



1ST SENSORFINT
INTERNATIONAL WORKSHOP

**SMART SPECTRAL
SENSORS FOR
AGRI-FOOD
QUALITY AND
PROCESS CONTROL**

30.09.2021 - 01.10.2021
PORTO, PORTUGAL

BOOK OF ABSTRACTS

ORGANIZATION / FINANCING ENTITIES



SPONSORS





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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 Abstract Book of our First International Workshop “Smart Spectral Sensors for Agrifood Quality and Process Control” (30th September- 1st October, Porto, Portugal).

This is the first event of the Action in which we are going to have the opportunity to share FACE-TO-FACE (but also providing a virtual access) ideas, knowledge, challenges, and reflexions about the important role of non-destructive spectral sensors in the control and monitoring of quality and authenticity in the food systems of the present and the future. It is obvious that Covid-19 has changed our life styles, everything around us has been affected, and in the case of the SENSORFINT Action everything has been more complex and unpredictable, sometimes making it very challenging to progress with the planned schedule.

But it is also true that the pandemic has reinforced the role that food production, its integrity and its assurance have in our life, making the advances in the digitalisation technologies to control them a key point in international research programs. Thus, it makes even more relevant our main objective, which is to build a vibrant and multidisciplinary network focused on the application of non-destructive spectral sensors to solve the demands of the industry regarding the assessment of food for quality, safety, authenticity or traceability, combining experience in research, manufacture, training and technology transfer to accelerate spectral sensor implementation through the food chain.



The use of sensors and technologies will enable the design of new intelligent quality control systems to achieve the new challenges of Industry 4.0 — a massive and instantaneous non destructive inspection of the food product to take decisions in real time from ‘field to the fork’, providing a unique digital print of the product and, therefore, a new digital labelling strategy with more complete information about the product for consumers, will be an essential aspect for the present and future of the food industry.

I would like to express my personal sincere thanks to the Local Organizers of this First SENSORFINT International Workshop (Antonio Silva Ferreira y Maria Lopes Cardoso), and to the Vice-Chair of this Action (Tom Fearn) for all the support, ideas and time dedicated to achieve this hybrid event. In addition, I would like to thank the keynote and the industry speakers for their kind availability from the beginning to collaborate. And of course I would like to thank the Core Group, the MC members and all the SENSORFINT participants for their support. Finally thanks to Cost for providing funds for this event.

Hoping all of you enjoy this workshop, the ideas and knowledge shared and of course the networking opportunities that it will open for us.



Signed: Prof. Dr. Dolores Pérez Marín

Chair of SENSORFINT (Cost Action 19145)



Preface by António Silva Ferreira

Universidade Católica Portuguesa, in Porto, and Faculty of Biotechnology, in particular, welcomes the 1st sensor FINT WorkShop devoted to debate the consequences of the arrival of emergent technologies described by our self-explanatory title “Smart Spectral Sensors for Agrifood Quality and Process Control”.

We propose to address the challenges and opportunities offered to food industry by the arrival of smart sensors in their production environment and supply chain, which enables real time data acquisition, bio-signals for quality and food safety. These disruptive tools are the drivers of change whith proper integration with robotics, digitization, 5G, automation, Internet of Things and artificial intelligence.

Following our tradition UCP aims to be on the front runner group and to provide the stage to an open debate together with relevant stakeholders on the food ecosystem, concerning what kind of resources, costs and what results are expected to be achieved with these disruptive technologies.



Signed: Prof. António Silva Ferreira

MC AND CORE GROUP MEMBER

SENSOR FINT 2021 – LOCAL ORGANIZER



TIME	30/09/2021 - THURSDAY
08h00	Check-in
09h00	OPENING SESSION
	Chairs: Jean-Michel Roger (France) & Ivan Štajduhar (Croatia)
09h15	KEYNOTE - HEINZ W. SIESLER On-Site Quality Control and Protection against Product Counterfeiting by Handheld Near-Infrared Spectrometers: Anytime, Anywhere by Anyone
10h00	ORAL PRESENTATION 1 - Christian Huck / University Innsbruck Principal Advances in Miniaturized NIR Spectroscopy Including Theoretical Attempts
10h15	ORAL PRESENTATION 2 - Irina Torres / University of Córdoba Near infrared spectral sensors for fraud detection in the almond industry
10h30	ORAL PRESENTATION - Marcus V. da Silva Ferreira / Universidade Federal Rural do Rio de Janeiro Portable near-infrared (NIR) spectrometer for prediction of carambola composition
10h45	Q&A
11h00	Coffee Break
	Chairs: Anna Sandak (Slovenia) & Marco Loschi (Switzerland)
11h30	ORAL PRESENTATION 3 - Jasenka Gajdoš Kljusurić / University of Zagreb Inspection of food quality by use of Near-infrared spectroscopy - modeling as an auxiliary or key tool
11h45	ORAL PRESENTATION 4 - Ana Garrido-Varo / University of Cordoba A long and exciting industry-university journey: the case of NIR-on line for the rendering industry
12h00	ORAL PRESENTATION 5 - Nils Kristian Afseth / Norwegian Institute of Food Towards in-process and on-farm applications of dry-film FTIR spectroscopy
12h15	ORAL PRESENTATION 6 - Miguel Vega-Castellote / University of Cordoba Food quality and safety assessment of spinach plants using a new generation NIR sensors along the food supply chain
12h30	ORAL PRESENTATION 7 - Cristina Alamprese / Università degli Studi di Milano Can NIR spectroscopy foster olive oil chain sustainability?
12h45	Q&A
13h00	Lunch
14h00	POSTER SESSION
	Chairs: Lola Pérez-Marín & Tom Fearn
15h00	INDUSTRIAL CASES
	INTRODUCTION
15h10	INDUSTRY CASE - PerkinElmer - MARTIN LAGERHOLM Balancing between robustness and accuracy, challenges and examples for NIR/MIR calibration
15h25	INDUSTRY CASE - Bruker Optik - ANDREAS NIEMOELLER Modern developments of FT-NIR and miniaturized MEMS based systems
15h40	Coffee Break
15h55	INDUSTRY CASE - Barilla - MICHELE SUMAN Hazelnut and apple products traceability through Near Infrared spectroscopy approach
16h10	INDUSTRY CASE - Aunir - ROCIO DONA GARCIA Investigating how wavelength ranges affect calibration performance in portable NIR equipment
16h25	INDUSTRY CASE - PortugalFoods - DEOLINDA SILVA Tech innovation in Portuguese agrifood sector
16h40	DEBATE Moderator: Manuela Pintado
17h40	Close
19h30	SOCIAL PROGRAMME - Gala Dinner (Sensor Fint2021 shuttle will be available)



TIME	01/10/2021 - FRIDAY	
	Chairs: Paolo Berzaghi (Italy) & Mecit Oztop (Turkey)	
09h00	ORAL PRESENTATION 8 - Wouter Saeys / KU Leuven A framework for bilinear calibration transfer based on transfer levels	
09h15	ORAL PRESENTATION 9 - Beatriz Carrasco / Chemometric Brain, S.L. An objective and easy-to-use NIR-based software for food quality control	
09h30	ORAL PRESENTATION 10 - Yannick Weesepeol / Wageningen Food Safety Research Keep it simple, stupid: photonics for industry and research, two worlds apart	
09h45	ORAL PRESENTATION 11 - Nicolò Pricca / Council for agricultural Research and analysis of Agricultural Economy Low-cost optical system for milk coagulation monitoring	
10h00	ORAL PRESENTATION 12 - Marina Cocchi / Università di Modena e Reggio Emilia A NMR-based foodomic approach to study Parmigiano Reggiano PDO cheese certification "Prodotto di Montagna Progetto Territorio"	
10h15	Q&A	
10h30	Coffee Break	
	Chairs: Vincent Baeten (Belgium) & Víctor Fernández (Spain)	
11h00	POSTER SESSION	
11h30	ORAL PRESENTATION 13 - Ana Rita Monforte / Universidade Católica Portuguesa Process Control in Flavour Generation: NIR as a tool to monitor key odorants formation	
11h45	ORAL PRESENTATION 14 - Jens Petter Wold / Nofima Optimal instrument design for in-line monitoring of heterogeneous foods by NIR interaction spectroscopy	
12h00	ORAL PRESENTATION 15 - Jose Blasco / Instituto Valenciano de Investigaciones Agrarias VIS-NIR hyperspectral imaging to detect internal damage in 'Rojo Brillante' persimmon using PCA and PLS-DA	
12h15	Q&A	
12h30	KEYNOTE - MOON KIM Line-scan multimodal spectral imaging for food safety and quality applications	
13h15	CLOSING SESSION + POSTER AWARD	
13h45	Lunch	
15h00	MC MEETING	IDEATION CORNER COST / Sensor Fint Lola Pérez-Marín - SensorFint Action Chair António Silva Ferreira - SensorFint Local organizer
15h15		Universidade Católica: multidisciplinary on campus João Pinto - Universidade Católica Portuguesa - Porto
15h30		Upcoming Funding Opportunities João Cortez - Universidade Católica Portuguesa - Porto
15h45		Industrial Tool Box Endress-Hauser Hammamatsu Siroco
16h30		Present challenges in industry Deolinda Silva - Portugal Foods
16h45		Debate Ana Machado da Silva - SONAE António Silva Ferreira - SensorFint Local organizer
17h30	SOCIAL PROGRAMME - Sunset	

KEYNOTE - HEINZ W. SIESLER

On-Site Quality Control and Protection against Product Counterfeiting by Handheld Near-Infrared Spectrometers: Anytime, Anywhere by Anyone

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Abstract

Recently, miniaturization of Raman, mid-infrared (MIR) and near infrared (NIR) spectrometers has made substantial progress, and marketing companies predict this segment of instrumentation will have a significant growth rate within the next few years. This increase will launch vibrational spectroscopy into a new era of quality control by in-the-field and on-site analysis.

While the weight of the majority of handheld Raman and MIR spectrometers is still in the ~1 kg range, the miniaturization of NIR spectrometers has advanced down to the ~100 g level, and developments are under way to integrate them into mobile phones. Thus, based on high-volume manufacturability and significant reduction of costs, numerous companies target primarily with NIR instruments a non-expert user community for consumer applications. Especially from this last-mentioned development, a tremendous potential for everyday life can be expected ranging from food testing to detection of fraud and adulteration in a broad area of materials (pharmaceuticals, textiles, polymers, etc.).



However, contrary to the exaggerated claims of many direct-to-consumer companies that advertise their “scanners of the future” by oversimplifying the measurements to “point-and-shoot” procedures with any deficiencies in sample presentation and sample heterogeneity being taken care of by “cloud evaluation of big data”, this presentation will provide an overview on the realistic application potential of these instruments.



KEYNOTE - MOON S. KIM

Line-scan multimodal spectral imaging for food safety and quality applications

Moon S. Kim

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Abstract

ARS research group in Beltsville, Maryland, has pioneered multimodal spectral line-scan imaging technologies for implementation in commercial food processing environments, such as wholesomeness inspection of broiler chickens on poultry processing lines. The research and development effort for the use of spectral line-scan imaging as a multispectral platform has been expanded to online safety and quality inspection of fresh produce. To achieve comprehensive online quality and safety inspection of fruits and vegetables, whole-surface sample presentation and imaging regimes must be considered. Because of the morphological shape differences between relatively round fruits and flat leafy greens, two independent methods have been developed to achieve whole-surface sample evaluation based on the use of a single hyperspectral line-scan imaging device on a processing line. In addition, a macro-scale Raman chemical imaging system was developed to implement high-throughput Raman imaging using a 785-nm line-laser. The line-scan Raman system accumulates hyperspectral data using a push-broom method for samples, and has been used to



authenticate powdered food ingredients and to detect chemical adulterants in powdered foods.

The research and development of line-scan multimodal spectral imaging technologies and methodologies for food safety and quality assessment and applications are presented.

INDUSTRIAL CASES - PERKINELMER

Balancing between robustness and accuracy, challenges and examples for NIR calibrations

Martin Lagerholm¹

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Partial Least Square Regression (PLSr) and Artificial Neural Network Regression (ANNr) have been used for decades in food applications with near infrared spectroscopic measurements. PLSr are more commonly used than ANNr. The author believes this is because ANNr is in general harder to understand, interpret and requires more data and more testing than PLSr. With a bad setup ANNr is at higher risk than PLSr especially if future data is not well represented in the calibration material (“extrapolation”). There are however many cases where this risk is low and where ANNr certainly is worth exploring.

This case study starts in parallel to reference [1] and then expand beyond pure accuracy into model robustness w.r.t. variations due to temperature, instruments (transferability) as well as regional effects. Wheat and Barley data from the Inframatic 9500 NIR Grain Analyzer (PerkinElmer/Perten) trimmed to the wavelength region 850:1050 nm is used. Given a reasonable amount of training data (5000 in this example) it will, by examples, be shown that ANNr is



- i) less sensitive and less dependent of data pre-processing
- ii) more accurate

as compared with PLSr.

Furthermore, the robustness of different models are investigated. The results will be hot of the printing press at the time of this talk but the author expects to find that the optimal model when only studying accuracy is not optimal when performance w.r.t. robustness is taken into account. Another expected find is that PLSr is a safe choice with decent accuracy and robustness but a well-tuned ANNr is often the better choice.

[1] Lagerholm M. A practical approach to ANN. Talk at 18th International Diffuse Reflectance Conference, 2016, Chambersburg, PA, USA.

Keywords: big data sets, non-destructive, NIR, food, wheat, barley, PLSr, ANNr, robustness, transferability.

INDUSTRIAL CASES - BRUKER OPTIK

Modern developments of FT-NIR and miniaturized MEMS based systems

Andreas Niemöller

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Near Infrared (NIR) is worldwide applied for routine analysis in agriculture, food, forestry, environmental, pharmaceutical, chemical, textile, cosmetics and many other industries and applications areas. The main aspect for the development of new hardware is reducing cost and size. This paper presents an overview of technical and practical aspects which need to be considered.

The field of spectroscopy is moving fast from the 80's where the first personal computers became available for laboratory devices. Especially for near infrared (NIR) spectrometers where chemometric evaluation approaches are mandatory, calculation power was essential.

Nowadays NIR benchtop, in-line and increasingly smaller and portable devices are in routine use in various industries and application fields using the main advantages of NIR analysis: almost no sample preparation, rapid analysis in seconds, no need of reagents, non-invasive and non-destructive and simultaneous analysis of multi-components. NIR is a secondary method and for quantifications a reliable calibration development with often hundreds of samples including a model validation step is required – similar is the work for an identification library. Beside the hardware costs



this is the only major investment in time and reference analysis to create a practical solution. Once this is finalized NIR is a work horse to cover the increasing number of samples resulting from today's higher quality control demands.

NIR instruments with many different technologies and setups are state of the art for various applications in routine quality control. What setup is used is a question of the application, the demanded accuracies, availability of ready-to-use calibrations, transferability and finally the price. The goal here was to highlight important aspects to be investigated, compared, and used for the final selection.

INDUSTRIAL CASES - BARILLA

Hazelnut and apple products traceability through Near Infrared spectroscopy approach

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Geographical origin of food products is nowadays a relevant aspect for high-quality characterization. The present study aims to assess geographical provenience of Italian hazelnut and apple products, by studying and comparing Near Infrared Spectroscopy (NIR) spectra of Italian and not Italian samples. A Design of Experiment, for training and validation sets building, was prepared, taking into account factors as harvesting year, variety, processing and percentage of peel. A total of n=32 dehydrated apple samples and n=24 processed hazelnut samples (both representative of several relevant countries from counterfeiting perspective) of 2020 harvesting year were analysed. Raw data were then elaborated and interpreted through multivariate statistical analysis, exploiting both unsupervised (Principal Component Analysis) and supervised (Partial Least Square – Discriminant Analysis), after an adequate pre-processing. This NIR approach consists of a limited or even inexistent sample preparation and provides for a good reproducibility when it is combined with the abovementioned statistical elaboration.



The overall strategy could be extended to other food chains traceability screening needs in the future.

Moreover, the final target would be to routinely apply it, deploying its exploitation at both industry quality control labs and raw materials reception points in order to systematically screen all the different lots which are delivered at production plants/lines.



INDUSTRIAL CASES - AUNIR

“Investigating how wavelength ranges affect calibration performance in portable NIR equipment”

The near infrared (NIR) spectroscopy is an analytical technique based on the interaction between matter and electromagnetic radiation in the range 780-2500nm. When analysing a sample by NIR a spectrum is obtained, and that is the result of the measurement of bands, overtones, and combination vibrations. That spectrum is specific to that material, and it is considered as its fingerprint.

