator system fitted with Rapid Content Analyzer (400-2498@2 nm, Si and PbS detectors) and the diode array Perten DA 7250 and Perten DA 7440 spectrometers (950-1650@2 and @5 nm, respectively, InGaAs detector array). Retsch AS 200 basic sieve shaker with analytical sieves was used to determine the particle size distribution.

Cluster analyses (CA) were performed to highlight the changes due to different parameters (egg content, mill). Based on these, 1) not only mills, but also degree of egg content can result in different particle sizes; 2) the mathematical treatments (normalizations, derivatives, etc.) and their combinations and sequences of application are able to eliminate the effects of light scattering to different degrees; 3) the optical differences between DA-based desktop and on-line devices are not significant, so calibration transfer is feasible.

Keywords: dried egg-pasta, particle size distribution, scattering, on-line NIR sensor

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Claudia Beleites

Open-Source Development of Portable NIR-Sensor Measurement Setups for Plant Leaves

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Project In4Food studies plant production in highly controlled environments, and NIR spectroscopic methods are developed for future quality control and monitoring as well as optimization purposes.

Small NIR sensors have become increasingly available. Also, readily available single-board computers such as the Arduinos, Raspberry Pis or similar that can be connected to normal PC hard- and software as well as to wide variety of sensors and actuators in general, plus the mechanical possibilities of affordable 3d printing together allow versatile adaptation of measurement setups to the precise needs of particular studies. This includes convenient automation of work-flows that has rarely been possible with the insular nature of bench-top spectrometers (or their portable counterparts) for fast-changing requirements such as usual in scientific research.

This convenience is of high practical importance: additional sensors allow for better characterization of samples (if only for “debugging” of the experimental data) and even saving the need to type (or copy/paste from an Excel-sheet) sample names by asking for a particular sample and confirming against a barcode frees human resources. In turn, larger or more complex experimental designs may be implemented with less need for curation and fewer errors.
We use a modular design strategy: small interoperable modules for various sensors and actuators focus on a particular task each. Parts/modules (both in a hardware and software sense) are combined into a setup for the experiment at hand, and easily adapted or re-assembled when the experimental needs change.

Our on-going work is publicly available at https://gitea.julius-kuehn.de/claudia.beleites

Keywords: free/open source software, open hardware, NIR spectroscopy, automation

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Marcello Vanzulli

QualiControl: Smart Cloud based NIR solutions for industry

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Nowadays, NIR solutions are mostly based on local or, in best cases, internal network services, with old, granitic and not-so-easy to use software. QualiControl is a modern, scalable, fast, flexible cloud solution, coupled with a Mobile App and a Web App and it is fully integrated with the Viavi MicroNIR.

The cloud allows the user to: create and manage other users, create new models and/or modify existing ones, configure the Viavi MicroNIR (number of scans, integration time, ...), see the results of the analysis in real time, make data driven decisions; all in one place. Moreover, the cloud offers several advantages: fast updates, it is a scalable service according to user needs, data loss is virtually impossible and available everywhere.

The UX that has been chosen is oriented to non-technical users, from top to bottom an unskilled user can configure himself the instrument and develop the models using the Web App in two manners: a guided way for skilled users, or with an automated model creator for untrained personnel; those solutions can be deployed to various users belonging to his organization; those models will be available into the Mobile App.

Keywords: NIR, cloud, chemometrics, data science, MicroNIR, Viav

VIRTUAL POSTERS
Innovation in process control by means of NDSS

Clara Barnés i Calle

Determination of hydroperoxides by near infrared spectrometry as a rapid procedure to evaluate oxidation susceptibility in fish

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Hydroperoxides are primary lipid oxidation products that can provide an early and accurate indication of the oxidative status of food products before sensory characteristics are affected. However, its analytical determination is challenging (Bou et al., 2008). The aim of this study was to evaluate the ability of near infrared spectrometry (NIRS) to determine the total hydroperoxide content in fish as a tool to rapidly estimate its susceptibility to oxidation.
To do so, hydroperoxides were enzymatically produced using lipoxidase from Glycine max (Merck KGaA, Germany) on emulsified linoleic acid to obtain a hydroperoxide stock solution (327µM), which was diluted in a control emulsion without enzyme to obtain 8^2 samples with concentrations ranging between 0 and 327 µM. Next, these emulsion systems containing hydroperoxides were combined with a fresh fish matrix (fish:emulsion, 1:2.25, w/v), obtaining fish-based samples with concentrations from 3^3 to 256 µM. Spectra were acquired using a high-performance Fourier Transform NIR spectrometer (Bruker Optik, Germany). Partial least squares regression was used to develop predictive models (PLS Toolbox, The MathWorks Inc., USA). PLS loadings were analysed to identify the most relevant wavelengths for the prediction of hydroperoxide content. First derivative of raw spectra resulted in satisfactory predictions of hydroperoxide content in both emulsion (R2=0.88; RMSEP=39.7 µM) and fish matrix (R2=0.84; RMSEP=28.0 µM) samples. The first PLS loading for the emulsion model showed three relevant regions at around 8770, 7560 and 7270 cm-1. For the fish-based model, similar regions were observed (8770, 7520 and 7200 cm-1) and spectral range between 4500 and 6500 cm-1, related to decomposition products such as aldehydes and alcohols, was not included since it could interfere in the prediction.
In conclusion, the obtention of a rapid procedure based on NIRS for evaluation of oxidation susceptibility and shelf life in fish seems feasible. However, more experimental work is needed.

Keywords: hydroperoxides, oxidation, shelf life, early detection, fish, quality.

