eman ta zabal zazu

IASIM 2024

BILBAO

IASIM
UV VIS NIR IR MS NMR um mm cm km

International Association of Spectral Imaging

6 – 10 July, 2024

2024.iasim.net

Videometer
HySpex by neo
Prediktera.
specim A Konica Minolta Company
INNO-SPEC
NEWTEC
Lightnovo
KAX Group Multivariate Analysis With Direction and Purpose
micampus residencias
International School Chemometrics 2024

Outline

Welcome to IASIM-2024

On behalf of the International Association for Spectral Imaging (IASIM), we are pleased to invite you to IASIM-2024, the ninth international conference in spectral imaging, which will take place in July 2024 in Bilbao, Spain.

The biannual IASIM conference is intended to provide a unified, open, cross-disciplinary and interactive forum for the exchange of information and ideas within the general spectral imaging community, regardless of the spectral or spatial range.

This conference will bring together speakers, contributors, attendees and exhibitors from a large variety of Scientific Communities (Food processing, pharmaceuticals, forensics, art, remote sensing, etc.) using a large variety of spectral imaging (microscopic, macroscopic or remote sensing) coupled to spectroscopic techniques (UV, visible, NIR, Mid-IR, Raman, etc). It will include three days of scientific sessions, with oral and poster presentations on spectral imaging research and applications. Pre-conference activities with several courses and workshops are also planned.

Technical sessions will include keynote presentations by invited speakers, contributed presentations, panel discussions from members of the imaging community, posters and exhibitors, promoting cross-talks and new ideas.

Paul Geladi – In Memoriam

On Saturday May 18, 2024 in Umeå, Sweden, at the age of 72, **Paul Geladi**, our Plenary Speaker at IASIM-2024, a reference for many of us, a good friend, and an outstanding person passed away suddenly.

Paul Geladi (born Belgium 1951) was Emeritus Professor in Chemometrics and still active in research projects dealing with Chemometrics, Vibrational Spectroscopy and Spectroscopic Imaging. He has a PhD in Analytical Chemistry from Antwerp University 1979. He has been teaching Experimental Design, Multivariate Data Analysis, Multivariate Calibration and Hyperspectral Imaging for a few decades. He is coauthor of three scientific books and more than 180 scientific papers. The number of citations is over 25000. He has been active in research in Seattle (WA) and Potsdam (NY), USA, Vasa, Finland, Stellenbosch, South Africa and Ås, Norway.

The IASIM scientific committee had planned several acts to honour his career and his wonderful attitude and person on Sunday 7th of July, before the cocktail hour.

Now, with a stronger reason, we will honour him, his way of seeing life and his eagerness to always have great and fantastic discussions.

Special Issue in Spectrochimica Acta A:
Molecular and Biomolecular Spectroscopy

Presenters of mature works will be encouraged to submit their manuscripts for publication in the special issue of Spectrochimica Acta: Molecular and Biomolecular Spectroscopy (IF: 4.4), subject to the normal peer review process. All details will be available on the conference website.

The submission system is ready for the special issue IASIM-2024.

The website for this journal is located at:

https://www.sciencedirect.com/journal/spectrochimica-acta-part-a-molecular-and-biomolecular-spectroscopy

To ensure that all manuscripts are correctly identified for inclusion into the special issue, it is important that **authors select VSI: IASIM-2024 Special Issue** when they reach the "Article Type" step in the submission process.

Please note that the deadlines associated with your issue will be as follows:

- Submission deadline (time by which all papers must be submitted; the system will be closed to new submissions after this date): **31 December 2024**

- Editorial/Review deadline (the time by which all papers must have received a final decision): **31 March 2025**

Committees

Scientific Committee

- **Aoife Gowen**, University College Dublin, Ireland
- **Ana Maria De Juan Capdevila**, University of Barcelona, Spain
- **Federico Marini**, University of Rome “La Sapienza”, Italy
- **Paolo Oliveri**, Department of Pharmacy, University of Genova, Italy
- **Cyril Ryckebusch**, LASIRE CNRS Université de Lille, France
- **Ludovic Duponchel**, LASIRE CNRS Université de Lille, France
- **Bosoon Park**, United States Department of Agriculture, Agricultural Research Service
- **Neal Gallagher**, Eigenvector Research, Wenatchee, WA, USA
- **Sergey Kucheryavskiy**, Aalborg University Esbjerg, Denmark
- **José Manuel Amigo Rubio**, IKERBASQUE, Department of Analytical Chemistry of the University of the Basque Country, Spain.
- **Costanza Cucci**, Institute of Applied Phyisics "Nello Carrara" IFAC-CNR, Florence, Italy
- **Michel Nieuwoudt**, Faculty of Science, Chemical Sciences, University of Auckland, New Zealand
- **Paul Williams**, Department of Food Science, Faculty of AgriSciences, Stellenbosch University, South Africa

Organizing Committee

- **José Manuel Amigo Rubio** (Chair), IKERBASQUE, Department of Analytical Chemistry of th University of the Basque Country, Spain.
- **Sergey Kucheryavskiy**, Aalborg University Esbjerg, Denmark.
- IBeA Team (Ikerkuntza eta Berrikuntza Analitikoa - Investigación e Innovación Analítica – Research and Innovation in Analytical Chemistry)


specim
A Konica Minolta Company
Advanced hyperspectral imaging solutions from VNIR to LWIR for leading-edge research and innovation.
Read more : www.specim.com


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inno-spec.de
is now part of the
Headwall Group
headwallphotonics.com
headwallphotonics.com
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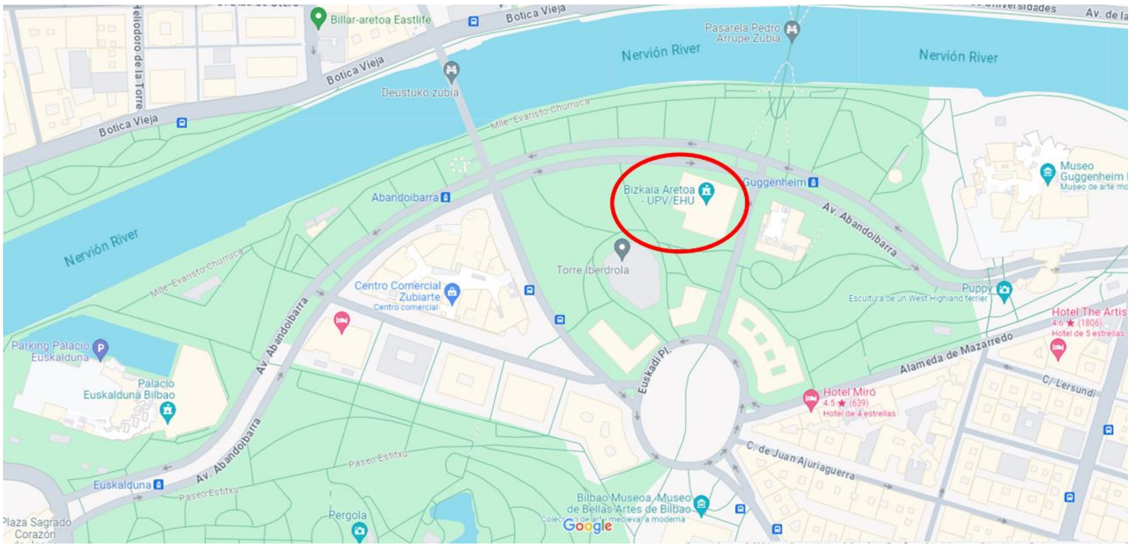
inno-spec.de
+49 911 376691-0

Venue

The conference will take place at the **Bizkaia Aretoa Building**. Kindly supported by The University of the Basque Country, this modern building is in the business center of Bilbao (**Abandoibarra Etorb., 3, 48009 Bilbo, Bizkaia**), easily reachable by bus, tram, metro and train, and surrounded by hotels, hostels and students residences.

Located five minutes walking from the emblematic **Fine Arts Museum of Bilbao** and other well-known museums, the Bizkaia Aretoa counts with more than 9000 m2 of fully prepared installations for comfortably running IASIM-2024.



The rooms assigned for the conference are:

- **MITXELENA:** Auditorium, with a capacity of more than 400 people. Conferences.

- **CHILLIDA and the terrace:** Coffee, lunch breaks and sponsor booths.

- **AXULAR:** Posters sessions.

- **BAROJA and LABOA:** Workshops.

All rooms are situated in the Bizkaia Aretoa, so there is no need to move to other locations during the conference time.

How to get to Bilbao

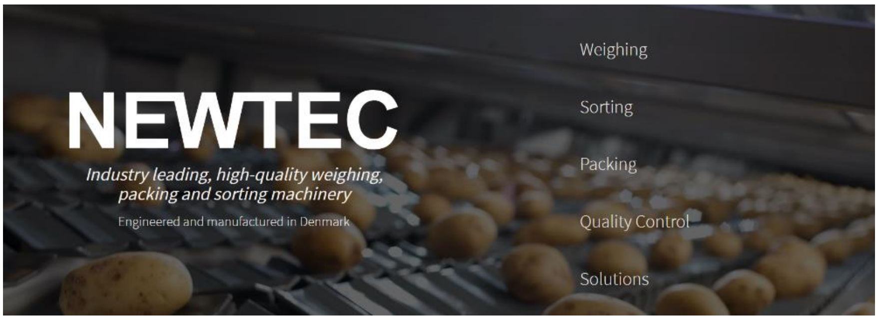
Bilbao is connected to the world through its international airport. Bilbao Airport is a day-type airport (closes from 00:00 to 05:00). But it has direct connections with the major airports in Europe (Madrid, Barcelona, Munich, Zurich, Frankfurt, Rome, etc.).

The airport is located behind the Artxanda Mountain. To get to the city, take a regular bus that departs every 30 minutes. It is around 4 euros, and the perfect occasion to buy the Barik card (3 euros that are reimbursable at your departure). You can also pay the ticket in the bus with credit card. However, if you feel tired and want to arrive directly at the hotel, a taxi ride takes around 25 minutes and costs 25-30 euros to the city center. One note, taxis are very safe! Don't worry about being cheated. Taxis are strongly regulated. Things can happen, but it is very unlikely.

Barik card

Barik is the public transportation card of Bilbao and the Bizkaia region. All public transportation (bus, trains, metro, tram, elevators, cable cars) is integrated. Therefore it is a piece of good advice to buy one upon your arrival. It can be bought (and recharged) at the city metro stations, some train stations, and Tobacco places. There is one place to buy it in the Arrivals of the Bilbao Airport. It costs 3 euros and it can be recharged whenever needed. You can return it when you leave, and the 3 euros will be returned to you.


IASIM BILBAO 2024
Meet our team at
IASIM BILBAO 2024
JULY 6–10
Let's find out together how our solutions can support your activities
Our unique solution portfolio includes:
MiniRaman
spectrometers and microscopes
Research-grade Raman
spectrometers and microscopes
Advanced Raman microscopes THOR
with polarization capacity
Lightnovo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Industry leading, high-quality weighing, packing and sorting machinery
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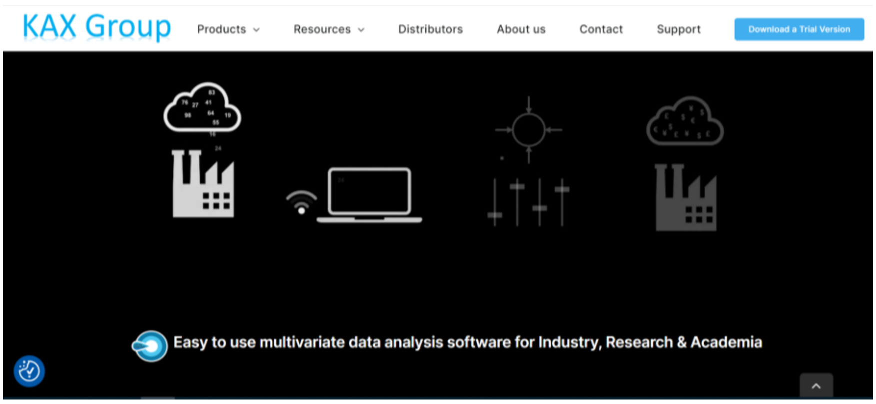
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Easy to use multivariate data analysis software for Industry, Research & Academia

Videometer A/S. Platinum Sponsor

SPECTRAL IMAGING: EXPANDING FOOD AND AGRI APPLICATIONS

Aske Schultz Carstensen[1], **Jens Michael Carstensen**[1]

[1]Videometer A/S, Hørkær 12B, 3rd, DK-2730 Herlev, Denmark

https://videometer.com/

E-mail: jmc@videometer.com

LED spectral imaging systems is a mature technology for a very rich and versatile analysis of food and agricultural products. When used together with cloud databases of images and quality traits it allows for an elegant handling of phenotypic variability as well as process variability, and machine learning models can be created, validation, updated, and deployed in an effective and efficient way. We will present examples of quality testing in seed and grain including purity, damages, and mycotoxin detection as well as examples of powder quality and food authenticity assessment.

Fig. 1. VideometerLab with autofeeder for a broad range of granular products including seed, grain, pellets, kibbles and more.

The multivariate analysis technique, normalized canonical discriminant analysis (nCDA) is used to optimize the application performance as well as to get information about the data/noise structure and importance of specific spectral ranges. The performance is illustrated on a number of real applications on contaminant detection in different materials. More examples and publications are found in [1].

References

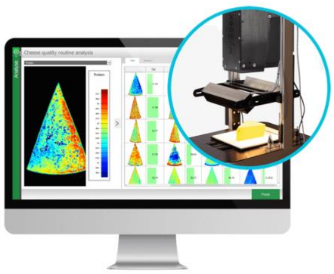
1. Videometer A/S, https://videometer.com/ (June 8, 2022)

HySpex and Prediktera AB. Platinum Sponsor

How to develop industrial applications from your research on hyperspectral imaging

Andreas Vidman, Prediktera AB
Lukasz Paluchowski, HySpex
https://www.hyspex.com/ - https://prediktera.com/
E-mail: lukas@neo.no

In this talk we will discuss the process of going from research and feasibility studies on a small scale, to an implemented full scale industrial application. Based on our experience, what are the typical challenges but also solutions, both from the aspect of the hardware; such as the camera and light source, and from the aspect of software and data processing; such as modeling, image segmentation, and integration with external process systems.



Specim. A Konica Minolta Company. Gold Sponsor

Advances and Applications of MWIR and LWIR Hyperspectral Cameras

Mathieu Marmion, PhD

Lead Application Specialist. Specim, Spectral Imaging Ltd.
mathieu.marmion@specim.com
+358 10 4244 451

The presentation will discuss the various advances and applications of the newly developed Specim MWIR and LWIR hyperspectral cameras, providing valuable insight into the capabilities of these solutions.

The capabilities of MWIR and LWIR hyperspectral camera range significantly impact both research and industry, as they can detect materials that are undetectable by other wavelengths.

The MWIR spectral range excels at detecting, for example, hydrocarbons, minerals, oil, contamination on metal surfaces, and even black plastics. LWIR hyperspectral imaging is adept at accurate mineral mapping and ordnance detection, and it can detect thermal anomalies and classify even gases.

The Specim MWIR and LWIR hyperspectral cameras utilize push-broom imaging spectrograph, with transmission grating and on-axis optics. The cameras are equipped with thermally stabilized optics and a cryogenically cooled MCT detector with a Stirling cooler.

specim

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Robust hardware and powerful software for successful industrial HSI applications

Christian Felsheim

Inno-spec (https://inno-spec.de/es/)

Join us at the inno-spec booth for a live demonstration of how to use our NIR system RedEye and the software PerClass Mira for industrial quality control.

In the past few years, HSI is becoming more widely used in industrial process analysis. Emerging fields of applications are food processing, pharmaceutical quality control, mining process control, or sorting of harvested produce. At the same time, HSI is applied to specific challenges in waste management, such as building site waste separation or textile sorting, in addition to the already mature technology of polymer recognition.

These applications require robust hardware to withstand harsh conditions, but also a reliable and flexible software to model and execute recognition and prediction algorithms for each specific implementation. The easy-to-use interface, efficient ways of model evaluation and adaption and the possibility of real-time deployment make the demonstrated software a perfect match for the ingress protected camera built for long-term 24/7 operation.

Christian Felsheim has a strong background in International Sales and Product and Business Management in Machine Vision. He joined Headwall in 2018, and after the acquisition of inno-spec into the Headwall group in 2024 is now leading the combined Sales & Product Management team.

INNO-SPEC

Lightnovo. Regular Sponsor

Optics miniaturization strategy without performance compromise for demanding Raman microscopy applications

Oleksii Ilchenko[1,2], Andrii Kutsyk[1], Yurii Pilhun[1], Danylo Komisar[1,2], Yaroslav Aulin[1,] Konstantinos Stergiou[1], Sofus Boisen[1], Anja Boisen[2]
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[2]Technical University of Denmark, Kgs. Lyngby 2800, Denmark
E-mail olil@lightnovo.com

We present a novel miniaturization strategy that allows us to create versatile compact Raman microscopes based on cheap non-stabilized laser diodes, densely-packed optics, and non-cooled small pixel size sensors. We demonstrate that the achieved performance is comparable with expensive and bulky research-grade Raman systems. Our miniaturization concept is based on real-time calibration of Raman shift and Raman intensity using a built-in reference channel that is independent of the main optical path (**Ilchenko 2024**). We have demonstrated the miniaturization of the device footprint down to 13x13 centimeters and achieved excellent sensitivity, low power consumption, perfect wavenumber and intensity calibration combined with high spectral resolution of around 7 cm-1 within the spectral range of 400-4000 cm^{-1}.

The high performance and vast versatility offered by our strategy facilitate simple integration into various applications. As examples, we show automated multiwell plate supported quantification of p-coumaric acid and Serine during fermentation by E. coli bacteria, high resolution Raman mapping, quantitative SERS mapping of the anti-cancer drug methotrexate and in-vitro bacteria identification by Raman mapping. We foresee that the proposed miniaturization strategy will allow realization of super-compact Raman spectrometers for integration in e.g. smartphones and medical devices.

References

Ilchenko 2024: Ilchenko O. et al., Optics miniaturization strategy for demanding Raman spectroscopy applications, *Nat. Commun.* (2024); In Press

NEWTEC. Regular Sponsor

The Development of a One-unit Hyperspectral Camera for VIS/SWIR

Bjarke Jørgensen

Newtec Engineering A/S, Odense, Denmark

E-mail bjarke@newtec.dk

The intention is to introduce the Oculus hyperspectral camera – a single push-broom camera covering the spectral range from 430nm to 1700nm.

Today, farmers and food producers optimize production value by sorting products based on parameters such as size, surface quality, and weight. This approach, unfortunately, only reveals information on the physical properties of the product, while valuable biochemical information, such as the content of sugar, starch, and amino acids, is not considered. Hyperspectral imaging in the Near- and Short-Wave Infrared region can reveal this type of information.

For over 25 years, Newtec has developed and produced optical sorting machines for potatoes and carrots. However, hyperspectral imaging is a versatile technique that can be utilized in fields such as biochemistry, heritage science, astronomy, plastic sorting, and geology.

Newtec is currently developing snapshot, push-broom, and plan-scanning hyperspectral cameras for Visible/Near Infrared/Short Wave Infrared (400-1700nm) and Long Wave Infrared (8-14µm). Specifically, a Long Wave Infrared Hyperspectral Camera [1], a Computed Tomography Imaging Spectrometer [2], and the Buteo, a tabletop setup equipped with Oculus and intended for research. An overview of the development process of the Oculus is provided along with stories of both success and failure.

[1] Jørgensen, A. et al. Surface temperature determination using long range thermal emission spectroscopy based on a first order scanning Fabry-Pérot interferometer, Optics Express, 2022/1/17, 30: p 2186-2196

[2] Huang, W. et al. The application of convolutional neural networks for tomographic reconstruction of hyperspectral images, Displays, 2022/9/1, p 102218

NEWTEC

KAX Group. Regular Sponsor

ImaJerI – What's in an Image?

Joonsup Lee, KAX Group, Sydney Australia.

E-mail joon@kaxgrp.com

KAX Group is an idea that became reality for its co-founders Brad Swarbrick and Rajani Davuluri in 2017. Having worked previously for a company that had a software package that was very adept at unscrambling data, they have a wealth of knowledge and experience in the field and have worked closely with some of the top companies in the world. Our flagship platform for Multivariate Data Analysis and Model Generation - VEKTOR DIREKTOR, began sales in 2019 and soon after in 2020 we released our process monitoring and control platform - ProaXesS. As a software company our partnerships with hardware manufacturers continues to grow with new instrument drivers added to our inventory each year. In 2023, ImaJerI was conceived as a plugin for VEKTOR DIREKTOR but the combined package was soon split into separate products to reduce the size of the software and began sales this year. ImaJerI incorporates the easy and intuitive user interface of VEKTOR DIREKTOR to analyse image and hyperspectral data with multivariate techniques. Currently the package includes all of the plotting and preprocessing features of VEKTOR DIREKTOR along with Image Correlation, Image PCA and Image PLS-DA at a competitive price.

KAX Group

Multivariate Analysis with Direction and Purpose

Social Event 01. Boat trip:

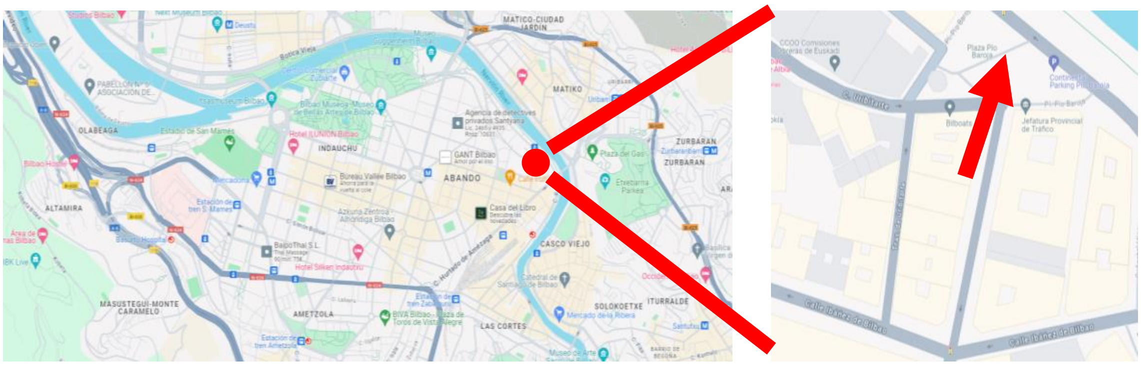
Have you looked at the IASIM-2024 logo? Look again!

At IASIM-2024 we do not want you to be lost. Therefore, our logo is a map of the iconic river of Bilbao, its bridges and the old town! This river, which is not a river but a estuarine, is crucial in the development of the city. And we want you to know it a little bit more! That is why we have thought that the best way to start IASIM-2024 is to get along with the river!

Join us for an unforgettable experience on a boat tour through the stunning Ría de Bilbao! Two vessels, hosting up to 80 passengers each, will showcase the rich history of the old Industrial, historical and modern Bilbao. As we cruise along the river, you will see iconic landmarks such as the Zubizuri Bridge, the historic Old Town and the Biscay Bridge. Highly prepared guides will provide fascinating stories, ensuring you do not miss any highlights. The comfortable seating and panoramic views will offer a perfect setting for relaxation and photography. This tour is an ideal way to start IASIM-2024 and discover the heart of Bilbao.

What should you do?

- We will meet on **Sunday 7th of July, at 13:40**, in Plaza Pio Baroja (https://www.google.es/maps/@43.2638618,-2.9257176,223m/data=!3m1!1e3?entry=ttu)(Tram stop Pio Baroja)



- Look for our logo (in our roll-up and our T-shirts) **and register**. You will be given your badge of the conference with the assigned boat number.

- Please, arrive in time to register with us! The boat will depart at 14:00!

- Enjoy!

Important:

- The trip will last 2h. Therefore, bring something to protect your head and sun protection is advisable.

- There will be a drink service on board (not included). Nevertheless, it is advisable to bring water ☺ (wine, beer and refreshment is waiting for you later in the welcome cocktail).

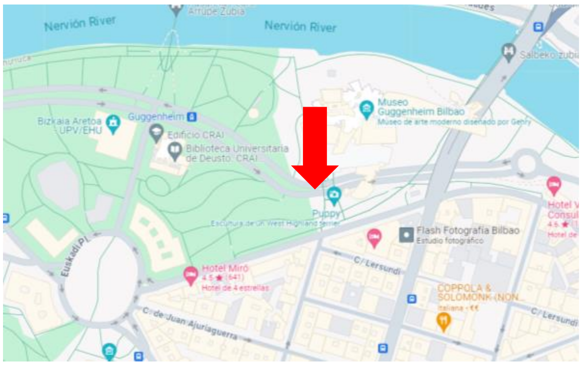
Social Event 02. Urdaibai:

Walk (or swim) in Urdaibai – Mundaka:

Urdaibai, Mundaka, and San Juan de Gaztelugatxe are three gems of the Basque Country, each offering unique and captivating experiences. Urdaibai Biosphere Reserve, a UNESCO World Heritage site, is a natural paradise with lush forests, tranquil wetlands, and diverse wildlife. This area is perfect for nature enthusiasts who can enjoy birdwatching, hiking, and kayaking in a serene and picturesque setting.

Mundaka, located within Urdaibai, is a charming coastal town renowned for its world-class surf break. Surfers from all over the globe flock to Mundaka to ride its legendary left-hand wave. The town itself is a delight, with narrow streets, traditional Basque architecture, and a lively local culture.

- We will meet at a point close to Bizkaia Aretoa on **Tuesday 9th at 16:30** to take the bus (see attached map of the meeting point - https://maps.app.goo.gl/UTCx2TCkQXoAqdcH8). There will be 4 busses waiting for us. And each one of you have an assigned bus. Therefore, be at the meeting point 10 minuntes earlier to register!



- At Mundaka, there are several options:

1) Four guides will walk you in the city and explain you the main features of Urdabai. You can join one of the groups!

2) You can go on your own: Directly to the beach or to the local bars to taste our wine.

- We will **depart for dinner at 19:30**. Be close to your bus 10 minutes earlier!

Dinner at ENEPERI restaurant:

Eneperi is a renowned restaurant offering traditional Basque cuisine with stunning views of the Bay of Biscay and San Juan de Gaztelugatxe, a small islet connected to the mainland by a narrow stone bridge and a winding staircase with over 200 steps.

Eneperi is a traditional and avant-garde cuisine blend together in a 1816 country house where guests can enjoy its restaurant, a beer house, a bar with its own pintxos as well as a museum surrounded by beautiful outdoor gardens.

We will enjoy a traditional basque dinner with local products and excellent wines from 20:00 until 23:00. Relaxing environment where the dress code only has a rule, do not be naked. Just come as you like and enjoy the company of all the IASIM-2024 people!

At 23:00 the busses will depart to Bilbao, leaving us at the Bizkaia Aretoa.

From that moment onwards until 8:30 next day… Well…

HYPER-Tools version 4

1st of October, 2024!

https://www.hypertools.org

Way faster and more interactive features!

Stand-alone / APP / code library (for analytical workflows)

More than 30 dataset! covering many scientific disciplines!

Free of charge!

Our Classics!

- Morphological, spatial and spectral preprocessing
- PCA, sPCA, fastPCA, fastsPCA, endmembers, MCR-ALS, Libraries, SAM
- Classification: SIMCA, PLS-DA, SVM, ANN
- Regression: MLR, PCR, PLS
- Analytical tools: Counting elements, highlighting shapes, etc...

New Methods!

- New preprocessing! (Cosmic spikes, baseline correction, etc)
- Fast PCA and fast sparse PCA implemented
- Target and untargeted anomaly detection

Conference program

All scientific activities will take place in the **Bizkaia Aretoa** (Abandoibarra Etorbidea, 3, 48009 Bilbo). The oral sessions will be located in the conference hall **MITXELENA**, while the poster session, exhibition, coffee and lunch-breaks in the annexed areas **CHILLIDA** and **AXULAR**. **Please wear you conference badge on during all sessions and events.**

	Sat. 6th July	Sun. 7th July
8:00	Doors Opening / Registration	
9:00	WS01	WS03
10:40	WS Coffee Break	
11:00	WS01	WS03
13:00	WS Break	
14:00	WS02	Social Event 01
15:40	WS Coffee Break	
16:00	WS02	Doors Opening Registration
17:00		Opening Hyperplenary Paul Geladi Welcome Cocktail (until 21h)
18:00	END	END

	Mon. 8th July	Tue. 9th July	Wed. 10th July
8:00	Doors Opening / Registration		
8:30	Conference Opening and Plan of the day		
8:40	Invited 01 Carolina Santos	Invited 03 Cristiane Vidal	Invited 04 Thomas Bocklitz
9:30	T0101	T0201	T0301
9:50	T0102	T0202	T0302
10:10	HySpex Prediktera	SPECIM	T0303
10:30	Coffee Break / Exhibition		
	Posters P1	Posters P1	Posters P2
11:00	T0103		T0306
11:20	T0104	T0204	T0305
11:40	T0105	T0205	T0304
12:00	T0106	T0206	T0307
12:20	NEWTEC	Kax Group	Lightnovo
12:30	Lunch Break / Exhibition / Posters		
	Posters P1	Change Posters	Posters P2
14:00	Invited 02 Jose Blasco	T0207	T0308
14:20		T0208	T0309
14:40		T0209	T0310
14:50	T0107		
15:00		INNO-SPEC	T0311
15:10	T0108		
15:20		Exhibition / Posters P2	Coffee Break Exhibition Posters P2
15:30	Videometer		
15:40			
15:50	Coffee Break Exhibition Posters P1		
			T0312
16:30			T0313
16:40	T0109	Social Event 02 Dinner (until 23h)	
16:50			T0314
17:00	T0110		
17:10			Awards IASIM-2026 Farewell
17:20	T0111		
17:30			
17:40	T0112		
18:00	Beer Break by KAX Group	END	END
20:00			

Keynote Speakers

Shedding light on Active Hyperspectral Imaging with Supercontinuum Sources

Carolina Santos Silva

Carolina obtained her PhD in Chemistry at the Federal University of Pernambuco (Brazil). She worked as a post-doctoral in the same institution (2018-2021), and at the University of Malta (2021-2022). She is a research scientist in the Optical Spectroscopy team at the VTT Technical Research Centre of Finland (since 2022). Her background includes the development of innovative analytical solutions to meet society's demands using optical sensors and chemometrics. Fields of application include forensic chemistry, food analysis, mining, etc.

How far can hyperspectral imaging uncover microplastics in the environment?

Cristiane Vidal

Cristiane is from the University of Campinas (UNICAMP), São Paulo – Brazil, where she did her Ph.D. in hyperspectral imaging combined with chemometrics for microplastic identification in beach sand, as well as for food fraud. She has a strong background in environmental analytical chemistry working as a Research Chemist for over 12 years at UNICAMP, collaborating with projects related to emerging contaminants in the environment and hyperspectral imaging acquisition and processing in many areas of study.

Photonic Data Science. The journey from vibrational spectroscopic data to knowledge

Thomas Bocklitz

Thomas studied physics at the university of Jena, and he received his Ph.D. in physical chemistry/chemometrics from the same university in 2011. In 2013 he became head of a junior research group “Statistical Modelling and Image Analysis” at the university of Jena. Since 2019 he is head of the research department “Photonic data science” at the Leibniz IPHT. His main research area is closely connected with the photonic data life cycle, which contains machine learning and chemometrics based modeling of photonic data. He has published more than 130 publications in peer reviewed journals and gave more than 50 invited talks on conferences. The work of Thomas Bocklitz was award with prestigious awards, like the Bruce Kowalski award in 2015, the Kaiser-Friedrich research-award in 2018 and the ERC Consolidator grant 2022.

Spectral measurements of agricultural products. Lights and shadows

Jose Blasco

Jose Blasco received his MSc (1994) and PhD (2001) in Computer Science at Universitat Politècnica de València. He worked for IBM Spain (1994-1996) as a system analyst before joining the Instituto Valenciano de Investigaciones Agrarias (IVIA), leading the Laboratory of Computer Vision in Agriculture. His research is focused on developing computer vision, spectral solutions, robotics, and precision agriculture applications for the agri-food sector. In 2014, he became the head of the Agricultural Engineering Centre of IVIA. Since 2012, he is charing the CIGR International Working Group on Image Analysis and Spectroscopy for Agricultural Products and Processes. He has participated in more than 40 research projects and 13 contracts with companies, obtained 8 patents, published 85 peer-reviewed, 40 extension papers, 20 book chapters and more than 180 contributions and talks at conferences. His work has received awards from the CIGR and EurAgEng.

Workshops

1. Image transformations

Sergey Kucheryavskiy

When: 6th of July, 9:00-13:00

Software needed: Python (3.10 or later), Visual Studio Code

This workshop is devoted to the basics of digital image processing — image transformations. We will start with brief overview about how digital images are represented, talk about vector and raster formats, compressions, etc. Then we will use Python notebooks and several additional packages (will install everything together on workshop) to learn how to load images, how to work with images as multidimensional arrays, how to do geometrical transformations, arithmetic transformations and convolution of digital images and, finally, how to make a chain of processing units and apply this chain to a batch of images. Most of the examples will be based using conventional RGB images, but, at the end, we will try to apply the learned skills to a hyperspectral images as well.

2. Hyperspectral and Multivariate Image Analysis

Neal B. Gallagher

When: 6th of July, 14:00-18:00

Previous knowledge needed: Principal Component Analysis (Multivariate Curve Resolution and Regression would also be useful).

Software: For those interested, instructor lead hands-on examples will be provided using [Solo + MIA_Toolbox] or [MATLAB and PLS_Toolbox + MIA_Toolbox]. Full demo versions can be downloaded at http://www.eigenvector.com/.

Hyperspectral imaging provides spatial and spectral information for an imaged sample or scene and multivariate image analysis provides tools for exploring and extracting information from measured images. After a brief introduction to hyperspectral imaging, the course will explain how images are represented in the MATLAB environment. Tools for image exploration will be introduced including principal components analysis, maximum autocorrelation factors, maximum difference factors, multivariate curve resolution and divisive cluster analysis. The course will finish by discussing decluttering and target detection. Decluttering used to enhance and refocus signals in an image, and target detection is used to detect specific analytes of interest within an image. The course content will be useful for those involved in chemical, food, forensics, pharmaceutical and medical imaging, and remote and standoff imaging.

3. Introduction to deep learning on spectral data

Artzai Picon Ruiz

When: 7th of July, 9:00-13:00

Software needed: Python (3.10 or later), Visual Studio Code

This workshop will focus on the use of Deep learning in spectral imaging. First, we will introduce the concepts of Deep learning and how it is applied to signal and spectral imaging for classification, regression or segmentation tasks. We will study which network architectures are more appropriate to each type of task and we will include concepts such as self-supervised learning and finetuning for the reduction of data requirements in these systems. We will apply what we have learned in a small use case.

Saturday, 6/07

08:00–09:00	**Doors Opening / Registration**
09:00–13:00	**WS01. Image transformations** Sergey Kucheryavskiy Baroja and Laboa Rooms
14:00–18:00	**WS02. Hyperspectral and Multivariate Image Analysis** Neal B. Gallagher Baroja and Laboa Rooms

Sunday, 7/07

08:00–09:00	**Doors Opening / Registration**
09:00–13:00	**WS03. Introduction to deep learning on spectral data** Artzai Picon Ruiz Baroja and Laboa Rooms
14:00–16:00	Social Event 01
16:00–17:00	**Doors Opening / Registration**
17:00–21:00	**Opening Honouring Paul Geladi** Welcome Cocktail (until 21h)

Monday, 8/07

7:30–8:30	**Doors Opening / Registration**
8:30–8:40	Conference Opening and Plan of the Day
	Session 1. Chair *Sergey Kucheryavskiy*
8:40–9:30 **I003**	**Shedding light on Active Hyperspectral Imaging with Supercontinuum Sources.** Carolina Santos
9:30–9:50 **T0101**	**A072. A direct comparison of a next generation hyperspectral camera to state-of-the-art** Martin Henriksen
9:50–10:10 **T0102**	**A052. Comparison of portable and bench-top spectrometers for short wave infrared reflectance measurements of soils and leaves** Giuseppe Capobianco
10:10–10:30	**Platinum 1. HySpex / Prediktera** **How to develop industrial applications from your research on hyperspectral imaging** Andreas Vidman, Lukasz Paluchowski.
10:30–11:00	**Coffee break / Exhibition** **Posters P1**
	Session 2. Chair *Cristiane Vidal*
11:00–11:20 **T0103**	**A150. MIR and NIR Hyperspectral imaging for food quality control** Federico Marini
11:20–11:40 **T0104**	**A058. Detection of Listeria monocytogenes on beef meat with NIR hyperspectral imaging** Rumbidzai Matenda
11:40–12:00 **T0105**	**A030. Cost efficient training of deep learning models for detection of contaminating grains in bulk oats** Emma Van Puyenbroeck
12:00–12:20 **T0106**	**A028. Detection of apple mouldy core and prediction of mycotoxin contamination using hyperspectral imaging** María Agustina Pavicich
12:20–12:30	**Regular 1. NEWTEC**
12:30–14:00	**Lunch Break / Exhibition** **Posters P1**

Session 3. Chair *Federico Marini*

14:00–14:50 **I004**	**Spectral measurements of agricultural products: lights and shadows** Jose Blasco
14:50–15:10 **T0107**	**A041. Chemometric strategies for the identification of adulterated oregano using NIR Hyperspectral Imaging** Rosalba Calvini
15:10–15:30 **T0108**	**A068. Multispectral Imaging as a Predictive Tool for Freshness in Whole Atlantic Cod: A Comparative Study with Sensory, Chemical, and Microbiological Analysis** Andrea Rakel Sigurðardóttir
15:30–15:50	**Platinum 2. VIDEOMETER** **Spectral Imaging: Expanding Food and Agri Applications** Aske Schultz Carstensen, Jens Michael Carstensen
15:50–16:40	**Coffee-break / Exhibition** **Posters P1**

Session 4. Chair *Jose Blasco*

16:40–17:00 **T0109**	**A007. On Chemometrics and Deep Learning when applied to Semantic Segmentation Classification** Marina Cocchi
17:00–17:20 **T0110**	**A027. Authentication of wholemeal content in bread using hyperspectral imaging and a quantification method based on pixel counting by classification** Miriam Medina García
17:20–17:40 **T0111**	**A025. Estimation of nutritional levels on citrus leaves using spectral imaging and machine learning techniques** Iván Blanco-Álvarez
17:40–18:00 **T0112**	**A043. Estimating the nutritional value of food through hyperspectral imaging** María José Sáiz-Abajo
18:00–20:00	**Beer Break supported by KAX Group, honouring Paul Geladi**

Tuesday, 8/07

7:30–8:30	**Doors Opening / Registration**
8:30–8:40	Conference Opening and Plan of the Day
	Session 5. Chair *Neal C. Gallagher*
8:40–9:30 **I002**	**How far can hyperspectral imaging uncover microplastics in the environment?** Cristiane Vidal
9:30–9:50 **T0201**	**A003. Quantification of wind turbine components for better recycling process** Ekaterina Galand
9:50–10:10 **T0202**	**A103 Early detection of water deficit stress in Eucalyptus spp. through VIS-NIR hyperspectral imaging technologies and multivariate analysis** Pamela Sanhueza
10:10–10:30	**Gold 1. Specim** **Advances and Applications of MWIR and LWIR Hyperspectral Cameras** Mathieu Marmion
10:30–11:20	**Coffee break / Exhibition** **Posters P1**
	Session 6. Chair *Ludovic Duponchel*
11:00–11:20 **T0203**	**A020. Classification of Phosphate Sedimentary Facies and Estimation of Carbonate-Fluorapatite Abundance Using Hyperspectral Infrared Imaging** Houda Lkhaoua
11:20–11:40 **T0204**	**A022. Remote Sensing For Asbestos Roofing Mapping: Mantua Case Study** Alice Aurigemma
11:40–12:00 **T0205**	**A115. Hyperspectral Pixel Unmixing with Large Spectral Libraries on Soils and Minerals** Jade Preston
12:00–12:20 **T0206**	**A113. H.E.I.M.D.A.L. Deploying a Computed Tomography Imaging Spectrometer camera system on a REXUS/BEXUS Balloon Mission** Mads Juul Ahlebæk
12:20–12:30	**Regular 2. Kax Group** **ImaJerI – What's in an Image?** Joonsup Lee
12:30–14:00	**Lunch Break / Exhibition** **CHANGE POSTERS P1 to P2**

Session 7. Chair *Paolo Olivieri*

14:00–14:20 **T0207**	**A059. The expanding horizons of essential information** Cyril Ruckebusch
14:20–14:40 **T0208**	**A006. Speeding up MCR-ALS by selecting the most influential pixels based on Combined Analyte Signal and randomized SVD** Sergey Kucheryavskiy
14:40–15:00 **T0209**	**A010. Automated Iterative Targeted Detection in Hyperspectral Imaging – Fast, Accurate Detection of Minor Target Signal in a Swamp** Neal B Gallagher
15:00–15:20	**Gold 2. INNO-SPEC**
15:20–16:10	**Coffee-break / Exhibition** **Posters P2**
16:40–23:00	**Social Event 2**

Wednesday, 10/07

7:30–8:30	**Doors Opening / Registration**
8:30–8:40	Conference Opening and Plan of the Day
	Session 8. Chair *Aoife Gowen*
8:40–9:30 **I001**	**Photonic Data Science the journey from vibrational spectroscopic data to knowledge** Thomas Bocklitz
9:30–9:50 **T0301**	**A016. Vis-SWIR Hyperspectral Microscopy of plasmonic color printed arrays** Mads Svanborg Peters
9:50–10:10 **T0302**	**A002. Integrating terahertz time-domain spectral imaging technique into agricultural and food bioprocess system: an innovative indirect in-situ processing quality sensing strategy** Yuqiao Ren
10:10–10:30 **T0303**	**A017. Detection and Analytics of Thin Surface Layers by Hyperspectral Imaging Techniques** Tom Scherzer
10:30–11:00	**Coffee break / Exhibition**
	Posters P2
	Session 9. Chair *Thomas Bocklitz*
11:00–11:20 **T0304**	**A080. Integration of an XRF-VNIR-SWIR hyperspectral imaging system with multiblock data processing for a non-invasive unveiling of Raffaello painting techniques** Giorgia Sciutto
11:20–11:40 **T0305**	**A146. Integrating Multispectral Photometric Stereo with Hyperspectral Imaging: A Unified Approach for Enhanced Surface Analysis and Spectral Insights** Alaitz Atxa Galdos
11:40–12:00 **T0306**	**A091. Magnificent colors in ancient Roman wall paintings. On-site Vis-NIR Hyperspectral Imaging in Ostia Antica Archeological Park** Costanza Cucci
12:00–12:20 **T0307**	**A021. Mapping water patterns during dehydration of nonvascular epiphytic communities through NIR hyperspectral imaging** Sara Gariglio
12:20–12:30	**Regular 3. LightNovo** **Optics miniaturization strategy without performance compromise for demanding Raman microscopy applications** Yaroslav Aulin
12:30–14:00	**Lunch Break / Exhibition**
	Posters P2

Session 10. Chair *Carolina Santos*

14:00–14:20 **T0308**	**A142. Transferring weights from RGB Large Visual Models into multispectral Deep Neural Networks** Pablo Galán
14:20–14:40 **T0309**	**A075. Joint CP Decomposition and Learnable Mapping for One-Shot Anomaly Detection in Hyperspectral Images** Gerardo Mora Jimena
14:40–15:00 **T0310**	**A029. Fusion, a novel and unique cloud-based platform for processing hyperspectral images using deep learning** Guillaume Hans
15:00–15:20 **T0311**	**A088 Solving the missing information problem in image fusion through single factorization unmixing analysis** Anna de Juan
15:20–16:10	**Coffee-break / Exhibition** **Posters P2**

Session 11. Chair *Anna de Juan*

16:10–16:30 **T0312**	**A097. Increasing spatial resolution in polarized Raman microscopy with tensor decomposition-assisted super-resolution** Andrii Kutsyk
16:30–16:50 **T0313**	**A037. Multivariate Exploratory Data Analysis of Mobility Patterns using Distributed Acoustic Sensing** Jose Camacho
16:50–17:10 **T0314**	**A065. Multivariate Curve Resolution of multltimodal multisample spectroscopic imaging analysis of tumor tissues** Romà Tauler
17:10–18:00	**Awards, IASIM-2026, Farewell**

I001. Photonic Data Science the journey from vibrational spectroscopic data to knowledge

Thomas Bocklitz[1,2]

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Photonics is being applied more frequently in various fields, including biology, medicine, and diagnostics. This increase in applications is due to improvements in experimental setups and the development of data science methods for photonic data. These methods enable the detection and extraction of biomedical information from subtle differences in biophotonic data. This information might be different, i.e. the prediction of tissue types, disease states or some properties of organisms such as eukaryotic cells or bacteria.

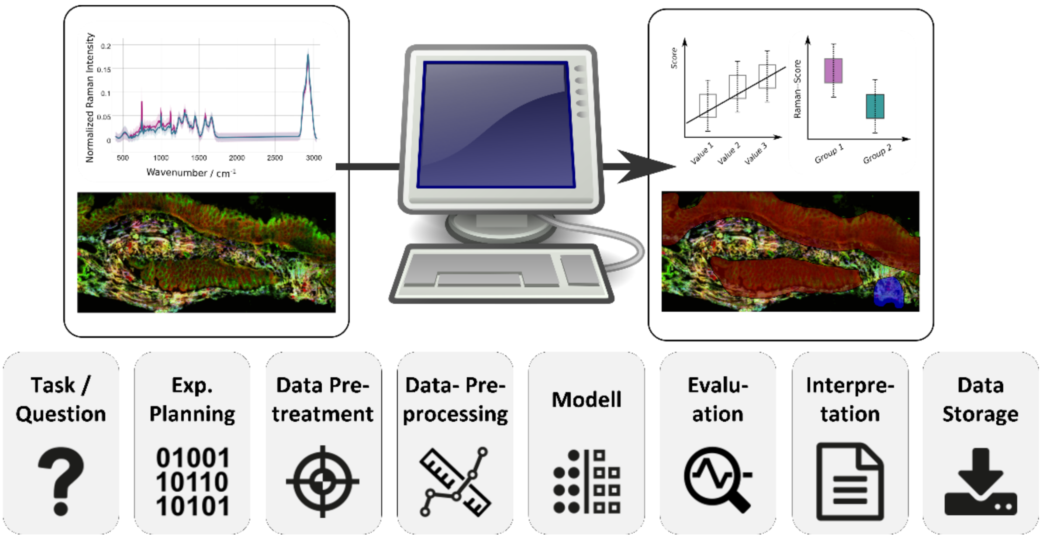

Figure 1. Data pipeline to translate spectral data and multi-contrast microscopic data into meaning full high level information.

To utilize the full potential of bio-photonic data, the whole data life cycle of photonic data from the data generation to the data analysis and to data archiving must be investigated in a holistic way. The data life cycle involves several important steps, including experiment design, sample size planning, data pre-treatment, solving inverse models of the measurement process, data pre-processing, chemometric and machine learning procedures for data analysis, model transfer methods, and transfer learning. These procedures and methods are combined in a data pipeline that standardizes the data and extracts reliable information.
We will present our recent studies on constructing data pipelines for biophotonic data especially for bio-medical Raman spectroscopy and multi-contrast microscopy. More specifically, we will discuss the possibility to use transfer learning for image based deep learning techniques (**Luo 2023**) and present a method to estimate the needed sample size for these transfer learning approaches (**Luo 2024**). Furthermore, a comparison of Siamese Networks with classical chemometric approaches and common deep learning methods like convolutional neural networks (CNNs) for Raman spectroscopic predictions of bacteria will be discussed (**Contreras 2024**). Finally, a newly designed Agnostic eXplainable Artificial Intelligence (XAI) approach Based

on Volterra Series will be presented (**Contreras 2023**), which can be used to visualize the basis of deep learning methods used to analyze spectral and image data.

References

Luo 2023: Luo, R.; Bocklitz, T.; A systematic study of transfer learning for colorectal cancer detection. Informatics in Medicine Unlocked, (2023) 101292. doi: https://doi.org/10.1016/j.imu.2023.101292.

Luo 2024: Luo, R; Guo, S.; Bocklitz, T. Sample Size Estimation of Transfer Learning for Colorectal Cancer Detection. Proceedings of the 13th International Conference on Pattern Recognition Applications and Methods – ICPRAM 2024, 841-851. doi: 10.5220/0012449500003654.

Contreras 2024: Contreras, J.; Mostafapour, S.; Popp, J.; Bocklitz, T. Siamese Networks for Clinically Relevant Bacteria Classification Based on Raman Spectroscopy. Molecules 29:5 (2024) doi: 10.3390/molecules29051061.

Contreras 2023: Contreras, J.; Bocklitz, T.; Agnostic eXplainable Artificial Intelligence (XAI) Method Based on Volterra Series. Proceedings of the 12th International Conference on Pattern Recognition Applications and Methods - ICPRAM (2023) 597–606. doi: 10.5220/0011889700003411.

I002. How far can hyperspectral imaging uncover microplastics in the environment?

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Mismanaged waste and high plastic consumption have led to massive and worrying plastic pollution worldwide. The impacts include hazards to aquatic and terrestrial lives and economic loss. The threat is posed by large plastics and those smaller than 5 mm, the microplastics (MP, 1 µm - 5 mm), which are contaminants of emerging concern. To measure the effectiveness of public politics regarding combating plastic pollution, there is a need to monitor the environment and create indicators, such as the temporal abundance of microplastics in a specific area of interest. However, accurate quantification to establish the pollution scenario and monitoring is difficult because of the MP size and widespread occurrence. From policymakers who have to manage plastic pollution to researchers who scientifically provide data on environmental impacts, there is a need for robust and reliable analytical methods (comprising sampling, sample preparation, detection methods for identification and quantification) to support research and decisions.

Hyperspectral imaging (HSI) operating with vibrational spectroscopy (Raman, mid and near-infrared) is being debated as a promising technology to increase sample analysis throughput to make environmental monitoring feasible, as it allows for the MP characterization based on their size, shape, and polymer identification simultaneously. This information is essential to assess MP impacts and fate.

The analytical technique and the instrumentation choice aiming at microplastic analysis highly depend on the environmental compartment studied and the experiment objectives. Investigations on the marine environment (Vidal 2021, Tsukada 2021), freshwater samples (**Figure 1)** in different water bodies in Brazil (Santos 2024, Sodré 2023), as well as in the atmosphere (Ferraz 2022) are presented to discuss MP spectroscopic analysis, their advantages, limitations, and practical aspects.

Finally, different approaches of chemometric analysis to identify MP are discussed, focusing on near-infrared hyperspectral imaging and how sample preparation, polymer material variability and weathering affect the HSI spatial and spectral dimension, as well as data interpretation.

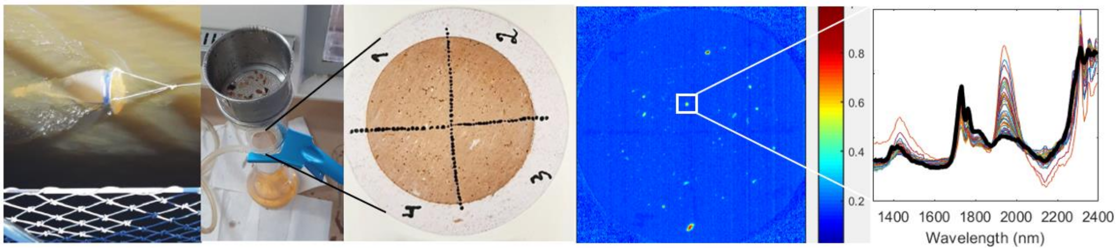

Figure 1. Microplastic analysis workflow, from the left to the right: freshwater sampling, sample preparation, extracted microplastics and remaining organic matter, illustration of spectral imaging analysis and microplastic detection confirmed through its spectral profile.

Acknowledgments are given to the INCTAA (FAPESP 2014/50951-4, CNPQ 465768/2014-8), the group working with hyperspectral imaging applied to environmental analysis, especially MP in the environment and oil spillage detection.

References

Vidal 2021: Vidal, C; Pasquini, C. A comprehensive and fast microplastics identification based on near-infrared hyperspectral imaging (HSI-NIR) and chemometrics. Environmental Pollution 285 (2021) 117251. DoI: https://doi.org/10.1016/j.envpol.2021.117251

Tsukada 2021: Tsukada, E; Fernandes, E; Vidal, C; Salla, RF. Beach morphodynamics and its relationship with the deposition of plastic particles: A preliminary study in southeastern Brazil. Marine Pollution Bulletin 172 (2021) 112809. DoI: https://doi.org/10.1016/j.marpolbul.2021.112809

Ferraz 2022: Ferraz, GM; Urban, RC. Quantification and characterization of microplastics in the atmosphere of São Carlos – SP. Master Dissertation, Federal University of São Carlos (UFSCar) – Brazil. Link: https://repositorio.ufscar.br/handle/ufscar/17419

Santos 2024: Santos, VS; Vidal, C; Bisinoti, MC; Moreira, AB; Montagner, CC. Integrated occurrence of contaminants of emerging concern, including microplastics, in urban and agricultural watersheds in the State of São Paulo, Brazil. Science of The Total Environment 932 (2024) 173025. DoI: https://doi.org/10.1016/j.scitotenv.2024.173025

Sodré 2023: Sodré, FF; Arowojolu, IM; Canela, MC; Ferreira, RS; Fernandes, AN; Montagner, CC; Vidal, C; Dias, MA; Abate, G; Silva, LC; Grassi, MT; Bertoldi, C; Fadini, PS; Urban, RU; Ferraz, GM; Schio, NS; Waldman, WR. How natural and anthropogenic factors should drive microplastic behavior and fate: The scenario of Brazilian urban freshwater Chemosphere 340 (2023) 139813. DoI: https://doi.org/10.1016/j.chemosphere.2023.139813

I003. Shedding light on Active Hyperspectral Imaging with Supercontinuum Sources

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Hyperspectral images (HSI) consist of a powerful type of data that has been used in different fields of knowledge for many years. The impact of this technology has been helping society to solve problems in several fields of knowledge (Khan *et al., 2018*). The majority of applications reported is related to passive hyperspectral setups, in which the ambient light plays an important role in the spectral acquisition, affecting signal integrity that can lead to spectral misinterpretation in certain scenarios. In contrast, active hyperspectral (AHS) systems use different types of light sources to illuminate the sample. Among the available sources to build an AHS system, the supercontinuum (SC) is the most commonly used, being initially reported in the late 90's (Johnson 1999) and enabling image acquisition in ranges such as VNIR, MIR, and SWIR. SC sources consist of a high-power laser that undergoes a nonlinear optical process allowing for the broadening of the spectral range. Although this spectral range is usually narrower when compared to passive systems, these broad and high-power light sources bring many advantages for the acquisition of hyperspectral images such as the ability to acquire spectra over long distances, in the dark, or even under adverse conditions. Those characteristics are usually limitations typically associated with traditional HSI systems but are overcome by AHS, making it a good alternative to be employed as a solution to problems related to mining, agriculture, defense, and a range of other applications. In this presentation, we will have an overview of how AHS equipment works, explore the abovementioned benefits and drawbacks of such systems, as well as assess some of the current applications.

References

Khan 2018: Khan, M. J., Khan, H. S., Yousaf, A., Khurshid, K., & Abbas, A. Modern trends in hyperspectral image analysis: A review. Ieee Access 6 (2018) 14118-14129. DoI: 10.1109/ACCESS.2018.2812999

Johnson 1999: Johnson, B., Joseph, R., Nischan, M. L., Newbury, A. B., Kerekes, J. P., Barclay, H. T., Willard, B. C., Zayhowski, J. J. Compact active hyperspectral imaging system for the detection of concealed targets. In Detection and Remediation Technologies for Mines and Minelike Targets IV. SPIE. 3710 (1999) 144-153. DoI: doi.org/10.1117/12.357002

I004. Spectral measurements of agricultural products: lights and shadows

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In the quest for more efficient and precise inspection methods, nondestructive spectral systems have emerged as a beacon of promise in various scientific and industrial domains. These systems, leveraging the properties of light, can analyse materials and products without causing any damage, making them a highly appealing option for a wide range of applications. Their unique ability to provide a rapid and accurate alternative to visual inspection methods sets them apart.

Automatic inspection systems were initially designed to replicate the human eye and, therefore, were based on colour cameras. These cameras, sensitive only to the three wavelengths humans can perceive (red, green, and blue), were developed to mimic the human eye and automate inspection tasks. They offer the advantage of obtaining information from a distance, regardless of product shape or size, and a vast array of algorithms for image processing, with specific hardware to accelerate image processing for millisecond inspection speeds. However, this technology is limited to the visible part of the electromagnetic spectrum. As an alternative, technology has paved the way for systems capable of capturing spectral information beyond human perception. This unique capability allows for simultaneous analysis of multiple product properties, enabling a more comprehensive and detailed evaluation than conventional methods. They also offer enhanced sensitivity and specificity in detecting specific product characteristics or properties, particularly in cases of chemical properties. This precision enables the detection of defects or anomalies, even at low or subtle levels, and the effective analysis of complex samples, such as mixtures or heterogeneous matrices. These features make them a versatile tool for various applications in diverse industries, including agrifood applications.