NIR analysis is fast, easy to use, requires little to none sample preparation, is non-destructive, allows multiple component analysis, allows large sampling size, handles high concentration, and all that capability makes it very attractive to many different industries. Recent developments in instrumentation have resulted in a growth of lower cost portable handheld NIR instruments capable of being taken onto farm or into a processing environment when samples can be analysed in-situ, making the technique even more attractive to industry but also creeping into the realms of the consumer fulfilling their requirement to understand more about the products they are buying and consuming.

This paper examines the performance of three commercially available NIR instruments using different technology and covering different wavelength ranges.



It looks at the Foss DS 2500 (400 – 2500nm) the Viavi MicroNIR (950 -1650 nm) and the trinamiX NIR (1450 – 2450nm). The performance was assessed using the same datasets of animal feed ingredients covering a range of nutrients including proximates, non-starch polysaccharides, amino acids, and phytate.

The findings show that for some nutrients the performance is very similar, and all instruments could be used to replace reference wet chemistry in these scenarios. However, this was not true of all nutrients and this paper examines the possible reasons behind this.

INDUSTRIAL CASES - PORTUGALFOODS

Tech innovation in Portuguese agrifood sector

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Technological innovation is a key factor for companies' success in the increasingly demanding global market. Introducing new technologies in the development of processes, products and services allows the incorporation of more innovation and diversification, and increases competitiveness of companies. The Portuguese agrifood sector has evolved towards a stronger incorporation of technology and knowledge in its product value chain. Industry 4.0 and Digital Economy have a presence in the sector, particularly concerning intelligent implementation of networks to link 'equipment with equipment' and 'equipment with people'. Companies mainly resort to solutions which allow integration of information flows between customers and production and, thus, product customization according to demand. Portuguese agrifood sector is dominated by SMEs with financial constraints that leads to slower transition. This is one of the sectors with the greatest potential to benefit from Industry 4.0, as it incorporates primary, secondary and tertiary activities, and presents a wide scope for the application of new concepts and diverse technologies.

[1] Silva D. Tech innovation in Portuguese agrifood sector. Talk at 1st SENSORFINT International Workshop, 2021, Porto, Portugal.

Keywords: industry 4.0, new technologies, digitalization, innovation, Portuguese agrifood sector.

ABSTRACTS

SF2021-10002 - Prediction of volatile compounds in Iberian dry-cured pork shoulders by Near Infrared Spectroscopy (NIRS) - Poster

Miriam Hernández-Jiménez - Universidad de Salamanca

Iván Martínez-Martín - Universidad de Salamanca

Inmaculada González-Martín - Universidad de Salamanca

Ana M. Vivar-Quintana - Universidad de Salamanca

Isabel Revilla - Universidad de Salamanca

Iberian dry-cured ham and shoulders are characterised by their intense and persistent aroma which is provided by volatile compounds generated from the degradation of lipids and proteins during processing (Andrés et al., 2004; García et al., 1991). These compounds depend on the raw material (racial purity and feed) and the dry-curing technology (Carrapiso et al., 2003; Ventanas et al., 1999). Volatile compounds are determinant for the odour and taste of the products. The evaluation of these quality characteristics is done by sensory analysis. The major drawback of this methodology is its high cost, as it requires qualified personnel and facilities. For this reason, the sector is looking for other alternatives to know the quality in a quick and easy way to implement in the industry. In the present work, the prediction of volatile compounds from the NIRS recording of the central area of the shoulder (brachiocephalic muscle) using a fibre-optic probe applied directly on the sample without any previous treatment has been proposed. Volatile compounds were analysed by Gas Chromatography Mass Spectrometry (GC-MS) in 60 dry-cured shoulders (30 pieces of 50% Iberian breed and 30 pieces of 100% Iberian breed with two different dry-curing processes). A total of 172 volatile compounds were determined, of which 10 were detected in 100% of the samples. It was possible to predict nine of these ten compounds using the modified partial least squares regression method (MPLS). The results of the correlation coefficients (RSQ) were between 0.607 for Benzeneacetaldehyde and 0.967 for 1-Pentanol.



The method was validated with a set of external samples with no statistically significant differences between the actual value and the one predicted by NIRS.

The results showed that is possible to predict these compounds in unknown samples.

Keywords: NIRS, volatile compounds , Iberian dry-cured shoulders.

Andrés, A. I., Cava, R., Ventanas, J., Thovar, V., & Ruiz, J. (2004). Sensory characteristics of Iberian ham: Influence of salt content and processing conditions. *Meat Science*, 68(1), 45-51. <https://doi.org/10.1016/j.meatsci.2003.08.019>

Carrapiso, A. I., Bonilla, F., & García, C. (2003). Effect of crossbreeding and rearing system on sensory characteristics of Iberian ham. *Meat Science*, 65(1), 623-629. [https://doi.org/10.1016/S0309-1740\(02\)00256-5](https://doi.org/10.1016/S0309-1740(02)00256-5)

García, C., Berdagué, J. J., Antequera, T., López-Bote, C., Córdoba, J. J., & Ventanas, J. (1991). Volatile components of dry cured Iberian ham. *Food Chemistry*, 41(1), 23-32. [https://doi.org/10.1016/0308-8146\(91\)90128-B](https://doi.org/10.1016/0308-8146(91)90128-B)

Ruiz, J., Ventanas, J., Cava, R., Andrés, A., & García, C. (1999). Volatile compounds of dry-cured Iberian ham as affected by the length of the curing process. *Meat Science*, 52(1), 19-27. [https://doi.org/10.1016/S0309-1740\(98\)00144-2](https://doi.org/10.1016/S0309-1740(98)00144-2)

SF2021-10675 - Front-face fluorescence allows inline estimation of multiple heat damage tracers in milk - Poster

Anna Zamora - Universitat Autònoma de Barcelona

Heather Taterka - Universitat Autònoma de Barcelona

Jinfang Liu - Universitat Autònoma de Barcelona

Carlos González - Universitat Autònoma de Barcelona

Noemí Ayala - Universitat Autònoma de Barcelona

Jordi Saldo - Universitat Autònoma de Barcelona

Manuel Castillo - Universitat Autònoma de Barcelona

During processing, milk is exposed to different intensities of heat treatment that can induce functional, nutritional and organoleptic changes, many of them undesirable. Various markers have been proposed: lactulose, furosine, etc., to evaluate thermal damage, but the analysis methods must be performed in a specialized laboratory, being laborious, expensive and slow.

Techniques for the determination of 5-hydroxymethylfurfural (HMF), sulfhydryl / thiol (-SH) groups, whey proteins (native, denatured bound to casein and denatured in the form of soluble aggregates), vitamins A, B2, and C, furosine, lactulose, and casein micelle particle size were implemented. Likewise, front-face fluorescence determination instrumentation and methods were implemented. Prediction models for a large number of thermal damage reference indicators were developed. Through the information extracted from the fluorescence analysis, eleven prediction models were successfully obtained for most traditional reference markers of thermal damage using a few fluorescence-based predictors. The most relevant models obtained were: 1) [-SH]: $R^2 = 0.92$, SEP = 0.01 $\mu\text{mol/L-cysteine L}$; 2) [HMF]: $R^2 = 0.94$, SEP = 6.54 $\mu\text{mol/L}$; 3) [lactulose]: $R^2 = 0.91$, SEP = 1.8 10^{-7} mol/L ; 4) [furosine]: $R^2 = 0.92$, SEP = 9.15 mg/kg protein ; 5) [native whey proteins]: $R^2 = 0.97$, SEP 35.3 $\mu\text{g/mL}$; 6) [denatured whey protein aggregates]: $R^2 = 0.70$, $R^2 = 134 \mu\text{g/mL}$; 7) [bound whey protein]: $R^2 = 0.98$, SEP = 38.7 $\mu\text{g/mL}$; 8) casein micelle size, $R^2=0.99$, SEP 2.77 nm ; 9) [ascorbic acid]: $R^2 = 0.95$, SEP = 0.72 ppm ; 10) [riboflavin]: $R^2 = 0.94$, SEP = 0.01 ppm ; 11) [retinol]: $R^2 = 0.87$, SEP = 2.47 $\cdot 10^{-2} \text{ mg/L}$. Results obtained encouraged usage of front-face fluorescence as a rapid method for thermal damage assessment in milk, which could contribute to the development of a new generation of low-cost, non-invasive optical sensors for dairy product process control.

Keywords: Front-face fluorescence; heat damage, tracer, milk.

The abstract does not contain any literature reference. I have included a short BIO. Dr. Castillo joined the Universitat Autònoma de Barcelona (UAB) as Associate Professor of Food Processing in 2009, where he has been recently promoted to Full Professor. He came from the University of Kentucky (UK) where he was Assistant Research Professor (Biosystems & Agricultural Engineering, BAE). Professor Castillo's research program focuses on the development of optical sensor technologies for food process control. Summarized scientific production track-record is as follows: Funded projects–37 (21 as PI); Competitive research funds received–2.5 million €; US Patents–2; EU patents – 1; EU patents under review–1; patent pre-evaluations -6; publications -321 (Refereed articles–73; Book chapters–5; Non-refereed articles–17; Conference papers–60; Presentations at conferences –oral & posters–166); Students advised–44 (6 postdoc, 10



PhD., 19 MS, and 9 TFG); International visiting scholars–22; Interns/part time employees–51; Presentations/invited conferences–35; International professors invited–18. His outstanding scientific contribution in the chemical and engineering sector of dairy products processing has been recognized with two prestigious international awards in the US (IDFA Research Award in Dairy Food Processing -ADSA, 2008- and Samuel Cate Prescott Award for Research –IFT, 2009-).

SF2021-13249 - Use of portable NIR instruments for commercial classification of Iberian pig in slaughterhouse - Poster

Víctor M. Fernández-Cabanás - Departamento de Agronomía. Universidad de Sevilla (Spain)

Alberto Horcada Ibáñez - Departamento de Agronomía. Universidad de Sevilla (Spain)

Iberian pork products are considered high quality, reaching high prices in the market. For this reason, over time, different analytical techniques have been used, including NIR spectroscopy; for the control of fraud in the meat industry. Recently, the development of portable NIR equipment has allowed several authors to develop predictive models that allow verifying that the product offered belongs to the commercial category associated with it on the label. The use of portable equipment is very advantageous, since it allows controls to be carried out outside the laboratory, and even in the slaughterhouse itself. In the first studies, models were developed to differentiate animals according to their diet, since those fed with natural resources such as acorns and grasses have better flavor (Pérez-Marín et al., 2009; Zamora-Rojas et al., 2012). With the change in regulation in Spain in 2014, the genotype of the animal was included in addition to the diet. With this new change in the regulations, it was necessary to determine if commercial categories could be assigned with portable equipment and which anatomical area (live animal skin, carcass surface, fresh meat and subcutaneous fat samples) was the most recommended for measurements at abattoir. Horcada et al. (2020) concluded that best assignments were obtained for NIRS measurements in the carcass surface and subcutaneous fat (75.9% and 73.8% of correct classification, respectively).

Moreover, 93.2% and 93.4% of carcasses were correctly classified according to feeding regimes by using the spectra from fresh meat and subcutaneous fat samples. In view of the present findings, portable NIRS could be used in commercial slaughterhouses as a tool to support the control of the official quality category assignment in Iberian pig carcasses.

Keywords: Iberian pork, handheld instruments, authentication.

Horcada, A., Valera, M., Juárez, M. & Fernández-Cabanás, V.M.. (2020). Authentication of Iberian pork official quality categories using a portable near infrared spectroscopy (NIRS) instrument. *Food Chemistry*, 318, p. 126471

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SF2021-14886 - VIS-NIR hyperspectral imaging to detect internal damage in 'Rojo Brillante' persimmon using PCA and PLS-DA - Oral Presentation

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Artificial vision inspection systems have been used in fruit to detect external quality. However, some mechanical damage to persimmon cv 'Rojo Brillante', caused during postharvest handling, is only visible when the fruit is peeled and therefore goes unnoticed during the postharvest inspection. This work uses hyperspectral imaging (450-1040 nm) to detect internal damage in meat without any external symptoms and, therefore, invisible to traditional systems. A total of 65 fruits were selected and artificially damaged on two opposite sides with a controlled force. The images of the fruit were taken just before and at 0, 1, 2 and 3 days after the induction of the damage, for a total of 650 hyperspectral images. To detect the damage caused by the hit, an image processing algorithm based on principal component analysis (PCA) was developed, capable of detecting differences in the pixels of the fruit that would identify any pattern and indicate the presence of the damage. With this algorithm, 90.0% of fruit without bruises and 90.5% of bruised fruit were detected. Later, using the mean spectrum of the pixels detected as bruised by PCA, a partial least squares discriminant analysis (PLS-DA) model was calibrated to determine when the fruit was damaged. As a result, 100%, 97.4%, 100% and 100% of the bruises corresponding to 0, 1, 2 and 3 days after the induction of the damage were correctly identified in an independent validation set. In addition, to obtain a graphical reference of the results, the detection and discrimination results given by the models were displayed on the image of the fruit. These results show the potential of the hyperspectral imaging technique to detect mechanical damage in the packaging lines of 'Rojo Brillante' persimmon and estimating the moment in which the damage occurred, thus predicting its evolution.

Keywords: invisible damage, fruit quality, computer vision, postharvest inspection.



SF2021-16578 - Principal Advances in Miniaturized NIR Spectroscopy Including Theoretical Attempts - Oral Presentation

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Near-infrared (NIR) spectroscopy nowadays is a mature and wide-spread analytical technique, valued for rapidness, flexibility and high-throughput capacity. It bears almost unparalleled practical value in diverse applications throughout analytical chemistry labs, various industries, agriculture, forestry, subjects involved in environmental monitoring and food safety institutions [1,2]. Despite gaining an ultimate value in several areas of application, certain limitations of this technique have been apparent that somewhat limited its further spread. However, recent few years have seen fundamental advancements in NIR spectroscopy, which decisively changed the potential for applications and our understanding of NIR spectra. Dynamic development of miniaturized spectrometers enabled a new array of applications [2,3]. On-site capable NIR spectrometers and unmanned aerial vehicle (UAV; i.e. drone)-mounted sensors are currently revolutionizing the applications of this technique. Development of ultra-miniaturized NIR spectrometers towards on-chip sensor will enable implementing these instruments in wearables and may ultimately place NIR spectroscopy as part of everybody's daily life [2,3]. On the other hand, advancements in methods for spectral data-analysis increase ones' understanding of the subtle spectral features, and enable better optimization of the analytical procedures [1]. Notable advances were made at the foundations of NIR spectroscopy, e.g. with the ability to theoretically predict absorption bands by quantum chemical simulations [4,5]. The advancements in basic science remarkably pushed the limits of interpretability of NIR spectra. Further, they enabled understanding of the instrumental difference in analytical applications and agile designing of the analysis towards specific compound.

Accompanied by a continuous refinement of established approaches, these factors decisively changed the potential for future applications of NIR spectroscopy. Combined advancements in fundamental research and technology bring a new perspective onto NIR spectroscopy.

Keywords: Miniaturization; Quantum chemistry; 2D-COS; Neuronal network algorithms.

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SF2021-16818 - Near infrared spectroscopy for the categorization of olive oils - Poster

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Virgin olive oil is an essential component of the traditional Mediterranean diet. Extra virgin olive oil is the most expensive and health-promoting of all the categories of olive oils and, because of this, it is a suitable target for fraudsters and particularly susceptible to be adulterated with cheaper vegetable oils or lower quality olive oils. This study sought to evaluate the viability of using near infrared spectroscopy (NIRS) to categorize olive oils as a function of their organoleptic evaluation. A total of 324 olive oils were evaluated by official tasting panels and classified as extra virgin olive oil (EVOO) (132 samples), virgin olive oil (VOO) (100 samples) and lampante olive oil (LOO) (92 samples), according to the Commission Regulation No 2568/91. Furthermore, analytical chemical information was also available for the categorization of olive oils (i.e., free acidity, peroxide index, extinction coefficients K232 and K270, and fatty acid ethyl esters).



NIRS analysis was carried out using a Foss NIRSystems 6500 SY-II spectrophotometer, working in the spectral range 400-2500 and using a transfectance cup. Partial least squares discriminant models were constructed to classify olive oils by category (EVOO versus VOO+LOO; EVOO versus VOO and EVOO versus LOO). The best models developed showed percentages of correct classification over the 75% in cross-validation, and over the 72% in external validation. The results obtained here should be considered the first step in the fine-tuning of NIRS for categorizing olive oils and detecting potential fraud, providing consumers with more reliable information.

Keywords: Extra virgin olive oil; fraud detection; NIR spectroscopy; categorization.

SF2021-17749 - An objective and easy-to-use NIR-based software for food quality control - Oral Presentation

Beatriz Carrasco - Chemometric Brain, S.L.