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Cristina Zomeño

Predicting pork belly firmness with a portable NIR device

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Pork belly firmness is an important quality trait because it determines the processing aptitude and consumer acceptability. Firmness is partially modified by the ratio of unsaturated to saturated fatty acids (FA), where a higher ratio produces softer bellies and is less favourable. A common method to assess this ratio is the iodine value (IV). The objectives of this study were to assess the feasibility of a NIR device to: (1) predict belly firmness based on the determination of IV and the subjective firmness of the subcutaneous fat and (2) classify bellies into firmness categories. A total of 18[2] bellies from pigs with different origin, diet, genotype, and sex were used. The subcutaneous fat from the central part of the belly was measured with a NIR SCIO 2.0 sensor (Consumer Physics, Israel). Five spectrums were obtained for each belly within the range 740-1070 nm. Two trained technicians scored firmness applying pressure with a finger in the same fat region using a 5-point scale (1: very firm; 5: very soft). Fatty acid composition of this fat region was determined by gas chromatography, and the IV was calculated using a stablished equation including all the unsaturated FA detected (Lo Fiego et al., 2016). Models were obtained with the Lab for SCIO software by pre-processing the spectra and applying PLS regression for the prediction models and RF algorithm for the classification one. Prediction equations for IV and subjective firmness had a RMSE of 2.03 and 0.57 and a R2 of 0.74 and 0.51, respectively. The classification model had an average sensitivity of 0.49 and discriminated 100% of bellies with extreme firmness categories. The obtained models can be useful for the meat industry for sorting bellies according to their firmness although further pre-treatments, spectral range and algorithms should be tested to improve their accuracy.

Keywords: belly, fatty acids, firmness, iodine value, pocket-sized NIR, pork

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Elena Fulladosa

In search to robust predictive models to determine the texture and ripening level of dry-cured ham

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A system able to evaluate the texture of dry-cured ham inline at the industry would be very useful to ensure and certificate the final quality of the product. Near infrared spectrometry (NIRS) have shown potential for the prediction of texture and pastiness defect (García-Rey et al., 2005) which are known to be related to the proteolysis index of the sample. Salt and water contents are also relevant parameters. The present study is aimed at identifying the NIR spectral bands that characterise dry-cured ham proteolysis. Prediction ability for proteolysis index, salt and water contents determination using different spectral regions has also been analysed. To do so, spectra from 125 dry-cured ham samples, with a wide range of proteolysis index, and with salt and water contents not correlated to this proteolysis index, were acquired using a high-performance Fourier Transform NIR spectrometer (Bruker Optik, Germany). Different mathematical pre-treatments were used to analyse the spectra and develop the predictive models. Regression coefficients of proteolysis index model using raw and normalized spectra show high negative values between 1680 and 1690 nm which corresponds with the absorption peak of amide group (CONH2) characteristic of proteins. Degradation of proteins occurring during proteolysis produces a decrease on this absorption band, as previously reported in cheese (Malegori et al., 2021). Predictive errors for the proteolysis index models developed using the complete spectra and this specific spectral range were 1.622 and 1.379% respectively. Salt and water contents could also be predicted with an error of 0.263 and 0.539%, respectively. These results show potential usefulness of this technology at the industry to estimate texture/ripening level of dry-cured ham from the measurement of proteolytic degradation level in combination with salt and water contents. However, more experimental work is needed to define their threshold values to define the different texture types.

Jakub Sandak

Using infrared spectra and molecular dynamic modelling for identification of valuable molecules in olive leave

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Currently, 4,5 million ton of olive leaves are produced annually in the world by the olive oil industry, present in southern Europe and along the Mediterranean coast. This recalcitrant biomass contains high added value bioactive chemical components. However, it represents a problem for both the farmers and the whole olive oil industry, who need to remove it from the fields and the olive oil mills. This biomass is nowadays underexploited, being burnt in the fields, given to the cattle or, in some cases, burned to produce energy.
The chemical composition of olive leaves vary depending on the species, local horticultural system or seasonal climate variations, among others. It results in high variation of the biomass suitability for the profitable biorefinery conversion. Circular bioeconomy and bio-based product development and production are becoming essential in the current transition from a fossil-based towards a new sustainable green economy. In this perspective, the possibility to valorise certain underexploited bio-based side streams and residues has huge advantages.
The goal of this research is to develop a reliable, low-cost and rapid methodology for the chemical composition determination directly in the field or sorting line. Different near infrared-based sensors and customized chemometric models were tested for this task revealing high suitability for routine application within frame of OLEAF4VALUE project. In addition an attempt for the direct interpretation of the infrared spectra was tested by means of adopting multiscale chemical-physical modelling of valuable compounds present in agricultural residuals.

Keywords: biomass, biorefinery, olive leaf, suitability, chemical-physical modelling

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Maria del Mar Giró Candanedo

Low-cost portable NIR spectrometers for fraud detection in fish

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Development of tools to control and prevent fraudulent practices and unfair competition by false labelling in the fish sector is a significant issue. In this sense, near-infrared spectroscopy (NIRS) has demonstrated its potential to identify changes associated with freezing-thawing practices.The aim of this study was to determine the ability of low-cost portable NIR devices to discriminate between fresh and thawed fish (submitted to one or two freezing-thawing cycles) and to different freezing conditions. For this purpose, a total of 25 mackerel were divided into four fillets and assigned to different freezing conditions (C0, kept at 4ºC; C1, frozen at -20ºC; C2, frozen at -80ºC; and C3, quick frozen at -20ºC in <45 min.). Water content and weight loss were determined, and NIR spectra were acquired using a portable spectrometer (SCiO, Consumer Physics, Israel) and an in-house spectrometer (NIRTA 2.0, Hamamatsu, Japan). Discriminant models were developed using partial least squares discriminant analysis (PLS Toolbox, Mathworks, USA) and validated. Results showed that SCiO and NIRTA are useful to discriminate between fresh samples and the same samples subjected to a differentnumber of freezing-thawing cycles, with an overall performance of 100%. This fact was attributed to the different water content present in the fish tissue after differen freezing-thawing conditions ($p<0.05$) that produces absorption changes around 980 nm associated with water (Qin et al., 2020). When measuring on frozen samples, discrimination performance was 92% and 100% for SCiO and NIRTA since the scattering of light is affected by the differential ice crystalline structure resulting from the different freezing conditions (Washburn et al., 2017). When measuring on thawed samples, discrimination was attributed again to the different water content ($p<0.05$) and structural alterations caused by the different freezing systems. We can conclude that low-cost spectrometers could be useful for food inspectors and consumers to assess product quality and prevent food fraud on-site. However, validation with independent samples must be done.