While spectral devices offer numerous advantages for product analysis, they also present specific disadvantages. Spectroscopic instruments must be properly calibrated and stabilised for accurate and repeatable measurements. However, measurements can be susceptible to environmental interferences that may vary over time, such as sunlight, humidity, and temperature, affecting the calibration of models trained under certain conditions. Additionally, in-line inspection requires a high speed of analysis since these systems are designed to monitor production quality, classify the product based on the estimated quality, and discard those that do not meet the minimum required standards. This high analysis speed necessitates rapid data acquisition, processing, and decision-making.

In the case of fruit inspection using spectral devices, the irregular spherical shape of the fruits makes achieving uniform illumination challenging. Another principal feature is the depth penetration of the light in the fruit skin to obtain internal properties such as total soluble solids, titratable acidity content, water content, phenols, tannins, etc. Moreover, the heterogeneous distribution of these compounds in the fruits makes it difficult to correctly select the measurement point, capture different measurements, or use imaging devices. Finally, the large variability among species, cultivars, origin or culture practices obligates the creation of robust predictive models or classifiers that are stable in time. This work explores different applications of spectral sensors to measure the quality of agrifood products, exploring the advantages and challenges for practical implementation.

A002. Integrating terahertz time-domain spectral imaging technique into agricultural and food bioprocess system: an innovative indirect in-situ processing quality sensing strategy

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The growing demand for high-quality agricultural and food products necessitates the development of various advanced, non-destructive sensing techniques for in-situ monitoring of processing quality (Liu, Pu, & Sun, 2017). However, certain bioprocesses, such as microwave vacuum drying, could be tough using existing real-time spectral imaging sensing methods because the quality attribute changes rapidly in the closed system under vacuum, and the interference from microwave rays during processing, could increase the noise in spectral images, which limits the application of existing spectral imaging sensors (Ren, Tong, & Sun, 2023). Terahertz time-domain spectroscopy (THz-TDS) imaging, known for its exceptional sensitivity to polar molecular, strong penetration ability for non-polar and dry materials, as well as the spectroscopic fingerprint feature, is explored for its potential in detecting and quantifying critical quality parameters, such as moisture content and polar molecule chemical composition, during various bioprocesses.

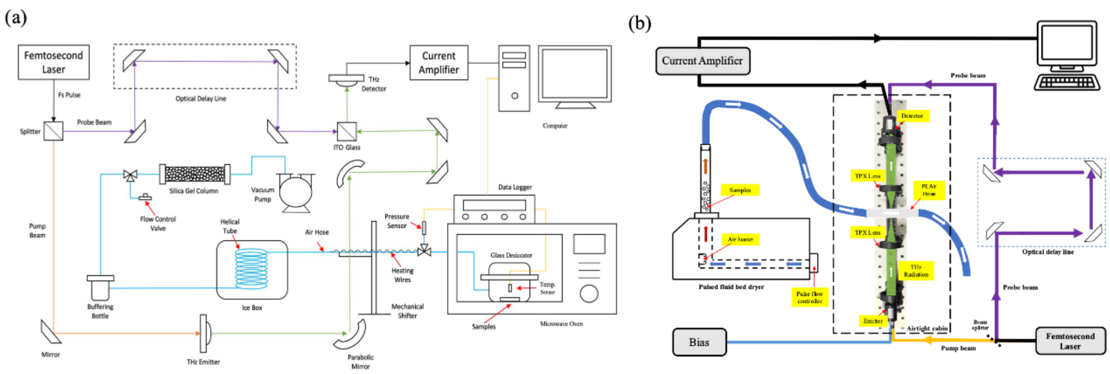

Figure 1. The schematic for the setup of the in-situ monitoring strategy for (a) microwave vacuum drying system and (b) fluid bed drying system

This study introduces an innovative indirect sensing approach by integrating THz-TDS imaging technique into agricultural and food bioprocess systems, namely microwave vacuum drying and fluidized bed drying, to conduct the real-time in-situ quality evaluations of dynamic vapor gas change and migration within the systems during the processing, and then predicting certain real-time quality attributes of products at different process stages. During the process, the THz radiation was guided to penetrate through non-polar material, part of the bioprocess system (Fig 1), and sensing the gas spectra change at different moments within the system. An advanced data signal processing process was successfully established, including conducting Fourier transforms of the time-domain spectra, absorbance and transmittance calculation, spectral integral values calculation, and advanced ML and DL-based chemometric analyses. The prediction models were built based on the processed THz spectra and corresponding reference attributes obtained by chemical analysis. The results demonstrate that THz-TDS can effectively identify subtle changes in product attributes, including real-time moisture content and moisture reduction, correlating closely with the result from conventional quality assessment methods.

This study underscores the feasibility of THz-TDS imaging in agricultural and food bioprocess systems and paves the way for its broader application in quality control. The integration of THz-TDS as an in-situ processing quality sensing strategy holds significant promise for enhancing food production processes' efficiency, reliability, and sustainability. Future work could focus on refining the technology for specific applications, scaling up the system, and integrating it with automated control systems for real-time quality management, and also to explore and develop similar methodologies on various attributes and bioprocess using THz-TDS imaging and other spectral imaging techniques.

References

Liu 2017: Liu, Y., Pu, H., & Sun, D.-W.. Hyperspectral imaging technique for evaluating food quality and safety during various processes: A review of recent applications. Trends in Food Science & Technology 69 (2017) 25-35. doi:10.1016/j.tifs.2017.08.013

Ren 2023: Ren, Y., Lei, T., & Sun, D. -W.. In-situ indirect measurements of real-time moisture contents during microwave vacuum drying of beef and carrot slices using terahertz time-domain spectroscopy. Food Chemistry, 418, 135943.

Ren 2024: Ren, Y., Zhu, X., Tiwari, B. K., & Sun, D. -W.. Terahertz time-domain spectroscopy imaging combined with convolutional long short-term memory neural network for In situ moisture reduction prediction of particle foods during pulsed fluidized bed drying. Journal of Food Engineering, 112183.

A003. Quantification of wind turbine components for better recycling process

Ekaterina Galand[1], **Noémie Caillol**[1], **Sandra Grimaldi**[2], **Nathalie Gibert**[2]
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[2] Arkema, Centre de Recherche Rhône Alpes, Rue Henri Moissan, 69491 Pierre Benite, France

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In recent years, demand for wind energy with lower ecological footprint has been rising steadily all over the world (Darwish 2020 and references therein). Consequently, the number of end-of-life wind turbines to be recycled will also increase over the years. Some parts of turbines could be easily recycled and recovered, while others, particularly the blades, are less so. In fact, the recycling of blades is complicated by the presence of fiberglass which create during grinding hazardous working conditions. Also, it is a low value material. With the development of new processes of fiberglass thermoplastic recycling (Cousins 2019) preventing hazardous risks, the quantification of blade constituents becomes necessary. However, no analytical methods for analysis and quantification of both fiberglass and polymer materials are described in the literature.

Hyperspectral imaging (HSI) is a widely used technique for analyzing polymer materials during sorting prior to recycling (Bonifazi 2023 and references therein). This technique associated with chemometrics models allows to distinguish different materials and to quantify them in composites. In addition, access to the spatial distribution heterogeneity is one major advantage of HSI when analyzing complex and/or multilayer materials. Hence, Axel'One in collaboration with Arkema has recently worked on wind turbines blade materials quantification using SWIR hyperspectral imaging with PLS modelling.

Images of 8 synthetic powders with variable materials content (Fiberglass, Polymer 1 as major polymer and Polymer 2 as additive), as well as bulk and ground real samples were acquired on Specim's SWIR camera with LabScan 40x20. Data analysis and modelling were performed on Breeze software of Prediktera. Firstly, a PCA was performed to evaluate data quality and to segment the image from the black background. Then, PLS models for each material were developed on pretreated spectra using Savitzky-Golay derivative.

No clear clustering of pixels was observed on PCA score plots, probably because of the large contribution due to sample height variability. Nevertheless, on the maximal variance images it was observed that PC1 describes Fiberglass/Polymer 1 content, while PC2 partially explains Polymer 2 content. In addition, we noticed that one of the samples had inconsistent values of scores compared to other samples. In fact, this sample containing important quantity of Polymer 2 was heterogeneous because of strong electrostatic aggregations of this polymer particles. For this reason, this sample was excluded from the calibration set.

PLS models obtained with 2 (Polymer 1) or 3 (Fiberglass or Polymer 2) latent variables correctly predicted the materials quantity on the image of the calibration set with RMSE < 1.5 % and confirmed the atypical signals for the one excluded as an outlier.

Models' test on real sample powder gives the expected values for this type of material. Models' test on bulk real sample (**Figure 1**) highlights sample heterogeneity with the distinguished layers for Polymer 2, which was expected. However, obtained values are quite different from those of the powder, especially for Fiberglass and Polymer 1. This inconsistency can probably be explained by several factors related to the sample morphology since the calibration is carried out on powders and not on bulk samples. In addition to its poor response in NIR spectra, fiberglass in bulk form reflects even less incident light.

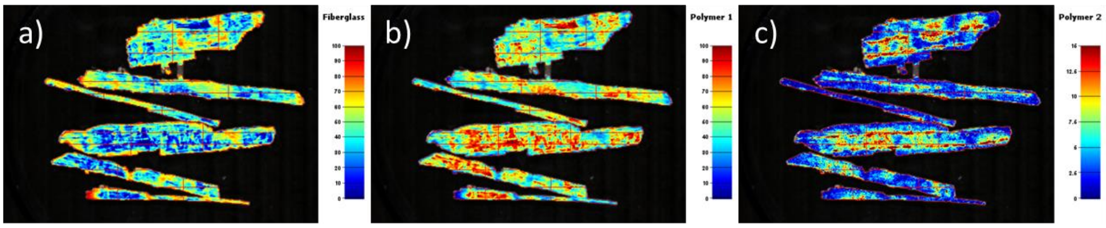

Figure 1. Models' validation on real sample for: a) Fiberglass, b) Polymer 1 and c) Polymer 2.

In conclusion, HSI technique combined with chemometrics allows quantification of different materials in wind turbine blades. Principal component analysis has revealed appropriate for anomalies detection while PLS modelling results for real sample crushed in powder form was in line with expectations. However, values obtained for the bulk form of real sample were incorrect in comparison with the powders. Still predictions correctly highlighted heterogeneity of bulk samples. Further work to adjust the calibrate from bulk samples is required.

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A006. Speeding up MCR-ALS by selecting the most influential pixels based on Combined Analyte Signal and randomized SVD

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Multivariate curve resolution by alternating least squares (MCR-ALS) is arguably one of the most widely used decomposition methods for spectral data. It enables researchers to reveal the contributions of individual chemical compounds and identify these compounds by resolving their spectra. The ALS is an iterative algorithm that loops through instructions (fitting two least squares models and applying a set of constraints) until the convergence criterion is met. This iterative nature makes the algorithm resource-demanding, particularly when non-negative least squares methods are employed for fitting. Consequently, the algorithm can be significantly slow when applied to the resolution of large hyperspectral images with hundreds of thousands of pixels.
This well-known challenge has prompted numerous researchers to address it over the last decade. One recent approach involves employing Singular Value Decomposition (SVD) and constructing a convex hull in a normalized score space (Ghaffari, 2019). The elements of the convex hull—referred to as essential pixels—form a truncated dataset to which MCR-ALS is applied. The number of essential pixels is much smaller than the original number of pixels, resulting in faster computations. While this approach is clear, straightforward, and quite efficient, it has a drawback: the efficiency of the convex hull algorithm diminishes when the number of dimensions exceeds three.
In this work, we propose an alternative solution that also relies on SVD but introduces two principal differences. Firstly, we suggest using randomized SVD decomposition, which accelerates the decomposition by one to two orders of magnitude (Kuckeryavskiy, 2018; Cruz-Tirado, 2022). This solution can be seamlessly integrated with the convex hull-based approach, further improving its speed. Secondly, we propose a novel method for identifying essential pixels—Combined Analyte Signal (CAS), recently introduced for subset selections (Pomerantsev, 2023). CAS is a generalization of the full distance concept from DD-SIMCA, applicable to multiblock datasets. The computation of CAS is rapid and independent of the ALS model's complexity, making it suitable for any number of pure components without sacrificing computational speed.
In this presentation, we will elucidate the theoretical aspects of the proposed approach and present experimental results based on simulated data as well as several real cases.

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A007. On Chemometrics and Deep Learning when applied to Semantic Segmentation Classification

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Real-time quality control of agri-food products by digital or multispectral imaging is more and more adopted in different industrial scenarios. However, most of the applications focus only on retrieving few parameters from the images, e.g. a specific color channel intensity, and relies on thresholding values which have to be tuned quite frequently. There is also a trend nowadays of implementing complex neural network architectures to solve certain issues that could be solved with simpler and less difficult to maintain and calibrate alternatives.
In this work, we aim at comparing chemometrics and Deep Learning approaches for patterns/objects identification on a difficult benchmark such as recognition of basil leaves and branches on RGB images acquired in-line with non-constant illumination conditions and varying coverage of the conveyor belt surface.
While this seems a perfect task to be solved by typical Deep Learning architectures and "blind" approaches in general, we will discuss how chemometrics-based image analysis and classification is also suitable and highlights that opening the box may reveal a certain degree of similarity between the approaches.

A010. Automated Iterative Targeted Detection in Hyperspectral Imaging – Fast, Accurate Detection of Minor Target Signal in a Swamp

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Hyperspectral imaging (HSI) is uniquely suited for detection of minor sources of signal in highly variable and spatially complex scenarios. As a result, HSI is an important analytical tool in process forensics, defect detection in surface analysis, quality control, and chemical and pharmaceutical process monitoring. The utility of HSI for detection of known target spectral signatures can be attributed to the following aspects associated with the sensing system. 1) Although target signal of interest may make only a minor contribution to the overall signal, it can dominate signal in single pixels. 2) HSI measures many pixels relevant for characterizing, and accounting for, interference (clutter) signal. 3) Clutter suppression algorithms (e.g., extended least squares [ELS] and generalized least squares [GLS]) can be easily identified and adapted on an image-to-image basis resulting in highly sensitive, image-specific target detection (Gallagher 2024). To improve detection sensitivity, local windowing approaches typically employ guard pixels to characterize clutter. However, windowed approaches are often very time-consuming and include clutter signal not relevant for the pixel under test. An alternative approach uses iterative target detection that has been demonstrated to be accurate for a stand-off application (Myers 2019, Gallagher 2024). This paper discusses an automated iterative target detection algorithm that is fast and accurate. The strategy improves detection sensitivity by removing detected pixels iteratively to maximize the ratio of target-to-clutter a.k.a., generalized likelihood ratio test. The concepts are demonstrated with an application using infrared HSI for the detection of plastic particles in sand (**Figure 1**) and melamine particles in wheat gluten.

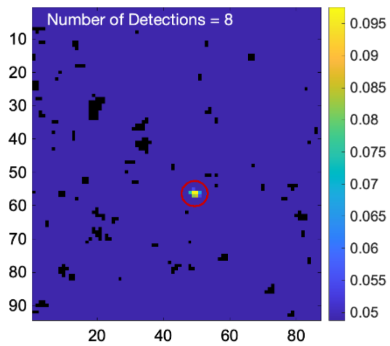

Figure 8. GLS target detection contributions, $\hat{c}$, saturated at $\hat{c} \in [c_{\text{lim}}, 2c_{\text{lim}}]$ for a detection limit based on a one-sided t-test at a 99% confidence limit. The region within the red circle corresponds to the location of an acrylonitrile butadiene styrene particle.

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A016. Vis-SWIR Hyperspectral Microscopy of plasmonic color printed arrays

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This work explores the intersection of hyperspectral microscopy imaging and plasmonic color printing arrays. Hyperspectral microscopy imaging involves capturing images at various wavelengths across the electromagnetic spectrum, allowing for detailed spectral analysis of the samples under study. Plasmonic color printing, on the other hand, utilizes the unique optical properties of plasmonic nanostructures to produce bright and customizable colors at the nanoscale (Roberts 2014).

This paper explores the applications of visible shortwave infrared (Vis-SWIR) hyperspectral microscopy in the context of plasmonic color printing arrays. The study focuses on metal-insulator-metal (MIM) configurations supporting gap-surface plasmons (GSPs) and investigates the spatial distribution of plasmonic resonances and the spectral response of nanostructures within the array (Roberts 2014). Our plasmonic color printing samples consist of square arrays of circular gold nanodiscs (NDs) with varying diameters on top of a continuous layer of SiO_2 and gold, enabling tunable color printing (**Figure 1**).

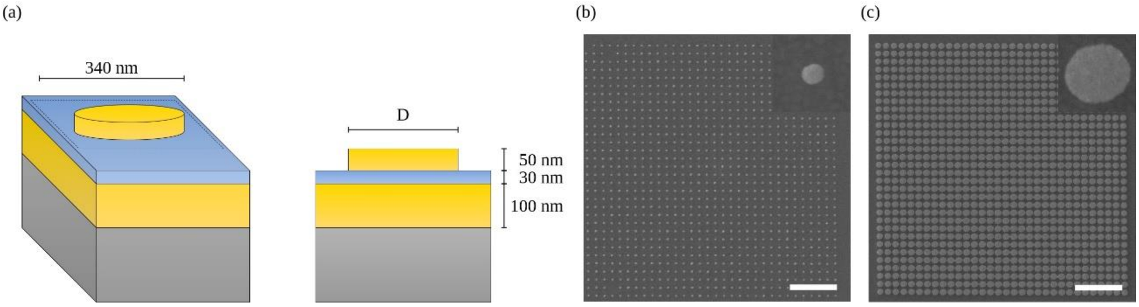

Figure 1. (a) Schematic view of a plasmonic color printed array with a periodicity of 340 nm, a gold ND with diameter D and thickness 50 nm on top of a layer of 30 nm SiO2 and 100 nm gold. Scanning electron microscopy (SEM) images of the 10.88 µm × 10.88 µm squares corresponding to (b) B and (c) H in Figure 2.b. Zoomed view of a single period in the top right corner. Scale bar in 2 µm.

We demonstrate the acquisition of detailed spatial and spectral information that shows the redshifting of the absorption peak with the increasing size of plasmonic NDs and identify the presence of fabrication errors and proximity effects in the arrays (**Figure 2**). Our custom hyperspectral microscopy setup comprises a Newtec Vis-SWIR Oculus hyperspectral pushbroom camera (Newtec 2024) mounted on an Olympus BX51 microscope with a Thorlabs translation stage. This work sheds light on the potential of hyperspectral microscopy for advancing our understanding and optimization of plasmonic color printing technologies.

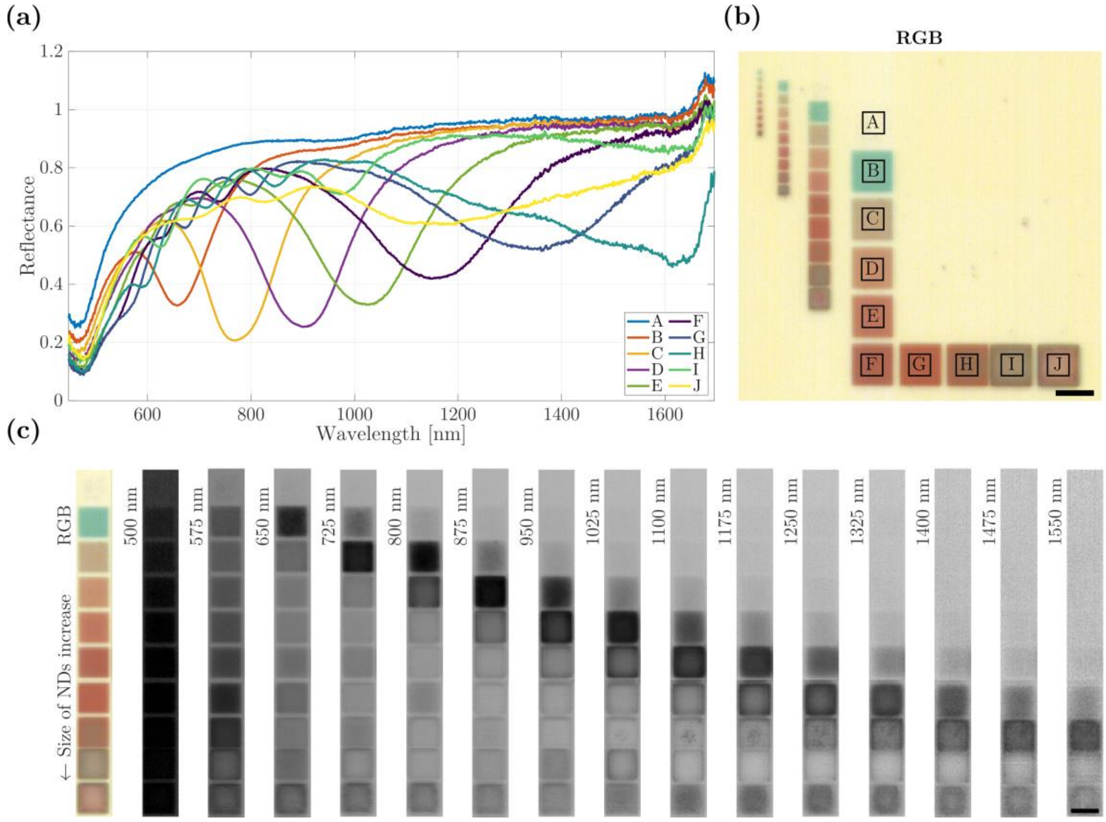

Figure 2. (a) Mean (average over blacks squares in (b)) reflectance spectra of the largest 10.88 µm × 10.88 µm plasmonic color printing squares from A-J as visualized in (b): RGB visualization of the reflectance data cube showing the four rows of plasmonic color printing squares. (c) RGB visualization and spectral bands from 500-1550 nm of the "unfolded" row of the largest 10.88 µm × 10.88 µm squares. Scale bars: 10 µm.

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A017. Detection and Analytics of Thin Surface Layers by Hyperspectral Imaging Techniques

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Thin surface layers with thicknesses between nanometers and a few micrometers are not only a field of intense basic and applied research. In fact, they are also widely used in numerous technical applications in order to generate or to modify specific functional properties of materials such as conductive, adhesion, non-reflecting, self-cleaning, barrier, reduced friction or catalyst layers. Application areas are extremely widespread and cover for example optics, microelectronics, optoelectronics, microfluidics or medicine as well as sensor, membrane, printing or textile technologies. Due to this broad range, a multitude of analytical methods is used for the characterization of thin surface layers. Infrared spectroscopic methods typically do not belong to the most sensitive methods used in surface analysis. Nevertheless, they have great potential at least for certain problems, in particular with respect to the spatial distribution of materials, structures or patterns on surfaces as well as the detection of inhomogeneity. This presentation will deal with the use of hyperspectral imaging techniques for the characterization of selected organic and inorganic layers in surface science and technology. It will include both microspectroscopic analyses carried out in a MIR microscope and large-scale NIR imaging used for technical process control.
Ion soft landing is a preparative mass spectrometry technique that allows deposition of intact polyatomic ions with well-defined composition and charge state on surfaces in high vacuum. The deposition of large numbers of ions onto supports has enabled fabrication of novel functional layers, which might be interesting for future applications in energy storage, catalysis, soft materials, or biology. Microspectral imaging was used to detect and to locate the deposited layers. An example shows **Figure 1**. A $[B_{12}I_{12}]^{2-}$

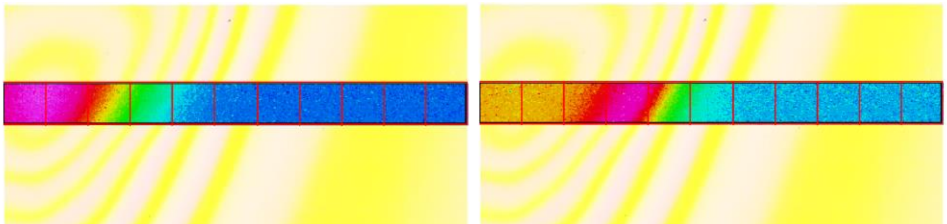

Figure 1. Spectral image of $[B_{12}I_{12}]^{2-}$ deposited on Au by ion soft-landing. Distribution of the bands at 940 cm^{-1} (left) and 2900 cm^{-1} (right).

complex was deposited on a gold substrate. The spectral image shows that there is no strict correlation between the visible yellow pattern and the distribution of the ions characterized by the breathing mode at 940 cm^{-1}, which are deposited in the center only. Another structure characterized by a CH absorption around 2900 cm^{-1} was found to form a ring around the deposited complex. It was identified as phthalate, which is used as plasticizer in the seals of the vacuum chamber. Due to the strong charging of the substrate during ion soft landing the plasticizer is deposited around the ion complex.
Poly(3,4-ethylenedioxythiophene) / polystyrene sulfonate (PEDOT:PSS) is a polyelectrolyte complex, which can be applied from aqueous suspensions for example by spin coating or gravure printing forming highly transparent conductive layers. For an effective control of such coating

and printing processes, particularly for control of the applied thickness, continuous in-line monitoring of the properties (e.g. by NIR hyperspectral imaging) of the deposited layers is inevitable. The reflection spectrum of PEDOT: PSS layers does not contain bands, but the overall reflectance in the range between 1320 and 1850 nm shows an extremely strong dependence on the thickness of the layers, which allows their use for quantitative measurements (**Figure 2a**). Calibration was carried out with reference data from white-light interferometry, ellipsometry and stylus profilometry. PLS models enabled quantitative imaging of the thickness distribution in PEDOT:PSS layers with a prediction error (RMSEP) of less than 10 nm (**Figure 2b**). Examples of the analysis of printed layers on PET film and other substrates will be shown as well (Daikos 2021).

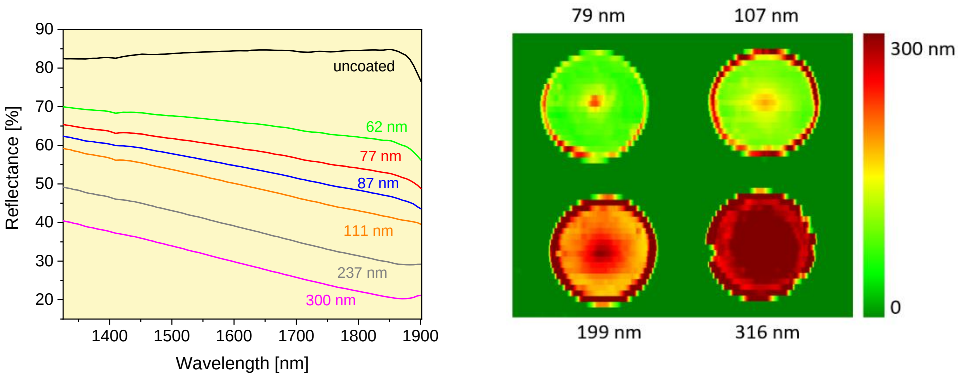

Figure 2. NIR spectra of PEDOT:PSS layers deposited on quartz with different thicknesses (left). In-line monitoring of the thickness of PEDOT:PSS layers on quartz discs by hyperspectral imaging (right).

Other examples discussed in this presentation will deal with the microspectroscopic analysis as well as the in-line monitoring of various printing processes.

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A021. Mapping water patterns during dehydration of nonvascular epiphytic communities through NIR hyperspectral imaging

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The present work is aimed at developing water maps for understanding how a micro-ecosystem composed by nonvascular epiphytic communities (mainly, lichens and bryophytes), manages water and, consequently, how the thalli can prolong water availability depending on the morphology of the species and the composition of the community itself. To achieve this aim, the water status of bark, lichens (crustose and foliose) and bryophytes was monitored by means of near-infrared (NIR) hyperspectral imaging (HSI), working in the spectral range from 1000 to 2500 nm (SWIR3 – Specim, Finland).
Pure communities, composed mainly by a single organism, were analysed alongside more complex samples containing two or three lifeform coexisting in the same ecosystem, for a total of 32 samples. All the micro-ecosystems were naturally supported by chestnut bark. Samples of non-colonised (or as less colonised as possible) bark were also analysed.
The samples were first submitted to a full hydration protocol, then let dry at room temperature (19°C) and humidity (41%) for about 12 h. During the dehydration, NIR hyperspectral images were acquired every 45 minutes. Then, two other acquisitions were performed to follow the samples until the full dehydration, getting a total of 17 sampling points and 544 images. Before each image acquisition the samples were weighed, and the weight was used to calculate their water status. The instrumental and data analysis protocol is visually represented in **Figure 1**.
Exploratory data analysis was performed on the images by means of principal component analysis (PCA), with the aim of comparing the drying trajectory in the orthogonal space defined by the lowest-order components with the dehydration curve. The study of these correspondences on pure communities opens the possibility to understand the water management of each organism and then to use such information in the study of more complex micro-ecosystems (binary and ternary samples). In practice this is done projecting these complex images in the PCA space defined by the pure samples and then producing false-RGB score maps.

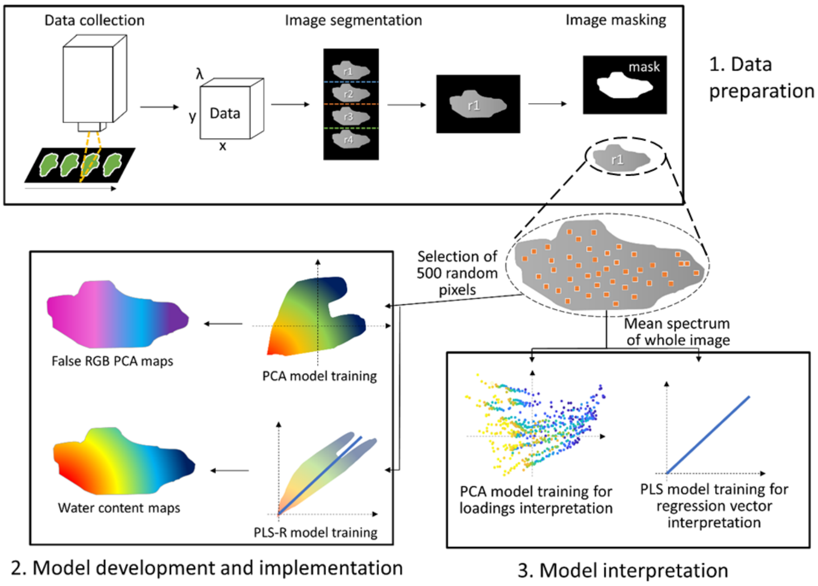

Figure 1. Data acquisition and processing pipeline

After the exploratory step, a supervised strategy is proposed, with the aim of extracting not only the water pattern inside the micro-ecosystem but also a numerical parameter expressing the water content in the different regions of interest inside a single map, as showed in **Figure 2**. This approach enabled to observe distinct behaviours between different types of communities inside a single sample.

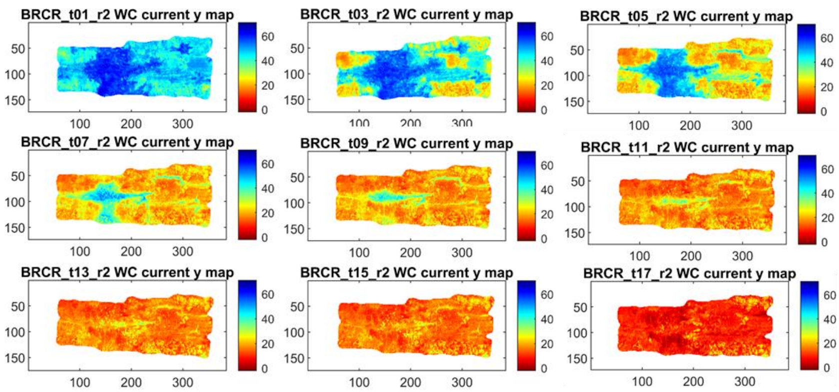

Figure 2. PLS water content maps along time for one of the binary samples.

The study of these communities and their relative behaviour in water stress condition plays a crucial role in understanding how these organisms are facing the climate change and the subsequent water scarcity or overabundance.

A022. Remote Sensing For Asbestos Roofing Mapping: Mantua Case Study

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Asbestos is still a common problem in a lot of Countries around the world. It was widely used during the 20th century thanks to its numerous physical and mechanical characteristics.
Nowadays, risks due to asbestos exposure are well known. Both the European and the Italian legislations banned the manufacturing, importation, processing and distribution in commerce of asbestos-containing products and recommended action plans for the mapping and safe removal of asbestos from public and private buildings (Bellagamba 2020). At international scale, this precautionary approach is expanding overseas, providing for its extensive and systematic removal. One of the most common and recurring risk situations worldwide is the presence of asbestos in cement roofing.
Aim of this work is to present a preliminary study concerning the application of remote sensing to asbestos cement roof mapping in Mantua (Italy) municipality, that has been chosen in consideration of the size and variability of its territory (i.e., urban, rural, and lake areas) and the presence of an extended industrial zone. This study has been realized using images collected, in August 2023, by WorldView 3, a multispectral sensor with high spatial resolution. The period was chosen to minimize cloud cover and to have maximum reflectance. Furthermore, the acquired wavelength cover Visible Near Infrared (VNIR) and Shortwave Infrared (SWIR) spectra, which are internationally considered suitable for the identification of asbestos cement (https://pubs.usgs.gov/of/2001/ofr-01-0429/spectra/; last accessed March 2023). For a proper images evaluation, Envi 6.0 software was utilized.
Each image was atmospherically corrected using QUAC (QUick Atmospheric Correction) algorithm. Two mosaics were then created both with VNIR and SWIR images. Afterwards, pan sharpening was applied to the SWIR mosaic in order to overlap it with the VNIR mosaic, thus allowing to work with one single image. Using ArcMap 10.8.2, a layer containing only the polygons of the buildings was extracted from the image in order to run the processing only on the roofs, making the elaborations easier and faster to perform. Moreover, spectral signatures studies were made for image classification obtaining specific ROIs used as reference to run different classification algorithms, which were then compared.
To test the accuracy of the classification, a confusion matrix was calculated based on 130 ground truth ROIs (10% of all detected roofing) that have been verified on site with specific surveys. The matrix showed an accuracy of 85%. The result of the study is reported in **Figure 1**.

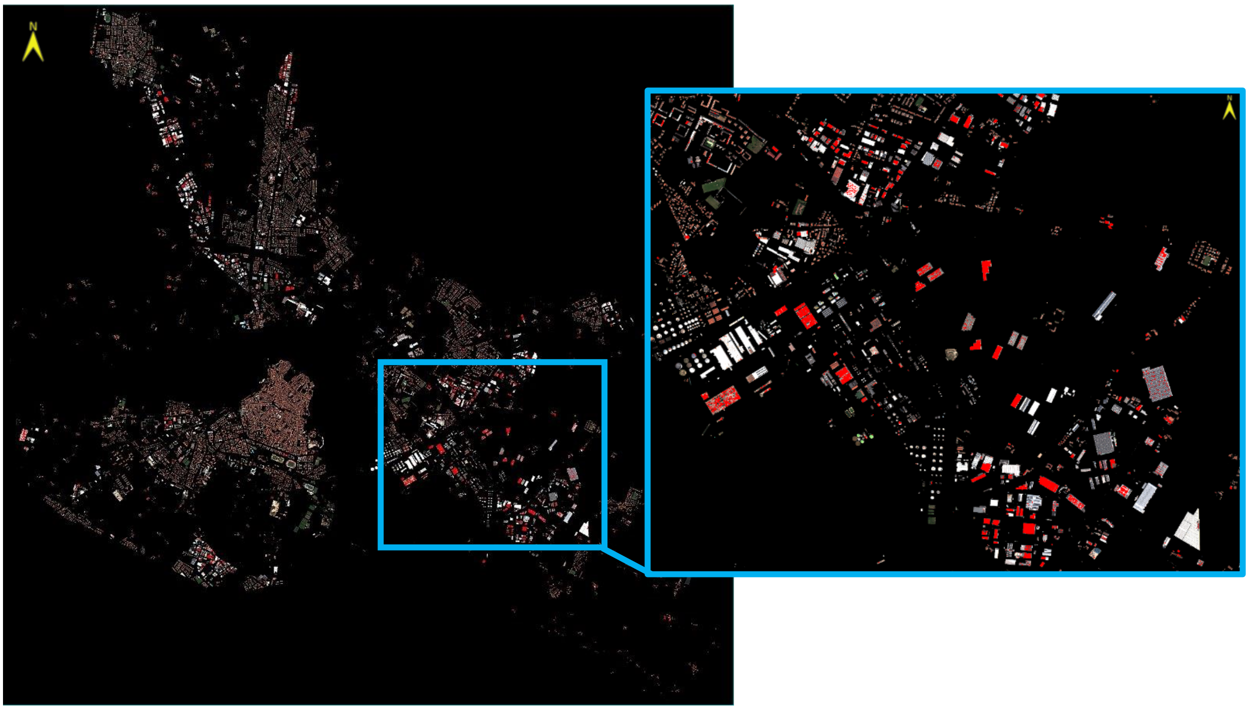

Figure 1. Studied area with a detail of some asbestos-cement roofing identified by the classification (in red).

The proposed approach can be considered as a representative case study, to calibrate an extended survey system of asbestos cement roofing to be also used at international scale. Such an innovative tool for managing the urban and natural environment allows, in fact, to perform analysis on large portions of territories in a relatively short time, contributing to improve the safety of operators involved in the risk assessment and remediation activities for a suitable land management.

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A025. Estimation of nutritional levels on citrus leaves using spectral imaging and machine learning techniques

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Proper nutrition is vital for fruit-producing plants such as citrus, as it affects both the quantity and quality of the fruit (Uthman 2023), as well as the farmer's income. However, excessive fertilizer usage to achieve this state can harm the environment. Balancing proper nutrition and optimal fertilization requires accurate diagnosis of the tree's nutrient levels. Currently, this is achieved through costly and time-consuming destructive ionomics analysis. This study proposes a new method that utilizes Vis-NIR hyperspectral imaging and machine learning models to estimate concentrations of macronutrients (N, P, K, Ca, Mg, Na, S) and micronutrients (Fe, Cu, Mn, Zn, B) in citrus leaves.

Several batches of spring sprouting leaves obtained from citrus trees cv. 'Clementina de Nules' (*Citrus clementina* Hort. Ex Tan.) mandarin were gathered monthly from April 2021 to January 2022. The images of the leaves were acquired with a hyperspectral imaging system in the range 500 - 980 nm with a spectral resolution of 10 nm, resulting in a total of 49 wavelengths. The images were corrected and processed to obtain the mean reflectance spectra of each leaf.

Then, the leaves were dried and grounded. The determination of organic N was performed using the Kjeldahl method and the other nutrients were determined by inductively coupled plasma optical emission spectrometry (ICP-OES). After an analysis of anomalies and outliers the number of samples selected for this study where 578, with each sample being a spectrum of one leaf and the reference values of the different nutrients analysed.

The prediction of the nutrient content was performed with the application of machine learning regression methods (Linear Regression (LR), Partial Least Squares (PLS), Random Forest (RF), Support Vector Machines (SVM) and Neural Networks (NN). Additionally, the study of the most meaningful wavelengths to predict each nutrient was performed using a Sequential Feature Selection (SFS) and Sequential Backward Selection (SBS) and finally optimization of hyperparameters and architectures were studied for each model.

The results from the most accurate models using all the wavelengths can be found in Table 1, while Table 2 shows the results obtained with the 6 best found wavelengths selected using the SFS and SBS methods.

Table 1. Results from the most accurate models using all wavelengths. MAE in Macronutrients is expressed in percentage, whether the MAE in micronutrients is expressed in parts per million or ppm.

	N	P	K	Ca	Mg	Na	S	Fe	Cu	Mn	Zn	B
Model	RF	NN	RF	RF	RF	RF	RF	NN	PLS	NN	RF	RF
MAE	0.14	0.02	0.17	0.45	0.07	0.01	0.02	8.32	0.70	4.80	7.56	3.31
R^2	0.59	0.61	0.58	0.71	0.53	0.49	0.53	0.83	0.30	0.52	0.57	0.77

MAE = mean absolute error

Table 2. Results from the most accurate models using 6 selected wavelengths. MAE in Macronutrients is expressed in percentage, whether MAE in the micronutrients is expressed in parts per million or ppm.

	N	P	K	Ca	Mg	Na	S	Fe	Cu	Mn	Zn	B
Model	RF	RF	RF	RF	RF	RF	RF	RF	RF	RF	RF	RF
MAE	0.18	0.02	0.19	0.48	0.07	0.01	0.02	11.78	0.70	5.77	9.13	3.76
R^2	0.45	0.55	0.51	0.69	0.40	0.45	0.42	0.58	0.22	0.34	0.40	0.72

MAE = mean absolute error

In most cases using all and the selected wavelengths, the most accurate models were using RF method. The results with the highest prediction accuracy using the full spectrum (Table 1) were found in the micronutrients Fe and B and in the macronutrient Ca, with R^2 values higher than 0.70 and MAE values of 8.32 ppm, 3.31 ppm and 0.45%. While the lowest accuracies were found on the micronutrients Cu and S.
When the models were built using only 6 wavelengths (Table 2), the accuracy of B and Ca remained similar to the model that used the full spectrum, with R^2 values of 0.69 and 0.72 and MAE values of 3.76 ppm and 0.48%, respectively. However, the accuracy of Fe model decreased. These results indicate that spectral imaging and machine learning models have the potential to assess citrus tree nutrition non-destructively, although their accuracy may vary depending on the specific nutrient and wavelengths used for analysis.

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A027. Authentication of wholemeal content in bread using hyperspectral imaging and a quantification method based on pixel counting by classification

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Wholemeal food products have become increasingly popular because of their numerous health benefits, leading to a growing market demand. Therefore, establishing quality control for these products is imperative to protect consumers of potential fraud. Despite bread being the most consumed wholemeal product, there is currently no European Regulation governing the labeling and content of wholemeal flour in bread, nor is there any official method to authenticate it compromising wholemeal bread quality on the market. Hence, the present study provides an environmentally friendly method based on hyperspectral imaging (HSI) combined with a novel quantification method based on pixel counting by classification (QPC) for authenticating the wholemeal flour content in bread. QPC methodology stemmed from the hypothesis that images captured from bread elaborated exclusively with a single kind of flour (white or wholemeal) contain spectral homogeneous pixels, whereas mixed bread presents a greater spectral heterogeneity. In both cases, bread is a homogeneous material. However, mixed bread exhibits dispersed particles into the matrix, which results in heterogeneity. These discernible particles, located in certain pixels, could be captured by HSI and quantified using the methodology proposed in this study.

To develop the presented methodology, 159 homemade breads were prepared using different proportions of white and wholemeal flour. These included breads prepared only with white flour, only with wholemeal flour and breads prepared with different proportions of both (flour mixed bread). The proportions in the mixtures included those usually found in marketed mixed wholemeal breads in Spain. One or two cereal varieties flours, including wheat, rye, oats and spelt were used to prepare each bread.

Bread samples were captured using a hyperspectral camera which measures in the spectral range from 384 to 1018 nm (VNIR). A region of interest (ROI) was selected to each sample and its pixel-spectra information was used to performer two screening analyses. Principal component analysis (PCA) and partial least-squares regression (PLS) were applied to explore the natural grouping of the sample ROI average spectra. Based on the screening results, two classification methods, partial least squares discriminant analysis (PLS-DA) and support vector machine (SVM), were applied to discriminate between ROI average spectra from samples only made with wholemeal flour than white flour. The classification models resulting from both methods were externally validated, and their quality metrics were compared to select the best one. In accordance with that, SVM model was selected to estimate the wholemeal composition of flour mixed bread by applying the QPC methodology. **Figure 1** illustrates an example of QPC application to a bread sample made with a 70% of wholemeal flour. In this case, randomly selected pixels from the sample were classified as wholemeal or white using SVM model and the proportion of wholemeal content was estimated by counting.

The methodology developed in this study was able to predict the wholemeal flour content in 48 flour mixed breads with a maximum deviation of 8 units (g wholemeal flour / 100 g flour) from the estimated value, irrespective of the type of cereal flours used in its production. This proves its potential as a solution to the current gap in the authentication control of this highly consumed product from an environmentally friendly perspective.

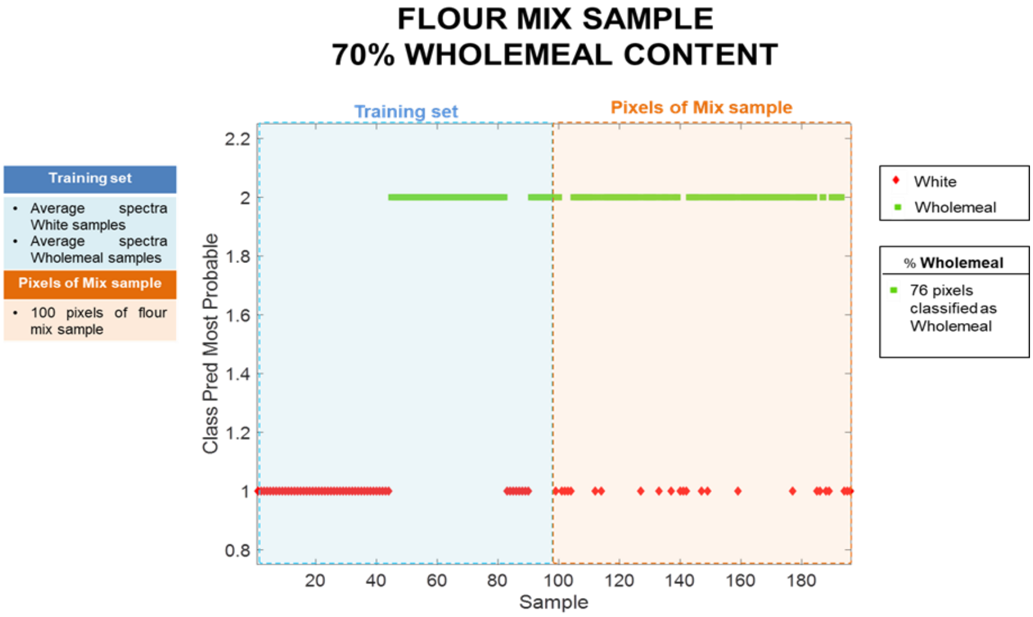

Figure 1. Example of QPC methodology applied to quantify wholemeal content in flour mixed bread.

A028. Detection of apple mouldy core and prediction of mycotoxin contamination using hyperspectral imaging

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The Food and Agriculture Organization estimated post-harvest losses of fruits and vegetables between 15% and 50%. For apples (*Malus domestica*), yield loss due to pathogen spoilage amounts to 70-80%. Mouldy core (MC) is a frequent post-harvest fungal disease in apples, manifesting as a rotten area inside the fruit without visible external lesions, making detection extremely difficult. MC is mainly caused by *Alternaria tenuissima*, capable of producing a wide range of secondary metabolites, many considered as mycotoxins (= toxic secondary metabolites produced by fungi). Since *A. tenuissima* is reported as one of the main causal agents of MC (Pavicich 2020) in apples worldwide and is hard to be detected, it imposes serious health risks, especially for young children. In recent years, efforts have been made to detect MC in apples with non-destructive methodologies (Genangeli 2022). However, none of the current methodologies to detect MC can correlate the infection with mycotoxin concentrations as the role of these metabolites in fungal physiology has not yet been elucidated. Since visual inspection of MC is not feasible for processing industries, and as mycotoxin exposure is mainly associated with processed products, the objective of this study was to detect MC using non-invasive reflectance spectroscopical images of fruits to link the MC to mycotoxin accumulation.
A total of 111 Golden Delicious variety apples were provided by PC fruit in Belgium and superficially disinfected for 10 min by drenching them in a 70% ethanol solution. We affixed QR codes to each apple and measured and their weight, height and diameter. Spore suspensions from six different *A. tenussima* isolates were prepared and 100 µl was aseptically injected through the calyx into the fruit core, resulting in a total of 60 infected apples. The remaining 51 apples served as control. All the apples were incubated in closed boxes at room temperature.
All apples were imaged in the horizontal and vertical position before infection by a hyperspectral spectrometry platform mounted on a horizontal rail with the Specim FX10 (400 – 1000 nm) and FX17 (900-1700 nm) cameras (Specim Spectral Imaging Ltd.; Oulu, Finland) (shown in **Figure 1**). Samples were illuminated overhead by six halogen lights at approximately 45° from the front and back of the camera target field. The distance from the target to the cameras, exposure time and focus were adjusted and kept stable throughout all experiments. In one image, multiple apples can be simultaneously imaged.

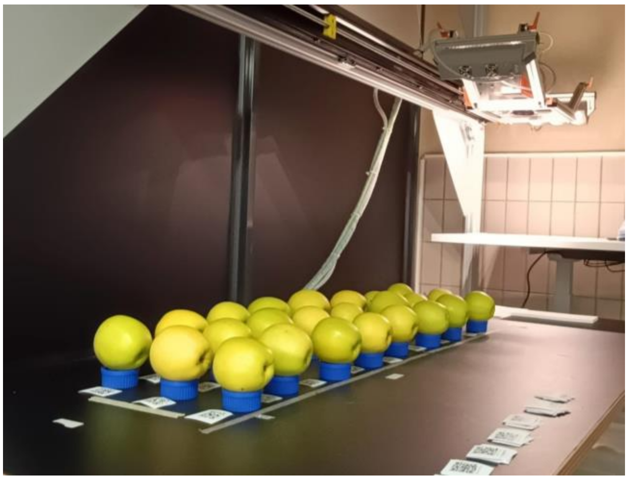

Figure 1. Set-up of hyperspectral cameras to image apples in horizontal position with their corresponding QR codes.

Hyperspectral images were taken at different time points post inoculation within 40 days. The images were processed using perClass Mira software and the mean spectra of each apple were extracted. On day 20, half of the apples were cut and visually inspected for MC. An extraction and LC-MS/MS in-house validated method was used to detect and quantify 10 *Alternaria* mycotoxins in the samples. The remaining apples were further incubated until day 40, when they were imaged and visually inspected for MC and mycotoxin contamination was determined. All data are being combined to build customized data fusion models that will be trained to predict fungal and mycotoxin presence from the first derivative of the reflection spectrum. These algorithms will not only classify a fruit as healthy or mouldy, but also will relate the lesion to the mycotoxins content. Thus, we will provide a hyperspectral imaging based tool to separate mouldy apples, reducing mycotoxin occurrence in apple products.

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A029. Fusion, a novel and unique cloud-based platform for processing hyperspectral images using deep learning

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Hyperspectral imaging is a highly versatile technology that presents tremendous potential for both industrial and remote sensing applications. It is currently being deployed across virtually all industries (agricultural, food, pharmaceutical, recycling, mining, forest, etc.) for feedstock monitoring, process optimization, quality control and cost reduction. Remote sensing optical applications, which historically have mostly exploited RGB and multi-spectral imaging, are also increasingly relying on hyperspectral imaging for earth observation with many companies (Planet, Pixxel, Orbital Sidekick, Sidus Space, Wyvern, etc.) planning to launch hyperspectral satellite sensors in the coming years. In 2022, the global hyperspectral imaging market was valued at USD 14.9 Billion and it is projected to expand to USD 51.2 Billion by 2032 (Market.us 2023). However, one of the main drawbacks of hyperspectral imaging is that it generates massive amounts of data that need to be handled and analyzed efficiently to provide value. This issue will only become more and more pronounced with the rise of new applications. To solve this problem, Metaspectral (Vancouver, BC) has, over the past few years, developed a novel and unique cloud-based platform and computing infrastructure, called Fusion (Metaspectral 2024), specifically designed to handle the vast amount of data coming from hyperspectral imagery and to process and analyze this information using state-of-the-art machine learning and deep learning algorithms. Fusion cloud-based platform presents several advantages in comparison with software running on a workstation. First, data is safely stored on the cloud with private access, does not consume local resources and can be seamlessly shared with colleagues and collaborators wherever they are. Second, all Fusion algorithms have been optimized for speed and memory efficiency. This coupled with the fact that cloud computing provides access to significant CPU, GPU and TPU resources give Fusion unparalleled capabilities. Third, the use of deep learning allows for the analysis of large datasets consisting of hundreds or thousands or hyperspectral images in a straightforward and scalable manner. Classification, regression, target detection and spectral unmixing models are available on the platform. Furthermore, for industrial applications, models developed on the Fusion cloud-based platform can be deployed on-site on the Fusion base-station allowing to visualize live inferences and effectively enabling real-time analysis. In this presentation, the usage of the Fusion platform and typical workflows for labeling data, creating datasets and building models will be illustrated using open-source data. Through these examples, it will be demonstrated that the Fusion platform can efficiently analyze a substantial amount of data and provide actionable insights from hyperspectral images.

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A030. Cost efficient training of deep learning models for detection of contaminating grains in bulk oats

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Computer vision based on instance segmentation deep learning models offers great potential for automating quality control of grains (Assadzadeh et al., 2022). Whereas distinguishing foreign objects is often relatively easy with the naked eye, it is much more difficult to distinguish highly similar products (e.g. good and bad quality, different variety). Spectral cameras measure a spectral fingerprint for each pixel in an image, allowing them to distinguish much more subtle differences (Lu et al., 2020). However, large amounts of labelled data are required to train supervised deep learning models. To overcome this limitation, in this research a new labelling technique is developed by 'tagging' the targets with fluorescent labels that make the targets 'light up' under UV illumination to efficiently generate ground truth segmentation masks. As these fluorescent labels are only visible in the UV range of the spectrum, the spectra in the Vis/NIR range can be used to discriminate grains from each other.

In this study, contaminating grains in bulk oats were detected. Oat (*Avena Sativa*) is a minor crop grain that is rich in essential nutrients such as proteins, lipids, vitamins, minerals and fiber, having the highest protein content among the major cereal grains. Moreover, it is a very interesting nutrient-rich grain for the human diet as it is associated with several health benefits such as lower blood cholesterol and reduced heart disease. In contrast to other major cereal grains, oat contains Avenins as gluten proteins, which are typically tolerated by people suffering from celiac disease (Erkinbaey, 2017). However, since oats are planted on neighboring fields with other cereal, gluten-rich grains and harvested with the same machines, the risk of contamination is high. As this is problematic for people with gluten intolerance, oat is not considered gluten-free. Because completely separate circuits are very expensive, there is a demand for automatic inspection of the purity of batches of gluten-free seeds.

To train the deep learning segmentation model, a cost efficient strategy was developed. The contaminating grains, more specifically spelt, were coated using a UV spray. Next, an RGB image with UV lighting was taken to capture the fluorescent tags. These labels could then be transferred onto the hyperspectral image. This allowed us to train a YOLO v5 deep learning-based model for hyperspectral image segmentation and to identify the most informative wavebands to classify spelt from oat.

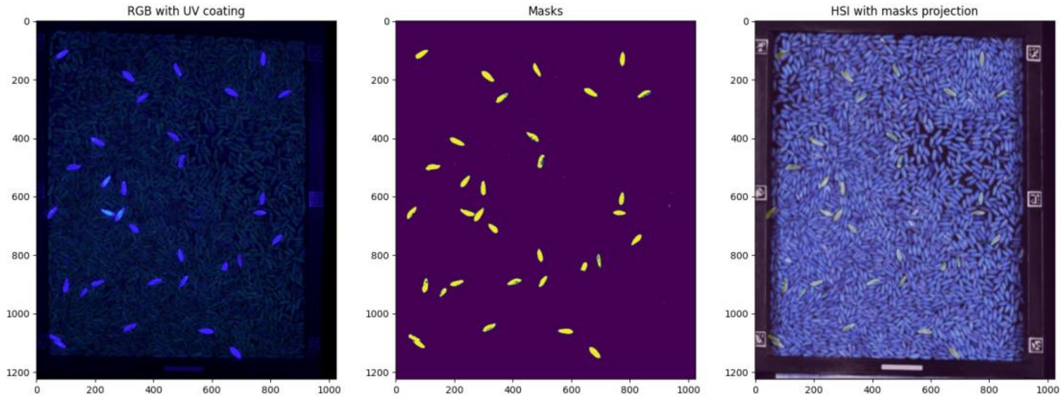

Figure 1. Overview of the UV tagging strategy. From Left to right: RGB image with UV coatings and UV light - the mask extracted from the UV tags – the mask projected on to the hyperspectral image.

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A037. Multivariate Exploratory Data Analysis of Mobility Patterns using Distributed Acoustic Sensing

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The study of human mobility in the urban context is important for applications such as understanding social behavior, traffic forecasting, urban and telecommunication networks planning and epidemic modelling (Barbosa 2018). The research on human mobility has experienced a boost thanks to the apparition of extensive geolocated datasets from mobile devices, but also to the management of COVID-19 (Hu 2021). In this context, an emergent sensing technology referred to as Distributed Acoustic Sensing (DAS) is gaining momentum (García 2023).

DAS technology is based on the Rayleigh back-scattering phenomenon occurring in an optical fiber when an interrogation light-wave faces its inhomogeneities. If a local perturbation occurs along the fiber, its refraction index will change locally providing a proportional change in the properties of the backscattered light-wave coming from the spatial point where the perturbation occurred. This capability of demodulating the magnitude and location of the stimuli affecting the fiber, converts optical fibers into arrays of sensors (1 *distributed sensor* occurring each 6-10 meters of fiber). Optical fibers already deployed in the cities become for DAS technology a dense network of distributed sensors capable of providing urban mobility patterns based on real data. Wide urban areas can be monitored during long time periods with no dependence on weather conditions, no need for massive maintenance of punctual sensors or preservation of anonymity. DAS registers have these traits: they are massively produced, they contain diversified energy footprints of overlapped mobility events, and they can be subjected to several types of noises. In addition, due to the highly dynamic properties of the ground solidary to the fiber along its deployment, each fiber's spatial locations will provide a different channel response to the same stimulus.