In the food industry, powdered products are about 40% of human consumption. Moreover, pure ingredients and powdered blends are used by food companies in the production of their final recipes. Quality control for these types of ingredients (and even for the final powdered products) is a challenge for most manufacturers as there are no specific methods that can provide reliable results. Adulterations and food safety failures are difficult to detect in these kind of products. Therefore, there is a real need to implement a methodology to perform quality control in a more reliable, faster and easier way, that can be conducted by any minimally trained technician, avoiding human error and providing reliable levels of identification and minimizing risks, while, at the same time, increasing a company's food-safety standards and establishing a precise and fully replicable quality-control process. NIR technology combined with chemometrics has proven to be a good alternative to perform inline and online quality control. With this technology, it is possible to analyze any powdered product, determining the composition, homogeneity and compliance of new samples. This technique provides the industry with an objective and reliable tool to ensure the composition and functionality of food products. In this work, we propose the use of Chemometric Brain software as a



service (Saas) to provide the industry with an easy-to-use, objective and automatic technique in order to perform more complete and accurate analysis of samples to ensure quality and food safety: identification, properties determination and even the composition in terms of ingredients and percentages, in case of blend products.

www.chemometricbrain.io

Keywords: Spectroscopy; Chemometrics; Cloud-based Software; Industry.

SF2021-19616 - Towards in-process and on-farm applications of dry-film FTIR spectroscopy - Oral Presentation

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Ulrike Böcker - Nofima - Norwegian institute of food, fisheries and aquaculture research

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Sileshi Gizachew Wubshet - Nofima - Norwegian institute of food, fisheries and aquaculture research

There is a continuous search for smart sensor systems that can potentially provide better means for exploring subtle chemical distinctions and minor chemical components than provided by near-infrared spectroscopy. Fourier-transform infrared (FTIR) spectroscopy is one of these alternatives that are providing new possibilities for detailed characterization, not only in research environments, but also in industrial settings. Today, FTIR spectroscopy is mainly used as a high-throughput approach in laboratory environments, but infrared technology is being developed at a steady pace, opening the

possibility to explore sampling approaches like dry-film FTIR spectroscopy and attenuated total reflection (ATR) as alternatives to the traditional transmission approach. By removal of water, the dry-film FTIR approach potentially provides better means for exploring detailed chemistry of liquid samples, and we have recently explored this approach for several applications. The first application is related to milk analysis as a tool to monitor the health status of a cow. We have shown how dry-film FTIR fingerprints of milk during the lactation period of a cow can give valuable information on features like energy balance and the likelihood of a cow entering subclinical ketosis, which is a condition that can affect health and reproductive performance in a negative way. The second application is related to the use of dry-film FTIR spectroscopy as an industrial tool to monitor quality features like average molecular weights of protein hydrolysates enzymatically produced from food processing by-products. Enzymatic protein hydrolysis is a growing industrial segment, and we have demonstrated FTIR as a valuable analytical technology for mapping product quality variations and subsequently for process optimisation. In the presentation, these two application areas will be discussed together with perspectives on the development of affordable smart sensor systems based on dry-film FTIR spectroscopy for in-process and on-farm applications.

Keywords: FTIR, in-process, on-farm.

Nils Kristian Afseth is a senior research scientist in Nofima – the Norwegian institute of food, fisheries and aquaculture research. He has more than 15 years of experience within applied vibrational spectroscopy and chemometrics for food analysis. Current major research interests include applied FTIR and Raman spectroscopy, and bridging vibrational spectroscopy and classical analytical technologies. Nils Kristian holds a MSc in organic chemistry and a PhD in Raman spectroscopy for food analysis.

SF2021-19925 - Food quality and safety assessment of spinach plants using a new generation NIR sensors along the food supply chain - Oral Presentation

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The horticultural sector demands fast and non-destructive analysis technologies to assure the quality and safety of agri-food products. The new generation of near infrared (NIR) spectral sensors enables to carry out a wide range of applications to meet the processing industry needs. In the past few years, our research group has focused on the study of the implementation of these sensors in the different steps of the food supply chain. Specifically, in this work, the potential of NIR spectroscopy for the prediction of the soluble solid content (SSC) and nitrate content in spinach plants in the growing fields and in the industry sorting lines was assessed using a portable handheld NIR spectrophotometer working in the spectral range 908-1676 nm (MicroNIR™ OnSite-W), suitable for the analysis in situ, and an online Fourier Transform (FT)-NIR instrument working in the spectral range 834-2502 nm (Matrix-F). Spectral data of spinach plants belonging to different cultivars, harvest dates, orchards and seasons was used to develop partial least squares (PLS) regression models for the prediction of the quality and safety parameters above mentioned. These models were later externally validated. Results showed that NIR spectroscopy can be used as a routine analysis tool to assess the spinach quality (SSC) both in the field and in the industry sorting lines. In addition, this technology enabled spinach plants to be classified both in situ and online according to their nitrate content, which determines their possible industrial destination (baby food production, preserved, deep-frozen or frozen spinach and fresh spinach) according to the European legislation (EC 1258/2011).

Keywords: Food quality; food safety; in situ; online; spinach plants.

Torres, I., Sánchez, M.-T., Vega-Castellote, M., Luqui-Muñoz, N., Pérez-Marín, D. (2021), Routine NIRS analysis methodology to predict quality and safety indexes in



spinach plants during their growing season in the field. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, 246, 118972. Torres I., Sanchez M.-T., Perez-Marin D. (2020), Integrated soluble solid and nitrate content assessment of spinach plants using portable NIRS sensors along the supply chain. *Postharvest Biology and Technology*, 168, 111273. Torres, I., Sánchez, M.-T., Entrenas, J.-A., Garrido-Varo, A., Pérez-Marín, D. (2019), Monitoring quality and safety assessment of summer squashes along the food supply chain using near infrared sensors. *Postharvest Biology and Technology*, 154, 21–30.

SF2021-20697 - The perks and ills of Vis-NIR spectroscopy in the assessment of “Algarve Citrus” ripening on-tree - Poster

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“Algarve Citrus” are non-climacteric Protected Geographical Indication (PGI) commodities. At harvest, fruit must observe minimal levels of juice content, soluble solids content (SSC) and maturation index (MI) [1]. These internal quality attributes (IQA) are currently determined in limited samples of fruit collected close to harvest, by standard destructive and time-consuming methods. Two commercial orchards of sweet orange (*Citrus sinensis* L. Osbeck ‘Newhall’) comprising 50 georeferenced trees, and located at sites (Quarteira and Paderne) with different edaphoclimatic conditions, were assessed for two consecutive years (four independent datasets). The spatiotemporal modelling of the mandatory IQA has shown a large variability within and among orchards, in addition to the negative correlation between firmness and MI [2]. The site-specific orchard management of citrus ripening would enable the best decision on their optimal harvest date. This warrants extensive samplings and an assessment in real-time. Visible-near infrared spectroscopy (Vis-NIRS) (680–1100 nm) was applied for monitoring, non-destructively, the ripening of ‘Newhall’ on-tree [3]. The spectral data acquired with a portable customized portable spectrometer was used to construct calibration models for the mandatory IQA and firmness, using PLS. Their robustness was assessed through the comparison of internal validation (IV: calibration and validation data sets homogeneously sampled from the whole data set) and external validation (EV: calibration and validation datasets corresponding to different orchards and/or years). Globally, SSC yielded the best performing model, followed by MI. Firmness yielded the worse model, and none was obtained for juice content. The results also showed that IV overestimated the models’ performance relatively to the realistic and stringent EV. Yet, when comparing the two validation approaches, a convergence of IV and EV performances was noticed for larger numbers of samples, and thus the potential for the future continuous model improvement through the inclusion of more orchards/years.

Keywords: Vis-NIRS; Ripening spatiotemporal variability; Optimal harvest date; Model robustness.



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SF2021-21651 - Portable near-infrared (NIR) spectrometer for prediction of carambola composition - Poster

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Fruit quality is often related to attributes, such as soluble solid content and acidity¹. Traditional analytical techniques for physicochemical quantification are costly and not environmentally friendly (involves the use of chemicals)². Hence, a quick and non-destructive evaluation of carambola quality using a portable near-infrared (NIR) spectrometer was proposed.

NIR spectra were acquired for 177 carambolas, and data was separated into 123 (70%) for the calibration set and 54 (30%) for the validation set. Predictive models were developed for soluble solid content (SST) and total titratable acidity (TTA) of carambola. These models were created using two different methods: Support Vector Machine regression (SVMR) and Partial Least Squares Regression (PLSR). Several pre-treatments were tested, and smoothing showed better performance for TTA, whereas the combination of 1st derivative and smoothing favored SST models. The SVMR models for SST and TTA presented coefficients of determination for prediction (R²P) of 0.66 and 0.73, respectively, and root mean square error (RMSEP) of 1.09 and 0.06, respectively. On the other hand, the PLSR models for SST and TTA (7 and 9 latent variables) showed R²P of 0.64 and 0.66 and RMSEP of 1.12 and 0.07, respectively. Similar findings were reported by some authors when applying NIR to other tropical fruits 3,4. Therefore, NIR seems to be a good method in combination with chemometrics for SST and TTA prediction in carambola fruit.

Keywords: carambola, spectroscopy, chemometrics.

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SF2021-24359 - FLUORESCENCE SPECTROSCOPY AS A TOOL FOR CIP-SYSTEM OPTIMIZATION: A PRELIMINARY STUDY - Poster

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Manuel Castillo - Universitat Autònoma de Barcelona

The major unit operation in the dairy industry is heat treatment. An unpleasant side effect to this unit operation is fouling, which is the formation of thermal materials from process fluids that deposit onto equipment surfaces. The CIP-system of a heat exchanger is responsible for the control of fouling. The objective of the research was to characterize the fluorescence profiles of four intrinsic fluorophores in the cleaning fluids of a milk plate heat exchanger (PHE), with the long-term goal of obtaining a reliable algorithm for identification of the end-point of cleaning processes, based on objective, inline, optical measurements of chemical composition changes occurring in the cleaning fluids of the CIP-system. Firstly, standard curves were created for each fluorophore (tryptophan, riboflavin, Maillard compounds and dityrosine), with the aim to set up the limits of the measuring technique. Then, right-angle and front-face fluorescence of cleaning fluid samples were assessed. Most of the samples had low fluorescence intensities results from all four fluorophores with some under the minimum detection level. However, the samples with water plus the alkali detergent, or water plus the enzyme detergent, had much higher fluorescence intensities from all four fluorophores. It was therefore assumed that there was type A fouling present in the milk PHE, which came loose due to an alkali or enzyme cleaning agent and was drained out of the PHE with the cleaning fluid. A non-destructive right-angle fluorescence sensor for inline monitoring of fluorescence intensities of these fluorophores in cleaning fluids, could provide useful information that can be used to improve cleaning operation process control.

Keywords: Right angle fluorescence; front-face fluorescence; fouling; cleaning-in-place.



Dr. A. Zamora has a BS in Environmental Biology (University of London) and a BS in Biology and Food Science (UB). During her PhD at UAB, on the use of UHPH as an alternative treatment of milk for cheese-making, she spent a research stay working with Prof. A. L. Kelly at UCC, obtaining the mention of “European Doctor” and “Extraordinary Doctorate Award”. She is currently working at UAB as researcher scientist and project manager. She has a broad experience in food processing and operation of pilot plant equipment, and a wide expertise in food chemistry and instrumental analysis. Dr. Zamora has participated in various R&D projects at European/national level (seven in the last 5 years). She is codirecting a PhD thesis on the application of FFFS for the determination of milk quality and a second PhD thesis on the application of light backscatter in the process control of meat emulsions production. She has directed 1 PhD, 12 MS, 2 end-of-degree students, and 8 internship scholars. With an h-index of 14, she has published 28 indexed papers and 30 contributions to congresses. She has also reviewed 13 manuscripts for peer-reviewed journals. Since 2015, she also became a member of the OPTICmizing research group, which allowed her to substantially expand her knowledge in photonics, where she has been instrumental on the development of a novel inline meat emulsion monitoring system (projects COMRDI15-1-0027 and ARP/1282/2018). She is currently the IP of the transference project “Estimación en línea del daño térmico en leche mediante fluorescencia front-face: Sistema multicanal compacto y automático para la adquisición de datos” (XIAVALTEC-2021-1-13).

SF2021-24905 - Usefulness of multi energy X-ray absorptiometry to determine salt content in commercial sliced dry-cured ham - Poster

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ISRAEL MUÑOZ - IRTA

PERE GOU - IRTA

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Technologies that enable precise labelling and verification of nutritional claims are of interest for food industry, especially in those products with an inherent variation of the composition. The objective of this study was to evaluate the feasibility of multi energy



X-ray absorptiometry technology for the determination of salt content in commercial sliced dry-cured ham in line at the industry. The use of different data treatment methods as well as the interference of overlapping of slices were studied. The potential of this technology to perform a verified salt reduced claim labelling was assessed in an industrial case study. To do so, an X-ray prototype system with a multi energy detector was used to scan 325 commercial sliced dry-cured ham packages at 110 keV with an intensity of 1.5 mA. The system acquired an image in which each pixel contained an X-ray energy spectrum of 128 channels (from 20 to 160 keV). Partial least squares regression (using the multi energy spectra) and Linear regression (using ratios from energy bands) were used to develop the predictive models, when selecting different regions of interest. PLSR models showed lower predictive errors (RMSE= 0.383%) than linear regression models (RMSE= 0.407%) for the prediction of salt content. Use of the entire image instead of regions of interest with similar thickness showed a better predictive capacity. Therefore, slice overlapping did not affect significantly the predictive capacity of the technology. With these predictive errors, when the production has a mean salt content of 5.6% and a standard deviation of 1.2%, the 5.5% of the production can be categorized as salt reduced with a classification accuracy of 91.3%. We can conclude that precise labelling and verification of nutritional claims of sliced dry-cured ham in line at the industry is possible.

Keywords: precise characterization, nutritional facts, salt, multi energy X-ray spectrometry.

SF2021-27887 - PREDICTION OF COOKING LOSSES OF MEAT EMULSIONS WITH A LIGHT BACKSCATTER SENSOR - Poster

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In the economy of meat industry, establishment of suitable emulsification conditions can control the destabilization of emulsions and consequently cooking losses. The purpose



of this research was to develop models for predicting cooking losses of meat emulsions produced at industrial scale. The intensity of peaks and inflection points of the spectra, and their ratios and mathematical transformations (inverse, square, and cube) were assessed as predictors. The optical response of meat emulsions depended drastically on the presence or absence of starch. Since its incorporation improves notably the stability of the emulsion by promoting the interaction between the main components of the batter, it is probable that the greater homogeneity of the emulsion with starch provided similar and reliable optical data overshadowing some strong predictors, which in the models seemed to be significant to predict the losses. However, very robust models with R^2 values > 0.999 were obtained with five and six statistically significant optical predictors for emulsions without and with starch, respectively. These results point out the potential of light backscatter technology as a control tool during the emulsification process in a continuous industrial emulsifier.

Keywords: Light backscatter sensor; meat emulsion; stability; cooking losses.

Dr. A. Zamora has a BS in Environmental Biology (University of London) and a BS in Biology and Food Science (UB). During her PhD at UAB, on the use of UHPH as an alternative treatment of milk for cheese-making, she spent a research stay working with Prof. A. L. Kelly at UCC, obtaining the mention of “European Doctor” and “Extraordinary Doctorate Award”. She is currently working at UAB as researcher scientist and project manager. She has a broad experience in food processing and operation of pilot plant equipment, and a wide expertise in food chemistry and instrumental analysis. Dr. Zamora has participated in various R&D projects at European/national level (seven in the last 5 years). She is codirecting a PhD thesis on the application of FFFS for the determination of milk quality and a second PhD thesis on the application of light backscatter in the process control of meat emulsions production. She has directed 1 PhD, 12 MS, 2 end-of-degree students, and 8 internship scholars. With an h-index of 14, she has published 28 indexed papers and 30 contributions to congresses. She has also reviewed 13 manuscripts for peer-reviewed journals. Since 2015, she also became a member of the OPTICmizing research group, which allowed her to substantially expand her knowledge in photonics, where she has



been instrumental on the development of a novel inline meat emulsion monitoring system (projects COMRDI15-1-0027 and ARP/1282/2018). She is currently the IP of the transference project “Estimación en línea del daño térmico en leche mediante fluorescencia front-face: Sistema multicanal compacto y automático para la adquisición de datos” (XIAVALTEC-2021-1-13).