Keywords: Near-infrared spectroscopy; Chemometrics; Fish quality; Consumer trust; Labelling.

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Mar Garrido-Cuevas

Suitability of a portable Near Infrared Spectroscopy sensor for its applicability to the on-site analysis of Extra Virgin Olive Oil

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Trends in the use of Near Infrared Spectroscopy sensors (NIRS) in the agri-food industry are moving towards the use of small size and low-cost spectrometers, suitable for on-site use. However, most of the existing commercial portable NIRS spectrometers were designed for process control within the pharmaceutical and chemical industries, and not for food applications. Therefore, before providing potential users with information on the suitability of a commercial portable NIRS sensor for a given food/ feed product, it is important to evaluate a number of key influencing factors (spectral signal repeatability, ease of cleaning, ease of on-site use). The aim of the present work is to provide scientific evidence on a commercial portable NIR sensor that provides absorbance readings between 908 and 1676 nm (every 6.2 nm) and is based on Linear Variable Filter (LVF) technology, for its suitability for on-site analysis of Extra Virgin Olive Oil (EVOO). A first step in the evaluation has been to compare three different liquid accessories possible for use with this instrument, which use different optical modes (transmission or transflectance) and different sample presentation modes. The task involves the evaluation of the spectral repeatability, sample preparation time, ease of cleaning and ease of use for on-site analysis of EVOO. Preliminary results show that collecting spectra in transflectance mode has some advantages over the transmission mode, such as ease of sample preparation or cleaning of the cup. However, the accessory for liquid analysis using the folded transmission mode offers a higher spectral repeatability, which is essential to obtain quality spectral data.

Keywords: Near infrared spectroscopy (NIRS), portable instruments, on-site analysis, extra virgin olive oil, liquid accessories.

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Mecit Oztop

Predicting the Crystallinity of MW-Vacuum Crystallized Sucrose by Time Doman NMR

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Sucrose production consists of many different unit operations and one of the most critical unit operation in the sucrose production is crystallization; which is a separation of sugar molecules from beet syrup. Sucrose crystallization is performed mostly by evaporation under vacuum in refined sugar industry. This operation is a considerably time-consuming step-in sucrose production, which limits production and it has a strong effect on product quality. Since microwave is a novel processing method that is infamous for providing drastic decrease in process times, it is hypothesized that combining this technology with a vacuum system might be a way to shorten crystallization of sucrose. In this study, sucrose was crystallized from the mother liquor of beet processing using microwave vacuum. The microwave power levels and the absolute pressure that are used for the crystallization were determined as 20,30 and 40% power and 260 mmHg pressure respectively, by preliminary studies. A non-destructive, TD-NMR has recently been shown to predict the crystallinity of sucrose samples. Solid echo sequence has been used and crystallinity of the sugars were calculated. The study showed that TD-NMR could be used to assess the quality of sucrose samples obtained through microwave vacuum technique.

Keywords: Sucrose, crystallisation, TD-NMR, MW vacuum

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Tiril Aurora Lintvedt

Raman Spectroscopy for In-line Estimation of Fatty Acid Features in Salmon Fillets

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In the food industry, smart in-line sensor systems are under constant development, aiming to effectively handle massive streams of food raw materials and products. Raman spectroscopy is gaining increasing interest for its chemical specificity. Recent feasibility studies show how the technique can be used to quantify fatty acids in muscle foods, water holding capacity in pork meat and mineral and bone contents in meat slurries. Furthermore, robust, and more low-cost Raman instrumentation has become available and paves the way for affordable and practical in-line sensor solutions in the food industry. The development of stand-off wide area illumination probes which utilize a defocused laser combined with multiple collection fibers is a cornerstone for Raman based in-line evaluation of food samples because of the insensitivity to smaller variations in working distance. This enables an in-line scanning strategy which facilitates more representative sampling of heterogeneous foods. In the current study, we employ such a probe and demonstrate the viability of an in-line scanning strategy for %EPA+DHA estimation in salmon fillets moving along a conveyor belt. One essential question was how to employ the surface scanning strategy to obtain a best possible predictive power. In general, Raman signals from food components can be of low intensity, and the signal to noise ratio (SNR) of the acquired spectra may be critical. This was also demonstrated in earlier work on %EPA+DHA estimation, where homogenized salmon samples were scanned at high speeds (Lintvedt et al., 2022). A successful scanning strategy must provide representative measurements for a whole fillet as well as obtaining adequate SNRs. For comparison, samples were also scanned by NIR hyperspectral imaging, which is another relevant method for fast stand-off measurements which undoubtedly has practical advantages over Raman but in return have lower chemical resolution.

Keywords: Raman spectroscopy, NIR hyperspectral imaging, In-line food evaluation, Representative sampling, Salmon, Omega-3 fatty acids

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Víctor Manuel Fernández Cabanás

Authentication of green asparagus of the Huétor-Tájar population variety by NIRS spectroscopy

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The Huétor-Tájar asparagus is regulated by a Specific Quality Denomination and by a Protected Geographical Indication within the European Union. In order to develop a qualitative model that allows discriminating this product from the commercial hybrids of green asparagus produced worldwide, NIRS spectra were collected from samples of freeze-dried shoots of 85 genotypes from Huétor-Tájar and 105 samples of hybrid asparagus from 35 cultivars.

The qualitative analysis model used in this work has been the discriminant analysis based on partial least squares regression (MPLS2). The discriminant models developed allowed to correctly classify 98.31% of the samples, with 1.69% of samples with uncertain classification.

