BOOK OF ABSTRACTS

SensorFINT Conference 2023 - Annual Workshop of the work group Chemometrics & Quality Assurance

by

GDCh AK Chemometrik und Qualitätssicherung

and SensorFINT Cost Action

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14195 Berlin

Preface by Dolores Pérez Marín

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 **Second International Conference** (5th – 7th June, Berlin, Germany) organised in collaboration with the Annual Workshop AK Chemometrik of the German Chemical Society (GDCh).

It is exciting to participate in this new SensorFINT event with the main objectives of sharing knowledge and enhancing our networking opportunities in the field of applying spectral sensors to food integrity issues. In particular, it is important to highlight how SensorFINT is collaborating in the dissemination of technological knowledge to the new generation of researchers and practitioners, and also to those coming from countries with a lower degree of technological development. In addition, it is very important to see the involvement of companies and the opportunities to exchange opinions, information, needs both in the scientific sessions, in the industrial round table, as well as in all the breaks and social events.

I would like to thank all of you, all SensorFINT members, for your collaboration and for making this possible again. Thanks, of course, to the keynote speakers and the session chairs. Special thanks to the Local Organisers (Claudia Beleites and Stephan Seifert) and to the Vice-chair (Tom Fearn) as well as to Marcel Dahms, the GDCh and the JKI for their dedication and support. Finally, thanks to Cost for funding SensorFINT and its activities.

Signed: Prof. Dr. Dolores Pérez Marín

Chair of SENSORFINT (Cost Action 19145)

ORGANISING AND SCIENTIFIC COMMITTEE

- Claudia Beleites, Chemometrix GmbH, (Germany), Local Organiser
- Stephan Seifert, Hamburg University, (Germany), Local Organiser
- Lola Pérez Marín, University of Córdoba (Spain), SensorFINT Chair
- Tom Fearn, UCL (UK), SensorFINT Vice-Chair

CONFERENCE PROGRAM

Day 1: Monday 05.06.2023

	08:30	Registration /Attendance list	
	09:00	Welcome	
	Session 1: NIR sensors for food integrity assessment ***Session chairs: Krzysztof Rutkowski and Christian Huck***		
1K	09:15	**Paolo Berzaghi**	**Portable Near Infrared instruments: available technologies, applications and limitations**
1O01	10:00	J.L. Aleixandre-Tudo	Prediction of astringency intensity during red wine fermentation using different spectroscopy techniques
1O02	10:15	José A. Entrenas	In vivo Assessment of Pelvic Fat in Pullet Broiler Breeders using Portable NIRS Sensors
1O03	10:30	Yuanyuan Pu	Standardisation of two NIR process probes with different cable lengths and comparison of its performance for the prediction of protein in milk protein concentrate
	10:45	**Coffee break**	
1O04	11:15	Mia Schutte	Antioxidant properties of roasted wheat using near-infrared (NIR) spectral data

1O05	11:30	Marina De Gea Neves	Differentiation of hazelnut crops and classification of fish populations by handheld NIR spectroscopy and PLS-DA
1O06	11:45	Mari van Wyk	Effect of sourdough dough yield (DY) and flour type on sourdough using near-infrared (NIR) spectra
1O07	12:00	Víctor Fernández-Cabanas	NIRS Evaluation of the lipid profile of Senegalese sole (Solea senegalensis)
1O08	12:15	Miguel Vega-Castellote	Light penetration of NIR radiation in watermelons with regard to soluble solid content determination
1O09	12:30	Stefka Atanassova	NIRS for nondestructive differentiation of fresh and frozen-thawed meat and fish
	12:45		Announcements
	13:00	**Lunch & Posters**	
	Session 2: Other non-destructive spectral sensors to solve food specific issues ***Session chairs: Antonio Silva Ferreira and Elena Fulladosa***		
2K	14:00	**René Bachmann**	**Spatially Offset Raman Spectroscopy in Food Control. The (challenging) way from laboratory to on-site analysis?**
2O01	14:45	Krzysztof Bec	Analytical Approaches for Quality Control and Authenticity Screening of Insect Protein-Based Food Products

2O02	15:00	G. Foti	Time Domain Reflectometry and chemometrics for bread dough characterization
2O03	15:15	Martin Kögler	Time-gated Raman spectroscopy: a promising tool for rapid and accurate bacterial identification
2O04	15:30	Nuri Cebi	Monitoring the effect of freeze-drying on discrimination of adulterated yogurts by using Raman spectroscopy combined with chemometrics
	15:45	 **Coffee break**	
	16:30	**Round Table: Industrial Session** • **Mario Krause, Carl Zeiss Spectroscopy GmbH** • **Julio Hernandez, Norsk Elektro Optikk AS** • **Martin Lagerholm, PerkinElmer** • **Marcel Dahms, Senorics GmbH** • **Daniel Graaff, Rheinlandkräuter** • **Vincent Baeten, Walloon Agricultural Research Centre** • **Anika Bockisch, Bio-PAT Network** **Moderation: Dolores Perez-Marin & Tom Fearn**	
	18:00	**Ice Breaker & Posters**	

Day 2: Tuesday 06.06.2023

	08:30	 **Attendance list**	
	Session 3: Sensor fusion for food safety and quality applications ***Session chairs: Marena Manley and Mecit Oztop***		
3K	09:00	**José Blasco**	**Hyperspectral imaging: A valuable tool for postharvest fruit quality inspection**
3O01	09:45	C. Demoitié	Assessment of vitreousness of durum wheat kernels using various HSI systems
3O02	10:00	Irina Torres-Rodríguez	Optimization of hyperspectral imaging acquisition for the quality assessment of sliced Iberian ham
3O03	10:15	Ebrahim Taghinezhad	Predicting Quality Properties of Pears During Storage Using Hyperspectral Imaging System
	10:30	 **Coffee break**	
3O04	11:00	Nikos Chorianopoulos	Multispectral Imaging (MSI) in combination with machine learning for the evaluation of microbiological quality and authenticity in several seafood
3O05	11:15	Hilmi Eriklioğlu	Early Detection of Chocolate Blooming by Using VIS-NIR Hyperspectral Imaging and Chemometric Techniques
3O06	11:30	L. Fiorani	Non-destructive laser spectroscopic sensing of organophosphate compounds

	12:00		
	12:50	**Lunch & Posters**	
	14:00	**MC meeting** (only for MC members)	**JKI tour & Posters**
	16:00	 **Coffee break**	
	Session 4: Combination of ICT and nondestructive spectral sensor signal to build decision support systems for the food industry ***Session chairs: Víctor Fernández and Luca Fioriani***		
4K	16:15	**Declan Delaney**	**The role of sensor data and data quality assurance in decision support systems**
4O01	17:00	Antonio Silva Ferreira	FieldOmics: Concept of a Smart Grape Sensor
4O02	17:15	Elena Fulladosa	Non-destructive spectrometric sensors for food labelling and consumers
4O03	17:30	Gonçalo Guedes	Toward Authenticity Port Wine using a Smart Sensor
	18:00	**Guided Walk through Dahlem**	
	20:00	**SENSORFINT DINNER**	

Day 3: Wednesday 07.06.2023

	08:30	**Attendance list**	
	Session 5: Chemometrics for spectral and non spectral data ***Session chairs: Stephan Seifert and Jean-Michel Roger***		
5K	09:00	**Hadi Parastar**	**Integrating design of experiment and machine learning to optimize HS-GC-IMS conditions**
5O01	09:45	Paul-Albert Anselm Schneide	Shift-Invariant Tri-linearity (SIT) - A new model for resolving untargeted GC-MS data
5O02	10:00	Federico Marini	Class-modeling: an overview
5O03	10:15	A. Deryck	Potential of local partial least squares methods for feed characterization
5O04	10:30	Ramin Nikzad-Langerodi	Multivariate statistical process control (MSPC): Quo Vadis?
	10:45	**Coffee Break**	
5O05	11:15	Alissa Drees	Rapid Determination of the Shell Content in Cocoa Products by FT-NIRS and Chemometrics
5O06	11:30	Justyna Grabska	Chemical interpretation of regression

			models and instrumental differences – the case of piperine analysis in black pepper
	STSM Session ***Session chairs: José Antonio Entrenas and Candela Melendreras***		
6O01	11:50	Ahmed Menevseoglu	Rapid detection of apricot seed adulteration in ground almond using FT-NIR spectroscopy combined with chemometrics
6O02	12:00	Mar Garrido Cuevas	NIRS technology and PLS-DA analysis for supporting EU Tasting Panels to classify Extra Virgin Olive Oils
6O03	12:10	Giorgia Stocco	Exploring the use of portable NIR and Raman spectroscopy for quality control of PDO hard cheeses
6O04	12:20	Arnaud Molle	Exploring the use of benchtop FT-NIR and portable Vis-NIR spectroscopy instruments for quality control of PDO hard cheeses
6O05	12:30	Alejandra Arroyo-Cerezo	Study of portable NIR instruments for virgin olive oil quality assurance
6O06	12:40	Lorenzo Strani	Identification of mountain food products' signature through different spectroscopic techniques
	12:50	**Closing**	

	13:05	**Lunch**

Keynote Lectures and Oral Presentations

1K: Portable Near Infrared instruments: available technologies, applications and limitations

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Portable near-infrared (NIR) applications refer to the use of compact and lightweight devices that can perform near-infrared spectroscopy measurements in the field or on-site, rather than in a laboratory setting. Portable NIR applications can be used for various purposes, such as analyzing the quality of agricultural crops and determining the nutritional content of food. The advantage of using portable NIR devices is that they allow for rapid and non-destructive analysis of samples, which can be useful in situations where time and resources are limited. The development of miniaturized and portable NIR devices has been facilitated by advances in technology, such as the use of low-cost and high-performance components, as well as the development of sophisticated algorithms for data analysis. In just a few years we have assisted at the launch of several sensors in the market, based on a variety of different technologies, all aiming at providing low cost, high performance instruments making NIR applications more accessible and affordable. Yet at the promise of vendors, there must be methods [**1**] to evaluate qualities and limitations of sensors. As there has been several review on the technical features (spectral band, resolution, signal to noise ratio) of some of the most popular sensors, this work will focus on the practical limitation related to sample presentation and homogeneity, calibration transferability and openness of prediction engines.

Discussion Question

What will be the role of portable sensors in the food industry?

References

[1] G. Gorla Author, Analytica Chimica Acta,1211:229900 (2022), https://doi.org/10.1016/j.aca.2022.339900

1O01: Prediction of astringency intensity during red wine fermentation using different spectroscopy techniques

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During red wine maceration phenolic compounds are released from the solid parts of the berries into the wine. Among these phenolics, tannins are the main drivers for the astringency perception which is one of the most appreciated attributes in red wines. Nevertheless, the astringency of the wines can be perceived as pleasant when smooth and high-quality tannins are present or unpleasant when tannins provide a harsh and bitter mouthfeel. Moreover other wine components also play a role in the perception of wine's astringency. For example, acids might enhance the astringency sensation, whereas sugars and alcohols decrease it. To ensure the quality of the wines produced it is therefore of special relevance to monitor the astringency intensity during maceration. However, the presence of sugars, masking the astringency perception, during the fermentation-maceration process makes the sensorial evaluation of the wines inaccurate. To overcome this, this work aimed at investigating the ability of spectroscopy techniques to quantify the astringency intensity of red wines during the fermentation process. Wines made over two vintages from several cultivars were used. A subsample of the wines was collected daily from each fermentation and fermented until dryness before the sensorial evaluation of the wine's astringency intensity. Spectral data was obtained with UV-Visible, NIR, MIR and fluorescence spectrometers. Overall, specialized per cultivar calibrations showed the best prediction accuracy. Spectral data obtained with a single excitation multiple emission fluorescence spectrometer predicted astringency intensity with an R^2val = 0.91 and a RMSEP = 0.174 (RMSEP% = 5.3). This study proved that spectroscopy and chemometrics can be used to predict astringency intensity during red wine fermentations serving as a valid monitoring tool to ensure wine quality.

Discussion Question

Can spectroscopy be used to quantify sensory attributes?

1O02: In vivo Assessment of Pelvic Fat in Pullet Broiler Breeders using Portable NIRS Sensors

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Efficient use and proper allocation of dietary energy in modern laying hens production systems are of increasing importance, as they lead to improved efficiency and more accurate control over production costs [1]. A significant indicator of adequate energy consumption during rearing is the amount of abdominal fat accumulated to prepare pullets coming into production. The most direct way to measure abdominal fat is to euthanize the animal and take the pelvis fat and weight. Another option is the palpation of the pelvic bones to assess the accumulation of fat and to know the readiness of the bird for light stimulation [2]. Nevertheless, the first method is highly invasive and only can be applied to a small number of birds from a flock, and the second one is very subjective. This study aimed to evaluate the potential of two portable Near Infrared Spectroscopy (NIRS) devices with different optical configurations, weight, and price — the MicroNIR™ Pro 1700 and the SCiO— for their ability to predict abdominal fat in living pullet broiler breeders using Partial Least Squares (PLS) regression. Results showed that NIRS handheld devices can provide a reliable, non-invasive, and easy to use by non-experts instrumental method to predict pelvic fat in pullet broiler breeders.

Discussion Question

Do you know any other running studies using portable /handheld NIRS devices for in vivo analysis of poultry?

References

[1] C. Souza, J.J.B. Jaimes, C.E. Gewehr. Poultry Science, Volume 96, Issue 6, Pages 1688-1695. 2017.

[2] P. Welten. Prepare your breeder hens for optimum production. Cobb-vantress. 2019.

1O03: Standardisation of two NIR process probes with different cable lengths and comparison of its performance for the prediction of protein in milk protein concentrate

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The main objectives of this study were to firstly, evaluate the spectral repeatability of two NIR probes (probe-1 (master probe) and probe-2 (satellite probe)) that had different fiber optic cable lengths (15 meters and 10 meters, respectively) attached to a FT-NIR instrument. Secondly to standardize the two probes for the measurement of protein in milk protein concentrate (MPC). In addition, the performance of calibration equations obtained for the prediction of protein in MPC was evaluated. Two different standardisation strategies, direct standardization (DS) and piece-wise direct standardisation (PDS) [1], were applied to a set of 10 cloning samples to reduce the spectral difference between the two probes. Once the best standardisation matrix was obtained, it was applied to the spectra recorded in probe-2. The results demonstrated that PDS performed better than DS to correct the spectral difference between the two different NIR process probes.

Discussion Question

Possible reasons for the differences between spectral signals produced by probe-1 and probe-2 ?

Reference

[1] Bouveresse, E., C. Hartmann, D. L. Massart, I. R. Last, and K. A. Prebble. "Standardization of near-Infrared Spectrometric Instruments." Analytical Chemistry 68, no. 6 (1996): 982-90. https://www.cobb-vantress.com/en_US/articles/prepare-your-breeder-hens-for-optimum-production/

1O04: Antioxidant properties of roasted wheat using near-infrared (NIR) spectral data

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Dry thermal treatment can be applied to wheat as a pre-treatment to increase antioxidant properties due to the occurrence of non-enzymatic browning [1]. Using near infrared (NIR) spectroscopy to measure total phenolic content (TPC) eliminates the need for the lengthy extraction process. The external parameter orthogonalisation (EPO) algorithm can be applied to NIR spectra to remove the effects of unwanted variation [2] such as moisture content. The use of EPO, standard normal variate (SNV) and 2nd derivative by Savitzky-Golay filtering (3rd polynomial; 15 points) were investigated individually and in combination to predict TPC from NIR spectra (1000-2500 nm) obtained from wheat roasted at 10 different temperatures. Due to the different roasting temperatures, moisture content varied greatly between the samples. EPO removes this unwanted moisture variation by projecting the spectra orthogonal to the spectral regions affected by moisture. Partial least squares regression (PLSR) models to predict TPC were developed using venetian blinds cross validation and the results are given as RMSECV and R^2. Savitzky-Golay 2nd derivative had the highest estimation accuracy (5.89 gallic acid equivalents (GAE); 0.85) followed by EPO (7.85 GAE; 0.84) and SNV (10.03 GAE; 0.77). When EPO was applied in combination with 2nd derivative and SNV, respectively the accuracy was best for EPO + 2nd derivative (5.72 GAE; 0.86) followed by EPO + SNV (7.48 GAE; 0.82). EPO applied to NIR removed the effect of unwanted moisture, making the PLSR models more robust for changes in total moisture content. Even better results were obtained when used in combination with Savitzky-Golay 2nd derivative allowing for improved prediction of TPC in whole wheat grain.