SF2021-35630 - Classification ability of low cost NIR sensors intended for consumers and stakeholders to discriminate fresh meat samples according to animal’s feeding regime - Poster

MARIA DEL MAR GIRO CANDANEDO - IRTA

CLARA BARNÉS - IRTA

JOSEP COMAPOSADA - IRTA

MARIA FONT-I-FURNOLS - IRTA

PERE GOU - IRTA

ELENA FULLADOSA - IRTA

Both consumers and industry are demanding low-cost tools to prevent fraudulent practices on animal feeding regime declarations. The aim of this study was to determine the ability of two low-cost NIR sensors intended for consumers to discriminate pork meat according to the animal’s feeding regime. Effect of the measurement’s location (inner and outer subcutaneous fat) was also evaluated using a high performance NIR spectrometer. For this purpose, fat samples from animals fed with Acorn (animals fed with grass and acorns in free range) (n=97) or Compound (animals fed with compound feed in an intensive system) (n=90) were used. The spectrometers used were the following: a portable low-cost smartphone-based spectrometer acquiring from 740 to 1070 nm (SCiO) (Consumer Physics, Israel), an on-line low-cost spectrometer acquiring from 600 to 1160 nm (Hamamatsu C14384MA-01) (Hamamatsu Photonics K.K., Japan), and a high-performance Fourier Transform NIR spectrometer acquiring from 12000 to 4000 cm^{-1} (833.3–2500 nm) (Bruker) (Bruker Optik GmbH, Germany). Spectra were acquired on a longitudinal section of the outer subcutaneous fat (Area 1) using all the sensors. Two additional locations, the outer layer (Area 2) and the inner

layer (Area 3) of a transversal subcutaneous fat section was also analysed using Bruker spectrometer. Results showed that classification scores were similar when measuring on the outer (75.8% and 70.5% in Area 1 and 2, respectively) or on the inner subcutaneous fat layer (82.5% in Area 3), although fatty acid composition is reported to be different [1]. Results showed that SCiO and Hamamatsu spectrometers could be also useful for the classification of fresh meat according to the animal's feeding regimes when measuring on Area 1, obtaining an overall classification accuracy on the validation set of 81.0% and 70.8%, respectively. This classification is possible because of the differences in the fatty acid profile attributed to the different feeding regimes as previously reported [2, 3]. Low-cost spectrometers intended for consumers and stakeholders could be useful for animal's feeding regime authentication on-site.

Keywords: fraud, feeding regimes, consumers, industry.

1.Daza, A., et al., Fatty acids profile of the subcutaneous backfat layers from Iberian pigs raised under free-range conditions. *FOOD SCIENCE AND TECHNOLOGY INTERNATIONAL*, 2007. 13(2): p. 135-140.2.Pérez-Marín, D., et al., A feasibility study on the use of near-infrared spectroscopy for prediction of the fatty acid profile in live Iberian pigs and carcasses. *Meat Science*, 2009. 83(4): p. 627-633.3.Zamora-Rojas, E., et al., Prediction of fatty acids content in pig adipose tissue by near infrared spectroscopy: At-line versus in-situ analysis. *Meat Science*, 2013. 95(3): p. 503-511.

SF2021-35668 - Inspection of food quality by use of Near-infrared spectroscopy - modeling as an auxiliary or key tool - Oral Presentation

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Davor Valinger - Faculty of Food Technology and Biotechnology at University of Zagreb, Croatia

Jasenka Gajdoš Kljusurić - Faculty of Food Technology and Biotechnology at University of Zagreb, Croatia

Tamara Jurina - Faculty of Food Technology and Biotechnology at University of Zagreb, Croatia

Maja Benković - Faculty of Food Technology and Biotechnology at University of Zagreb, Croatia



Near infrared spectroscopy (NIRs) found its first agricultural application 60 years ago in grain moisture measurements. NIR spectroscopy absorbs radiation at molecular vibrational frequencies occurring for the O–H, N–H, S–H, and C–H groups related to moisture, protein, and/or fat content of a wide variety of food products, bioactive compounds in foods, and food waste. Furthermore, it has the potential to detect origin (like olive oil or wines) and/or purity (as adulterated foods). This has promoted NIRs as a non-destructive, rapid tool used for scanning not only in the laboratory but as well on the spot (of breeding, sales, control). Depending on the device used, the NIR spectrum of the scanned sample results in a large set of data (absorbance at a given wavelength) and it is necessary to apply one or more multivariate (MVA) methods to extract significant data from the spectra. Data processing of NIRs spectra includes spectral pre-processing, calibration modeling, and linear/nonlinear modeling. Pretreatment is often used for reduction of noise and unwanted spectral factors that could potentially be used in the construction of calibration models. Unfortunately, pretreatment (spectrum pretreatment) is not unique and is often based on the experience of researchers. This presentation will give an example of an “inappropriate” application of the MVA and some examples of efficient application in prediction of wastewater constituents, detection of honey and butter adulterations and quantification of bioactive compounds in olive leaves. Presented MVA tools will be focused on Principal Component Analysis, Partial Least Squared Regression modeling, and Artificial Neural Network modelling.

Keywords: modeling; NIR spectroscopy; food.

Jurinjak Tušek, A., Benković, M., Malešić, E., Marić, L., Jurina, T., Gajdoš Kljusurić, J., Valinger, D., (2021) Rapid quantification of total dissolved solids, total phenolic and antioxidant activity of dried root vegetable extracts using near infrared spectroscopy. *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*. 261, 120074 <https://doi.org/10.1016/j.saa.2021.120074> Kim, S.Y., Čurko, J., Gajdoš Kljusurić, J., Matošić, M., Crnek, V., López-Vázquez, C.M., Garcia, H.A., Brdjanović, D., Valinger, D. (2021) Use of near-infrared spectroscopy on predicting wastewater constituents to facilitate the operation of a membrane bioreactor. *Chemosphere*, 272, 1298899 ISSN 0045-6535, <https://doi.org/10.1016/j.chemosphere.2021.129899> Valinger, D., Longin, L.,



Grbeš, F., Benković, M., Jurina, T., Gajdoš Kljusurić, J., Jurinjak Tusek, A. (2021) Detection of honey adulteration - the potential of UV-VIS and NIR spectroscopy coupled with multivariate analysis. *LWT - Food Science and Technology*. 145, 111316. <https://doi.org/10.1016/j.lwt.2021.111316>

Kazazić, S., Gajdoš Kljusurić, J., Radeljević, B., Plavljančić, D., Špoljarić, J., Ljubić, T., Bilić, B., Mikulec, N. (2021) Comparison of GC and NIR spectra as a rapid tool for food fraud detection – the case of butter adulteration with different fats. *Journal of Food Processing and Preservation*, 2021;00:e15732. <https://doi.org/10.1111/jfpp.15732>

Gajdoš Kljusurić, J., Jurina, T., Valinger, D., Benković, M., Jurinjak Tušek, A. (2019) NIR Spectroscopy and Management of Bioactive Components, Antioxidant Activity and Micronutrients in Fruits in Fruit Crops - Diagnosis and Management of Nutrient Constraints (ed. A. K. Srivastava & Chengxiao Hu) Elsevier. pp r. 95-110. ISBN: 978-0-12-818732-6 <https://doi.org/10.1016/B978-0-12-818732-6.00008-3>

SF2021-37116 - Overview of applications of VIS/NIR spectroscopy developed in CEOT for monitoring fruits and plants - Poster

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Ana M. Cacavo - CEOT – Centro de Eletrónica, Optoeletrónica e Telecomunicações, Universidade do Algarve

Dário Passos - CEOT – Centro de Eletrónica, Optoeletrónica e Telecomunicações, Universidade do Algarve & Departamento de Física, Faculdade de Ciências e Tecnologia, Universidade do Algarve

Andreia M. Afonso - CEOT – Centro de Eletrónica, Optoeletrónica e Telecomunicações, Universidade do Algarve & Duas Siglas, Lda.

Rosa Pires - CEOT – Centro de Eletrónica, Optoeletrónica e Telecomunicações, Universidade do Algarve

Sandra P. Cruz - CEOT – Centro de Eletrónica, Optoeletrónica e Telecomunicações, Universidade do Algarve

Jaime Martins - CEOT – Centro de Eletrónica, Optoeletrónica e Telecomunicações, Universidade do Algarve



Natália T. Marques - CEOT – Centro de Eletrónica, Optoeletrónica e Telecomunicações,
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Maria D. Antunes - MED - Instituto Mediterrâneo Para a Agricultura, Ambiente e
Desenvolvimento, Universidade do Algarve

António Brázio - Calibrafruta, Lda., Souto da Carpalhosa, Leiria-Portugal

Thomas Panagopoulos - CinTurs - Research Centre for Tourism, Sustainability and
Well-being, Universidade do Algarve

This presentation describes the applications of visible-near infrared spectroscopy, developed at CEOT, with the aim of monitoring various internal fruit quality parameters and making early detection of diseases in trees. Some of the more representative investigations are described briefly in this poster: 1. Early detection of mealybug infestation on tomato plants [1] 2. Detection of asymptomatic trees infected with Citrus Tristeza Virus through spectroscopic measurements in leaves [2] 3. Assessment in-tree of internal quality parameters of citrus: model robustness and optimal harvest date forecast [3] 4. Development of a benchtop instrument for the assessment of internal quality in fruit (in collaboration with companies Calibrafruta and MCM Systems) 5. Development of an optical module for the in-line assessment of internal quality in automated fruit sorters (in collaboration with companies Calibrafruta and MCM Systems) 6. Investigation of Deep Learning tools for the interpretation of spectroscopic data in agriculture produce [4]

Keywords: Vis/NIR spectroscopy; internal fruit quality; plant diseases; orchard monitoring.

[1] Canario, David, et al. "Detecting early mealybug infestation stages on tomato plants using optical spectroscopy." *European Journal of Horticultural Science* 82.3 (2017): 341-348. [2] Afonso, Andreia M., et al. "Identification of asymptomatic plants infected with Citrus tristeza virus from a time series of leaf spectral characteristics." *Computers and Electronics in Agriculture* 141 (2017): 340-350. [3] Cavaco, Ana M., et al. "Validation of short wave near infrared calibration models for the quality and ripening of 'Newhall' orange on tree across years and orchards." *Postharvest Biology and Technology* 141 (2018): 86-97. [4] Dário Passos, Puneet Mishra, "An automated deep



learning pipeline based on advanced optimisations for leveraging spectral classification modelling”, *Chemometrics and Intelligent Laboratory Systems*, Volume 215, 2021, 104354, <https://doi.org/10.1016/j.chemolab.2021.104354>

SF2021-37467 - Authentication of margarines and related fat-spread products by spatially offset Raman spectroscopy - Poster

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Ana María Jiménez Carvelo - Department of Analytical Chemistry, Faculty of Sciences, University of Granada

Luis Cuadros Rodríguez - Department of Analytical Chemistry, Faculty of Sciences, University of Granada

Margarine is a water-in-oil solid emulsion derived from vegetable and/or animal fats. Current EU legislation states that the designation margarine should be restricted to those products containing a fat content ranged from 80% to 90% and a milk fat content of no more than 3%. In addition, there are other related-products with fat contents less than the limits mentioned, which could be generically named as 'fat spreads' or just 'spreads' [1]. There are several commercially available types of fat-spreads and its composition depends on the country where it was produced. Recent trends in the margarine/spread market include blends of 'healthy' vegetable oils with low trans and saturated fatty acid contents (for example, high-oleic sunflower, canola or olive), as well as the addition of plant sterols. For other hand, nowadays, there is great concern among the consumers regarding the fat content of foods. Foods with a low fat content are increasingly sought after. Therefore, within the category of spreadable fats, such as butter or margarine, a wide variety of these products are available [2,3]. The question is whether these products actually contain the percentage of fat that is stated on the label. Currently, the official gravimetric method requires fat extraction after an acid hydrolysis step. This is a destructive method and there is no other officially recognized method for measuring this content without the need to handle the sample. Therefore, in this study is shown the application of fingerprinting methodology using spatially offset Raman spectroscopy (SORS) to develop a fast analytical method in combination with

data mining/machine learning tools to develop and perform an analytical protocol to control the quality/safety of margarines and fat-spreads from different origins (EU and non-EU) and to verify label compliance of these products.

Keywords: Spatially offset Raman spectroscopy (SORS); chemometrics and data mining; margarines and fat-spreads analysis; food quality.

[1] Regulation (EU) No 1308/2013 establishing a common organization of the markets in agricultural products, OJ02013R1308-EN-003.001-223 (consolidated version 01.08.2017), Brussels, 2017.[2] M. Arellano, I.T. Norton, P. Smith, Specialty oils and fats in margarines and low-fat spreads, in: G. Talbot (Ed.), Specialty Oils and Fats in Food and Nutrition – Properties, Processing and Applications, Woodhead Publishing / Elsevier, Cambridge, 2015, ch. 110, pp. 241–270. DOI: 10.1016/B978-1-78242-376-8.00010-7.[3] N.W.G. Young, P. Wassell, Margarines and spreads, in: G.L. Hasenhuettl, R.W. Hartel (Eds.), Food Emulsifiers and their Applications, third ed., Springer Nature, Cham, 2019, ch. 13, pp. 379–405. DOI: 10.1007/978-3-030-29187-7_13.

SF2021-38064 - An inline optic sensor technology to determine milk pH in yogurt manufacturing - Poster

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Anna Zamora Viladomiu - Universitat Autònoma de Barcelona

Isabel Achaerandio Puente - Universitat Politècnica de Catalunya

Manuel Castillo Zambudio - Universitat Autònoma de Barcelona

Accurate determination of yogurt fermentation end-point (i.e., the end of the fermentation process at pH = 4.6) is essential for yogurt manufacturing. As a result of the high complexity of milk fermentation induced by lactic acid bacteria, an inadequate fermentation end-point selection could significantly compromise manufacturing cost and the final yogurt quality. Currently, acid coagulation to produce yogurt in the industry is monitored from discontinuous pH measurements that are measured manually every 10-15 minutes, a laborious and inaccurate technique. This work evaluates an in-line optical method that allows continuous determinations to predict the pH progress



during yogurt fermentation in order to eliminating the need to take periodic samples. The method uses a NIR light backscatter probe that works at 880 nm. A pilot-scale experiment was designed with five replicates to study the effects of three different levels of milk fat (0.2 g / 100 mL, 1.6 g / 100 mL, and 3.6 g / 100 mL) with a concentration of 3.7 g / 100 mL protein in yogurt fermentation at 43 °C. The results showed that the optical sensor technology was suitable for inline monitoring of yogurt acidification. The inline optical pH prediction models were successfully validated with standard error of prediction values of 0.004, 0.001 and 0.006 pH units and coefficients of variation of 0.086, 0.021 and 0.123% for skimmed, semi-skimmed and whole milk, respectively. Continuous, pilot plant validation of the prediction model improved the results of previous lab-scale work. It can therefore be said that the method seems to have a promising future at the industrial level by facilitating the monitoring of the yoghurt fermentation process.

Keywords: pH, inline, monitoring, optic sensor.

The abstract does not contain any literature reference. I have included a short BIO.Dr. Castillo joined the Universitat Autònoma de Barcelona (UAB) as Associate Professor of Food Processing in 2009, where he has been recently promoted to Full Professor. He came from the University of Kentucky (UK) where he was Assistant Research Professor (Biosystems & Agricultural Engineering, BAE). Professor Castillo's research program focuses on the development of optical sensor technologies for food process control. Summarized scientific production track-record is as follows: Funded projects–37 (21 as PI); Competitive research funds received–2.5 million €; US Patents–2; EU patents – 1; EU patents under review–1; patent pre-evaluations -6; publications -321 (Refereed articles–73; Book chapters–5; Non-refereed articles–17; Conference papers–60; Presentations at conferences –oral & posters–166); Students advised–44 (6 postdoc, 10 PhD., 19 MS, and 9 TFG); International visiting scholars–22; Interns/part time employees–51; Presentations/invited conferences–35; International professors invited–18. His outstanding scientific contribution in the chemical and engineering sector of dairy products processing has been recognized with two prestigious international awards in the US (IDFA Research Award in Dairy Food Processing -ADSA, 2008- and Samuel Cate Prescott Award for Research –IFT, 2009-).