It should be noted that no sample of the Huétor-Tájar population variety was classified as a global hybrid and vice versa. This result could be of great interest for the control of the productions regulated by the specific denomination of this crop.

Keywords: Asparagus, NIRS, authentication

Giorgia Stocco

Rapid and non-destructive determination of Ca and P in milk using WDXRF

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Calcium (Ca) and phosphorus (P) are two important minerals in milk, playing an essential role in human nutrition (Manuelian et al., 2018). Concentration of Ca and P in milk is then extremely important in the coagulation process, as they bond together to the casein micelles, influencing curd structure and stability and eventually to the quality of cheeses (Malacarne et al., 2014). Milk is routinely analysed for main components (Fat, Protein and lactose) by mid infrared spectroscopy and attempts to use the same technique for minerals have shown limited performances (Toffanin et al., 2015). X-ray fluorescence (XRF) is used as rapid and non destructive spectroscopic technique specific in the determination of elements. Thirty samples were collected from single cows at different very diverse dairy farms in Northen Italy. Triplicates were placed in 50ml vials and stabilized with the addition of Bronopol. One sample was sent to commercial lab for mineral determination by ICP-OES, one sample was frozen and stored at -20 °C for backup and the third subsample was scanned on a wavelength dispersive XRF (WDXRF) instrument (S6 Jaguar, Bruker AXS, Milan). Samples were poured in cups over thin prolene X-ray film, placed in the scanning chamber saturated with Helium and scanned at 30KV for P determination and at 50KV for Ca determination, with total scanning time of 3 minutes. Calibrations were developed using Spectra.Elements Advance v.^{3} software of Bruker. The results of this study shows that prediction models using XRF spectroscopy was excellent for Ca and P, with coefficients of determination greater than 0.90, RPD greater than 3.5 and SECV of 32 and 52 mg/kg for Ca and P respectively. WDXRF is a valuable method at improving the evaluation of milk quality for mineral composition which can be used to improve coagulation properties of milk.

	Chemical Composition					WDXRF calibration				
Trait	n.	Min	Max	Mean	SD	RSQ	SEC	Slope	Bias	RPD
Ca (mg kg-1)	30	1000	1800	1234.67	151.92	0.96	31.46	0.93	-3.93	5.12
P (mg kg-1)	30	900	1610	1094	149.15	0.93	52.68	0.81	-11.13	3.82

Keywords: Mineral determination, Wavelength Dispersive X-ray fluorescence (WDXRF), Calcium, Phosphorus, milk coagulation

Acknowledgements: First Author gratefully acknowledges receiving funding from programme name (POR FESR 2014-2020: PG/2019/916776).

Real-time methodologies for processing NDSS data

Jana van Rooyen

Application of ASCA to characterise eff ects of roasting temperature, -time and milling method on SWIR spectral data of whole and milled wheat

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Dry thermal treatment to modify wheat starch has been increasingly investigated. Structural changes of starch in heat treated wheat affects the molecular order, pasting properties, and retrogradation (Van Rooyen et al., 2022). Analysis of variance simultaneous component analysis (ASCA) partitions variation and interprets these partitions with SCA (Smilde et al., 2005). ASCA was used to investigate the effect of roasting and milling on whole wheat and flour shortwave-infrared (SWIR) spectra by assessment of statistical significance and characterisation of the contributing spectral features. A full factorial experimental design included three roasting temperatures, three roasting times and two milling methods. SWIR spectral images (1000-2400 nm) were collected from roasted wheat and subsequent milled samples. The factors 'roasting temperature' and 'milling method' had significant effects ($p<0.05$) on the samples, visualised by SCA. 'Roasting time' was statistically not significant ($p=0.06$), however it could have notable effect in practice. The high temperature affected starch (i.e. partial gelatinisation) and protein (i.e. denaturation) structures to a greater extent compared to intermediate and low temperatures. The intermediate temperature affected starch structures and moisture content more compared to the low temperature. The most prominent difference between the two milling methods was observed as changes in starch, protein, moisture (Quadrumat) and fibre (Perten). The absence of bran particles in the Quadrumat milled flour was responsible for the difference in protein structures. Protein denaturation was confirmed by an increment in Rapid Visco Analyser (RVA) peak viscosity as roasting severity increased (1753-2036 cP). Changes in starch structures resulted from starch damage. ASCA applied to SWIR whole wheat and flour spectral data effectively characterised the significant effect of roasting on wheat starch and protein structures.

Advances in decision support systems for efficient control in the food supply chain

Irina Torres Rodríguez

In situ authentication of Iberian pork meat using Near infrared spectroscopy

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Iberian pork meat, which is considered a seasonal product, has exceptional organoleptic, sensory and nutritional characteristics, making it a gourmet product. The high prices and consumers' demand are the main incentive for the Iberian pork products being exposed to frauds and mislabelling. This problematic raises the need to search analytical alternatives that enable to guarantee the integrity of the Iberian pork meat in a fast and non-destructive way. The author´s group has developed extensive research aimed to provide industry, producers and consumers with an analytical method based on Near Infrared Spectroscopy (NIRS) to guarantee the labelling of Iberian pork products. The aim of this work is to evaluate the viability of a low-cost and portable NIR sensor to guarantee the authenticity and integrity of Iberian pork meat both in terms of breed purity and freshness. To achieve this, fresh and frozen-thawed Iberian pork tenderloins from pure and cross-bred animals were analysed using the MicroNIRTM Pro 1700, which works in reflectance mode in the spectral range 908 – 1676 nm. Different models were developed using partial least squares discriminant analysis (PLS-DA) to classify Iberian tenderloins according to freshness and breed purity. These results confirmed that NIR spectroscopy provides a reliable method to guarantee, in situ, the integrity of each individual piece of Iberian pork meat, opening new opportunities of control at the different points of the meat production process and increasing the sampling capability.

Keywords: Iberian pork meat, portable NIR sensor, integrity authentication, fresh meat authentication, breed purity.