An example of outcome of a DAS sensor is shown in Figure 1 (left): It corresponds to a multivariate time series that spans the space of deployment of the fiber. We believe the study of DAS signals is intimately related to that of spectral imaging. In a recent conceptual experiment (Martínez 2023), we deployed a dark fiber of an approximate length of 1 Km at the University of Granada, Spain. The area monitored corresponds to a neighborhood of apartments adjacent to the university dependencies, with variations of traffic density and types of mobile events along the day. In an initial exploration of the data, we identified three canonic types of movement categories: cars, pedestrians, and buses. Discriminative features like the Hjorth parameters (activity, mobility and complexity) and the approximate entropy were extracted for the three types of events. The resulting data was subject to a Multivariate Exploratory Data Analysis with

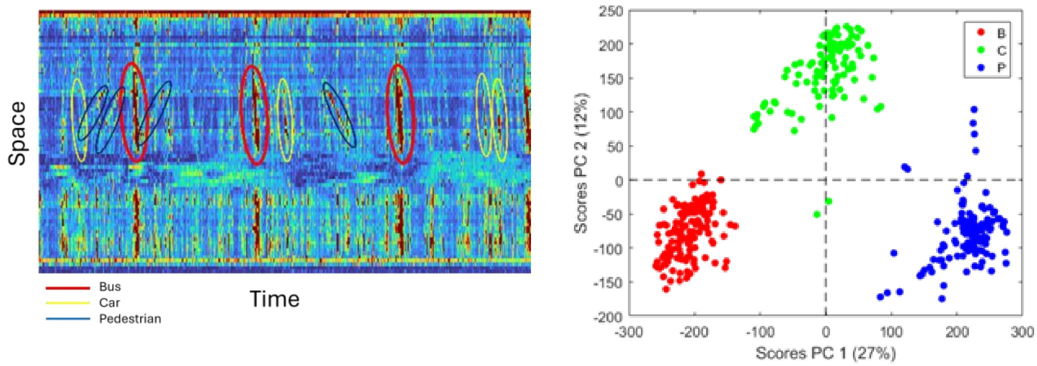

Figure 1. Example of output from a DAS sensor, where the space spans the fiber length and time corresponds to time series measurements (left), and example of PCA score plot distinguishing types of movements (right).

PCA (Figure 1 (right)) and PLS-DA, which allowed us to identify a suitable moving window for future real-time analysis.

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A041. Chemometric strategies for the identification of adulterated oregano using NIR Hyperspectral Imaging

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According to a recent technical report by the European Commission's Science and Knowledge Service (JCR), dried oregano leaves resulted to be one of the most frequently adulterated herbs, with 48% of adulterated samples (Maquet 2021). Common adulterants include olive leaves, sumac, strawberry tree and myrtle, whose dried and ground leaves are visually identical to oregano.
In this study, we assessed the utility of Near Infrared Hyperspectral Imaging (NIR-HSI) as a rapid and non-destructive analytical technique capable of authenticating oregano samples. Indeed, thanks to the possibility of coupling both spatial and spectral information from a sample, NIR-HSI is particularly suitable for characterizing heterogeneous matrices like authentic and adulterated oregano (Amigo 2015).
To this aim, we analyzed a sample set composed of authentic oregano samples, the most frequent pure adulterants (i.e., myrtle leaves, sumac leaves, strawberry tree leaves and olive leaves) and oregano samples adulterated with different percentages of the considered adulterants, for a total of 49 samples. Three replicate images were acquired for each sample using a line scanning NIR-HSI camera working in the 980 – 1660 nm spectral range.
Firstly, multivariate classification models were calculated to differentiate authentic oregano from pure adulterants. Class Modelling (CM) classification methods like Soft Independent Modelling of Class Analogies (SIMCA) are typically recommended to face authentication issues like the one considered in this study (Rodinova 2016). However, the high heterogeneity of authentic oregano class as well as its partial overlap with pure adulterants resulted in poor classification performances, with special concerns on the model specificity. As a valid alternative, we applied a soft discriminant algorithm, named Soft Partial Least Squares Discriminant Analysis (Soft PLS-DA), that combines the advantages of CM and Discriminant Analysis (DA) methods (Calvini 2018). Indeed, like DA methods, Soft PLS-DA maximises the differences between the considered classes even when they overlap. At the same time, Soft PLS-DA allows to potentially detect samples adulterated with herbs not previously considered for model development, which is a typical feature of CM methods.
Soft PLS-DA allowed to obtain satisfactory classification performances in discriminating spectra of authentic oregano and pure adulterants, with a classification efficiency value in prediction equal to 92%.
Finally, to have a final assignment of the acquired samples as authentic or adulterated classes, both SIMCA and Soft PLS-DA models were applied to each image, obtaining the corresponding percentage of pixels predicted as oregano (PPO%). Based on PPO%, a threshold value was set to differentiate authentic and adulterated oregano samples.
Despite both SIMCA and Soft PLS-DA allowed to achieve high sensitivity values for authentic samples, relevant differences in the classification performance were found considering the ability of the two algorithms in recognising adulterated samples. As a matter of fact, SIMCA

failed in the identification of most adulterated oregano samples, while Soft PLS-DA correctly recognised as adulterated all the samples with adulterant concentration equal to or higher than 10%. This value can be considered as a limit of detection of NIR-HSI for the identification of adulterated oregano, which can be acceptable since adulterants are generally added in higher percentages to gain an economic advantage.
In addition, the outcomes of this study suggest that soft discriminant approaches represent an effective and powerful classification strategy in the frame of authentication issues, overcoming the limits of both CM and DA methods.

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A043. Estimating the nutritional value of food through hyperspectral imaging

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Determining the nutritional value of foods is important for the food industry to allow for accurate package labelling and appropriate packaging conditions, as well as the development of new food products and innovation of existing ones. In addition, knowing the composition of foods in terms of nutrients and energy content is essential for the construction of food composition databases, which are essential for designing therapeutic diets and formulating population dietary guidelines, amongst other uses (Sociedad Española de Nutrición (SEN), 2017).
Current methods to quantitatively characterize food composition and determine its energy value, are based on analytical chemistry. However, these conventional methodologies are slow processes that require chemical products and trained technicians, moreover, they are destructive processes in which the analyzed food cannot be recovered, and sometimes expensive materials are needed (Ingle, P.D., Christian, R., Purohit, P., Zarraga, V., Handley, E., Freel, K., & Abdo S. 2016).
Hyperspectral imaging (HSI) techniques use different wavelength ranges, such as ultraviolet (200-400 nm), visible (380-800 nm), VIS-NIR (400-1000 nm), NIR (900-1700 nm), and short-wave infrared (970-2500 nm) for optical sensing of different types of samples (Lohumi, S., Lee, S., Lee, H., & Cho, B. K. 2015).
Despite recent progress in the field of food technology, there is still a growing interest in finding faster, cheaper and nondestructive techniques for determining the nutritional composition of foods. With the incorporation of artificial intelligence (AI) and machine learning (ML) models in the equation, this problem is being progressively solved.
We hypothesize that the nutritional value of heterogeneous food products can be readily measured instead by using hyperspectral imaging systems combined with mathematical models previously fitted with spectral profiles.
One hundred and eighteen (118) samples from different food products were collected for building the predictive models using their hyperspectral imaging data as predictors and their nutritional values as dependent variables.
The results obtained in this work show that it is possible to predict the energy and nutritional values in processed complex foods, without being grinded or procesed, using hyperspectral imaging systems (both NIR and Vis-NIR), combined with artificial intelligence machine learning methods.
The best performance was for estimating the protein content with a RMSE of 1.02 and a R2 equal to 0.88 in a test set, following by moisture (RMSE of 2.21 and R2 equal to 0.85), energy contain (RMSE of 21.84 and R2 equal to 0.76) and total fat (RMSE of 2.17 and R2 equal to 0.72). The performance with carbohydrates (RMSE of 2.12 and R2 equal to 0.61) and ashes (RMSE of 0.25 and R2 equal to 0.38) was worse.
The advantage over other analytical methodologies is that the sample does not need to be grinded or extracted, it is a rapid and non-destructive analysis, and the system can be easily used by non-expert users. This result could be of great interest in hospitals, nursing homes and school canteens to measure the nutritional value of a given dish in real time and before delivering the meal to the patient or school canteen users.

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A052. Comparison of portable and bench-top spectrometers for short wave infrared reflectance measurements of soils and leaves

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Shortwave infrared (SWIR) spectroscopy has received widespread interest as a method to complement traditional soil and leaves analysis (Van Leeuwen 2009). Recently available portable SWIR hyperspectral imaging systems (HSI) also offer potential for on-site applications, thanks to the achieved spectral data quality.
In this paper performances of the NIREOS HERA portable FT-SWIR unit in comparison with SISUchema XL benchtop detection device have been evaluated in terms of spectral characteristics and variance detected through principal component analysis (PCA).
The proposed comparative approach is based on the acquisition, in the short-wave infrared range (SWIR: 1000-1700 nm), by both the two hyperspectral devices of dried vine and olive leaves and soils coming from the same areas, followed by the correlation of the spectral collected signatures, in the SWIR range, with the micro- and macro-nutrients detected, on the same samples, by X-ray micro fluorescence. Furthermore, the prediction maps showing the distribution of macro- and micro-nutrients in the samples were obtained and compared with those resulting by HSI. The achieved results suggest as the portable HSI FT-SWIR unit can have great potential for on-site applications.

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Acknowledgements
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A058. Detection of *Listeria monocytogenes* on beef meat with NIR hyperspectral imaging

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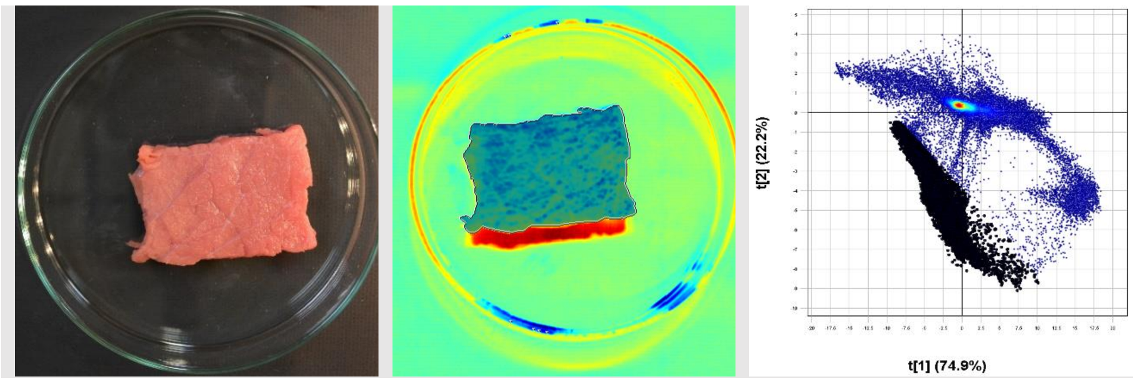
There is a growing interest in rapid and sensitive detection of foodborne bacteria to ensure food safety and reduction in food waste. Globally, it is estimated that 30% of all food produced results in food waste with 7% attributed to microbial spoilage of meat and meat products (Lipinski 2020). The current methods of analysis are laborious and often provide retrospective information. This is not ideal in fast-paced environments such as meat processing plants where decisions must be made promptly. In this study, near infrared hyperspectral imaging (NIR-HSI; 900-1700 nm) was applied for the discrimination of *Listeria monocytogenes* contaminated/spiked beef meat and non-contaminated meat. Fresh beef steaks from the M. *Longissimus thoracis et lumborum* muscle were inoculated with *L. monocytogenes* serotype 4b (suspended in saline) containing approximately 100 cfu/ml. Hyperspectral images of meat samples stored at 4 ^{o}C were acquired using a line scan NIR-HSI imaging system (SpecimFX17, Spectral Imaging Ltd., Oulu, Finland), over six days. Principal component analysis with three principal components (PCs) was used to select the region of interests by retaining the scores associated with the beef samples (Figure 1).



(a1) (a2) (b)

Figure 1. (a1) Digital and (a2) score image of meat samples and (b) the corresponding principal component analysis score plot showing PC1 (75%) and PC2 (22%). These were used iteratively to select the regions of interest (i.e., the surface of the meat).

Following the removal of the background and bad pixels, partial least squares discriminant analysis (PLS-DA) was used to discriminate between three classes: spiked, saline-treated, and non-treated samples. Various pre-processing techniques, including standard normal variate and Savitzky-Golay smoothing (1st derivative, 2nd order polynomial with 11 points) were applied for scatter correction and noise reduction. The results showed that partial distinction was achievable, with classification accuracies ranging from 63% to 81% for the three classes over time. Further classification, using support vector machines (SVM) and PLS-DA to discriminate between *L. monocytogenes* inoculated samples over time, showed excellent classification accuracies exceeding 98%. In both cases, the average sensitivity and specificity values surpassed 90%. Spectral information revealed that the primary wavebands responsible for the discrimination were associated with protein (1166 nm, 1690-1696 nm) and carbohydrates (1370-1410 nm) and their association with moisture in the meat samples (Workman and Weyer 2007). The findings suggest that NIR-HSI holds the potential for detecting *L. monocytogenes* on beef meat and discriminating from non-contaminated meat.

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A059. The expanding horizons of essential information

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The identification and retrieval of essential information has recently emerged as a very useful and valuable approach for compressing spectral and hyperspectral imaging data before the application of multivariate curve resolution (linear unmixing) methods. Essential spectra encompass the most linearly dissimilar spectra measured, which, by themselves, enable the lossless reproduction of the entire set of collected data in a convex linear way. This brings advantages in terms of computational time and facilitates challenging analytical tasks such as the detection of minor species. The selection of essential information is applicable to various types of data and is particularly versatile, *i.e.*, it can be performed after any linear transformation of the investigated measurements.
In this presentation, we start by extending the concept of essential information to the Fourier domain. This permits the independent assessment of the "essentiality" of every individual spectral profile registered, paving the way for data acquisition procedures based on the content of essential information encoded by, *e.g.*, each single pixel in Raman hyperspectral imaging. We then broaden the core principles of this approach for the reduction of trilinear datasets and highlight the benefits that this strategy can bring in domains like multiway fluorescence imaging or polarized Raman microscopy.

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A065. Multivariate Curve Resolution of multltimodal multisample spectroscopic imaging analysis of tumor tissues

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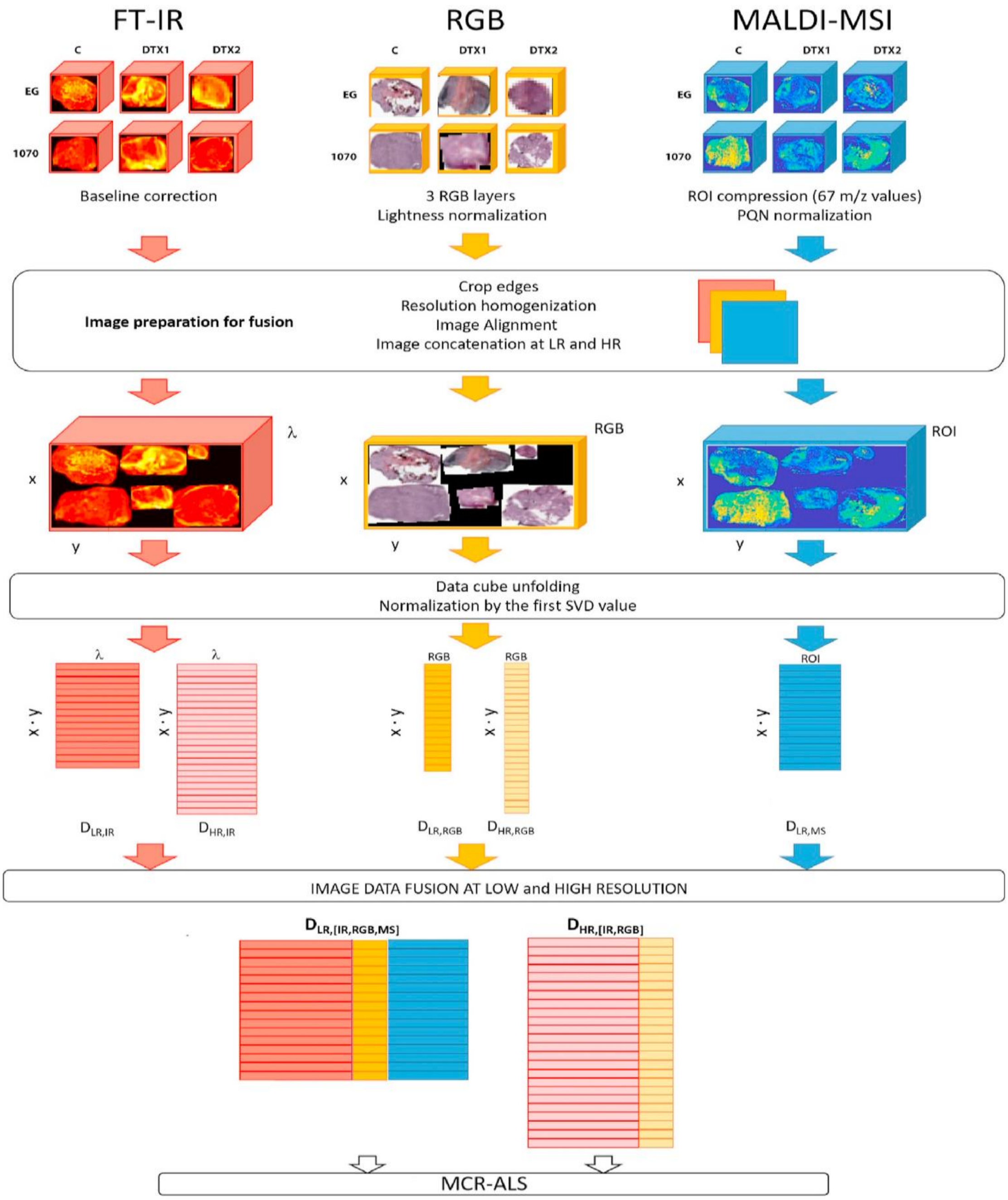
Chemical imaging aims to analyse molecular patterns in tissues or surfaces, providing high-resolution images with rich molecular information. This is particularly useful in biomedicine, where specific molecular patterns can aid in understanding pathological traits. Traditional staining techniques may miss certain patterns, but chemical composition analysis can reveal novel insights. In this study, a new chemometrics approach was proposed to analyse six tissue slices from two types of tumours (EG and 1070) with varying sensitivity to the drug docetaxel. By employing MALDI-TOF mass spectrometry imaging (MSI), FT-IR hyperspectral imaging, and hematoxylin/eosin staining, the study combined multiple imaging techniques. The extensive spectral data generated was organized and analysed using multivariate curve resolution (MCR), revealing distinct chemical patterns in specific tumour areas. Specifically, this study will explore two key areas: first, the simultaneous Multivariate Curve Resolution (MCR) analysis of chemical images acquired at varying spatial resolutions, resulting in incomplete multimodal multisampling datasets (image data fusion); and second, the utilization of non-negative constraints when missing data blocks are present within alternating least squares optimization algorithms. This approach proves to be a powerful tool for extracting chemical information from fused image datasets obtained from various spectroscopic imaging techniques, offering insights into tumour characterization and drug response [Bedia 2021, Bedia 2022].



Graphical representation of the different pre-processing steps of image data arrangement and fusion (see Bedia et al., 2021,2020).

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A068. Multispectral Imaging as a Predictive Tool for Freshness in Whole Atlantic Cod: A Comparative Study with Sensory, Chemical, and Microbiological Analysis

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This study investigates the potential of using multispectral imaging (MSI) techniques to predict the quality of whole gutted Atlantic cod throughout its shelf life during storage on ice. By capturing progressive changes in the optical properties, we aim to develop a non-invasive, real-time method for assessing the freshness of whole cod. This method has the potential to improve quality control in the seafood industry, reducing waste and ensuring consistent product quality. Alongside MSI, systematic sensory evaluation was conducted using the Quality Index Method (QIM) scale, complemented by traditional chemical and microbiological analyses, providing comprehensive degradation profiles throughout the storage duration.

The MSI systems, VideometerLab 4 and VideometerLite (TMF 2) (Videometer A/S, Herlev, Denmark), were used to capture the MSI images. The VideometerLab 4 can capture images at 19 different wavelengths, ranging from 365 nm to 970 nm. The VideometerLite is a portable, easy-to-use imaging device with 13 wavelengths between 365 and 850 nm.

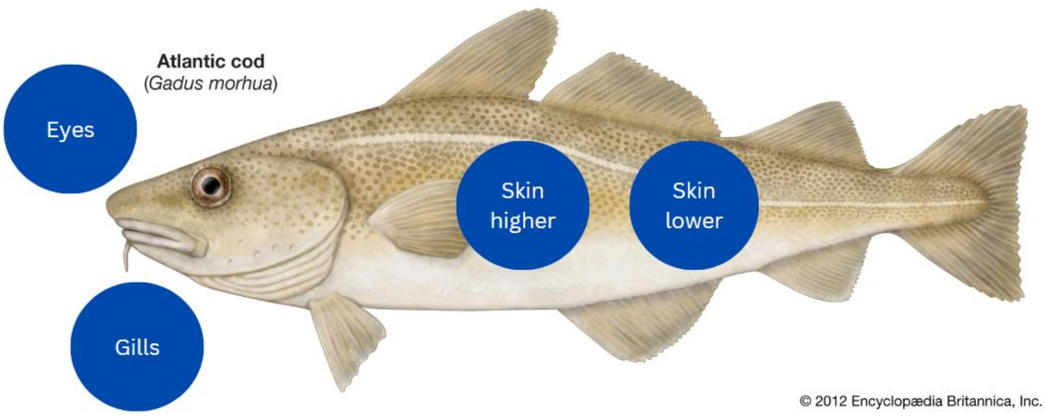

Figure 1 Overview of image capturing. Image adapted from "Atlantic cod," by Encyclopedia Britannica, 2012.

During the study, 110 fish were imaged, and 30 of those fish were imaged over the entire storage period. Images were taken of the eyes, gills, and two regions of the skin (**Figure 1**). Concurrent with the MSI imaging, eight reference sampling events were conducted. In these sessions, each cod specimen underwent sensory evaluations by eight specially trained panelists using the QIM method. This sensory evaluation method records and rates individual quality factors, which are then aggregated into an overall quality index, a metric linearly correlated with storage time on ice, thus providing an estimate of shelf life and remaining freshness (Martinsdóttir et al., 2001). Alongside the sensory evaluations, chemical and microbiological analyses were conducted.

These included measuring the total volatile basic nitrogen (TVB-N) of muscle and the total viable count (TVC) of fish muscle and skin.

Preliminary analysis using Partial Least Squares Regression (PLSR) showed promising correlations between MSI data and overall QIM scores, with spectra on skin showing a good correlation between both the total QIM score (R^2_{cv} = 0.77, RMSECV = 2.85) and individual quality factors for the skin, such as stiffness (R^2_{cv} = 0.96, RMSECV = 0.13). While the analysis of spectra of the eyes, which encompassed the whole eye, showed a strong correlation with distinct quality factors such as eye form (R^2_{cv} = 0.91, RMSECV = 0.21), the correlation with the overall QIM score was not as strong (R^2_{cv} = 0.35, RMSECV = 5.29). Further analysis into specific regions of the eye, notably the pupil, demonstrated a good correlation with the overall QIM score (R^2_{cv} = 0.71, RMSECV = 3.28), highlighting the pupil's distinct contribution to the freshness assessment. These initial findings underscore the potential of MSI in assessing the freshness of whole fish.

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A072. A direct comparison of a next generation hyperspectral camera to state-of-the-art

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Hyperspectral camera technology is advancing rapidly, and this study seeks to compare a state-of-the-art industrial dual-camera setup to a single-camera system employing the latest chip technology (IMX990 from Sony). The hyperspectral cameras are compared over both the Visual and Short-Wave Infrared range (400-1700 nm) of the electromagnet spectrum. The spectral range and resolution, as well as spatial parameters and spectroscopic information are quantified with comparable optics, electronics, and test targets. Generally, enhanced spectral detail and reduced noise were observed for the new generation compared to its peers as seen in **Figure 1**.

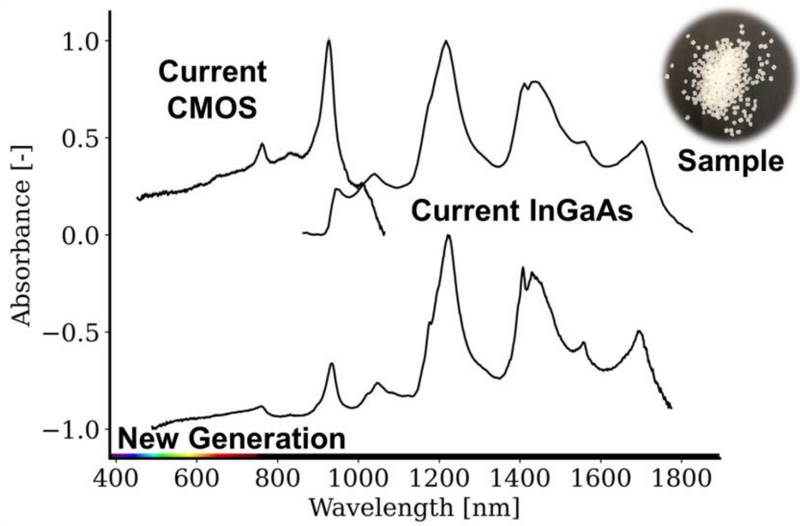

Figure 1. Spectral comparison of polyethylene, acquired with both the current state-of-art hyperspectral cameras and the new generation hyperspectral camera.

The presentation will go through, how the cameras are calibrated (Henriksen 2022), followed by quantification of performance via Modulated Transfer Functions and spectral Signal-To-Noise ratios, finally, several industrial relevant plastic types are measured to highlight the relevance of this technological advancement. Key findings are better signal-to-noise ratio, more reliable crossover regions, simplicity compared to alignment in multimodal systems, clearer spectral features and enabling a more detailed spectral assignment. The overall improvement, its industrial implications and where our research is heading will be touched upon in the end of the presentation.

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A075. Joint CP Decomposition and Learnable Mapping for One-Shot Anomaly Detection in Hyperspectral Images

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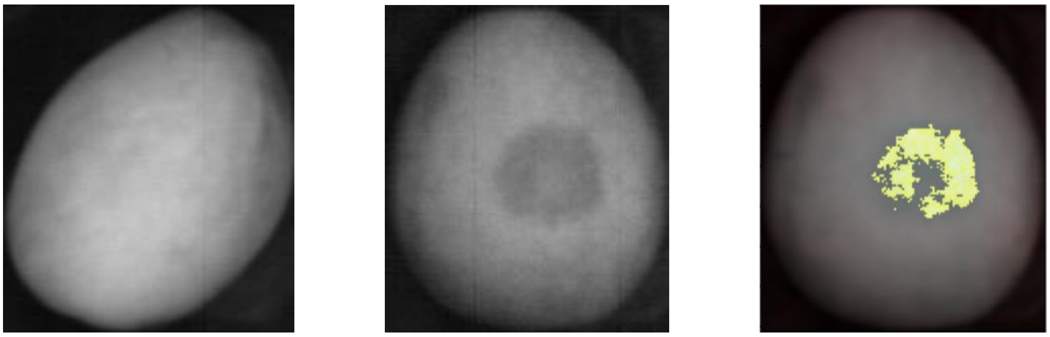
Anomaly detection in hyperspectral images (HSIs) is a crucial task with applications in agriculture, surveillance, and environmental monitoring. HSIs, which capture detailed spectral information across numerous bands, can reveal subtle anomalies that may not be visible in conventional RGB images. However, the high dimensionality of HSIs and the scarcity of labeled anomalous samples pose significant challenges for anomaly detection algorithms.
In this presentation, we introduce a novel one-shot anomaly detection method designed to address these challenges. Our approach is rooted in tensor decomposition (TD), a powerful mathematical framework that allows us to analyze hyperspectral images (HSIs) in their natural three-dimensional structure (two spatial dimensions and one spectral dimension). This is in contrast to traditional methods that often flatten or vectorize HSIs, potentially losing valuable spatial-spectral relationships. TD methods, such as the Canonical Polyadic (CP) decomposition, decompose the HSI tensor into simpler components, revealing underlying patterns and structures within the data. While TD has been used before for anomaly detection in HSIs (Zhang, 2016), these methods have primarily focused on finding small, distinct targets within a uniform background.
Our focus, however, is on detecting anomalies as general deviations from a normal or control sample. We achieve this by jointly performing CP decomposition on both the anomalous and control HSIs, along with a learnable mapping function that aligns the spectral factor matrices of the two tensors. The learnable mapping function, inspired by the work of Lu et al. (2017), aims to bridge the domain gap between the anomalous and control images by transforming the spectral signatures of the control image to match those of the anomalous image. The proposed method's objective function is formulated as follows:

$$\min_{\substack{A_A,B_A,C_A,A_C,B_C,C_C \\ \Phi}} \left\| X_A - [[A_A, B_A, C_A]] \right\|_F^2 + \left\| X_C - [[A_C, B_C, C_C]] \right\|_F^2 + \lambda \left\| A_C - \Phi(A_A) \right\|_F^2$$

where X_A and X_C represent the anomalous and control HSIs, respectively, and $[[A, B, C]]$ denotes the CP decomposition with factor matrices A (corresponding to spectral mode**)** and B and C (spatial modes). The mapping function $\Phi(*)$ is a shallow neural network that learns a nonlinear transformation between the spectral factor matrices A_A and A_C. The regularization parameter $\boldsymbol{\lambda}$ controls the trade-off between the reconstruction error and the mapping error. This optimization problem is solved through gradient descent, as opposed to the conventional ALS approach for CP, to allow the joint optimization of the neural network's Φ parameters. To detect anomalies, we compute the pixel-wise mean squared error (MSE) between the reconstructed anomalous $X_A^* = [[A_A, B_A, C_A]]$ and the mapped HSI $X_{A\to C}^* = [[\Phi(A_A), B_A, C_A]]$. Anomalies are identified as pixels with high reconstruction errors, indicating a significant deviation from the normal spectral behaviour.



(a) (b) (c)

Figure 2. *Results from rank 30 Joint CP with NN mapping* $(\lambda = 10^{-4})$*, HSIs displayed at 941 nm. (a) Control (b) Anomalous (c) Top 5% errors*

We evaluate our method on a dataset of hyperspectral images of plums (210 bands, VIS-NIR), where the anomalies are represented by early bruises caused by controlled impact, visible only in the NIR range. Our results demonstrate that the proposed method can effectively detect bruises at early stages, using only one control image **(Figure 1).** We also found that the use of a neural network as the mapping function allows us to capture nonlinearities in the spectral transformations, leading to improved anomaly detection performance compared to a linear mapping function.

In conclusion, our one-shot anomaly detection method based on joint CP decomposition and learnable factor matrix mapping offers a promising solution for identifying anomalies in HSIs. By leveraging both spectral and spatial information and incorporating a nonlinear mapping function, our method can accurately detect subtle anomalies in challenging scenarios with limited reference data. Future work will focus on developing automatic thresholding techniques and exploring the application of our method to other types of HSIs and anomaly detection tasks.

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A080. Integration of an XRF-VNIR-SWIR hyperspectral imaging system with multiblock data processing for a non-invasive unveiling of Raffaello painting techniques

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A urgent issue in cultural heritage investigation consists of the need for acquiring information regarding the in-depth distribution of organic and inorganic components, without any invasive sampling. To address this requirement, a new analytical set-up, able co-register VNIR, SWIR, and XRF spectral data, was exploited in combination with a multivariate and multiblock data processing strategy, for the analysis of multilayered paintings.
The instrument simultaneously records X-ray fluorescence (XRF,1.4-40 keV) data, together with visible & near-infrared (VNIR, 380–1100 nm) and short-wave infrared reflectance (SWIR, 1100–2500 nm) spectra, obtaining elemental and molecular information from superficial to subsurface layers across the investigated area. Data from these three spectral ranges were co-registered, thus inherently saved with high spatial coherence.
The chemometric strategy applied efficiently reduced data and extracted valuable information from the three different spectroscopies. For an effective data visualization and inter-correlation assessment, the approach combined principal component analysis (PCA), brushing, correlation diagrams, and maps within and between spectral blocks, using both low-level and mid-level data fusion. Correlation diagrams and maps are particularly useful for reconstructing a stratigraphic structure without sample collection. They account for inter-correlations among data variables, characterizing possible component combinations at the same depth level.
The method was applied to the extraordinary painting of San Sebastiano attributed to Raffaello Sanzio (1483-1520) and exhibited at the Accademia Carrara (Bergamo, Italy), to obtain information on the mixtures of artist pigments and techniques, while preserving the integrity of the artwork. In particular, it was possible to uncover the painting technique used for the background, which relied on the presence and superimposition of different layers composed of malachite, azurite, and lapis lazuli to modulate the color shade and tonality of the landscape and sky.

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A088. Solving the missing information problem in image fusion through single factorization unmixing analysis.

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Image fusion faces many challenges due to the platform-to-platform differences in terms of scanned area, spatial resolution, sample orientation or spectroscopic dimensionality. Indeed, when coregistration among images is carried out, there are many platform-specific pieces of information that do not find equivalence in the other imaging systems employed.
Unmixing analysis of data structures coming from image fusion improves significantly the characterization of the sample constituents due to the complementary spectroscopic (chemical) information. Algorithms such as Multivariate Curve Resolution-Alternating Least Squares (MCR-ALS) are particularly useful for this purpose since multiset analysis allows for the construction and interpretation of structures formed by data blocks coming from different scanned samples by different platforms (Tauler 2020). However, the classical application of MCR-ALS in this framework requires complete multisets that enclose equivalent pixel information, i.e., the same scanned area with the same spatial resolution for all coregistered images fused. This strong requirement forces downsampling images to the pixel size of the platform with the lowest spatial resolution and working only with the scanned area that is common to all images.
Using all available spectral and spatial information in image fusion necessarily implies working with pieces of information that will not find an equivalent definition in all platforms, i.e., the incomplete multiset generated will have full blocks of missing information linked to non-common scanned areas and/or to pixels with small sizes that can only be attained by some platforms (see F. 1).

For complete multisets, MCR-ALS works iteratively using a single factorization to obtain the basic bilinear model in equation 1:

$$\mathbf{D} = \mathbf{C}\mathbf{S}^{T} + \mathbf{E} \qquad (1)$$

where **D** is the initial multiset data with blocks of spectra from different samples and imaging platforms, **C** and $\mathbf{S}^T$ are the matrices related to concentration profiles (which can be turned into distribution maps) and to the concatenated pure multiplatform instrumental responses of the components of interest, respectively, and **E** is the matrix of model residuals.

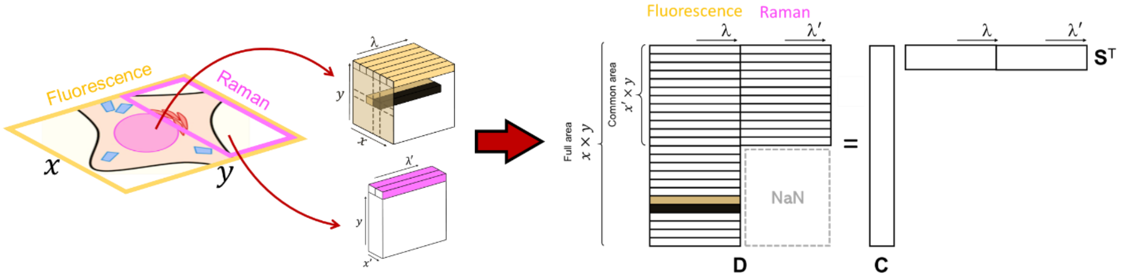

Figure 1. Illustrative example of an image fusion of hyperspectral images with different scanned areas, where the full sample area is scanned by fluorescence imaging and only a small region by Raman imaging. The incomplete multiset formed has an empty block, related to the sample area not scanned by Raman (set as Not-A-Number, NaN), and a complete fused region where both signals are available for each pixel. Nevertheless, this information allows recovering the full bilinear model.

Incomplete multisets can be analyzed either using imputation approaches to recover the full structure or working with only the available information, which often implies using algorithms that perform and combine multiple factorizations on complete submultisets to obtain the global bilinear model sought (Piqueras 2018).

The new approach proposed allows analyzing incomplete multisets by MCR-ALS with a single factorization and without performing data imputation. The new methodology exploits that **C** and $\mathbf{S}^T$ can be calculated in a least-squares manner one row at a time (eq. 2) and one column at a time (eq. 3), obeying the following formulations of the bilinear model:

$$\boldsymbol{d}(i,:) = \boldsymbol{c}(i,:)\mathbf{S}^T + \boldsymbol{e}(i,:) \qquad (2)$$

$$\boldsymbol{d}(:,j) = \mathbf{C}\boldsymbol{s}^T(:,j) + \boldsymbol{e}(:,j) \qquad (3)$$

Following these formulations and using only the non-missing values of every **D** row and the matching columns of $\mathbf{S}^T$, the **C** matrix can be obtained one row at a time (eq. 2). Likewise, with the non-missing values of every column of **D** and the matching rows of **C**, the full $\mathbf{S}^T$ matrix can be obtained one column at a time (eq. 3). Working in this way, no data imputation is needed and a single factorization provides the global bilinear model sought (Gómez-Sánchez 2024).

The approach is tested in diverse simulated and real image fusion problems to show that the algorithm adapts to any data configuration, pattern and percentage of missing values.

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A091. Magnificent colors in ancient Roman wall paintings. On-site Vis-NIR Hyperspectral Imaging in Ostia Antica Archeological Park

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The applications of Hyper-Spectral Imaging (HSI) in the field of Cultural Heritage (CH) have exponentially increased over the last decade, with a significant growth of publications which demonstrates the technique's multiform capabilities for non-invasive analysis and augmented visualization of artworks. Beside the well-rooted applications of HSI in museum contexts, an emerging research branch aims at transferring the know-how gained from HSI technology for artworks into the archaeological research. This is a challenging task, due to technical issues and, more importantly, to a lack of in-field experimentation. A pioneer study carried out in Pompeii demonstrated a huge potential of reflectance HSI, implemented in the extendedVIS-NIR-SWIR range, for investigating - extensively and non-invasively - painted surfaces and inscriptions in archeological contexts (Cucci 2020). However, this campaign was carried out with complex and costly remote-sensing technology, based on avionic instrumentation, which remained an isolated application.
Recently, thanks to the development of a new generation of compact HSI cameras the scenario has changed. Despite their lesser technical performances, these devices can open new applicative perspectives. Within this framework, portable reflectance HSI technique in the Vis-NIR range has been proposed as an innovative methodology for non-invasive investigations of polychrome surfaces and wall paintings in Ostia Antica archeological Park.
The ancient city of Ostia was the harbor of Rome, thus mirroring the Roman civilization history. Today Ostia is one of the largest archaeological areas in Italy, and hosts several exceptionally preserved wall paintings, covering a temporal arc from the 2nd century BCE to the 5th century CE. This makes this site a unique, open-air laboratory for investigating the evolution in time of Roman paintings, along with their changes in styles, materials and pictorial techniques, from the Republic era to Late Antiquity. An ambitious research program, currently on-going, was undertaken in 2019 with the goal of systematically investigating the walls paintings of the city, using a non-invasive and multi-analytical approach, with both routine analytical methods and novel tools (Blümich, 2021). Among these, in March 2023 portable HSI technique was also included. A HSI compact camera (Specim IQ), operating in the 400-1000nm range with 2 nm spectral resolution was used for measurements on walls paintings of selected houses, which were also analyzed with other non-invasive techniques. The HSI data were exploited for both spectroscopic analysis and augmented visualization of the polychromies. The issues of illumination and calibration can limit the applicability of the technique and measurements were acquired in a variety of settings to test different operative conditions. Overall, the results demonstrated the suitability of HSI technique not only for identifying pigments, but also for mapping materials distribution on the wall surfaces. This resulted particularly important for a fast detection of anomalous and non-original zones, such as undocumented restorations. In addition, HSI data elaboration (e.g. PCA, MNF) enabled enhancement of details that are not visually evident (e.g. faded decorations) and visualization of hidden structures. The most significant outcomes of the first HSI experimentation carried out in the Ostia archeological area will be presented, with a discussion on open issues and future perspectives.

Figure 1. HSI measurements campaign on wall paintings in the "Giove and Ganymede" house Ostia Antica Archeological Park

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A097. Increasing spatial resolution in polarized Raman microscopy with tensor decomposition-assisted super-resolution

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Polarized Raman microscopy is a valuable tool for the non-destructive analysis of anisotropic materials (e.g., for the 2D and 3D orientation mapping of polycrystals – **Ilchenko2019**). The spatial resolution in far-field Raman microscopy is limited by the Rayleigh criterion and its further increase is commonly achieved using complex instrumental techniques such as tip-enhanced Raman spectroscopy (**Kawata2017**). Nonetheless, for such resolution enhancement. it is alternatively possible to exploit computational approaches which do not require complex instrumentation. Chemometric assisted super-resolution image restoration, for example, has already been successfully used for this purpose (**Offroy2015**, **Wintrauer2020**, **Li2021**). Here, the basic idea is to use chemometric methods (like multivariate curve resolution or principal component analysis) to decompose or factorize the data at hand, decrease their original dimensionality and perform super-resolution restoration on the resulting single-component images. Polarization Raman maps can be regarded as trilinear data and, therefore, PARAFAC can be used for the aforementioned factorization step (**Miron2019**). PARAFAC is attractive because it guarantees unique decomposition under mild conditions **(Kolda2009)**. In this work, we used PARAFAC for the analysis of polarization Raman maps of different polycrystalline samples (such as nanodiamonds and calcite) with further super-resolution image restoration (Figure 1). This allowed us to obtain richer information regarding the physicochemical properties of spatial heterogenous samples as well as resolved polarization Raman profiles that can be used for the determination of the orientation of polycrystalline structures.

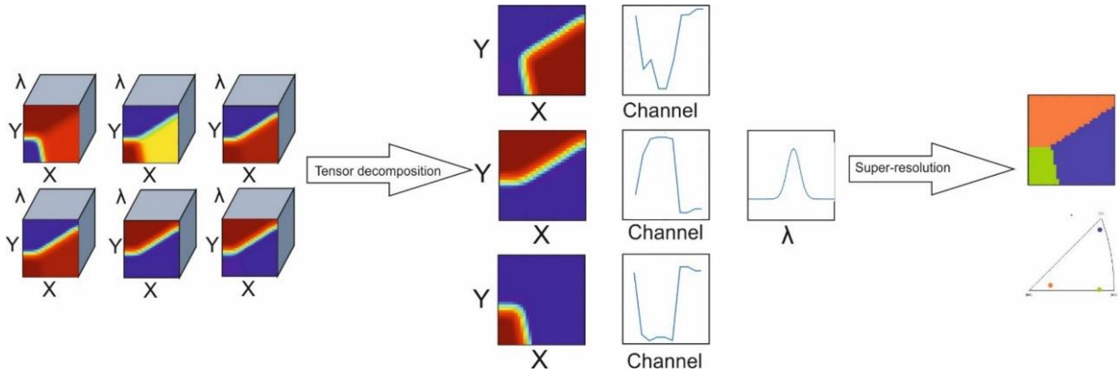

Figure 1. Tensor decomposition-assisted super-resolution pipeline.

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A103. Early detection of water deficit stress in *Eucalyptus spp.* through VIS-NIR hyperspectral imaging technologies and multivariate analysis

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Early detection of water stress in *Eucalyptus spp (E. globulus, E. nitens)* is a crucial challenge for the forestry industry. In this sector, eucalyptus production is especially important, given its large presence in the central and southern regions of Chile. The development of a tool to anticipate water stress situations in these species could have a significant impact on the efficiency and sustainability of the forestry industry, contributing to its resilience to the challenges of climate change.

In the context of the study of water stress in *Eucalyptus* plants, physiological analyses and multispectral analyses to calculate vegetative indices play an essential role in understanding how water scarcity affects the development and performance of these species. However, the specificity of these methods can be limited. This work aims to solve this problem through the development of more direct, efficient, and accessible methodologies to detect water stress in *Eucalyptus spp.* and to evaluate plant recovery after the stress period, with the purpose of contributing to breeding programs. For this purpose, different clones of *Eucalyptus spp*. were subjected to water-deficit stress, in contrast to a control group, in order to evaluate the capabilities of artificial vision techniques for the detection of the level of stress produced in plants, through the use of hyperspectral images in the VIS-NIR range.

Spectral data were obtained from different areas of the plant on days 3, 7 and 10 of stress, using the Pika-L hyperspectral camera, Resonon (Inc), with a spectral range of 400 -1000 nm and spectral resolution of 3.9 nm. The pre-processing of the images, particularly the masking step, was performed using the HyperTools V.3.0, followed by exploratory analysis using Principal Component Analysis (PCA) and finally using Partial least squares-discriminant analysis (PLS-DA) to obtain a predictive model to predict stress level expressed in days. Chemometric analysis was developed using MATLAB R2013a (Mathworks Inc) and PLS_Toolbox (Eigenvector Inc).

PCA analysis evidenced distinctive clustering of the data according to stress, depending on the sampling days, separating samples from day 10 from the others (days 3 and 7) (Figure 1). When examining the loadings matrix, it is concluded that this differentiation is attributed to the contributions of the bands at 701 and 385 nm, which are associated with chlorophyll and flavonoids, respectively (1,2). These findings indicate that day 10 samples show a stress response with an increase in flavonoid production, while days 3 and 7 show a disparity in chlorophyll content that separates them from the rest of the group.

Furthermore, the predictive model exhibited a prediction error of 2% (Table 1), which places it in an advantageous position with respect to the vegetative indices, because it allows us to identify signs of stress from the seventh day of water deficit, even before they are visible in the plants. Besides, PLS-DA was useful to reconstruct images of plants to detect zones with a estimated level of localized stress (Figure 2).

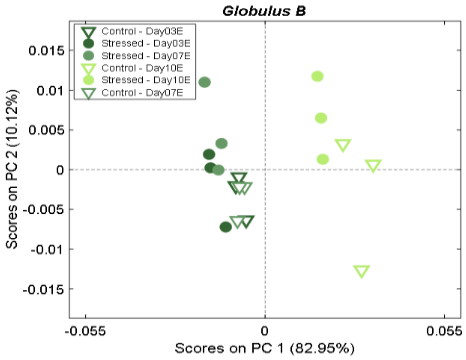

Figure 1: PCA with second derivative and 15-point smoothing for *E. globulus* clones in different stress states according to their sampling day.

Table 1: Confusion matrix for PLS-DA model with three classes, representing the level of stress according to the sampling day.

	Validation Set		
	Actual Class		
Predicted	*Day03*	*Day07*	*Day10*
Day03	15	0	0
Day07	0	16	0
Day10	1	0	16
Unassigned	0	0	0
Err	2%	0%	2%

This predictive tool was used to reconstruct images of plants with different levels of stress, where, in addition to verifying their stress condition, an approximation of the spatial distribution of stress in the plant can be made, as shown in Figure 2.

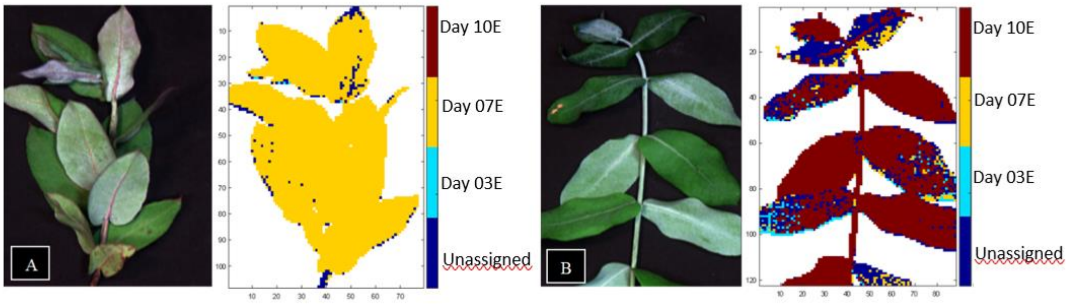

Figure 2. Image reconstruction by PLS-DA model. Globulus day 7 of stress (A) and Globulus day 10 of stress (B).

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A113. H.E.I.M.D.A.L.
Deploying a Computed Tomography Imaging Spectrometer camera system on a REXUS/BEXUS Balloon Mission.

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The H.E.I.M.D.A.L. (Hyperspectral Environmental Imaging Measurements Differentiating between Areas of Localized specimen) team is participating in the Balloon Experiements for University Students 34/35 project of the **REXUS/BEXUS** (https://rexusbexus.net/, last accessed April 2024) programme, and will fly on vehicle: BEXUS 35 with a planned launch in October 2024. The H.E.I.M.D.A.L. experiment consists of a Computed Tomography Imaging Spectrometer (CTIS) and an RGB camera, provided and developed by NEWTEC Engineering A/S. The experiment is both a technology demonstrator and a scientific mission. The flight will test the hyperspectral snapshot imaging system in the harsh environment of the stratosphere following tests in the Mars Simulation Laboratory at Aarhus University in DK, able to simulate stratospheric conditions. The scientific goals include differentiating between vegetation types including Norway Spruce (Picea Abis) and Scotch Pine (Pinus Silvestris), two specific pine tree species.
The CTIS images recorded will be reconstructed both on-board and post flight using both a deep convolutional neural network (Huang 2022, Ahlebæk 2023) and more traditional methods like the Expectation Maximization (EM) algorithm (Shepp 1982).
The preliminary design of the experiment is visualized in **Figure 1** and shows all camera modules and the electronics box.

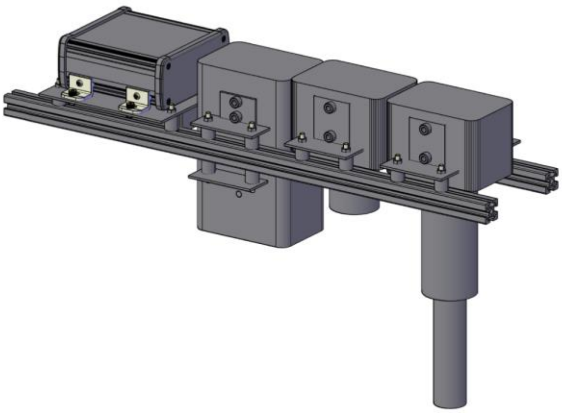

Figure 3. Visualization of the experiment mounted on aluminium extrusions. From left to right: The electronics box, the camera computer module, the RGB module and the CTIS module.

I will present the experimental design, the imaging processing and the scientific applications that arise with hyperspectral imaging on stratospheric platforms.
The REXUS/BEXUS Programme allows students from universities and higher education colleges across Europe to carry out scientific and technological experiments on research rockets and balloons. Each year, two rockets and two balloons are launched, carrying up to 20 experiments designed and built by student teams.

Both the REXUS and BEXUS vehicles are launched from Esrange Space Center in Northern Sweden.
The team consists of bachelors-, masters- and PhD students from the University of Southern Denmark (SDU) and Aarhus University (AU), from engineering (Electronics, Mechanical and Software), physics and Biology and is supervised by associate profs. Christoffer Karoff (AU), Rene Lynge Eriksen and Mads T. Frandsen (SDU)

Figure 4. The H.E.I.M.D.A.L. team after successfully presenting at ESTEC in the Netherlands.

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REXUS/BEXUS: The REXUS/BEXUS programme is realised under a bilateral agency agreement between the German Aerospace Center (DLR) and the Swedish National Space Agency (SNSA). The Swedish share of the payload has been made available to students from other European countries through the collaboration with the European Space Agency (ESA).

A115. Hyperspectral Pixel Unmixing with Large Spectral Libraries on Soils and Minerals

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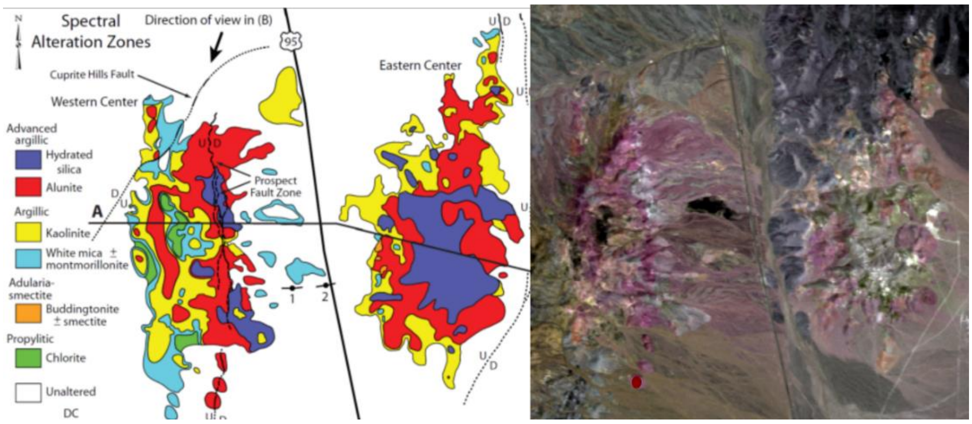
Hyperspectral unmixing is the process of determining the individual materials present and their abundances at the pixel location from the spectrum. This is a fundamental process for hyperspectral image processing, and the basic method is linear regression with the coefficients providing the abundances. However, unmixing with a large library requires inverting a non-invertible matrix when there are more spectra in the library than bands in the image. This problem is magnified in the case of mineral spectra, where intimate mixtures require nonlinear methods. Thus, regularization of some type is a necessity for hyperspectral unmixing when the materials present are not known a priori (Borsoi 2021).

In this talk we investigate the use of major statistical regression models which can be used for unmixing. In these models, coefficients represent the abundance of the respective minerals and the model selection process is used to identify the minerals that are present out of a large library. We consider parametric regression models that are linear and higher-order polynomial to model the multiple photon-material interactions. Regularization comes in the form of a penalty on model size, or some approximately equivalent mathematical formulation (Li,2019). Thus, we consider ordinary least squares regression, ridge regression, lasso regression, elastic nets, Bayesian model averaging methods, and stepwise regression (Gault, 2016).

Our pure material spectra are from the USGS spectral library along with additional spectra we collected with an ASD Field Spectrometer, and the mixed-material spectra are from the USGS library as well as mixed-material spectra we collected. For ground-truthed image pixel spectra, we use AVRIS imagery over the well-studied Cuprite Nevada. Figure 1 displays an image of the dataset as well as a mineral location considered for detection (Swayze, 2014).



(a) (b)

Figure 1. Figure 1 shows approximate mineral locality of the Cuprite Hills dataset. The red dot in Figure1(b) indicates the location of one of the pixels we are unmixing with high amounts of alunite (Swayze, 2014).

We evaluate approaches using multiple criteria (see Table 1 for preliminary results). First, we determine if the model presents the correct materials with reasonable abundances. Second, we verify the provided nonzero abundances for materials are actually present in the observed pixel.

Third, we evaluate the model provides some evidence of accuracy, for example low error. Additionally, we discuss runtime and practical considerations, but because these are dependent on optimized implementations, we do not include this as a formal evaluation metric. While we provide rigorous evaluation metrics for all models and datasets, our goal is not just a bake-off to find the best performer or class of top performers. We provide an algorithm taxonomy for the methods we present and discuss how the various models incorporate the physical-chemical phenomenology in the spectral mixing.

Table 1. Table 1 compares the techniques in terms of model accuracy, abundance non-negativity and model size.

	OLS	Ridge Regression	Lasso Regression	Stepwise Regression	Bayesian Model Averaging
Non-negative Abundances?	No	No	Yes	Yes	Yes
Model Size	480	480	7	3	6
Mineral Detected?	Yes	No	Yes	Yes	Yes
RMSE	0.001	0.007	0.005	0.006	0.005

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A142. Transferring weights from RGB Large Visual Models into multispectral Deep Neural Networks

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In the constantly evolving field of computer vision, the role of foundational models has gained increasing importance. These foundational models, often pre-trained on large-scale datasets, serve as a versatile starting point for fine-tuning and subsequent adaptation across a wide variety of computer vision tasks. Their impact extends to diverse applications, including segmentation, image classification, and image generation, where they have demonstrated remarkable performance and generalization capabilities.
While foundational models have proven to be highly effective in the realm of RGB images, their application in the multispectral domain remains limited. Multispectral images, which capture a wide spectrum of light, provide information beyond what can be seen in RGB images. However, the unique characteristics of multispectral data, such as high dimensionality and spectral variability, present new challenges that foundational models, primarily trained on RGB images, may not be equipped to handle.
In light of this, our research aims to evaluate the performance and adaptability of foundational models, specifically DINOv2 (Oquab 2023), in the multispectral domain for downstream tasks. We focus on image segmentation which involves dividing an image into multiple segments or regions, each corresponding to different objects or parts of objects. We use the Agriculture-Vision dataset which is a combination of processed and labeled images (Chiu 2020), and raw, unprocessed agricultural images. Both subsets contain images featuring a variety of spectral channels, including red, green, blue, and near-infrared (NIR).
Our research has focused on the creation of a model based on DINOv2 that transfers the existing knowledge from RGB weights to a multispectral neural network. This has resulted in an improvement in the performance, compared to training a segmentation model entirely from scratch.