SF2021-39571 - A NMR-based foodomic approach to study Parmigiano Reggiano PDO cheese certification “Prodotto di Montagna Progetto Territorio” - Oral Presentation

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P. Becchi - Dept. Chemical and Geological Sciences, Università di Modena e Reggio Emilia (IT)

S. Michelini - Consorzio del Formaggio Parmigiano Reggiano, RE (IT)

V. Pizzamiglio - Consorzio del Formaggio Parmigiano Reggiano, RE (IT)

F. Savorani - Dept. Applied Science and Technology (DISAT), Politecnico di Torino (IT)

M. Cocchi - Dept. Chemical and Geological Sciences, Università di Modena e Reggio Emilia (IT)

The feeding system represents one of the main factors driving hard-cheese composition, thus determining differences in nutritional value and characteristic properties. The Parmigiano Reggiano PDO certification “Prodotto di Montagna Progetto Territorio” establishes an additional and more stringent quality assessment [1] with respect to the legal requirements for mountain products, as ruled by Reg. UE 1151/2012. This high added value product plays an important role in supporting the sustainability of the mountain areas where it is produced, offering revenue opportunities for local economy. It is thus of great interest to investigate the identity traits of the product to support the quality label and, on the other hand, to develop an analytical methodology to assess its authenticity. In this preliminary study, a comprehensive NMR-based foodomic approach was used to investigate the compositional profile of the Parmigiano Reggiano “Prodotto di Montagna Progetto Territorio” in comparison with conventional Parmigiano Reggiano PDO. NMR spectroscopy can detect low-molecular weight metabolites which may bring valuable information useful to reveal differences between the two denominations. In this study, a traditional full-spectra analysis was first carried out and the capability of distinguishing the two categories was assessed; then, the focus was moved to metabolites identification by using a Multivariate Curve Resolution (MCR) interval-based procedure [2] aimed at resolving and extracting chemical features from



the spectra. These features were then joined in a new dataset and analysed, comparing the obtained results with the traditional approach. The resolved features were also compared with the NMR profiles provided by the spectral reference library of Chenomx NMR Suite, with the goal of validating the signal assignments. Parmigiano Reggiano “Prodotto di Montagna Progetto Territorio” samples resulted well differentiated with respect to conventional Parmigiano Reggiano PDO samples, in terms of amino acids and oligopeptides content, which are the markers showing the highest discrimination potential.

Keywords: mountain product; foodomics; ¹H-NMR; MCR.

<https://www.parmigianoreggiano.com/product-guide-seals-and-marks#5> (last accessed 22/07/2021)². Winning, H.; Larsen, F.H.; Bro, R.; Engelsen, S.B. Quantitative analysis of NMR spectra with chemometrics. *J. Magn. Reson.* 497 2008, 190, 26–32, doi:10.1016/j.jmr.2007.10.005.

SF2021-42192 - Keep it simple, stupid: photonics for industry and research, two worlds apart - Oral Presentation

Yannick Weesepeel - Wageningen Food Safety Research

Martin Alewijn - Wageningen Food Safety Research

Judith Müller-Maatsch - Wageningen Food Safety Research

Saskia van Ruth - Wageningen Food Safety Research, Wageningen University, Queens University Belfast

New photonic sensing concepts for agro-food are popping up here, there and everywhere for application in industry and research. Interestingly, both areas seem to have different philosophies in the sense of the required technological complexity of the solutions developed. Nevertheless, as movie director Denis Villeneuve stated: “In contradiction and paradox, one can find truth”. In industry, increasingly cheaper photonic sensors with customized housing are being developed. Therefore, these applications are driven by commercial interest and rely on proven technologies like fluorescence, UV-visible or narrow-range near-infrared sensing.



Here, the intended applications are mainly defined spots in a production chain for a single product and a single analyte with high sample throughput and simple multivariate statistic solutions. A major drawback here is that the system is only designed for a limited set of analytes and possible product defects, at relatively high abundance or concentration. A specific spectral database needs to be developed for each application and analyte, ramping up development costs. In research the opposite development is visible: the concept of a universally applicable photonic sensor is seen as the holy grail. This 'sensorem omnimodus' is equipped with the utmost wide wavelength range detectors or imagers (i.e. UV to far IR) and have an array of different light sources enabling orthogonal sensing (i.e. fluorescence). These hyphenated sensors combined with a suitable data-fusion approach result in a wider application in detectable analytes and concentration range. Motivators for this strategy are that spectral databases can be built in a more 'sustainable' way and tackle the complexity of the food product market. A drawback is that such sensors are complicated to construct at higher costs and will more easily suffer from technical difficulties. Therefore, we deconstruct and explain these apparently incompatible interests and explore where both sides need each other by using recent examples from both sides.

Keywords: industry application, universal sensor.

Yannick Weesepeel studied food science and graduated from Wageningen University in 2014. He works since 2014 at WFSR, Institute of Food Safety as a project manager and researcher in the team Authenticity and Nutrients. He is primarily involved in test-casing and developing hand-held, low-cost optical devices for food safety and food authenticity cases. Furthermore, he works on projects where next-generation optical devices are developed. Current research activities on food authenticity and fraud are based on Weesepeel's involvement in EU-PhasmaFOOD where a next-generation optical device is developed, tested and validated for food safety and authenticity applications. Next to that, he is involved in developing next-generation optical devices for edible oil authentication in collaboration with the industry. Other projects, concerning food authentication and adjacent areas comprise, imaging methods (RGB, multi/hyperspectral) for tuna authenticity and estimation, usage of low-cost scanners for assessment of forbidden substances and developing tools to estimate total food intake.

SF2021-42799 - A secure and integrated platform for acquisition, storage, visualization, and analysis of spectral data - Poster

Abhilash Nair - DOSCON AS

Harsha Ratnaweera - Norwegian University of Life Sciences

The ubiquity of internet-enabled devices and low-powered communication hardware has encouraged researchers and engineers to adopt real-time monitoring rather than offline data collection. Several commercial and open-source components, available in today's market, can be used to set up stations for real-time spectral data acquisition. The multitude of physical components, incompatible communication protocols, and lack of standardization (for both hardware and software) pose a significant challenge in system integration. This work presents a secure, integrated, and user-friendly digital platform for storage, real-time analysis, and visualization of spectral data. The digital platform also provides an integrated module to deploy AI and ML algorithms, written in commonly used scientific programming languages such as Python or MATLAB. The system performance is demonstrated with a case study where several water-quality parameters are estimated in real-time using scanning UV-Vis spectral data.

Keywords: IoT, realtime monitoring, scanning UV-Vis.

Nair, A. M., Hykkerud, A., and Ratnaweera, H. (2020). A Cost-Effective IoT Strategy for Remote Deployment of Soft Sensors - A Case Study on Implementing a Soft Sensor in a Multistage MBBR Plant. *Water Science and Technology*. 81(8), 1733–1739. doi:10.2166/wst.2020.067. Carreres-Prieto, D., García, J.T., Cerdán-Cartagena, F. and Suardiaz-Muro, J. (2020). Wastewater Quality Estimation Through Spectrophotometry-Based Statistical Models. *Sensors*, 20 (19), 5631. doi:10.3390/s20195631. Guo, Y., Liu, C., Ye, R. and Duan Q. 2020. Advances on Water Quality Detection by UV-Vis Spectroscopy. *Applied Sciences*, 10(19), 6874. doi:10.3390/app10196874.

SF2021-45397 - In-situ determination of the fatty acid profile of in-shell and shelled almonds using a handheld NIRS sensor - Poster

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María-Teresa Sánchez - Department of Bromatology and Food Technology, ETSIAM, University of Cordoba, Campus of Rabanales, 14071 Córdoba, Spain.

Irina Torres - Department of Animal Production, ETSIAM, University of Cordoba, Campus of Rabanales, 14071 Córdoba, Spain.

José-Antonio Entrenas - Department of Animal Production, ETSIAM, University of Cordoba, Campus of Rabanales, 14071 Córdoba, Spain.

Dolores Pérez-Marín - Department of Animal Production, ETSIAM, University of Cordoba, Campus of Rabanales, 14071 Córdoba, Spain.

Lipids are one of the major compounds in almond kernels and are related to their nutritional quality. In addition, the fatty acid composition of almonds can provide information on the state of the fruits and their shelf-life. This work sought to offer an alternative non-destructive technique to measure in-situ the fatty acid composition of almonds when the product is received by the industry and during the postharvest storage. For this purpose, 135 in-shell and shelled almond samples collected during the 2018-2019 harvesting season and belonging to different cultivars, were analysed in static and dynamic modes using a handheld near infrared (NIR) spectroscopy sensor. The NIR instrument used is based on the diode array technology and works in reflectance mode in the spectral range 950 – 1650 nm. To predict the fatty acid content, in particular the composition in palmitic, stearic, oleic and linoleic acids, modified partial least squares regression models were developed using NIR spectra with different combinations of signal pre-treatments (derivative and scatter correction methods). The results obtained confirmed that NIR spectroscopy is a suitable alternative to measure the fatty acid profile both in in-shell and shelled almonds in different steps of the food supply chain.

Keywords: In-shell and shelled almonds; Shelf life and nutritional quality; Handheld NIRS sensor; In-situ analysis.

Fernández-Cuesta, Á., Fernández-Martínez, J. M., Socias i Company, R., Velasco, L. 2013. Near-infrared spectroscopy for analysis of oil content and fatty acid profile in almond flour. *European Journal of Lipid Science and Technology*, 115, 211–216.

SF2021-46098 - Use of a pocket-sized NIR device to determine fatty acid composition of pork bellies - Poster

Michela Albano - IRTA

Josep Comaposada - IRTA

Albert Brun - IRTA

Joel González - IRTA

Cristina Zomeño - IRTA

Begonya Marcos - IRTA

Juan Florencio Tejeda - UEX

Marina Gispert - IRTA

Maria Font-i-Furnols - IRTA

Belly is an important cut from pig carcasses. Its quality is mainly defined by its firmness, which depends on the amount and composition of the fat tissue. Thus, the determination of fatty acid composition in pork belly would be essential for defining its technological, sensory and nutritional quality. The aim of the present work is to evaluate the use of a portable NIR device to determine the fatty acid composition of pork bellies. For this purpose, 137 bellies from pigs differing in their origin, diet, genotype and sex, have been collected in order to ensure a great variability in their fat content and fatty acid profile. Fat content was determined with computed tomography device (HiSpeed Zx/I, GE, Spain). The subcutaneous fat from the central part of the belly was measured with a NIR SCIO 2.0 sensor (Consumer Physics, Hod HaSharon, Israel). Five spectrums were obtained for each belly at 1 nm interval over the spectral range 740 and 1070 nm. A Samsung Galaxy Core Prime phone with Android 5.1.1. software was connected via Bluetooth to the sensor. A fat sample from the same region was analyzed by gas chromatography (Sandler and Karo, 1992) to determine its fatty acid composition. Spectra were analyzed with the Lab for SCIO software, pre-processed (SNV and 1st Derivative) and averaged for each belly. Prediction equations were obtained applying a PLS regression. Bellies had a fat content of 54.3±15.1%. Regarding fatty acid composition, bellies had a 36.0±2.3% of saturated (SFA), a 50.2±3.0% of monounsaturated (MUFA) and a 13.9±3.1% of polyunsaturated (PUFA) fatty acids. Prediction equations had a RMSE of 1.4, 1.7 and 1.5% and a R² of 0.62, 0.64, 0.78 for

SFA, MUFA and PUFA, respectively. Other data pre-treatment or spectral range selection is needed to improve the accuracy of the prediction. Financial Support: RTI2018-096993-B-I00(BellyQTech)

Keywords: firmness, fatness, portable device, online measurements.

Sandler, S.R.; Karo, W. Source book of Advanced Organic Laboratory Preparations; Academic Press: Cambridge, MA, USA, 1992; ISBN 0126185069.

SF2021-46581 - Evaluation of spectral handheld devices for assessing fish freshness and quality in comparison with standard methods and non-targeted metabolomics - Poster

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Fish is a highly perishable food commodity and therefore, freshness is a key element in the assessment of fish quality. To date, there are many different tools available to characterize freshness. These techniques are based on sensory, physical, chemical and microbiological methods [1-5]. However, these methods are time-consuming, retrospective and expensive. These limitations have initiated an interest in Near Infrared (NIR) spectroscopy approaches for assessing fish freshness and quality and now the focus lies on the application of portable and handheld devices. Analysis with this technique is rapid, non-destructive and comparatively low in cost. Additionally, no chemical reagents and sample preparation are required and several analytes can be determined simultaneously [6]. The current study investigated the potential of three different handheld NIR spectrometers (TellSpec, SCiO, MicroNIR) to monitor freshness of Austrian organic carp and trout fillets after 1, 3, 6 and 9 days of storage at +4 °C. Discriminant and class modelling approaches (OPLS-DA and DD-SIMCA) were used to determine which device provides the best classification abilities. Furthermore, the fish were analyzed with commonly used methods and non-targeted metabolomics by

dynamic headspace - gas chromatography - time-of-flight mass spectrometry (DHS/GC-TOFMS). The results from the different methods were correlated with the NIR data in order to be able to better understand and interpret the obtained spectra and by using only the highly correlated wavelengths some chemometric models could be improved. Within this study, handheld NIR spectrometers could discriminate carp fillets according to its age with high sensitivity and specificity. However, for trout samples, both classifications methods did not lead to satisfactory model performance. It has been proven that NIR handheld technologies can be a useful tool for fish quality assessment, especially for screening processes. For more accurate results, confirmatory analysis based on one of the commonly used spoilage indicators is required.

Keywords: fish freshness; NIR; handheld spectrometer; multivariate data analysis.

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SF2021-49304 - Stimuli Responsive Polymeric-Materials as Sensing Platforms - Poster

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Mihai Brebu - "Petru Poni" Institute of Macromolecular Chemistry, Romanian Academy

Food spoilage occurs mainly under microbiological action that significantly decreases the shelf-life of foodstuffs and can negatively impact the human health if not properly addressed. Oxidation, which among others induces alteration of flavor and color, vitamin degradation and lipid rancidity, is also a common process occurring in food spoilage. Therefore, the new trend in fighting against food spoilage is to include antimicrobial and antioxidant agents into food packaging materials. Products derived from plants that are rich in bioactive compounds can induce antimicrobial and antioxidant properties. However, most bioactive compounds have limited stability in the

presence of environmental factors, undergoing processes such as volatilization, oxidation, photo- / thermal- degradation. Therefore, protection and stabilization in formulations is needed and interactions with the matrices have to be adjusted to achieve controlled release of the active principle. When a beneficial interaction between packaging, environment, and food occurs, the bioactive compound is released in a controlled manner [1]. In this regard, stimuli responsive polymeric materials gained a great attention due to their versatility in developing sensitive food packaging. Among them, pH sensitive chitosan offers many advantages as matrix for incorporating various bioactive agents ensuring the release by triggered processes [2]. In our study presents several methods for fixation of bioactive principles into polymeric materials and the evaluation of their impact on the food spoilage. Discussion will be made on various active principles, different polymeric matrices and fixation techniques. These systems could act as proactive sensing platforms for retarding food spoilage.

Keywords: responsive polymers; bioactive agents; food packaging.

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SF2021-50403 - Multivariate Control charts to monitor an industrial pesto sauce production process - Poster

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Alessandro D'Alessandro - University of Modena and Reggio Emilia, Barilla G. e R. Fratelli

Marina Cocchi - University of Modena and Reggio Emilia

Caterina Durante - University of Modena and Reggio Emilia

In the last years, food companies have been under high pressure due to the increasing of demand coupled with consumers requests for high quality, healthy and environmentally friendly products. Barilla, one of the biggest Italian food companies, pays particular attention on those topics, planning its food production processes accordingly. One of the most popular Barilla product is pesto, a typical sauce made by basil, garlic, parmesan cheese, extra-virgin olive oil and other ingredients mixed together. Basil is the most important ingredient in pesto production, as its features highly affects the quality of the sauce in terms of sensorial characteristics (taste, color, odor, etc.) [1]; for this reason, an accurate control of the very first steps of the process, where the basil plants enter in the production line, is fundamental to obtain an high quality final product. In this context, a camera was installed on one of the conveyor belts installed inside Barilla's plant, acquiring RGB images and extracting information about plants color and defects. Moreover, other parameters are monitored, such as temperature, pH and moisture, in order to have a broader pool of information for the process control and to evaluate the best process operative conditions. The main objective of the work was to assess in-line and in real time the quality of basil plants taking into account different basil suppliers, varieties and harvesting, computing PCA-based Multivariate Statistical Process Control (MSPC) charts.

Keywords: Multivariate Statistical Process Control, Basil, RGB imaging.

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SF2021-50572 - Use of Hyperspectral Imaging to Determine Protein Content in Sugar Beet Leaves - Poster

Hilmi Eriklioglu - Middle East Technical University

Ali Can Karaca - Yıldız Technical University

Mecit Öztop - Middle East Technical University



Today, valuation of byproducts is a quite important area in food industry. Effective use of discarded food parts which are considered as wastes, is beneficial for both customers and producers. It was found out that sugar beet leaves can be a good plant protein alternative and it can be a potential substitute for milk, soy and meat proteins. Protein content of the beet leaves could be affected from many factors and it is usually determined by chemical methods. Nondestructive methods that could help to determine protein content on field could be great to be used by beet sugar producers. Hyperspectral Imaging (HSI) technique could be a perfect tool for that purpose. HSI is a nondestructive and rapid spectra analysis method which gives opportunity to work with nonhomogeneous samples. HSI can cover three regions (UV-Vis-NIR) of the electromagnetic spectrum, which can be very informative on natural substance analysis for both qualitative and quantitative perspective. In this study, three different leaf samples from sugar beet were collected and their image was acquired by using a Vis-NIR hyperspectral camera covering the wavelengths from 400 nm to 1000 nm. Differences between leaf samples were observed for both visible and NIR region. This preliminary work with the integration of further calibrations and data analysis techniques shows HSI method can be used to analyze protein content of sugar beet leaves.