Type of presentation: Oral Presentation

Jasenka Gajdoš Kljusurić

Near infrared spectroscopy as authentication tool of protect design of origin for Dalmatian wine produced from grape Maraština

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The chemical composition of wine is highly influenced by the terroir, the viticultural area where vine interacts with the agronomic practices and environment (cultivar, geographic position, soil, climate conditions of a vineyard, along with the vineyard management). In accordance with EU Regulation (1308/2013) three viticultural areas in Dalmatia (Northern Dalmatia (ND), Dalmatian Hinterland (Dh) and Central and Southern Dalmatia (CSD)) can have protected designation of origin (PDO).

This study is aimed to analyse the wine composition and investigate if they can be marked by chemical finger-prints from a given terroir by measuring the colour and standard chemical composition of wines produced from the grape from Vitis vinifera L., 'Maraština', harvested from 11 vineyards located in three different viticultural subregions of Croatian Adriatic region. Near infrared spectroscopy (NIRS) was used to examine the effectiveness of differentiating wines by regions with assistance of NIRS combined with chemometrics (Balbino et al., 2022).

Differences were detected in the colour and physicochemical parameters, where the wines produced from the grape harvested in the hinterland had significantly lover pH (3.14 vs 3.45 and 3.43 in CSD and ND), but significant higher values for total dry extract (TDEDh= 23.80 g L-1 vs TDECSD= 20.14 g L-1 & TDEND= 21.4 g L-1). NIR spectra of wines were coupled with physicochemical and colour data to investigate the quantitative ability in relating NIR spectra with the wine characteristics based on the grape growing region. The principal component regression was used to construct the calibration models based on NIR spectra and standard physicochemical and colour data showing high prediction ability of all studied parameters (R2 of 0.98, RPD of 6.8).

NIRS has indicated the relation of the regionality and wine composition, proving that even in a small data set, it provides exceptional opportunities in monitoring the quality and authenticity of wine.

Keywords: NIR spectroscopy, Maraština, wine, PDO, chemometrics

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Regulation (EU) No. 1306/2013 of the European Parliament and of the Council on the financing, management and monitoring of the common agricultural policy and repealing Council Regulations (EEC) No. 352/78, (EC) No. 165/94, (EC) No. 2799/98, (EC) No. 814/2000, (EC) No. 1290/2005 and (EC) No. 485/2008.

José Antonio Entrenas de León

Ready to use vs specific NIRS calibrations for determination of chemical parameters of Processed Animal Proteins (PAPs) meals

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The authors' group, in close cooperation with the rendering industry, has scientifically demonstrated the feasibility of NIRS technology for the determination of chemical and nutritional parameters of Processed Animal Proteins (PAPs) meals, using instruments with very different hardware and software, installed either at line or on-site. However, based on our experience, the availability of "ready to use" calibrations are of paramount importance for a massive uptake -by the rendering and feed industries- of the existing NIRS knowledge. Theirs use, will allow to the instrument buyers to get predictions from the day one after its installation. Nowadays, instrument providers and several NIRS analytical service companies are offering those type of calibrations. Although the existence of "ready to use" calibrations are an excellent first approach, for the spread of NIRS technology, they lack the precision desired by the users for the specific PAPs they manufacture or buy as animal feed ingredient. In fact, most of the existing "ready to use" calibrations for the analysis of PAPs have not been scientifically validated for their general applicability to the very different PAPs produced by each specific rendering plant. The main goal of this work is to contribute to scientific validation of "ready to use" calibrations for their applicability to PAPs produced by a rendering plant located in Southern Spain.
For this purpose, a total of 347 PAPs from the mentioned Spanish rendering plant have been analysed in two diode array NIR instruments: the DA7440 suitable for on-line analysis, and the DA7250, an at-line instrument, both marketed from the same commercial company (PerkinElmer Inc). Results will be shown about the predictive ability of "specific" PLS calibrations - for the prediction of the moisture, crude protein (CP) and ashes of PAPs- versus the use of "ready to use" calibrations.

Keywords: ready to use calibrations, specific calibrations, NIRS, protein animal by-products meals

Type of presentation: Oral

Liudmil Antonov

Near Infrared Diffuse Reflectance Spectroscopy with Partial Robust M- Regression(PRM) as Sensory Tool for on-line Control of Biscuit Dough Production

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Biscuit dough mixing is a critical stage in the breadmaking process that affects biscuit quality. The mixing step must ensure a uniform distribution of ingredients (water, sucrose, fat, and flour). Developing a monitoring sensor for the biscuit dough mixing process is crucial for effective quality control. Most online systems are based on the indirect survey of biscuit dough rheological properties changes using torque and consistency probes. Non-invasive near-infrared spectroscopy (NIRS) offers a possibility for fast measurement times that simultaneously deliver critical sample properties like water, sucrose, fat, and flour. Developing the NIR sensor with a fiber optic probe positioned inside the mixer is important for further automation of the industrial mixing process.

In the present study, we investigate the ability of the diffuse reflectance NIR spectroscopy to monitor the real biscuit doughs data in the wavelength range (1100–2500 nm). The presence of a vertical outlier and some leverage points in that data set may cause an unreliable calibration model with misquantified components. As a solution, we propose using Partial Robust M-regression (PRM) (Serneels et al., 2005) to determine fat, flour, sucrose, and moisture content. PRM has been combined with different pre-processing techniques such as first derivative Savitzky Golay algorithm (D1), standard normal variate (SNV), multiplicative signal correction (MSC), and the combinations of MSC and SNV with first derivative (D1+SNV, D1+MSC). The obtained results are comparable with pre-processing in the literature using the first differences according to Marx and Eilers. The optimal pre-processing for every component (water, sucrose, fat, and flour) was found. PRM regression improves the performance compared with the results of classical PLS1 regression.

Together with the facility of NIR technology to be implemented in the process engineering, these improvements make it ideal for the quality control of the bread dough mixing process and other food manufacturing processes.