Discussion Question

How can the principle of external parameter orthogonalization (EPO) preprocessing, as applied to NIR spectra, be explained to non-chemometricians?

References

[1] E.E. Çelik & V. Gökmen, *Journal of Cereal Science*, *93* (2020), https://doi.org/10.1016/j.jcs.2020.102978

[2] J.M. Roger, F. Chauchard & V. Bellon-Maurel, *Chemometrics and Intelligent Laboratory Systems*, 191–204 (2003), doi:10.1016/S0169-7439(03)00051-0

1O05: Differentiation of hazelnut crops and classification of fish populations by handheld NIR spectroscopy and PLS-DA

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Hazelnuts are widely used in the food industry to produce butter, chocolate, ice-cream, dairy products, confectionary and baking, and can also be added to yoghurts, breads, cereals, and liquors. The oxidation process is the main degradation factor in food containing oil and fat and therefore, the control of storage, shelf life and annual harvest has shown enormous importance both in the industrial production chain and in supplier analysis. In order to test the feasibility of discrimination between hazelnuts harvested in two successive years of cultivation, the handheld trinamiX NIR spectrometer was used in tandem with PLS-DA calibration (Fig. 1). The sensitivity value of new samples was 90% while their specificity was 100%.

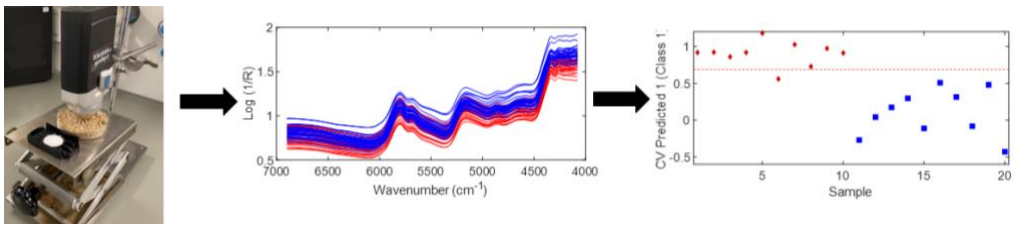

Fig. 1. Experimental set-up of hazelnut-powder measurement, spectral data, and PLS-DA results (red: 2021 crop, blue: 2022 crop)

For the second application 142 otoliths from two different fish populations (Northern Component (NC), and Southern Component (SC), of the Central Baltic Herring) were measured with the NeoSpectra NIR scanner and subsequently analyzed by PLS-DA. The model achieved for both classes sensitivities (CV) and accuracy results >82%, thereby demonstrating the potential of the technique as a rapid screening tool (Fig 2).

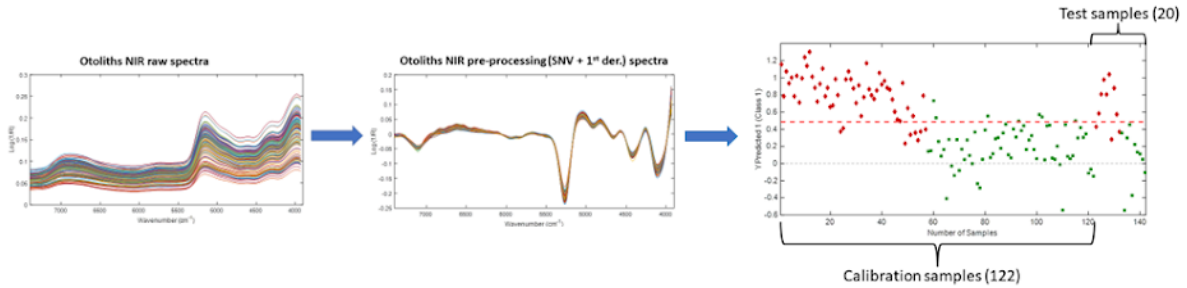

Fig. 2. Raw (left) and preprocessed (SNV + 1st derivative)(center) NIR spectra of 142 otolith samples and PLS-DA calibration and validation developed thereof (right).

Discussion Question

Sample presentation/number of replicate spectra; minimum number of samples for the PLS-DA.

1O06: Effect of sourdough dough yield (DY) and flour type on sourdough using near-infrared (NIR) spectra

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Sourdough bread consumption has increased dramatically due to an increase in consumer demand for clean-labels and artisan products. Many bakers prefer stoneground flour for baking sourdough bread due to its texture and sweet nutty flavour (Cardinali *et al*., 2022). This study aimed to assess the effect of stoneground and roller-milled flour on Type I (DY 160) and Type II (DY 220) sourdough using near-infrared (NIR) spectral data, pH measurements and total titratable acidity (TTA). NIR spectroscopy measurements can allow bakers to monitor sourdough pH throughout the fermentation process to obtain the desired end product. For each sourdough, absorbance spectra were acquired from 1000–2500 nm every fourth day for 28 days. The use of SNV, MSC, external parameter orthogonalisation (EPO) and MSC combined with Savitsky-Golay (SG) 1st derivative (2nd polynomial; 15 points) were investigated to predict pH. PLS regression models were developed using full-cross validation. RMSECV and R^2 were used to indicate the accuracy of the model. For pH, MSC combined with SG 1st derivative had the highest accuracy (0.056; 0.64) followed by MSC (0.064; 0.61), SNV (0.064; 0.61) and EPO (0.073; 0.50). The coarse stoneground flour exhibited a higher average value for pH and TTA compared to the other flours. This may be attributed to the elevated bran content in the former. PCA biplots showed an association between sourdough dough yield (Type) and pH and TTA values of the respective flours. Specifically, Type I sourdough was found to be associated with elevated pH levels, while Type II sourdough was linked to increased TTA values, irrespective of the flour used. The use of pH and TTA measurements in combination with NIR spectroscopy can provide a rapid and non-destructive method to monitor sourdough fermentation progress.

Discussion question

How does one determine the optimal parameters (component) when EPO is used as a pre-processing method during NIR model development?

References

Cardinali F, Garofalo C, Reale A, et al 161, 111796 (2022)

https://doi.org/10.1016/j.foodres.2022.111796

1O07: NIRS Evaluation of the lipid profile of Senegalese sole (Solea senegalensis)

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The consumption of fish is often associated not only with the high organoleptic quality of seafood products, but also with health benefits for the consumer. Most of these benefits are due to the properties of the animal fat, so it is of great interest to be able to determine its lipid profile quickly and, if possible, non-destructively.

In this context, Near Infrared Spectroscopy (NIRS) can be very useful as it has demonstrated its ability to rapidly (usually within seconds) estimate the lipid profile of a wide variety of animal and plant products.

In the aquaculture facilities located at the IFAPA El Toruño Center, different families of sole have been studied with diets in which fish fats and meals are partially replaced by other more sustainable raw materials of vegetable origin, with the aim of improving their lipid profile (Project PR.FEM.PPA201900.001). Considering that the reference analyses used to determine the lipid profile of fish samples are slow and produce residues that could be highly contaminating if not properly handled, it is of great interest to evaluate the feasibility of estimating the lipid profile using benchtop NIR instruments.

In the present study, the feasibility of using one of these instruments to obtain information on the quality of animal fat was analyzed. The models developed with analytical data expressed on the basis of muscle dry weight would make it possible to estimate quickly and with acceptable precision the content of majority fatty acids, as well as saturated fatty acids (SFA), n3-HUFA and the n3/n6 ratio, which would be very useful for the nutritional characterization of aquaculture products.

Discussion Question

What are the units for lipid profile expression that best correlate with NIR spectra?

1O08: Light penetration of NIR radiation in watermelons with regard to soluble solid content determination

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Near infrared (NIR) spectroscopy is well known as a fast and non-destructive technology for the internal quality determination of horticultural products. Particularly, in the case of watermelons, although some studies have shown promising results for the evaluation of their internal maturity, there is a need to assess the penetration depth of the NIR light into these intact fruits with thick rind. This could provide a better understanding of the correlation between the spectral information taken in the watermelon's rind and the reference data obtained from different portions of the flesh. Consequently, this study sought to assess the penetration of the NIR light through the watermelon's rind and to determine the soluble solids content (SSC) in the flesh of intact fruits. To that end, an NIR device working in interactance mode in the 761–1081 nm range was used. Two different distances between the light source and the field of view of the interactance instrument were tested (10 and 28 mm) in order to assess the influence of the optical measurement geometry in the results. For the light penetration assay, spectral information was taken from watermelon slices of different thicknesses placed upon a block of coconut fat. The contribution of the watermelon and coconut fat to the captured signal was assessed by means of the multivariate curve resolution (MCR) method. Clear penetration depth differences could be seen between the assays carried out using the 10 mm and the 28 mm distance. For the prediction of the SSC, the partial least squares (PLS) regression method was used, and excellent results were obtained, being the obtained results highly dependent on the instrument's optical measurement configuration used.

Discussion Question

Do you always consider how deep the NIR light is traveling into your sample when developing applications using this technology in fruits?

1O09: NIRS for nondestructive differentiation of fresh and frozen-thawed meat and fish

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Rapid and reliable analysis of meat and fish quality would be highly desirable both for the manufacturers and consumers. The results of two experiments, related to the application of NIR spectroscopy to the discrimination of fresh and frozen pork meat and fish will be presented. In the first experiment, pork samples from chilled meat were used. Slices of the meat with a thickness of 1.5-2 cm and a weight of about 55-60 g were prepared and placed in Petri dishes. Carp (Cyprinus carpio) weighing from 400 g to 800 g was used in the second experiment. From each fish, two test pieces were cut from the dorsal and ventral regions. Each meat and fish sample was measured as fresh, after a single freezing in a freezer at -18^{0}C for a period from 15 to 45 days with subsequent thawing and after a second freezing and thawing. NIRS measurements were performed by NIR Quest 512 spectrometer (Ocean Optics, Inc.) in the region 900-1700 nm using a reflection fiber-optics probe. Fish samples were measured from the skin side. SIMCA models for discrimination of fresh and frozen-thawed meat and fish were developed using two/third of the samples and different spectral data transformations. The rest of the samples were used as a validation data set.

Differences were found in the spectral data of fresh and once or twice frozen-thawed meat and fish samples. The best models for the discrimination of pork samples showed a recognition rate from 96 to 100% for the calibration data set and from 91 to 99% for the validation set, respectively. The models for dorsal fish samples discriminate correctly from 82 to 89% of validation samples, and the model for ventral regions samples from 76 to 91%, respectively. A reason for the slightly lower accuracy obtained for the fish samples is probably the presence of a scaly covering on some of the carp.

From the obtained results we can conclude that NIR Spectroscopy has the potential for fast and non-destructive discrimination not only between fresh from frozen-thawed pork meat and carp fish but also distinguish between once or twice-frozen samples.

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2K: Spatially Offset Raman Spectroscopy in Food Control. The (challenging) way from laboratory to on-site analysis?

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Spatially Offset Raman Spectroscopy (SORS) is a specialised Raman technique focussing on through barrier measurements. Despite the lower Signal intensity compared to other Raman techniques, this makes SORS to a potential interesting analysis method for foods. Beside optimization of analysis costs and times, sustainability is an urgent topic in food control. Through packaging measurements would allow withdrawing only foodstuffs from circulation that are conspicuous, while the other products can remain on the market. Up to now, food control works with random sampling, which leads to food losses in the case of faultless foods. Nevertheless, it is a long way from promising results in laboratory to the final application in on-site analysis. At the state laboratory of Schleswig-Holstein currently authenticity verification of vegetable oils and fish as well as analysis of the microbiological profile of chicken meat are main research topics for the use of SORS. Analytical, matrix problems and challenges in data evaluation are discussed and possible ways of handling these difficulties were shown. Furthermore, an outlook on the current state of analytics in routine on-site analysis is given.

Discussion Question

What are good methods to decide which optical spectra a suitable for analysis in heterogeneous foods?

2O01: Analytical Approaches for Quality Control and Authenticity Screening of Insect Protein-Based Food Products

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The future of food supply is becoming increasingly dependent on alternative protein sources due to rising concerns about the environmental impact of traditional livestock farming practices. Insect-derived protein is emerging as a promising alternative, as it offers a more sustainable and efficient way to produce protein. However, the growing popularity of this protein source has also created a need for effective methods to ensure quality control [1].

Our quantitative study focused on developing rapid and efficient on-site analysis methods for protein content in artisanal insect bars using miniaturized NIR spectrometers. We evaluated the performance of four different spectrometers, including a benchtop and three miniaturized devices, using PLSR and GPR calibration methods and data fusion concept. Our results demonstrated that miniaturized NIR spectrometers, particularly those with GPR calibration (Figure 1), could provide an effective method for the prediction of the protein content in insect protein-based energy bars.

In addition to the quantitative study, we also conducted a qualitative analytical study that aimed to discriminate between insect-derived protein flour and wheat protein in energy bar products. Since wheat protein is less expensive for retail and small enterprises, having an easily accessible tool for authenticity screening is crucial. We compared the feasibility of NIR spectroscopy, ATR-IR, and a portable Raman instrument (equipped with fluorescence mitigation technology) in discriminating between insect-derived protein flour and wheat protein. Our findings suggested that all three techniques could provide effective methods for discriminating between the two types of protein; however, NIR spectroscopy showed decisive lead in analytical performance and practical factors in such scenario.

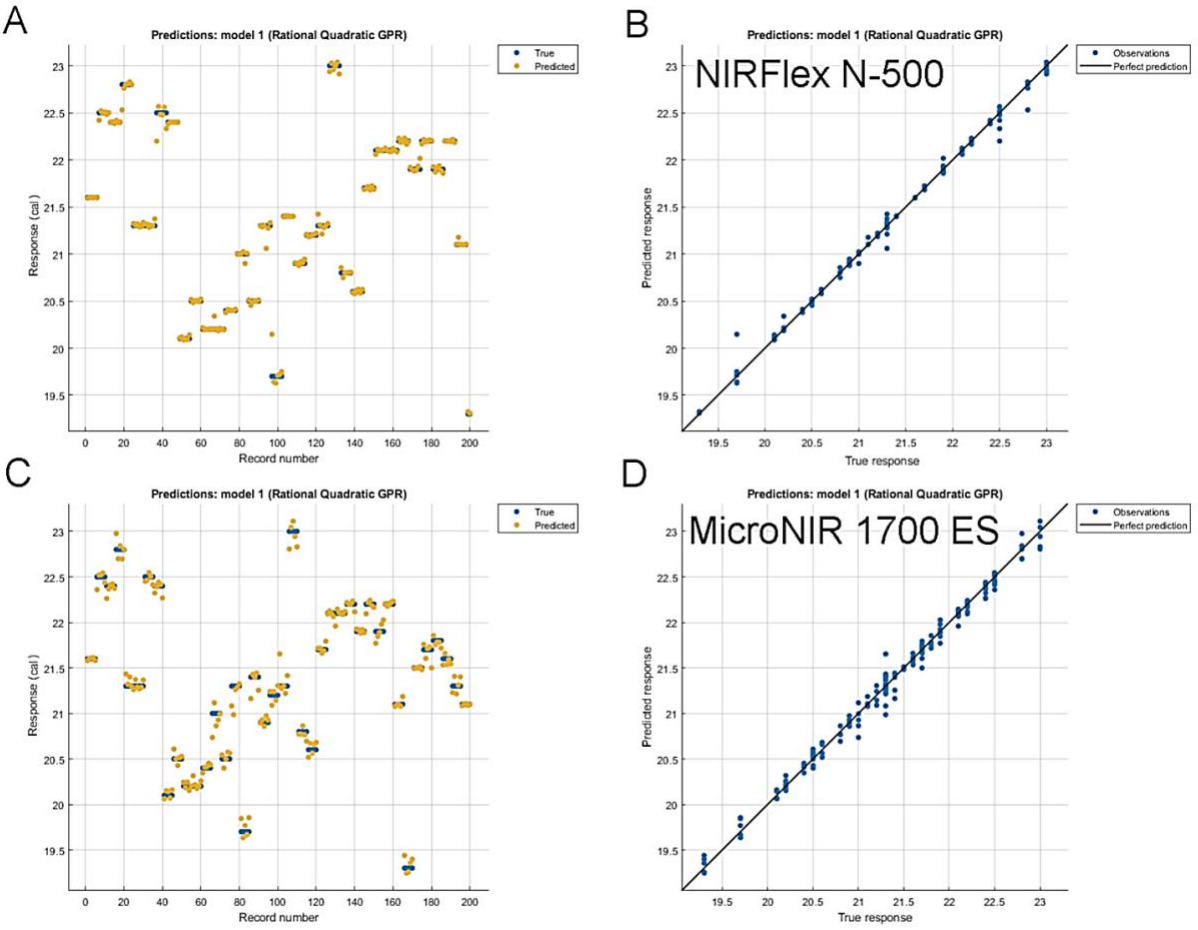

Figure 1. The fit of the GPR model to the calibration set of milled samples for (A,B) benchtop and (C,D) miniaturized MicroNIR 1700 ES spectrometer. (A,C): response plot; (B,D): predicted vs. true response plot.