Keywords: Hyperspectral Imaging (HSI), Sugar Beet Leaf, Protein, Spectra, Vis-NIR.

SF2021-51561 - Recalibration as a major tool to improve Vis-NIR spectroscopy-based calibration models performance in the non-destructive assessment of 'Ortanique' ripening on-tree - Poster

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Visible-near infrared spectroscopy (Vis-NIRS) calibration models for internal quality attributes (IQA) of fruit may lack enough robustness. This means that the IQA predictions may diverge from what is expected when the fruit originates from new orchards, producers or years not included in the calibration dataset. The most recommended solution is to gather a significant set of observations, covering several years and growing conditions [1]. However, there are many reasons, namely, atypical climate conditions in a particular harvest season, which may reduce significantly any model's performance and challenge its robustness, even when properly validated. In this work, two 'Ortanique' (*Citrus reticulata* Blanco x *Citrus sinensis* (L) Osbeck) orchards were assessed throughout the harvest season, and calibration models were built for several IQA of interest in the citrus industry [2]. Calibration models were built for each orchard individually and for the two together. Predictions for the fruit of one orchard were made based on the calibration models built for the other orchard. The results varied according to the IQA under study. In particular, there was a large deviation in the predictions for the maturation Index (MI), a key parameter for the harvest decision. Two recalibration strategies were investigated in order to reduce the prediction error to an acceptable level. Recalibration involves the assessment of a small fraction of new samples by standard destructive methods. The first procedure is bias correction, which is equivalent to add to the predictions the difference between their mean and the measured mean IQA. The second procedure, called "spiking", corresponds to the introduction of the recalibration samples in the dataset and the subsequent construction of a new calibration model. The results showed that both approaches generate good



results and lower the prediction error to an acceptable level, requiring only the destructive evaluation of a few fruits.

Keywords: Algarve Citrus”; Vis-NIRS; Ripening on-tree; Models’ recalibration.

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SF2021-53501 - Identifying infant formula from different origins using imaging analysis - Poster

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Sara W. Erasmus - Food Quality and Design Group, Wageningen University and Research

Saskia M. van Ruth - Food Quality and Design Group, Wageningen University and Research

This study explored if stage one infant formula products produced in different countries have unique colour signatures. The relationship between the chemical composition and CIE L*a*b* colour values were investigated.



Single parameters indicated that there were some differences between products from different continents according to the colour signatures. Carotenoids likely influenced the b^* values, while the combined analysis of colour data and chemical composition increased the possibility of sample identification from different origins.

Keywords: colour, IRIS, Colorimeter, colorChopper.

Aprèa, E., Bergamaschi, M., Betta, E., Bovolenta, S., Romanzin, A. and Gasperi, F., Utilizzo dell'occhio elettronico per la valutazione del colore e delle occhiature di montasio prodotto in Malga, *Italian Journal of Dairy Science and Technique* 66(2015) 39-44. Ayustaningwarno, F., Fogliano, V., Verkerk, R. and Dekker, M., Surface color distribution analysis by computer vision compared to sensory testing: Vacuum fried fruits as a case study, *Food Research International* 143(2021). <https://doi.org/10.1016/j.foodres.2021.110230>BBC. "Fake baby milk formula scare hits Malaysia." Retrieved 14 December, 2017, from <https://www.bbc.com/news/business-42348254>. Boue, G., Cummins, E., Guillou, S., Antignac, J. P., Le Bizec, B. and Membre, J. M., Public health risks and benefits associated with breast milk and infant formula consumption, *Crit Rev Food Sci Nutr* 58(2018) 126-145. <https://doi.org/10.1080/10408398.2016.1138101>Briones, V. and Aguilera, J. M., Image analysis of changes in surface color of chocolate, *Food Research International* 38(2005) 87-94. <https://doi.org/10.1016/j.foodres.2004.09.002>Calderon, F., Chauveau-Duriot, B., Martin, B., Graulet, B., Doreau, M. and Noziere, P., Variations in carotenoids, vitamins A and E, and color in cow's plasma and milk during late pregnancy and the first three months of lactation, *J Dairy Sci* 90(2007) 2335-2346. <https://doi.org/10.3168/jds.2006-630>"A factory packaging fake baby formula shuts down in Spain, shocks China." Retrieved 24 April, 2018, from https://news.cgtn.com/news/3d3d414d7759444d77457a6333566d54/share_p.html. Cheng, N., Barbano, D. M. and Drake, M. A., Effect of pasteurization and fat, protein, casein to serum protein ratio, and milk temperature on milk beverage color and viscosity, *J Dairy Sci* 102(2019) 2022-2043. <https://doi.org/10.3168/jds.2018-15739>Feng, J., Liu, Y., Shi, X. and Wang, Q., Potential of hyperspectral imaging for rapid identification of true and false honeysuckle tea leaves, *Journal of Food Measurement and Characterization* 12(2018) 2184-2192. <https://doi.org/10.1007/s11694-018-9834-0>.



SF2021-56634 - Detection of Agrifood Originated Mature Bacterial Biofilms by Near Infrared Spectroscopy - Poster

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Marta Sampayo Iglesias - ASINCAR (Asociación de Investigación de Industrias Cárnicas del Principado de Asturias)

Natalia Prado Marrón - ASINCAR (Asociación de Investigación de Industrias Cárnicas del Principado de Asturias)

Martín Hervello Costas - ASINCAR (Asociación de Investigación de Industrias Cárnicas del Principado de Asturias)

Juan Díaz García - ASINCAR (Asociación de Investigación de Industrias Cárnicas del Principado de Asturias)

Felipe Lombó - Department of Functional Biology, Faculty of Medicine, University of Oviedo

Pelayo González González - ASINCAR (Asociación de Investigación de Industrias Cárnicas del Principado de Asturias)

IntroductionIn food environments, biofilm matrixes become reservoirs of bacteria and enhance their resistance to environmental stresses that are commonly encountered in food processing. Biofilms are extremely difficult to remove and control and cause enormous problems in food facilities. NIRS is suggested as a useful, rapid, and noninvasive tool for biofilm detection [1-2].
AimThis study is aimed to investigate the possibility of detection of mature biofilms by NIRS on two common food contact surface types.
Material and MethodsIn this study, a detection model for single species, mature biofilms has been developed. The studied biofilms, made of *E. coli* CECT434 and *S. enterica* CECT4594 which are commonly present bacterial species in food industry surfaces, were generated on coupon surfaces made of high density polyethylene (HDPE) and stainless steel. The biofilms were analysed by near infrared spectroscopy (NIRS) coupled with spectral pretreatment methods and chemometric classification models to detect presence/absence of biofilms. Crystal violet assay was done to cross-validate biofilm detection.



Results: The results show that it was possible to build successful classification models on mature biofilms generated by common foodborne pathogens, *E. coli* and *S. enterica* (over 88% for HDPE and over 95% for stainless steel) by aid of staining and image processing techniques. Conclusions NIRS coupled with chemometrics was found to be a promising method for biofilm detection on HDPE and stainless steel surfaces. The studies can further be extended to other surfaces and bacteria.

Keywords: NIRS, detection, agrifood, biofilm.

Rossi C, Chaves López C, Serio A, Goffredo E, Goga BTC, Paparella. A Influence of incubation conditions on biofilm formation by *Pseudomonas fluorescens* isolated from dairy products and dairy manufacturing plants. *Italian Journal of Food Safety*, 2016, 5, 57-932) Oliveira MMM, Brugnera, DF, Alves E, Piccoli RH. Biofilm Formation by *Listeria Monocytogenes* on Stainless Steel Surface and Biotransfer Potential. *Brazilian Journal of Microbiology*, 2010, 41, 97-106.

SF2021-59209 - Optimal instrument design for in-line monitoring of heterogeneous foods by NIR interaction spectroscopy - Oral Presentation

Jens Petter Wold - Nofima

Marion O'Farrell - SINTEF Digital

Jon Tschudi - SINTEF Digital

Near-infrared spectroscopy (NIRS) is widely used for in-line analysis in foods. Previously, we have developed tailor-made in-line solutions, where NIRS and hyperspectral imaging have been combined to handle rather complex samples: e.g. fat in salmon fillets, meat content in brown crabs, and protein in chicken fillets. However, NIRS has the potential to be used on even more complex samples, such as individual measurements of whole intact potatoes and whole fish at high speed. Such samples are extremely heterogeneous, are covered with skin, and optical sampling depths of 10-15 mm are required for good results. We are now developing NIRS for such applications, studying performance in process lines to bring instrumentation and applications a significant step forward. We present the results obtained by a novel prototype NIR instrument designed to probe deep into complex food samples at high speed.



The instrument is based on interaction measurements, which are done without physical contact, with a distance of approximately 20 cm between the instrument and samples. It measures rapidly, up to 50 measurements per second, and enables several interaction distances to be recorded for each measurement. An increased interaction distance generally leads to deeper optical sampling, that is, a larger share of the measured signal is from deeper regions in the samples. Examples of this will be shown for different food products. Since these small differences in optical measurement geometry influence the depth of sampling, they also largely affect accuracy of the calibration models for heterogeneous food products. Examples will be shown for in-line determination of dry matter in potatoes and fat in whole salmon, where an optimal choice of interaction distance can improve accuracy with 30% versus a less optimal distance.

Keywords: In-line NIRS, interactance, optical design, high speed.

Dr. Jens Petter Wold is a senior research scientist at Nofima AS, Norwegian Food and Fisheries Research Institute, Norway. He has a PhD in Food science and biospectroscopy from The Norwegian University of Life Sciences in Ås, Norway. He has published more than 100 scientific papers within the field of rapid and non-destructive quality assessment of foods and is specialised within fluorescence, near-infrared and Raman spectroscopy, including hyperspectral imaging. He has contributed to a successful on-line NIR hyperspectral imaging system (QVision 500) which is used worldwide for in-line food quality control. Jens Petter is now director of SFI Digital Food Quality (www.digifoods.no), a centre for research driven innovation.

SF2021-61477 - Low-cost optical system for milk coagulation monitoring - Oral Presentation

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In the Italian dairy context, D.O.P. productions (such as Grana Padano) and small dairies, where non-standardized raw milk is processed in small coagulation vats, play an important role.

These production processes are difficult to standardize and it is only the cheesemaker who establishes the timing of the process. In order to overcome these criticalities, a low cost prototype spectrometer has been realized and validated for the on-line monitoring of the milk coagulation process and the identification of the beginning of the casein gel formation (clotting time), a technological parameter on which depend the timing of the cutting. In order to realize an inexpensive tool, the optical bench of the sensor is composed of LED sources in the near infrared region and an InGaAs photodiode placed inside a probe (called phototube) for immersion in the milk. The modulation of the LED source, the acquisition and initial processing of the signal are managed by Arduino™ DUE controller. The prototype was developed with diffuse reflectance geometry that allows a use directly in the vat in contact with the coagulant mass and to easily clean the instrument. The data acquired by the microcontroller and transferred directly to PC, are related to the variation of backscattering during the process of casein micelles aggregation and subsequent formation of casein gel, the relative curve can be easily processed to identify the gelification time. The system has been validated by performing micro-coagulations on a laboratory scale monitoring in parallel the process both with the prototypal system and with a mechanical lactodynamograph and with a commercial optical system, obtaining a r^2 compared to the mechanical reference system equal to 0.86 and a cost reduction compared to the commercial optical system equal to a scale of 1:100.

Keywords: “milk coagulation”, “on-line process monitoring”, “Arduino controller”, “NIR LED”.

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SF2021-62620 - DEVELOPMENT OF NEAR INFRARED SPECTROSCOPY MODELS FOR MONITORING POLYMERIC ADHESIVES USED IN CORK INDUSTRY FOR TECHNICAL CORKS' MANUFACTURE - Poster

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C. Mariana Machado - Cork Supply Portugal

António C. S. Ferreira - Cork Supply Portugal; Universidade Católica Portuguesa - Centro de Biotecnologia e Química Fina

Polyurethane adhesives are widely used in many industries such as automotive, plastics, pharmaceutical, cork, among others. In their production, the polyol hydroxyl functional groups are cross-linked with monomeric molecules containing two or more isocyanate functional groups [1]. As far as food safety aspects are concerned, the presence of residual precursors of isocyanate groups and the possible by-products formation, such as aromatic amines, are regulated since their presence can represent a hazard for human health. Food-grade polyurethane adhesives are used in cork industry for the manufacture of the technical cork stoppers, to promote the agglomeration of cork granules [2]. Cork stoppers, used as wine closures [3], are food contact materials and should not represent a risk to human health. Therefore, control the migration of compounds from cork stoppers and/or of their constituents to wine is of great importance since the transference of unwanted substances can make it less safe for consumption. Near infrared spectroscopy is a rapid and non-destructive technique for process monitoring, which associated with chemometrics represent an accurate and reliable technique to routine quality control applications [4]. In this work, the NIR spectra of different polymeric adhesives used in the manufacture of technical corks were obtained and PCA and PLS-DA analysis were performed. The results obtained show good discrimination of the different adhesives with precision values above 90% and proportion of samples incorrectly classified below 0.1%. Therefore, the proposed model is a potential candidate for real time process control that requires rapid and reliable techniques to ensure the conformity of the product.

Keywords: Isocyanate adhesives; Near infrared spectroscopy; Chemometrics; Cork adhesives.



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SF2021-63481 - A framework for bilinear calibration transfer based on transfer levels - Oral Presentation

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Wouter Saeys - KU Leuven

The success of transferring calibration models contributes to diminishing the costs and waste involved in building models for new instruments or environments. Several methods have been proposed in the last two decades to successfully transfer models between instruments[1][2]. However, in many applications, the transferred models using state-of-the-art methods did not render models with satisfactory performance or models with highly noisy regression coefficients. We have elaborated a unified framework for transferring multivariate calibration models, defining the problem as transferring models at the level of the instrument variation and/or at the level of the Xy relationship. This framework allows to position state-of-the-art methods for calibration transfer such as (Piecewise) Direct Standardization[3], Orthogonalization[4], [5] Joint PLS[6] and more recent proposals such as Domain Invariant PLSR [7] with respect to each other in order to analyze the conditions under which they will provide a successful transfer. We present applications of calibration transfer in light of the proposed framework for agrofood studies involving handheld devices.

Keywords: Instrument variation, Xy relation, NIRS, model transfer.

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SF2021-66728 - Feasibility of near-infrared spectroscopy for the analysis of legume flours - Poster

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Iván Martínez-Martín - Higher Polytechnic School of Zamora. Universidad de Salamanca

Isabel Revilla - Higher Polytechnic School of Zamora. Universidad de Salamanca

Ana M. Vivar-Quintana - Higher Polytechnic School of Zamora. Universidad de Salamanca

In recent years there has been a growing interest in incorporating legumes into different foods through its transformation into flour.



The success of legume flours as a food ingredient depends on their functional characteristics. These properties are mainly related to proteins and complex carbohydrates such as starch, fibres, pectins and mucilages. In addition, other parameters such as water, salts, sugars and fats can affect their functionality. All these factors make it necessary to carry out a large number of analyses on the different flours in order to establish their behaviour when they are used as ingredients in other foods. NIRS technology could be a suitable technique for the research and development of a novel analytical method for the determination of both the nutritional composition and the prediction of the techno-functional properties of legume flours. In the present work, lentil, pea, chickpea and soybean flours have been analysed by near infrared spectroscopy. The NIR measurement of the flour samples was performed by using Foss NIR System equipment. The measurement was taken by the direct application of remote reflectance optic fiber. with a spectral range of between 1100-2000 nm. The spectral information identifies four characteristic absorption bands in all the legume flours analysed. The first band is located between 1150 and 1250 nm corresponding to the C-H bond (second overtone bands). The second is between 1400 and 1700 nm corresponding to the N-H and O-H bonds (first overtone bands). The third between 1700 and 1800 nm corresponding to the C-H bonds (first overtone bands). The last band is between 1900 and 2000 nm and is related to N-H and O-H bonds (combination bands). Lentil, pea and chickpea flours present very similar spectra. Soybean flour, despite presenting the same absorption bands, presents differences in all of them with the other flours analysed.