Keywords: NIR, outliers, leverage points, PRM

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Madalina Belous

Evaluation of Plant Bioactive Compounds Activity and Stability by Spectroscopic Methods

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Plants are a very important source of bioactive compounds with applications in various domains, from health and wellness, cosmetics and pharmaceutics, to food packaging and agriculture. The large variety and complex composition of bioactive principles derived from plants offer important advantages compared with their synthetic counterparts (Stoleru and Brebu, 2021). However, they also have some limitations, such as susceptibility to loose of activity due to oxidative, thermal or light- induced degradation. Therefore they are rarely used directly and carriers are often used or they are added to inert matrices to induce them bioactivity. Compatibility and interactions between the natural compounds and the carrier/matrix affect their bioactivity and bioavailability (Stoleru et al., 2021). Spectroscopic methods are useful tools for characterisation of the materials containing natural compounds. They can offer information on the fixation and stabilization of compounds in matrices and also on their release behaviour. Changes in bioactivity can be also determined. Incorporation of bioactive principles and their related bioactivity will be presented for plant derived products such as essential oils, cold pressed vegetal oils, and dried solvent extracts used in food related applications.

Keywords: spectroscopy, bioactive principles, food applications

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Sebahattin Serhat Turgut

Use of chemometrics for decision support in food quality assurance: an example study for tea blending

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Due to the rising development of computer and sensor technologies and the fact that they are more cheaply accessible, the feasibility, pace, and amount of data collected in the food industry are increasing day by day. These collected data are used as an aid in decision-making processes for many different purposes such as safety management, stock management, process management and optimization, economic evaluation, environmental impact evaluation and quality assurance. One of the methods that can be used for quality assurance is the take advantage of non-destructive sensors and chemometric approaches. Within the scope of the present study, a simple chemometric approach by Turgut et al. (2021) that can be utilised in the calculation of tea blend prescriptions will be exemplified. High UV-Vis spectral similarity (which is also the indicator for the likeliness of product quality) can be obtained with the tea mixtures prepared with the sample application, compared to the targeted tea samples.

Keywords: tea, quality, decision-support

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Tassos Koidis

Detection of offal adulteration in minced beef products using Near-Infrared (NIR) spectroscopy

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Adulteration in meat products is always one of the significant frauds, with intentional or economically reasons driving its occurrence. Due to the nature of the ground beef and the adulterants involved this is not easily detectable, and it is also unsafe for the downstream supplier or the end consumer. The current DNA based detection method can achieve high precision but is costly, cumbersome, and time-consuming. Near-Infrared (NIR) spectroscopy, as a non-destructive and rapid technique, can explore the differences between authentic and adulterated products based on the variance of the detailed profile, which will significantly shorten the time to identify the unknown problem. NIR has proved that it can quickly detect adulteration of minced meat products (Leng et al., 2020). However, previous work focused on adulteration from exogenous sources, and little evidence on the adulteration of ground meat from endogenous sources. Therefore, this work uses NIR in untargeted reflection mode to detect adulteration of minced beef including different animal-derived adulterants (beef offal such as liver and heart). Minced beef products are made from the less desirable cuts (chuck), which is often labelled as "lean ground beef" and used for blending it into burgers and meatballs. In this study a battery of machine learning methods are used to train the calibration models of the NIR signals (Partial Least Squares-Discriminant Analysis Support Vector Machine-Discriminant Analysis, Classification and Regression Tree and Back Propagation Artificial Neural Networks). Results have shown that the NIR can distinguish between pure and adulterated samples very well (accuracy >80%). The overall quality parameter (KAPPA) was also used to evaluate the classification model (Jiménez-Carvelo et al., 2017). Overall, NIR has the potential to achieve the designed requirements of online/remote, real-time/testing platform for minced beef authenticity.

Keywords: Near-Infrared, Mixture adulteration, Meat, Chemometrics, Machine learning

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Matching scientific progress to industrial needs – alternative strategies for knowledge transfer

Dr. José Blasco

A non-destructive method to measure the light penetration depth and optical properties of “Rojo Brillante” persimmons

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Hyperspectral imaging is commonly used to estimate the quality of fruits and vegetables. Reflectance and transmittance are specific to each biological tissue, and their values are linked to its chemical composition and physical characteristics. However, these properties are influenced by other extrinsic factors, such as the instrumentation or the light source, which can reduce their reproducibility (Lu et al., 2020). Estimating the theoretical light penetration depth could be helpful to validate the non-contact methods, such as hyperspectral imaging, as accurate tools for assessing quality properties based on optical properties. A non-destructive protocol, based on the spatially resolved spectroscopic principle (Sun et al., 2021), was developed to estimate the light penetration depth in persimmons for all bands in the range 450-1050 nm, in steps of 10 nm. Backscattering images of intact persimmons (‘Rojo Brillante’) of similar size were obtained. The light was produced by one halogen lamp and concentrated on a single point. The absorbance (μa) and scattering (μ’s) coefficients from Farrell’s diffusion theory (Lorente et al., 2015) were calculated using the backscattered light measured at different distances from the incident point at each spectral wavelength. A destructive experiment was performed to obtain the actual light penetration depth. Each fruit was cut into pieces of different controlled thicknesses and placed on a dark surface. For every set of fruit pieces, hyperspectral images were acquired. The reflectance was measured for each thickness and wavelength, obtaining the actual light penetration depth. Linear regression was used to relate the penetrability depth results from both protocols (theoretical and real), showing a high relationship ($R^2>0.8$ and RPD>2.5) for the range 610-1050 nm (persimmon is red), confirming that our non-destructive protocol based on hyperspectral imaging technique to estimate the light penetration depth and the optical properties of persimmon is accurate.