Discussion Question

How can small and medium-sized enterprises be encouraged to adopt non-destructive sensors, such as miniaturized NIR spectrometers, ATR-IR, and portable Raman instruments, for efficient quality control and authenticity screening of insect protein-based food products?

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2O02: Time Domain Reflectometry and chemometrics for bread dough characterization

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Time Domain Reflectometry (TDR) has recently emerged as a cheaper alternative to more expensive optical spectroscopy-based sensing techniques for the characterization of different food matrices in a broad range of applications [1]. By applying a step-like voltage signal to a food sample, it probes its dielectric properties. Such time-domain signal, in fact, has an ultrabroadband spectrum in frequency domain (with a cutoff frequency of approximately 5 GHz) and thus is capable of exciting the vibrational modes of polar molecules such as water. In this work the potential of this sensing technique, coupled with chemometric methodologies, was explored for the determination of the salt content in bread doughs prepared with different procedures (manual as well as automatic kneading). Several pre-processing methods were tested, ranging from more basic ones such as Standard Scaling and Mean Centering to more advanced, such as Fast Fourier Transform (FFT). The obtained results showed that Partial Least Square Regression (PLSR), in combination with simple pre-processing methods, allows to achieve high values of R^2 with a relatively low Root Mean Square Error (RMSE). We compare these results with those obtained with NIR technique where similar values of R^2 and RMSE were obtained. Our findings demonstrate the potential of TDR technology as an alternative to NIR for bread dough characterization and for other applications where the material under test contains polar molecules and costs represent a constraint.

Discussion Question

Do you expect this technique to be able to discriminate fatty acids?

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2O03: Time-gated Raman spectroscopy: a promising tool for rapid and accurate bacterial identification

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This study aimed to investigate the potential of time-gated Raman spectroscopy to identify common pathogenic bacteria in clinical settings and food spoilage. Six bacterial pathogens namely *A. baumannii, E. coli, P. aeruginosa, S. aureus, S. pneumoniae,* and *K. pneumonia*. were obtained from NordLab, Oulu, Finland. A PicoRaman M2 Time-gated Raman spectrometer (TimeGate Instruments, Oulu, Finland) with a state-of-the-art SPAD detector and a 532nm laser was used to collect Raman spectra from bacterial droplets. The preprocessed spectra were fed to a principal component analysis (PCA) to identify different bacteria. Surface-enhanced Raman spectroscopy (SERS) measurements were also collected for reference purposes. The results showed that time-gated Raman spectroscopy significantly reduced background fluorescence, allowing for the detection of unique Raman signals from bacterial cells. Each of the six bacteria was successfully identified through PCA analysis with 4 principal components. In contrast, SERS spectra were found to exhibit reproducibility issues. This study highlights the potential of time-gated Raman spectroscopy as a sensitive, auto-fluorescence suppressing, and specific technique for rapidly detecting and identifying common pathogenic bacteria, without the need for plasmonic effects. This technique could be a valuable tool for clinical diagnostics, as well as monitoring bacterial growth and metabolism in industrial and environmental settings.

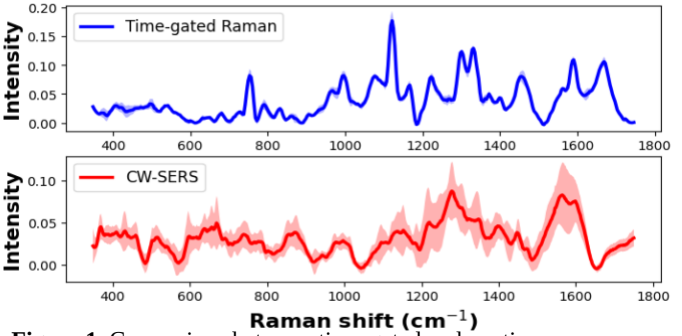

Figure 1. Comparison between time-gated and continuous-wave (CW) SERS spectra collected from *E. coli*.

Discussion Question

How can time-gated Raman spectroscopy be further optimized and developed as a reliable and practical tool for the rapid detection and identification of bacteria in clinical, industrial, and environmental settings?

2O04: Monitoring the effect of freeze-drying on discrimination of adulterated yogurts by using Raman spectroscopy combined with chemometrics

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Today, food adulteration and contamination problems are increasing an alarming trend across the world. In this research, Raman spectroscopy was used to determine the effect of freeze-drying on the discrimination of control yogurts from starch, flour, and adulterated yogurt samples. Spectral ranges of 585-646, 844-882, 1058-1103, 1290-1344, 1400-1460, 1640-1673 and 1725-1746 cm^{-1} were selected for discrimination in the hierarchical cluster analysis (HCA). Freeze-drying process considerably improved the spectral properties and discrimination pattern of control yogurt samples. The rheological behavior of the aqueous samples was evaluated, and rheological behavior was determined to be directly proportional to adulterant concentration (% w/w). Results highlighted the usefulness of freeze-drying prior to the Raman analysis in the context of evaluated samples. Raman spectroscopy combined with chemometrics can be used as an effective, rapid, green, robust cost-effective and high-throughput screening method in the food industry.

Acknowledgment

This project was funded by Yildiz Technical University Scientific Research Project Unit (YTU-BAP) under Project No: FBA-2021-4301.

Discussion Question

With the chemometrics method applied in this study, only freeze-dried yogurt samples could be discriminated from adulterated ones. Which chemometrics methods would you recommend to be used for discrimination of yogurt samples without any preprocessing or drying.

3K: Hyperspectral imaging: A valuable tool for postharvest fruit quality inspection

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Unlike conventional colour images, hyperspectral imaging (HSI) based systems capture information in multiple spectral bands. This feature makes HSI an important tool in inspecting postharvest fruit quality as it provides detailed information about invisible or internal properties, such as chemical composition, ripeness, presence of invisible damage and other factors, leading to early decisions about processing, sorting, storing and marketing the fruit, increasing supply chain efficiency and reducing food waste.

These images are analysed by techniques that extract relevant information from the hypercubes. Chemometrics is commonly used to relate spectral data to fruit characteristics. Regression techniques are used to predict the composition or concentration of certain compounds, allowing the estimation of properties such as acidity or sweetness or the shelf life based on estimated ripeness. In contrast, classification techniques can separate fruits according to quality attributes, such as the presence of damage, to sell them at different prices, at different moments, or target specific markets. Selection of the most important bands related to specific problems is another of the major applications of HSI in fruit inspection. Recently, deep learning techniques are also being used to analyse hyperspectral images in fruit problems, as they can learn complex patterns in the data, improving the accuracy in detecting fruit characteristics.

A major problem with statistical models applied to fruit inspection is their enormous variability and seasonal dependence. The same fruit variety can have different characteristics depending on the crop management, the soil, or annual variations in the climate, making it difficult to build general models or maintain their performance over time. This work explores some works at IVIA, applying hyperspectral imaging to practical fruit postharvest problems.

Discussion Question

Despite their usefulness, the many works found in the scientific literature and some success stories, why are they not widely implemented in the postharvest industry?

3O01: Assessment of vitreousness of durum wheat kernels using various HSI systems

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The vitreousness of kernels is one of the major factors used to assess of the quality of durum wheat intended for the food industry. Hyperspectral imaging (HSI) has previously been claimed as a promising alternative to the tedious visual inspection still used to grade batches [1]. HSI systems can vary in terms of acquisition technology, wavelength range and usability. The study aims to compare the classification performances of three visible-near infrared (Vis-NIR) equipment (HySpex VNIR-1800, Specim IQ and HinaLea 4200) and one NIR device (IMEC snapscan) based on partial least square-discriminant analysis to distinguish non-vitreous from vitreous wheat endosperm at the pixel-level. Further analyses were performed on two systems to validate their ability to determine the vitreousness of a batch at kernel-level in parallel with the reference method. Due to setup limitations, Vis-NIR cameras were compared on a limited spectral range (440-700 nm); the entire usable range was kept for the NIR camera (1125-1672 nm). The same sample sets of calibration and validation were used for each instrument to guarantee fair comparison. Models were developed from manually selected ROIs following principal components analysis. This process proved to be a more effective method of selection than applying a mask. While all cameras performed similarly with classification errors of prediction ranging from 7.8 % to 11.4 %, the best performances were obtained with the Specim IQ. The NIR range was not necessary to improve the predictions at pixel-level. However, individual kernels classification tested on various wheat batches performed better with the NIR camera.

Discussion Question

What advantages do HSI systems provide compared to conventional spectroscopy to assess the vitreousness of kernels?

Reference

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3O02: Optimization of hyperspectral imaging acquisition for the quality assessment of sliced Iberian ham

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Iberian ham has exceptional organoleptic, sensory and nutritional characteristics, being considered a gourmet product. To guarantee the consumer demands in terms of quality and authenticity, non-destructive analytical alternatives are needed. Hyperspectral imaging (HSI) records both spatial and spectral information, facilitating the characterization of heterogeneous samples, such as the Iberian ham. Nonetheless, a crucial aspect to obtain a high-quality dataset for the non-destructive assessment of any agricultural product is the optimization of the acquisition procedure. The aim of this research was to compare various acquisition settings to optimise the image quality without compromising the measurement time. For this aim, sliced Iberian ham samples of different categories were analysed – with and without packaging – using a hyperspectral imaging system working in the spectral range 900 – 1700 nm. To compare each configuration, the RMS statistic was calculated, and the spectral repeatability results were evaluated. Furthermore, given the importance of having representative spectral libraries to develop robust equations, especially in the case of products as heterogeneous as Iberian ham, the selection of different regions of interest was also evaluated.

Discussion Question

Which are the key factors for the analysis of sliced cure ham using HSI?

3O03: Predicting Quality Properties of Pears During Storage Using Hyperspectral Imaging System

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The utilization of Vis/NIR spectroscopy for estimation of the pear fruit chemical properties such as pH, titratable acidity (TA), soluble solids content (SSC), and Vitamin C during the storage period (different times and temperatures) is examined in this paper. Different pre-processing techniques were applied to the spectra to improve the accuracy of the prediction models. The results indicated that the S.G.+MSC+D2 pre-processing method accurately predicted the fruit's pH (rp=0.95, SDR=4.9). Conversely, the S.G.+MSC+D1 method accurately forecasted the TA (rp=0.98, SDR=9.6). Moreover, the study also investigated the significant effect ($p<0.05$) of storage period and temperature on the pear fruit's chemical properties. The findings revealed that the pH of the fruit increased with the storage period and temperature increase, whereas the TA decreased. In addition, it explains that as the storage period and temperature increase, the pear fruit loses its original characteristics, and its soluble solids and vitamin C content decrease. In conclusion, the study highlights the potential application of Vis/NIR spectroscopy for non-destructive and rapid monitoring of pear fruit's chemical properties during storage under varying temperature and time conditions. The results confirm findings from previous research on the impact of storage conditions on fruit quality.

Discussion Question

Why had been used different conditions of storage in this research?

3O04: Multispectral Imaging (MSI) in combination with machine learning for the evaluation of microbiological quality and authenticity in several seafood

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The expansion of Aquacultural sector and the automation of many procedures, enhances the need for implementing rapid, real-time technologies for seafood quality and authenticity assessment. In brief, shellfish, finfish and seaweed samples (n=2200) of various microbiological quality, species, origin and form were analyzed using different Multispectral Imaging devices provided by Videometer (Herlev, Denmark). Different machine learning classification and regression models (e.g., Partial Least Square - Discriminant analysis (PLS-DA), Support Vector Machines and/or Extra Trees) were generated and validated for the discrimination of the products based on geographical origin, species and/or form as well as for the estimation of their microbiological quality. Concerning fish, accuracy scores higher than 90% were recorded for the discrimination of seabass and seabream fillets, while the developed models exhibited a satisfactory performance in predicting microbial population (R^2>0.70, RMSE<0.9). In shellfish, 86 and 98% of mussel samples were grouped correctly based on their origin (Greek vs Spanish) and form (fresh/thawed). The results of the regression model for the prediction of the microbial counts in brown seaweed indicated a good prediction performance on the external test dataset. This work has been co-funded by the projects DiTECT (861915) and TraceMyFish (ERA-NET Cofund BlueBio) (Grant Agreement number 817992).

Discussion Question

Contribution of feature selection to the development of more efficient predictive models, customization of the device to specific foodstuff and integration of the method in an automated monitoring system.

3O05: Early Detection of Chocolate Blooming by Using VIS-NIR Hyperspectral Imaging and Chemometric Techniques

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Chocolate blooming is one of the main issues in the chocolate industry. There are two types of blooming, fat blooming and sugar blooming. When blooming occurs, customer satisfaction significantly decreases because of the unpleasant look and undesired texture. The reason for blooming is generally lack of tempering or poor storage conditions. Since blooming occurs over time, it is not easy to detect it, especially in the early stages. Therefore, it is necessary to develop tools to monitor chocolate blooming before visible signs and predict the blooming time and type. VIS-NIR Hyperspectral imaging (HSI) is a non-destructive imaging technique that can reveal differences related to the physical and chemical structure of samples. In this research, commercial chocolate samples were collected and melted to produce untampered chocolate to evaluate HSI technique for early detection and location of blooming. All samples were remolded into coin size tablets and hyperspectral images were taken for 30 days using line scan Pika L 400 to 1000 nm ranged hyperspectral camera (Resonon Inc). It is known that improving prediction accuracy requires chemometric approaches such as KNN, SIMCA, Class TREES, artificial neural networks [1]. These methods were applied using a ROI of tempered and untampered samples to create a predictive model of blooming detection by sample and by pixels. Results showed that spectral signatures were different between tempered, untampered chocolate and different storage times. Several chemometrics methods showed high performance, but artificial neural networks predicted correctly 99% of the samples using Savitzky Golay (SG) preprocessing.

Acknowledgements: Authors gratefully acknowledge receiving funding from European Union's horizon 2020 research and innovation programme under grant agreement (#101008228).

Discussion Question

What are the chemometric approaches that suit best with hyperspectral imaging.