Table 1. Results

Backbone	Decoder	Weights	mIOU	mIOU thr	mF1	mF1thr
U-Net	U-Net	-	0.2955	0.3168	0.4081	0.4514
DinoV2	Linear	RGB	0.29	0.31	0.42	0.46
DinoV2	U-Net	RGB	0.3966	0.4145	0.5412	0.5661

From the obtained results, we can conclude that using a foundational model and transferring the initial weights from RGB to the multispectral domain yield better outcomes than simply training a segmentation model from scratch.

Building on our successful implementation, we plan to extend our work to leverage both the labelled and unlabelled multispectral data. Our future work aims to fine-tune DINOv2 in a self-supervised manner, using both the unlabelled and the training labelled multispectral data. This fine-tuning process will enable DINOv2 to better adapt to the peculiarities and inherent challenges of multispectral data, potentially enhancing its performance in downstream tasks.

This research has been supported by the Elkartek Programme, Basque Government (Spain) (SMART-EYE, KK-2023/00021 (P. Galan & A. Picon) and BEREZIA, (KK-2023/00012) (A. alvarez-Gila and Leire Benito))

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A146. Integrating Multispectral Photometric Stereo with Hyperspectral Imaging: A Unified Approach for Enhanced Surface Analysis and Spectral Insights

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Hyperspectral Imaging (HSI) and Multispectral Photometric Stereo (MPS) (1; 2) techniques rely on the analysis of light-surface interaction, but approach it from different perspectives. On the one hand, HSI focuses its attention on analysing the subtle changes in radiance and reflectance spectra at each pixel, which depends on the chemical composition of the imaged object. On the other hand, Photometric Stereo (PS) (3; 4; 5) aims to recover the normal vector field of the object surface (and indirectly the 3D shape) by exploiting the image intensity variations produced when illuminating the object from different directions. MPS extends the underlying principle of traditional PS to overcome its time-multiplexing approach, by using a different wavelength light source for each direction to achieve a one-shot measurement. However, in MPS, the wavelength-dependent reflectance of the surface introduces a systematic bias on the estimation of surface normals. Therefore, spectra variations in which an HSI system is based, pose a challenge for PS, complicating the integration of both technologies into a unified set-up and constraining the utilisation of their combined data for a comprehensive analysis of the imaged object.
Typical scenarios require either a detailed spectral analysis or precise surface geometry recovery. However, in certain applications, combining both fields can provide deeper insights into the imaged object. For example, in the metal manufacturing industry, surface defects have a deep influence on a wide range of physicochemical properties that affect, for example, the corrosion resistance of the material and the mechanical properties. Another example lies in the field of cultural heritage preservation, where performing a geometrical and chemical characterisation enables conservators to conduct historical studies, plan conservation treatments, etc. (6). Although there are several works based on MPS, they are mainly focused on dealing with the wavelength dependent reflectance and on improving the accuracy of the estimated geometry in a single shot, and they do not further exploit the acquired spectral information.
In this work, we present our ongoing efforts to develop a method that integrates multispectral photometric stereo (MPS) with hyperspectral imaging to simultaneously acquire geometric and spectral data of observed surfaces. We describe the devised imaging system, based on a linear hyperspectral camera and different wavelength LED light sources, and we present some preliminary results that show the potential of the proposed method. Figures 1, 2 and 3 show the results obtained for one of the samples.

ACKNOWLEDGMENTS

This work was partially funded by Basque Government (KK-202300021 ELKARTEK 2023/2024)

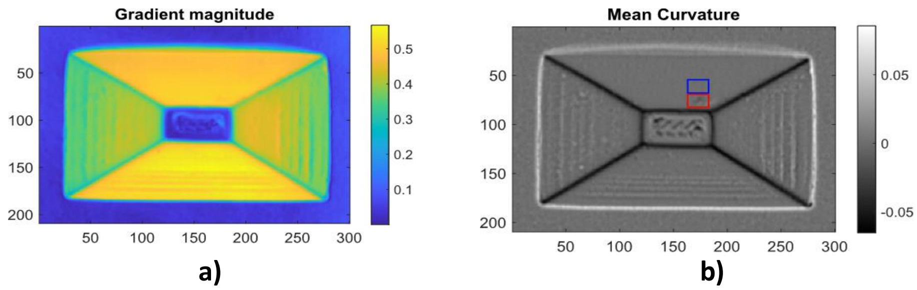

Figure 1. Truncated pyramid 3D printed in PLA. **a)** Surface gradient magnitude plot. **b**) Mean curvature plot. Regions enclosed by blue and red squares correspond to PLA and a foreign body inclusion. The geometrical imperfections in the topand lateral faces remaining after a sanding operation are visible.

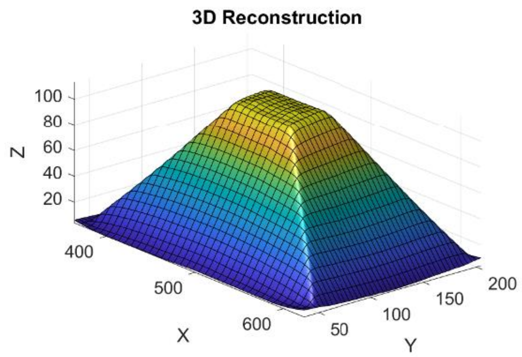

Figure 2. Truncated pyramid 3D printed in PLA. 3D reconstruction

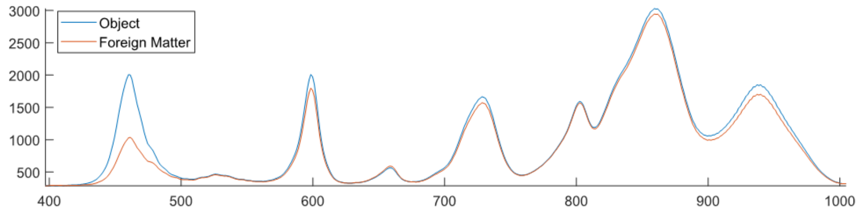

Figure 3. A foreign body inclusion in one of the truncated pyramid faces can be detected from the spectral signature. Meanspectra of PLA and foreign body inclusion regions corresponding to the blue and red squares in Figure 1 – **b)**.

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A150. MIR and NIR Hyperspectral imaging for food quality control

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Food quality control encompasses topics such as the detection of adulterations, contaminations, frauds, the verification of the safety of use and genuineness, and of labeling compliance, including the possibility of tracing the origin (botanical, animal, geographical) of the food. In this context, the use of hyperspectral imaging, especially in the infrared region, which is particularly rich in contributions from the food constituents, represents a promising tool supporting producers, consumers and regulatory entities, due to its ability to couple a detailed spectroscopic signature at each pixel with the possibility of characterizing the spatial distribution of specific molecules or families of substances.
At the same time, foods are rather complex matrices and their composition is influenced by many sources of variability, so that their characterization and authentication may profit from the integration of the complementary information from different spectroscopic platforms. Based on these considerations, in the present communication, the use of a combined MIR and NIR hyperspectral imaging system in the context of food quality control will be presented and discussed. Attention will be focused on one hand on the different information brought by the different platforms and on the other on the way near and mid infrared data can be integrated through data fusion strategies for improving model performances.
Examples will involve the characterization of rice samples, quality control of coffee beans and, more extensively, the results obtained within the framework of the National project Agritech, where the use of MIR and NIR hyperspectral imaging for tracing the whole supply chain of specific food products was investigated.

A005. Infrared spectroscopy: Alternative method for assessment of trace elements and mineral composition in soil

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Agricultural product provenance is emerging as a major concern globally for consumers, food industries, and regulatory bodies due to product safety issues, fraudulent relabeling of products, and a desire by consumers to know the origin of the products. Australia, having reputation as a provider of high-quality products such as beef, wool, wheat, cotton, diary, wine etc. being able to verify the product geographic origin is a key requirement for protecting the high-quality brands of Australia. Product provenance has been studied using various analytical techniques including DNA traceability, stable isotope analysis, and trace element analysis. However, the common methods that are used to analyse the isotopes and trace elements such as isotope ratio mass spectrometry (IR-MS), Inductively coupled plasma optical emission spectroscopy (ICP-OES) are cost intensive, required special sample preparation, and require special training in the sample analysis.

The main objective of our work is to develop an easy, low cost, user friendly, robust, and efficient method to analyse the composition of agricultural products and identify their product origin. Plants derive their mineral content from soil type and parent material, soil fertilization, botanical origin, pollution, and production year. Some elements are directly linked to geology and subsequently weathered soil parent materials of the area and are minimally influenced by different production methods and harvest year. Therefore, the elemental profile measured in agricultural products will reflect the composition of bioavailable and mobilized nutrients present in the underlying soils where they were grown. As the initial step, we analysed the trace elemental and isotope composition of bulk soil and soil fractions (including fine fraction and coarse fraction), using ICP-OES, XRF and XRD characterization methods. The Soil samples were collected from six different sites of South Australia (named as FP1-FP6) and were analysed for the elemental (Figure 1a), and mineral (Figure 1c) composition. The NIR and MIR spectra were collected from the same samples (Figure 1b) and PLSR code is being developed using XRF, ICP-OES results as the reference data set. In future, we will use the short and mid infrared spectra to identify the trace elements in a sample, which has the potential to become a key technique underpinning food origin and traceability.

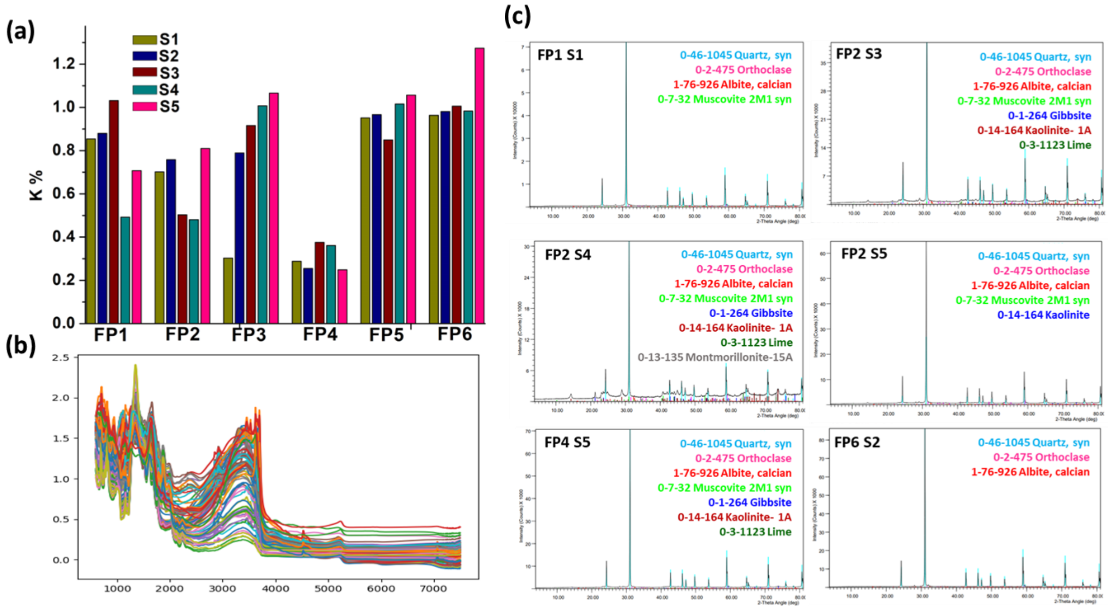

Figure 1 The elemental composition and mineral composition was analysed using XRF and XRD respectively. The soil samples were further analysed using NIR in order to develop a prediction method. (a) Potassium concentration of the soil samples, (b) mineral composition of the soil samples collected from sites FP1-FP6. (c) MIR spectra of soil samples.

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A011. New automatic cosmic spikes removal algorithm for Raman images

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In this study, a new algorithm for automatic detection and removal of cosmic rays in hyperspectral Raman Images is presented. Charge-coupled device (CCD) detectors employed in Raman instruments occasionally suffer from spikes caused by the unexpected impact of cosmic rays, which generate artifacts in the acquired spectra, thus adding information not chemically related to the analyzed material.

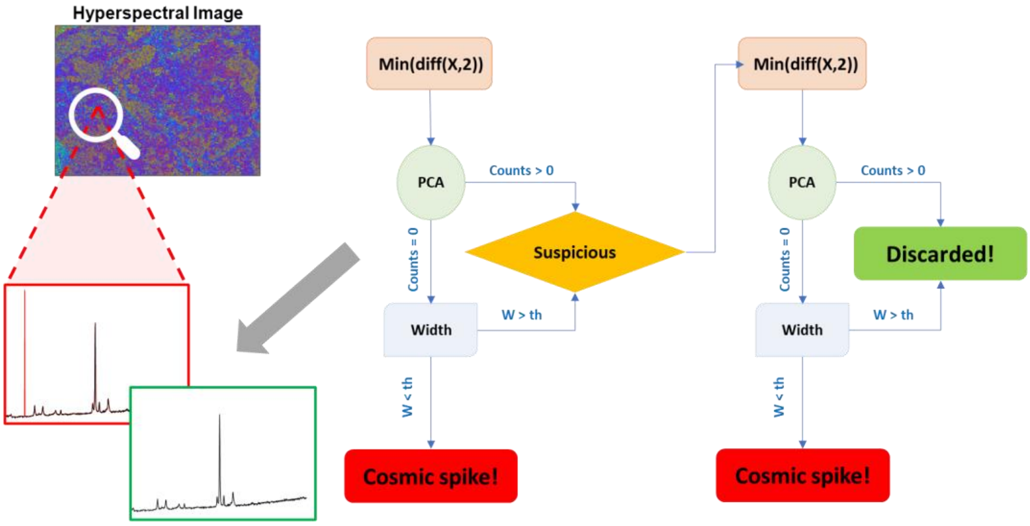

Figure 1. Schematic representation

The algorithms that are already available in the literature, such as Width of Features or Nearest Neighbour[1], among others, require a final supervision by the user of every detected candidate. We propose an iterative approach that combines simple but effective operations such as the use of derivates, exploratory analysis, correlations and peak width assessment, which enables the identification of suspicious candidate wavenumbers of being cosmic rays artifacts and their automatic elimination. The algorithm shows a high detection ability independently of whether the image has been processed or not. The proposed algorithm has been tested with Raman hyperspectral images containing cosmic rays of different shapes and intensities, and the overall performance was assessed taking into account false negatives (undetected spectra containing cosmic spikes) and false positives (real vibrational modes corrected as if they were artifacts), resulting in a promising ability to discriminate cosmic spikes from real Raman vibrational modes without user supervision. The algorithm has been developed in MATLAB environment and implemented in HYPER-Tools version 4.0[2,3], a freely available toolbox for hyperspectral image analysis.

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A014. Systematic investigation on long-term device drift for Raman spectroscopy

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Raman spectroscopy provides the unique fingerprints of molecular components under measurement by indirectly detecting molecular vibrations [1]. The capability of Raman spectroscopy has been largely enhanced by machine learning techniques, which translate the spectral fingerprints into interpretable knowledge. Nowadays, Raman spectroscopy has been largely applied in biological, medical, and clinical investigations. To push it into clinical applications, however, is by large hindered by the substantial variations between different devices. Even the same device may show significant drift over time [2, 3]. The device-relevant spectral variations often disable a machine learning model built on one to be applied on data from a different device or the same device but measured at a later time. A systematic investigation of such variations is in urgent need.

In this study, 13 substances were measured weekly as quality control references over 10 months on one Raman setup to investigate the instrumental variations and the time-dependence of the variations. The 13 substances were selected to be stable and span a broad range of solvents, lipids, and carbohydrates. From each substance 50 Raman spectra were acquired every measurement day. All spectra were preprocessed to remove spikes and fluorescence baselines. We compared the performance of calibrating the wavenumber axis with different standards [4]. Thereafter, we characterized the spectral variations of each substance over the measurement period based on the intensity variations as well as the correlation coefficient and the clustering properties across measurement days. With this, we aim to discover and characterize the time-dependent device variations, as important knowledge preparation to find a better way of spectral standardization in Raman spectroscopy to push it forward in real clinical applications.

Acknowledgements

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A015. A hyperspectral thermal imager based on a low order scanning Fabry-Pérot interferometer

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The long-wave infrared (LWIR) regime can be used to probe the vibrational states of many different compounds. Common techniques for this include Fourier Transform Infrared (FTIR) and Attenuated Total Reflectance (ATR) spectroscopy. Frequently, these methodologies are limited to single point or, in some cases, line-scan (push-broom) measurements. Consequently, relative movement between the sample and the instrument is required to acquire spatial information. This makes some samples impractical or unfeasible for measurement. A spectral scanning imager alleviate this problem as it images the entire scene simultaneously, hereby obtaining the spatial information. The spectral information is then acquired by imaging the scene repeatedly while filtering different parts of the spectrum.

We have developed a hyperspectral imager sensitive to wavelengths in the range from 8 µm to 14 µm. It is a spectral scanner, which combines an uncooled microbolometer-equipped thermal camera with a scanning Fabry-Pérot interferometer (SFPI) as illustrated in **Figure 1**. We have previously demonstrated that this imaging system is capable of distinguishing between materials and subsequently predicting the surface temperature of samples by applying material-specific temperature models (Jørgensen 2022). The SFPI consists of two semi-transparent dielectric mirrors, and the separation between the two determine the distribution of wavelengths transmitted to the camera. This way, the SFPI functions as a variable bandpass filter, and by continuously acquiring images, while the mirror separation distance is increased, a hyperspectral image is formed. During the acquisition of the 150 images making up the hyperspectral image, the mirror separation distance is increased from ≈ 3 µm to ≈ 13 µm. This is enough to cover the first transmission order of the SFPI as well as most of the second and part of the third order. The hyperspectral image has with dimensions of 1024×768×150 (height × width × depth).

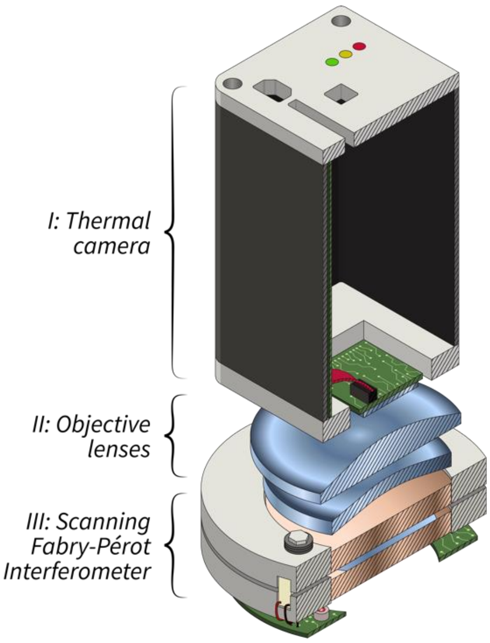

Figure 1. Schematic of hyperspectral LWIR imaging system (not to scale).

This presentation will include a technical description of how the hyperspectral imaging system functions. What components make up the camera, how are the mirrors controlled throughout data acquisition, and how can the recorded spectral information be used for material classification by simple chemometric techniques.

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DoI: https://doi.org/10.1364/OE.441798

A019. Opening new avenues for hyperspectral imaging analysis within BASF

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The project is being conducted by BASF, a leading chemical company, and aims to analyze the potential applications of infrared (IR) hyperspectral imaging technology in improving the quality, efficiency, and accuracy of product identification and quantification. The effectiveness of IR hyperspectral imaging will be determined, along with exploring its benefits and limitations in selected applications. The project addresses the relevance to customer needs and strategic goals, as customers seek cost-effective solutions to optimize production processes and reduce wastage. Technical risks, such as limited spectral range or resolution, and challenges in integrating IR hyperspectral imaging systems into existing production lines, will also be considered. IR hyperspectral imaging has the potential to provide detailed and comprehensive analysis of materials and components, enabling accurate and fast identification and characterization. Its non-destructive nature is advantageous in industries where preservation of product integrity is crucial. Real-time data capture and analysis using IR hyperspectral imaging can facilitate proactive decision-making, leading to improved efficiency and productivity. However, there are technical risks involved, including the complexity and computational intensity of hyperspectral data analysis, sample (in)homogeneities, calibration challenges, and maintaining accuracy over time. Integration with existing production lines may require modifications or adaptations. Limitations in hardware and equipment, such as spectral range, resolution, or sensitivity, may impact the technology's effectiveness in specific use cases. Environmental and experimental conditions, such as lighting variations and ambient temperature, can affect performance and reliability. Addressing these factors and ensuring consistent performance under different conditions pose technical challenges. The project's deliverables include identifying the viability of using hyperspectral IR cameras in several use cases and developing chemometrics models for exploration, classification, and quantification of desirable parameters. Additional work packages involve validation through orthogonal analysis methods (e.g. lab-grade IR and/or NMR spectroscopy), evaluation of different types of IR cameras and technical alternatives. Ultimately, the project aims at providing a solid technical performance assessment that judges its use for the respective operational divisions. Local implementation of developed workflows will be conducted, and potential transfer to other BASF global operational divisions will be explored. By determining the feasibility and effectiveness of IR hyperspectral imaging in product analysis and sorting, this project has the potential to significantly enhance production processes and minimize errors in various BASF fields.

A026. Application of Short-wave Infrared (SWIR) Spectral Imaging for Analysis of UV-induced Polyurethane Degradation

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With the extensive use of Polyurethane products in various sectors, such as outdoor material applications, medical device manufacturing, and automotive industries, it is critical to assess the degradation of these materials. Evaluating the impact of polymer degradation, particularly due to UV exposure, is crucial for understanding its potential effects on environmental sustainability, human health, and the efficiency of recycling processes(Patti & Acierno, 2020). Our study specifically investigates changes in PU material under UV degradation to assess the polymer products and the polymer degradation products (Henriksen et al., 2022).

In our experiment, we aimed to study the UV degradation of PU material across a 16-day period. Initially, four PU samples, each measuring 4.5 by 3 centimeters, were prepared within plastic petri dishes. Due to the time series nature of the study, spectral measurements were taken at four-day intervals using a SWIR (short-wave infrared) camera to collect spectral information. This resulted in a dataset encompassing days 0, 4, 8, 12, and 16, making up five time points. The hyperspectral images obtained were converted into point spectra for analysis in MATLAB. The data was then divided using different training approaches: 70% for training and 30% for validation (All the data were integrated and labelled in a one-to-one manner, then randomized in an upset fashion. Subsequently, the top 70% of the data was selected as the training set, and the remaining 30% was designated as the test set), as well as 5-fold cross-validation. A Random Forest classification model was trained to categorize the different point spectra according to their respective time points. This process allowed us to analyze the degradation over time and further study the extent of degradation of the PU material.

The SWIR camera captures the changes in the spectra of the PU materials caused by UV degradation. Once collected, these spectral datasets are used to train a Random Forest classification model, which could categorise the material into different levels of degradation (represented by the number of days in this model).

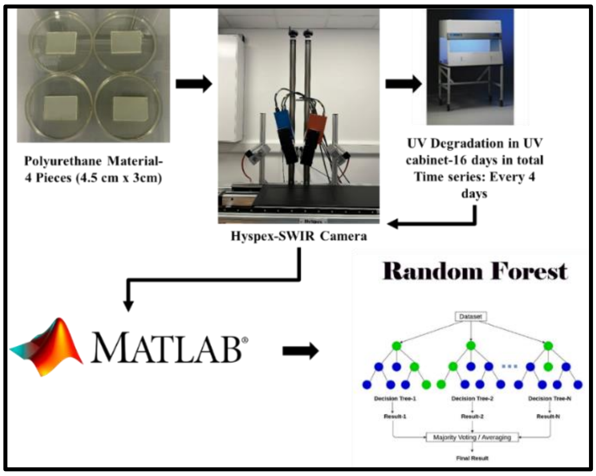

Fig.1. Flowchart on the experimental & data analysis process.

In our study, various preprocessing techniques were applied to Random Forest models for classifying PU material under UV degradation across time series data. Different preprocessing methods, including SNV, Savitzky-Golay (SG) derivatives, and Multiplicative Scattering Correction, were applied to the dataset before train and test the model. The model consistently achieved high accuracy, with Multiplication scattering correction preprocessing reaching up to 99.59% accuracy in 70/30 Training validation method and 100% accuracy in K-fold cross-validation. This highlights the robustness of the Random Forest approach in spectral classification under varying preprocessing conditions.

Our methodology demonstrates high accuracy and offers a non-destructive approach for assessing material durability, which is crucial for quality control in various industrial applications. This research highlights the potential of integrating spectral imaging and advanced analytical techniques in the field of material degradation. The findings of this study contribute to the advancement of spectral imaging and machine learning in the field of material science, particularly in the monitoring and analysis of polymer degradation.

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A032. *INSIDE* – IN-DEPTH CHEMICAL MAPPING: NIR&XRF SPECTRAL IMAGING FOR NON-INVASIVE 3D ANALYSES

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The two-year research project *INSIDE*, funded by the Italian Ministry of Universities and Research – MUR as a frame for the “PRIN 2022” call, involves three Italian universities: Genova, Bologna and Torino. The project is aimed at revolutionising the concept of hyperspectral imaging (HSI) in the near-infrared (NIR) and X-ray fluorescence (XRF) spectral domains, evolving from a surface analytical technique to an in-depth 3D spectral tomography (**Figure 1**).

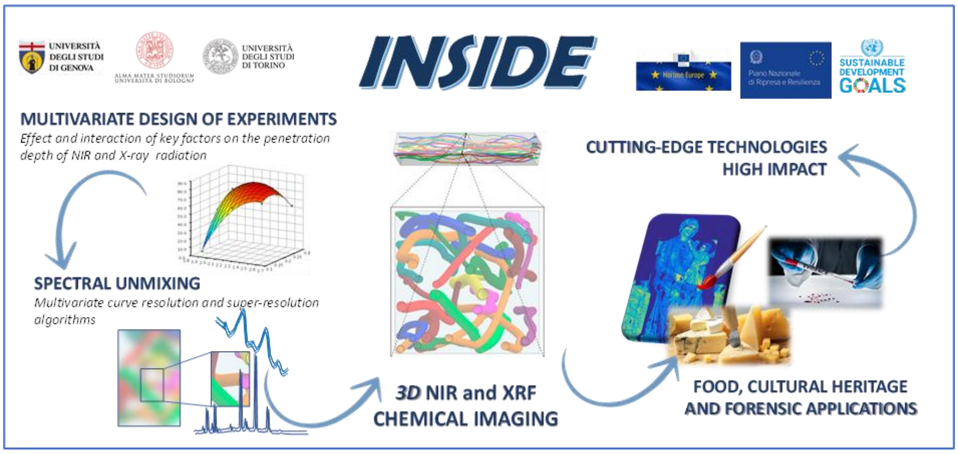

Figure 1. General scheme of the INSIDE research project

To this aim, the project will investigate on the penetration depth of incident NIR and X radiations and will exploit this property to obtain highly informative 3D NIR and XRF spectral images of heterogeneous samples.

The impact of such a cutting-edge analytical solution will be exploited and validated in three main application fields: food analysis, cultural heritage, and forensic sciences.

After a systematic literature analysis of research studies published on this topic, for a comprehensive recognition of the state of the art, key factors affecting the penetration depth of NIR and X radiations, as well as their interactions, will be investigated by application of multivariate design of experiments (MDOE). Moreover, applying proper sampling design techniques will ensure the collection/preparation of samples capable of guaranteeing maximum representativity and the development of analytical strategies characterised by an effective capacity to address the predetermined targets. During these initial phases, *ad hoc* samples, with a well-defined stratigraphy, will be designed and built employing a multi-material 3D printer, using polymers with distinct spectral signatures.

Multivariate unmixing strategies – including multivariate curve resolution (MCR) and super-resolution algorithms – will be applied for efficiently gathering 3D chemical information from hyperspectral data.
Confirmatory analyses will be performed to validate the analytical protocols developed by using scanning electron microscopy (SEM), gas chromatography-mass spectrometry (GC-MS) and ultra-high performance liquid chromatography tandem mass spectrometry (UHPLC–MS/MS).
Suitable tools for 3D graphics will be implemented for the conversion of deconvoluted NIR and XRF hyperspectral information into 3D chemical maps, including the development of a stand-alone app with a user-friendly GUI, which will be distributed to the project stakeholders for testing, and will demonstrate the way forward for establishing new opportunities in research and industrial sectors.

Acknowledgement
Financial support provided by the Italian Ministry of Universities and Research – MUR (Research Project PRIN 2022 n. 20223WBTH8, CUP: D53D23008950006) is gratefully acknowledged.

A034. Hyperspectral imaging and chemometrics for analyzing biodegradable plastics.

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Polymers widely available worldwide, such as cassava starch, have sparked researchers' interest due to their structural properties for the production of biodegradable films, meeting current demands for environmental sustainability. However, due to their hydrophilic nature, investigations involving lipophilic components are necessary. These components not only contribute to barrier properties but also impart bioactive characteristics. The characterization of these materials involves analyses that require considerable time and technical knowledge. In this context, this study focuses on development of hyperspectral imaging as a tool to characterize bioplastics based on cassava starch, cellulose, and essential oil of oregano (OEO) at concentrations of 25%, 50%, and 75%.

Ninety-seven samples were analyzed, and the images were acquired in the spectral range of 1700 to 2500 nm. Principal Component Analysis (PCA) was employed to explore the behavior of the NIR-HSI data and identify potential trends to better guide subsequent steps.

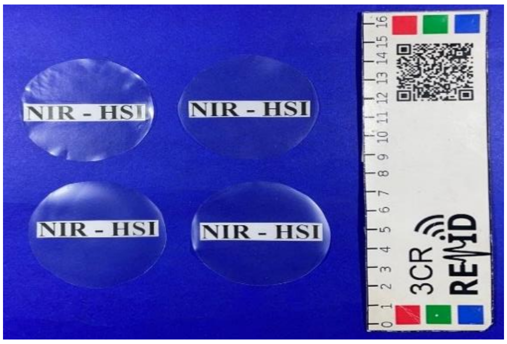

Figure 1. Biodegradable films based on cassava starch, cellulose, and oregano essential oil.

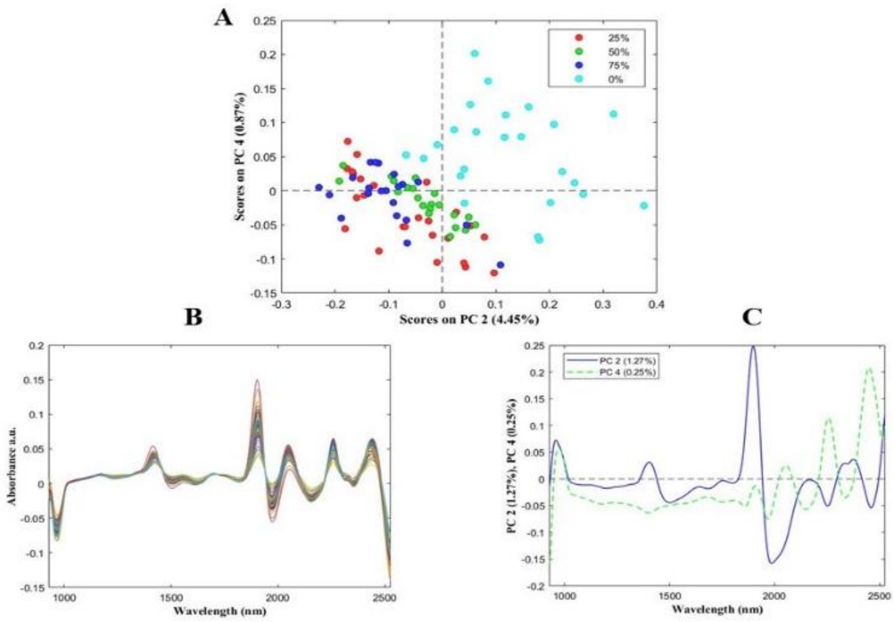

Figure 2. Principal Component Analysis based on the content of OEO (A), pre-processed NIR-HSI spectra (SNV) (B), and loadings plot (C).

As observed, the results revealed clustering of samples with added OEO, distinguishing them from control samples formulated solely with carbohydrates. The significant similarity between formulations may be attributed to similar concentrations of OEO. Although PC2 explained only 4.45% of the total explained variance, it allowed for better differentiation between samples compared to PC4. We also note that sample scores on PC2 shifted from positive to negative as OEO was added to the formulations. This suggests that the combination of NIR-HSI with chemometric tools is sensitive to the organic compounds present in the films, providing a rapid and non-invasive analytical system to assess the behavior of bioplastics in different formulations. Further analysis will be performed regarding the samples mechanical properties, as they are related to the chemical composition, thus making HSI a valuable tool for this task.

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A042. Exploratory Data Analysis of Seismic Data using Distributed Acoustic Sensing and Principal Component Analysis

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The study of seismology and vulcanology is fundamental for public security in areas with active volcanoes and high earthquake activity. Knowing the nature of this phenomena is crucial to be able to predict their occurrence and minimize the effects of these natural disasters. In September 2021 La Palma Island in the Canary Islands suffered the volcanic eruption of Tajogaide (Taddeucci 2024). The intensity and duration of this eruption had no known precedent. The disaster caused by this event made evident that it was necessary to develop new knowledge and technology in this field. A Distributed Acoustic Sensor (DAS) was monitoring the island of La Palma with a fiber of 40 km covering part of the Island and its submarine surroundings during the eruption. It registered the seismic activity around the volcano, generating a vast amount of seismic data. Those registers, in conjunction with the invaluable work of INVOLCAN experts who generated catalogues of occurring volcano-seismic earthquakes, are an attractive source of information to understand the under-going seismic processes.

DAS is a technology based on the Rayleigh back-scattering phenomenon that occurs in an optical fiber when a known light-wave called "interrogation" light-wave faces an inhomogeneity in the optical fiber. Vibrations solidary to the fiber cause local changes in its refraction index, and therefore produce changes in the characteristics of the back-scattered pulse. Current state-of-the-art DAS technologies can, analyzing the back-scattered pulse, locate the stimulus with precision along the fiber and measure its intensity. This way, DAS technology has been used for several years to monitor seismic and volcano-seismic activity taking benefit of its long monitoring range and robustness (Lindsey 2017). DAS optical fibers can be thought of as an ultra-dense network of punctual sensors, having one sensor every 6 to 10 meters of fiber. We can see an example in Figure 1.

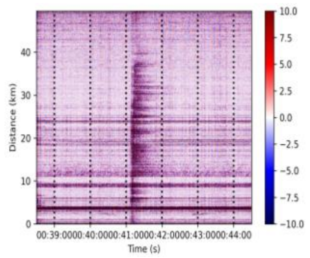

Figure 1. Normalized strain-variation amplitudes for the 40 kms of fiber (spatial sampling 10m, freq. sampling 100Hz)

Acoustic signals contain rich information, but in a way that is hard to interpret. This is why signal preprocessing is always necessary. By preprocessing we can obtain different features from the signals that we can then study. However, this is no easy task, as the potential myriad of features can be overwhelming. We can study them one by one, but this can lead to incorrect or incomplete interpretations, as many phenomena are contained not in one variable of our problem, but in many of them at the same time. To make sure that we are looking at the data the right way, we need a multivariate approach, that considers every variable and observation at the same time (Benítez 2018).

Principal Component Analysis (PCA) is a widely used exploratory approach for multivariate data, as it makes no initial assumptions regarding the data, making for a good first modelling and visualization. This type of analysis has led to interesting initial results in our exploratory analysis. We labeled every window of our signals as "EQ" if it contained an earthquake, "Noise" if it showed energy in frequencies up to 5Hz and “Other” if it showed energy in frequencies between 5 and 10Hz. Windows not meeting any of these criteria received the label “Unknown”. Applying a FFT to our data with a frequency discretization of ~0.4Hz and discarding the lowest two frequencies we obtained the PCA model shown in Figure 2. This model suggests that frequencies around 2.76Hz are the most important ones for detecting earthquakes. It also shows that some of the windows labeled as Unknown have some structure in them that is dominated by frequencies under 1.6Hz.

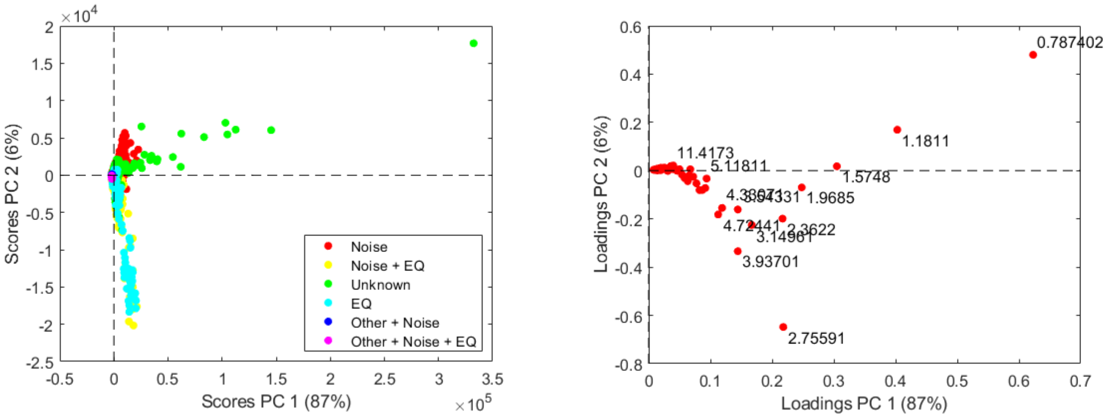

Figure 2. Scores and Loadings plots of a 2 PC model of the FFT coefficients of every time window in ten DAS sensors. Points on the Scores plot correspond to different windows. The number next to the points on the loading plot correspond to the frequency of the FFT coefficient in Hz.

With the information provided by PCA we managed to pinpoint the unexpected behavior that the PCA analysis suggested in the original data. In Figure 3 we can see the anomaly in the original signal. That is, we can see how part of the signal classified as “Unknown” shows an unexpected amount of high energy at low frequencies. While further investigation of the reason for this phenomenon is required, PCA proved to be excellent at pointing us in the right direction to do so from early on. The result in Figure 2 represents one of the several analyses to be presented in the proposed poster. Our middle term goal is to analyze the entire length of the volcanic event (several months).

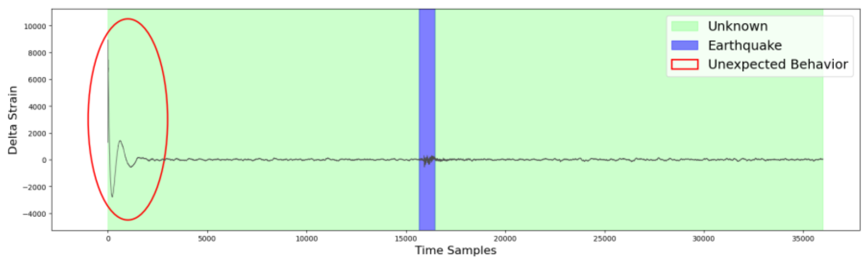

Figure 3. Signal measured by one of the sensors containing earthquake and unknown portions. In red we see the unexpected behavior that the PCA analysis suggested.

Acknowledgements:

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A045. Uncovering sea pollution: microplastics monitoring in marine salt using hyperspectral imaging

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The massive use of plastics in industry, coupled with the headache of managing its discards, constitutes one of the main problems worldwide today. Plastic discards accumulate in seas and oceans where it undergoes a fragmentation process due to exposure to UV light and ambient temperature. These plastic fragments of tiny sizes are called microplastics and they present more than 70% of the waste present in the seas. Addressing this challenge requires efforts in research, policy-making and public awareness to mitigate the adverse effects of microplastics on marine biodiversity and ecosystem health. In response, several international organizations have developed action plans for the monitoring, mitigating and preventing of these pollutants.

The aim of the present study is developing an analytical method based on hyperspectral imaging to monitor the presence of microplastics along the Andalusian Mediterranean coast as a means of pollution control. To achieve this, samples of marine salt were collected from salt works in the study area. Salt works act as a high-scale natural "preconcentrators", in which microplastics from seawater were accumulated during the salt extraction process. Consequently, the sea salt would serve as an indicator of microplastics present in seawater.

Sea salt samples images were captured using a hyperspectral camera which measured in two spectral ranges: from 400 to 1000 nm (VNIR) and from 900 to 1700 nm (SWIR). Additionally, five of the most commonly plastics used in the industry were selected as microplastic standards (polypropylene, polyethylene, polystyrene, polyvinyl chloride and polyethylene terephthalate). They were acquired from chemical manufacturers and from industrial products composed of them (caps, packaging, bottles, etc.), and they were crushed to reach microplastics size. Salt from inland salt works was selected as a 'salt blank' (microplastics-free). The image of microplastics standard and salt blank was also captured. As exploratory analysis, principal component analysis (PCA) was performed using pixel-spectra information of the region of interest (ROI) selected on the microplastics and microplastic-free salt standard samples. Support vector machine (SVM) was applied to build a classification model capable of discriminating between sample pixel-spectra which contain salt or any kind of microplastic. SVM model was used to detect those pixels that contained microplastics in marine salt samples and to identify which kind of microplastic it was, reflecting their presence in seawater.

A046. Making uneven illumination EVEN: automatic Evaluation and Enhancement for multimodal microscopy

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Uneven illumination affects all measurements acquired by optical microscopes and strongly impacts large multicolor and nonlinear images, generating vignetting and mosaicking artifacts and impeding the correct analysis of the measurements (Chernavskaia 2017, Smith 2015). Uneven illumination can be effectively reduced by various state-of-the-art methods, but an established workflow for the evaluation of raw and processed images is still missing (Chernavskaia 2017, Smith 2015, Peng 2017). We present EVEN: an informed machine learning method for the Evaluation and Enhancement of images affected by uneven illumination. EVEN is based on a Linear Discriminant Analysis model trained to classify images with and without uneven illumination. It employs quality metrics designed to characterize vignetting, mosaicking artifacts, and quality features of experimental measurements. We applied EVEN to generate optimized corrections of three-channel multimodal measurements of human head and neck tissue slices (Lai 2023). The trained model builds an automatic quality ranking for the single-channel corrections and predicts the optimized multimodal image. EVEN can be used to detect vignetting in raw images, tune the parameters of single correction methods and select the best inputs for further processing and analysis tasks, such as image registration and segmentation.

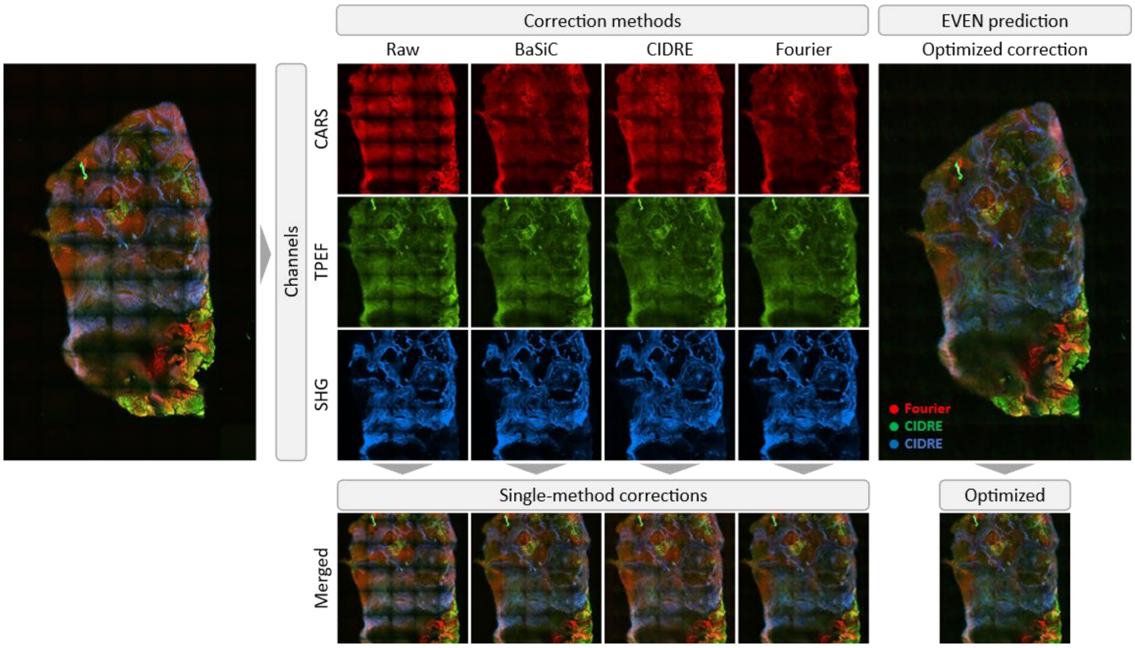

Figure 1. EVEN optimization of a multimodal measurement. Each channel of the raw image is corrected with three different methods: BaSiC (Peng 2017), CIDRE (Smith 2015) and Fourier method (Chernavskaia 2017). Our method generates the optimized multimodal image for this specific case.

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A047. Active hyperspectral pushbroom imager for conveyor belt applications

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Hyperspectral imaging with short wave infrared (SWIR) wavelengths for qualitative or quantitative analysis of product on a moving conveyor belt typically employs commercially available grating spectrograph-based cameras. There are certain challenges when using these cameras. With high-speed conveyor belts, high power halogen light sources are required to be placed close to the conveyor belt, which can be impractical due to mechanical restraints, heating of the product and optics getting dirty. Furthermore, the current cameras offer a fixed spatial resolution, requiring sometimes multiple cameras to cover a wide conveyor belt with high resolution. The price of the system has also been a limiting factor for the wide scale employment of hyperspectral imaging in industry. In this work, we present an alternative way of hyperspectral imaging for conveyor belt applications. Instead of broadband illumination and spectral resolving at the camera side, we use broadly tunable laser source and a monochromatic camera. This approach has many potential benefits. First, any high-resolution SWIR camera can be used. Second, since the laser light is very controllable, the light source and the camera can be placed much further from the conveyor belt. Third, the developed tunable light source can be operated at very rapid speed of over 100k channels per second, and the user is allowed to pick the relevant wavelengths for each application. Furthermore, since only a single wavelength band is used for illumination at any given moment, there is no excess heating on the target.
The tunable broadband laser source is based on in-house developed compact and low cost supecontinuum light source (Kääriäinen 2021). The light source covers wavelengths between 1200 nm - 2500nm. Microelectromechanical (MEMS) tunable Fabry-Perot interferometer (FPI) filter (Antila 2010) is used to filter the broadband laser light, to allow a single wavelength band to be transmitted at an instance. The bandpass wavelength of the filter is tuned by electromechanically adjusting the gap between the two mirrors forming the Fabry-Perot cavity. Powell lens is used to form a line illumination pattern on the target. Finally, the 2048-pixel SWIR line sensor is used with a simple objective lens to image the area being illuminated. FPGA software is used to switch the transmission wavelength for each successive camera frame.
The proposed active hyperspectral pushbroom imager has the potential to result in a flexible, low-cost alternative to commercial grating spectrograph hyperspectral cameras for conveyor belt applications. Future work includes validation of the system on an industrial conveyor belt for qualitative and quantitative analysis.

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A055. Laser-Induced Breakdown Spectroscopy (LIBS) analysis: Study of Classical Regression and Deep Learning Methods

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Laser-Induced Breakdown Spectroscopy (LIBS) is a rapid and precise method for measuring elemental concentrations in various samples. It utilizes laser-induced plasma to analyze the spectral signatures of elements, enabling versatile applications in numerous fields (Nicolini 2020) (Pasquini et al. 2007).

This research explores the LIBS spectra using a well-established classical regression technique called Partial Least Squares (PLS) and Deep Learning (DL) approach. The main challenge for developing predictive models was the variation of electron density and temperature of the plasma, which can completely modify the spectra. Therefore, besides PLS, we tried implementing more advanced tools such as CNNs. The aim was to provide insights into the predictive capabilities of PLS and CNNs in predicting the concentration of 24 elements within the LIBS spectra.

The study employed a training set comprising 20000 simulated LIBS spectra and a test set containing 5000 simulated LIBS spectra. These datasets were used to develop and evaluate the predictive PLS and CNN models. Given that the simulated spectra were generated without baselines, the only pre-processing step applied to the simulated LIBS data was normalization to the [0, 1] range. However, the models were also trained and tested with the original data (without normalization) to make the study more comprehensive.

For DL, a simple CNNs with six convolutional layers was designed. The PLS models were also trained using the simulated LIBS spectra, with different numbers of PLS components utilized.

The performance of the models was evaluated based on their stability and accuracy in predicting the concentration of the 24 elements within the test set. Our findings suggest that DL outperformed classical regression in predicting the concentration of presented elements within the simulated test LIBS spectra. The DL model showed greater stability and higher accuracy in predicting concentrations of elements. Overall, this study provides important insight into the application of DL in LIBS analysis as a powerful and stable tool for accurate and reliable elemental analysis.

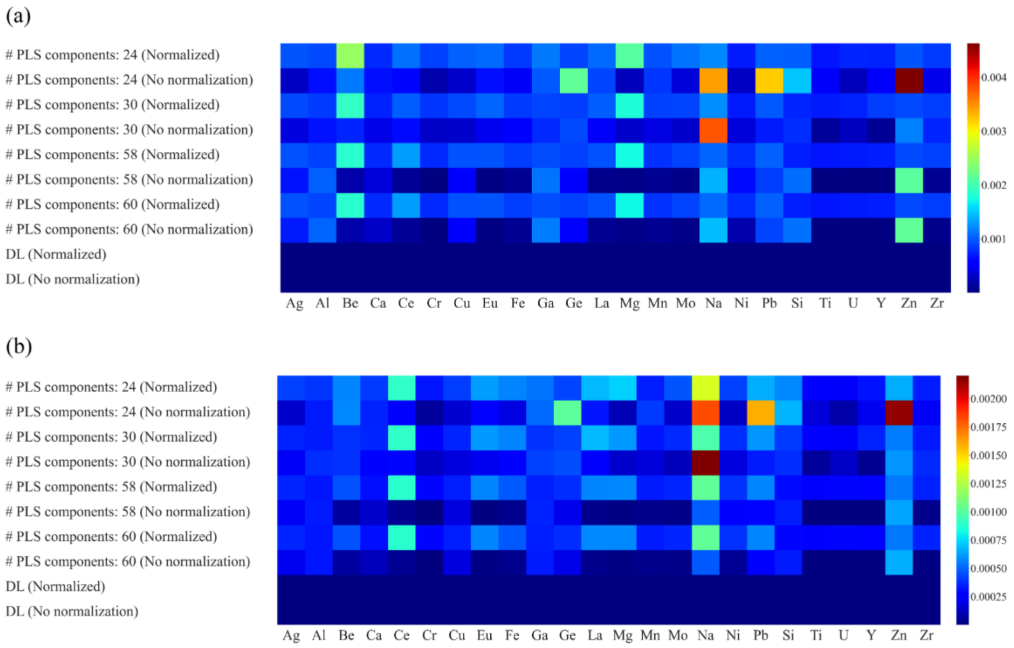

Figure 1. Analyzing the predictive model stability and performance for element concentration prediction using PLS and DL approaches. (a) Represents the Interquartile Range (IQR) values as a crucial indicator of the stability of the predictive models, where the dark blue colour associated with CNNs model denotes lower IQR and, consequently, signifies their outperformance over the PLS models with higher stability. (b) Illustrates the median values of the obtained Mean Squared Error of Prediction (MSEP) per element for the simulated LIBS spectra utilized as the test set. The dark blue colour proves the developed CNNs model's superior prediction accuracy performance.

Acknowledgement

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A056. Alzheimer's classification via hyperspectral Raman imaging on specific zones of dried biofluids

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Raman spectroscopy combined with machine learning has the potential to revolutionize medical, biochemical, and biological research. Alzheimer's disease (AD), so far an incurable neurodegenerative disorder, presents a major health challenge. Building on previous research (Xu 2023), our study aims to explore the potential of Raman spectroscopy in AD detection, offering a new perspective within the traditional drop coating deposition Raman (DCDR) method.

Our research proposes a different approach that utilizes hyperspectral Raman imaging to improve the understanding of the biochemical composition of biofluids. This approach, in which spectra are captured for each pixel of an image (Amigo 2019), provides valuable insight into the spatial distribution of sample components, yielding unique spectral fingerprints indicative of the sample's biochemical composition. This approach has the potential to improve the predictive accuracy of AD significantly.

One microliter each of human plasma (PL) and cerebrospinal fluid (CSF) from 15 volunteers (**Table 1**) were prepared for subsequent hyperspectral data acquisition using a confocal Raman microscope (Renishaw inVia Qontor). Hyperspectral images were taken from the circular pattern (⌀ ~1400 µm) of dried droplets with 750 to 950 spectra per droplet, respectively.

Table 1. Statistical distribution of the dataset. SD: standard deviation

Sample type	Healthy (PL/CSF)	Preclinical AD (PL/CSF)	Prodromal AD (PL/CSF)	Male/Female	Age (mean ± SD)
15 Plasma / 15 CSF	5/5	5/5	5/5	12/18	65.2 ± 2.3

Figure 1 shows an exploratory analysis by Fuzzy C-means (FCM) clustering of PL and CSF samples, using the freely available version 3 of HYPER-Tools (Mobaraki 2018). Interesting differences associated with characteristic AD peaks can be particularly observed in the centers of these clusters. PL samples (top 15 images) exhibit a more uniform spectral distribution all over the drop with less apparent differentiation among clusters. Conversely, CSF samples (15 bottom images) show a spectral distribution that facilitates the identification of distinct regions for classification modeling. By constructing independent models for each region, we better understand the optimal DCDR zones for discriminating between healthy and AD individuals. This understanding directly contributes to the identification of molecular signatures associated with AD. Our results underline the importance of hyperspectral zone-specific Raman analysis and show its potential not only for the detection of AD, but also for the classification of other diseases.

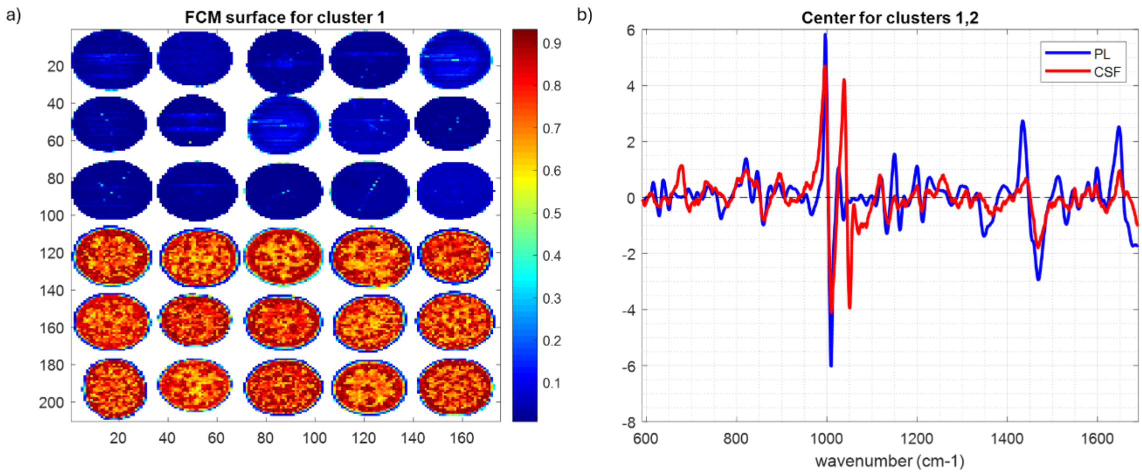

Figure 1. a) FCM clustering of PL (upper 15) and CSF (lower 15) samples. b) Loadings from the cluster centers.

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A057. Impact of Color Transformation Methods on Image Registration

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Medical imaging is essential for diagnosing diseases and understanding their underlying mechanisms. Traditional staining methods such as Hematoxylin and Eosin (H&E) have long been used in histopathology to visualize tissue morphology and specific cellular components. However, recent advancements in imaging technologies have introduced new techniques that offer additional insights beyond classical staining.
Combining multiple imaging techniques within one device makes it possible to capture various molecular and cellular components related to the tissue composition and organization. In this study, we used multimodal imaging that generates images with three channels: red for coherent anti-Stokes Raman scattering (CARS), blue for second harmonic generation (SHG), and green for two-photon excited fluorescence (TPEF). Integrating these modalities provides a more comprehensive understanding of tissue characteristics(Bocklitz et al. 2016).

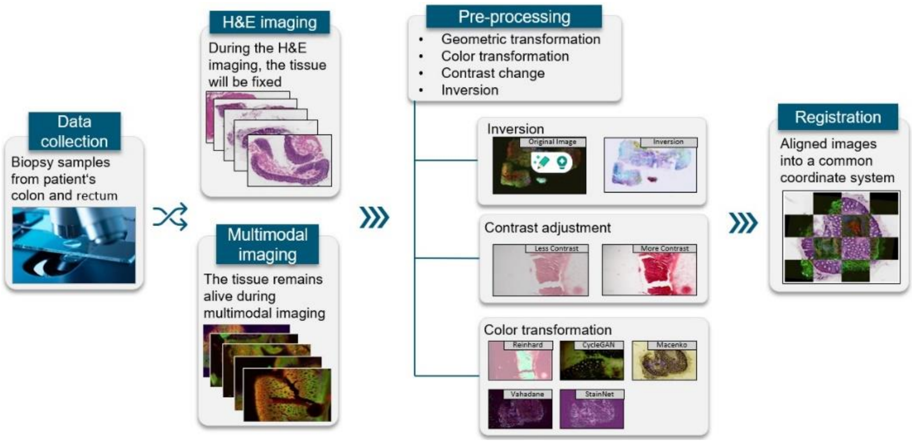

Figure 2. Workflow for image registration: Data collection, preprocessing, and final registration step for accurate alignment.