Keywords: Penetrability depth, Persimmon, Scattering, Absorption, Optical properties

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Dijana Blazhekovikj Dimovska

Determination of polycyclic aromatic hydrocarbons (PAHs) in commonly consumed smoked fish

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Smoking is one of the oldest methods of fish preservation, combining the effects of salting, drying, heating, and smoking. Smoke is a good preservative since it contains bactericidal and antioxidant properties. Depending on the smoking method, the amount of carcinogenic compounds in smoke varies. PAHs often function as a carcinogenic group found in smoked products and always be identified for their composition. Several PAHs compounds represent carcinogenic especially for smoked fish. The EU Scientific Committee on Food (SCF) has identified 15 PAHs compounds as carcinogenic genotoxic i.e. Benzo[a]anthracene, Benzo[b]fluoranthene, Benzo(j)fluoranthene, Benzo[k]fluoranthene, Benzo(a)pyrene, Benzo(ghi)perylene, Chrysene, Cyclopenta[cd]pyrene, Dibenz[a,h]anthracene, Dibenzo[a,e]pyrene, Dibenzo[a,l]pyrene, Dibenzo[a,i]pyrene, Indeno[1,2,3-cd]pyrene, and 5-Methylchrysene. This research aimed to determine the content of polycyclic aromatic hydrocarbons (PAHs) in five samples of smoked fish, namely trout (Salmo trutta), tuna (Thunnus albacares), mackerel (Scomber scombrus), salmon (Salmo salar) and mullet (Mugil cephalus), processed in a smoking kiln, and collected from markets of different countries (Kosovo, Italy, United Kingdom, and Greece). The levels of these compounds were determined by a GC/MS technique in smoked fishery products. The content of all identified compounds, in individual fish species, was below the permissible limits following European regulations for the maximum permitted amount of polycyclic aromatic hydrocarbons in smoked products.

Keywords: polycyclic aromatic hydrocarbons, smoked fishin

Dilip Sing

Rapid quality assessment of Andrographis paniculata using a developed portable infrared spectroscopy instrument

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Andrographis paniculata (Kalmegh), is a popular medicinal plant in India, which is expansively used in Ayurveda, Unani and Siddha medicines as home remedy for various diseases like upper respiratory infections, fever, sore throat, hepatitis and other chronic and infectious diseases(Jayakumar et al., 2013) . The main active constituent is andrographolides and its quantitative determination is crucial for the assessment of its quality. The feasibility of estimating of andrographolides and gradation of Andrographis paniculata leaves by near-infrared (NIR) spectrometry has been demonstrated by our laboratory (Sing et al., 2021). However, NIR spectrometers used in this study and also those available in the market and suitable for such purposes are expensive and non-portable.

The goal of this study was to develop a portable near-infrared (NIR) spectrometer for quality assessment of Andrographis paniculata based on their andrographolides content. The portable NIR spectrometer was developed using a tungsten halogen lamp, a concave mirror, a prism mirror and a diode array detector. A customized graphical user interface (GUI) was developed by creating and using wrapper DLLs on MATLAB App Designer®. The software controls the measurement process and executes the calibration and prediction algorithms. The prototype was made standalone by incorporating a single board PC with a touch screen display, which enabled portability of the assembled device for on-site use.

A set of 40 Andrographis paniculata samples has been used in this paper and calibration models have been developed using Partial Least Square Regression (PLSR). The PLSR model developed using first derivative pre-processed data yielded R2P, RMSEP and RPDP values of 0.99, 0.08 and 8.7[1] respectively. The results demonstrate the efficacy of the portable NIR spectrometer for estimation of andrographolides in the Andrographis paniculata samples. The spectrometer can be used for other marker molecules in plants and their products by suitable modifications in the software.

Keywords: Portable NIR, GUI, Andrographis paniculata, PLSR

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Maria Tarapoulouzi

Discrimination of Halloumi cheese samples regarding species' origin

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Halloumi cheese belongs to the category of white brined cheese, and it is originated from Cyprus. The traditional cheese of Cyprus has become known throughout Europe and internationally with a significant economic interest, without obtaining any PDO or PGI status yet. To enhance the protection of authentic and high-quality Halloumi cheese is crucial.
Therefore, the development of a method, capable of determining and identifying the adulteration of Halloumi cheese due to mislabeling regarding species' origin of milk was the target of our research, and the first publication was in 2020 (Tarapoulouzi et al., 2020) with a database of various Halloumi cheese and milk samples.
Today, we present a model produced based on Halloumi cheese samples only. Spectra were taken using Fourier Transform Infrared (FTIR) Spectroscopy. Prior to the spectroscopic measurements, all the samples were pre-treated with lyophilization (freeze-drying). The spectra were analyzed with SIMCA by applying Hierarchical Cluster Analysis (HCA), as well as Orthogonal Projection to Latent Structures - Discriminant Analysis (OPLS-DA). The final model has been validated to ensure that the utilized chemometric methods do not predict randomly.
Future studies include the establishment of a novel approach with sensor application for more rapid control, of course based on the method proposed here.

Keywords: Halloumi cheese, spectroscopy, FTIR, chemometrics, OPLS-DA, species' origin.

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Sara Chumillas Lidón

A collaborative platform economy to accelerate the democratization of NIR-based quality control in the food industry

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Around the world, mounting pressure on food systems because of increasing food fraud, new consumer demands, and geopolitical crisis, has highlighted the need for transparency and traceability in the industry. In the age of digital technologies, the food industry has been using NIR (Near Infrared) technology due to its many advantages over traditional food analysis methods: cheaper, faster, non-destructive, efficient, and replicable. At the same time, the development of cheaper and higher performing desktop and portable equipment, leads to believe that the implementation of NIR technology in quality control systems of food companies still has a long way to go.

Despite the advances in the field, the application of NIR technology still necessitates expert personnel to deploy their knowledge into the creation of models and calibrations, making this the largest barrier to adoption of the technology. Meanwhile, universities, research centres and wet labs with NIR application experience, have been limited in their ability to disseminate the knowledge since no shared channel for distribution of models, calibrations and additional services exists.