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3O06: Non-destructive laser spectroscopic sensing of organophosphate compounds

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Organophosphate compounds are used for insecticides and pesticides to improve crop productivity. Unfortunately, they can enter the trophic chain via feed and food, posing a severe risk to human health. In addition, organophosphate compounds are used as chemical warfare agents (nerve toxins). Although banned by the Chemical Weapons Convention, Sarin and Novichok were used in Syria in 2013 and the UK in 2018, respectively. For these reasons, rapid field detection of organophosphate compounds is highly desirable. In this regard, non-destructive laser spectroscopic sensing can be a sensitive and specific tool for rapidly detecting organophosphate compounds in a real-world scenario. LPAS (laser photoacoustic spectroscopy) has been applied since 2017 to assess the safety and authenticity of fruit juices, oil, oregano, milk, pollen, rice (flour and cereals), saffron, and seafood. In a typical system, a tunable laser is modulated at a sound frequency and injected into a resonant cell where it strikes the sample under investigation, which absorbs the incident radiation, undergoing an increase in temperature and volume, thus producing a pressure wave. Typically, sound detection is performed by a microphone connected to a lock-in amplifier, and data analysis is performed using chemometric techniques. This paper reports on recent updates to an experimental system, focusing on acoustic resonance, and the first tests on detecting nerve agent simulants.

Discussion Question

Regarding the detection of pesticides in food, what are the standard and innovative techniques?

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4K: The role of sensor data and data quality assurance in decision support systems

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Decision Support Systems (DSS) play a pivotal role in current agriculture, food processing and distribution chains to benefit resource sustainability, security, safety and waste management of food. Such systems may employ prediction models, real time data from sensors and logistical data to present best possible actions given a current scenario. The importance of quality data which underlines and drives the recommended actions made in DSS is clear. Data quality may be measured via a number of metrics including accuracy, reliability, completeness and timeliness. Increasingly, real time DSS for food supply chains are harnessing the real time capabilities of networked sensor devices in decision making. While the integration of sensor devices can improve data completeness and timeliness, these sensors may introduce unreliable or inaccurate data. In this talk we explore the role of sensors in the food supply chain and how they can be integrated within DSS while maintaining data quality assurance.

4O01: FieldOmics: Concept of a Smart Grape Sensor

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The advent of precision viticulture has led to increased automation and monitoring for grape and wine quality improvement, crop management optimization, regulatory compliance, and cost reduction. Access to metabolic information of vines, such as grape composition, is crucial for effective grape maturation and wine quality management. However, the lack of non-destructive technology for measuring multiple vine and grape metabolic parameters has posed challenges in implementing advanced management strategies, as seen in other agro-industrial biotechnology areas.

Data processing and multivariable integration of spectroscopy enable prediction of grape quality during maturation and operational adjustments under changing conditions. This approach reduces overall viticulture process variability and allows for segmentation of grape quality for different types of wine with distinct sensory characteristics. The integrated system enables planning of viticulture operations and wine production using monitored data, segmentation of treatments by grape varieties and wine types, and improvement of quality based on data.

The proposed Smart Grape Sensor (SGS) for decision-making should include automation of spectroscopy data processing in the database, integration of field and laboratory-collected information using augmented reality techniques for field image visualization, classification of grape quality and chemical composition based on field images, monitoring and development of decision support methodologies, and visualization of results from various wine management strategies.

The method of acquiring spectra in the field should consider factors such as collection of information on spectral variation in each shot, spectral variation of grape bunches, spectral variation of bunches in different plants, and definition of spatial and temporal resolution.

Discussion Question

Cost of equipment and operations.

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Authentication and Environmental Investigations. Chemosensors. *In press*

4O02: Non-destructive spectrometric sensors for food labelling and consumers

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In recent years, new consumer demands have been established, increasing the need to improve food processing and to create new products with added value based on the new quality standards. The use of nutritional claims such as 'salt reduced' may have competitive advantages for companies and enables consumers to adopt healthier diets according to their needs. However, these claims and nutritional facts are sometimes not precise and should be verified to avoid exceeding the error tolerance limits recommended by the European Union. Likewise, consumers also demand information regarding the quality of foods and the truthfulness of the information on the label. In this sense, one of the challenges of the CCLabel project was to develop and evaluate different non-destructive spectrometric sensors (NDSS) based on X-ray and infrared spectroscopy and hyperspectral imaging to characterise food in the industry (for process optimization or precise labelling) and for consumers (to evaluate nutritional composition and quality of foods in situ) to stimulate a personalized nutrition and a more rational food choice.

A summary of some of the actions undertaken during the execution of the project to achieve this challenge are reported to show the potential of NDSS. Specifically, a study of the use of multienergy X-ray spectrometry for precise labelling at dry-cured ham industry which showed classification errors between 0 and 10% depending on the case study; a feasibility study of bench-top and low-cost near infrared spectrometric instruments to determine salt content in canned tuna which demonstrated the usefulness of these devices for process optimization; and an evaluation of the ability of commercial and developed in-house miniaturized low-cost sensors for consumers to determine the fresh/thawed fish quality with a classification performance between 88% and 96%.

Discussion Question

What do you think about the adoption of NDSS by consumers? How should this be implemented?

4O03: Toward Authenticity Port Wine using a Smart Sensor

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The authenticity assessment of Port wine is of critical importance to ensure the quality and integrity of this renowned liqueur wine. Spectral sensors, such as Fourier-transform mid infrared (FT-MIR) spectrometers and near-infrared (NIR) spectrometers, have emerged as valuable tools for authenticity assessment due to their non-destructive nature, rapid data acquisition, and ability to provide information on the chemical composition of wine. Authenticity classification using spectral sensors can help identify potential adulteration, detect counterfeit products, and ensure compliance with legal regulations. Accurate classification of Port wine authenticity is crucial for protecting consumers' interests, maintaining the reputation of Port wine producers, and safeguarding the economic value of this premium product. Therefore, the development and application of spectral sensors for authenticity classification in Port wine is a significant area of research with practical implications for the wine industry.

The combination of spectral sensors with artificial intelligence (AI) techniques, such as neural networks (NN), holds immense potential for authenticity classification in Port wine. Spectral sensors provide large amounts of data on the chemical composition of wine, while AI algorithms, specifically NN, can process and analyze this data to accurately classify wines based on their authenticity.

One bottleneck in spectroscopy to transfer data from one spectrometer to another. Recent advances in artificial intelligence (AI) have made it possible to transfer data between spectrometers with a high degree of accuracy. The model learns to identify the underlying patterns and relationships between the spectra, and can then be used to transfer calibrations.

These models can be used to detect various types of adulteration, such as blending with cheaper wines, addition of unauthorized additives, or mislabeling of wine origin.

The integration of spectral sensors with AI techniques can enable rapid and reliable authenticity assessment, helping to safeguard the quality and reputation of Port wine in the market.

The main objective of this work is to develop a set of digital filters for data curation, allowing for real-time database loading and data visualization, as a step towards creating a "smart sensor" that can override operation supervision. The model system chosen for this study is Port wine, which represents a complex matrix with changes in chemical profile over time. Initially, spectra were collected using a benchtop FT-(M)IR spectrometer, which provided consistency for comparison of the digital filters' performance.

Samples were divided based on “Port wine” and “Not Port wine”. The distances between new samples and the center of the PCA (T2 Hotelling) and between the plane of the PCA and the new samples (Q Residual) were used in conjunction with the digital filters. If a sample's Q Residual and T2 Hotelling values were outside the model, and the evaluation of physical-chemical parameters determined in the samples, were considered out of expected ranges, the samples were considered outliers and discarded. Results that were obtained represent an accuracy and specificity of 90%.

Current work has been developed to improve the transferability of the AI-based models for model transfer.

Discussion Question

What are the operation cost?

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5K: Integrating design of experiment and machine learning to optimize HS-GC-IMS conditions

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Headspace gas chromatography-ion mobility spectrometry (HS-GC-IMS) plays a major role in the areas of both targeted and non-targeted analysis [1]. However, due to the non-linear behavior of IMS and its highly complex ion chemistry, existing methodologies to find optimum experimental conditions are of limited applicability. Our research suggests that one possible way to overcome these issues is the integration of strategies from machine learning or deep learning (ML/DL). To this end, a novel combination of design of experiment (DOE) and ML/DL techniques is presented here, with saffron as a case study [2]. A rotatable circumscribed central composite design (CCD) is used to design five effective HS-GC-IMS factors, including sample amount, headspace temperature, incubation time, injection volume and split ratio. Then, different linear (i.e., multiple linear regression (MLR) and partial least squares (PLSR)) and non-linear (i.e., support vector machine (SVM) and artificial neural network (ANN)) ML/DL models are applied to predict GC-IMS responses (total peak areas and number of detected peaks) in individual and combined forms. The results showed outperformance of DOE-ML over the traditional modeling approach. Emphasis is placed on interpretation of factor effects and finding optimal conditions, as these are crucial for an assessment of the goodness and robustness of the models developed.

Discussion Question

How can we calculate factor effects and optimal procedure conditions in the case of non-linear models?

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5O01: Shift-Invariant Tri-linearity (SIT) - A new model for resolving untargeted GC-MS data

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Parallel Factor Analysis (PARAFAC) and its extension PARAFAC2 are widely used methods and applications of PARAFAC2 to untargeted data analysis of hyphenated gas chromatography with mass spectrometric detection (GC-MS) has been very successful [1]. This is attributable to the ability of PARAFAC2 to account for retention time shifts and shape changes in chromatographic elution profiles. Despite its usefulness, the most common implementations of PARAFAC2 are considered quite slow. Furthermore, it is difficult to apply constraints (e.g., non-negativity) to the shifted mode in PARAFAC2 models. Both aspects are addressed by a new shift-invariant tri-linearity (SIT) algorithm, proposed in this paper. It is shown on simulated and real GC-MS data, that the SIT algorithm is 20 to 60 times faster, than the latest PARAFAC2-ALS implementation and the PARAFAC2-Flexible coupling algorithm [2]. Further, the SIT method allows implementation of constraints in all modes. Trials on real world data indicate that the SIT algorithm compares well with alternatives. The new SIT method achieves better factor resolution than the benchmark in some cases and tends to need fewer latent variables to extract the same chemical information. Although SIT is not capable of modelling shape changes of elution profiles, trials on real world data indicate a great robustness of the method even in those cases.

Discussion Question

What are the pitfalls in untargeted analysis of LC-MS data?

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5O02: Class-modeling: an overview

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Many chemometric applications in the field of analytical chemistry, in general, and in spectroscopy-related problems, in particular, involve some sort of classification, i.e., the prediction of one or more qualitative attributes of samples, based on the measured data. In this context, class-modeling techniques, which aim at describing one particular category at a time, are, in principle, best suited to deal with situations such as food authentication or process control, where the classification problem is almost always asymmetric, with one category of interest being well characterized and representatively sampled (e.g., a food product with PDO origin or, in the case of process data, the so-called Normal Operating Conditions), while the alternative (made of everything that is not that specific group) is almost always under-represented by definition and highly heterogeneous. Despite this, such approaches are not as popular as the discriminant ones and largely underused.

In this communication, the fundamentals of class modeling [1] will be illustrated, with representative examples, together with some possible extensions to the multi-blòck context, where multiple data matrices are used to characterize the analyzed samples.

Discussion Question

Why is class-modeling still underused? What can we do to make it more widespread?

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5O03: Potential of local partial least squares methods for feed characterization

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Feed characterization is critical for optimal growth and health of production animals, but the variation in nutrient concentrations in feed products poses a significant challenge. Near-infrared spectroscopy (NIRS) combined with chemometrics appears to be a promising, rapid, and non-destructive technique for the reliable prediction of forage composition. Our goal is to develop more accurate and efficient NIRS-based predictive models for key parameters describing the quality of fresh green fodders and silages.

To achieve this goal, NIR spectra of four agricultural feed products (fresh green fodders, pre-wilted grass silage, direct-cut grass silage, and whole maize plant silage) were measured with the Aurora NIR spectrometer. Classically global partial least squares (PLS) techniques are used for the creation of predictive models for such products. But because they fail to account for local variability, they may be limited in accuracy and reliability. We thus investigate published local PLS methods to address this issue and improve feed characterization with NIRS.

Predictive models were developed for eight parameters characterizing the feed products' quality. In addition to a global PLS, four local PLS methods were tested: the local PLS regression[1], the local PLS regression on global PLS scores[2], the locally weighted PLS regression[3], and the locally weighted PLS regression on global PLS scores. This study explores the performances of those PLS techniques for feed characterization.

Discussion Question

Could local methods fully replace global methods in the future?

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5O04: Multivariate statistical process control (MSPC): Quo Vadis?

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MSPC is an umbrella term for data-driven approaches to process monitoring that are widely used in the process industry and manufacturing [1]. This contribution aims at giving a high-level overview on (latent variables-based) MSPC from a chemometrics perspective, including some real-world examples on its application. Furthermore, some important limitations, recent developments and open challenges will be discussed. Thereby, the focus will be put on causality, an important pre-requisite for extracting decision support from MSPC models, and the application of MSPC for federated analysis/modeling of value chains involving multiple companies/stakeholders [2].

Discussion Question

How can we use PCA/PLS-based MSPC models for optimizing industrial processes and value chains towards increased sustainability?

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5O05: Rapid Determination of the Shell Content in Cocoa Products by FT-NIRS and Chemometrics

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The determination of the cocoa shell content is of interest because a high shell content can cause a reduction in the quality of cocoa products. Consequently, we aimed to develop a routinely applicable method for the quantitation of shell material in cocoa nibs. For this, 51 fermented cocoa samples of different varieties from 14 cocoa growing countries covering the crop years 2012–2017 were acquired. Admixtures of cocoa nibs with shell material were prepared in a range of 0–20% cocoa shell and subsequently analysed by Fourier transform near-infrared spectroscopy (FT-NIRS). Support vector machine regression models were created, which enabled the prediction of the cocoa shell content in a mixing ratio range of 0–20% with an RMSE of 2.05% and a R^2 of 0.88 and in a range of 0–10% with an RMSE of 1.70% and a R^2 of 0.72. This predictive capability suggests that the presented method is suitable for rapid determination of cocoa shell content in cocoa nibs. In addition, it was demonstrated that the method is applicable to other relevant cocoa matrices, as the prediction of the shell content of several industrial cocoa masses by the FT-NIRS-based model showed good consistency with the prediction by liquid chromatography–mass spectrometry. This emphasizes that FT-NIRS combined with chemometrics has great potential for the determination of cocoa shell content in cocoa nibs and cocoa masses in routine analysis, such as incoming inspection.

Discussion Question

How can representative samples for calibration of a new model be created in a complex matrix without an available “zero sample” and no reliable reference method (e.g. shell content in chocolate)?

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5O06: Chemical interpretation of regression models and instrumental differences – the case of piperine analysis in black pepper

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Interpreting near-infrared (NIR) spectra is challenging due to the complex convolution of individual overtones and combination bands. Anharmonic quantum mechanics computations have become increasingly practical for simulating NIR spectra, and we evaluated effective approaches for this problem. Using piperine as an example, we compared two time-efficient approaches to simulate the NIR spectrum and identified the complex structure of its bands, which are mostly binary combinations [1]. We also assigned the NIR bands of piperine and used them to interpret the performance of two partial least squares (PLS) regression models built to describe piperine content in black pepper samples. We compared models developed from spectral data sets obtained with a benchtop laboratory instrument (NIRFlex N-500) and a miniaturized spectrometer (microPHAZIR). Although both spectrometers capture the most significant NIR absorption of piperine, they have profound instrumental differences. Our conclusion was that the stationary spectrometer is more selective in capturing chemical information, resulting in the laboratory FT-NIR spectrometer and narrow-waveband miniaturized spectrometer having different performances in analyzing piperine content in black pepper.

Discussion Question

How can we improve the interpretation of complex NIR spectra from natural products like piperine, which have overlapping and convoluted bands, and what are the potential applications of this in pharmaceutical and food industries?