The alignment and comparison of different image types, such as H&E and multimodal images, poses challenges. Image registration becomes essential to establish a common reference frame for accurate comparisons. This process as shown in **Figure 2** transforms images into a unified coordinate system, addressing geometric distortions and ensuring coherence in features.
Despite availability of various co-registration methods, disparities in information content, color representation, and geometric distortions complicate image registration. To overcome these challenges, color transformation becomes essential. By adjusting the color distribution of one image to match the other, accurate and meaningful comparisons can be made. This study delves into evaluating various color transformation methods for the alignment of H&E and multimodal images. To identify color transformation methods that produce stable and reliable results, we evaluate their performance and stability.

After preprocessing the multimodal images by inverting them to ensure consistent color representations across all image types, as you can see in **Figure 3**, we applied a range of color transformation methods, including Reinhard, Vahadane, Macenko, CycleGAN, and StainNet, before performing image registration. For registration, we employed the Lucas-Kanade optical flow method, using keypoint detection and matching functions such as BRISK, SIFT, ORB, AKAZE, Harris, and Shi-Tomasi corner detection(Zingman et al. 2024). After registration, we extracted windows from the registered images and performed a second keypoint detection step within this workflow. We measured the distances between the detected keypoints and computed statistical metrics such as median distance, median angles, numbers of good and bad matches to assess the stability of the color transformation.

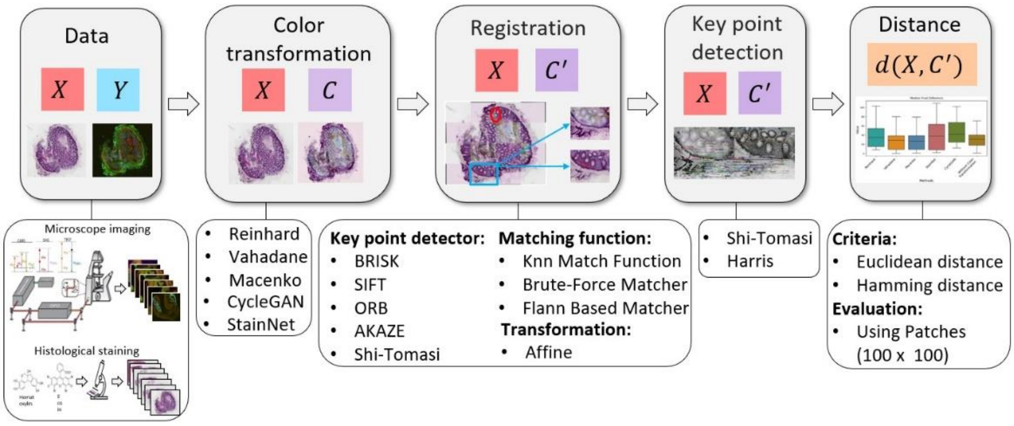

Figure 3. Conceptual Workflow: Assessing color transformation's impact on registration through data gathering, transformation, co-registration, keypoint detection, and stability evaluation steps.

Ultimately, our goal is to improve medical imaging analysis by identifying optimal color transformation approaches. By bridging the gap between different imaging modalities, we aim to improve diagnostic accuracy and advance medical research.

Acknowledgment
This work is supported by the BMBF, funding program Photonics Research Germany (FKZ: 13N15466, 13N15706, 13N15710, 13N15715, 13N15719) and is integrated into the Leibniz Center for Photonics in Infection Research (LPI). The LPI initiated by Leibniz-IPHT, Leibniz-HKI, UKJ and FSU Jena is part of the BMBF national roadmap for research infrastructures.

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A062. Rapid detection of tyre wear particles by multiblock hyperspectral imaging

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The unbridled worldwide production of synthetic polymers, which began in the 1950s, and the related mismanagement have resulted today in a critical and urgent social, economic and environmental challenge. Thus, microplastic (MP) pollution is currently detected in all the main environmental compartments. Although MP pervade all the ecosystems, their detection, quantification, and characterization is still nowadays one of the biggest technological challenges, representing a current analytical issue.

A new environmental threat arises from tyre wear particles (TWPs). Despite of the various approaches available, there is recognition of the crucial need for reliable analytical strategies for the qualitative and quantitative assessment of TWPs in the environment.

Spectroscopic techniques like infrared (IR) and Raman are usually not suitable for studying TWPs, due to the high levels of highly adsorbent carbon black present. Consequently, the analytical characterization of TWPs typically relies mainly on elemental analyses or mass spectrometry-based techniques.

Exploiting the high potentialities of hyperspectral imaging systems for the detection of MP, the present research is focused on the application of a new analytical set-up, able to co-register X-ray fluorescence (XRF, 0–48 keV) data, together with visible & near-infrared (VNIR, 400–1100 nm) and short-wave infrared reflectance (SWIR, 1100–2500 nm) spectra, with a single scanning head. Image pixels from the three spectroscopies are spatially aligned to facilitate the combination of the spatial-spectral information from the three ranges.

The innovative instrument was applied on TWPs laying on cellulose filters after filtration from EtOH dispersions. Tyre particles were produced from 4 different tyres (Bridgestone Potenza, Continental WinterContact, Kleber Viaxer and Flken Azenis) using a planner plough. The obtained fragments were then milled with liquid nitrogen in an ultracentrifuge mill and sieved to < 0.3 mm.

While TWPs are known to be characterized by specific elemental signatures, the mentioned inherent challenge in analyzing TWPs, due to their black color, poses difficulties in VNIR and SWIR reflection modes. Despite this, employing VNIR spectroscopy was proven to be a fruitful approach, enabling the rapid and efficient identification of particles according to their reflectance values with respect to the white background. Exploiting these values, masks were created in the visible domain and used to isolate XRF signals specifically from areas where TWPs were present, enabling the recognition of particles, even when not directly visible in XRF maps. An in-house Matlab routine was created to automatically extract the XRF spectra, to count particles and to obtain information on their dimensions.

Furthermore, the extracted XRF spectra offer a wealth of compositional data that can be subjected to further analysis using advanced multivariate techniques, such as principal component analysis (PCA). These techniques provide researchers with a robust tool for assessing the composition and uniformity of tyre wear particles, enabling them to discern subtle variations and patterns within the data.

Acknowledgment

Authors would like to acknowledge financial support from Italian Ministry for University and Research (MUR). Research Project PRIN 2022 (P20227N5YZ) DIORAMA: “A deep dive into the study of microplastics in aqueous matrices”.

A066. Prediction and mapping of degradation degree in acrylonitrile-butadiene-styrene (ABS) and high impact polystyrene (HIPS) using near-infrared hyperspectral imaging

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Sensing technologies for identification and sorting of waste plastics are widely used in recycling plants, as several commercial solutions have become available during the past years (Yang 2023). NIR sensors are the most versatile, enabling sorting of plastic waste by polymer type, detection of additives or contaminants. However, sorting plastic by polymer type and additive content alone is not enough to ensure the quality of the recycled plastic. Without a proper quality control, the recycled plastic cannot be used in its original application, leading to a depreciation of value, and preventing a true circular economy. One important quality parameter is irreversible chemical aging due to plastic degradation (Alassali 2018).

In this work, we used near-infrared hyperspectral imaging and chemometrics to model the ageing time in acrylonitrile-butadiene-styrene (ABS) and high-impact polystyrene (HIPS). We generated artificially aged ABS and HIPS samples by realizing thermal degradation at 120, 150 and 180 °C, and recorded their hyperspectral images using a commercial short-wave infrared (SWIR) camera. We developed partial least squares (PLS) regression models to predict the degradation time. The PLS models were calibrated and cross-validated using average spectra of the preprocessed images. The evaluated preprocessing methods were: standard normal variate (SNV), 1st derivative and asymmetric least squares baseline removal (AsLS). A subset of the samples was characterized in terms of MFI, impact strength and differential scanning calorimetry-oxidation induction time (DSC-OIT).

We achieved optimal determination coefficients of cross-validation (R^2CV) in the PLS models for prediction of degradation time of 0.8056 and 0.8355 for HIPS and ABS, respectively. Figure 1 shows the heatmaps of degradation time across the pixels, using the optimal PLS models, along their corresponding histograms. The heatmaps clearly show the difference in degradation degree of the two samples, despite the broad width of the histograms.

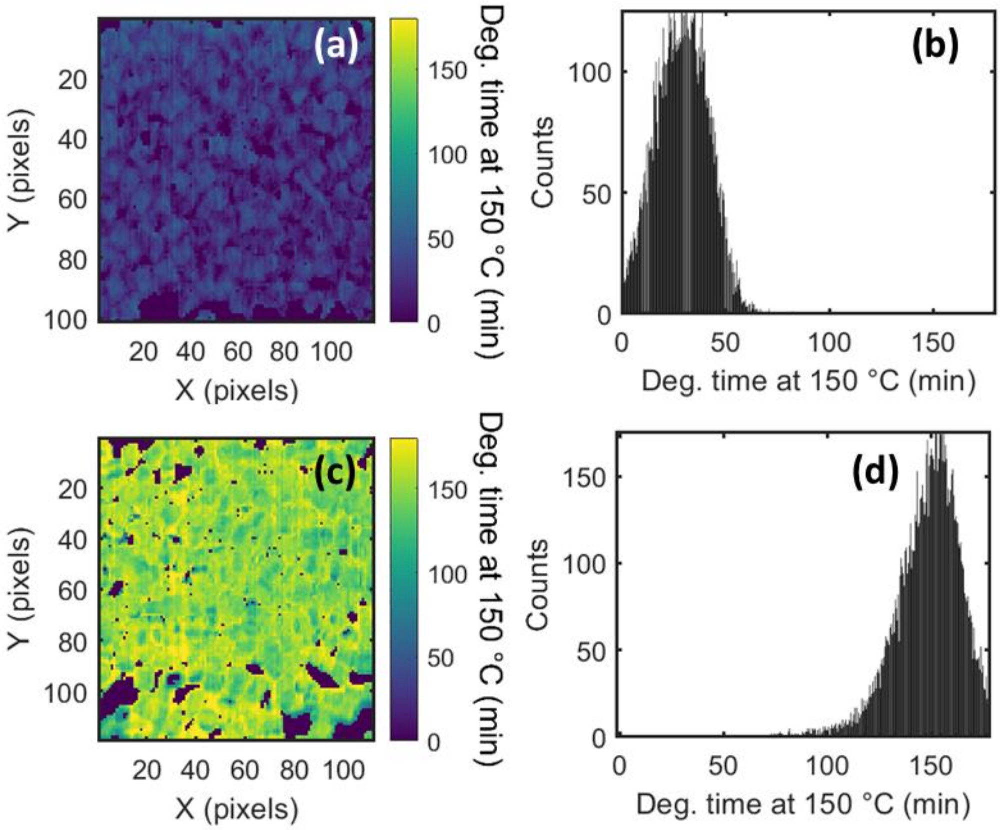

Figure 1. Pixel-wise prediction for degradation time for HIPS. Heatmap of the degradation time at 30 min (a) and 160 min (c). Histograms of the degradation time at 10 min (b) and 160 min (d).

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A069. Identification, mapping, and quantification of asbestos minerals in NOA and ACM using NIR hyperspectral scan imaging: preliminary study

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As well known and widely scientifically demonstrated, asbestos within serpentinite outcrops (Naturally Occurring Asbestos-NOA) or artificial materials (Asbestos Containing Material-ACM) represents a serious threat for human health. This makes the definition of rapid and accurate *in situ* asbestos detection and quantification of primary importance, although such analytical objectives still represent very challenging tasks. Indeed, the recognition and quantification of the different fibers has a crucial importance in order to evaluate the specific toxicities, disposal protocols, and possible preventive measures.

Since the production and installation of ACM was banned (1989 in US, 1992 in Italy, 2005 in Europe), significant efforts have been dedicated to the characterization of the six types of asbestos encountered in NOA or ACM (chrysotile, amosite, crocidolite, tremolite, actinolite, and anthophyllite) using laboratory analytical approaches, such as X-ray diffraction (XRD), thermal analysis, Fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM-EDX), and other (Accardo 2014, Viti 2010). Conversely, just a few works were recently reported on the potential of *in situ* fiber characterization using portable Raman and XRF spectroscopies (Petriglieri 2021, Bloise 2018). Furthermore, promising analytical perspectives in terms of effectiveness, cost reduction, and portability of the instruments also appear to come out from IR spectroscopic techniques, such as SWIR-HSI (Short-Wave Infrared-Hyperspectral Imaging) (Bonifazi 2024).

Here, we aimed at extending the latter approach through the development and testing of a novel portable NIR-HSI tool, which was tested in combination with Laser Induced Plasma Spectroscopy LIPS-HSI. NIR-HIS was based on high resolution spectroscopy (res. 0.52 nm) over a range of about 170 nm around the OH overtone bands (about 1370-1410 nm), highly focusable excitation source, compact XYZ translation stages, and dedicated homemade software in LabView™ programming environment. The vibrational data measured with this system along with the geochemical patterns provided by LIPS-HSI allowed to discriminate different asbestos minerals and to define the conceptual bases for their quantification. Reflectance NIR and LIPS scan chemical imaging with a spatial resolution <50 m was compared with the results of the traditional petrography in order to evaluate the actual potential of the former.

The overall data collected show the the possibility of characterizing asbestos in NOA or ACM directly *in situ*, through chemical mapping providing qualitative and semi-quantitative information on the fiber contents.

Acknowledgements

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A070. Application of Raman Hyperimaging for Bio-Fluid Spots Segmentation and Characterization on Cotton Supports

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Within the domain of forensic sciences, the detailed analysis of bio traces discovered at the scene of crimes emerges as a key topic(Wickenheiser, 2021). This meticulous examination encompasses the study of various substances, such as body fluids, and can provide valuable insights into criminal investigations. By scrutinizing these biological traces, forensic experts can identify potential suspects, establish links between individuals and crime scenes, and unravel crucial details to reconstruct events accurately. This process involves employing advanced techniques like DNA analysis(Chong et al., 2021), serology, and toxicology to extract vital information that helps in piecing together the intricate puzzle of criminal cases(Wickenheiser, 2019). Such scrutiny not only plays a pivotal role in solving crimes but also serves as a cornerstone in ensuring justice is upheld through scientific rigor and evidence-based conclusions. The analysis of these traces usually involves a sequence of extraction steps. These techniques can be optimized according to the unique characteristics of the trace being examined if it is possible in advance to establish its nature. This is also of particular importance since most of the aforementioned analytical methods are destructive and hamper the possibility of making counter-analyses or replicated measurements on samples that have been already analyzed. Moreover, conventional diagnostic approaches to perform such preliminary discrimination do not allow the analyst to perform a significant profiling on the recovered evidence and evaluate the molecular composition beneath the sample surface. Therefore, the necessity to deconvolute the mixture components on the collected evidence is crucial in forensics since a partial, limited, unrepeatable examination of the traces jeopardizes the comprehensive characterization of crime evidence. Chemometric tools can aid in providing the two key requirements that must be fulfilled to allow this. Firstly, by means of a precise spot localization, with the aim of selecting only regions of the sample that can be associated with a biological residue instead of the support on which they are found. Secondly, through a correct spot characterization, differentiating the type of biological residue represented in the segmented spot.

Notably, Raman spectroscopy has emerged as a valuable technique for characterizing both biological fluids(George et al., 2022), whether in their desiccated or liquid states, on cotton-based supports(Zapata et al., 2022). Its proven efficacy underscores its significance in the realm of forensic investigations and with this work we intend to propose and assess its applicability for the preliminary scrutiny of biological traces on cotton supports. This has been carried out by applying a segmentation procedure, based on Soft Modelling of Class Analogy (SIMCA)(Vitale et al., 2023) with the intent of selecting informative pixels that have a different spectral composition from the underlying support. Moreover, an assessment on the possibility of differentiating four of the most common biological fluids (i.e., blood, urine, saliva and sperm) has been conducted by comparing the segmented regions using Principal Component Analysis (PCA).

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A074. Characterisation of brick quality using hyperspectral imaging

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Brick is a durable and widely used construction material. The production of new bricks is a highly energy demanding process due to the high temperatures required during the burning of clay. This process is inherently associated with emissions, driving the high embodied emissions of bricks compared to other building materials. By reusing old bricks and ensuring a longer lifetime for the material, it is possible to save emissions. However, a quality control of the old bricks must be performed to guarantee the required physical characteristics. The goal of the present study is to investigate if hyperspectral imaging can be used as a non-destructive characterization technique for bricks, thus facilitating reuse of brick in the construction sector.

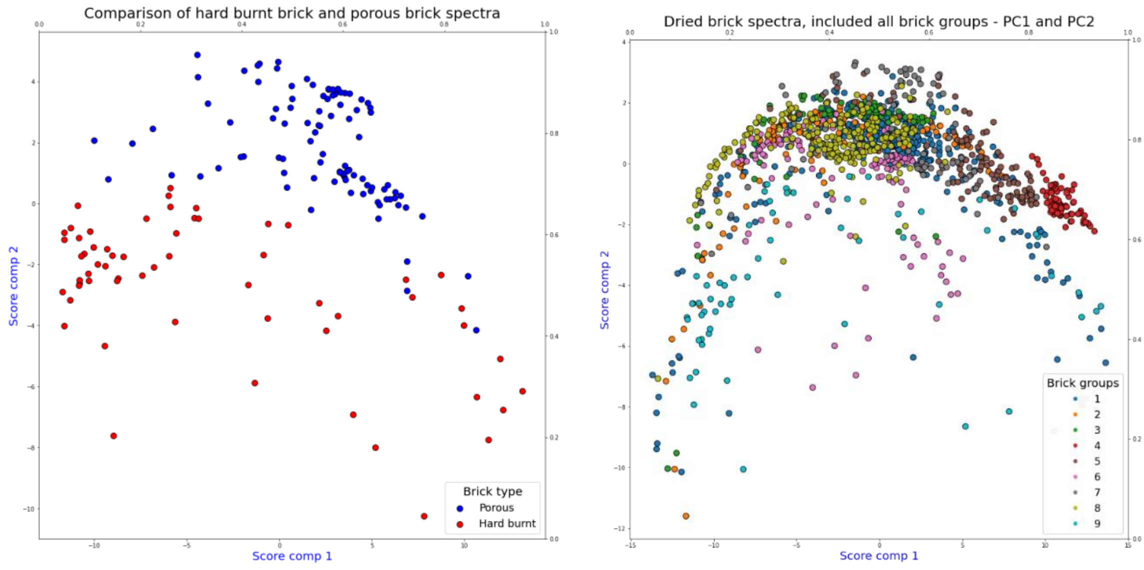
A set of 61 bricks from seven different building sites, consisting of nine types of brick, were scanned with a hyperspectral SWIR camera (hyspex.com). The bricks were scanned in both raw condition and after drying. After preprocessing, twelve mean spectra were calculated per brick based on sectioning of the image. An explorative Principal Component Analysis (PCA) indicated that two groups of bricks could be distinguished, between porous and hard burnt bricks. Figure 1a depicts the score plot of PC1 versus PC2 of the mean spectra of the bricks. Moreover, as shown on the score plot in Figure 1b, the PCA also showed that some groups of bricks had correlated spectral features, whereas others not.

An additional set of 63 bricks, from the same seven building sites, was sent for testing in an independent lab, where their physical properties were determined by standard non-destructive and destructive measurement techniques, resulting in a range of values characterizing the nine different groups of brick. Application of PCA to the brick property dataset, showed that it was possible to distinguish low from high quality brick, based on properties like compressive strength, dry density and water absorption.

A classification of the various groups of bricks have been tested on the hyperspectral images, both using the porous/non-porous characteristics as truth values, and based on values of water absorption and compressive strengths from the physical measurement data set.

The raw version of the bricks studied with the hyperspectral camera had different values of water content. This affects the absorption at the typical water wavelengths around 1450nm and 1950nm, as well as the scattering effect of the light from the bricks' surface. To better understand and correct for these effects, two bricks, one porous and one hard burnt, were soaked in water for 24 hours, then weighed and scanned with the SWIR hyperspectral camera continuously through the drying process. This data set is used to study how signal from scattered light changes during the drying process, and to study the signal from free and bound water over time, using the optimised version of the Extended Multiplicative Signal Correction (EMSC) as described in Stefansson (2019). The difference between the spectrum of a wet and dry samples was also used as input constituent spectrum to the EMSC of the data set of the 61 bricks to see if the amount of the free and bound water in the samples could be modelled and corrected for, as an alternative to drying the bricks.

b)



a) *b)*

Figure 1a) Biplot comparing the spectral properties of hard burnt and porous brick, coloured in red and blue, respectively. 1b) Biplot comparing the distribution of spectra from all 9 brick groups. For both 1a) and 1b) the spectra are preprocessed with Savitsky-Golay and SNV.References

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A076. Microplastics detection in seawater using 2D Raman mapping of a filter (membrane) with residue

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Nowadays, microplastics (MPs) – synthetic particles less than 5 mm in size – are widely present in the environment, and seen as a potential global threat to biodiversity, food safety and public health (**Pitchel 2023**). The problem is especially acute for seawater, since it is one of the main sources of foodstuff, and, at the same time, it accumulates a huge amount of plastic waste. As a result, MPs have already been found in the tissues and organs of many marine species, as well as in sea salt. To control and correct the situation, it is necessary the systematic extensive monitoring of MPs in seawater is including their size/type distribution, spreading over the water area/depth, weathering, degradation, interaction with chemical pollutants etc.
Raman spectroscopy is an effective analytical technique for this task (**Pitchel 2023**). It is a rapid, non-contact and non-destructive method that uses monochromatic light to excite molecules in a material, and the spectrum of inelastically scattered light (Raman spectrum) to recognize the types of these molecules, intra- and intermolecular bonds. The method has high selectivity and sensitivity, allowing to identify different types of MPs, even if their number are low, they are mixed, or the irrelevant (matrix) components are present. In addition, one can observe minor changes in the MPs chemical composition and structure. Combination with scanning optical microscopy (Raman microscopy) yields the distribution of locally measured Raman spectra over the sample (hyperspectral imaging) that in turn can be used for simultaneous visualization of the MPs chemical composition, geometry and spatial distribution (chemical imaging).
Our Raman microscope can perform the analysis of MP at a very small footprint so it can be used in portable labs on ships in the ocean.

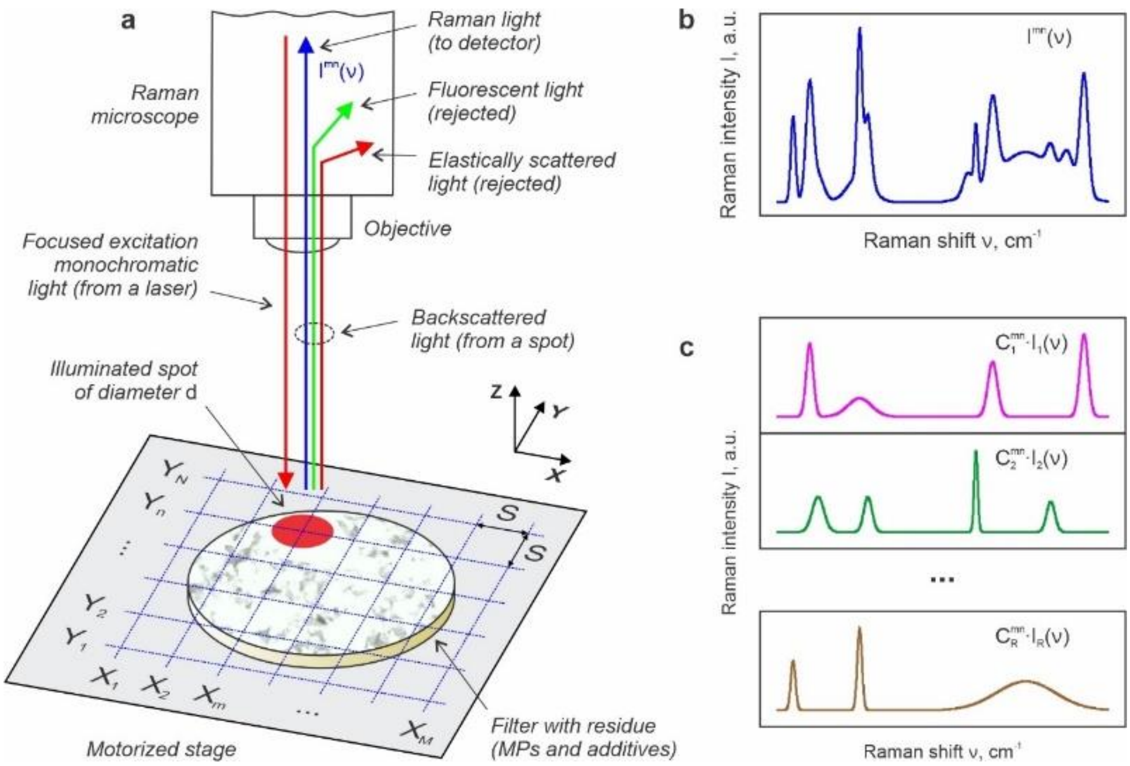

Figure 1. 2D Raman mapping: (a) general measurement scheme;(b) model Raman spectrum for the mixture "obtained" from one illuminated spot;(c) "pure" Raman spectra for individual components present within the spot

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A077. Salts vs Angels: Revealing the Battle

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This work concerns the study of murals preserved in the Valencia Cathedral, known as the Angel Musicians, which were painted in the 15th century. Re-discovered in 2004, are considered the first example of Renaissance-style painting in Europe outside of Italy, prior to Sistine Chapel. Although the paintings, executed in *buon fresco*, were restored after their discovery in 2007; some issues related to the emergence of salts (efflorescences) and the lifting of the polychrome began to appear again in 2014. To comprehend the extent of damage induced by the formation of soluble salts, non-destructive analytical techniques such as Raman spectroscopy in conjunction with NIR-Hyperspectral imaging were employed. Portable in-situ Raman analysis was utilized to identify the salts involved in the deterioration process. The spectrometer was outfitted with a 785 nm excitation laser and had a maximum nominal laser power of 300 mW. The laser power settings ranged from 10% to 30%, and all spectra were captured within a spectral range of 100 to 2200 cm-1. Each measurement was set to 1-3 seconds, with the number of accumulations ranging between 10 and 20. It was determined that the primary salts adversely affecting the paints were potassium and sodium nitrate, alongside calcium sulphate and calcium carbonate salts. Furthermore, hyperspectral imaging was used to expand the point-by-point analysis conducted with Raman spectroscopy to encompass the entirety of the paint layer. Consequently, the ultimate objective is to generate detailed damage maps delineating the areas affected by salts, while also identifying regions relative to each type of salt.

For the preliminary analysis, a study is being conducted on an image obtained from the area exhibiting the most striking form of deterioration. The analysis and processing of the hyperspectral image spectra are being carried out using HYPER-Tools v3.0 (freely available at https://www.hypertools.org) (Mobaraki 2018). Exploratory analysis using Principal Component Analysis (PCA) revealed a clear separation between salt-affected and unaffected areas. For instance, the use of various preprocessings, such as Savitzky-Golay smoothing with a window of 11 and a polynomial degree of 2 successfully identified the areas affected by salts from the unaffected ones in the PC8 scores (0.04% of explained variance). Furthermore, by cropping the annular region, two principal components were identified, effectively separating two distinct salt-affected zones.

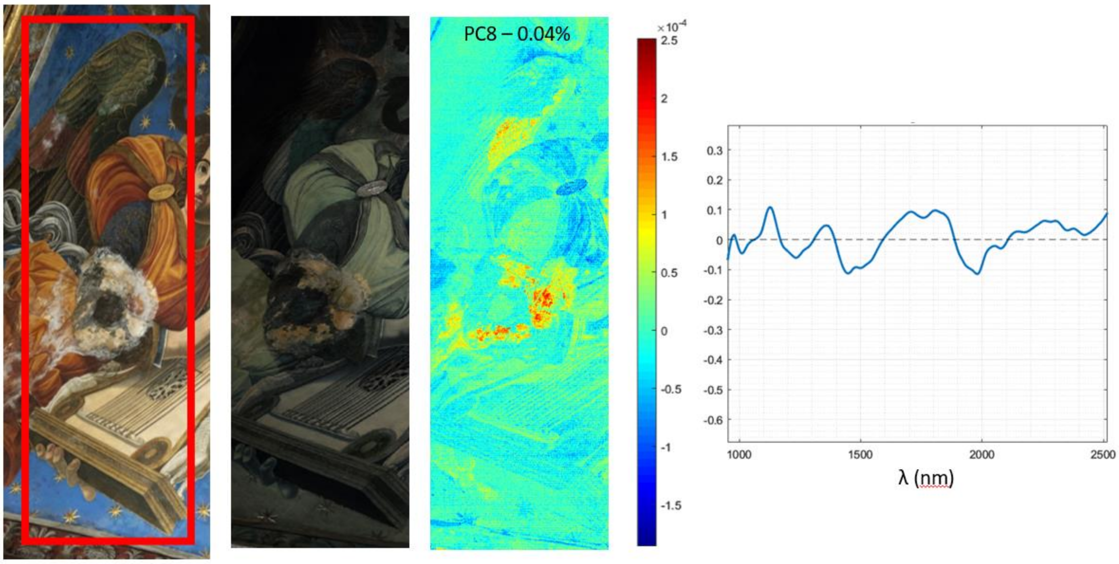

Figure 1. From left to right: photograph of the analysed painting with the area analysed by NIR-Hyperspectral image highlighted; RGB false colour image of the NIR-Hyperspectral image; PC8 Scores and Loadings.

With these preliminary results, a distinction is demonstrated between the NIR spectra of the salts and the rest of the paint components. The next steps will involve measuring standards of the salts identified with Raman spectroscopy and utilizing correlation methods to attempt the identification of each salt in the hyperspectral images.

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Acknowledgement

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A078. Untying the Knots: Exploring Analytical Challenges in Hyperspectral NIR Imaging of Textiles

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The identification of textile fibers holds immense significance due to their status as major international commodities, integral components of cultural heritage, and physical evidence in forensic investigations (Peets, 2019). Moreover, the recognition and sorting of textile material is extremely important for reuse and recycling as it could guarantee added value of the recycled material (Cura, 2021). In particular, within the context of recycling, the wide variety of fibers used in textile production inherently complicates the process of analysis and identification. In addition, textile samples represent very complex materials both for their chemical composition and physical characteristics. The chemical information is mainly related to the raw material, dyes, and chemical treatments. Optical and physical characteristics could be related to thickness, surface texture, colour, and transparency. In the last decades, special attention has been drawn to spectroscopic analytical techniques as a fast-non-destructive option to obtain meaningful information about textiles (Peets, 2019; Quintero Balbas, 2022; Bonifazi, 2022).
In this study, samples of different textile compositions (i.e., cotton, polyester, elastane, linen) and reflectance properties were analyzed with a Specim SWIR camera (Specim, Spectral Imaging Ltd., Oulu, Finland (**Figure 1**) using halogen lamps and a NKT Photonics Supercontinuum light as sources. The camera covers a spectral range of 1000-2500 nm. Different spatial resolutions were investigated to emphasize the varied issues that could arise depending on the samples. The challenges due to the nature of the sample surface, such as particle size, brightness, colour, and the possibilities offered by the camera and acquisition configuration, have been evaluated. Moreover, tests with different resolutions and optical focus have been carried out. As a reference identification for the materials, Raman spectra were acquired using an InnoRamanTM portable spectrometer (B&WTEKINC, Newark, USA) coupled to a microscope (20x and 50x magnification) and provided with 532 nm laser and CCD detector (Peltier cooled)), and external reflectance spectra were acquired with the Agilent 4100 Exoscan FTIR portable spectrometer (Agilent Technologies, Santa Clara, CA,USA) with a diffuse reflectance sampling interface. Spectra interpretation and multivariate analysis allowed a better understanding of the issues in the identification of materials. Data exploration has been carried out with Principal Component Analysis and clustering techniques. Multivariate Curve Resolution has been evaluated unmixing spectral components of the textiles.

Figure 1. Some textile samples, example of acquisition process, and image of sample with elastane

Acknowledgment
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A079. MCR-ALS image analysis of climate variables spatio-temporal dynamics in the Iberian Peninsula

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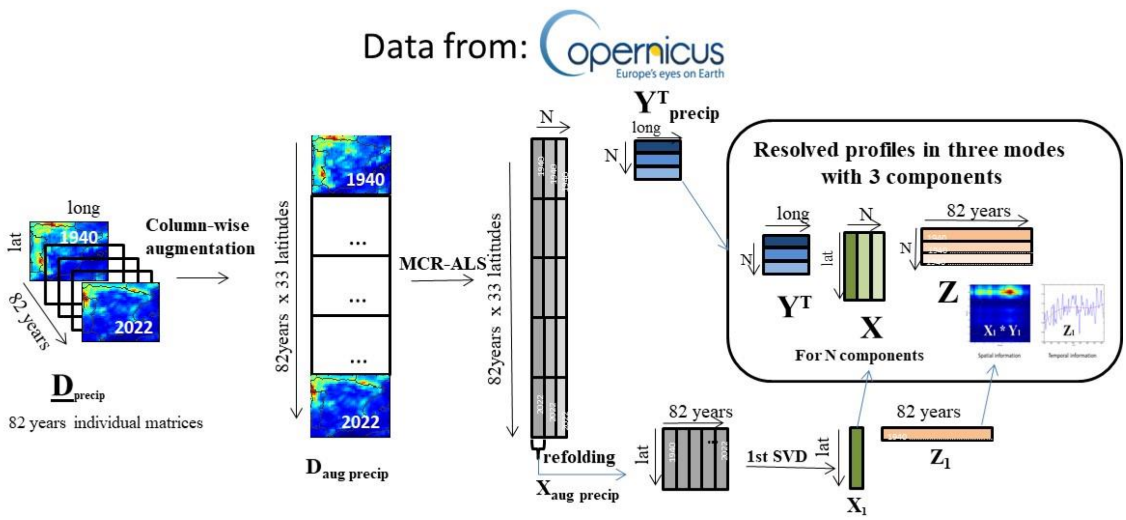
Multivariate Curve Resolution-Alternating Least Squares (MCR-ALS)[1,2,3] is applied to the image analysis of the spatial-temporal dynamics of climatic variables, such as total precipitation and temperature, across the Iberian Peninsula. The geographical region is represented by a grid of 33 latitude bands spanning from 36º to 44º North and 53 longitude bands ranging from -9º to 3º East. Climatic data were converted into rasterized image data matrices, where each pixel corresponds to a geographical area of 0.25º x 0.25º, roughly equivalent to about 28 x 28 km of the Iberian Peninsula. Within these pixels, monthly temperature and precipitation values were aggregated over an 80-year period, sourced from the European Centre for Medium-Range Weather Forecasts (ECMWF) project[4]. Our investigation facilitates the extraction of insights into the spatial-temporal dynamics of climatic variables over the Iberian Peninsula. Specifically, we identified precipitation zones exhibiting shared patterns across pixels within defined geographic areas and track temporal trends over the 80-year period under scrutiny. Temperature changes confirmed the increasing trend observed for the last years.



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A084. Advancing Aluminum Recycling: Unwanted insert detection in aluminum parts with Innovative hyperspectral imaging solutions"

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The recycling of aluminum is crucial for environmental sustainability and energy conservation, yet the industry faces a significant challenge that undermines these benefits: the contamination of aluminum scrap with inserts of various materials. These inserts, composed of different metals or non-metals, degrade the quality of the recycled aluminum, affecting its properties and limiting its applications. The presence of such contaminants not only diminishes the value of recycled aluminum but also compromises its role as a sustainable alternative to primary aluminum production. Addressing this issue necessitates the development of advanced detection and separation techniques to ensure the purity and usability of recycled aluminum, thereby reinforcing the material's economic and environmental advantages. In a previous publication (De la Peña 2023), we introduced an artificial intelligence model based on spectral information to tackle the intricate challenges of scrap segmentation. Building upon that foundation, we present a paradigm-shifting advancement in our methodology, steering away from the conventional pixelwise classification approach and embracing a holistic hyperspectral imaging strategy. This innovative approach involves predicting the complete hyperspectral image in a single shot, thereby overcoming the limitations of pixelwise classification, and providing a more comprehensive solution to the complex nature of ferrous scrap materials.

This advancement is particularly pivotal for real-time applications and the processing of extensive datasets, where reduced complexity translates to accelerated decision-making. Beyond efficiency gains, our holistic hyperspectral imaging approach allows our model to capture the global context and intricate relationships within the entire image. This expanded understanding of material composition at a broader scale contributes to improved accuracy in material segmentation. This new approach has been validated in an industrial use case for the detection of different types of unwanted inserts in aluminum parts.

Specifically, we use the model proposed in (Zheng 2020), dubbed FPGA, to process spectral and spatial information from two different hyperspectral cameras, Specim FX10 and FX17. The former operates in the 400-1000nm range, and the latter in the 900-1700nm range, and this allows to capture the spectral signatures of various materials in scrap mix.

The research provides a detailed overview of the steps involved in generating, preprocessing, and labeling a hyperspectral image dataset for identification of different types of unwanted inserts in aluminum parts, prior to their recycling for the generation of secondary aluminum from fractions from end-of-life vehicles. The dataset consists of 364 acquisitions (172 for FX10 and 192 for FX17) of scenes with different aluminum parts of different quality and shape with six types of unwanted inserts such as copper, foam, ferric, rubber, brass and plastic (Figure 5). The resolution of the images obtained with the FX10 camera is 640x640x448, and for the FX17, it is 640x640x224. The dataset was generated taking advantage of the material characterization set-up of Tekniker, depicted in Figure 4. The set-up consists of a circular conveyor belt, 2 hyperspectral cameras, 500w halogen lighting and a PC with NVIDIA GeForce 4070 12GB GPU.

The dataset was normalized using white and black balance, and labeled using a web-based annotation tool. The work also discusses the noise reduction and normalization methods applied to the hyperspectral data. These include Savitzky-Golay smoothing, dead pixel and spike removal, and standard normal variate and multiplicative scatter correction. These methods are used to account for spectral variations and enhance the classification accuracy.

Figure 4: Material characterisation set-up in Tekniker facilities

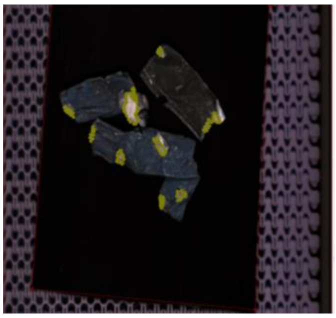

Figure 5: Labelled unwanted insert example

In our previous work (De la Peña 2023), the model obtains an inference time of 29.7 seconds using the original resolution analysing all pixels and an inference time of 0.75 seconds when the image size is reduced by 64 times. With this new holistic approach an inference time of less than 0.1 seconds is achieved with both cameras. Figure 6 illustrates the confusion matrix derived from training sessions utilizing FX10 captures, where an F1 score of 70% was attained. Conversely, Figure 7 presents the confusion matrix resulting from training with FX17 captures, achieving a 57% F1 score. For both datasets, the training partition comprised 80% of the data, with the remaining 20% allocated for evaluation purposes. Notably, the confusion matrices for both training scenarios indicate a predominance of high recall rates, consequently leading to diminished precision and adversely impacting the overall F1 score. Future research will prioritize enhancements in model precision.

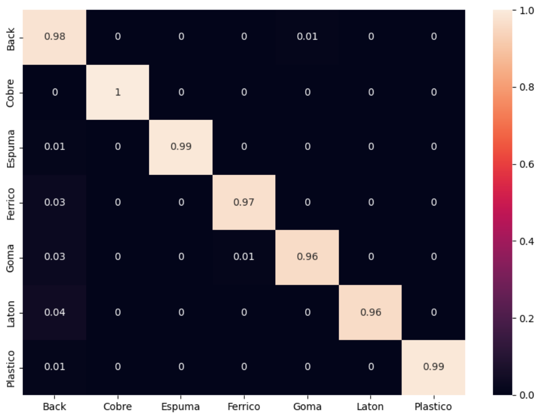

Figure 6: Fx10 confusion matrix

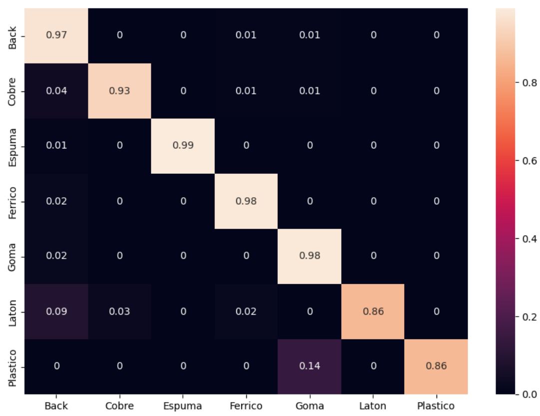

Figure 7: Fx17 confusion matrix

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A085. Comparative Analysis of Spatial and Spectral Features for Addressing Challenges in Hyperspectral Imaging of Historical Documents

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Preserving and interpreting historical documents often involves overcoming challenges posed by obscured text due to additional layers such as binding materials or overlaid paper. While hyperspectral imaging has proven valuable for revealing hidden texts (Snijders 2016), achieving legible results remains a challenge, complicating cultural and historical studies (**Figure 1**). Moreover, distinguishing text on different layers of paper proves difficult with conventional spectral unmixing techniques, which fail to detect textual data on different layers as independent components. As dismantling these manuscripts is not feasible, the absence of ground truth data regarding text appearance limits the possibility of applying data-driven approaches.

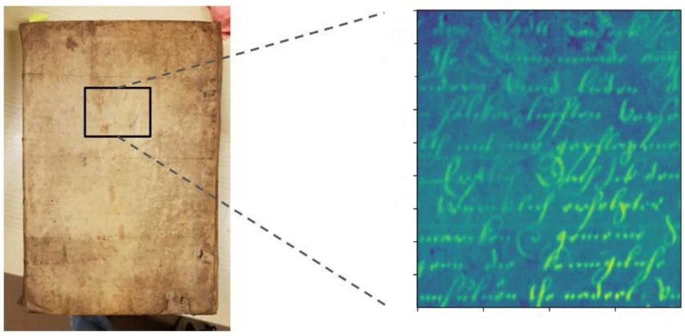

Figure 1. Principal Component Analysis (PCA) applied to the hyperspectral scan of a historical book binding reveals the hidden text. However, the revealed text is not legible to manuscript specialists.

As the first step towards addressing these challenges, we undertake a comparative study of spectral and spatial features of hyperspectral scans between covered and exposed documents, simulating bound manuscripts through fabricated test samples. Thorough analysis of spectral and spatial features of covered documents compared to uncovered ones is conducted, laying the groundwork for building deep learning models capable of detecting and separating different layers of textual data. Furthermore, to study the effect of covering on the textual legibility, relevant Digital Image Quality Assessment (DIQA) measures were applied to selected hyperspectral bands of samples before and after covering. This study contributes to advancing our understanding of hyperspectral imaging for historical document analysis and lays the foundation for improving computational techniques for text extraction and layer separation.

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A086. A pigment of your imagination – Illusive Red Ochres and NIR Imaging

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Prehistoric Rock art and the use of pigments (ochre) have been given a lot of attention in Archaeology and Geology as images and colours gives us a different angle into prehistoric people's imagination (Erdogu 2011, Wreschner et al 1980). Ochres, based on compounds of iron, manganese, calcium or carbon can be investigated in many different spectroscopic ways (Linderholm et al 2015, Horn et al 2020). Iron oxides, in the form of hematite, are the base pigment for making red ochre and is the pigment of choice at least since the era of Neanderthals and was used in burials and later on for painting (Roebroeks et al 2012).
However, in Scandinavia red ochre is found in settlements, graves and as rock paintings. A problem that archaeologists encounter is that all red stains (non-figurative colourings) are not intentionally made, but some of them may well be. So how do we differentiate natural stains from human made ones?
Benefits of imaging in these contexts are obvious (Bayarri et al 2019), and one could say that images deserve imaging. Even so, sediments and soils that harbour ochre pigments are better represented as images due to the heterogeneity of samples and heterogenous materials i.e. sediments may be better understood in more detail. In this presentation we will provide examples to show how NIR spectral imaging is an advantageous technique to use.
Samples of ochre pigments from various archaeological contexts in Scandinavia were collected for analysis. Spectroscopic analysis was conducted using near-infrared (NIR) spectral imaging technique. The NIR spectra of the pigments were compared to reference spectra of known ochre sources and natural bedrock materials. Hyperspectral images were generated with a HySpex SWIR-640 imaging system to visualize the distribution and composition of the pigments on different substrates.
The analysis of ochre pigments using NIR spectral imaging revealed distinct spectral signatures characteristic of iron oxides, particularly hematite, confirming their presence in archaeological samples (Figure 1). By comparing the spectra of the pigments to reference spectra of known ochre sources and natural bedrock materials, we were able to differentiate between intentional pigment applications and natural staining. Furthermore, the use of hyperspectral imaging provided detailed spatial information, allowing for a better understanding of the distribution of ochre pigments within sediments and soils. This highlights the effectiveness of NIR spectral imaging as a valuable technique in archaeological investigations, particularly in elucidating the use of pigments in prehistoric societies and distinguishing intentional cultural deposits from natural phenomena.

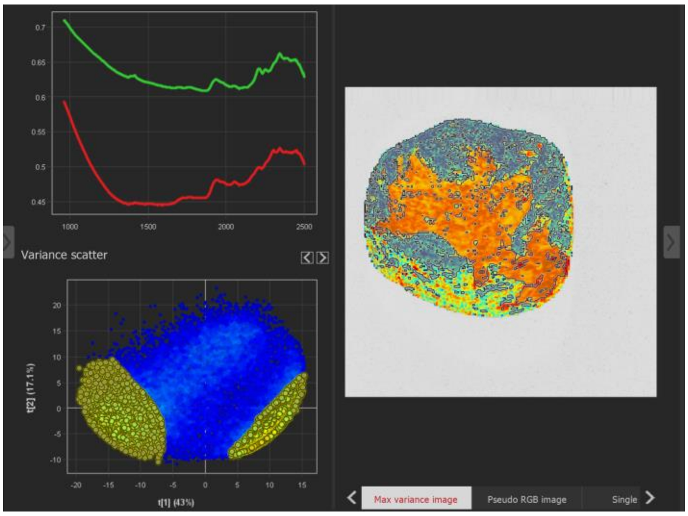

Figure 1. NIR mean spectra of pigments (red) and bedrock (green) with PC score image and score plot.

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A087. Hyperspectral imaging for the inline quality control of painted wood

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Surface treatment with coatings not only gives wood products a desired structure and colour but also protects the wood surface against weathering for prolonged service life. The performance of a surface coating is strongly dependent on the film-forming mechanism and the film thickness. An insufficient dry film thickness reduces the durability of coated panels during weathering which shortens the lifespan and the maintenance intervals. Excessive film thickness, on the other hand, increases the chemical consumption, the costs and the environmental load associated with the production of coated panels. Wood as a heterogeneous substrate with high surface roughness adds extra complexity, making it difficult to achieve a homogeneous coating with specified film thickness.
Today's quality control methods for coated wood panels are based on random checks and manual operations. Several methods to determine the wet and dry film thickness exist and have been standardized. However, these methods are either not applicable for online measurements, are destructive, or do not provide spatially resolved information.
The scope of the present pilot project is to investigate hyperspectral imaging as a tool to evaluate the quality of coated wooden panels. If successful, this method may replace manual quality control operations based on random checks to attain: (1) less laborious and thus more efficient operations; (2) an automated inspection of all pieces that go through the line, which will ensure consistent quality of the products; and 3) better accuracy of measurements that will provide the basis for smoother quality and product optimization.
Samples of Norway Spruce (*picea abies*) with dimensions 500mm x 150mm x 25mm, with two different colours (white and wood stain) and two different thicknesses have been scanned with a hyperspectral camera from hyspex.com in the SWIR (short wavelength infrared region, 1000-2500nm). First a set with three samples of each was selected from batches in the industry, scanned, weighed and analysed. Then a second independent set from new batches was prepared, scanned, weighed and analysed for validation. Dry coating thickness was also determined destructively using the wedge cut method and a microscopic assessment with a pain inspection gauge in order to verify the hyperspectral measurements. Finally, samples with wet film were investigated to study the potential of integrating hyperspectral imaging as process control in early stages.
The images of the samples were down sampled into mean spectra of size 5x5 pixels. Examples of mean spectra of the different colours and thicknesses are shown in Fig. 1. In Fig. 2 is depicted the microscopic image of a region of one of the samples. PLS-DA classification resulted in 96% (wood stain) and 99% (white paint) correctly classified pixels on the first dataset, and correspondingly 90% and 94% correctly classified pixels on the second data set. Preliminary results on wet film also indicates that measurements can be carried out directly in the production line.

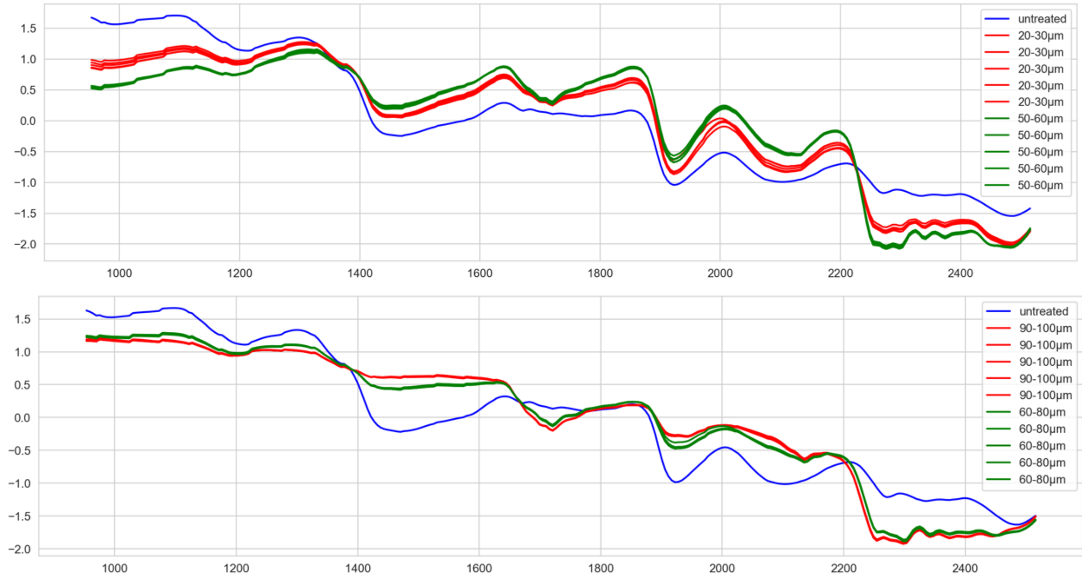

Figure 1. Mean spectra of non treated and painted samples with two ranges of coating thickness of wood stain (upper panel) and white paint (lower panel).

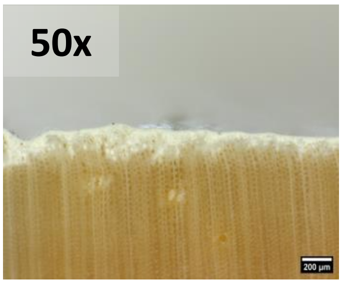

Figure 1. Example of a microscope image for individual assessment of coating thickness.

A089. Molecular and morphological characterization of Microplastics recovered from the *Urdaibai* Biosphere (Basque Country, Spain) Using Imaging Raman Analysis

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Microplastics (MPs) are considered contaminants of emerging concern (CECs) because of their role as propagation vectors of hazardous pollutants. Evaluating their impact in the nature starts with the assessment of their presence in the different environmental compartments [1]. Thus all around the world, a huge amount of monitoring studies take place aimed to determine the MPs presence in waters, sediments, soils and air media.

As such, this work is focused on evaluating the MPs impact suffered along the natural biosphere of the *Urdaibai* estuary (Basque Country, Spain). Thus, a monitoring study was conducted to assess for the first time this micro-pollutant presence in sediment matrices that are a known contaminant sink. The seasonal campaigns covered 6 sampling points following the river course (*i.e.*; Maier, Karramarro, Depuradora, Tejera, Txakarramendi and Arteaga). Once the samples were collected, they underwent the established treatment by filtration, flotation, and digestion methods [2] to recover the target particles in the range of interest (240 – 500 µm). Then, the molecular and morphological characterization was performed through a novel methodology based on Imaging Raman analysis, handling the drawbacks associated with such matrix due to the common fluorescence effect caused by their inherent composition (organic matter, feldspar, or clays, among others) [3].

The imaging data collected allow the automatic quantification of at least seven types of plastics (PE, PET, PP, PS, PVC, PMMA and PC), being the PE and PET concentration levels the highest ones detected. The particles found were successfully registered according to their color, dimensions, and shapes to provide further information in the field. Moreover, Arteaga, Txakarramendi and Tejera were pointed out as hot spot areas with alarming values of particles per kilograme. In contrast, Depuradora point located after the water treatment plant showed the lowest number of particles, evidencing the level of efficiency of its working system. Further analyses are on going to deeply discuss the influence of the seasonal effect in accordance with the anthropological activity of each area.

Acknowledgements: This work has been financially supported by the Spanish Ministry of Science and Innovation (MCIN) project PLASTEMER (PID2020-118685RB-I00), by the Basque Government project "Consolidated Research Group 2022-2025 (IT1446-22) and by the European Regional Development Fund (FEDER). T. Maupas gratefully acknowledges his predoctoral grant contract from the University of the Basque Country (UPV/EHU). U. Uribe-Martinez also thanks the Consolidate Group (IT1446-22) project from the Basque Government for her predoctoral contract.

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A092. Performing VIS-NIR hyperspectral imaging of pelagic fishes: evaluation of experimental critical factors for direct analysis

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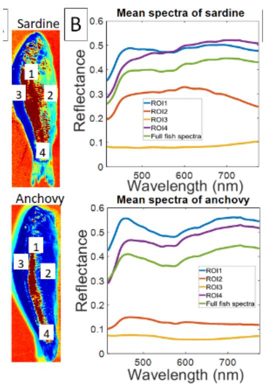
The determination and identification of fish species, as well as characterization of diverse compounds in pelagic fishes play a crucial role in the fishing industry, food research and management of marine resources. Traditional methods for identification of species, rely heavily on the expertise of the observer or including DNA barcoding and meta-barcoding methods[1]. Despite advances, both traditional morphological taxonomy and molecular barcoding, including polymerase chain reaction method (PCR) require laborious laboratory work. This implies the need for a taxonomist with intensive training in microscopy and meristic to identify phenotypic structures, or a technician specialized in performing PCR and sequencing reactions for barcoding. Thus, the need for a more objective and efficient methodology for accurate identification and characterization of pelagic fish species has become pressing. Hyperspectral imaging offers a promising solution by providing information not only on the visible colors of fish, but also on wavelengths in the ultraviolet and near-infrared ranges in a rapid way and with minimal sample preparation or direct analysis, overcoming the limitations of the traditional techniques when dealing with large numbers of fish. Despite this, its use in the animal kingdom is poorly described and there are not many applications described in the literature[2].

This work proposes the use of hyperspectral imaging (HSI) technique in the VIS-NIR region (400-1100 nm) to evaluate diverse factors affecting the HSI analysis of fishes, under a multivariate overview, in order to improve the ability to capture and record fish spectral information, with a particular focus on pelagic fish. The study includes the evaluation of specific morphological regions of interest (ROIs) in fish images for evaluation of intrasample spectral variability of fishes, the study and assessment of fish freshness, as well as the study of the fish refrigeration storing for long time on spectral characteristics. Four pelagic species including anchovy (*Engraulis ringens*), sardine (*Sardina pilchardus*), hake (*Merluccius Gayi Gayi*) and silverside (*Basilichthys australis*) were used. Diverse multivariate techniques such as principal component analysis (PCA), regression by SVM (SVM-R) and discriminant - partial least squares (PLS-DA), were applied for these purposes. Comparative study of morphological ROI allowed us to conclude that there are considerable differences between spectral characteristics of different fish zones. Lateral zones and dorsal region, near the tail, are the most representative zones to describe the entire fish (Figure 1). Thus, it is not necessary to evaluate the complete fish information since these ROIs provide the same spectral information as that given by a complete image for each individual, in addition to having 10 times less weight of data to facilitate chemometric analyses by reducing the capacities that computers must have. The freshness

study shows that there is a decrease of the intensity of the spectral bands when fishes are analyzed over time, and prediction of this freshness as “time after capturing” was possible by HSI by SVM-R, with 7.5% of relative error of prediction. Regarding the spectral differences produced by freezing, results showed that there are notorious differences between the measurement of fresh and thawed fishes, where the band at 940 nm assigned to the second overtone of O-H bond in water, plays a fundamental role (Figure 2). Successful prediction of the freezing time by PLS-DA (100% of correct classification) was also possible.
Thus, ROI, freshness and freezing sample pretreatment should be considered as critical factors since results have demonstrated their effects in spectral characteristics of fishes. Finally, HSI considering these factors supported with multivariate analysis, made possible a differentiation between the studied species.

Fig. 1 Evaluation of morphological ROIs in fishes by HSI.