Keywords: legume flour, NIR.

Phetkhaeo, T., Klaithin, R., Theanjumol, P., Kunasakdakul, K., Thanapornpoonpong, S., Vearasilp, S. (2012). Comparison of Sample Preparation Methods on the Infected Corn Seed Detection by NIR Spectroscopy. *Journal of Natural Science*, 11, 243-249. Rambo, I., Ferreira, M.M.C., Melo, P.M., Santana, C.C., Bertuol, D.A., Rambo, M.C.D. (2020). Prediction of quality parameters of food residues using NIR spectroscopy and PLS models based on proximate analysis. *Food Science and Technology*, 40, 444-450. De Ron, A. M., Sparvoli, F., Pueyo, J. J., & Bazile, D. (2017). Editorial: Protein Crops: Food and Feed for the Future. *Frontiers in plant science*, 8, 105. <https://doi.org/10.3389/fpls.2017.00105>



Lastras, C. Revilla, I. González-Martín, M.I., Vivar-Quintana, A.M. (2021). Prediction of fatty acid and mineral composition of lentils using near infrared spectroscopy. *Journal of Food Composition and Analysis*, 102, 104023. <https://doi.org/10.1016/j.jfca.2021.104023>.

SF2021-67726 - Implementation of multivariate and machine learning algorithms in Python for quality control of virgin olive oil using near infrared spectroscopy - Poster

Maria del Mar Garrido-Cuevas - University of Cordoba

Ana Garrido-Varo - University of Cordoba

Dolores Pérez-Marín - University of Cordoba

Generally, NIRS instrumentation is accompanied by proprietary software for chemometric analysis of NIR data. Recently, some works have started to use open-source tools, such as R and Python, but the development status is still in its infancy (Dixit et al., 2015; Torniainen et al., 2020). These open-source tools offer benefits such as transparency, customization, easier access and lower cost. This work tries to generate information on the potential of the open-source Python software for the implementation of multivariate algorithms and signal pre-treatment methods for the development and validation of NIRS models applied to the prediction of the quality of olive oils. For this goal, 492 olive oil samples were analyzed in a portable NIRS Linear Variable Filter (LVF) instrument. The results obtained show that the routines developed in Python produced similar information on the predictive quality of the equation for acidity ($r^2v = 0.625$; $SEP = 0.107$) that the one obtained with WINISI ($r^2v = 0.714$; $SEP = 0.080$), a very common software in NIRS analysis of agri-food products. The differences found between the prediction statistics could be attributed to different strategies for the detection and elimination of outliers.

Keywords: Near infrared spectroscopy (NIRS), Virgin Olive Oil (VOO), Python, PLS regression.

Dixit, Yash & Casado, Maria & Cama-Moncunill, Raquel & Cullen, P.J & Sullivan, Carl. (2015). Near Infrared Data Analysis Using R : Live Streaming Graph Generation and Processed Data Visualisation. *NIR news*. 26. 15-17. 10.1255/nirn.1544. Torniainen,



Jari & Afara, Isaac & Prakash, Mithilesh & Sarin, Jaakko & Stenroth, Lauri & Töyräs, Juha. (2020). Open-Source Python Module for Automated Preprocessing of Near Infrared Spectroscopic Data. *Analytica Chimica Acta*. 1108. 10.1016/j.aca.2020.02.030.

SF2021-70616 - Evaluation of an FT-NIR transreflectance probe for predicting protein and lactose contents in milk protein concentrate - Poster

Yuanyuan Pu - Food Chemistry and Technology Department, Teagasc Food Research Centre, Moorepark, Fermoy, Co. Cork, Ireland

Dolores Pérez Marín - Faculty of Agriculture & Forestry Engineering, Department of Animal Production, University of Cordoba, Campus Rabanales, Ctra. Nacional IV-Km 396, 14071 Cordoba, Spain.

Norah O'Shea - Food Chemistry and Technology Department, Teagasc Food Research Centre, Moorepark, Fermoy, Co. Cork, Ireland

Ana Garrido-Varo - Faculty of Agriculture & Forestry Engineering, Department of Animal Production, University of Cordoba, Campus Rabanales, Ctra. Nacional IV-Km 396, 14071 Cordoba, Spain.

The dairy sector is one of the biggest agri-food sectors in Ireland, with 85% of its total dairy outputs being exported worldwide [1]. Several government reports have stated that for the Irish dairy industry to improve its productivity and competitiveness, integration of process analytical technologies (PAT) in dairy manufacturing is required [2, 3]. Project “NIR4Dairy”, is a European collaboration between University of Cordoba (Spain), Teagasc (Ireland) and a leading Irish dairy company. The main aim of the project is to evaluate an emerging in-line NIR sensor (a process transreflectance probe connected to a multiplexed FT-NIR spectrometer) in a milk processing plant. Milk protein concentrate (MPC) powder or milk protein isolate (MPI) powder, is a high-protein ingredient frequently used in the applications of infant nutrition, protein-fortified foods and, weight management products. A prediction model for “real time” monitoring of lactose and protein in MPC post membrane filtration is essential for ensuring an optimal process is achieved. This presentation introduces the research work currently being carried out, which includes: (1) optimization of instrument settings and



sample presentation to obtain high-quality spectra, (2) calculation of spectral repeatability limit in order to make decisions whether samples are to be re-scanned or not, (3) calibration development for quantification of lactose within a low concentration range (0.07-0.3%) in MPC. Current on-going studies include development of a protein model for MPC retentate that has a protein content ranging from 16.0% to 17.5% and a calibration transfer model between two FT-NIR instruments.

Keywords: Milk Protein Concentrate; FT-NIR Probe; Lactose; Protein.

1.Enterprise-Ireland. Dairy and Ingredients-A key part of Ireland’s food heritage, now contributing to global dairy markets. 2021; Available from: <https://www.enterprise-ireland.com/en/Start-a-Business-in-Ireland/Food-Investment-from-Outside-Ireland/Key-Sectors/Dairy-and-Ingredients/>.2.Teagasc. Teagasc Technology Foresight 2035-final report. Available from: <https://www.teagasc.ie/media/website/publications/2016/Teagasc-Technology-Foresight-Report-2035.pdf>.3.DAFM-Ireland. FoodWise 2025. 2020; Available from: <https://www.gov.ie/en/publication/a6b0d-food-wise-2025/>.

SF2021-72436 - Process Control in Flavour Generation: NIR as a tool to monitor key odorants formation - Oral Presentation

Ana Rita Moforte - Universidade Católica Portuguesa

António César da Silva Ferreira - Universidade Católica Portuguesa

Sensors suitable to monitor chemical reactions leading to the formation of potent odorants in foods and consequently enabling process control are on increasing demand. In the present work, real time kinetic analyses were made by developing new methodologies combining near infrared spectroscopy (NIR). These were applied to study the dynamics in phenylacetaldehyde formation through a number of reactions, namely (i) glucose and phenylalanine, (ii) gallic acid and phenylalanine and iii) gallic acid, phenylalanine and glucose. Phenylacetaldehyde as well as other reaction intermediaries were monitored during 60 min with a frequency for data acquisition of 3 spectra/min. A 10 minutes’ reaction intervals samples were collected and target analysis was performed using mass spectroscopy.



For comparison, the spectral data were analyzed in a conventional way fitting kinetics for specific wavelengths, and then by multivariate alternative least squares (MCR-ALS) method for modelling spectral data with quantification of reaction compounds, and perform deconvolution of spectral data. The method developed allows to unlock chemical information related with specific compounds present in the reaction. Different reaction rates were observed according to the perturbation, i.e. metals addition, temperature increasing and substrate class. A database for feature comparison has been developed to classify each new set of “individuals” taking into account their ability to form potent odorants. In conclusion, the method allows for a real time, high-throughput and low-cost analysis for process monitoring.

Keywords: NIR, FLAVOUR, AROMA.

SF2021-72456 - Near infrared spectral sensors for fraud detection in the almond industry - Oral Presentation

Irina Torres - ETSIAM, University of Córdoba

María-Teresa Sánchez² - ETSIAM, University of Córdoba

Miguel Vega-Castellote - ETSIAM, University of Córdoba

José-Antonio Entrenas - ETSIAM, University of Córdoba

Dolores Pérez-Marín - ETSIAM, University of Córdoba

Nowadays, one of the common frauds the almond industry faces is the presence of bitter almonds in sweet almonds batches. In this sense, this research group has carried out an extensive research aimed to provide the producers and the industry with a non-destructive technology, such as the Near Infrared Spectroscopy (NIRS), to detect adulterated almond batches. Thus, the main goal of this research was to assess the potential of near infrared (NIR) sensors to be implemented at the key steps in the industry for the instantaneous detection of adulterated sweet almond batches. These research works carried out were focused on the amygdalin content quantification, the detection of bitter almonds along the industrial process and the identification of non-compliance sweet almond batches. For this purpose, sweet and non-sweet – including bitter almonds and mixtures - almond batches were analysed using three NIR instruments with different features and optical designs: the Aurora and the



MicroNIR™ Pro 1700, suitable for the analysis in situ, and the Matrix-F for the implementation online. Different chemometric treatments were applied, such as Partial Least Squares, Partial Least Squares Discriminant Analysis and Shewhart control charts. The results confirmed that NIRS technology could be an extremely useful tool for the non-destructive identification of adulterated sweet almond batches in the processing industry, both on receipt and on the sorting lines, ensuring to the industry the integrity of the almond batches processed. It must be stressed that the NIRS instrumental development and evolution, based on a new generation of sensors, which combine reduced size, portability, robustness and stability, have been essential to obtain these achievements.

Keywords: Almond batches; bitter almond detection; NIRS portable sensors; online almond authentication.

SF2021-73292 - Towards Online Quality Monitoring of Chocolate Spread - Poster

Alexandros Xanthopoulos - Catholic University of Portugal

António César Silva Ferreira - Catholic University of Portugal

Cacao spreads are products of major significance in the global food market, formulated to fulfil the pleasure expectations of consumers. Despite being considered stable, the temperature conditions through long distribution and storage periods may cause negative alterations in their organoleptic characteristics. Until now, any quality degradation which occurs after the packaging is impossible to be detected unless the product is destroyed and analysed by sensory evaluation specialists. This study investigates the feasibility of substituting the traditional sensory analysis with a spectrometric device. In that direction, a data-driven approach was adopted and the results of sensory evaluation on thermally degraded samples were used for the calibration of spectroscopic data. Three cacao spreads underwent thermal treatment, for 5-time intervals. The samples were separated into 2 independent sets (calibration and validation) and for the validation set a fourth product was added. Ten experienced but not trained assessors evaluated the products according to their preference and ranked the degraded samples according to the perceived level of quality deterioration from



consumer's perspective. Except for the quantitative results, the assessors also declared the qualitative attributes of degradation which pointed at rheological alterations, fat oxidation and Maillard reactions. NIR spectroscopic data were received directly from the bottom of the sample container without any product invasion. The measurements on the same samples demonstrated satisfactory repeatability and PCA showed excellent decomposition. PLSR models were developed for each product. Furthermore, a "universal" PLSDA model were developed in order to classify the samples into "good" or "bad" quality. The results demonstrated excellent sensitivity, however, the model's robustness is in doubt due to the low amount of data. The study concludes that the concept of using spectroscopic devices for real-time instrumental sensory evaluation is feasible, however, additional sensory and NIRS data is needed for further model enrichment and development.

Keywords: NIRS, chocolate, chemometrics, sensory.

Biancolillo A, Preys S, Gaci B, Le-Quere JL, Laboure H, Deuscher Z, et al. Multi-block classification of chocolate and cocoa samples into sensory poles. *Food Chem.* 2021;340:127904. Cen H, He Y. Theory and application of near infrared reflectance spectroscopy in determination of food quality. *Trends in Food Science & Technology.* 2007;18(2):72-83. Chapman J, Elbourne A, Truong VK, Newman L, Gangadoo S, Rajapaksha Pathirannahalage P, et al. Sensomics - From conventional to functional NIR spectroscopy - Shining light over the aroma and taste of foods. *Trends in Food Science & Technology.* 2019;91:274-81. Davis AMC, Franklin JG, Grant A, N.M. G, Shepherd R, Fenwick GR. Prediction of chocolate quality from near-infrared spectroscopic measurements of the raw cocoa beans. *Vibrational Spectroscopy.* 1991;2:161-72. Giusti AM, Bignetti E, Cannella C. Exploring New Frontiers in Total Food Quality Definition and Assessment: From Chemical to Neurochemical Properties. *Food and Bioprocess Technology.* 2007;1(2):130-42. Gunaratne TM, Gonzalez Viejo C, Gunaratne NM, Torrico DD, Dunshea FR, Fuentes S. Chocolate Quality Assessment Based on Chemical Fingerprinting Using Near Infra-red and Machine Learning Modeling. *Foods.* 2019;8(10). Lemarcq V, Van de Walle D, Monterde V, Sioriki E, Dewettinck K. Assessing the flavor of cocoa liquor and chocolate through instrumental and sensory analysis: a critical review. *Critical Reviews in Food Science and Nutrition.* 2021:1-17.



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SF2021-74655 - Exploring Deep learning as a tool to enhance Chemometrics and analysis of VIS-NIR spectra of agriculture produce - Poster

Dário Passos - CEOT—Center for Electronics, Optoelectronics and Telecommunications, University of Algarve, Portugal & Physics Department, Universidade do Algarve, Portugal

Puneet Mishra - Wageningen Food and Biobased Research, Wageningen, the Netherlands

Jaime Martins - CEOT—Center for Electronics, Optoelectronics and Telecommunications, University of Algarve, Portugal

Rui Guerra - CEOT—Center for Electronics, Optoelectronics and Telecommunications, University of Algarve, Portugal & Physics Department, Universidade do Algarve, Portugal

Non-destructive food quality assessment is becoming more and more common due to the improvement of small hand-held spectrometers and machine learning modelling. Over the last 6 years, Deep Learning’s (DL) popularity has been rising meteorically due to its successful applications in the fields of computer vision and natural language processing. This research boost has enabled a large community of models and APIs that are now started to be absorbed by other research fields, such as Physics and Chemistry. The main goal of the present project is to explore the potential of DL methodologies in the areas of Chemometrics and Vis-NIR Spectroscopy with a special emphasis in its application to the characterization of plant biological tissues (e.g. fruit, vegetables, grain, etc.). The application of DL to spectral data analysis requires exploration of

different neural network architectures, model's interpretability techniques, quantization of the data set's size influence, etc. So far, in the areas of spectroscopy and spectral analysis, our team has explored data augmentation techniques by combining classical chemometric pre-processing methods with DL models [1], automatic DL model optimization techniques [2], calibration transfer between different spectrometers [3] and between different acquisition scenarios [4] based on DL transfer learning, and finally, fusion of different data types [5]. These initial works provided encouraging results because the DL-based models developed were able to attain state-of-the-art results in the characterization and prediction of internal quality properties of several produce (e.g. dry matter content and soluble solid content in mango fruit and pear, classification of different wheat grain species, etc). Publicly available data sets of produce spectra are not easy to find and its one of the current limitations. We try to overcome this hurdle by producing our own spectral data sets (pears, oranges and kiwi) and by establishing collaborations (Wageningen Food and Biobased Research, the Netherlands and the College of Biosystems Engineering and Food Science, Zhejiang University Hangzhou, China).

Keywords: Deep Learning; Chemometrics; Vis/NIR spectroscopy; Transfer learning.