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6O01: Rapid detection of apricot seed adulteration in ground almond using FT-NIR spectroscopy combined with chemometrics

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This study aimed to develop prediction models based on FT-NIR spectroscopic techniques combined with chemometric tools for the detection of apricot seed in ground almond samples. Almonds are one of the most expensive nuts with high economic value. Due to its high economic value, it has become more prone to adulteration. Apricot seed is one of the adulterants in ground almond as they have very similar appearance. In addition, the apricot seeds can contain high content of amygdalin which can cause cyanide poisoning. The samples (n=68) were purchased from local grocery stores in Türkiye. Ground almond samples were mixed with ground apricot seeds (1-50% w/w) at different concentrations. Spectra were collected using a portable FT-NIR and a benchtop FT-NIR spectrometer. Spectral data were analyzed using SIMCA to classify the samples, and PLSR to predict adulterant level. In addition, conditional entropy (CE) algorithms were used to predict adulterant levels and select wavenumbers associated with the prediction models. SIMCA and CE models showed 100% accuracy. FT-NIR spectroscopy combined with PLSR showed great potential to detect apricot seed adulteration in ground almond, as standard error prediction (SEP) was as low as 3.96 with R^2>0.96. Despite some disadvantages, overall, FT-NIR spectroscopy with chemometrics is simple, rapid, and an inexpensive tool to detect ground almond adulteration.

Discussion Question

What is the advantage of using conditional entropy algorithms?

6O02: NIRS technology and PLS-DA analysis for supporting EU Tasting Panels to classify Extra Virgin Olive Oils

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Delegated Regulation (EU) 2022/2104 (EU) stablishes standards that can be applied to all the Virgin Olive Oils (VOOs) subject to international trade. The standards include, among others, that the competent authorities should carry out conformity checks based on a risk analysis, in order to maximize the protection of consumers. Conformity tests should include physico-chemical and organoleptic characteristics assessed by panels of selected and trained tasters. The last word in the classification and labelling of VOOs is the result of the Panel Test. However, during the last ten years, the scientific community has highlighted several drawbacks on its application such as its subjectivity, cost and reproducibility[1]. The present work shows preliminary results on the potential of NIRS technology to support Panel Test to categorize Extra Virgin (EVOO) and Virgin Olive Oils, the two most difficult categories to distinguish due to overlapping organoleptic attributes. A total of 100 samples from both categories, extra vigin (EVOO N=50) and virgin (VOO, N=50), were analyzed in a monochromator instrument that provides absorbance readings between 400 and 2500 nm. Multivariate models were developed to classify olive oil samples by category (EVOO vs. VOO), using PLS-DA, obtaining an average percentage of correctly classified samples in external validation of 75%. The preliminary obtained results confirm the viability of the NIRS technology and PLS-DA to complement the work of the Panel Test for the classification of EVOO and VOO categories. Further research is in progress to evaluate novel non-targeted multivariate approaches and using a greater collection of samples of both categories.

Discussion Question

NIRS and discriminant approach could provide a cost-effective method for olive oil classification?

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6O03:Exploring the use of portable NIR and Raman spectroscopy for quality control of PDO hard cheeses

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The objectives of this study were to 1) investigate the feasibility of using a portable near infrared (NIR) spectroscopy instrument and a Raman benchtop microscope on Grana Padano (GP) and Parmigiano Reggiano (PR) PDO cheese samples, 2) test the use of spectra derived from the two instruments to discriminate the PDO cheeses and the ripening time, 3) develop calibration models for predicting chemical composition and texture properties, and 4) explore the potential of integrating signals from NIR and Raman spectroscopy, as further tool related to the quality of these PDO cheeses. A total of 18 cheese samples were collected from 6 dairy plants: 3 belonging to GP and 3 to PR PDO chains. For each dairy, 3 ripening times were selected: 12, 20, 36 for GP and 12, 24 and 36 months for PR. A portable NIR instrument (spectral range: 948-1,652 wavelength × cm^{-1}) and a confocal Raman microscope (spectral range: 50-3,700 relative wavenumber × cm^{-1}) were used to acquire spectra on 3 locations of the paste and 2 of the crust, for each cheese sample. Calibration equations were developed using a Bayesian approach with a random cross-validation [80% calibration; 20% validation set] by using the NIR and Raman spectra from the paste and the crust, separately. The same CV procedure was performed on the merged spectra from the two instruments, prior standardization. All the procedures were repeated 5 times per each trait. Overall, for the spectra of the paste, cheese moisture was predicted with similar accuracy by both instruments, whereas Raman outperformed NIR for fat and protein with a coefficient of determination (R^2_{VAL}) and root mean square error in validation ($RMSE_{VAL}$) of 0.74 and 1.69 for fat and 0.50

and 2.49 for protein, respectively. NIR spectra were much more effective for texture traits, with R^2_{VAL} ranging from 0.25 to 0.59. As regards to the spectra of the crust, they showed better prediction accuracy than the paste only in few cases, depending on the trait and the instrument considered. Integration of signals from NIR and Raman spectra led to intermediate prediction accuracy between the two instruments, indicating that the combined information from both techniques provides a more comprehensive characterization of the sample compared to using either technique alone, even though it depends on the instrument considered. On the other hand, the integration of signals was much more successful for the prediction of the age and label of the cheese, resulted in better prediction accuracy (75 and 91% correct assignment) compared to using the techniques alone. This could suggest synergic effects derived from the data fusion, or improved signal-to-noise ratio, which may help to provide more accurate and comprehensive analysis of the sample. The positive outcomes achieved with this study highlight the feasibility of using spectra for the quality control of these PDO cheeses, and besides the incorporation of additional cheese samples in the dataset, further investigation and validation strategies would be necessary to confirm the underlying reasons for the observed results. The study is part of the Short-Term Scientific Mission included within the WG2 of the CA19145 COST Action: Innovation related to the integration of several NDSS signals for critical issues in food integrity.

Discussion Question

Which other validation strategies and data fusion approaches can be investigated?

6O04: Exploring the use of benchtop FT-NIR and portable Vis-NIR spectroscopy instruments for quality control of PDO hard cheeses

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The aims of this study were to 1) investigate the possibility of combining the spectra from two IR instruments to create calibration models for predicting chemical composition, color, and texture properties, in Grana Padano (GP) and Parmigiano Reggiano (PR) PDO cheese samples and 2) compare the prediction accuracy between instruments by selecting common spectral intervals. A total of 18 cheese samples were obtained from 6 dairy plants, with 3 plants being part of GP and 3 plants belonging to PR PDO chains. Each dairy plant provided 3 samples, each one with a different ripening time as follow:12, 20, and 36 months for GP, 12, 24, and 36 months for PR. Spectral data were acquired on 3 locations of the cheese paste and 2 locations of the cheese crust for each sample, using a portable Vis-NIR instrument (350-2500 nm) and a benchtop FT-NIR instrument (11000 to 4000 cm^{-1}, corresponding to 900-2500 nm). Calibration equations were built using a Bayesian model on a calibration set (80% of samples randomly selected) and validated on the remaining 20% of the samples. The same modeling approach was used on the paste and crust spectral sets, independently. The spectra were centered and scaled to 0 mean and unit variance before fitting the models. In a first approach, the spectral sets of the two instruments were used separately (one model for each instrument), in a second approach the spectra were merged (unique model for spectra together). In a third approach the spectra were split into three separate bands and separate models were fitted as follows: 350–900 nm (Vis-NIR), 900–1900 nm (both instruments), and 1900–2500 nm (both instruments).

Whereas the comparison between the prediction based on Vis-NIR and FT-NIR showed expected dispersed results, this study showed that the fusion of spectra covering different spectral ranges could significantly improve the accuracy for the prediction of chemical

composition, texture, and color. Furthermore, the selection of the spectral interval could be "trait-specific". As an example, the selection of the interval between 1900 and 2500 nm allowed to improve of the coefficients of determination of the validation ($R^2_{VAL)}$ for the prediction of protein from 0.34 to 0.85 using the FT-NIR crust spectra, whereas the integration of signals from the two spectrometers allowed to improve the R^2_{VAL} for the prediction of fat from 0.35 to 0.55, while maintaining the same prediction error. Similar improvement can be reached for all the studied traits by selecting the most informative spectral interval and combination of spectra. The findings of this study also suggest that a non-destructive examination of the cheese rind may yield valuable insights into the composition, color, and texture of the cheese interior. Specifically, the higher R^2_{VAL} and lower $RMSE_{VAL}$ values obtained from the analysis support this assertion. This may lead to the development of novel quality control techniques based on crust spectral signature, avoiding opening an entire wheel and performing lab-based analyses. The study is part of the Short-Term Scientific Mission funded within the WG2 of the CA19145 COST Action: Innovation related to the integration of several NDSS signals for critical issues in food integrity.

Discussion Question

Is there alternative way to fuse the spectral data and split the spectral range to optimize the prediction accuracy?

6O05:Study of portable NIR instruments for virgin olive oil quality assurance

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Virgin olive oil (VOO) is often subject to food fraud, which poses economic and health risks. Current regulations require multiple physicochemical and sensory analyses, which involves the use of complex and time-consuming techniques to determine the quality of the VOO [**1**]. Therefore, faster and less invasive methods are needed to detect potential fraud. NIR spectroscopy is a powerful solution that can provide a large amount of physicochemical information about a sample in a short time [**2**]. In addition, the existence of portable NIR instruments offers the possibility to develop a multi-parametric method for VOO characterization. This requires studying the potential of portable NIR instruments and the development of suitable calibrations. The aim of this work and of the STSM performed was to study the potential of two low-cost portable instruments to be used in the quality control of VOO. An initial study was carried out to obtain the optimal configuration for oil samples measurements, and a spectral repeatability study of both instruments. Subsequently, a set of 200 oil samples were measured for development of PLS calibrations to predict the values of physicochemical parameters of interest for VOO (acidity, peroxides, K232, K270 and 7 fatty acids). The results demonstrated the capability of miniaturized NIR instruments for rapid and non-invasive screening of VOO in control laboratories. This work was possible thanks to a SensorFINT STSM carried out during May, June and July 2022 at the University of Padua with Professor Paolo Berzaghi that allowed Alejandra Arroyo-Cerezo to learn the NIR technique and improve chemometric skills.

Discussion Question

How to ensure portable instrument are used correctly?

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6O06: Identification of mountain food products' signature through different spectroscopic techniques

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Food producers that operate in mountain areas, despite the high quality of their products, struggle in competing on the market due to the difficult production conditions related to the landscape. For this reason, European Community has defined a quality label, called "Mountain Product", in a regulation reserved for food products produced and processed in mountain areas, with the aim to support the economy in underprivileged areas [1]. Among others, Parmigiano Reggiano cheese, one of the most renowned Italian food product with a PDO (Protected Designation of Origin) label, has a vast part of production that takes place in mountain areas. The MOUNTAIN-ID research project (https://www.mountainid.unimore.it), to which the current work is related, has the main objective of developing analytical methodologies to conjugate identity, sustainability, and value for some mountain products. In fact, the "Mountain Product" label is not yet popular among consumers, which is why there is an interest by food producers to promote these products as well as to protect their authenticity. The present work aims to correctly detect and classify, among different Parmigiano Reggiano samples, the ones characterized by the mountain denomination as well as additional requisites as established by the producer consortium [2], i.e." Prodotto di Montagna - Progetto Territorio Consorzio" ("Quality Project - Mountain Product"). To this aim, different spectroscopic techniques, namely ^{1}H-NMR, NIR and Raman, were coupled with chemometric tools, such as data fusion, variable selection and classification techniques.

Discussion Question

What would it take to make chemometric methods officially used for food authentication?

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P01: Agri-food waste as source of valuable materials

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Agricultural residues are naturally available lignocellulosic biomass, with high carbon content that can be converted into valuable products (e.g. biochar, bio oils, biofuels). These residues represent all the materials left after harvesting and processing of food crops including stalk, husk, shell, hull, seeds, etc. Here we present the characterization of five types of agricultural residues such as husk pellets, stalks, hulls, shells and seeds as a preliminary step to determine their potential use as source of valuable compounds (e.g. sugars, phenolic compounds, flavonoids). The extractives complex composition explains the antioxidant activity, with fast scavenging of DPPH radicals, especially for hulls and shells – Figure 1. The PCA and hierarchical clustering used for exploratory data analysis offered the possibility to combine multiple information obtained from detailed characterization of samples into a global view of the system. That allows observing and distinguishing similarities and differences among samples originating from various sources.

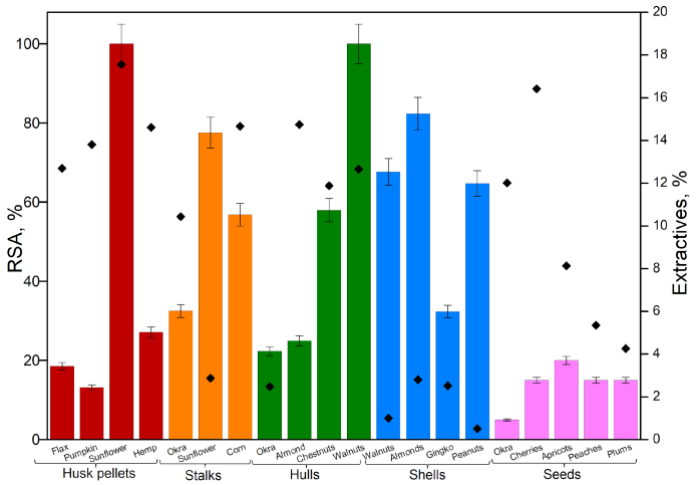

Figure 1. Radical scavenging activity of extractives from different types of agri-food wastes

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P02: Evaluation of sample presentation on intact food analysis using miniaturized Near Infrared Spectroscopy devices

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Miniaturized Portable Near Infrared Spectrometers (NIRS) are low cost and easy-to-use alternatives for quality and safety control in the food industry. There are several applications in the bibliography related to this topic. However, not too many have been implemented at industrial level. In this sense, sample presentation and scan collection strategies are critical, to obtaining a valuable spectra of intact samples and develop a chemometric model able to assess the quality and/or safety of food products.

This work will present the results of different NIR assays carried out to evaluate quality and safety of oils and pasteurized breast milk samples using: a) two miniaturized NIR instruments, a microNIR and a homemade NIR device [2]; b) different scanning modes and c) several sample presentation strategies adapted to common sample preservation.

Discussion Question

Importance of window size of miniaturized NIR spectrometers for scanning intact food products to quantify compositional parameters.

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P03: Detection of Food Fraud Using FTIR

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Food fraud is a significant issue that encompasses a wide range of fraudulent activities. The globalization of trade makes fraudulent activities easier to implement and have a more significant impact on consumer trust in food industries and authorities. Therefore, preventing fraudulent practices is essential for businesses related to the food industry, food authorities and consumers. The need for food defense to be included in the food industry by policy makers and operational managers as part of an integrated approach to food supply chain integrity at every level (local, national, and international) is critical. Surveillance and control of food supply chains are crucial in mitigating and preventing food fraud. Thus, rapid detection with low-cost, non-invasive, and online methods is particularly important. Spectroscopy-based sensors coupled with machine learning approaches are potential solutions for this purpose. Several studies have been published on this topic by our scientific group [1-7]. Fourier transformed infrared spectroscopy (FTIR) coupled with machine learning (ML) approaches has been used for the discrimination of fresh from frozen/thawed beef [7]. A similar approach was used for the investigation of various food fraud scenarios. FTIR data were collected and split to training vs. testing set (ca. 70 - 30%, respectively) and partial least square discriminant analysis (PLSDA) was applied. The examined cases are the discrimination of fresh from frozen/thawed chicken (n= 450), of beef muscles (n= 330) and of origin (i.e., Greek vs. abroad) (n= 90). Meat adulteration with cheaper substitutes is also an issue, especially when there are no morphological characteristics to differentiate between different types of meat, such as in minced meat. To address this, beef was adulterated using pork in raw (n= 210) and cooked (n= 171, n= 171) minced meat. Accuracy scores were obtained >78% for the test sets indicating the potential for the detection of food fraud using FTIR. Further investigation and data exploration is required to draw firm conclusions (e.g., investigation of important features, use of external validation). This work has been funded by the project DiTECT (861915).