With these challenges in mind, at Chemometric Brain we have developed a SaaS (Software as a Service Solution) and collaborative platform with the goal to accelerate the democratization of NIR-based quality control in the food industry through the dissemination and promotion of the knowledge generated (i.e., spectra libraries, qualitative models, and quantitative calibrations) by public/private research institutions in a model that rewards the knowledge creators.

https://www.chemometricbrain.io/

Keywords: NIR, SaaS, platform, food, qualitative models, quantitative calibrations

Tiziana Cattaneo

Evaluation of the effect of different soil fertilizers on rice plants using a hyperspectral imaging system

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Municipal solid waste can be adequately treated producing sewage sludge (SS), rich in organic and inorganic plant nutrients, and exerting beneficial effects on soil properties (Donatello and Cheeseman, 2013). Soil samples were collected at the Penati Farm (Basiglio, Italy). After drying, sifting, and mixing with three different SSs (R10 sludge; carbonate of defecation; defecation plaster), soils were used for a pot experiment (15 kg each) from April to July 2021. The greenhouse experiment (5 treatments) was carried out at the University of Milan, for the assessment of the impact of innovative fertilizers on rice (Oryza sativa L. var. Sirio CL) plants. SSs were compared with unfertilized soil (control) and mineral fertilizer. The amount of urea and fertilizers were calculated to provide the same total nitrogen for each treatment. Alterations in physiological performance of the plant growth using spectroscopic indices obtained by hyperspectral imaging system data were studied. Selecting 1[1] spectral bands, the values of four indices highly correlated with chlorophyll (chl) content were calculated on 330 images: NDVI, Chlred-edge, MCARI, TCI (Ranghetti et al., 2020). From images of the indices, the average indices were calculated from three sub-samples in different areas of each leaf. The differences between the treatments did not indicate statistical significance in any of spectral indices. Similar results were obtained from VIS-NIR spectra (400-1000 nm). A positive correlation was found between NDVI, MCARI and TCI, while the Chlred-edge index showed a negative but significant (p-value <0.001) correlation. As expected, the highest correlation value was found between NDVI and Chlred-edge (R = 0.935; R2 = 0.874). These results indicated that the chl content was not affected by the administration of SSs as alternative fertilizers, suggesting that the treatments did not reduce plant health compared to chemical fertilizer.

Keywords: rice, fertilizers, hyperspectral imaging, plant health, physiological performance.

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Tiziana Cattaneo

NIR calibrations to predict stress related parameters in rice plants fertilised with sewage sludge

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Sewage sludge (SS) from municipal solid waste is rich in organic and inorganic plant nutrients. When adequately treated, SS can be used as fertilizers with beneficial effects on soil properties (Donatello and Cheeseman, 2013). The impact of this kind of innovative fertilizers was evaluated on rice plants (Oryza sativa L. var. Sirio CL) and compared to standard soil nutrition. A pot experiment (30 pots) was carried out with five treatments: unfertilized soil (control), soil with the addition of urea, soil with SS treated with: CaO; CaO + CO2; CaO + H2SO4. The amount of urea and SS were calculated to provide the same total nitrogen level for each treatment. The control did not receive any nitrogen fertilization. Biochemical analyses and non-destructive NIR analyses were carried out at tillering stage, booting and panicle emergence on the last fully expanded leaf. The NIR spectra were collected in reflectance mode using a portable MicroNIR OnSite-W spectrometer (VIAVI Solutions S.r.l., Italy) in the spectral region between 900 and 1600 nm. For each pot, 60 spectra were acquired. The raw spectra and the results of Principal Component Analysis showed evidence of minimal differences in NIR spectral profiles between treatments. A good separation resulted between the first stage of growth and the following development stages. Partial least square analyses showed good prediction ability for chlorophyll (CHL) content and ascorbic acid/dehydroascorbic acid ratio (AsA/DHA). The model for CHL showed good performance in independent validation (R2val=0.87). The model for AsA/DHA ratio showed R2Xval = 0.89 but did not give the same performance in independent validation (R^2 val = 0.64). These preliminary results, besides confirming the potential of SS as alternative fertilizer for rice, suggested the usefulness of NIR as a fast and non-destructive technique for the simultaneous prediction of multiple parameters related to physiological state of the plant.

Keywords: rice, sewage sludge, NIR, PLS, chlorophyll, AsA/DHA ratio

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Nežka Sajinčič

Learning about NDSS through video – Evidence-based guidelines for effective instructional videos for a smooth transition into industry

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Non-destructive spectroscopic sensors (NDSS) are an innovative and highly useful group of tools that have a potential to considerably improve the food industry. Research and development are reaching the point where these laboratory-bound technologies can be implemented directly in the field, allowing the industry to apply them and put them into practice. However, widespread adoption of new technologies requires effective knowledge transfer, which means that people must first learn what these innovations can do and how to use them properly.

The COVID-19 pandemic brought many face-to-face meetings and training sessions to a standstill and highlighted the possibilities of online learning that will outlast the period of constraints. Although more sophisticated learning technologies now exist, recorded instructional videos remain one of the most popular and consistently used mediums for both formal and informal learning because of their ease of use, convenience, flexibility, and effectiveness (Islam et al., 2020). However, not all instructional videos are created equally, so it is important to know how to design educational videos that promote learning by knowing which features contribute positively to knowledge transfer and which do not (Fiorella and Mayer, 2018; Mayer et al., 2020).

Drawing on theories of learning with multimedia such as Cognitive Load Theory (Sweller et al., 2011), Cognitive Multimedia Learning Theory (Mayer, 2014), and the Cognitive-Affective Theory of Learning with Media (Moreno, 2006), we will present evidence-based guidelines for making effective educational videos. Using the topic of non-destructive spectral sensor applications for in situ analysis as an example, we will demonstrate some ways to improve instructional videos with the goal of accelerating the transfer of knowledge from academia and facilitating the implementation of NDSS in the food industry.

Keywords: instructional video, multimedia learning, instructional design, video demonstrations, knowledge transfer

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