Fig. 2. PCA applied to fresh and thawed samples for



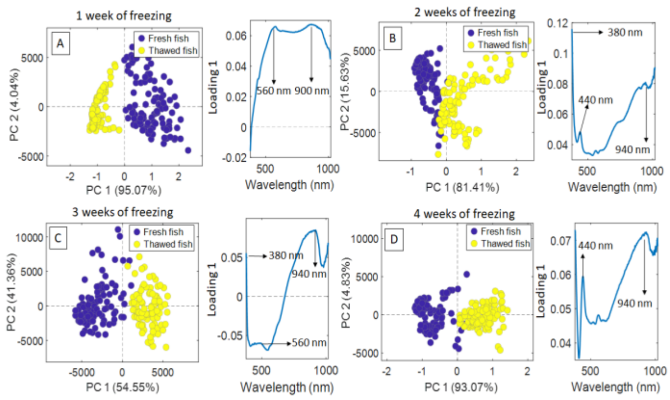


Fig. 1 Fig. 2

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A093. Adaptable Multipurpose Calibration of Hyperspectral Pushbroom Cameras

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This work presents an innovative an adaptable approach to calibrating hyperspectral images (HSI) generated using a pushbroom setup. The proposed method provides a solution for calibrating spectral, intensity, and spatial information, while also offering precise details regarding the system's spectral and spatial resolution, all in a single scan. This is realized through the creation of a single calibration board equipped with all the necessary information for the multipurpose calibration, inspired by previous research endeavors. (Henriksen, ML 2022)
Calibration of spectral information is done using an array of LEDs spanning the entire Vis-SWIR range, allowing for a simple construction of the wavelength array covered in the HSI. Intensity inaccuracies arising from uneven lighting across the imaged object and variations in sensitivity on the camera sensor is all calibrated using a highly reflective white reference made with material such as TiO_2 or PTFE based RESTAN. Given the nature of the pushbroom method spatial calibration is required to maintain an accurate aspect ratio within the image. This is achieved using a simple checkerboard pattern.
The calibration board is further equipped with an MTF line-pattern and a laser diode to accurately determine both the spatial and spectral resolution of the given HSI setup.
The calibration procedure is done using a python-based software embedded with an object detection AI trained to accurately extract all the necessary information from the imaged calibration board. The object detection AI makes the calibration process highly adaptable as it allows for accurate calibration of pushbroom systems of varying field of view (FOW) and scan speeds.
The method is evaluated using the Newtec Vis-SWIR Oculus hyperspectral pushbroom camera (Newtec 2024) showing excellent outcomes (**Figure 1**). These results are demonstrated for images captured at various speeds and with differing FOW.

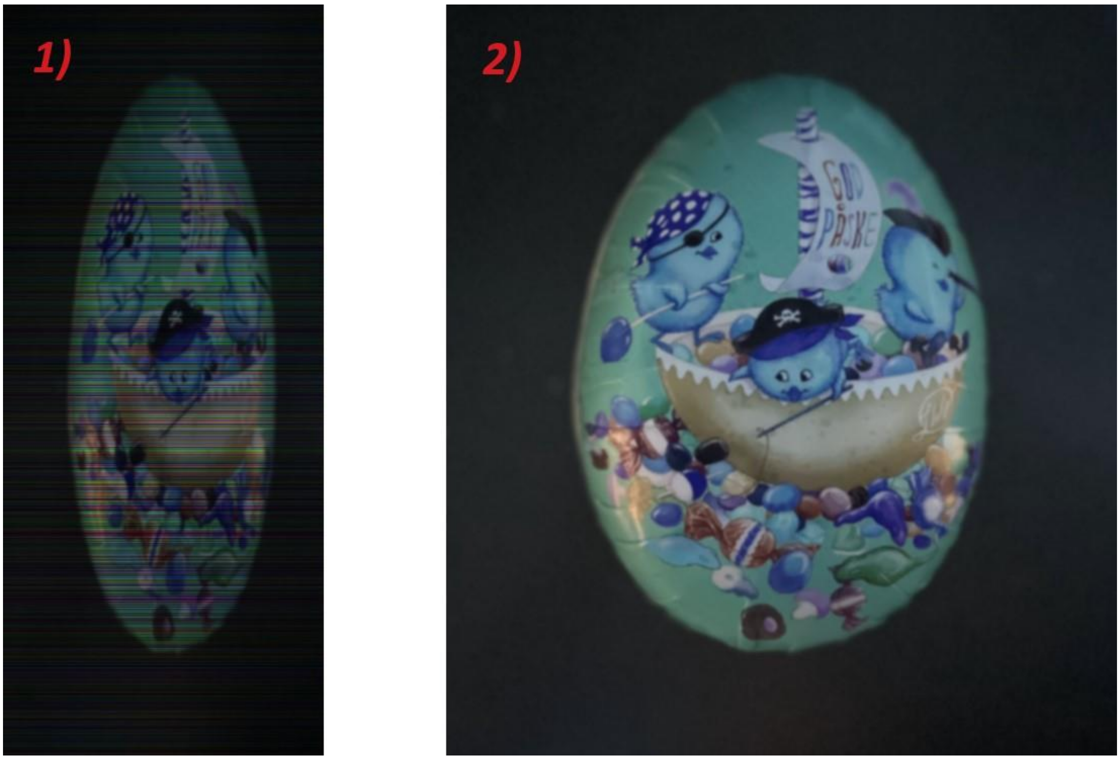

Figure 1. 1) RBG representation of a hyperspectral image of a Danish easter egg before intensity and spatial calibration. 2) RBG representation after intensity and spatial calibration have been applied.

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A096. Mobile, ground-based VNIR-SWIR hyperspectral imaging for cultural heritage applications. Towards the study of complex architectural surfaces.

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The application of hyperspectral imaging (HSI) in the cultural heritage field is consistently growing, as evidenced by the increasing number of studies from worldwide research groups. Applied for monitoring, high-quality documentation, as well as non-destructive characterization of materials in works of art, HSI has been proven to be an extremely versatile method for investigating different typologies of artworks (Striova et al. 2020). The most commonly examined spectral range is the visible and near-infrared (VNIR) between approximately 400 and 1700 nm, which can provide spectral information about compounds such as pigments and other materials used in works of art. The adjacent short wave infrared range (SWIR) up to approximately 2500 nm is instead less explored, even though it provides significant additional information (Cucci et al. 2019). In this region, overtones and combination bands of fundamental vibrations can be used for spectroscopic classification and/or identification of organic and inorganic compounds. In addition, the increase of the penetration capability as a function of the wavelength can allow the visualization of hidden information beneath the upper visible layer, e.g. underdrawings. Despite HSI is today well-established for investigating several types of polychrome surfaces, a significant research gap lies in the systematic application of HSI for studying architectural surfaces with complex geometries on site. In this paper, we present the application of a dual-sensor Hyspex VNIR-3000N/SWIR-384 system with a motorized biaxial rotation stage on a mobile tripod and an integrated illumination system to study in-situ the wall paintings of the Magdalen Chapel of the church of St. Emmeram in Regensburg (Germany). The push-broom imaging spectrometer system covers a broad spectral range from 400 to 2500 nm, at a spectral resolution of 2 nm in the VNIR and 5,45 nm in the SWIR. The biaxial rotation stage enables simultaneous scanning with both scanners, while its portability makes it more versatile than the commonly used systems with a fixed X-Y scanning stage (Cucci et al. 2016).

The wall paintings of the Magdalen Chapel present a complex stratigraphy made of four different painting phases dating from the 12th to the 17th century. Due to the fragmentary state of conservation of the paintings and a partial uncovering in the 1980s (intentional removal of younger phases during a restoration), all phases are simultaneously visible today. This results in an iconographic, stylistic, and material patchwork. The mostly curved surfaces of painted niches and vaults of the chapel further add technical challenges to the complexity of the context. The HSI system was applied to understand and discriminate the artistic materials employed for each phase, allowing their preliminary identification and mapping. First, we optimized the image acquisition and data pre-processing workflow. Secondly, the data were geometrically corrected using rectified photogrammetric images. In order to interpret the spectroscopic data and study the influence of stratigraphy and layering on the signal, reference measurements were acquired on ad hoc produced mockup paintings that simulate historic techniques. Informed by this spectral reference database, the HSI data were key to shedding light on the pigments palette. Moreover, the high spatial and spectral resolution permitted a data-based visualization of the painting phases. The results were validated with a digital mapping by a wall painting conservator. The application of VNIR-SWIR HSI and the optimized workflow contributed to the understanding of the artistic technique of this highly complex and unique heritage site, opening the venue for future implementations in the conservation-restoration praxis.

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A101. Advances in External Reflection FT-IR Mapping: Exploring the Potential of a NIR-MIR Instrumentation and Multivariate Data Handling for Painting Investigation

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In recent years, the investigation of paintings through external reflection Fourier Transform Infrared (ER-FT-IR) spectroscopy has evolved from traditional point analysis to the comprehensive mapping system. However, the state-of-the-art techniques are constrained by several limitations including the complex interpretation of reflectance profiles, high operating costs and limited spatial resolution. These issues, compounded by long acquisition times, highlight the imperative for continued development to improve the applicability and effectiveness of ER-FT-IR mapping techniques in cultural heritage analysis (Rosi 2019).

To open the new possibility of ER-FT-IR mapping in Mid-IR region, the current research focuses on the development and application of a custom-made system for painting investigation. The system operates in the near-infrared (NIR) and mid-infrared (MIR) region (5500-650 cm^{-1}), integrating capabilities across two regions enhances the analytical power, allowing for deeper penetration and the revelation of stratigraphic details.

This mapping system assembled the Agilent Cary 630 portable FT-IR spectrometer with the high-precision motorised stage, providing a cost-effective solution while enhancing analytical capabilities and efficiency. Analyses on laboratory-prepared mock-up paintings have been performed, including varnished sample. To achieve a reasonable balance between data acquisition time and the quality of information retained for advanced data processing explorations, several denoising methods have been tested. By reducing the interference, denoising prevents the obscuration of spectral information. This process ensures the subtle and significant details within the data are accurately captured and analysed. The combination of applying inverse PCA and wavelet has proven efficient for denoising, maintaining the intensity and position of spectral features, enhancing the clarity and interpretability of spectra. Comparisons have been performed on both single spectrum and the entire data cube.

Chemometric based multivariate image analysis techniques have thus been conducted on the denoised data to navigate the interpretation of the complex reflectance profiles obtained by the system. Multivariate curve resolution-alternating least squares (MCR-ALS) was carried out for additional depth to the analysis. By decomposing the complex spectral information of the mock-up painting into meaningful components, MCR-ALS facilitated a more understanding of the painting's composition and stratigraphy (Rutan 2009).

With a particular focus on the impact of advancements in denoising techniques, the capabilities of the system are extended and promise the further research and applications in the non-invasive study and conservation of cultural heritage materials.

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A105. Threshold of pathogenicity: Hyperspectral imaging and multivariate analysis in detecting *Fusarium circinatum* in seeds

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Detecting *Fusarium circinatum* in radiata pine seeds is critical for forest health and management (Sanchez-Lucas & Boa, 2022). In this investigation, we employed hyperspectral imaging coupled with Principal Component Analysis (PCA) and Multivariate Curve Resolution with Alternative Least Square (MCR-ALS) to discern the spectral differences in seeds subjected to a range of *Fusarium* inoculum concentrations. The hyperspectral camera, operating between 400-1000 nm, captured data over five days. Subsequently, an image mosaic of 1600*900 pixels was compiled for each treatment and observation day, enabling a comprehensive evaluation of the seeds' spectral responses to the varying *Fusarium circinatum* concentrations over time. The study's pivotal finding is that the pathogenicity threshold detectable via HIS in the first day is $2.7x10^5$ conidia/mL. Below this threshold, *Fusarium's* impact on spectral signatures remains indistinguishable (Figure 1).

The significance of the first principal component and component MCR was particularly noted in the 430-450 nm wavelength band, critical in differentiating between the degrees of infection and establishing a quantifiable spectral threshold for pathogenicity. The development of prediction models is currently in progress. This study advances the domain of plant pathology by establishing a hyperspectral-based threshold of pathogenicity for *Fusarium circinatum* in seeds, facilitating early detection and precise quantification of infection levels. The identified spectral markers and threshold values contribute significantly to the toolkit for forest health practitioners, promising enhanced decision-making in the management and prevention of *Fusarium*-related diseases in pine forests (Feng et al., 2019).

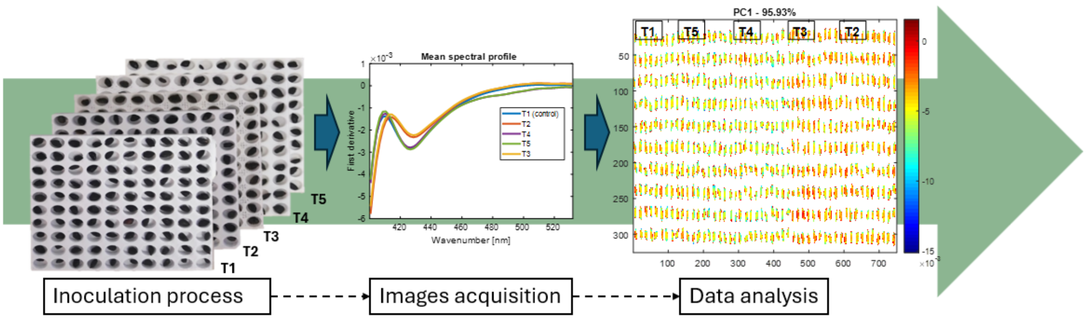

Figure 8 Setting pathogenicity thresholds for *Fusarium* in pine seeds.

Acknowledgement

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A108. Resin curing degree monitorization for Liquid Resin Infusion process using NIR Hyperspectral Imaging

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This study evaluates the use of Near-Infrared Hyperspectral Imaging (NIR-HSI) for monitoring the curing degree of composites made via Liquid Resin Infusion (LRI), emphasizing the importance of accurate curing in determining the mechanical integrity of the final products. It reviews existing in-line monitoring methods, optical, electrical, and acoustic, as categorized by (Kyriazis et al., 2022), noting their various limitations in integration, environmental susceptibility, and intrusiveness, particularly in high-value sectors like automotive and aerospace where embedding sensors could compromise part integrity. Optical methods like Raman Spectroscopy, though detailed, face practical application challenges, while electrical methods e.g., dielectric sensors by (Wu et al., 2023)) are impacted by conditions such as humidity. This research leverages NIR-HSI alongside chemometric analysis to offer a non-destructive, real-time evaluation of the curing process, potentially surpassing existing methods in providing comprehensive quality control for composite material production.
Our methodology involves a NIR Hyperspectral camera (Specim FX17e) combined with halogen lighting, mounted on a robotic arm for dynamic scanning of 200x280 mm flat composite parts during manufacture with carbon fibers and Hexcel RTM6 epoxy resin via the Liquid Resin Infusion (LRI) technique. Data collection spanned the entire three-hour curing process for one part, capturing images every two minutes through heating and isothermal stages. For two additional parts, full curing was achieved, but monitoring covered only initial phases, thus data suggests they were partially cured. The dataset comprises three parts (**Table 1**): Part A with 98 hyperspectral images for a complete curing overview, Parts B and C with 50 and 19 images, respectively, all with (1200, 640) spatial dimensions and 224 spectral bands (900-1700 nm range). Dielectric sensor monitoring on Parts A and C provided ground truth for chemometric regression models.

Table 1. Manufactured composite parts with their respective monitoring information.

Part	Number of Hyperspectral images	Cure status	Dielectric sensor
A	98	Totally cured	Yes
B	50	Partially cured	No
C	19	Partially cured	Yes

Our analysis begins with pre-processing of the hyperspectral images, a mandatory step prior of the application of other processing techniques (Vidal and Amigo, 2012), including spatial correction to define regions of interest (ROIs) and spectral correction using Standard Normal Variate (SNV) transformation to mitigate the effects of light scattering (Amigo et al., 2015). In **Figure 9** we show the mean spectrum of each acquisition after applying spatial and spectral preprocessing.

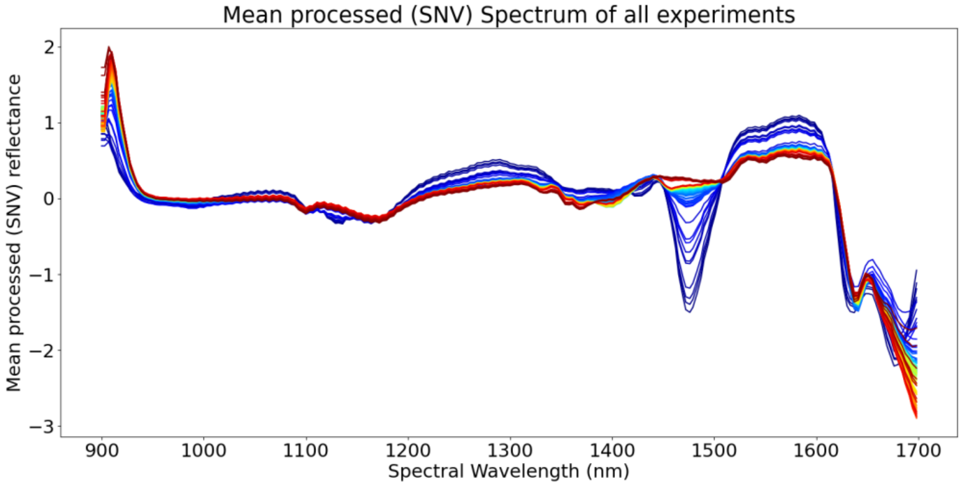

Figure 9. Mean spectrum after preprocessing of each acquisition of part A.

Then, we employ chemometric methods, specifically Partial Least Squares Regression (PLS-R) and Principal Component Regression (PCR), to create a cure degree model using the data acquired in part A manufacturing.

The application of Hyperspectral Imaging (HSI) has proven to be an effective tool for monitoring the curing level of composite materials. One of the key advantages of using HSI is its ability to generate spatial maps that offer detailed insights into the curing process without necessitating direct contact between the sensor and the manufactured part. This non-invasive approach opens up new avenues for in-line monitoring of composite manufacturing.

Looking ahead, our future work will aim to extend this research to include other materials, such as glass fibers, and different resin types like vinylester or polyester. Additionally, we plan to investigate the monitoring of non-flat parts and analyze setups that are not fully transparent, such as those incorporating extra breathers. Further validation and calibration of this method through more extensive testing will also be a crucial part of our continued research, ensuring its applicability and reliability across a broader range of manufacturing scenarios.

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A109. Near-infrared hyperspectral imaging to reveal moisture content in wood under static loading conditions

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The relationship between wood and moisture content is complex and can lead to a range of issues, such as cracking due to dimensional changes and fungal degradation (Kocaefe et al., 2015; Thybring et al., 2020). Wood expands in response to increased moisture content, but this swelling can be controlled by applying static loads that compress the wood fibers and reduce their ability to absorb moisture to some extent (Widehammar, 2004). The determination of moisture content under static loading conditions and varying relative humidity is important for ensuring the effective use of wood in service applications. For this, specialized fixtures were designed to apply static loads on woodblocks in both the radial and tangential directions during conditioning. Near-infrared hyperspectral imaging and partial least squares regression (Geladi and Kowalski, 1986) were used to quantify the change in wood moisture content under static loading conditions, see Figure 1.

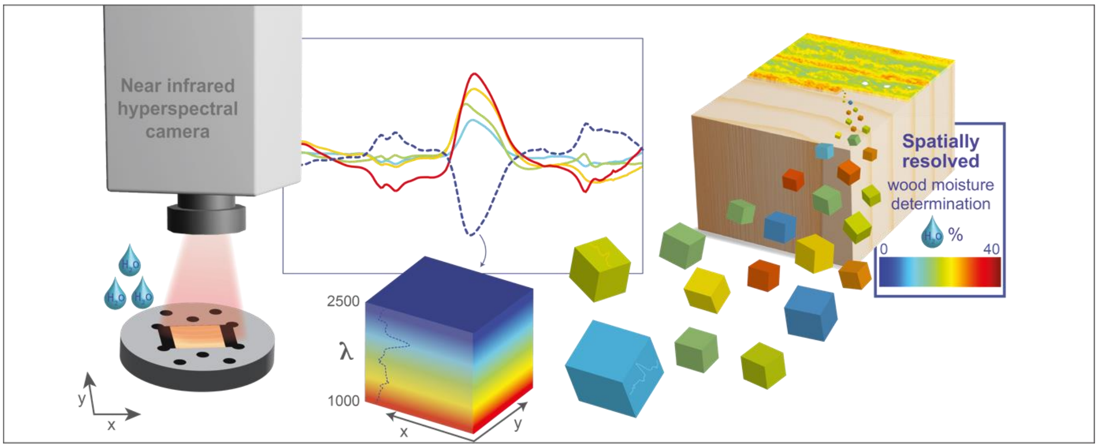

Figure 1. Graphical abstract to illustrate the use of hyperspectral imaging to determine the moisture content in wood under static loading conditions

The developed model accurately predicted moisture content within the range of 0-95% relative humidity, with high precision and minimal error. The predicted results were complemented with gravimetrically measured moisture content using automated sorption balance.
Our results indicated that static loading on wood limits the amount of moisture uptake that occurs when relative humidity increases. However, this effect may not be significant enough to entirely prevent moisture uptake, and the amount of static load required to limit moisture uptake may cause the wood to become permanently deformed, resulting in other mechanical failures. Overall, our study evaluated the change in moisture content of wood under restricted swelling and varying relative humidity conditions.

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A110. Raman based crystallography on the payroll of the solar cells development

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Raman spectroscopy can provide advances in the thin film characterization technology, as it can be widely employed to study absorber materials for photovoltaics, especially promising antimony chalcogenide materials: Sb2Se3, Sb2S3. The anisotropic properties of Sb2S3 imply that the optoelectronic properties are highly contingent on the crystallographic orientation (Jin 2020, Zhao 2020), making it a perfect candidate for investigation with polarization Raman microscopy In practice, achieving precise control over the preferred orientation, particularly the orientation, during Sb2S3 film synthesis presents a significant challenge. The synthesis processes often result in polycrystalline films with random crystallographic orientations, limiting the exploitation of the material's inherent advantages and hampering device performance. For instance, the champion Sb_2S_3 solar cell device reached an efficiency of 7.5%, well below its theoretical limit of 29% (Choi 2014).

In our recent work, we present the analysis of the distribution and alignment of crystallographic orientations in Sb2S3 films through quantitative Raman-based crystallographic orientation mapping (qRICO) (Ilchenko 2019). Our novel experimental design allows for the simultaneous recording of 16 polarization channels from each sample point, without the need for sample rotation. This enables the definition of crystallite orientation with high precision.

Another important approach presented in this work involves measuring the crystallographic orientation of sub-resolution grains in Sb2S3 polycrystalline films using super-resolution image restoration methods. This allows for fast and precise measurement of the crystalline structure, enabling a rapid feedback loop for synthesis and thereby facilitating the development of technology.

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A119. In-line analysis of flame retardants in polyolefins via industrial hyperspectral imaging and machine learning

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A small portion of the global plastic waste generated is currently recycled and reintroduced into the economy (Plastics Europe 2023). A sustainable option is to employ a circular model in which plastics are mechanically recycled. However, plastic recycling is challenged due to the presence of harmful additives in the plastics and the need for technological advance of an inline analysis of plastic waste (Hennebert 2022).
The aim of this work is to develop an in-line quality control tool that employs an industrial short-wavelength infrared (SWIR, 955-1700 nm) hyperspectral imaging system (HSI, Newtec^{TM}) and machine learning techniques to identify and quantitatively estimate critical flame retardants such as ammonium polyphosphate (APP), aluminium trihydrate (ATH), and melamine (MEL) in low-density polyethylene (LDPE) and polypropylene (PP), respectively.
Plastics with varying APP, ATH, and MEL content are compounded and characterized by elemental analysis, FTIR, differential scanning calorimetry (DSC), and thermogravimetric analysis (TGA). Finally, continuous functions based on both SWIR band area ratios and principal component analysis (PCA) are applied to document and determine APP, ATH, and MEL concentrations in polyolefins.
The results shows that the PCA model outperforms the band area ratio model for all flame retardants SWIR spectra (Amariei 2023a, Amariei 2023b). SWIR spectra of ATH samples in the range from 955-1700 nm are presented in Figure 1, as an example. The modelling achieved good predictions between measured and predicted: (i) APP concentrations ranging from 24.3 - 1.5 wt% in LDPE (R^2 = 0.98) and 20.0 - 1.7 wt% in PP (R^2 = 0.97). (ii) ATH concentrations ranging from 22.9 - 1.6 wt% (R^2 = 0.95) in LDPE and from 24.0 - 2.5 wt% in PP (R^2 = 0.94); (iii) MEL concentrations ranging from 23.3 - 2.0 wt% in LDPE (R^2 = 0.98) and 21.0 - 1.7 wt% in PP (R^2 = 0.97).

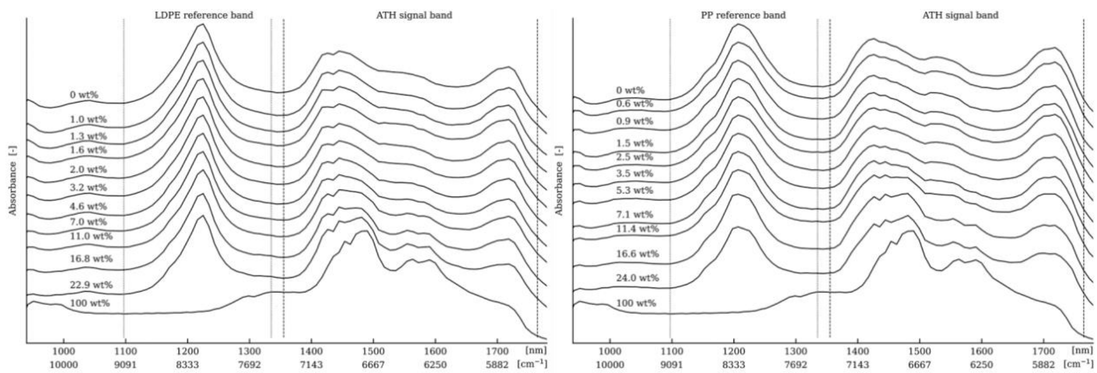

Figure 1. SWIR spectra of the ATH pure (100 wt%) and ATH compounded samples with: LDPE (left) and PP (right). Each spectrum is the mean of 375 spectra, are normalized and shifted for clarity.

This study shows that an industrial HSI (955 -1700 nm) coupled with PCA based modelling can be successfully applied for in-line detection and quantitative prediction of ATH, APP, and MEL flame retardant in LDPE and PP. The presented method is a fast, non-destructive, and in-line tool for detecting and quantifying additives content in the plastics waste streams, providing new solutions on industrial recycling and processing technologies of inorganic and nitrogen-based flame retardants in plastics.

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A122. High-speed tracking of mixing and coalescence dynamics in optically controlled airborne droplets

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Airborne microdroplets serve as unique chemistry reactors in various natural and industrial processes, including combustion engines (Sazhin 2016), atmospheric phenomena (Dobson 2000:), emulsions, biochemistry, to mention a few. Experimental platforms capable of manipulating and characterizing these microenvironments are in demand (Jayaweera 2020). Optical and acoustic traps (Watanabe 2018, Power 2012) have enabled gentle manipulation and enhanced understanding of droplet dynamics in air with minimal interference. This study contributes to the advancement of optical tools in this field by introducing a dual-steerable optical trap for on-demand trapping and collision of droplets while imaging their interaction at high speed (Fig. 1). The trap effectively maneuvers two 10 µm radius glycerol droplets into a controlled collision and stabilizes their positions during coalescence. A high-speed phantom camera captures their interaction, while the coalescence region is analyzed spectroscopically using a fiber-coupled spectrometer.

This platform is designed for conducting in-droplet bio-chemistry experiments in airborne environments. As a proof-of-principle, we dyed each droplet with a fluorophore (ATTO532 and ATTO550, donor and acceptor dye respectively) to facilitate Förster resonance energy transfer (FRET) upon contact and mixing. By examining the spectrum of the droplets upon coalescence together with frames from the high-speed camera, we tracked the mixing dynamics with a time resolution of 86 µs. Our findings revealed that the dyes concentrated at the surface of the droplets, and approximately half of the molecules mixed abruptly within a time scale below our experimental resolution. This was followed by steady diffusion over seconds, characterized by an exponential decay trend.

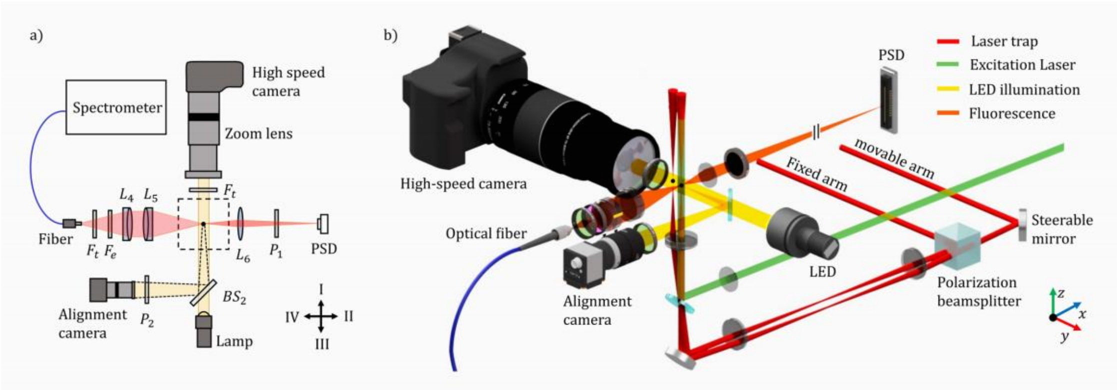

Figure 1 a) Top view of the coalescence experimental chamber (marked with a dotted square), featuring the lens (L), polarizer (P), beamsplitter (BS), filter (F), and position-sensitive detector (PSD). The chamber includes four ports labeled with Roman numerals: I for high-speed camera imaging, II for active stabilization using PSD feedback to the laser trap, III for illumination and alignment, and IV for spectral acquisition. b) Simplified CAD design of the optical system illustrating the two-trap configuration and the excitation source for facilitating FRET.

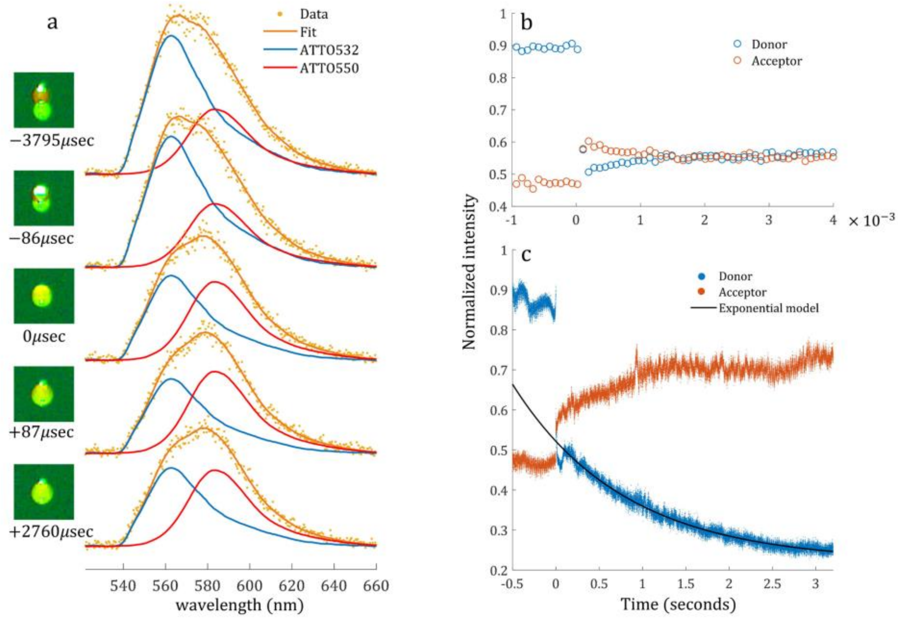

Figure 2 a) Correspondence within the high-speed imaging and the spectral footprint (in yellow the total fluorescence response, and blue and red the decomposition into the contributions from each flurophore) the onset of coalescence is set as the zero-time reference. b) Normalized fluorescence intensity of each dye around the collision onset. c) Long-term dynamical view of the coalescence of two droplets. The solid black line is a mono-exponential decay fit with a time constant of $\sim$ 1.3 sec.

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A123. Optical heterodyne microscopy for characterization and imaging of operating spin Hall nano-oscillator networks

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Spin Hall nanooscillators (SHNO), composed of magnetic film stack nanoconstrictions, hold promise for the emerging field of neuromorphic computing (Grollier 2020, Zahedinejad 2020). In this work we demonstrate a specialized Optical heterodyne detection (OHD) setup (fig. 1a) for quick characterization and imaging of such devices. A NiFe SHNO subjected to a magnetic bias *H* is stimulated electrically with an RF+DC source (fig. 1b). The magnetic response of the device modulates an incident probe beam via the Magneto-Optical Kerr Effect (MOKE). Subsequently, the optical signal is detected by a 40 GHz photodetector and analyzed using a Vector Network Analyzer (VNA), which measures the input/output coherent ratio (S_{21}). The acquisition is limited by the VNA filter requirements (10-100 Hz), with a frequency resolution in the kHz range. Spatial resolution is 300 nm approximately (diffraction limit).

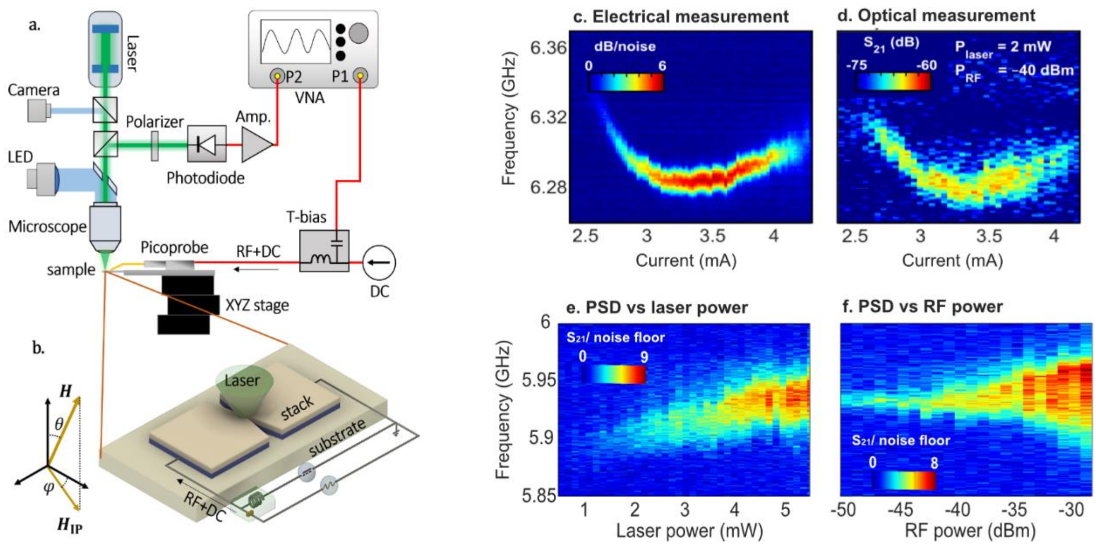

Figure 1 a. Experimental setup, red lines represent electrical connections, in blue the LED illumination, and in green the laser path. **b.** Reference axis and SHNO device representation. In **c.** and **d.** electrical vs optical measured PSDs, respectively. **e.** and **f.** show the influence of the laser and RF inputs on the PSD.

Fig. 1(c-f) shows typical power spectral densities (PSD) measured both electrically and using OHD (for comparison), as well as the influence of the laser (P_{laser}) and RF (P_{RF}) power on the measurement bandwidth and signal intensity.

OHD offers direct access to phase information. In Fig. 2, we present imaging of a system comprising two synchronized oscillators in their four possible phase-binarized states. Parametric injection at twice the operational frequency f_0 enables this binarization (Houshang 2022). This novel method provides a simple and cost-effective alternative to traditional magnetic imaging techniques, such as Brillouin Light Scattering (BLS) or time-resolved MOKE. It eliminates the complexity in the optical layout and mechanical isolation requirements. Furthermore, this simplicity could facilitate miniaturization into an embedded reading device akin to a laser-head reader, making it appealing for end-user industrial spintronics applications beyond the proof-of-principle presented here.

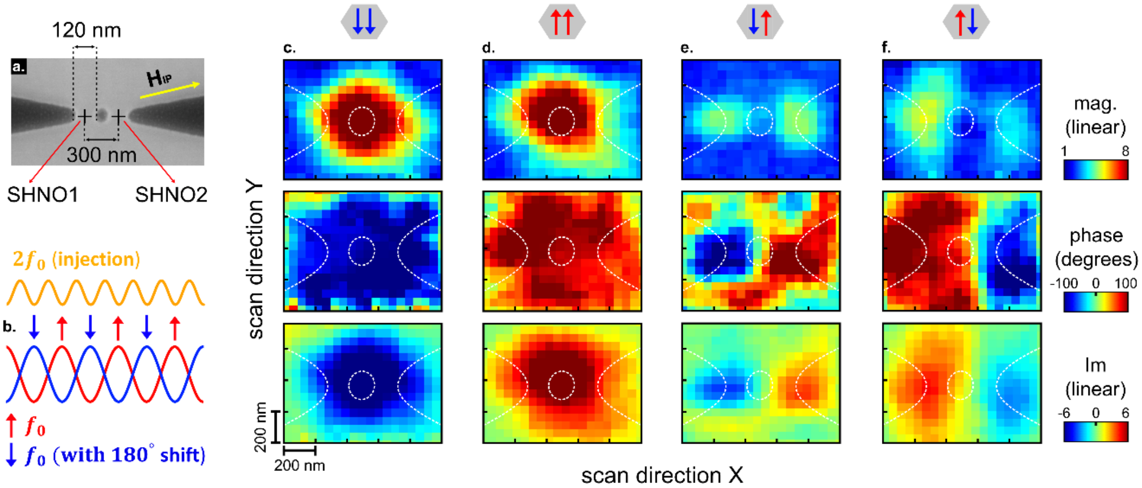

Figure 2 a. Electron imaging of the 2-SHNO network, H_{IP} represents the direction of the in-plane operational magnetic bias. **b.** Parametric pumping scheme for phase binarization. **c-d**. Magnitude, phase and imaginary (Im) imaging of the system and its four possible states. Out-of-phase and in-phase states are represented by ↓ and ↑ symbols, respectively.

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A137. Monitoring cell line evolution via Raman spectroscopy and machine learning

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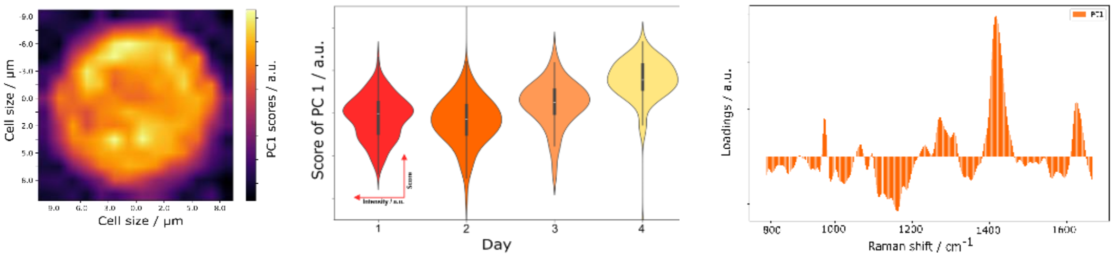
Human cancer cell lines are an indispensable tool in research, serving as a valuable resource for understanding cancer biology and drug testing. Despite their crucial role, too little emphasis has been placed on studying the changes that human cancer cell lines undergo during culture (Iuchi 2020). Nevertheless, it is well documented that changes in cell state that occur over time strongly influence the observed behavior of the cells, which can have an impact on the reproducibility of in vitro assays and drug response. (Ben-David 2018). These previously widely accepted limitations have in turn remained unresolved because there are no techniques that can routinely monitor the fitness of cells over time. (Sigle 2023). With the help of Raman microspectroscopy in combination with machine learning, we want to solve exactly this problem for the characterization of individual cells. Raman spectroscopy is an excellent tool for this task as it provides insights in terms of spectral information into encapsulated cell content and, due to its non-invasive and label-free nature, enables the measurement of living and non-fixed cells (Butler 2016). That way, we have developed a method to study a Hek 293T cell population by acquiring hyperspectral images and individual spectra of single cells and analyzing their vibrational changes during their evolution in vitro over one month.

The parameters of the experimental setup we used to acquire hyperspectral images were selected based on successful protocols validated in previous studies (Horgan 2021). Raman spectra were taken with the Renishaw® inVia™ confocal Raman microscope using a laser wavelength of 785 nm laser, a 50x long-distance objective, and a grating with 1200 L/mm. A demountable cuvette from Hellma® Analytics with a beam path of 0.01 mm, consisting of two Suprasil® quartz glass plates, served as the sample holder. A dataset of hyperspectral images of single cells was acquired at 5 µm resolution to identify key Raman peaks associated with cellular components, which is considered a crucial step. The raw spectra were preprocessed via a defined routine in the Python environment, followed by principal component analysis (PCA) with the corresponding scikit-learn function, revealing the important features and information hidden in the hyperspectral images. As an example, Figure 1 (a) shows the values of the first principal component (PC1) of one hyperspectral image from an individual cell candidate. The distribution of the PC1 values across the measured area shows clear differences between the cell (bright colors, high PC1 values) and its surroundings (dark colors, low PC1 values).



(a) (b) (c)

Figure 1. (a) Values of PC1 across the cell based on its hyperspectral Raman image.
(
b) Distribution of PC1 by days of the map dataset. (c) Loadings of PC1 of the whole map dataset.
Those differences show that we can clearly distinguish between the Raman signals of cell and background. The result shows us that the acquisition of single-point Raman spectra of several individual cells (n = 100) can provide information about the overall condition of the cell culture even at a lower resolution (> 20 µm). Performing this workflow over a longer period could therefore be used to study the evolution of the cell line in culture. Accordingly, the cell line was cultured for one month and the measurements were carried out on four selected days. The PC1 scores grouped per measurement day can be found in **Figure 1** (b) and the corresponding loadings of the whole single-point map dataset are shown in **Figure 1** (c). The results of this work offer a promising opportunity to monitor the heterogeneity and evolution of cell lines over extended culture periods. In comparison to the time-consuming nature of conventional sequencing-based techniques, our method represents an efficient, fast, and cost-effective alternative for the investigation of cell line evolution. The overall objective of our work is to improve the reproducibility and reliability of in vitro tests in the field of cancer research and drug development.

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A151. Safety, repeatability and deferability in crime scene documentation and material qualification in the framework of the EU H2020 RISEN Project

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Forensic investigations require efficient and precise execution, even when time is limited. Emerging technologies such as 3D reconstruction and forensic sensors offer investigators valuable support in the detection, visualization, identification, and on-site interpretation of traces. In this contex we introduce the Real-tIme on-site forenSic tracE qualificatioN (RISEN) H2020 project (grant agreement No. 883116) as an innovative framework for forensic investigations.

The primary objective of RISEN is to advance forensic analysis by enabling investigators to securely capture data without contamination of the crime scene, to provide timely and entirely objective analyses based on highly credible evidence, without overlooking latent evidence to securely communicate and visualise information between stakeholders, and to maintain a comprehensive digital record of the crime scene for subsequent evaluation.

In this poster communication we present a novel approach for forensic analysis of "post-blast" crime scenarios using both conventional UV-VIS and FT-IR spectroscopy and portable Hyperspectral Imaging (HSI) to potentially discriminate between detonation cord and electrical cables at the scene.

These materials are often found together at crime scenes following ATM bombings, and their in-situ differentiation using contactless techniques could potentially streamline the crime scene collection activities of law enforcement personnel in the future.

On the other hand, the same methodological approach has also been used to differentiate bloodstains when it is necessary to distinguish them from other fluids of the same colour.

The proposed methodology is based on the use of unsupervised and supervised chemometric tools (PCA and PLSDA) to the data acquired by the multispectral camera. The SPECIM IQ hyperspectral used for the experimental activities is a portable camera, battery-powered equipped with a linear scanning hyperspectral imager which acquires reflectance spectra in the range 400-1000 nm producing images of 512 x 512 pixels. These images are then processed with a custom-developed Python software to visualize the results then transferred to the RISEN API.

The objective is to analyse the spectral response of a range of materials commonly encountered at crime scenes that may be mistaken for biological traces (such as tomato juice, lipstick, ketchup, chocolate, etc.) on different substrates (white fabric, black fabric, wood, PVC, ceramic, etc.). This analysis will then be used to provide a score associated with the presence of blood or other materials potentially useful for the investigation.

The determination of the score is of paramount importance, as it provides investigators with a reliable output that enables the discrimination of useful from non-useful traces in the course of criminal investigation activities.

A169. Machine learning driven methodology for enhanced nylon microplastic detection and characterization

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In recent years, the field of microplastic (MP) research has evolved significantly; however, the lack of a standardized detection methodology has led to incomparability across studies. Addressing this gap, our current study innovates a reliable MP detection system that synergizes sample processing, machine learning, and optical photothermal infrared (O-PTIR) spectroscopy. This approach includes examining high-temperature filtration and alcohol treatment for reducing non-MP particles and utilizing a support vector machine (SVM) classifier focused on key wavenumbers that could discriminate between nylon MPs and non-nylon MPs (1077, 1541, 1635, 1711 cm^{-1} were selected based on the feature importance of SVM-Full wavenumber model) for enhanced MP identification. The SVM model built from key wavenumbers demonstrates a high accuracy rate of 91.33%. Results show that alcohol treatment is effective in minimizing non-MP particles, while filtration at 70 °C has limited impact. Additionally, this method was applied to assess MPs released from commercial nylon teabags, revealing an average release of 106 particles per teabag. This research integrates machine learning with O-PTIR spectroscopy, paving the way for potential standardization in MP detection methodologies and providing vital insights into their environmental and health implications.

A001. Hyperspectral imaging for *Prunus* genomics and breeding

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Plant breeding is a scientific discipline focused on developing superior cultivars using principles of genetics and genomics. Plant breeders employ crossbreeding and advanced molecular techniques to improve traits of interest such as yield, resistance to pathogens, and environmental adaptability. Modern crop breeding approaches are based on genotyping (DNA sequencing) and phenotyping (study and quantification of plant traits) to identify useful genetic associations that accelerate and make economically efficient and viable breeding programs. In the last decade, large progress has been made in plant breeding through the development of new genomics technologies. However, the acquisition of large phenotypic data is the current breeding bottleneck because phenotyping processes are tedious, time-consuming, and expensive. The development of high-throughput phenotyping platforms (HTPP) for the screening of large biological datasets such as plants, leaves, fruits, seeds, and more, in the field or in the lab is being carried out by plant breeders. In this sense, hyperspectral imaging is being introduced in HTPPs to detect and quantify abiotic, biotic, and quality traits in plants. Hyperspectral imaging allows phenotyping tasks not invasive and destructive, to monitor processes over time, and to be scalable for large datasets where the alternative approaches are not viable economically. We present the first data and approaches using hyperspectral imaging in *Prunus* breeding programs. *Prunus* includes many important crop species as cherries, plums, apricots, almonds, and peaches. Here, we present several applications such as the use of hyperspectral imaging for predicting quality traits in almond seeds and the quantification of plant disease damages.

A009. Enhancing Image Analysis: Utilizing the Successive Projection Algorithm for Unmixing from Chemicals to Interstellar Clouds

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Hyperspectral imaging, as a non-invasive analytical technique, captures images across a wide range of contiguous variables from the same scene, preserving both **morphological** and **chemical information** associated with samples. This technique is widely studied in chemistry, spanning diverse fields such as pharmaceutical analysis, material science, environmental monitoring, and analytical chemistry [1]. This method offers spatial and chemical insights into samples, overcoming the spatial limitations of single-point spectroscopy. Furthermore, **Faraday Tomography** is a recent technique that provides tomographic information on magnetized astrophysical objects like galaxies, quasars, and galaxy clusters using polarized radio emission. The interstellar medium -contains gas, magnetic fields, and relativistic electrons. Relativistic electrons emit synchrotron radiation, which is partially linearly polarized. As this radiation propagates through the interstellar medium, it undergoes Faraday rotation, resulting in a complex combination of **emission at different distances** with **varying degrees of rotation.** This can be detected and analyzed using telescopes and Fourier transformation into Faraday spectra. Most telescopes record a hyperspectral image instead of a single sightline. The resulted cube for a single data is visualized as Figure 1a.
While hyperspectral images yield rich information, its **high-dimensional** data poses processing challenges. **The resulting signal is a mixed information** and needs further **unmixing** [1]. Spectral unmixing is an inverse problem aimed at automatically retrieving the signatures of different materials in the observed scene, known as endmembers, and quantifying their relative proportions, referred to as fractional abundances, within each pixel of the image [1]. The **Successive Projection Algorithm** (SPA) introduced by M. C. U. Araujo in **2001**, is a forward selection method that mitigates variable collinearity, enhancing the predictive accuracy of Principal Component Regression by selecting 20% of variables [2].

a b

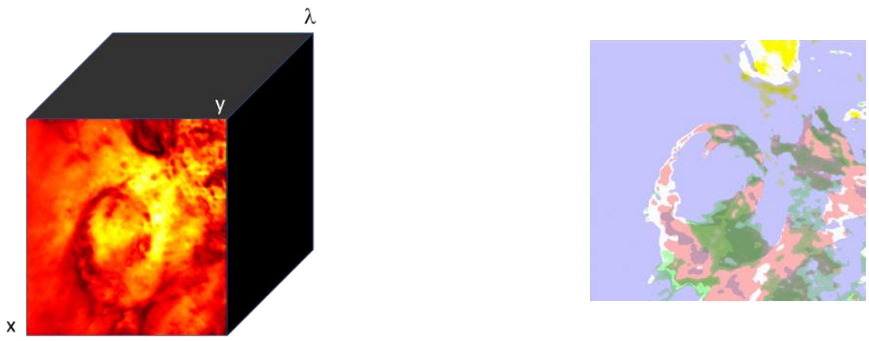

Figure 1. The mean image of a Faraday Tomography image and the resulted fractional abundances by SPA are presented in a and b, respectively.

While most literature reports on **SPA** focus on **variable selection** for improved quantification and classification, a single report in 2008 demonstrated SPA's utility as **an endmember extraction algorithm** in two case studies, namely the AVIRIS Cuprite cube and Probe-1 imagery for Baffin Island, where image endmembers were validated against ground truth data [3]. In this study, we harness the power of the Successive Projection Algorithm as a rapid and precise endmember extraction technique, aimed at unraveling the pivotal role of endmembers in hyperspectral imaging with a focus on its applications from chemistry to Faraday Tomography. We conduct an in-depth analysis of several hyperspectral images using SPA alongside other endmember extraction methods for comparative purposes. The presented Faraday Tomography data in Figure 1a was analyzed by SPA and the resulted fractional abundances are visualized. Our findings, visualized in data abstract spaces, underscore SPA's robustness and repeatability, as it accurately delineates the edges of the data inner polygon in the spectral space even in the case of minor component. These edges represent the most independent signatures of various materials within the data, with corresponding fractional abundances situated at the boundary of the data outer polygon in the dual space. Notably, SPA operates without the need for parameter tuning and consistently outperforms other methods in terms of speed and accuracy across multiple comparisons, underscoring its reliability and stability.

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A031. Near-infrared hyperspectral imaging and chemometrics to classify different rice varieties

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Hyperspectral imaging (HSI) is a non-destructive, highly informative analytical technique that provides both spectral and spatial information about the analysed samples. The advantages of this technique allow its application in many fields [1], one of which is the agro-food field. In this context, the possibility not to compromise samples and avoid their manipulation or descruction during the analyses is of particular interest, because it prevents wastes and allows to re-use the food samples.
As another advantage, HSI allows to analyse a large number of samples, making it is possible to eventually obtain their chemical fingerprint. Moreover, an additional source of information comes from the morphological features extracted from the images: it is possible not only to discriminate samples based on their chemical profile, but also considering structural parameters. In the present work, HSI was used to analyse 47 different rice varieties.
For each variety, one image with 15 rice grains and one image with 100 grains were taken. For this purpose, a NIR-HSI camera (SPECIM FX17, Finland) connected with a motorized scanning bed (LabScanner Setup 40×20 cm) was used. The images were pre-processed to remove light scattering and optical effects due to the round shape of the camera's lenses. The data were then converted from reflectance to absorbance and merged to obtain an individual data file gathering the information from both collected images (15 and 100 grains).
In order to handle the complex and plentiful amount of information, this technique is usually combined with multivariate analysis and deep-learning tools [2,3]. Multivariate data analysis was applied to inspect and model the data under MATLAB environment. Firstly, Principal Component Analysis (PCA) was used to gather a general idea of the information carried by the samples, both for spectral and morphological features. Then, different classification methods were applied to build robust and reliable models aimed at distinguishing among the varieties, with the perspective of counteracting food-fraud. To do that, Partial Least Squares-Discriminant Analysis (PLS-DA) and hierarchical classification models were exploited. The obtained results provided interesting insights into the chemical and structural differences occurring among the rice varieties under examination, which could also be clustered into macro-groups according to their similar morphological and spectral features.

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A033. Early detection of Brown Marmorated Stink Bug punctures on pears using NIR Hyperspectral Imaging

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Halyomorpha halys, commonly known as Brown Marmorated Stink Bug (BMSB), has recently emerged as an invasive insect pest of global importance. In Europe, the Emilia-Romagna region was one of the affected areas in which BMSB caused dramatic losses to pear orchards due to punctures on harvested fruits (**Maistrello 2017**). Moreover, BMSB late damages, i.e. the punctures inflicted on fruits near harvest, determine internal suberifications and necrosis of the fruit pulp, which are not visible to the naked eye. If these damages are not promptly detected at post-harvest, they may promote the spread of pathogens compromising the freshness of sound fruits during storage.

In the frame of the EU Project HALY.ID, NIR HyperSpectral Imaging (NIR-HSI) was evaluated as a possible post-harvest sorting system method for the detection of late damages caused by BMSB on pears, which are not detectable using cameras working in the visible range.

To this aim, pear fruits of two varieties (*cv.* Williams and *cv.* Abate Fétel) were collected from an organic orchard in Carpi (Modena, Italy) during summer 2022 and summer 2023. About half of the collected fruits were exposed to BMSB specimens for one week before harvesting, while the remainder fruits were used as control samples. The hyperspectral images of the collected fruits were acquired in the 1156-1674 nm range at eight subsequent times, over a period of six weeks from the day of harvesting. Considering both harvest years, about 1000 hyperspectral images were acquired for each variety. In addition, also the RGB images of unpeeled and peeled pear samples were acquired following the same procedure. Indeed, the RGB images were used to visually classify the fruits based on damage type and intensity.

A preliminary exploratory analysis performed on a subset of representative hyperspectral images using Principal Component Analysis (PCA) enabled the identification of damages. However, a clear identification of the Regions of Interest (ROIs) ascribable to punctures resulted troublesome, due to their highly irregular shapes and blurred edges between sound and damaged areas.

To address this issue while analyzing all the images altogether, a data dimensionality reduction approach based on Common Space Hyperspectrograms (CSH) was adopted (**Calvini 2018**). This step allowed the conversion of each image into a CSH, a signal obtained by merging in sequence the frequency distribution curves of PC score values, Q residuals and Hotelling T^2 derived from a global PCA model.

The data dimensionality reduction step was followed by image-level classification coupled with variable selection using interval Partial Least Squares – Discriminant Analysis (iPLS-DA) (**Nørgaard 2000**). The features selected by iPLS-DA were then visualized back into the original image domain, leading to the identification of the ROIs ascribable to punctured areas in an automated and objective way.

Starting from the identified ROIs, a dataset of representative spectra belonging to both punctured and sound areas was built for the development of pixel-level classification models and the selection of the most relevant spectral regions.

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A035. Exploring Block Term Decomposition for enhanced hyperspectral images analysis

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Tensor-based decomposition methods have long been established as robust methodologies in chemometrics, offering powerful tools for analyzing complex data structures (Acar 2008, Smilde 2005). Their utility extends to the analysis of hyperspectral images, where the simultaneous exploration of spatial and spectral domains within a data cube is essential. Canonical Polyadic Decomposition (CPD) and Tucker decomposition (Kolda 2009) are prevalent techniques in image analysis in the context of tensor-based methods. However, CPD's imposition of rank 1 on each factor may be overly restrictive, whereas Tucker offers greater flexibility by allowing different ranks for each factor, however suffering from rotational ambiguity.
Positioned between these methods is Block Term Decomposition (BTD) (De Lathauwer 2008), the implementation which benefits from imposing a rank = 1 on one factor and allows a rank ≠ 1 for the other two factors, i.e., LL1-BTD (see **Figure 1**), preserving the uniqueness property of CPD. BTD allows modelling complex spatial structure related to a single spectral signature. BTD can be suited, then, to analyze hyperspectral images where the spatial structure of different spectral components are properly described with different factorization, as in the case of the presence of minor components, or those components that have a very similar spatial distribution but a different spectral signature or vice versa. In this work, we explore the adoption of BTD for analyzing benchmark hyperspectral datasets, confronting its performance with CPD as well as spectral unmixing method applied on unfolded hyperspectral data cube. Leveraging algorithms from the Tensorlab Toolbox (https://tensorlab.net, last accessed March 2024) and various alternatives within the MATLAB environment (The MathWorks, Inc. Natick, MA 01760-2098, USA), we conduct a comparative evaluation. Constraints and parameters choices are discussed, and results demonstrate that the LL1-BTD could be a promising approach for the analysis of hyperspectral images. This study offers insights into the utility of tensor-based decomposition methods in addressing the challenges posed by hyperspectral data.