Discussion Question

The presence and the kind of fraudulent action on a food product is unknown in real life. Should the methods include detection of different scenarios, such as adulteration,

mislabeling to prevent-mitigate food fraud actions? (an holistic approach-an holistic method, but how possible it is?)

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P04: Volatile compounds analysis coupled with with machine learning for the rapid quality assessment of chicken meat

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The determination of volatile compounds (VOCs) in tandem with machine learning could contribute to rapid and reliable quality assessment. This study aimed to the investigation of applying gas chromatography-mass spectroscopy (GC-MS) and e-nose in combination with different machine learning algorithms to estimate the microbial load in chicken fillet, regardless of the part of the carcass originating from. Chicken thigh and breast fillets (n=240) were aerobically stored at different temperature conditions for specific time intervals and were microbiologically analyzed for the determination of aerobic plate counts (APC). Solid phase microextraction (SPME) combined with GC–MS and e-nose analysis were also performed for the estimation of VOCs. Different machine learning regression models (Partial Least Square, Multilinear, Bayesian, k nearest neighbors, Support Vector Machines, Random Forests and Extra Trees regression) were generated and validated to assess the correlation between GC-MS, e-nose and microbial data. Both GC-MS and e-nose showed satisfactory models' performance using specific algorithms. Tree-based algorithms were more efficient in predicting the microbial populations with both analytical technologies as indicated by the performance indices on the validation dataset (slope a; 0,98 and 0,83, R^2; 0,94 and 0,69, RMSE; 0,27 and 0,63 for the GC-MS and e-nose, respectively). This work has been funded by the project DiTECT (861915).

Discussion Question

Although these techniques can contribute to rapid and reliable quality assessment compared to conventional ones can be also used as the basis for the development of efficient miniaturized and portable sensors.

P05: Optimizing spectral repeatability of vacuum packed and unpacked cured Iberian ham using two on-line NIRS instruments

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The acquisition of high-quality spectral data is a key aspect in the development of any Near-infrared Reflectance Spectroscopy (NIRS) application. Nowadays, the instrumental development of NIRS technology has made NIRS *"on-line"* instruments suitable for analysis at different critical points in the food industry. Nevertheless, the existing commercial instrumentation was not developed for any specific food product. Therefore, before to take decisions about what instrument to buy for a given food application is important to scientifically evaluate and optimize them. The aim of the present work was to evaluate the repeatability of the spectral signal provided by two *"on-line"* NIRS devices of very different optical configurations (FT- NIR and Diode Arrays) for analysing sliced cured Iberian pig ham (packaged and unpackaged) and to optimise the methodology of analysis in each case. This evaluation was carried out using eleven samples from different commercial categories and different producers. The quantification of the spectral repeatability was done by using the Root Mean Square (RMS) statistic [1,2], which allows to evaluate the differences and similarities between different spectra of the same sample.

Discussion Question

How can we use the findings of this study to improve the accuracy and efficiency of NIRS analysis in the sorting lines of the Iberian ham industry?

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P06: Effect of conching of dark chocolate on near-infrared (NIR) spectral data

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During conching, a crucial step in chocolate manufacturing, chocolate is exposed to long term heat treatment combined with constant mixing. Mixing is important for the development of flavour and aroma, rheological modification, and appropriate texturing of the chocolate mass (Toker et al., 2019). It is best described as the process in which particle size is reduced, followed by coating of particles in molten fat. This results in a final product that is more homogeneous and free flowing (Augusto & Bolini, 2022). As dark chocolate conching has not been studied with near-infrared (NIR) spectroscopy to date, this study aimed to examine the effect of different conching times on particle reduction in dark chocolate samples as measured by NIR spectral data. Spectra were collected after conching on the melted and solid chocolate using a Viavi handheld MicroNIR device. A clear trend in conching time was seen in the directions of PC1 and PC2 for the melted and solid chocolate, respectively. PLS regression models were developed to predict conching time on 5-point smoothing and SNV pretreated spectra of both the melted and solid chocolate using full-cross validation. RMSECV, R^2 and RPD values obtained for conching time (representing particle size) models for the melted chocolate (10 PLS factors) were 15.84 min, 0.85 and 2.62. Higher accuracies were obtained for solid chocolate with 8 PLS factors (7.02, 0.98 and 6.84). This work illustrates the potential of using NIR spectroscopy as a process analytical technique for monitoring conching during chocolate manufacturing.

Discussion Question

What potential limitations should one be aware of and what role can near-infrared (NIR) spectroscopy serve in enhancing our understanding of chocolate quality?

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P07: Monitoring of high moisture extrusion process using Near infrared spectroscopy

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A strategy to reduce meat consumption and promote the consumers' adherence to more sustainable healthy diets is to develop products that can replace meat in a meal context. High moisture extrudates (HME) are textured proteins (from different alternative protein sources) designed to mimic the properties, texture, nutritional profile and appearance of whole-muscle meat, which can be used to elaborate meat alternative products. HME can be produced using high moisture extrusion, but it is a complex process, and many factors can influence the characteristics of the final product. Thus, the use of non-destructive spectrometric sensors (NDSS) for inline monitoring is essential to understand the process and for supporting early warning and automatic decision-making protocols at the food industry. This study is a preliminary work on the monitoring of high moisture extrusion process during production of Fava bean extrudates when using different extrusion conditions (Temperatures and powder feeding rates). A laboratory-scale co-rotating and intermeshing twin-screw extruder (Process 11, Thermo Fisher Scientific Inc., Waltham, MA, USA) was used. Extrusion conditions were a temperature of 145 or 155 ºC and a solid concentration of 40, 45 or 50%. Spectra were recorded at the different positions of the cooling die on a Fourier Transform NIR spectrometer model Matrix-F duplex (Bruker Optik GmbH, Germany) using an optical probe (QR600-7-VIS125BX, Ocean Optics B.V, Germany) previously adapted to the extruder. Temperature was also recorded (Novus, Barcelona, Spain). Spectral data were analyzed using Principal component analysis. Results showed different spectral profiles when using different extrusion conditions. Temperature variations were important on the different positions and their effect on the spectra needs to be subtracted using spectral pretreatments. Monitoring of the process is feasible but more experimental work is needed to develop models that can provide early information on the texture and composition of HME to optimize the process. The use of other spectrometric sensors should also be investigated.

Discussion Question

How can NDSS help industry on the development of HME and meat alternatives?

P08: Advancing Strawberry Quality Assessment with a Portable Vis-NIR Spectrophotometer and Reflectance Quality Index (RQI)

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The fruit and vegetable industry faces significant challenges in reducing food losses and extending shelf-life. This study aimed to develop a novel approach to assess optimal shelf-life and minimize food losses in strawberries using a portable spectrophotometer and Vis-NIR reflectance-based fruit quality index. A total of 96 strawberries (Fragaria ananassa) were stored at different temperatures (5, 15, 25, and 35 °C) with 60% relative humidity for 15 days. Various quality parameters, including colour, firmness, weight loss, appearance, and microbial quality, were evaluated every three days during storage. Kinetic models were used to describe the changes in weight loss, appearance colour, and firmness. Vis-NIR spectroscopy was employed to establish a Reflectance Quality Index (RQI) for determining fruit quality during storage, reducing the number of wavelengths to a lower set of representative independent variables. A very good fit was obtained (R^2 = 0.95), demonstrating the feasibility of both methods for evaluating quality. Calibration and prediction models were created using modified partial least squares (MPLS) regression method with cross-validation, to predict quality indicators of strawberries, including appearance, weight loss, L*, a*, b* colour parameters, and firmness. This study presents a novel approach for assessing the shelf-life of strawberries based on time and storage temperature using a portable spectrophotometer, which can be a valuable tool for the food industry to minimize food losses and ensure optimal fruit quality.

Discussion Question

What is the feasibility of using a portable Vis-NIR spectrophotometer and Reflectance Quality Index (RQI) to assess the shelf-life of strawberries, based on time and storage temperature, and minimize food losses in the fruit and vegetable industry?

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P09: A novel approach to identify the “age” of saffron (C. sativus L.) using fluorescence spectroscopy in tandem with chemometrics

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Saffron, the dehydrated red flower stigmas of *Crocus sativus* L., is an elegant spice of high economic value in global trade due to its low yield and laborious production. Mislabeling and substitution with inferior quality products are quite common in its supply chain highlighting a continuous need for upgrading the official screening methods with highly selective, sensitive but also rapid and cost-effective tools. In this view, fluorescence spectroscopy (FLS) presents an attractive alternative for direct, non-invasive analysis compared to other non-destructive spectroscopic techniques but applications to saffron are scarce [1]. In this study, we investigated the potential of exploiting FL measurements to extract diagnostic information about the “age” of traded saffron. Our experimental design involved reference fresh samples of various qualities and mixtures with aged saffron that were used for calibrations against the level of admixture or other quality attributes of commercial importance. The challenges of acquiring accurate FL spectral measurements in situ either with a portable sensor or with a benchtop spectrofluorimeter along with choosing the “best” chemometric algorithms are discussed.

Discussion Question

Novel quantitative chemometric approaches in solving authentication problems

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P10: Differenting persistent and sporadic *Listeria monocytogenes* : FT-IR Applicability

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Listeria monocytogenes (*Lm*) is a ubiquitous, Gram-positive intracellular pathogen with high mortality rates among immunocompromised individuals. Certain strains of *L. monocytogenes* are routinely isolated in food processing environments (FPEs) - persistent strains – while others are only encountered sporadically. One explanation for this recurrent isolation may be the presence of heterogeneous subpopulations, with some capable of withstanding adverse conditions encompassing high salinity, low temperature, and low pH, along with other FPEs-related stressors. Hence, we set out to evaluate the suitability of Fourier Transformed Infrared Attenuated Total Reflectance (FTIR-ATR) spectroscopy to discriminate between the fittest persistent isolates from the remaining sporadic subpopulations. 72 *Lm* isolates, persistent and sporadic, were grown under various food-associated stressors (pH, TºC, %NaCl). After reaching late exponential phase the cell pellets were collected and analysed trough FTIR-ATR spectroscopy. The gathered spectra were then analysed and PLS-DA classification models were elaborated to correctly discriminate both groups. From the gathered spectra, FTIR analysis has shown promising results in differentiating persistent and sporadic isolates belonging to the same serogroup (IVb, I/IIa and I/IIb).

Discussion Question

Risk Management and mitigation

References

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P11: Prediction of the hazelnut content in the cocoa hazelnut pastes by using FTIR and Raman Spectroscopy

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In this research, two different hazelnut species (classical and wrinkle) were roasted at the temperatures of 130, 140, 150 and 160^{0}C for 30 minutes. Cocoa hazelnut pastes were prepared representing industrial production by using couverture chocolate and the roasted hazelnuts at the ratio of 90%, 70%, 50%, 30%, 20% and 10% w/w.

FTIR spectrometer (Bruker, Germany) and Rigaku Raman spectrometer (Wilmington, MA, ABD) was employed in spectral acquisition. The OPUS software (version 7.2) was used to build calibration curves. The spectral ranges of 1495-815 cm^{-1} and 1450-1340 cm^{-1} was used to build calibration curves by using the spectral data of FTIR and Raman, respectively.

Results showed that FTIR and Raman techniques could be effectively used for prediction of the hazelnut content of cocoa hazelnut pastes. The R^2 values higher than 0.90 was obtained by using both techniques. However, more favorable results were obtained by using FTIR technique.

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P12: Using Chemometrics to Tackle Honey Issues in Albania

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Throughout the research conducted in Albania to tackle honey issues, for instance, adulteration and the process of investigating the botanical origin of honey, but also the characterization of different types of unifloral honeys and the production in different parts of Albania; chemometrics played a significant role. From the simplest tools, i.e descriptive analysis, correlation and then multivariate analysis, like PCA (*Principal Component Analysis*), it was possible to reduce the number of parameters in honey (*consider that the parameters measured in honey and sugar ratio are a large number* [1]), and make a better judgment in authenticating honey in terms of composition (*dilution of honey with cheap sugar syrups*), classifying unifloral honeys (*the botanical origin*) [2]. Also, it was possible to discriminate honey produced in different districts of Albania (*for the determination of geographical origin*) [3] through dendrograms and PCA – ensuring fast and reliable results.

Discussion Question

What are the drawbacks of chemometric tools (models created) to authenticate food?

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P13: Spectral identification of therapeutic allergen products

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Raman spectroscopy is a widely used technique in the quality control of pharmaceutical products. Inelastic scattering of laser light generates unique fingerprints of chemical compounds which allows for the identification of products and potential quantification of active components.

The spectroscopic analysis of biomedicines like vaccines or therapeutic allergen products introduces new challenges as these products show inherent variability and contain excipients that strongly contribute to the spectral signal [1-3]. Therefore, standardization in experimental and analytical protocols is particularly relevant. Spectral pre-processing affects each analysis's outcome. We show that Raman spectroscopy can distinguish between near-related bee and wasp therapeutic allergen products from different manufacturers with varying sensitivity and specificity depending on the details of prior pre-processing. Using machine learning and statistical techniques based on different models, we found that completely processed Raman spectra from bee and wasp venoms can be differentiated with accuracies above 95%. While baseline correction had a major impact on the separability of spectra, unprocessed spectra showed a high variance obfuscating relevant spectral differences. Our results demonstrate that Raman spectroscopy can serve as a method to distinguish between therapeutic allergen products and offers a proof-of-concept for the applicability of Raman spectroscopy in the quality assurance of biomedicines. Further improvements and standardization in experimental protocols and spectral analysis are required to ensure robust and reliable predictions.

Discussion Question

Which algorithms are recommended to accomplish a robust and reliable pipeline for Raman spectroscopy analysis?

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P14: Deep neural network-based method applied to confocal microscopy images of PDO cheeses

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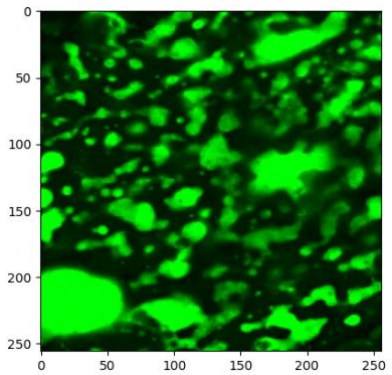
The main goals of this study were to 1) investigate the feasibility of using a confocal scanning laser microscope (CSLM) on Grana Padano (GP) and Parmigiano Reggiano (PR) PDO cheese samples, and 2) explore the potential of applying deep neural network-based method (DNN) to the CLSM images for predicting the PDO type and the age of the cheese, as further tool related to the quality of these labeled cheeses. A total of 18 cheese samples were collected from 6 dairy plants: 3 belonging to GP and 3 to PR PDO chains. For each dairy, 3 ripening times were selected: 12, 20, 36 for GP and 12, 24 and 36 months for PR. A confocal scanning laser microscope (Leica Microsystems CMS GmbH, Germany) operated with Ar/He-Ne laser excited at 488 nm and 559 nm with a 63X oil immersion objective was used for the fat and protein distribution, after staining the samples with Nile Red (fat) and Fast Green FCF (protein). On average, each cheese sample provided 22 images, with a minimum of 15 and a maximum of 45. The round fat droplets (green) within a continuous protein phase (red), were differently distributed between the two PDO cheeses and among ripening times. To explore the potential of applying DNN method to the CLSM images, only green-channel images (N = 130; 69 from GP, 61 from PR) were chosen (Figure 1a). Image data were normalized and augmented before being analyzed in a DNN model with three 2D convolutional layers (relu activation function) followed by MaxPooling and Dropout layers and a final dense layer (sigmoid activation). The learning rate was 5e-4. The DNN model had 85,089 parameters and was run for 200 epochs. In total, 25 images (13 from GP and 12 from PR) were used for validation. The average accuracy was 0.928 in the training set, meaning that the model can learn the underlying patterns and features from the CLSM images to make accurate

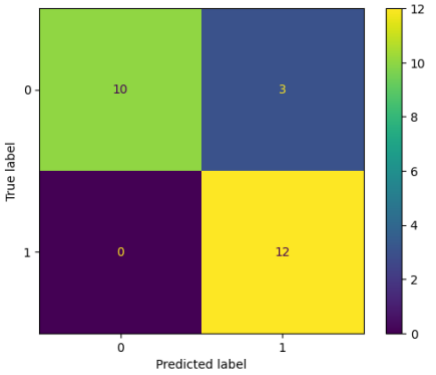
predictions, whereas the accuracy was 0.844 in the validation set (Figure 1b). This suggests that the model performs good on the data as well.