1. Puneet Mishra, Dário Passos, "A synergistic use of chemometrics and deep learning improved the predictive performance of near-infrared spectroscopy models for dry matter prediction in mango fruit", *Chemometrics and Intelligent Laboratory Systems*, Volume 212, 2021, 104287, <https://doi.org/10.1016/j.chemolab.2021.104287>.
2. Dário Passos, Puneet Mishra, "An automated deep learning pipeline based on advanced optimisations for leveraging spectral classification modelling", *Chemometrics and Intelligent Laboratory Systems*, Volume 215, 2021, 104354, <https://doi.org/10.1016/j.chemolab.2021.104354>
3. Puneet Mishra, Dário Passos, "Deep calibration transfer: Transferring deep learning models between infrared spectroscopy instruments", *Infrared Physics & Technology*, 2021, 103863, <https://doi.org/10.1016/j.infrared.2021.103863>
4. Puneet Mishra, Dário Passos, "Realizing transfer learning for updating deep learning models of spectral data to be used in new scenarios", *Chemometrics and Intelligent Laboratory Systems*, Volume 212, 2021, 104283, <https://doi.org/10.1016/j.chemolab.2021.104283>
5. Puneet Mishra, Dário Passos, "Deep multiblock predictive



modelling using parallel input convolutional neural networks”, *Analytica Chimica Acta*, Volume 1163, 2021, 338520, <https://doi.org/10.1016/j.aca.2021.338520>

SF2021-79770 - Prediction models of Pitaya’s shelf life using NIR and E-nose systems - Poster

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Ingrid Alves de Moraes - Universidade Estadual de Campinas (UNICAMP), São Paulo, Brazil

Douglas Fernandes Barbin - Universidade Estadual de Campinas (UNICAMP), São Paulo, Brazil

Pitaya is fruit rich in micronutrients and it has been consumed due to its benefits for health, such as improving digestion and reducing cholesterol. Its use in the industry has also been widely spread. However, the fruit short shelf life is a common problem that restrict its use (Wu et al. 2019). Electronic Nose (E-nose) is an equipment that mimics the olfactive cells of mammals that was projected to identify and classify odors (Pearce 2003). Following the same trend of non-destructive techniques, Near Infrared Spectroscopy – NIRS is based on the vibrational forces of organic chemical molecules and its interaction with the radiation of infrared spectrum (Basantia; Nollet; Kamruzzaman, 2018). Therefore, these two techniques have been proposed to predict the shelf-life of pitaya based on titratable acidity (TA). Partial Least Squares Regression (PLSR) was used to model the relationship for each of the analysis (NIRS and E-nose) with the TA of Pitaya fruit. The region responsible for the picks in the spectra was 1000 nm and 1440 nm which could be related to organic acids, which for pitaya is represented by malic acid (C₄H₆O₅). The mean reference analysis values for each day were (Day 0 (0.36 ± 0.06), Day 7 (0.22 ± 0.003), Day 14 (0.15 ± 0.012), Day 21 (0.15 ± 0.018), Day 25 (0.11 ± 0.015) g/g malic acid) that correspond to the values found in the literature 0.20 g/g malic acid (Wu et al. 2019). For the E-nose system the pre-treatment used was the mean center. It explains the selectivity towards the molecule of malic acid due to its OH group.



The analyzed PLS regression methods for NIRS and E-nose system showed good prediction models with RMSEP of 0.038 and 0.031, respectively. The use of NIRS and E-nose system combined with chemometrics can be used in the industry to distinguish the different stages of pitaya, which would facilitate the selection of these fruits to specific use and products, which includes their selection for marketplace, as well as processed products such as ice cream, jelly, and juice.

Keywords: E-nose, NIR, PLSR, Pitaya.

WU, QIXIAN. Et al. (2019). “Comparative Volatile Compounds and Primary Metabolites Profiling of Pitaya Fruit Peel after Ozone Treatment.” *Journal of the Science of Food and Agriculture* v.99 (5): 2610–21. <https://doi.org/10.1002/jsfa.9479>. BASANTIA, N. C.; NOLLET, L. M. L.; KAMRUZZAMAN, M. (2018) *Hyperspectral Imaging Analysis and Applications for Food Quality*. CRC Press, p.175-193 (Food Analysis and Properties). ALANDER, J. T. et al. (2013) A Review of Optical Nondestructive Visual and Near Infrared Methods for Food Quality and Safety. *International Journal of Spectroscopy*, v.2013, p. 1–36, 24 mar. 2013.

SF2021-81704 - Low cost NIR spectroscopy to support Agri-food in Agroecology - Poster

COUSIN philippe - Senseen

HUSSON Olivier - CIRAD

The poster will present the key measurement for Agroecology as seen as a major approach for sustainable agriculture leading to sustainable production, resilient food to climate change and final better food quality. Importance of measuring Oxydo-reduction potential (eH, Redox potential) and Ph will be presented together with new innovative method using low cost Near Infra Red scanner. Ongoing activities and success stories will be given for Cereal, rize, Wine yards.

Keywords: NIR spectroscopy, Agroecology.

Innovative measurements to drive sustainable agriculture: the agroecology case. P Cousin, D. Dumet O.Husson . M Rollet V Levavasseur ICFAE 2021 food and agriculture engineering - May 2021.



Bünemann, E. K.; Bongiorno, G.; Bai, Z.; Creamer, R. E.; De Deyn, G.; de Goede, R.; Fleskens, L.; Geissen, V.; Kuyper, T. W.; Mäder, P.; Pulleman, M.; Sukkel, W.; van Groenigen, J. W.; Brussaard, L. "Soil quality – A critical review". *Soil Biol. Biochem.* 2018, 120, 105–125, doi:10.1016/j.soilbio.2018.01.030. Van Bruggen, A. H. C.; Semenov, A. M. "In search of biological indicators for soil health and disease suppression." *Appl. Soil Ecol.* 2000, 15, 13–24, doi:10.1016/S0929-1393(00)00068-8. Moebius-Clune, B. N.; D.J., M.-C.; Gugino, B. K.; Idowu, O. J.; Schindelbeck, R. R.; Ristow, A. J.; Es, H. M. van; Thies, J. E.; Shayler, H. A.; McBride, M. B.; Kurtz, K. S. ; Wolfe, D. W.; Abawi, G. S. *Comprehensive Assessment of Soil Health Laboratory. The Cornell Framework; Edition 3.2.*; New York, 2017; ISBN 0967650763. Cardoso, E. J. B. N.; Vasconcellos, R. L. F.; Bini, D.; Miyauchi, M. Y. H.; dos Santos, C. A.; Alves, P. R. L.; de Paula, A. M.; Nakatani, A. S.; Pereira, J. de M.; Nogueira, M. A. "Soil health: Looking for suitable indicators. What should be considered to assess the effects of use and management on soil health?" *Sci. Agric.* 2013, 70, 274–289, doi:10.1590/S0103-90162013000400009. Husson, O.; Brunet, A.; Babre, D.; Charpentier, H.; Durand, M.; Sarthou, J.-P. J. "Conservation Agriculture systems alter the electrical characteristics (Eh, pH and EC) of four soil types in France". *Soil Tillage Res.* 2018, 176, 57–68, doi:10.1016/j.still.2017.11.005.

SF2021-82768 - Grana Cheese monitoring by low cost pocket size near infrared sensor - Poster

Xueping Yang - University of Padua

Giorgia Stocco - University of Parma

Paolo Berzaghi - University of Padua

Both Parmigiano Reggiano e Grana Padano PDO are semi-fat cheeses with strict rules about maximum fat content. Cheese producer must remove some cream in order to stay within the limits of fat content. Near infrared spectroscopy(NIRS) is able to monitor the cheese quality, but high cost of NIR instruments limits its use for many small producers. This study aimed to evaluate the performance of NIR calibrations to predict the quality of fresh grana cheese with a low cost pocket instrument. Grana cheese wheels (n.176) from different plants were sampled and scanned at 5 spots using a digital light processor



instrument (DLP; AlbaNir, GraiNit srl, Italy; DLP) covering the range 950-1650 nm. Samples were placed in plastic bag, frozen at -20 C till analysis. Each sample was analyzed for Moisture, Protein (Nx6.38) and Fat. Test set samples were selected by Kennard Stone algorithm, and calibration development was performed using the software R Version x64.4.1.0, based on algorithms Mathematical spectral pre-treatments included, Standard normal variate, Detrend, Savitzky-Golay (SG) first derivative with a window size of 7 point. The performance of the prediction models was evaluated by the r^2_{val} , Bias and Standard Error of Prediction (SEP), Moisture had very good prediction performances both in calibration, then confirmed also with the test set with SEP and r^2_{val} of 0.90 and 0.97 and RPD >5. For Protein and Fat calibrations had good accuracies with error below 1%, for both DM and as is basis. However, r^2_{val} of DM basis were 0.51-0.55 indicating a small range of variation of the dataset. In the future, we will have to concentrate in expanding the data sets including samples with a broader composition. In conclusion, the study shows that a low cost DLP handheld can quickly detect the quality of fresh cheese by cloud computing. The low cost would allow small producer to monitor the quality of their production improving yield and profitability.

Keywords: Cheese quality, NIR.

Da Costa Filho, Paulo Augusto, and Pascal Volery. "Broad-Based versus Specific NIRS Calibration: Determination of Total Solids in Fresh Cheese." *Analytica Chimica Acta*, vol. 544, no. 1-2 SPEC. ISS., 2005, pp. 82–88, doi:10.1016/j.aca.2005.03.022. Revilla, I., et al. "Texture Evaluation in Cheeses by NIRS Technology Employing a Fibre-Optic Probe." *Journal of Food Engineering*, vol. 92, no. 1, Elsevier Ltd, 2009, pp. 24–28, doi:10.1016/j.jfoodeng.2008.10.022.

SF2021-83218 - A long and exciting industry-university journey: the case of NIR-on line for the rendering industry - Oral Presentation

Ana Garrido- Varo - Faculty of Agriculture & Forestry Engineering. University of Cordoba. Spain

Jose A. Entrenas- de León - Faculty of Agriculture & Forestry Engineering. University of Cordoba. Spain

Maria del Mar Garrido-Cuevas - Faculty of Agriculture&Forestry Engineering.



University of Cordoba. Spain

Dolores C. Pérez-Marín - Faculty of Agriculture&Forestry Engineering. University of Cordoba. Spain

The uptake by the industry of the existing knowledge about the online NIR analysis is being much slower, compared to the acceptance of the at-line analysis. There are several reasons for this. One of them is the need to adapt the instrumentation and accessories to each process. Another one derives from the need to have specific calibrations for each desired control point, and the differences that exist even within the same agro-industrial process are well known. Lastly, but not less important is that the instrument suppliers generally do not have the capacity to offer turnkey solutions, so the implementation should be undertaken in the framework of R & D projects with the participation of the industry, instrument suppliers, and specialists in NIR and process engineering. The Research Group of the authors since 2001 has been in close collaboration with the largest Spanish rendering plant. After years of developing applications for protein and rendered animal fats, in the framework of different research projects (Garrido et al., 2005; De la Haba et al., 2006; Garrido et al., 2008), it was clearly demonstrated the feasibility of NIRS for the chemical and nutritional NIR analysis of the animal byproducts produced. That innovation in the quality control helped to the industry to expand to new markets, because of its supremacy against other rendering plants, concerning the amount and quality of the analytical information provided to the buyers. In 2010 the company expressed its willingness to explore the opportunities to implement NIRS on-line. Again after a feasibility study undertaken by the authors' group (Garrido et al., 2018), the company decided to invest in a on-line project. The history of the exciting travel realized together, for moving from at line to on line analysis in the rendering plant will be summarised in the Conference.

Keywords: At-line, on-line NR analysis, rendering, protein animal byproducts.

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SF2021-88113 - Classification of Iberian dry-cured pork shoulders according to breed and dry-curing process using NIRS technology - Poster

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The Iberian pig is an autochthonous breed from Spain which provides exceptional characteristics to its derived products due to the quantity and capacity of fat infiltration in the muscle fibres. For this reason, racial purity is a determining factor in the quality of this type of product. Thus, the hams and shoulders produced can be classified according to the purity of the breed of pig as "100% Iberian" and "75% or 50% Iberian" (crosses with Duroc). The sector is looking for non-destructive techniques such as Near Infrared Spectroscopy (NIRS) to classify pieces according to feed, breed or curing process as it is easy to use, accurate and robust and can be implemented online. In this study, NIR spectroscopy coupled to a fibre optic remote reflectance probe has been used. The analysis was performed by applying the probe directly on the fat of the tip of the piece (non-destructive sampling) as well as on slices. Spectra were recorded in the



1100-2000 nm range. The aim was to discriminate samples according to racial purity or curing process. For this purpose, samples of 60 controlled shoulders (30 from 100% Iberian acorn-fed pigs and 30 from 50% Iberian acorn-fed pigs) cured at two different temperatures were analysed. Spectral differentiation is performed using the residual RMS X method combining different scatter and mathematical treatments. After optimisation of the pre-treatment, correct classification percentages according to breed of 95% in calibration and 90% in validation were obtained using the spectra of fat, while using the spectra of slices the values were 83 and 75%. In the case of treatment, a correct classification of 73% and 75% for fat and 90% and 61% for slices was achieved for calibration and validation respectively. These preliminary conclusions will have to be confirmed by analysis of a larger number of samples.

Keywords: NIRS, breed, dry-curing process, pork shoulders.

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SF2021-89540 - Is there a possibility to differentiate beet vs cane sugar by spectrophotometric methods? - Poster

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Sucrose is a widely used food ingredient. There are two main sources that sucrose can be obtained, while sugar cane is dominating 80% of the world market 20% of sucrose is produced by using sugar beet. Although beet and cane sugar both are sucrose based, differentiation of the source of sucrose can be very difficult by chemical methods. Plant source and production processes may give different results when inspected by various spectroscopic methods like Isotope ratio-mass spectrometry (IRMS), nuclear magnetic resonance (NMR) spectrometry and different types of optical spectroscopy (UV-VIS-NIR) even though sucrose molecules are same. Differential Scanning Calorimeter has also been used for that purpose. In this study sucrose samples from both sources and nine different countries were measured for potential use of spectrophotometric techniques. Absorbances of 25% (w/w) sucrose water solutions were measured in the region 200-1380 nm and differences in spectral signatures were observed in 200-600 nm region. For statistical data analysis of obtained spectra, principal component analysis (PCA) was used. As a result of this preliminary work, it was shown that the representation of the measured spectra in the three-dimensional space of the principal components makes it possible to differentiate sources of sucrose.

Keywords: Sugar cane, sugar beet, spectroscopy, sucrose.

SF2021-89641 - HOW IS INFLUENCING PAKAGING FOOD SAFETY? - Poster

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According to some global studies a 40 percent of our food is wasted. Food is wasted at every point along the food chain: on farms and fishing boats; during processing and distribution; in retail stores and restaurants; at home; and after it enters our trash cans¹. It's a general preoccupation among the management of waste – how can it be reduced. Related with this topic, active packaging improves food organoleptic properties, extends food shelf life, and increases food safety². Active principles

contained into packaging materials can be released, either into food or headspace, in a controlled manner initiated by a trigger (pH, NH₃) developed in early stages of food spoilage aiming to prolong the self-life. The aim of this study is to produce a food quality evaluation system that can be linked with a physico – chemical trigger. The trigger can be linked to microbial, chemical, and organoleptic properties alteration of some studied foods. FTIR spectroscopy and gas chromatography will be used as laboratory methods for identification of food spoilage products. The method represents a new opportunity for food industry producers regarding the extended shelf life foods, reducing food alteration and food waste.

Keywords: food waste, extended validity, sensors, safety food.

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SF2021-89757 - Can NIR spectroscopy foster olive oil chain sustainability? -

Oral Presentation

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Thinking of sustainable development as “development that meets the needs of the present without compromising the ability of future generations to meet their own needs”, it is clear that green chemistry can play a pivotal role for sustainability of agri-food chains, by providing on-line techniques for automatic evaluation of food quality and optimization of food processes, while minimizing the use of hazardous materials, decreasing energy and water usage, and maximizing efficiency (Kirchhoff, 2005). This presentation aims at demonstrating the usefulness of NIR spectroscopy (NIRS) as a green chemistry tool in fostering olive oil chain sustainability. In particular, key applications of NIRS for olive ripening evaluation, extra virgin olive oil (EVOO) process guidance and authenticity assessment are presented. An objective and automatable method for olive maturity evaluation and the prediction of moisture, oil content, soluble solids, total phenolic content, and antioxidant activity of intact olives based on NIRS is proposed. Thirteen cultivars were harvested at different ripening stages along three years and analysed for maturity index and composition. Partial Least Squares-Discriminant Analysis (PLS-DA) classification models for olive ripening degree prediction were developed using FT-NIR spectra collected in diffuse reflectance (12,500-3,600 cm^{-1} ; 8 cm^{-1} resolution; 32 scans), reaching sensitivity and specificity of 79% and 75%, respectively. The same spectra were used to develop PLS regression models for prediction of chemical characteristics, obtaining R^2_{pred} ranging from 0.68 to 0.77, and low RMSEP values. As for EVOO authentication, FT-NIR spectra of 197 olive oil samples were collected (12,500-4,000 cm^{-1} ; 8 cm^{-1} resolution; 16 scans) and used for calculation of PLS regression models, considering the whole fatty acid ethyl esters content range (0.92-111.63 mg/kg) or a reduced range (0.92-50 mg/kg). The best models were obtained with the reduced range, reaching a R^2_{pred} of 0.85 and a RMSEP of 4.63 mg/kg. Acknowledgements: This work has been supported by AGER 2 Project (Grant n° 2016-0105).

Keywords: NIR spectroscopy; non-destructive method; olive oil; sustainability.

Kirchhoff, M.M., 2005. Promoting sustainability through green chemistry. Resources, Conservation and Recycling, 44, 237–243. doi:10.1016/j.resconrec.2005.01.003



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all participants the contribution!*



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