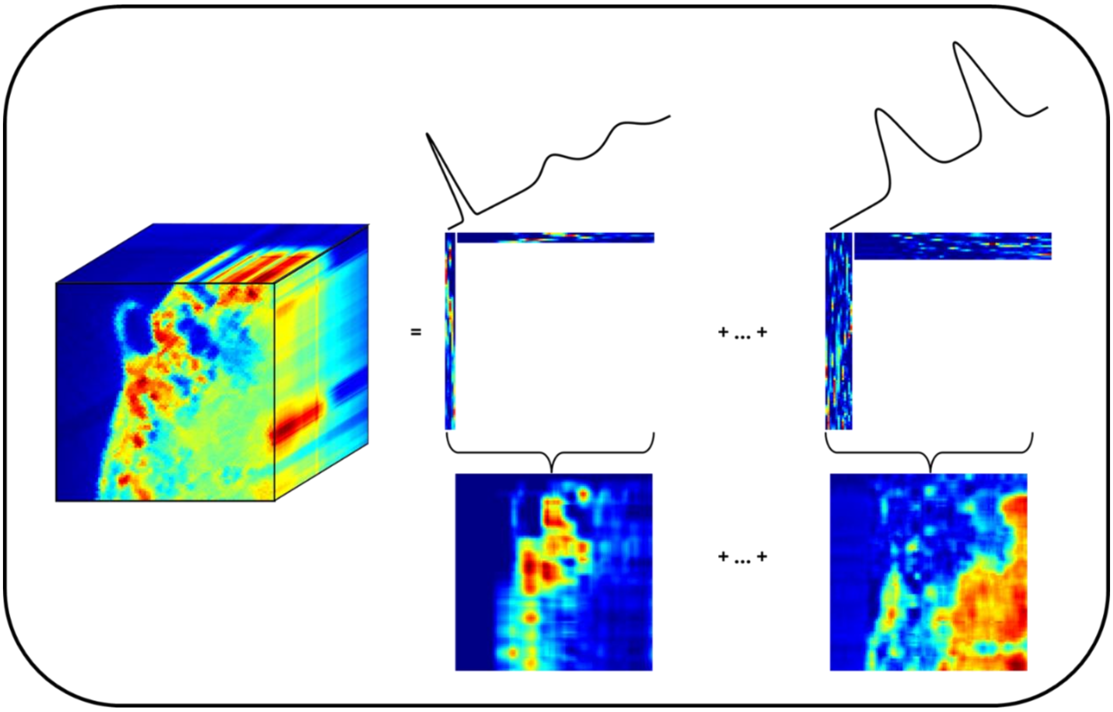

Figure 1. Hyperspectral data cube is decomposed as the sum of outer product of a component matrix (the two spatial dimension factor matrices of equal rank ≠1) and a vector (rank = 1, which is the spectral factor).

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A036. How data incompleteness affects factor ambiguity in MCR analyses

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Pure component factorizations in MCR analyses typically apply to complete spectral data sets as stored in rectangular matrices. Sometimes parts of the data are missing (due to sensor failure, etc.) or the data set is composed of different data subsets that cannot be cast into a common rectangular matrix form. A common approach is to consider the largest complete submatrix (by neglecting the incomplete rows or columns) and to apply the MCR analysis to that submatrix only. However, such an approach ignores all the "in-between data" that is between the largest complete submatrix and the incomplete original matrix (see Figure 1).
We present an approach how to extract chemical information from this "in-between data". The focus of our approach is to reduce the factor ambiguity of the pure component factors derived from the submatrix by exploiting this additional information. Our method differs from other approaches by computing all feasible solutions of the factorization problem instead of a single one.

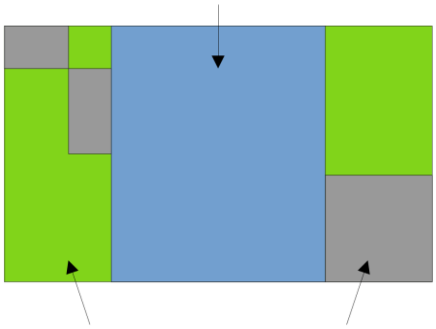

Figure 1. Matrix with marked missing data (gray) and the resulting largest complete submatrix (blue) as well as the remaining "in-between data" (green).

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A038. Hyperspectral imaging to bread authenticity: grain type identification for quality assurance

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The everlasting search for healthier alternatives to modern day foods has opened the door to an increasing number of frauds, with many of them being directed towards labeling products in a way that misleads the consumers. The problem is as follows: bread can be made from a variety of flours, (e.g. wheat, oats, spelt, rye), and there is currently no official European quality control method to authenticate the variety flour used in its production. Therefore, to combat this problem, the present study seeks to discover whether discrimination of breads made from flours of different grains, is possible using an analytical environmentally friendly method based on hyperspectral imaging (HSI).

Bread samples analyzed in this study were composed of flour from three different varieties of grains: wheat, spelt and oat, and their analysis were made with hyperspectral imaging. More specifically, two cameras were used: the first one with spectral range from 400 to 1000 nm (VNIR) and a second one with a spectral range of 900 to 1700 nm (SWIR). All of the bread samples were homemade, with them being prepared with both white and wholemeal versions of each type of flour. Once the bread was made, samples were prepared for the HSI capturing process by drying and grinding it into small particles. In total 78 samples were captured, pre-processed and examined via exploratory analysis applying principal component analysis (PCA) and partial least-squares regression (PLS) methods using average spectra from the selected region of interest (ROI) of each sample. In the SWIR spectral range, samples demonstrated a natural clustering into "wheat" and "not wheat" groups. Subsequently, partial least square analysis discrimination (PLS-DA) and support vector machine (SVM) were employed as supervised analysis methods to classify the samples according to the variety of grain from which they were prepared (wheat, spelt and oat).

The application of hyperspectral imaging combined with the aforementioned multivariable analysis methods is expected to provide an analytical method capable of authenticating the grain variety flour used in bread production, serving as a quality control method of this product.

A039. Spectral discrimination of sorghum (*Sorghum bicolor* (L.) Moench) genotypes for high throughput phenotyping and selection

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There is need to rapidly develop crop varieties that able to sustain food production to meet food demands of an increasing global population in a changing climate. Remote sensing has immense potential for high throughput phenotyping of the agronomic and physiological traits that can be used in selection of elite lines for productivity, adaptability and/or biotic and abiotic stress tolerance in crop breeding programs (Araus et al 2018, Jones et al 2020). This is especially important for crops such as sorghum that are important for food security and livelihoods of millions of people across the world.

Therefore, in the aim of this study was to use remote sensing for spectral characterization and discrimination of 20 sorghum genotypes. Spectral reflectance and narrow band vegetation indices were used in detecting variations in morphological traits (leaf length, leaf width, leaf area, plant height, number of leaves and chlorophyll), colour of grain, and variety type at vegetative and maturity growth stages. Multivariate analysis of variance, t-tests, principal component analysis and clustering methods were used to analyze the spectral data and vegetation indices (Bheemanahalli et al 2023).

Our results showed that the morphological traits were all higher at maturity stage than at vegetative stage as expected but varied widely between the evaluated genotypes. Of all indices, 8 and 9 of the evaluated vegetation indices showed significant differences between genotypes ($p<0.05$) at vegetative and maturity stages, respectively. There were no distinct differences between hybrid and OPV varieties at vegetative stage but at maturity the OPV genotypes had higher reflectance in the visible and near-infrared regions of the spectrum. Higher reflectance was obtained for the white-grained varieties in the visible but lower in the NIR at vegetative stage, while at maturity the white grained genotypes had higher reflectance (Figure 1).

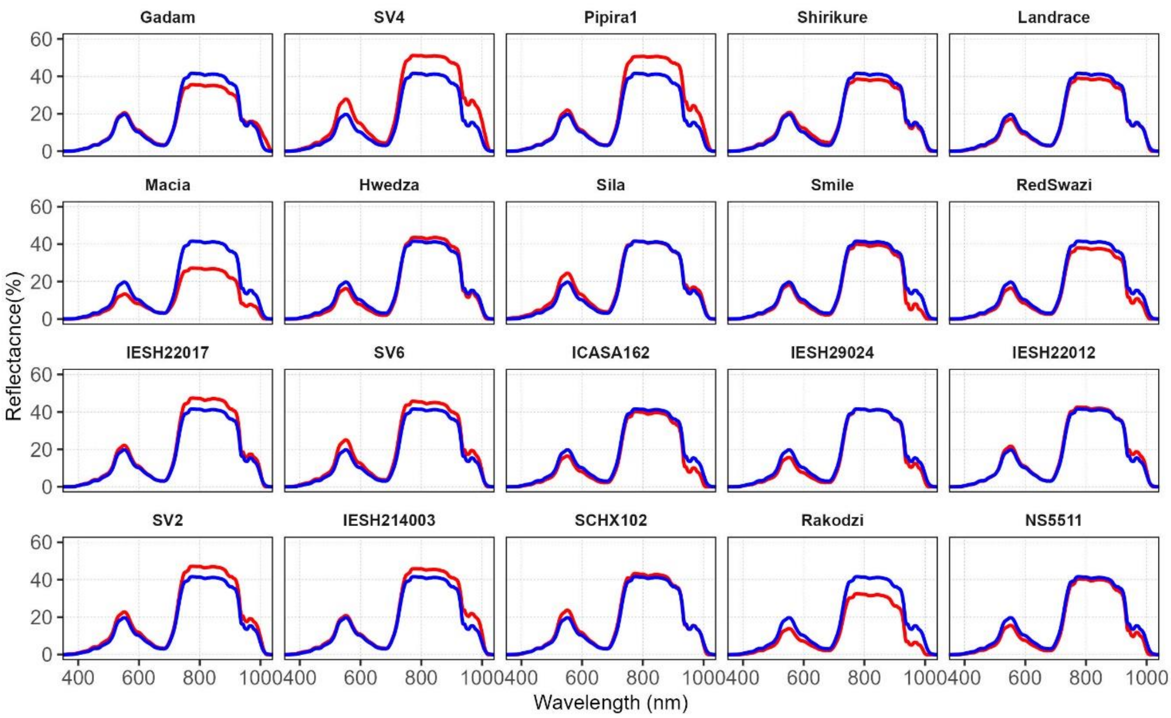

Figure 1. Spectral response curves of the 20 sorghum genotypes at vegetative and maturity stages in the VIS/NIR spectrum.

Three principal components had eigenvalues greater than one, and explained 90% of the variation for both the vegetative and maturity stages. Sorghum genotypes were clustered based on the spectra and vegetation indices. Four clusters are detected from the dominant vegetation indices at vegetative stage while these increased to five at maturity stage. We conclude that there is a potential for spectral data to be used in discrimination of sorghum genotypes as an effective tool for related to sorghum genotype selection in crop improvement.

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A044. Early detection of ovine pregnancy status in milk through portable NIR spectroscopy

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One of the major challenges facing sheep farming is being able to determine as early as possible when a ewe is pregnant. In addition, the sooner the animal's pregnancy status is known, the sooner subsequent matings during that time will be avoided. During these months, the priority must be the care of the animal to avoid abortions caused by pathologies or management errors. Often, an abortion not only results in the death of the fetus but also the mother herself. The earlier and more effective the detection of pregnancy, the more efficient and profitable the farm management will be, avoiding significant economic losses.
The current method used to determine the status of a sheep relies on ultrasound scans. The process begins with the estrus synchronization of the ewes using the sponging technique (day 0), 16 days later the ewe is inseminated (day 16). After 10 more days (day 26), a ram is introduced to increase the chances of pregnancy. Finally, on day 61, an ultrasound is performed to confirm whether the ewe is pregnant or not. Throughout the process, the composition properties of the milk they produce are altered.
Based on this fact, and combined with the support of various research studies on the use of spectroscopy technology for predicting different components in milk (Holroyd, S.E. 2013 and Melfsen, A., Hartung, E., & Haeussermann, A. 2012) and the incorporation of machine learning (ML) models, the present study on early detection of ovine pregnancy status in milk through VIS-NIR (400-1000 nm) and NIR (900-1700 nm) spectroscopy arises.
Tracking is done on 2 groups of 50 ewes, taking milk samples at the beginning of the process (day 0 before sponging), day 16 (after insemination), and day 26 (after mating) to build predictive models of binary classification using their spectral data as predictors and their pregnancy status as the dependent variable (on day 61, ultrasound is performed to determine pregnant ewes).
The best classification result for detecting pregnant ewes was obtained on day 26 with an accuracy of 0.74, a precision of 0.56, and a recall of 0.71 in the test set (20% of the total number of ewes). On day 16, the results were worse, but would still correctly isolate 54% of the pregnant ewes, assuming the loss of a second opportunity for pregnancy through mating of the 31% of ewes not in pregnancy (calibration performed with group 1 of ewes and test validation with group 2).
This study leads us to believe that the use of portable NIR technology could be a very useful tool in detecting and understanding the pregnancy status of ewes, allowing for more than half of the pregnant females to be isolated on day 16 or knowing their number, and, on the other hand, on day 26 correctly classifying 74% of the group. Consequently, the mating process on day 26 could be focused only on non-pregnant animals since pregnant animals could be identified by NIR measurement of milk on that day.
The significant advantage this technology would provide is the speed of analysis and anticipation of ultrasounds, allowing for more efficient and profitable decision-making.

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A050. Authentication of ripened sausages according to the animals rearing system by NIR hyperspectral imaging

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Rearing system, breed, geographical origin are some of the quality features able to drive consumer's choice in meat and meat products purchase. The same aspects are marketing leverage from the producer's side. However, the compliance of a specific product with the declared - or supposed - quality features is mostly of a documentary nature, resulting in a possible distrust. Indeed, according to the Alert and Cooperation Network, meat and meat products are the third most reported category concerning non-compliance and suspicions fraud notifications, mostly related to faulty labelling or claims (European Union, 2023). Bearing this framework in mind, both authorities and consumers could profit from the development of rapid, non-destructive solutions to certify meat and meat products with claims of quality. In a previous study (Totaro 2023) it was shown that Near InfraRed Spectroscopy (NIRS), coupled with chemometrics, allowed to classify the rearing system of animals by using only the fat portion in unprocessed meats. However, when moving to processed products, minced and fermented such as ripened sausages, the things start to get complicated. Indeed, these products have usually highly non-uniform surfaces, with both fat and lean portions irregularly mixed and the analysis of the fat portion by single spot NIRS is often technically impossible. In the attempt to overcome this issue, in this work NIR HyperSpectral Imaging (HSI) was tested. A total of n = 12 different sausages obtained from both extensive (n = 7) and intensive (n = 5) declared rearing systems of the pigs were collected. The hyperspectral images were acquired using a HERA hyperspectral camera (Nireos SRL, Milan, Italy), in the range 900 - 1700 nm. A total of eighteen images were acquired (3 random positions × 3 salami slices × 2 replicates). The camera was controlled by the HERA ANALYSIS App software that, after proper corrections, allows to export the normalized images. These were imported and processed using Matlab R2021a (The MathWorks, Inc., Natick, MA, USA) and HYPER-Tools (Mobaraki 2018) version 3 (freely available at https://www.hypertools.org/; last accessed January 2024). After background removal and data exploration, K-means clustering was used to separate the pixels of each sample into two clusters (fat/lean) (**Figure 1A**).

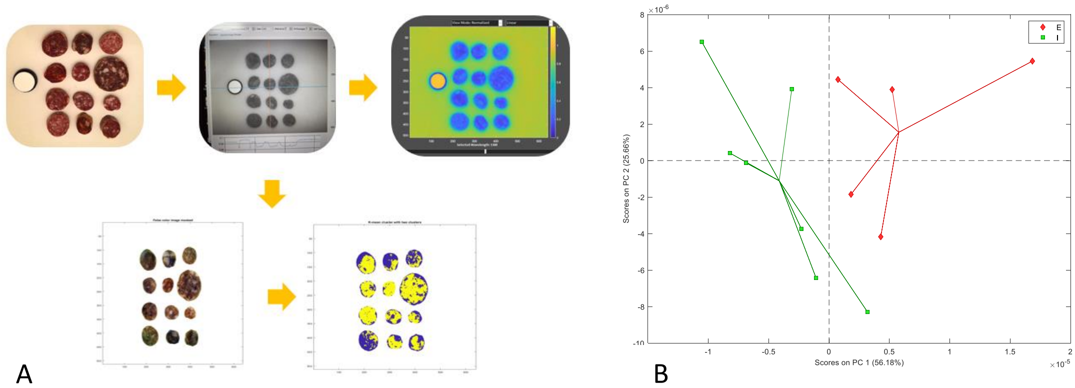

Figure 1. A) Image acquisition and processing; B) PCA score plot.

Then, the NIR signal of the sole fat pixels of each salami was averaged and preliminarily subjected to Principal Component Analysis (PCA) after proper preprocessing. By means of PCA a distinct clustering of the samples according to the declared rearing system was highlighted into the scores plot (**Figure 1B**), highlighting a great potentiality of the applied technique. As next step, an authentication model by Soft Independent Modelling of Class Analogy (SIMCA) will be calibrated and tested.

This research was carried out within the Agritech National Research Center and received funding from the European Union Next-GenerationEU (PIANO NAZIONALE DI RIPRESA E RESILIENZA (PNRR)–MISSIONE 4 COMPONENTE 2, INVESTIMENTO 1.4—D.D. 1032 17/06/2022, CN00000022). This manuscript reflects only the authors’ views and opinions, neither the European Union nor the European Commission can be considered responsible for them.

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A053. Hyperspectral imaging applied to monitoring of plants during the phytoremediation of arsenic-rich soils

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Arsenic (As) is a highly toxic, carcinogenic metalloid widely spread due to anthropogenic activities such as pesticides, industrial waste and smelting and to natural sources related to soils of volcanic origin that can contaminate groundwater. To date, highly expensive approaches are involved to respect the European limits of As in drinking water and soil. In addition, further research is needed to investigate the possibility of using innovative, non-invasive and fast monitoring methods to prevent As contamination. This framework developed a low-cost and eco-sustainable strategy using the hyperaccumulator *Pteris vittata* fern as a biosensor in As-contaminated soil (Antenozio 2022). This work aims to investigate the use of the hyperspectral imaging (HSI) technique in the shortwave infrared region (SWIR: 1000 – 2500 nm) to monitor As accumulation over time in pinnules of *Pteris vittata* plants grown in a volcanic, naturally As-rich soil. X-ray micro fluorescence semi-quantitative analyses have been carried out on the pinnules to confirm the presence of As in plants and its increase over time in plant tissues. The results demonstrated as the proposed strategy, based on spectroscopic data acquisition followed by chemometric analysis, is very promising to develop future on-site monitoring of the phytoextraction process in plants grown on contaminated soil.

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A054. DIFFERENTIATION OF *LISTERIA MONOCYTOGENES* SEROTYPES USING NEAR INFRARED HYPERSPECTRAL IMAGING

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Among the severe foodborne illnesses, listeriosis resulting from the pathogen *Listeria monocytogenes* exhibits high fatality rates of up to 30% in hospitalised immune-suppressed individuals (Gray et al. 2018). This study investigated the application of near infrared hyperspectral imaging (NIR-HSI) for the classification of three *L. monocytogenes* serotypes. The *L. monocytogenes* serotypes 4b (ATCC 23074), 1/2a (ATCC 19111) and 1/2c (ATCC 7466), which attribute to most listeriosis clinical cases, were grown on Brain Heart Infusion agar for single colonies. After incubation, a HySpex short wave infrared pushbroom imaging system was used to collect images in the spectral range of 950-2500 nm and principal component analysis (PCA) was used to detect and remove unwanted pixels of the petri dish, agar, and background pixel noise. Pre-processing techniques as standard normal variate and the Savitzky-Golay smoothing (1^{st} derivative 2^{nd} order polynomial with 11 points) were applied for scatter correction and noise reduction. The PCA results indicated that PC1 and PC3 accounted for 62% and 7% of the total variation respectively (Figure 1) and three clusters could be noticed, with a clear separation between *L. monocytogenes* 1/2a and *L. monocytogenes* 1/2c along PC3. An overlapping of the three serotypes along PC1 was attributed to the similar carbohydrates and proteins found in the bacterial cell wall.

Classification was achieved using partial least squares discriminant analysis (PLS-DA) utilizing both the full and reduced (after wavelength selection) spectra. The PLS-DA results revealed classification accuracies exceeding 80% for all the bacterial serotypes for both training and test set data. Based on test data, sensitivity values for *L. monocytogenes* serotype 4b, 1/2a and 1/2c were 0.69, 0.80 and 0.98, respectively when using full wavelength data. The reduced wavelength model had sensitivity values of 0.51, 0.87 and 0.98 for serotype 4b, 1/2a and 1/2c, respectively. Results were indicative of the inability of the model to correctly identify *L. monocytogenes* 4b. The most relevant bands for serotype discrimination were identified to be around 1490 nm (associated to proteins) and 1580-1690 nm (associated to carbohydrates) based on both principal component loadings and variable importance in projection scores (Osborne 1993; Williams et al. 2019).

The outcomes of this study demonstrate the feasibility of utilizing NIR-HSI for detecting and classifying *L. monocytogenes* serotypes on solid growth media. Based on this perspective, it is recommended that this method be used as an early detection system. The models developed could be complimented with traditional microbial assessment techniques to further confirm and give a comprehensive assessment of bacterial classification. Furthermore, while the current models demonstrate effective classification, integrating quantification methods should be considered to provide valuable insights into bacterial levels, strengthening the utility and applicability of the models.

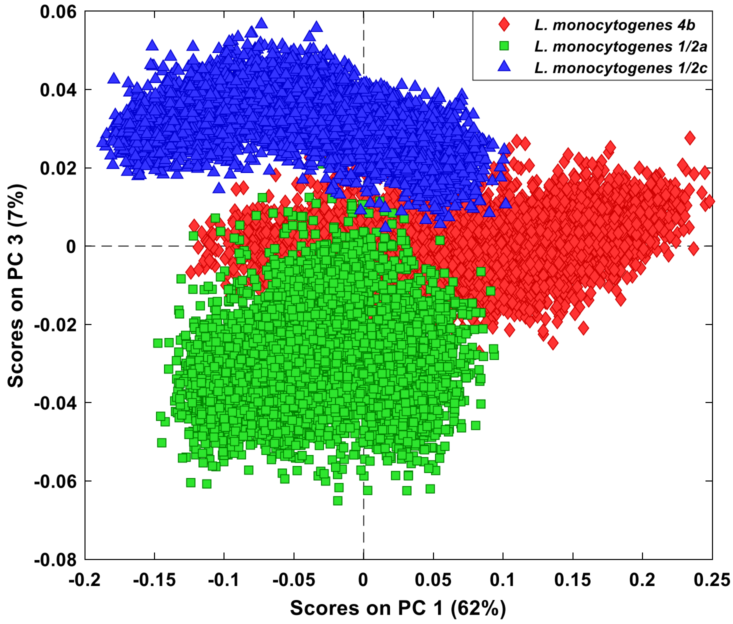

Figure 1. PCA score plot of PC1 and PC3 contributing 69% of total variance for *Listeria monocytogenes* serotype 4b (red), 1/2a (green) and 1/2c (blue) with minimal separation observed.

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A060. Detection of common bunt disease in wheat kernels and ears using visible and near-infrared hyperspectral imaging

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Common wheat bunt (mainly *Tilletia caries*) is a highly pathogenic fungal disease that affects crops yield and quality. Infected ears are characterized by a ruffled appearance revealing at maturity short, dark and rounded kernels. Bunt-affected kernels are filled with millions of spores which are easily released during harvesting and storage, and can thus contaminate the soil and surrounding healthy kernels. This disease is a major problem in organic farming because of the absence of effective disinfection treatments (Bataille *et al*., 2023).

In recent years, near-infrared hyperspectral imaging (NIR HSI) has shown its potential to detect impurities and contaminants such as ergot bodies (Vermeulen *et al.*, 2013) in cereal batches. Therefore, a method based on NIR HSI was first developed to detect common bunt in wheat kernels. Samples measurement were taken on the linescan hyperspectral camera SWIR XEVA (SPECIM, Finland) working in the spectral range from 1100 to 2400 nm and coupled with a conveyer belt (BurgerMetrics, Latvia). A dichotomous classification tree based on five partial least square discriminant analysis (PLS-DA) models was used to detect successively healthy kernels, whole affected kernels, burst affected kernels, clusters of spores and wheat impurities in a sample. Bunt spores exhibit a spectral profile showing a high lipid content allowing a discrimination from healthy kernels in this spectral range.

Following kernels analysis, the differentiation of healthy and diseased wheat ears using imaging was assessed in the laboratory similarly to the study on the Fusarium Head Blight disease detection on winter wheat ears (Vincke *et al*., 2023). In 2022 and 2023, wheat ear samples were collected before harvest from bunt inoculated test plots and stored in micro-perforated plastic bags after the visual assessment of the health status. Individual ears were measured with the linescan hyperspectral cameras FX10 [400-1000 nm] and FX17 [900-1700 nm] (SPECIM, Finland) combined with a sample tray (21 cm × 40 cm) mounted on a motorized linear translation stage (Labscanner, SPECIM, Finland). In a first approach, image analysis consisted of the development of a PLS-DA model to distinguish healthy from affected ears based on the average spectra of each ear. A comparison of the classification performances shows that the NIR camera provides slightly better results, yet similar, to those of the visible/NIR camera (**Table 1**). The latent variables loadings reveal that wavelengths related to water and starch content in the NIR region of the spectrum measured by those cameras are important for the discrimination.

Table 1. Performances of the classification models developed from the average spectra of the ears measured with FX10 and FX17 over the entire spectral range of the camera and over a reduced range of interest.

Camera	Spectral range	Latent variables	Preprocess	Sensitivity (validation)	Specificity (validation)	Error of classification (validation)
FX10	410 – 990 nm	4	Savitzky-Golay 1st derivative (2,7)	86.2%	88.5%	12.7%
	900 – 990 nm	2		84.5%	96.2%	9.7%
FX17	965 – 1682 nm	5		81.9%	98.5%	9.8%
	1055 – 1229 nm	3		85.3%	97.7%	8.5%

In a second approach, PLS-DA models were developed and applied at pixel level to discriminate the different parts of the ears, namely the awns, leaves and stem, and the parts containing healthy and infected kernels. This method allows for the detection of partially affected ears still containing healthy kernels. The models developed had a classification error at pixel level in validation of 17.8% for FX10 and 8.3% for FX17 for the distinction of healthy and affected areas. Although both models were effective for differentiating at ear level, the FX17 model generated fewer classification errors at pixel level.

Following laboratory analysis, HSI will now be investigated as a potential phenotyping tool applied directly in the field to estimate more easily and accurately the extent of bunt disease infestation in a common wheat plot. If results in fields are conclusive, this method could also be used as part of research to evaluate the tolerance of cereal varieties to bunt or the effectiveness of seed protection products on plants before harvest.

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A061. CHEMOMETRIC APPROCHEAS TO INVESTIGATE MULTIBLOCK HYPERSPECTRAL DATA IN THE FRAMEWORK OF FORENSIC BIOLOGICAL EVIDENCES

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From a forensic perspective, the analysis and identification of biological fluids using traditional techniques (e.g., forensic alternate light source) presents difficulties due to critical conditions, such as complex heterogeneous sample matrices and/or degradation effects. Nowadays, the development of new techniques allowing to detect latent biological traces in a selective and non-destructive way is an urgent research issue in the forensic framework of crime scene investigation.

The present study explores the potential of a multiblock platform (IRIS, XGLab SRL – Bruker Nano Analytics) that simultaneously acquires X-ray fluorescence (XRF, 1.4 - 40 keV) data together with visible & near-infrared (VNIR, 380 - 1100 nm) and short-wave infrared reflectance spectra (SWIR, 1100 - 2500 nm), in combination with chemometric methods, for the effective identification of dehydrated biological fluids. Several biological fluids, produced by different donors, were submitted to the investigation: such as blood, urine, semen, and saliva, deposited on wood specimens and analysed at different deposition times.

The objective of this study is two-fold: (i) to identify and localize the presence of biological fluids on the substrate, and (ii) to distinguish among specific fluids. To exploit the complementary information embedded in the different hyperspectral data blocks, a multivariate strategy based on Principal Component Analysis (PCA) and Multivariate Curve Resolution - Alternating Least Squares (MCR-ALS) was implemented for the processing of each data block and of all the three low-level fused arrays.

Chemometric strategy proved highly effective in the recognition and discrimination of biological fluids via highly informative chemical maps. The utilization of a low-level data fusion approach was crucial for distinguishing between different biological fluids, particularly due to the similarities in vibrational bands and elementary information observed in certain fluids (e.g., urine and saliva).

A063. Towards an automated seed purity analysis of cereals using machine vision

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Introduction

Seed purity is among the most essential factors determining the quality of seeds for the production of plants, and determination of this aspect is a prerequisite for the sale of agricultural seeds within the EU (Council Directive 66/402/EEC 1966). The International Seed Testing Association (ISTA) provides guidelines for many types of seed analysis including *analytical purity* and *other seeds by number* (ISTA 2024). Both types of analyses require highly specialized lab-technicians to classify each seed according to species. A task that is both labour-intensive and repetitive. This is why, in recent years, more researchers have been looking into automatable methods for these types of analysis of which machine vision seems to be the most promising (ElMasry 2019).

Objective

To develop a model based on multispectral imaging to be used for seed purity analysis and determination of other species in samples of cereals meant for seed certification within the EU. A special focus will be on analysis of wheat and barley as these species constitute the largest amounts of cereals produced in Denmark. This contribution represents a snapshot of the development of said model as the study is still in progress.

Methods

Imaging system: The method is based on the Videometer SeedLab (Videometer A/S, DK-2970, Hørsholm, Denmark) multispectral imaging system which includes an autofeeder, conveyer belt and a robotic arm. Images are captured of each seed from a single top down angle at 19 wavelengths: 365, 405, 430, 450, 470, 490, 515, 540, 570, 590, 630, 645, 660, 690, 780, 850, 880, 940 and 970 nm. Through segmentation, each seed / piece of dockage is saved as an individual blob for further identification performed by the classifier.

Sample materials: The training set consists of the 16 species listed in **table 1** including cereals, weeds regulated in cereals within the EU, and the most common weeds found in samples of cereals harvested in Denmark. Each species is represented by between 668 and 11.509 seeds. The training set also includes dockage.

Classification: Blobs are classified in two steps: in the first step the blob are classified as either a weed seed, a cereal grain or a piece of inert material (dockage); in the second step the blobs are classified to the species level within its identified category. The classifications in both steps are performed by random forest classifiers utilizing 24 morphological, 16 textural, 4 color and 35 multispectral features for a total of 79 features.

Results

Table 2 shows the total accuracy of each of the nodes in the classification process, estimated from a fivefold cross validation on the training set. The accuracy of the initial classification into the categories weeds and cereals is 99,57 %. Further classification into the specific weeds and cereal done with an accuracy of 99,78 % and 99,35 % respectively. The total accuracy of the entire model is 99,67 %.

Table 2. Species included in the training set.

Species
Barley (*Hordeum vulgare*)
Durum (*Triticum durum*)
Naked oat (*Avena nuda*)
Oat (*Avena sativa*)
Rye (*Secale cereale*)
Spelt (*Triticum spelta*)
Triticale (*xTriticosecale*)
Wheat (*Triticum aestivum*)
Barren brome (*Bromus sterilis*)
Black bindweed (*Fallopia convolvulus*)
Cleavers (*Galium aparine*)
Corn-cockle (*Agrostemma githago*)
Field pansy (*Viola arvensis*)
Scentless mayweed (*Tripleurospermum inodorum*)
Soft brome (*Bromus hordeaceus*)
Wild oat (*Avena fatua*)

Table 3. Performance of the different nodes in the model expressed in accuracies based on fivefold cross validation on the training set.

	Initial node	Weed node	Cereal node	Entire model
Accuracy	99,57 %	99,78 %	99,35 %	99,67 %

Conclusions

The classification accuracies look promising so far. As the study is still ongoing there will be further improvements to the classification model, including more species of weeds and the introduction of classes within the category *inert matter*.

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A067. The effect of particle size on NIR spectral profiles: how to understand and manage light scattering

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One of the principal advantages of near infrared spectroscopy (NIR) is to acquire instrumental signals without sample preparation (extraction, filtration, concentration, etc.) but this interesting opportunity can hide an underrated effect: the unwanted spectral distortions caused by radiation scattering of solid samples. The impact of these distortions on spectral modelling was already underlined and several chemometric data pretreatments were suggested, trying to mitigate the impact of these spectral phenomena. However, a comprehensive and designed study of these effects is still missing, in particular when focusing on the significance of distortions along the different spectral bands. Commonly applied (and namely effective) data pre-treatments do not always take into account the wavelength dependency of the effects due to particle size, which may cause signal distortions. For instance, diffuse absorbance spectra A=log(1/R) are often obtained for turbid or opaque samples from measured reflectance spectra R. When such absorbance spectra are preprocessed with additive methods (e.g. derivatives) and modelled by additive subspace methods such as PCA and PLSR, different sources of light scattering variation may cause problems, due to different changes in effective optical path length, angular distribution of reflected light and response linearity to specular reflection and constituent. Conventional mixed-additive-and-multiplicative preprocessing methods (e.g. SNV (standard normal variate), MSC (multiplicative signal correction) and EMSC (extended multiplicative signal correction) can alleviate some of these problems, but not all.
With the goal of better understanding such a fundamental phenomenon, a working group is being constituted with the interest of collecting spectral data from absorbing and non-absorbing material with a variation of particle size and relative amounts. This working group was constituted under the umbrella of a wider project, the TREx-modelling – Transmission and reflection Explained – under the coordination of Prof. Harald Martens.
The first dataset that was collected, was design by means of multivariate design of experiment (MDOE) and makes use of a *per se* non-absorbent, but slightly hygroscopic, substance (NaCl) and a substance with a typical NIR signal (sucrose), considered at three particle size levels (1.3- 2 mm; 1-1.3 mm; 0.7-1 mm) and in three different mixture proportions (33%+66%; 50%+50%; 66%+33%). A total of 33 samples were prepared and NIR spectra (from 1000 to a maximum of 2500 nm) were acquired with a benchtop (NIRFlex, Buchi), a portable (MicroNIR, VIAVI Solutions) and an imaging (SWIR 3, Specim) spectrophotometer. The dataset has been submitted to spectral visualization and principal component analysis (PCA), to highlight the information related to the proportion of the absorbent material, and the unwanted distortions, due to particle size. From this preliminary research emerged that the factor "salt particle size" causes baseline shift, the factor "sugar particle size" causes spectral shape deformation (See Figure 1) and the different proportions between the two substances lead to baseline drift of spectral signal. Mathematical transformations such as SNV and various versions of EMSC were applied

on the spectral signals to evaluate their effect. Also, the removal of spectral variables most influenced by the physical properties of the analyzed sample was evaluated.

The association of spectral visualization and data exploration, followed by a quantitative evaluation of the effect's significance, was demonstrated to be a valuable approach to understand the impact of the factor under study and to choose the optimal spectral pretreatments.

If the results obtained from this initial case-study will be confirmed with other datasets, the final outcomes would support the analytical chemist in the choice of how to acquire spectral data (mainly balancing spectral region and particle size) and which algebraical transformation apply, depending on the own goal: quantify an absorbent substance, determine particle size of an absorbent substance or characterize a material from both a physical and chemical perspective.

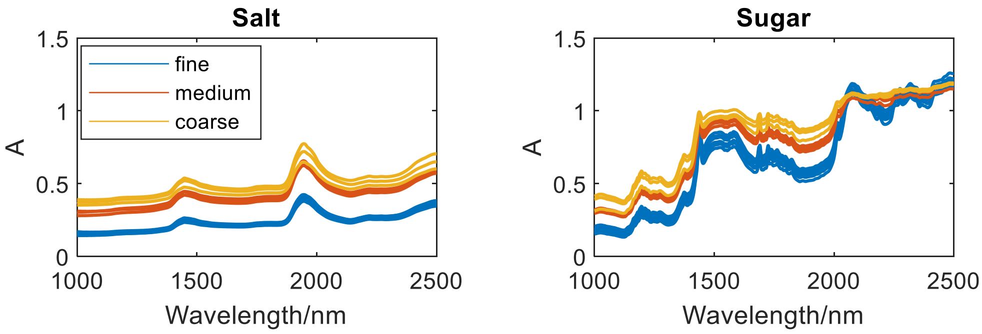

Figure 1: Diffuse NIR absorbance spectra of pure salt and sugar samples with different granulometries ranging from 0.7 to 2 mm

A082. Prediction of lipid content in black soldier fly larvae by NIR-Hyperspectral imaging and chemometrics

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The continuous expansion of the global population compels the food industry to explore new, sustainable sources of food. In this context, new technologies are available in the market, such as insect-derivate products, cultured meat and vegetable-derivates products. Insects are one of the promising sources of protein and lipids to help meet the demand for nutrients in the population, either through direct consumption by humans or through their incorporation into animal feed **(Nieto et al., 2023)**. Among the eight insects approved by the EU for animal feed (excluding ruminants) (**Commission Regulation (EU) 2021/1925** of November 5, 2021), the larva of the black soldier fly (*Hermetia illucens*) stands out. This larva has the ability to produce high-quality lipids (17 – 49%) and protein (29 – 45%) from organic agricultural residues. Therefore, its use aligns with the principles of the circular economy and environmental sustainability, contributing to the strengthening of food security objectives. Therefore, the quality control of macronutrients in black soldier fly larvae is essential in order to optimize the production.

The near infrared spectroscopy (NIRS) is a powerful technique to monitor and predict macronutrients, such as protein and lipids, in several food matrices. When we integrate a computer vision system with NIRS (Near-Infrared Spectroscopy) technology, we obtain hyperspectral images (HSI), which can capture both chemical (internal) and physical (external) information of the analyzed material **(Vidal & Amigo, 2012)**. By processing the information obtained from NIR-HSI using chemometric methods such as Partial Least Squares Regression (PLSR) or Support Vector Machine Regression (SVMR), we can create robust mathematical models to predict the concentration of the modeled analyte.

The objective of this work was implemented a NIR-HSI system coupled chemometrics to predict the concentration of lipids in black soldier fly larvae.

A total of 18 batch (50 g) of black soldier fly larvae samples were collected from local producer in São Paulo (Brazil) during years from 2020 and 2021. Then, intact larvae samples were imaged using a SisuCHEMA SWIR hyperspectral camera (Specim Spectral Imaging Ltd, FIN-90571 Oulu, Finland), in the spectral range 928–2524 nm with 6.23 nm intervals (256 wave channels). Next, samples were grounded and lipids were extracted using black dyer method. The total of lipids (%) was calculated by using gravimetric approach. For data analysis, PLSR and SVMR were implemented using PLS_Toolbox (Eigenvector Research, Inc. 196 Hyacinth Road, Manson, WA 98831, USA) for the Matlab 2020a environment (The Mathworks, Inc. Natick, MA 01760-2098, USA).

The results of chemometric approach are showed in **Figure 1**. SVMR model performed slightly better than PLSR model, with RMSEP values of 5.7% and 4.8%, respectively. Likely, this is due to the higher complexity of SVMR compared to PLSR. Nevertheless, we can observe that both models can be useful for predicting the lipid content in black soldier fly larvae. Finally, it is important to mention that the spectra were obtained without destroying the larvae, which may facilitate on-site monitoring of lipid accumulation in the larvae associated with the larval feeding system.

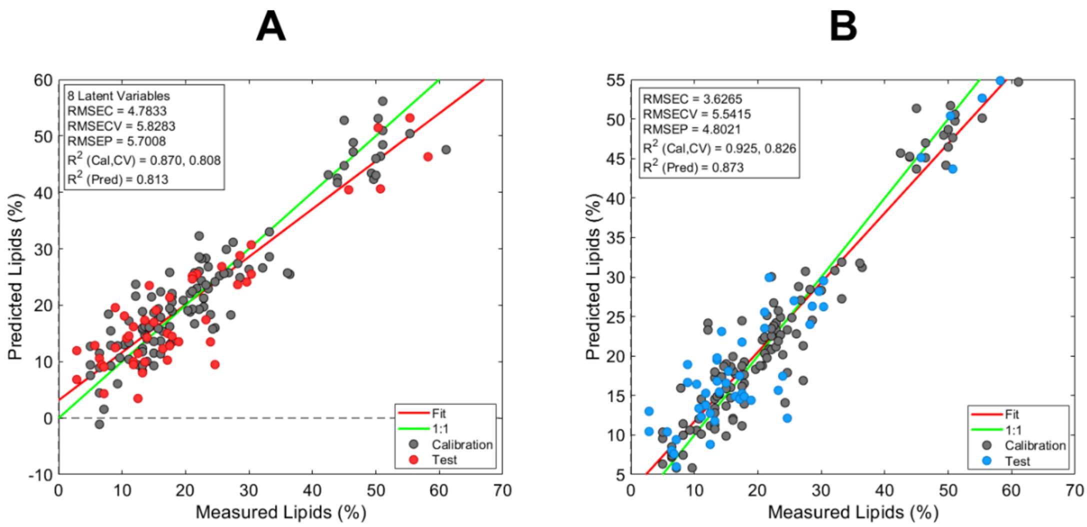

Figure 1. Prediction of the lipid concentration (%) in black soldier fly larvae using PLSR (**A**) and SVMR (**B**) models

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A083. Detection of Insects in Wheat Grains: A MCR-ALS and FDA Approach Using Hyperspectral Imaging

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The detection of insects present in large grain shipping sites are becoming crucial to reasoning out a possible treatment to protect them from a massive infestation, which could lead to significant financial losses. This study is oriented to show that hyperspectral imaging combined with a multivariate data processing pipeline can be used to detect insects in wheat.
Our approach utilizes two hyperspectral cameras: one operating in the spectral range of 400 to 1000 nm (HySpex VNIR-1800), and the other covering the range of 1000 to 2500 nm (HySpex SWIR-384). This dual-camera setup allows for comprehensive spectral coverage, facilitating the extraction of detailed spectral information.
In our multivariate data analysis strategy, we employ a combination of multivariate curve resolution-alternating least squares (MCR-ALS) [De Juan 2010] and factorial discriminant analysis (FDA) [Hand 1985]. MCR-ALS is utilized to extract chemically significant spectral signatures and generate distribution maps of wheat and insect images. The resulting MCR scores serve as input for FDA to distinguish pixels corresponding to wheat grains or insects. Additionally, insect identification is achieved using Multivariate Imaging Analysis-Toolbox functions.
Our methodology is tested on images captured by the individual cameras separately. Subsequently, data from both cameras are merged using a fusion imaging strategy. By combining data from multiple hyperspectral cameras, we aim to improve the accuracy and reliability of insect detection and quantification. Comparison of results from individual MCR/FDA models and the fused model will be provided to assess the efficacy of each approach.
Preliminary results are very encouraging that promote further investigation to propose the strategy studied as a good approach for the detection of insects that could help to reinforce insect control at the main shipping sites.

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Hand 1985: Hand, DJ. Discrimination and classification. Biometrical Journal. 27:2 (1985) 148. DoI: https://doi.org/10.1002/bimj.4710270204

A094. Brix and pH Prediction of Grapes using Snapshot Hyperspectral Computed Tomography Imaging Spectroscopy

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In this work, we use a recently developed snapshot Hyperspectral Imaging (HSI) system based on a Computed Tomography Imaging Spectrometer (CTIS) with convolutional autodecoder data reconstruction to determine Brix and pH values in table grapes using a Partial Least Squares Regression (PLSR) model. We compare the performance of the CTIS system with a state-of-the-art line scan HSI system by imaging 200 grapes on both systems while measuring the Brix and pH values of the grapes directly using a refractometer and a pH-meter. Brix and pH are key parameters for determining both table grape and wine grape quality.

HSI enables the analysis of the reflectance spectra across the entire grape skin area, providing the maximum amount of information about the grape's chemical composition, including its sugar content (Biano 2012, Gomes 2021). The previous HSI studies used a line scan HSI with grapes put on a conveyor belt.

In this work we employ a newly developed CTIS system with a spectral range from 600-850 nm (Ahlebæk 2023). We compare the CTIS system performance with a state-of-the-art line scan Oculus HSI system with a visible shortwave infrared (Vis-SWIR) spectral range from 532-1655 nm (Newtec 2024) (**Figure 1**).

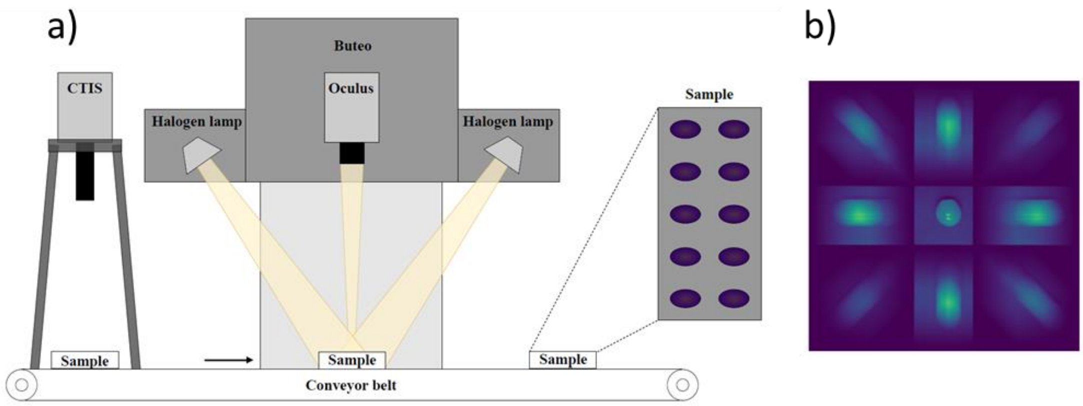

Figure 1. a) Experimental setup for hyperspectral imaging of grapes with both line scan and snapshot HSI systems, b) CTIS image of a grape (false colors).

The standardized mean reflectance spectra for both the line scan and snapshot hyperspectral cameras are visualized (**Figure 2**). From the figure there are no noticeable variations in the spectra that appear to explain the Brix differences.

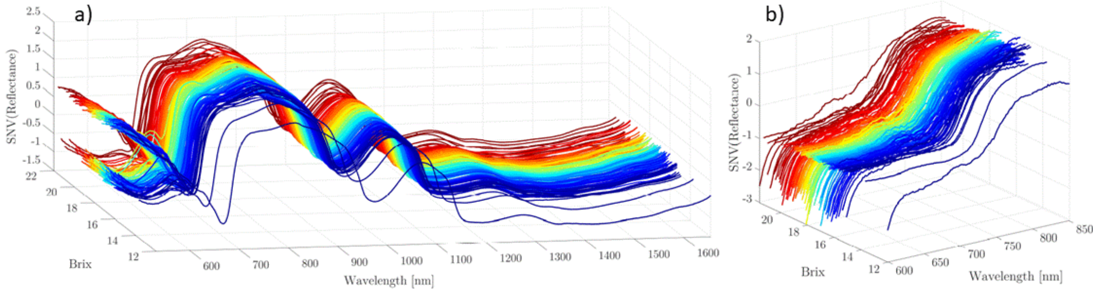

Figure 2. (a) Standardized mean spectra of grapes from (a) line scan and (b) CTIS datacubes.

For each of the investigated cases, a predictive PLSR model that correlates the spectral information with the Brix and pH values was constructed. A 10 K-fold cross-validation was performed with 20 PLS components, resulting in an MSE_{Brix} = 0.17 Brix for the full spectral range 532-1655 nm line scan HSI and for a reduced spectral range 600-850 nm line scan HSI an MSE_{Brix} = 0.41 Brix was obtained and using the same spectral range 600-850 nm with the CTIS camera an MSE_{Brix} = 0.98 Brix was obtained.

We find a good correlation between the spectra recorded by the CTIS camera and the direct measurements. Combined with the durability and portability of the CTIS camera this opens a range of promising in-field applications such as field robotics.

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A095. Data volume reduction strategies of near-infrared hyperspectral imaging to discriminate meat from different cattle feeding systems

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Food waste is in the spotlight as it involves a misuse of both monetary and physical resources. One possible solution is that farm animals take advantage of by-products that are inedible to humans. In view of a future label that ensures circular economy practices, this project aimed to evaluate the potential of near-infrared hyperspectral imaging (NIR-HSI) and data volume reduction strategies to discriminate meat from two cattle feeding systems.

In this study, 23 entire young bulls were used. Twelve were provided a barley and straw-based (BS) diet while eleven were supplied a novel feed incorporating 37.4% vegetable by-products (VBPR). After a fattening period of 139.73 ± 18.54 d, the animals were slaughtered, and seven steaks from the posterior *longissimus lumborum* were obtained from the left-side carcass of each animal, vacuum packaged, and kept under refrigerated conditions. After 7 d of aging and 20 min of blooming, one steak was scanned on both sides with a Xenics hyperspectral camera (Model Xeva-1.7- 320, Leuven, Belgium) and an InGaAs detector of 320 x 256-pixel resolution (spatial resolution: 0.75 mm; spectral resolution: 3.14 nm). The camera was coupled to an ImSpector N17E spectrograph (Specim, Spectral Imaging Ltd., Oulu, Finland) in the 900 – 1,700 nm spectral range. The OPT-000107 Xenics lens (SWIR, f/1.4, Leuven, Belgium) with a focal length of 16 mm were used. The scanning speed was set to 7 mm/s while the integration time was 2,000 µs. Meat quality was also evaluated by reference methods (i.e., color, instrumental texture, and intramuscular fat, protein, and collagen content).

Prior to chemometric modelling, images were normalized and spikes were removed. After fat extraction from the steaks (both exterior and marbling), the complete dataset only considering the lean pixels (100% of the pixels from 46 images; 2 images per steak per animal) consisted of two matrices of 837,856 x 207 and 233,713 x 207 for Train and Test (78:22), respectively. To manage computational load and the curse of dimensionality, 25% of the pixels were randomly selected, reducing the matrixes to 209,468 x 207 (Train) and 58,430 x 207 (Test) (25%px). Afterwards, the ReliefF feature selection algorithm was applied to reduce the information further and shorten data processing times (Roffo, 2016). The ReliefF basis lies on the assignment of feature quality, therefore, the two nearest neighbors (one of each category) are examined. Then, a weighted vector is calculated according to the potential to discriminate near samples in the target groups (25%px+ReliefF). Additionally, variable selection was performed in terms of interval Partial Least Squares (iPLS), using 10 intervals limited to 1 wavelength interval size (25%px+iPLS). Subsequently, the PLS-Discriminant Analysis (PLS-DA) was conducted as a discriminant approach with the software PLS_Toolbox 9.3. under MATLAB R2023b.

The classification results differed depending on the feeding groups (**Table 1**). The BS meat was discriminated with a rate >79% in the Test, regardless of the data reduction strategy, while VBPR lean pixels were a challenge for the PLS-DA models (<55.35%). Most of the meat quality analyses did not reveal statistically significant differences between meat from cattle fed the two diets (*P*-value>0.05), except for total collagen content (*P*-value<0.05, data not shown). Hence, despite no clear differences in most of the conventional meat quality parameters, hyperspectral imaging was able to capture a chemical variation between both steak groups.

Table 1. Partial Least Squares-Discriminant Analysis metrics of the pixel-wise models.

Dataset	Pre-process	LV	%CC Train		% CC CV		%CC Test		Time (min: s)
			BS	VBPR	BS	VBPR	BS	VBPR	
25%px	SM+MC	4	84.12	54.14	84.10	54.14	**80.58**	54.33	3: 55
25%px+ReliefF	MC	1	82.61	51.81	82.56	51.83	80.20	54.26	**0: 12**
25%px+iPLS	MC	5	83.94	55.61	83.93	55.61	79.67	**55.35**	0: 41

%CC, Percentage of samples correctly classified; LV, Latent variables; CV, Cross-validation; px, Pixel; SM, Smoothing, MC, Mean center; BS, Barley and straw; VBPR, vegetable by-products; min, Minute; s, Second.

Despite the classification performance of the data volume reduction strategies was similar, they contributed to shortening processing times. By extracting the most prominent features with the ReliefF algorithm (X_{Train} = 209,468 x 2, X_{Test} = 58,430 x 2), the analysis time was reduced by 95% compared to 25%px, while the proportion of well-classified samples remained practically stable. Likewise, the selection of 10 variables by the iPLS method (1,063 nm, 1,141 nm, 1,373 nm, 1,593 nm, 1,621 nm, 1,671 – 1,678 nm) reduced the computational time by 83% compared to 25%px (X_{Train} = 209,468 x 10; X_{Test} = 58,430 x 10). Further studies considering the fat pixels would be warranted to potentially enhance the classification performance. In a real-time application, minimizing the time required for data processing is of utmost interest. Therefore, the application of data volume compression and reduction strategies is key for the real-time application of NIR-HSI in the meat industry.

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A098. Analysis of Vegetation Chemistry Using Feature Importance in Hyperspectral Images

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The levels of nitrogen, potassium, phosphorus, carbon, lignins, cellulose, and water in vegetation are important indicators of plant health and specifically are useful for determining management actions that are needed such as increase water supply, soil conditioning, sun exposure, and fertilizer type and quantity. Spectroscopy has been used to estimate these levels [**Fan 2019, Taha 2022**], but only in controlled single-species situations such as from leaf samples in a single orchard.

In this study, we present methods for estimating levels of these nutrients using Hyperspectral imaging using machine learning. For this study, we used vegetation data available in the ECOSTRESS spectral library [**Baldridge 2009, Meerdink 2019]** which includes chemistry information for these quantities. We also collected vegetation spectra using an ASD Field Spectrometer along with LAQUAtwin ion meters.

We test around 40 of regression algorithms using Python, including parametric, tree-based, Bayesian, and neural networks. The best-performing methods include ridge, ridge (cross validated), lasso lars (cross validated), Bayesian ridge, LGBM, poisson regressor, huber regressor, and random forest as the regression , with initial results for predicting water content shown in Table 1.

Table 1. Results of top 8 models using all 2151 bands.

Model	RMSE, Water Content
RidgeCV	7.44
Ridge	7.78
ExtraTreesRegressor	7.79
XGBRegressor	7.85
LGBMRegressor	7.97
HistGradientBoostingRegressor	8.03
RandomForestRegressor	8.12
LassoLarsCV	8.13

The top-performing methods all incorporate regularization of some form. To both potentially improve prediction performing and to provide further insight into spectra features that are important for predicting these quantities, we computed multiple feature-selection methods, including genetic algorithm (GA), sequential forward selection (SFS), principal component analysis (PCA), Shapley, and feature importance with ridge (cross validated) and XGBoost. A plot of feature importance, along with vegetation spectra for multiple water-content level, is shown in Figure 1.

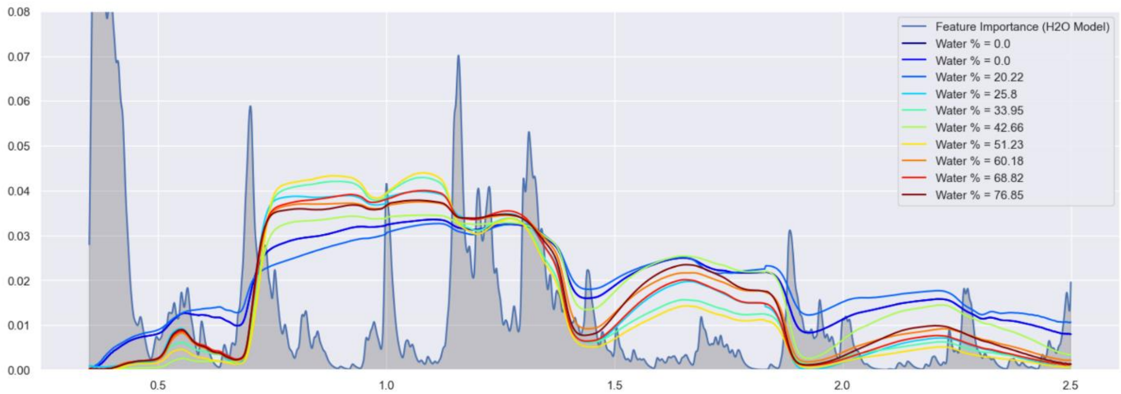

Figure 1. Feathers (Bands) that are most important in predicting water content.

We investigate the accuracy of the various regression machine learning methods for estimating these quantities, investigate the feature (band) importance for the different methods, and relate the bands with high importance to chemical relevance of the important bands to specific compounds in the vegetation. We investigate the explainability of the various regression methods to determine the how and why the different methods are effective, particularly with respect to the bias-variance trade-off, the meaning of parameters in parameterized methods, and degrees of regularization needed.

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A099. Bayesian Sampling Methods for Material Identification and Parameter Estimation In Hyperspectral Imaging

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Bayesian sampling is the process of iteratively computing a series of models, with parameters that change across the models. The goal is to develop a probability distribution for the parameters. This can be used to improve accuracy, for example by generating an ensemble of models created by sampling the parameter values from the inferred distributions. It can also be used for robust inference with quantified uncertainty. In this presentation, we discuss Bayesian sampling for processing hyperspectral imagery in general, and then present specific implementations using Bayesian model averaging for neural network material identification method and a Bayesian model averaging for linear unmixing with validated identification of minerals down to 2-3% abundance for minerals in Nevada related to Lithium mining.