Figure 1. Fast Green FCF (lipids) image of cheese sample and confusion matrix of DNN results on the validation set (where: 0=GP, 1=PR).

a – Fast Green FCF channel image



b – DNN confusion matrix



Further steps, such as regularization techniques or increasing the amount of training data, may be necessary to mitigate the overfitting and improve the model's performance on unseen data. The study is part of the Short-Term Scientific Mission included within the WG2 of the CA19145 COST Action: Innovation related to the integration of several NDSS signals for critical issues in food integrity.

Discussion Question

What are the benefits of artificial intelligence in confocal imaging related to food?

P15: In-field analysis of nutritional value in perennial ryegrass

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Rapid analysis of quality parameters in forage breeding would allow for quicker selection of perennial ryegrass varieties with desirable nutritional components [1]. Faster generation of nutritional value data could be achieved at field using a tractor-mounted NIRS instrument, greatly increasing the number of phenotyped grass selection candidates. The biggest challenge in prediction using in-field collected NIRS data is caused by the presence of high water content in samples [2]. In 2022, 618 sward plots of perennial ryegrass *Lolium perenne* L. were scanned upon cut with an in-line NIR portable spectrometer. Matching grass samples were obtained for laboratory NIRS measurements on dried and milled material. The analysis of saliency maps for prediction of digestibility traits: NDF (neutral detergent fiber) and OMD (organic matter digestibility), showed that wavelengths in the water region contribute highly to the prediction based on dried samples, as opposed to models built with spectra obtained on fresh biomass.

Discussion Question

Is the choice of digestibility estimate (NDF vs OMD) crucial for prediction accuracy using in-field NIRS measurements on fresh biomass?

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P16: Classification and characterization of truffles with ^{1}H NMR and random forest methods

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Due to the large price differences between truffle species, this food is particularly susceptible to food fraud. Therefore, methods are being sought to ensure the determination of the taxonomic species of truffles. NMR spectroscopy is promising for this purpose as it provides fast and reproducible results. However, since NMR spectra are complex, chemometric methods are needed for their evaluation. In this study, we show that the machine learning approach random forest (RF) can be used for both classification and characterization of truffle samples. For the latter, we apply Surrogate Minimal Depth (SMD), an RF-based variable selection method that considers the mutual impact of the variables on the classification model [1]. In addition, we also use SMD to analyze the relationship between variables to identify groups that provide similar information for classification. These can be attributed to the same metabolites, but also to different metabolites whose interaction in metabolic pathways is already known. In this data, intermolecular relations were identified and associated to several amino acids and sugars among other metabolites, which then were consequently identified in shared metabolic pathways.

Discussion Question

Should we apply machine learning models without analyzing how these methods obtain their results?

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P17: Moving Block Model (MBM) and Aquaphotomics for monitoring dehydration process

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Two dehydration experiments were carried out using a solar dehydration plant commercially available: Italo BASE+ (G-teK s.r.l., Carpi, Modena, Italy), located in the small farm Ca' dal Saggia (Pavia, Italy). The tests were carried out on apple slices (*Red Delicious* and *Fuji* varieties; 1.5 mm thickness). A total of 650 spectra were recorded in reflectance mode by a MicroNIR On-site W™ (VIAVI Solutions Italia S.r.l., Monza, Italy) portable spectrometer with the MicroNIR Pro ES 1700 software until the end of the processes (55 hours). NIR spectra were collected every five minutes by placing the probe, thermally insulated, directly over a sample slice. Spectra were pre-treated by applying the 2nd derivative Savitzky–Golay filter (2nd order polynomial fit and 21 points) and the multiplicative scatter correction (MSC) [1]. After normalisation, aquagrams were calculated from the spectral data. The Moving Block Model (MBM) was applied to the data using block sizes of 5 and 65 spectra. The combination of information from the two chemometric instruments, MBM and Aquagrams, can be useful for defining and predicting the end of the dehydration processes. The choice of the proper size of blocks is crucial to gain a good predictive power of the MBM. Aquaphotomics approach was considered more reliable than MBM, as not further investigations for its optimisation and application at industrial level should be needed. Aquaphotomics was selected to set up a system, named Aqua-Control, to monitor in real time the progress of the drying process.

Discussion Question

Do different matrices and different processes need to build dedicated aquagrams?

References

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P18: Anomaly detection in fermentation processes by online GC-IMS exhaust gas monitoring and chemometrics

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Gas chromatography hyphenated to ion mobility spectrometry (GC-IMS) is a powerful, two-dimensional separation and detection technique for volatile organic compounds (VOC). Low detection limits (low ppbv), high selectivity and robust operation characterize it as an ideal tool for headspace non-target screening of complex sample materials without prior enrichment [1]. Fermentation exhaust gas is available without manual sampling or process interference. The aim of this study is to screen volatile metabolites online by GC-IMS and combine the obtained “fingerprints” with chemometric data analysis to predict parameters that are difficult to measure directly, such as the presence of contaminations. This talk presents results from an offline proof-of-concept study, which demonstrates that E. coli, S. cerevisiae, L.brevis and P. fluorescens can be categorized simply by VOC profiling as a first step towards detecting contaminations. Further, the transition to online measurements with a prototypic GC-IMS device and first results towards anomaly detection are shown.

Discussion Question

How do you handle serially autocorrelated data?

References

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P19: Carbon resistant catalysts for syngas production over Ru supported on $CaZr_{0.85}Sm_{0.15}O_{3-\delta}$ perovskite prepared by auto-combustion method

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The increasing worldwide CO2 emission into the atmosphere, amounted at 40 metric gigatons CO2 per year. Ideally, the purpose is to produce added-value from conversion of CO2, mitigating CO2 emissions. Among different process from conversion CO2, DRM is a promising green technology able to raise the commercial value of syngas mixture. However, the DRM technologies starting from pioneering studies on gasification effects showed suffering from carbon deposition able to fast deactivate the catalyst due to the relatively low H/C ratio. It is therefore necessary to propose appropriate operating mixture where catalysts are coking resistant, able to ensure long-term stability, preferably at low doses of catalyst and low temperatures. In this context several transition metals including Ni, Co, Ru, Rh, and Pt were adopted for DRM and Ni-based catalysts and related bimetallic metals: Ni-Fe, Ni-Co have attracted most attention owing relatively activity and low-cost also if it is not preferable due to fast deactivation due to carbon deposition, metal oxidation, as well as particle sintering. Some basic support of catalyst surface plays a role on the activity and durability, considering several routes of activation C-H. In order to mitigate the above problem of carbon deposition, Ru doped samarium on calcium zirconate $CaZr_{0.85}Sm_{0.15}O_{3-\delta}$ was proposed as a valid alternative to the rapid deactivation process. Self-oriented gel-combustion technique for the synthesis of ruthenium doped samarium zirconate is reported using glycine as fuel at temperature (150-350°). In this work the catalytic properties and composition of ruthenium doped $CaZr_{0.85}Sm_{0.15}O_{3-\delta}$ (RxCZSm with x = 0.5, 1.5, 3.0 wt %) are studied as a thermally resistant composition. Then, characterization methods such XRD, TPR, SEM, XPS and the use of a methane dry reforming laboratory scale set-up are presented. Time on stream tests of 50 hours were conducted in a fixed bed bench scale reactor in a temperature range of 550-850°C. The catalytic activity toward dry reforming gives a remarkable efficiency in term of

conversion (~ 90%), syn-gas H_2/CO molar ratio and stability. Furthermore, as highlighted by SEM images, these combined RxCZSm catalysts showed an outstanding resistance to the coking formation and Ru metal sintering, constituting a promising alternative to the current use of Ni catalysts.

Discussion Question

The role of crystallinity and amorphous phases in the chemo sensors analysis

P20: Predicting frying times in recently fried potato fries using imaging spectroscopy and Partial Least Squares Discriminant Analysis (PLSDA)

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A new method was developed to classify frying times of recently fried potato fries using imaging spectroscopy and chemometrics. Ninety frozen potatoes, round cut, pre-fried in sunflower oil, were finally fried for 3 and 5 minutes, then cooled for 10 minutes and immediately measured by a spectral camera (Specim FX17, spectral range: 937.33 nm to 1718 nm). All images were converted to .mat format in MatLab using an inhouse developed function. Then, spectra were extracted from the images, from core and crust, using Hypertools version 3 in MatLab. Typical chemometrics analysis was performed in R version 4.2. Samples were distributed in two classes according to the frying time: class 1 (3 minutes) and class 2 (5 minutes). Three classification models were calibrated and validated: a) One model to classify 3 min from 5 min fries using 90 spectra from the cores, b) One model to classify 3 min from 5 min fries using 84 spectra from the crusts, c) One model to classify cores from crusts, using all measured spectra (not shown here). The best models were achieved using PLSDA, results can be seen in Table 1. Core: SNV, then 12 variables selected by CovSel, PLSDA with 8 latent variables (LV). Crust: Detrend, then 14 features selected by CovSel, PLSDA with 12 LV. Both models presented high accuracy of validation, 0.89 and 0.92 for core and crust, respectively. Sensitivity and specificity, were 1.0 and 0.81, respectively, for class 1 in core; and 0.83 and 0.95, respectively, for class 1 in the crust model. Thus, both models presented potential as a fast alternative methods to classify recently fried potato fries using imaging spectroscopy and chemometrics.

Discussion Question

What is the advantage of imaging spectroscopy over non-imaging spectroscopy? Which chemicals contribute to the spectral differences? What is the best pre-processing method for this data, and why? What is the best performance measure?

Model	Set	Real/predict	3 min	5 min	Sensitivity	Specificity	Precision	Accuracy
CORE	Calibration	3 min	16	3	0.84	0.93	0.84	0.95
		5 min	3	41	0.93	0.84	0.93	
	Validation	3 min	11	0	1.00	0.81	0.79	0.89
		5 min	3	13	0.81	1.00	1.00	
CRUST	Calibration	3 min	19	3	0.86	0.97	0.95	0.98
		5 min	1	36	0.97	0.86	0.92	
	Validation	3 min	5	1	0.83	0.95	0.83	0.92
		5 min	1	18	0.95	0.83	0.95	

Table 1: Classification metrics of the prediction in the validation set.

P21: Non-invasive optical sensing film for smart food packaging

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Food safety is one of the most important points for human health protection strategies and the food and agriculture industry. Smart packaging accomplishes the isolation of products from the outer atmosphere to extend their shelf life and is capable of giving information about the microbiological and physicochemical properties of the product during storage and commercialization. The use of these packages improves traceability and also is able to extend food shelf life. In this way, we propose a non-invasive, easy to use, rapid and low-cost system composed of a sensitive film based on a nanoMOF (metal organic framework) [1] as colorimetric and luminescent indicator of biogenic amines presence in food samples. The presence of biogenic amines in non-fermented foods is usually undesirable and is related to microbial spoilage. The developed film is attached to the inner surface of the food package, in contact with the inner atmosphere, and a smartphone is used to register the color and fluorescent change of the nanoMOF film in presence of biogenic amines. The system has been applied to the monitoring of fish freshness sealed in a package and stored into a controlled environment.

Discussion Question

Could the use of smart food packaging minimize the food loss and waste and not mislead the consumer about the quality status of a product?

References

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P22: Sensomics approach to uncovering the aroma of bitter-tasting herbal liquors

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In assessing the quality of food and beverages, a new scientific discipline that unravels sensor properties at the molecular level is the sensomics approach. In this work, near-infrared (NIR) spectroscopy is related with the sensorial characteristics of samples, with the aim of determining the aromatic imprint of samples in the vibrational spectrum 900-1700 nm. Sensory evaluation of six bitter herbal liqueurs was carried out by two groups of panelists (expert and consumer) and color parameters were measured and NIR spectra were recorded with the portable device. The comparison of the mean values of the total sensory ratings of samples did not differ significantly for the expert and consumer panels ($p<0.05$), and the color measurement showed uniformity for ¾ of samples. The analysis of the main components for the sensory properties of the brightness and color of the samples determined the connection between the sensory evaluations of the expert panel and the following color parameters: Croma, a* and b*. Applying partial least squares regression, NIR spectra with alcohol content in bitter liquors were successfully calibrated and validated for the portable device (RSEP=0.67 %). Sensory at the molecular level was confirmed by models for evaluating the odor and taste characteristics of expert and consumer panels, using sample recording with two NIR devices. The mentioned sensor characteristics of both panels were successfully validated and the qualitative and quantitative potential was confirmed.

Discussion Question

Potential of the portable NIR devices.

References

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P23: LACTAI: Comprehensive control of cheese making through AI

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Cheese is a globally recognized product that is marketed for its wide range of varieties and versatility of use. According to the FAO, global cheese imports are expected to reach 3.5 million tons by 2023 [1]. Cheese industry faces two major problems in the production process. Firstly, the difficulty of standardizing the process and the final product, due to the high variability of the raw material and the subjectivity associated with production variables. Secondly, the high energy and water costs. Optical sensor technology, unlike conventional analysis techniques, is robust, versatile, fast, non-destructive, environmentally friendly, and can be successfully applied to monitor and control critical stages of processing. This technology, coupled with machine learning tools, can optimize processes and resource usage, increase and standardize product quality, and accelerate the transition towards sustainable and innovative production. In this work, a near-infrared light scattering sensor measuring at 880 nm, a digital camera, and a light source were coupled to a 10-L cheese vat. Real-time coagulation monitoring was performed using the NIR light scattering signal, and the inflection point of the curve was multiplied by a constant factor to estimate the optimal cutting time of the curd. Whey separation was monitored for 90 min by taking constant images of the mixture of whey and curd inside of the vat, and a moisture curve was constructed by taking curd samples at 5 or 10-min intervals. To predict humidity, a Convolutional Neural Network was applied; transfer learning technique based on the EfficientNetB0 architecture and pretrained weights in ImageNet were used, with freezing/unfreezing layers and a linear activation function at the output. The model was validated with the obtained data, resulting in an RMSE of 0.0113%.

Discussion Question

What are the limitations of using artificial intelligence tools coupled with optical sensor technology?

References

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P24: Predicting rheological characteristics of meat emulsions with a VIS-NIR sensor

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The measurement of the complex dynamic shear modulus (*G**) enables the determination of the interaction between dispersed and continuous phases of meat emulsions, which affects the quality of the final product and jeopardizes profitability of meat industries due to cooking losses. The purpose of this research was to develop optical models for predicting *G** of meat emulsions produced at industrial scale.

Rheological analysis was performed through dynamic oscillatory tests with a Rheo Stress 1 (Haake; MPC/DC60 and PP60 probe) at 21 °C with a frequency sweep range of 1-100 Hz at a maximum strain of 0.01% obtaining *G** at 10 Hz. Light backscatter measurements between 300 and 1100 nm were performed with a HR4000 fiber optic spectrometer coupled to a LS-1 halogen bulb (Ocean Optics, Inc.) and communicated with a double-jacketed sample holder through two fibers of ~600 µm diameter. After optical data processing, the Maximum R2 procedure of the Statistical Analysis System (SAS®) was used to generate algorithms and, for the best model, a cross-validation with REG procedure of SAS® system was performed.

Model V was the best since it explained 99.1% of the variability observed in *G**, yielded 3.99% of error and only needed 5 predictors. Cross-validation of this model showed R^2 of 0.972 and CV of 4.03%. Considering the formula, meat emulsions with and without starch were characterized by different types of predictors. They notably tended to be more informative in emulsions without starch where an exceptional prediction was obtained with only one predictor.

These results point out the potential of VIS-NIR light backscatter technology as a tool to predict relevant rheological parameters during meat processing.

Discussion Question

Why does starch worsen the optical response in the VIS-NIR area?

P25: Determination of Lycopene Content of Dried Tomato Products(Snack Bar and Leather) by Using NIR Spectroscopy and Hyperspectral Imaging Techniques

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Tomato and tomato based products are commonly consumed around the world and specifically in Mediterranean region. Tomato is a rich source of lycopene which has high antioxidant capacity and health benefits for human beings. Therefore, lycopene content of the product is an important parameter for human diet. Development of green methods for measurement is a big concern to decrease the usage of chemicals. Scientists worked on several nondestructive, fast and easy techniques such as FT-Raman, Near inferred (NIR) spectroscopy for lycopene content of different tomato based product. However, for NIR spectroscopy high moisture is a problem since water can dominate spectra .Dried tomato products such as snack bar and leather could be more suitable products to make a calibration by using NIR spectroscopy. Also, the drying techniques affect the content and distribution of lycopene in these products. Hyperspectral imaging (HSI) technique is also convenient to detect lycopene for non-homogenous samples since whole samples could be measured and pixel based detection is possible [1]. There is no study for lycopene measurement in tomato based snack bar and leather by using and (HSI) and NIR spectroscopy. In this research, tomato based snack bar and leather samples were produced with different lycopene content at different drying conditions. Lycopene calibrations were done by using HSI and NIR spectroscopy. A line scan (push broom) hyperspectral system (MS Macrosystem, Nederland) was used in this work which covers the wavelengths from 400 nm to 1000 nm. The chemical reference method based on UV-spectra was applied at 503nm. The objective of this study is using NIR spectroscopy and HSI to obtain calibration for lycopene content of snack bar and leather.

Keywords: Tomato, lycopene, NIR, hyperspectral, imaging,

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Discussion Question

Can lycopene content be determined in dried tomato products by using HSI and NIR spectroscopy

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P26: Evaluation of the spectral repeatability of olive oil analysis using Near infrared spectroscopy

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As an indispensable diet product in Mediterranean regions, olive oil is well welcomed due to its sensory characteristics of fine aroma and pleasant flavor combined with nutritional value of specific composition such as oleic acid, sterols, and rich phenolic compounds. Rapid detection of the quality parameters is an important tool to control the nutritional quality of olive oil. Near infrared (NIR) spectroscopy was widely used in the detection of the quality parameters in olive oil due to its rapid, low cost, non-destructive, environmentally friendly measurement, and greater penetrative power. In this study, three different NIR instruments (DairyQuant GO with the wavelength of 671.82-2702.70nm, GrainNit with the wavelength of 900-1700nm and 1350-2150nm) were used to analyse the olive oil samples from various regions, and the root mean square (RMS) statistic were calculated to evaluate the spectral repeatability. This has been used for the optimization of the analysis of olive oil, previously to the development of models to predict the quality parameters in olive oil.

Key words: Olive oil; near infrared spectroscopy; spectral repeatability of olive oils analysis; root mean square

P27: Screening procedure for control of cannabinoids based on a portable FT-NIR tool and chemometrics

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The global use of cannabis for medicinal, recreational and industrial purposes, combined with changes in legislations, have increased the demand for efficient and cost-effective analytical methods for quality control. This study explores the use of portable FT-NIR combined with chemometrics for rapid and accurate discrimination of cannabis samples based on their pharmacological (CBD), psychotropic (THC) content, as well as for differentiating industrial hemp and by-products (leaves and stems). Four types of fresh hemp (*Cannabis sativa* L.) samples were utilized: Type A) Futura 75 variety, which is certified by the EU for high-quality CBD and THC levels below 0.2%. Type B) served as a positive control with THC levels above 0.2%. Type C) comprised by-products (leaves and stems), which were used as a negative control. Type D) industrial hemp was utilized for fiber and grain production with low CBD content and no THC content. To validate the presence of target compounds (CBD, CBDA, THC, and THCA) an extraction procedure was done from samples type A, B, and C and compared with standards using liquid chromatography (UHPLC-MS/MS) [1,2]. Spectral signals were obtained using a portable FT-NIR and a Benchtop NIR (used as reference) and divided into two sets of data: one for calibration (N=100, sieved samples) and another for validation of the models (N=20, samples in their natural state). Signal pre-processing and outlier removal routines were applied, including Extended Multiplicative Signal Correction (EMSC), Standard Normal Variation (SNV) correction, Savitzky-Golay 1st and 2nd derivatives, and vector normalization. Discriminatory models (PLS-DA) were designed based on cross-validation and RMSECV results. Results exhibit that the portable FT-NIR device presents a correct validation model, accurately categorizing all sample types with 7 LVs. The model shows high coefficients of determination (R^2 Cal) and minimal cross-validation error values (RMSEcv), indicating robustness and similarity to the Benchtop device's values. This

promising procedure effectively discriminates cannabinoids in fresh hemp, providing reliable predictive results.

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P28: A food safety application of VIS-NIR Spectral Imaging and chemometric exploratory methods: detection of E. coli Biofilms on Aluminum surfaces

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Food contamination due to uncontrolled growth of bacterial cells is a major concern in production facilities. These cells give rise to formation of biofilms, more persistent and resistant forms of microorganism communities, on food contact surfaces and cause further problems. Biofilms are composed of organic substances as various types of lipids, carbohydrates, and proteins [1-3]. *Escherichia coli*, a human pathogen, is one of the most common biofilm producer species in food production environments [4].

Hyperspectral imaging has a potential use for hygiene monitoring for microbiological safety considerations [3]. This study explores the applicability of visible and NIR imaging for the detection of *E.coli* biofilms, by comparing two exploratory methods, Principal Component Analysis (PCA) and Independent Component Analysis (ICA). With a data split of 20% for validation, this approach was found successful to differentiate the biofilms spectra from those of control negative group, with different mean spectra and cluster centers.

Discussion Question

Can food industry be fully monitored in a similar way that pharmaceutical industry is, considering the possibility to adapt of Process Analytical Technology applications?

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P29: The integrity of coffee in Serbia: State-of-the-art, gaps and need for knowledge transfer

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In Balkan region, including Serbia, traditional black coffee is a very popular beverage, consumed several times a day [1]. In the context of hramonization of Serbian with the EU legislation [2], a new 'Rulebook on the quality of raw coffee, coffee products, coffee substitute and related products' has been adopted by the Ministry of Agriculture in December, 2020 [3]. In May 2022, the implementation of the Rulebook began, which required producers to clearly declare the presence of each substitute on the coffee label. Coffee is a complex beverage containing more than 1000 compounds, thus, many different techniques have been investigated in order to verify its integrity. These include microscopy, chromatography and spectroscopy associated with advanced data processing tools, such as chemometrics and machine learning, and DNA-based methods. Each of them exhibit certain advantages and limitations [4, 5]. Nevertheless, it should be underlined that, although it strongly demands labeling the presence of peas, chicory, rye, barley, soybeans or any other commonly used coffee substituent, the novel regulation does not propose official control methods for verifying the product authenticity on the market, except for standard methods for quality assessment (such as the content of moisture, caffeine, ashes etc.). According to [4], efficient low-cost methods are still not available, and classical optical microscopy is still used for purity assessment in many countries, although it can be unreliable depending solely on visual inspection of an analyst.

Discussion Question

In order to protect the consumers from possible fraud, it is necessary to identify or develop applicable state-of-the-art authentication methodologies in the research sector, and to transfer and implement those in the lab sector, aiming to monitor the quality of all coffee types available in the market. Are there any available yet?

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P30: Hyperspectral imaging (HSI) combined with Chemometrics tools as a new analytical approach to authenticate the wholemeal bread

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The production and sale of wholemeal bread are subject to varying regulations across different countries worldwide. For instance, there are no unified European regulations governing the chemical composition of this product, which means that each member state has its own quality control measures in place. To illustrate it, in Spain, in order to label bread as "wholemeal bread" according with the the Spanish food regulations, it must contain 100% wholemeal flour. If the percentage is lower, it should be labeled as "x% wholemeal bread" Nevertheless, Denmark regulations mandate that this type of bread must contain at least 30% wholemeal flour to label as “wholemeal bread”. These disagreements combined with the absence of an official analytical methodology for quality control of wholemeal bread contributes to the difficulty of authenticating this product, posing a significant challenge.

This communication presents a non-invasive analytical methodology to authenticate the wholemeal based on acquisition of hyperspectral imaging (HSI) combined with chemometrics tools. HSI offers the opportunity to generate a visual representation or a "picture" of the material system being studied. It is a sustainable technique that does not require the use of solvents or reagents and eliminates the need for time-consuming sample pre-treatment stages. The HYPERTools package in MATLAB environment was used to develop a classification and quantification model (PLS-DA and PLS-R). The classification model was built to discriminate between to class: (i) Bread made from more than 50% wholemeal flour; (ii) Bread made from a smaller or no percentage wholemeal flour. After that, a quantification model was developed to determine the percentage of wholemeal flour used in the bread production.

P31: Single spot NIR and NIR imaging. What is needed when?

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The interest in monitoring food and food processes led to installing on/in-line or in-situ Near Infrared (NIR) sensors that, coupled with chemometrics, can allow the acquisition of timely quality information on food commodities.

One of the main aspects that the industry is concerned with is the possible product heterogeneity and which could be the appropriate NIR device to assess its quality. When the material is suspected to be heterogeneous, NIR hyperspectral cameras might be desired instead of NIR classical single-spot spectrophotometers. However, it is not clear yet, and it would be useful to assess the extent to which NIR hyperspectral camera is needed and which one is the spatial information that a single spot classical NIR device can capture.

Here, we present a case study concerning the industrial production of *pesto alla genovese* sauce in Barilla G. e R. Fratelli S.p.A food company (Italy). The work aims to define the application range of a single-spot NIR spectrophotometer and a NIR hyperspectral device for classifying different pesto sauces. Two aspects are evaluated and discussed: the area of interest to consider for the HSI technique and what the NIR single spot is actually measuring.

Discussion Question

When do heterogeneous samples really need Hyperspectral Imaging techniques?

P32: Terahertz spectroscopy in agro-food quality evaluation: potentials and limitations

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Terahertz spectroscopy is an emerging optical technique that utilizes the radiation between the microwave and the infrared regions of the electromagnetic spectrum. The introduction of commercially available benchtop and handheld THz spectrometers has resulted in a wide range of applications in various fields, particularly in materials science, pharmaceuticals, and biomedical engineering. In this poster, agro-food applications of THz spectroscopy are presented. These applications exploit the sensitivity of THz spectroscopy towards intermolecular vibrations and relaxations that occur in the picosecond timescale. In the THz frequency, water exhibits very strong absorption. Thus, many food applications of THz spectroscopy are about the direct moisture content determination. Water dynamics studies have also been performed and provided insights about the hydration states of food. THz spectroscopy can also probe lattice vibrations that involve the collective motion of atoms or molecules within the crystal lattice structure. This sensitivity has allowed the monitoring of the phase transitions in confectionary products and of the breakdown of the starchy endosperm in grains. THz spectroscopy is also particularly useful for studying collective molecular vibrations. Food adulterants and contaminants like melamine, talc, aflatoxins, and some pesticides have been finger-printed in the THz region and have been quantitatively measured using THz spectroscopy. There remain some challenges that hinder the acceptance of THz spectroscopy as an analytical tool in the food industry: A practical disadvantage is the cost of acquiring and maintaining a spectrometer. Many of the reported THz-based quantitation methods have limits of detection that are unacceptable for trace analysis. The presence of water in food can also be disadvantageous as it can lower the sensitivity of the technique towards other analytes.

Discussion Question

Survey the food industry for sectors where the potential of THz spectroscopy as an analytical technique can be realized.

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P33: Early detection of infection by *Penicillium digitatum* in oranges using hyperspectral imaging and machine learning

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Fungal infections are a main concern in fruit packing houses since a single infected fruit can spread the infection, causing severe losses. Hence, early detection is crucial. Fluorescence induced by UV light is commonly used to detect infected fruits, but it can harm the eyes and the skin. Hyperspectral imaging and chemometrics have already been used to detect early infected fruits, but novel deep-learning approaches can improve the detection. In this work, 50 oranges 'Navelate' were inoculated with *Penicillium digitatum* and another 50 oranges were inoculated with distilled water as a control. After the inoculation, the fruits were stored at 20 ºC and 90 % relative humidity. Images were taken daily from the inoculation for four days, using a Vis-NIR pushbroom system (900-1700 nm). A total of 500 images were captured, corrected using white and dark references, cropped to the size of the fruit and divided into a train (60% of the images), validation (20% of images) and independent test (20% of images) datasets. A customised convolutional nerual network (CNN) was designed, composed of 3 convolutional layers (16, 32 and 64 filters and a kernel size of 3), followed by 3 max-pooling layers (pool size 2) and two final dense layers for classification of 128 and 1 neuron (with sigmoid activation function) which was trained for 800 epochs with a binary cross-entropy loss function. It was possible to correctly classify 100% of the control oranges and 80% of the inoculated ones from the second day, demonstrating that it is possible to detect asymptomatic infected using this technology.

Discussion Question

Is there a relationship between the depth to which the light penetrates and the anticipation in detecting internal damage? How important is the intensity of light?

P34: Is the VIS/NIR technique suitable for determining maturity and quality of peaches at harvest and after storage?

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Within the project, the usefulness of two devices (DA meter, Sintéleia, Italy, and CP Pigment Analyzer PA1101, Control in Applied Physiology GbR., Germany) for the nondestructive assessment of maturity and quality of the following peaches cultivars: 'Royal Glory', 'Redhaven', 'Harrow Beauty, and 'Supechsixteen' was determined. Measurements were done at harvest and after storage. Both devices use VIS/NIR spectroscopy and the following indices were gathered: the DA index (DA meter) - calculated using formula DA=A670-A720 (A670 and A720 are absorbances at 670 and 720 nm), and Normalized Difference Vegetation Index calculated as NDVI=(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 (CP Pigment Analyzer). In the case of CP Pigment Analyzer signal at wavelengths in the range from 400 nm to 1100 nm was also gathered. Besides the nondestructive measurements, the following standard quality parameters were measured: fruit weight, ethylene and CO_2 production, skin and flesh colour, fruit firmness, soluble solids content, and titratable acidity. The sensory analyses were also performed.

After harvest the fruits were divided into "maturity" classes, using the DA meter. Fruits of particular classes were placed in single-layer boxes and stored under regular, controlled, or MAP conditions. The results of the experiment indicate that the VIS/NIR spectroscopy is very useful for the prediction of the harvest date of peaches and/or sorting fruits for "ripening" classes before and after storage. The distinguished "ripening" classes are also recognized by sensory evaluation.

During fruit maturation and ripening fruit firmness and acidity decreased, but soluble solids content increased. Skin (background) and flesh colour changed (yellowing). Also all non-destructive indices steadily changed. The rate of changes depended on storage conditions and cultivar.

The non-destructive methods based on VIS/NIR spectroscopy are suitable for the estimation of soluble solids content, acidity, and firmness of peaches.

Keywords: peaches, nondestructive, VIS/NIR, ripening, quality, sensory evaluation, storage

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