In previous work (Basener 2022), we showed that neural network models can be very effective at identification of materials from spectra, including showing that the spectral features are learning by the network in the weights. An plot of weights learned by a neural network along with the spectrum are shown in Figure 1. We also showed that Bayesian methods provide quantification of uncertainty (Preston and Basener 2022) and improve accuracy through model averaging. In this presentation, we show the effectiveness of these methods for identifying materials in hyperspectral imagery using the Forest Radiance dataset. In contrast to other deep learning hyperspectral methods which often train and test on a single image (Paoletti et al 2018), our method enables training on a spectral library of known spectra and applying to an image.

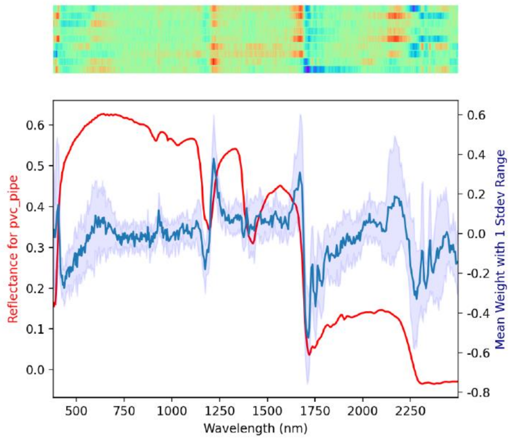

Figure 2A PVC spectrum (red) along with distribution of weights in the network associate with detecting this material (blue and included heatmap above).

We present how model averaging can produce accurate low-abundance identification of materials in a hyperspectral image. Using a custom model-search method, we produce probabilities that can correctly discriminate between target spectra and similar confusers, and additionally produce sub-pixel plots of the spectra for visual confirmation. An example showing detection and identification of a lithium-related mineral at 2% abundance in the mountainous regions of Nevada, USA, is shown in Figure 2.

Figure 3 A region of interest (ref, left) and spectral plots (right) for a low-abundance detection and identification of leidolite using Bayesian model averaging unmixing.

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A100. The Potential Use of the VIS-NIR and NIR Hyperspectral Image as A Non-Destructive Method for Early Detection of Chilling Injury in Zucchini

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Zucchini is a chilling sensitive product although it is often held at temperatures below 5 °C during the distribution chain. For this reason, rapid and early detection of zucchini previously stored at chilling temperatures would allow the correct reallocation of this fruit to the correct temperatures or the early withdrawal of chilled fruit from the market in the worst case. This research aimed to explore the potentiality of hyperspectral imaging for the early detection of chilled fruit. To this scope zucchini fruit (cv. Asso) were stored at 2 °C, and 12 °C for 9 days, soon after harvest. Hyperspectral images were taken at 2, 6, and 9 days of storage. The spectral scanner (version 1.4, DV srl, Padova, Italy) had a spatial resolution of 1000 × 2000 pixels (Vis-NIR) and 600 × 320 pixels (NIR), both with a 5 nm spectral resolution. In addition, chilling injury (CI) was assessed according to the presence of yellow discoloration of the flesh area and surface pitting, evaluated after one additional day at room temperature to allow symptoms to develop. Supervised classification models were developed using Partial Least Square Discriminant Analysis (PLS-DA) on hyperspectral data to classify zucchini fruit based on storage temperature. Raw spectra were pre-processed with different combinations of spectral preprocessing techniques, and the dataset was divided into two groups (70% for calibration, and 30% for validation). The result shows that with VIS-NIR spectra was possible to discriminate chilled fruit with accuracy of 90, and 92% in calibration and prediction, respectively, already after 2 days of chilling temperature. Accuracy increased to values higher than 98 % with an increase in the length of storage. The model obtained with NIR spectra allowed 100% accuracy in prediction, for fruit stored for 9 days but lower performance with fruit stored for shorter periods, if compared to VIS-NIR. These results demonstrate the potential use of hyperspectral imaging techniques to early detect chilling injury in zucchini fruit.

Keywords: Hyperspectral images, Zucchini, VIS-NIR, NIR, PLS-DA.

A102. The Potential Application of Visible-Near Infrared (Vis-NIR) Hyperspectral Imaging for Classifying Typical Defective Goji Berry (*Lycium barbarum* L.)

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Goji berry is acknowledged for its notable medicinal attributes and elevated free radical scavenger properties. Nevertheless, their susceptibility to mechanical injuries and biological disorders reduces the commercial diffusion of the fruit. A hyperspectral imaging system (HIS) line scanner (Version 1.4, DV srl, Padova, Italy) was employed to identify common defects in the Vis-NIR range (400-1000 nm) possessing a spatial resolution of 27.9 pixels/mm^2 and 5 nm of spectral resolution. The sensorial evaluation of visual appearance was used to obtain the reference measurement of defects, with a total of 4 classes, 3 for defective fruit and one for sounds. A supervised classification model employing PLS-DA was developed with the integration of a Covariance Selection algorithm (CovSel) for variable selection and validation through an rDCV approach encompassed 10 cancellation sets of groups in the outer loop, 8 cancellation sets of groups in the inner loop, and as many as 50 double cross-validations (DCV) runs. Before the construction and validation of the model, the spectra underwent pre-treatment, including Multiplicative Scatter Correction (MSC), second derivative (Savitzky-Golay, 15 points windows, 3rd order polynomial), and finally mean centering. The classification model demonstrated superior performance when only 2 classes (sound and defective were used, achieving an accuracy of 94.9%. However, when extended to a more complex task of classifying fruit into four categories, the model exhibited reliable results but with lower accuracy. These results indicate that a method based on hyperspectral visible-NIR can be implemented for the online sorting of defective goji berries.

Keywords: PLS-DA, multivariate-analysis, defective goji, hyperspectral imaging, non-destructive

A104. Vis-NIR hyperspectral imaging and multivariate analysis as a tool for the assessment of sugar beet chemical variation during storage

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In the sugar beet industry, beets undergo approximately two months of storage in field clamps before sugar production, with a growing consideration to extend this period (Gruska et al. 2022). Significant chemical changes during storage such us decrease in sucrose content and an increase in glucose, fructose, raffinose, N-amino and betaine content have been reported (Kenter & Hoffmann 2009). Conventional methods for assessing sugar biomass quality (e.g. refractometry, polarimetry, and chromatography) are typically time-consuming, labor-intensive, and destructive. Thus, there's a crucial need for rapid, non-destructive techniques for accurate sugar beet quality assessment. Hyperspectral imaging (HSI) is a technique widely used for quality analysis in various food matrices (Sun 2010). Our objective is to employ Vis/NIR hyperspectral imaging along with chemometric tools for the assessment of sugar beet chemical variation during storage. The samples were subjected to storage at 20°C for a period of 0 to 90 days (t_0, t_{30}, t_{45}, t_{60}, t_{75} and t_{90}). On each day of analysis, a cross section was made in the center of beets, to immediately acquire images with the Pika-L (Resonon) camera (400 to 1000 nm). Each image was preprocessed using the Graphical User-friendly Interface (GUI) Hyper-Tools v.3.0 (Mobaraki & Amigo 2018). Principal Component Analysis (PCA) was applied to the average spectrum of each image and to each pixel of the unfolded image. Partial Least Square Discriminant Analysis (PLS-DA) classification methods was applied to assess the ability to predict the freshness of the sugar beets, expressed as storing time. In addition, Multivariate Curve Resolution - Alternating Least Squares (MCR-ALS) was used to evaluate sample homogeneity and to identify beets zones more susceptible to storage. The PLS_toolbox v.9.0 (Eigenvector Research, Inc., Wenatchee, WA) and MCR-ALS GUI 2.0 Toolbox (Jaumot et al. 2015) were used. After two months of storage, alterations in the appearance of the beets were observed, where a brown coloration started to appear. In PCA, good class separation by storage time has been obtained, shown in Figure 1. High classification accuracy rates (>70%) were achieved in the PLS-DA model for both training and external validation. After applying MCR-ALS, two MCR components were resolved with high percentages of explained variance (99.9%) and low error rates (2.3 to 3.5%) According to the maps of relative concentrations, one component corresponds to the inter-ring zone (IRR) (whitish coloration) and the other to the central ring (CR) and the rings (R) (slightly brownish coloration) (Figure 2). Variations in pure spectra due to storage were evaluated respect to the storage period. These results argue for the potential application of advanced spectroscopic techniques in the assessment and monitoring of quality during storage, with far-reaching implications for sugar production
and alternative applications.

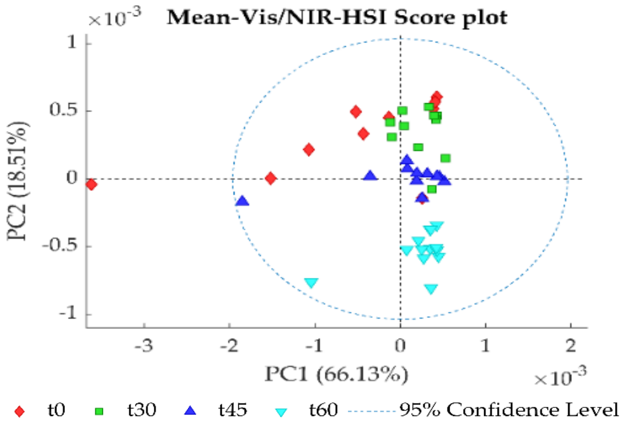

Figure 1. Score plots of mean HSI spectra of sugar beets subjected to storage.

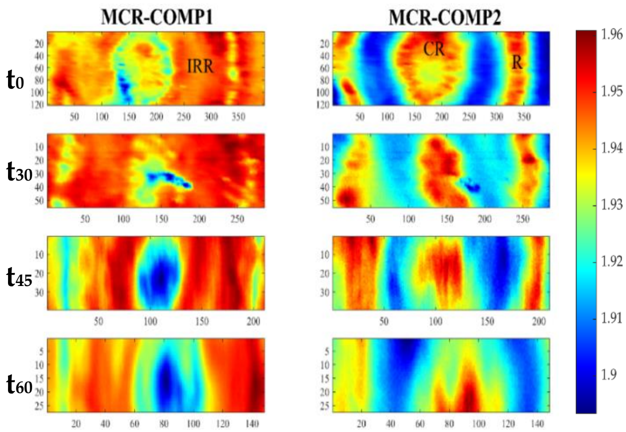

Figure 2. Relative concentration maps for the two MCR-ALS components determined in Vis/NIR HSI of sugar beet

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A106. Use of hyperspectral imaging to help in the identification of the Mushy Halibut Syndrome

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Introduction:
Mushy Halibut Syndrome (MHS) is a condition affecting Greenland halibut that is characterized by an abnormal opacity and texture of the flesh, rendering it flaccid and jelly[1]. The manifestation of MHS significantly impacts fish quality, leading to substantial economic losses for fishermen and producers due to the degraded market value of their products[2]. Typically, the syndrome is not detected until post-filleting, resulting in product devaluation and consumer dissatisfaction[3], thereby posing a major challenge for the seafood industry. Currently, there is no standard method for early MHS detection.
In previous studies, we evaluated the feasibility of hyperspectral imaging as a non-invasive technology for the characterization and early identification of MHS[4,5]. We explored two methods: estimating chemical composition through spectral unmixing and using Partial Least-Squares Discriminant Analysis (PLS-DA) for supervised classification. While the spectral unmixing method showed limitations, PLS-DA proved highly effective for MHS detection. However, the observed trend in the reference chemical measurements indicated that fish affected by MHS exhibit reduced fat, dry matter, and protein levels in their muscle tissue. Therefore, in this work we evaluate the feasibility of the identification of MHS based on the prediction of the fish's chemical composition from the spectral data.
Materials and methods:
The instrumentation used in this work was the Maritech Eye, a hyperspectral imaging system tailored specifically for the seafood industry. The Maritech Eye includes an interactance lighting system and a hyperspectral camera (HySpex Baldur V-1024N), which covers the spectral range from 485 to 960 nm. The principle of interactance illumination involves measuring light following its multiple internal scatterings within the sample, thereby enabling the extraction of details on the chemical composition that goes deeper than just the surface[6].
In this study, 32 Greenland halibut fillets provided by Royal Greenland were selected at the production site and scanned using the previously described hyperspectral instrumentation. These samples were chosen based on varying degrees of MHS affection to ensure a broad representation of chemical composition variability within the cohort. Subsequent biochemical analyses were conducted in a laboratory to quantify the fat, dry matter, and protein content in the fillets.
The prediction of the chemical composition in terms of the spectral data was performed using Partial Least-Squares Regression (PLSR). Before PLSR, the images were calibrated using a flat-field calibration, converted to pseudo-absorbance, and normalized using Standard Normal Variate (SNV).

Results:
The results of the estimation of the chemical composition from the spectral data are shown in Figure 4. Competitive predictions are obtained in cross-validation for dry matter and fat, with

high coefficients of determination (0.8 and 0.82) and low RMSE (2.4 and 1.78). However, the results for the prediction of proteins are not accurate (R^2_{CV}=0.39).

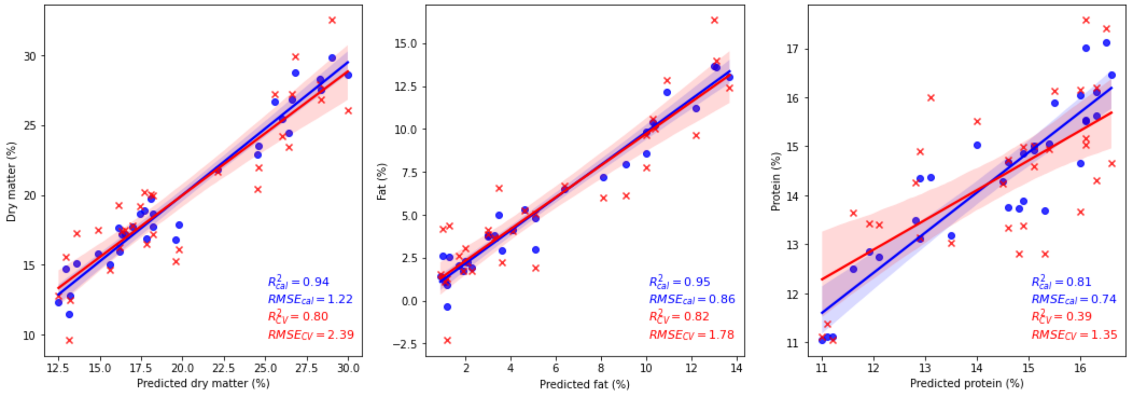

Figure 4: PLSR results on estimating the chemical composition of the Greenland halibut.

Conclusions:

In the past, we proved that the use of supervised classification based on the spectral data was adequate for the identification of MHS non-invasively. In this work, we show that the prediction of the chemical constituents that are relevant for the identification of the MHS from the spectral data is also possible. In future works, we further explore the use of this chemical data for the identification of MHS.

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A107. Exploring multivariate curve resolution coupled with deep learning for hyperspectral imaging data: from quantitative analysis in biological tissues to qualitative analysis in plastic samples

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The importance of employing innovative data analysis methods for hyperspectral imaging is crucial, particularly for complex studied samples where traditional analytical techniques may struggle to capture the detailed chemical composition and spatial distribution patterns. Plastics play an important role in numerous sectors, yet their efficient utilization and recycling necessitate a comprehensive understanding of their chemical composition and distribution patterns. This study aims to contribute to the development of data-driven solutions that support the sustainable management and utilization of plastics within a circular economy paradigm. Thus, we investigated the efficacy of combining multivariate curve resolution (MCR) with deep learning (DL) techniques for the analysis of hyperspectral imaging data. The focus is on transitioning from quantitative analysis in biological tissues, which was successfully achieved in our previous research in quantifying chlordecone in mouse liver, to qualitative analysis in plastic samples. In our prior work, MCR was effectively utilized as a quantitative labeling method, producing quantitative labels for hyperspectral image pixels, as depicted in Figure 1, which were then used as samples for training a DL regression model (Golpelichi, 2023). In this research, we adapted our MCR-DL framework to the qualitative analysis of plastic samples to effectively study chemical composition and distribution patterns within these samples using hyperspectral imaging data. Thus, we applied our MCR labeling approach, this time for the qualification of pixels according to the type of plastic or non-plastic material included in the samples. For the next step, we trained convolutional neural networks (CNNs) on pixel-level data using MCR-labeled data, enabling the accurate identification and mapping of chemical compounds in plastic samples. The results obtained reveal that our proposed MCR-DL framework can be applied to different types of hyperspectral imaging data from biological or chemical samples using either qualitative or quantitative approaches.

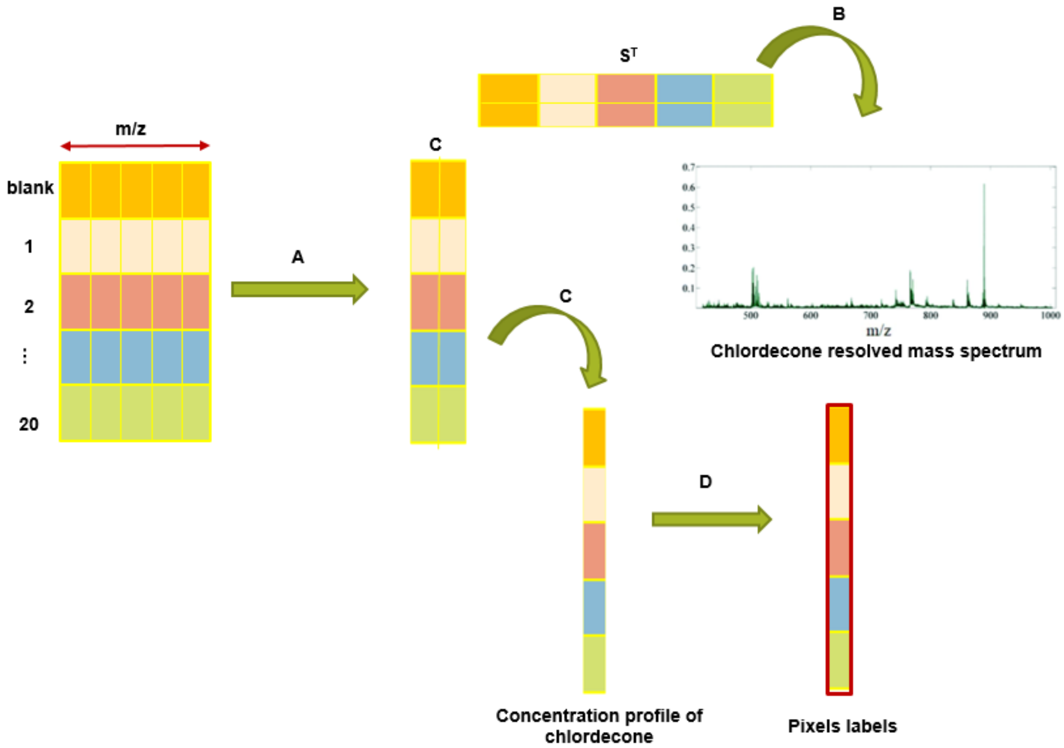

Figure 1. Multivariate pixel labelling procedure. (A) MCR-ALS analysis. (B) Identification of chlordecone resolved mass spectrum. (C) Assigning the concentration profile corresponded to chlordecone. (D) Pixel labelling (Golpelichi 2023).

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A111. Unravelling the secret of chocolate: multivariate analysis of hyperspectral images for spectral discrimination of cocoa content.

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The food and confectionery industry is constantly faced with the challenge of maintaining high quality standards in its products, satisfying the demands of an increasingly demanding and diversified market. In this context, differentiation and quality control become critical aspects to ensure product excellence and consumer loyalty. One of the most emblematic products in this industry is chocolate, whose quality and sensory characteristics depend to a large extent on factors such as cocoa concentration and the presence of additional flavours [1]. However, the diversity of brands and varieties on the market makes it difficult for producers and consumers to discern between high and low quality products.

This work use hyperspectral imaging (HSI) technique in the VIS-NIR region (400-1100 nm) as a technique for evaluating and classifying chocolate samples differing in cocoa content. To fully exploit the potential of HSI for chocolate analyses, the data were evaluated by multivariate analysis of spectra. Principal Component Analysis (PCA) and Partial Least Squares Discriminant Analysis (PLS-DA) were employed as multivariate techniques.

The present project focuses on the evaluation and differentiation of chocolates of three different commercial brands purchased from the Chilean trade characterized by variations in their cocoa concentrations and presence of additional flavors. To preserve the identity of the brands we have designated them as Brand 1,2 and 3 and are shown in Table 1 with the cacao concentration and the flavor respectively.

Table 1: Samples analyzed by hyperspectral camara.

	Brand 1	Brand 2	Brand 3
Sample 1	34% cacao	70% cacao	62%
Sample 2	66% cacao	70% cacao mint flavor	62% cacao mint flavor
Sample 3	71% cacao	82% cacao	72% cacao orange flavor

Preliminary results indicate that the use of hyperspectral cameras combined with PCA allows for differentiation among different chocolate brands. Tablets of chocolate with no visual differences but varying in cocoa content are successfully distinguished, as is showed in Figure 1. The Scores plot shows the separation of samples based on their cocoa content for Brand 1. In the Loadings plot, certain spectral bands are highlighted as significant for each type of sample. These bands are responsible for the observed separations, such as the high correlations for Brand 1 with wavelengths near 787-791 nm, and for Brand 2 with wavelengths near 402-432 nm. Brand 3, on the other hand, exhibits spectral regions between 993-1006 nm with high correlation. Furthermore, this technique enables discrimination among samples with the same cocoa concentration but differing in any additional flavor added during the manufacturing process. Additionally, performing PLS-DA analysis revealed through the confusion matrix that the percentages of correct classification reached 100% in the best models. This demonstrates a tool capable of quickly and non-destructively determining differences in samples.

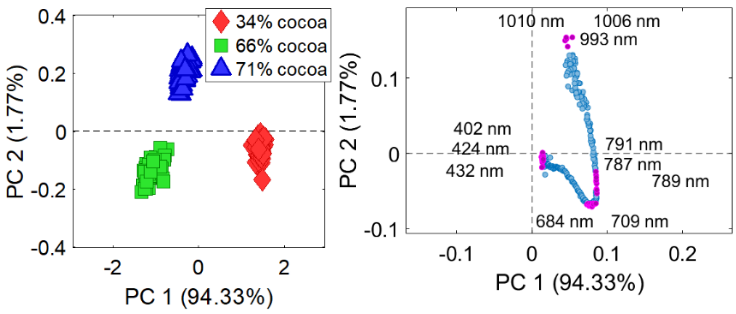

Figure 1. PCA performed on spectra obtained from mark 2 On the left we can see the graph of Score 1 vs Score 2. In the figure on the right we can see the Loadings 1 vs Loadings.

The usefulness and effectiveness of multivariate analysis of hyperspectral images for the discrimination of chocolates of different brands, cocoa concentrations and additional flavors is confirmed. This approach offers a powerful tool for quality control and product differentiation in the chocolate industry. In addition, distinctive spectral patterns have been identified that allow differentiation between chocolates of different brands and sensory characteristics. These patterns provide valuable information on product composition and quality.

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A112. Potential of Hyperspectral Imaging for Differentiating Conventional and Free-Range Chicken Meat of South African origin

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This study investigated the feasibility of using short-wave infrared (SWIR) (930 – 2500 nm) Hyperspectral Imaging (HSI) technology and chemometrics to distinguish between conventional and free-range chicken meat samples obtained in South Africa. In a similar study (Xiong 2015), the fusion of spectral and image texture data yielded excellent classification accuracy (> 90 %) when analysing free-range and non-free-range chicken meat.

To enhance the potential of HSI as an adjunctive measure against food fraud, a comprehensive classification model was developed to simulate real-world complexities. This model encompassed both free-range (FR) and non-free-range (NFR) categories, incorporating retail chicken samples derived from diverse commercial chicken genetics (Aviagen® and Cobb®). These samples were sourced from various producers over a span of two years, providing a broader perspective for analysis.

Images were acquired with a HySpex SWIR-384 hyperspectral imaging camera and analysed using Prediktera Breeze and Evince software (Prediktera AB, Umeå, Sweden). Samples were placed on clean black 160 gsm A5 sheets. A PCA image segmentation model was trained on pixels relating to the black paper background, after which the selection was inverted and shrunk by 1 pixel to obtain sample-only images.

Preprocessing was applied as follows (Jia 2020): Firstly, the first 11 and last 11 wavelength variables were removed to reduce the effect of sensor noise. Secondly, 4th order Savitzky-Golay smoothing was applied. The left and right windows were both set to three to remove as much noise as possible without eliminating the small CH_2 peaks at 1725 nm and 1765 nm. Thirdly, multiplicative effects were reduced by applying Standard Normal Variate (SNV). Lastly, the data was mean-centered.

The dataset (n = 132) was segregated by chicken cut, namely drumsticks, wings and thighs. Each measurement was assigned a class label; either free-range (FR) or non-free-range (NFR). The FR/NFR classification performance of each chicken cut was determined separately and therefore 44 samples were used in each model. 66 % of data was assigned to the training set, and 34 % was assigned to the test set. Three classification algorithms were applied to each group, namely Partial Least Squares - Discriminant Analysis (PLS-DA), Soft Independent Modelling of Class Analogies (SIMCA) and Stochastic Dual Coordinate Ascent (SDCA). In general, using four PLS-DA latent variables yielded a good balance between model complexity and predictive power. The average test set F-scores of both classes are summarised in Table 1.

Table 4 Average test set F-scores for classifying chicken samples as FR or NFR

	Wings	**Thighs**	**Drumsticks**
PLS-DA	79.8 %	53.0 %	95.7 %
SIMCA	90.9 %	80.4 %	67.4 %
SDCA	54.2 %	90.6 %	95.7 %
Average	75.0 %	74.7 %	86.27 %

Given these results, only drumsticks were used for subsequent analyses, in which the methodology was refined, and the sample count and variety (in terms of chicken genetics and producers) increased.
To understand the underlying physicochemical differences between free-range and non-free-range chicken samples, total moisture, protein and lipid contents were determined. Because most of the pixels in the hyperspectral images related to chicken skin, the skin and meat were analysed separately. When using two-tailed heteroscedastic t-tests, significant differences were found between the moisture content of the meat ($p = 0.012$) and the lipid content of the skin ($p = 0.049$) at a 95% confidence interval.

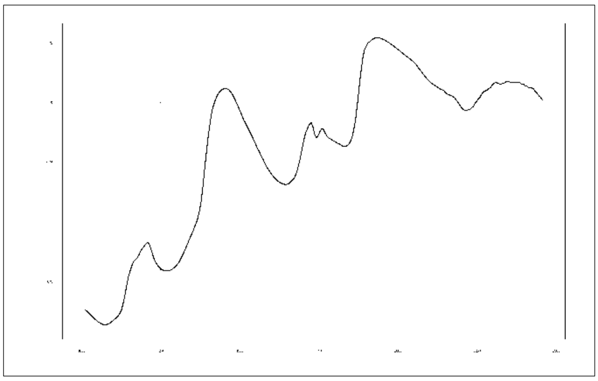

Figure 1 Typical pseudoabsorbance spectrum of chicken

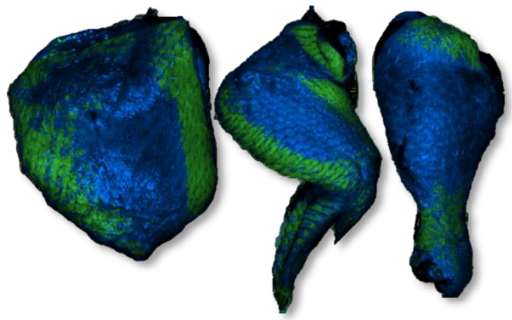

Figure 2 Pixel prediction image of NFR chicken cuts, with FR pixels in green and NFR pixels in blue

Hyperspectral Imaging continues to show great potential for food analysis. So far, this study has shown that in smaller, less diverse datasets, differentiating between free-range and non-free-range chicken cuts with high accuracy (> 90 %) is achievable. However, to prove its ability as an industry-ready measure against food fraud a very large and diverse dataset is required. Performing conventional chemical analyses alongside spectral imaging is recommended for an enhanced understanding of the physicochemical and spectral characteristics of the food product. Spectral imaging is reaching maturity and the abundance of chemometric methods at users' disposal makes increasingly rapid and accurate analyses easier than ever before.

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A114. Advancements in non-destructive detection of avocado damage using hyperspectral imaging technologies

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To ensure the optimal quality of avocados, it is critical to discern the subtle shifts in their composition, which often elude visual detection (Metlenkin 2023). Our study harnesses hyperspectral imaging (HSI) integrated with Principal Component Analysis (PCA) to delineate the intricate spectral profile of 'Hass' avocados across various post-impact intervals. Analysis of PCA score plots within a 400–1000 nm spectral range (Figure 1) revealed distinct spectral signatures indicative of immediate and progressive post-impact alterations, reflecting changes in the fruit's surface attributes. Critical wavelengths identified by PCA loadings emerged as significant indicators of damage, providing a swift, non-invasive technique for ongoing monitoring of the fruit's condition. Additional multivariate analyses are under exploration. These insights underscore the capability of HSI to supplant conventional, invasive methods, heralding a significant leap forward for the avocado sector. Ongoing research is dedicated to enhancing these models, steering us toward more accurate and sustainable quality control measures (Lorente, D 2012).

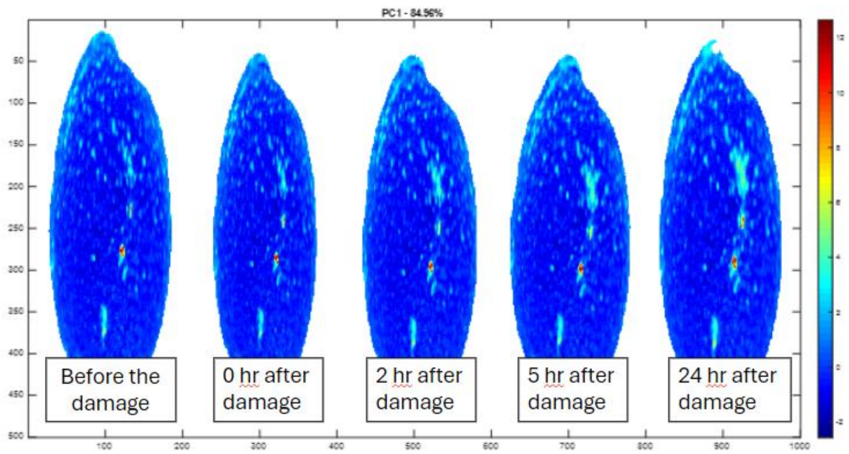

Figure 5 Score plot of and avocado at different times before and after damages.

Acknowledgement

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A118. Comparison of generalized least squares and multivariate curve resolution for detection of microplastics via near infrared hyperspectral imaging

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The lack of standardized analytical techniques for the detection and characterization of microplastics in environmental media is a well-known problem. Near-infrared hyperspectral imaging (NIR-HSI) holds promise for microplastic monitoring due to its speed and less extensive requirements for sample preparation compared to hyperspectral imaging with middle infrared and Raman spectroscopy.

This study aims to compare two chemometric algorithms—generalized least squares (GLS) and multivariate curve resolution-alternating least squares (MCR-ALS)—with respect to their ability to identify and characterize microplastics via NIR-HSI in sand, a heterogenous environmental matrix. Generalized least squares analyzes the entire image using a weighted classical least squares model to take clutter, i.e. non-target signal, present in the image into account (Gallagher et al., 2024). MCR-ALS optimizes data sets based on sensible initial guesses, such as known or expected target spectra, to provide chemically meaningful results given selected constraints (de Juan et al., 2014). Other classification techniques that have been applied to NIR-HSI for microplastic detection, including PLS-DA, SIMCA, support vector machines, and artificial neural networks, have been demonstrated to have shortcomings that lead to over- and underestimates of microplastic abundance (Goyetche et al., 2023).

This research was tackled by collecting NIR-HSI images of sand spiked with microplastics of known size and polymeric identity. The images were collected using a SPECIM SWIR hyperspectral camera (SPECIM, Oulu, Finland) in the spectral range from 1000 – 2500 nm and the chemometric analyses were carried out using MatLab 2022b (MathWorks, Natick, MA, USA) and PLS_Toolbox (Eigenvector Research, Inc., Manson, WA, USA). This comparison of two chemometric techniques furthers our understanding of their applicability to the detection of microplastics via NIR-HSI. In doing so, the promise of NIR-HSI as a valuable addition to the analytical toolbox for microplastic detection and characterization may be realized.

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A120. The story of kiwifruit trauma: seeing beyond the surface with Near Infrared Hyperspectral Imaging

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Kiwifruits can easily suffer damage during picking, harvest handling, transport, or other forms of mechanical stress. This issue is inconsistent with marketing requirements and may result in significant economic and reputational losses (Hou 2012). In this contest, the study aims to assess the feasibility of rapidly detecting occurrence and progression of mechanical damage on kiwifruit by a non-destructive technique: Near Infrared Hyperspectral Imaging (HSI).
A representative sample of kiwifruits from the green cultivar produced in different countries (Spain and Portugal) was collected from local sellers in Bilbao, Spain. The samples were stored at room temperature (25 ± 1 °C). Various types of fruit damage were investigated through impact tests, compression tests, and their combination. Reference techniques were employed to assess destructive parameters such as pH, soluble solid contents, and titratable acidity. Hyperspectral data were acquired using a SWIR camera (Specim, Spectral Imaging Ltd., Oulu, Finland) (**Figure 1a**) at different sampling time after inducing the damage. The acquired spectral data were analyzed using HYPER-Tools 3 software (Mobaraki 2018). Interesting challenges arise from the physico-chemical characteristics of kiwi, including the brown colour of the peel, its opacity, and the high-water content, which may complicate HSI analysis (Liu 2023). Thus, several steps were considered to identify similarities between chemical and physical changes in the fruit images and the progression of mechanical damage. First of all, preprocessing techniques such as derivatives and scattering removal were tested. Then, principal component analysis (PCA) and K-means clustering models were developed. Finally, the relationship between moisture and the reference parameters with time was investigated (**Figure 1b**).
The developed method could aid in preventing damaged fruits from entering the fresh market while facilitating alternative uses such smoothies' preparation.

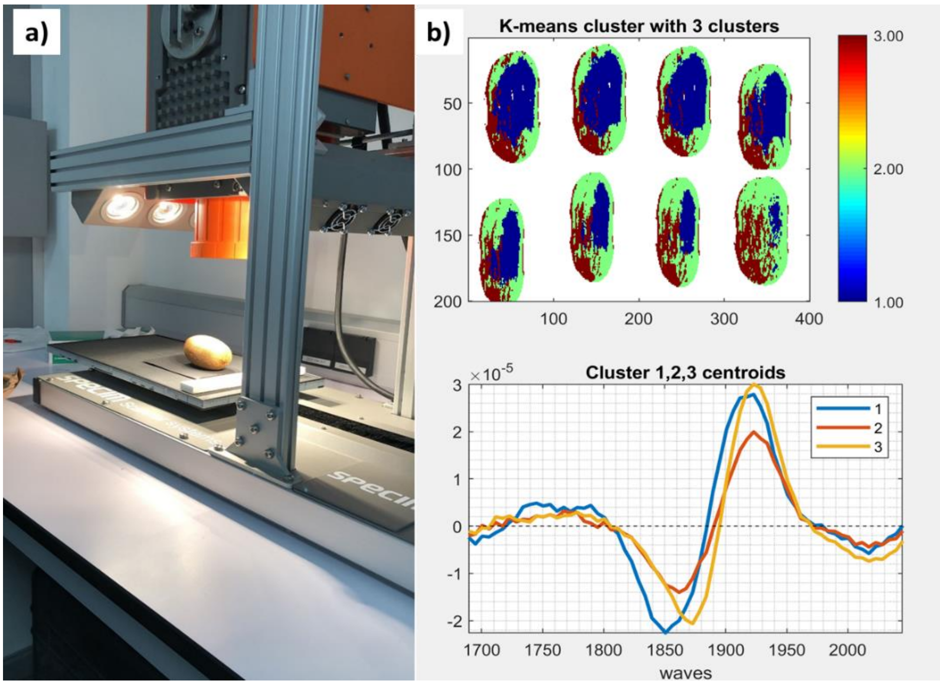

Figure 1. a) Example of the acquisition process. b) Example of results obtained from K-means clustering analysis on a restricted range of wavelengths. Upper: distribution of the clusters. Bottom: centroid of the cluster

Acknowledgement

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A128. Detection of Adulteration in Saffron using NIR-HSI

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Saffron (Crocus Sativus L.), is a time-honored spice with a rich history of medicinal and therapeutic applications in various nations globally. Despite its high market value and growing demand, the cultivation of Saffron is restricted due to its specific agro-climatic growth requirements. This limitation often leads to deceptive practices by merchants to satisfy market needs and gain substantial financial profits. That is why, in the current global trade environment, verifying its quality and its possible adulteration is crucial (Koocheki 2020, Maquet 2021, Kumari 2021).
Near Infrared Hyperspectral Imaging (NIR-HSI), a non-destructive and rapid method, joined with multivariate data analysis strategies (like Principal Component Analysis and Multivariate Curve Resolution) has shown promising results in visualizing the spatial distribution of chemical components, thereby enabling the identification of adulterants(Amigo 2008). The combined use of these techniques has demonstrated a powerful ability to detect and visualize adulteration in Saffron, paving the way for more effective quality control measures in the spice industry (Cruz 2009).
For this purpose, this study explores the efficiency of NIR-HSI coupled with chemometric techniques such as PCA and MCR-ALS for detecting and visualizing adulteration in Saffron.
The results of this study highlights the potential of NIR-HSI as robust tools in the fight against food fraud, ensuring the authenticity and quality of high-value products like Saffron. Future research will focus on refining these techniques and exploring their applicability to other food products.
Keywords: Saffron, Adulteration, Near-Infrared Hyperspectral Imaging, Principal Component Analysis, Multivariate Curve Resolution, Food Fraud, Quality Control, Authenticity.

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A132. Early detection of potato sprouting by near infrared hyperspectral imaging

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The sprouting of potato tubers is an inevitable physiological phenomenon which naturally occurs more or less quickly after their harvest when their vegetative rest has passed. To ensure long-term preservation, the use of cold is not sufficient and anti-germinative treatments are necessary. Early detection of potato sprouting (before the white spot appears) would reduce the use of preventive treatments by optimizing their application. In this study, we show that infrared hyperspectral imaging can be used to early detect potato sprouting.

1. Materials and method

This study was carried out using tubers from 6 different potato varieties (Amandine, Agata, Bintje, Charlotte, Franceline et Lady-Claire). For each variety, 20 tubers were selected. The sprouting evolution of each tuber was followed over time for 6 weeks, with approximately two days of analyses by week. A preparation phase consisted of identifying 81 sprouting eyes which will be followed over time. During all the study, the potatoes were stored in optimal germination conditions, i.e., at high temperature (close to 20°C) and at saturated humidity.
Sample images were acquired using the SPECIM FX17 hyperspectral camera in the infrared range (from 900 to 1700nm). With a spectral and spatial resolution of 3nm and 640 pixels respectively, this camera is based on push-broom technology. A conveyor is used to move the samples under the camera. Each side of the tuber was scanned.
Reference data are visual observations. Each day of analyses, before being scanned with the camera, the presence or not of a white spot is noted for each sprouting eye.

Data processing was carried out with Matlab environment (R2020a, The Mathworks Inc. Natick, MA 01760-2098, USA).
First, reflectance spectra were transformed in absorbance spectra. Then, using spatial and spectral information, the area corresponding to a followed sprouting eye was manually cropped and the mean spectrum calculated. A database of 162 average sprouting eye spectra associated with information on the presence or absence of a white spot and with temporal information was generated.

Using Duplex algorithm, the database was split into 2 sets: 108 spectra to build the classification model and 54 spectra to test it.
A selection of 30 discriminative wavelengths was done using Support Vector Machine Recursive Feature Elimination (SVM-RFE). SVM-RFE classifies the wavelengths from the least discriminating to the most discriminating using criteria derived from the coefficients in SVM models (**Yann 2015**). An SVM model was applied to classify each eye in 2 groups: “the stage to be detected” (the day of analyses before the day when a white spot is visible) and “dormancy” (the days of analyses preceding the stage to be detected and having an interval of at least 3 days of analyses with it) (**Figure 1**).

Day 1	Day 2	Day 3	Day 4	Day 5	Day 6	Day 7	Day 8	Day 9
Dormancy	Dormancy	Dormancy	Dormancy				Stage to be detected	White spot

Figure 1. Example of the groups assigned to a sprouting eye whose white spot appeared on the 9th day of analysis.

2. Results

Model performances were evaluated on the test set. The classification results are shown in the confusion matrix in **Table 1**. They are encouraging, 81.5% of followed spouting eyes are well classified. Eyes which are in the stage to be detected are better predicted than dormant eyes (93% and 70% of good classification respectively). This means that it is more likely that anti-germinative treatments are used too early than too late.

Table 1. Classification results on validation set

		Model	
		Dormancy	Stage to be detected
Reference	Dormancy	19	8
	Stage to be detected	2	25

3. Conclusion

This feasibility study shows the potential of infrared hyperspectral imaging to early detection of potato sprouting. In future work, it would be interesting to verify these performances on other harvest years and in storage conditions closer to real conditions (approximately 8°C and 80% humidity), slowing down the physiological evolution of the tubers.

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A133. Internal quality and colour prediction of blood oranges using NIR hyperspectral imaging

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Blood oranges are increasingly attracting attention due to their vibrant internal and external red colour and the health-enhancing properties attributed to their elevated levels of anthocyanins. However, not all blood oranges exhibit the same internal red colour intensity. Some fruits have dark red flesh, while others appear mostly in a typical orange colour. Most prized blood oranges are those with rich red colour inside, so finding a non-destructive method for distinguishing between oranges with dark and light red interiors would greatly interest the industry. Additionally, the flavour of these fruits is influenced by their sweetness, acidity, and anthocyanin content, making these factors crucial for consumers. Hence, this study aims to predict the internal colour, total soluble solids (TSS), anthocyanins, and titratable acidity (TA) of blood oranges using hyperspectral imaging. 400 'Sanguinelli' blood oranges from the 2023 season and another 400 from 2024 were used in the experiments. Images of each fruit were taken using a pushbroom NIR hyperspectral camera (Headwall NIR R-Series camera, Bolton, Massachusetts, USA) in the spectral range from 900 to 1700 nm, with 5 nm of spectral resolution. A custom high-performance lighting system was built to avoid saturation while providing more light intensity and uniformity throughout the fruit. It comprises a white semicylindrical dome with 18 halogen lamps of 55 W, 12 V (LLB477 Lucas Lighting, Itasca, IL, USA). On each side, nine lamps are distributed from bottom to top, as shown in **Figure 1 left**.

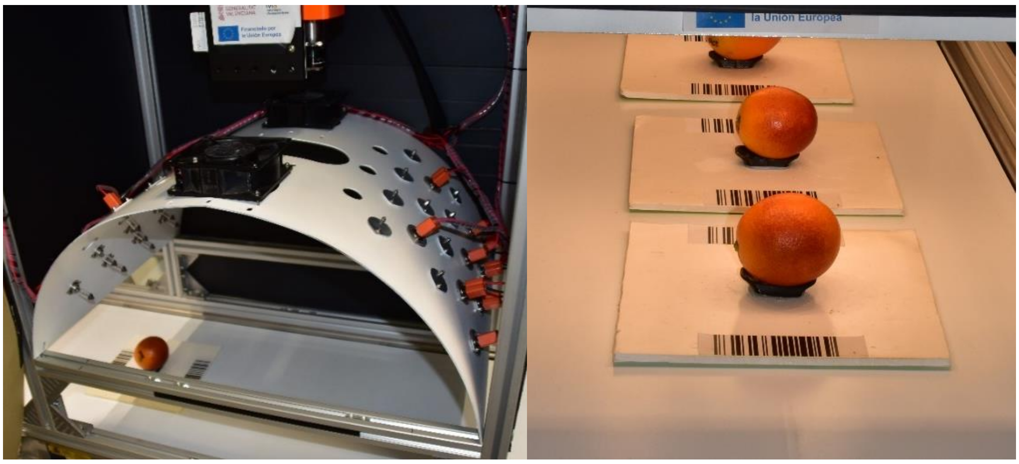

Figure 1. HSI and imaging system (left), and samples being imaged with the imaging system (right)

The average spectrum of each fruit was extracted from the images. Measurements of TSS, anthocyanins, and TA were conducted for each orange, as well as the internal and external colour of the oranges using a colourimeter (D65, 2°) (Konika Minolta CR-400, Chiyoda, Tokio, Japan). Data was divided into a training set (70 %) and an independent test set (30 %). Due to the lack of uniformity in the internal colour of the fruits, two scales were decided: a 3-point hedonic scale consisting of orange, mid-red, and intense red (**Figure 2**) and a 2-point hedonic scale (consisting of orange and red). Later, the data was divided into a training set (70% of the data) and an independent test set. (30%).

Figure 2. Different internal colours of blood oranges

Preliminary results suggest the feasibility of classifying blood oranges based on the intensity of red colour in the pulp, achieving a 57% accuracy for the 3-point hedonic scale using a Support Vector Machine (SVM). However, with the 2-point hedonic scale (light/dark), a 69% accuracy was reached using a machine learning model based on decision trees (Extra Trees Classifier). Additionally, a coefficient of determination (R^2) of 0.57 was obtained to predict TSS using SVM. Lower R^2 values were observed for predictions of TA and anthocyanins, indicating limitations in predicting these parameters. Thus, hyperspectral imaging could separate fruits that do not meet the minimum required internal colouration for consumers who expect dark red blood oranges. However, further studies are needed to determine the depth at which HSI reflectance can provide internal information.

Aknowledgments

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A141. Dynamic spectral contribution for LIBS image synthetic generation

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On the last years, deep learning techniques have revolutionized computer vision and AI giving them the capabilities for complex characterization. In the case of complex tasks, such as quantitative analysis of LIBS (Laser Induced Breakdown Spectroscopy) spectral data, Deep Learning models show better performance compared to other regression methods (Van den Eynde 2023) as they can easily map the non-lineal relationships and external factors (sensor parameters, noise…). As a counterpart, they require large amounts of annotated data requiring high cost or limited availability. One solution to this is the use of synthetic data. Some work has been made by employing the NIST LIBS database (Kramida 2019) to generate additional synthetic spectra theoretically but without reflecting sensor or process characteristics (Finotello 2023). In this work, we propose a novel method for the generation of synthetic spectra based on real data. Initially the proposed method was based on the linear combination of pure element samples to create mixtures as a function of the concentration of each element. It was observed that the contributions of the intensities of each wavelength to the linear combination were not uniform, resulting in a non-optimal representation of the spectral mixtures. For this reason, it was decided to adapt the method by adding a dynamic factor where each wavelength has a different weight depending on the concentration of the elements in the mixture as defined in equation (1).

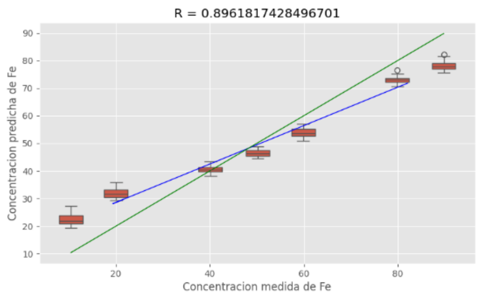
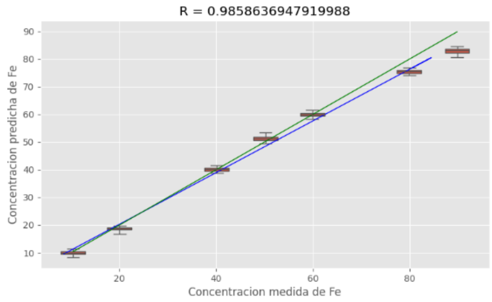
$$y_\lambda = \sum_{n=1}^{N} C_n \cdot \hat{y}_{n_\lambda} \cdot K_{n_\lambda} \qquad (1)$$

Where N is the number of components, C_n, the concentration of component n, $\hat{y}_{n_\lambda}$ is the intensity of the pure spectrum signal of component n at wavelength λ and K_{n_λ} is the dynamic contribution factor of the n component at wavelength λ. K_{n_λ} is calculated as a linear polynomial coefficient that best fit spectral reconstruction with pure and mixture samples with known concentration by minimizing a reconstruction mean squared loss function as defined in (2).

$$argmin\ (loss(y\_true_\lambda, \sum_{n=1}^{N} C_n \cdot \hat{y}_{n_\lambda} \cdot K_{n_\lambda})) \ (2)$$

For the validation of this method, a public dataset of binary mixtures of Fe and Co was used (Vrabel 2023). It was composed of 9 samples of different concentrations and samples of pure Fe and Co. The difference of concentrations in the mixtures is about 10% from one to another. Each sample is composed of 50 spectra between the wavelengths of 243 nm to 410 nm. All Pure Spectra and all spectra with concentrations of 30% Fe - 70% Co and 70% Fe - 30% Co was used for estimating the dynamic factors by applying (2). After that, we generated a set of 10 synthetic spectra with different concentrations by using (1). These samples train a regression model using the partial least squares (PLS) method. The validation was done using the Fe and Co mixture samples that have not been used as reference (Concentration 30% Fe - 70% Co and 70% Fe - 30% Co) and can be observed in Table1 where we compare results of the PLS with only real samples, synthetic samples generated linearly and the proposed method.

Table 1. Results of a PLS model over testing samples

Method	Synthetic images (Linear)	Synthetic images (Proposed)
R	0.90	0.99
MAE	7.63	2.24
Figure		

As it can be seen, the proposed method leaded to a better performance in quantification for the PLS model. In the future, the method will be validated over deep convolutional neural networks regressors to verify the benefit of synthetic sampling on data eager models.

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A155. Non-Destructive Analysis of Hazelnut Oxidation in Different Environment Plastic Packaging Using Near-Infrared Hyperspectral Imaging

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Hazelnuts hold significant social relevance due to their cultural, economic, and nutritional importance across various regions worldwide and, particularly, in the Mediterranean area. Economically, hazelnuts contribute substantially to the agricultural sectors of Mediterranean countries, supporting thousands of jobs from farming to export. Nutritionally, hazelnuts are prized for their high content of healthy fats, proteins, vitamins, and minerals, promoting heart health and reducing risks of chronic diseases. This combination of cultural heritage, economic value, and health benefits make hazelnuts a vital crop. This is why understanding the shelf-life and degradative mechanisms of these fruits and its derivatives is paramount for the development of the hazelnut industry (López 1997).

Oxidative rancidity is a significant determinant of the shelf life and consumer acceptability of hazelnuts, driven by lipid oxidation that affects both nutritional value and sensory properties. Traditional assessment methods for lipid oxidation are chemical and destructive, posing limitations for continuous quality monitoring in the food industry (Pannico 2015). This research aims to advance the non-destructive testing capabilities by utilizing near-infrared (NIR) hyperspectral imaging technology to monitor the oxidation process in hazelnuts stored in plastic bags over a period of two months.

NIR hyperspectral imaging, spanning wavelengths from 1000 to 1700 nm, was employed to obtain spectral data from packaged (in plastic bags) hazelnuts non-destructively at intervals of 2-3 days. Different condition bags, specifically prepared for this study replicating commercial hazelnut bags, were studied. These conditions considered different environments used in packaging: air, nitrogen and vacuum (e.g. **Figure 1**); as oxidative, inert and non-reactive conditions, respectively. In addition, half of the bags were stored in ambient-temperature and exposed to natural light, and the other half in constant 20ºC and dark conditions, to maximize oxidation-process differences. Three bag replicates were imaged and studied for each condition, which contained 12 raw shelled hazelnuts, randomly sampled from the same original batch. Using this strategy the impact of oxidative degradation of the hazelnuts on their organoleptic properties was explored.

Figure 1. Raw hazelnuts packaged in a plastic bag using a vacuum environment.

Results from this study, expanding what other authors have proposed (Pannico 2015; Moscetti 2015), demonstrate that NIR hyperspectral imaging can be effectively used as a non-destructive method to study and potentially predict the oxidation process of in-bag dry-fruits. This technique facilitates proactive interventions in storage and packaging processes, ultimately enhancing product quality and extending shelf life. The integration of hyperspectral imaging into routine quality assurance workflows promises to adapt the nut industry to modern green chemistry principles by providing a rapid, environmentally friendly, and economically viable method for ensuring nut quality.

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A156. Quantifying leaf age and nutrient concentrations in citrus through Vis/NIR hyperspectral imaging

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Overusing fertilisers can strain farmers economically and jeopardise the sustainability of agriculture in the short and long term. Therefore, designing farming systems that minimise input dependence is vital to promote sustainable practices. An effective fertilisation strategy for citrus trees involves closely monitoring the nutritional needs throughout their growth cycle and adapting fertiliser applications accordingly. But, achieving optimal fertilisation requires precise knowledge of the nutritional status of the plants. The analysis of leaves using complex and costly ionic methods has been the norm for assessing nutrient levels, as leaves serve as nutrient reservoirs for developing organs. However, the accuracy of such analyses depends heavily on selecting the appropriate leaves, as reference tables for the nutritional diagnoses of citrus were created for leaves of spring sprouting from 7 to 9 months. An alternative technique for nutritional diagnosis of planta is hyperspectral imaging (HSI), which has shown promise in other crops. Hence, this study aims to explore whether citrus leaves from various vegetative cycles can be distinguished using Vis/NIR hyperspectral imaging and quantifying the concentrations of key nutrients such as nitrogen (N), phosphorus (P), potassium (K), and calcium (Ca).
Hyperspectral images of the leaves were captured every 10 nm in the spectral range of 500 - 980 nm, with a spatial resolution of 1392 x 1040 pixels. This was achieved using two liquid crystal tunable filters. Illumination within a hemispherical dome was provided indirectly by 12 halogen spotlights. Images were corrected with white and dark references. Each hyperspectral image comprised eight leaves. To obtain the mean spectrum of each leaf, a principal component analysis (PCA) was first conducted to generate a PC image emphasising the contrast between the leaves and the background. The PC 1 image was then selected for further processing. It underwent min-max normalisation to scale intensity values within the range of [0, 1] and was then binarised using the Otsu method. Finally, a morphological opening operation was applied to eliminate noisy pixels. Following image acquisition, the leaves were subjected to ionomic analysis through standard destructive methods. N was determined using the Kjeldahl method (Bremner, 2016), while other nutrients were quantified using an inductively coupled plasma optical emission spectrometer (ICP-OES).
ANOVA and Tukey's least significant difference multiple comparison tests were conducted on the reference data obtained from ionomic analysis to identify significant differences between the two vegetative cycles of the leaves. Partial least squares discriminant analysis (PLS-DA) was employed to differentiate between old and young leaves, using the mean spectra as X variables and leaf classes (young and old) as Y variables. PLS regression (PLS-R) was used for nutrient prediction, with mean spectra as X variables and nutrient concentrations as Y variables. Standard normal variate (SNV) was applied to reduce scatter. In total, 880 leaves were included in the analysis, with 66.7 % for training and cross-validation and the remaining 33.3 % for external validation. The ten most crucial wavelengths for predicting each nutrient were determined using weighted regression coefficients (BW) extracted from the PLS-R models with the optimal number of latent variables (LV). The scores were mapped onto the space delineated by the first two principal components (PCs), explaining 92.3% of the total variance (88.0% from PC1 and 4.3% from PC2). Two groups could be mostly separated using the PC1 (Figure 1), corresponding to the age of the leaves. The discrimination between young and old leaves using PLS-DA achieved

a success rate of 99.5 %, which suggests the efficacy of this technique in accurately classifying leaves based on their age.

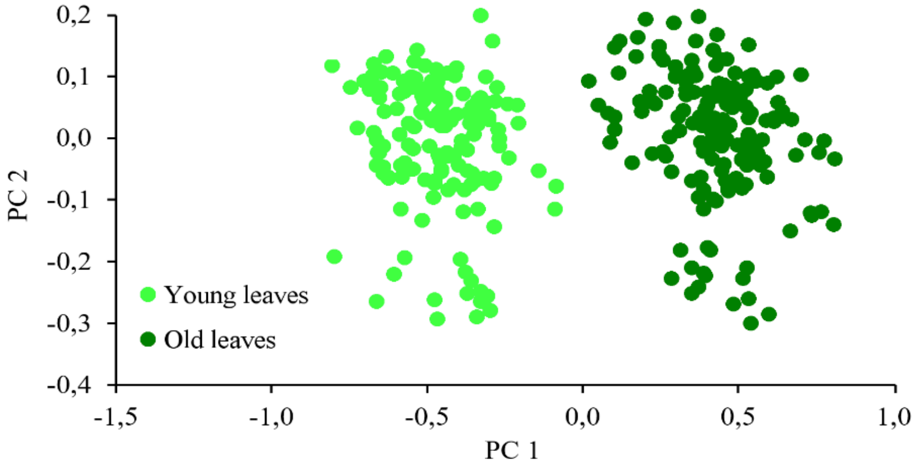

Figure 1. Scores of the first two PCs of PCA.

Table 1 shows the results of predicting the concentration of the studied nutrients in the leaves using all and the ten selected bands.

Table 1. Results of prediction of nutrient using all and selected wavelengths.

Nutrient	LV	CV		Test (full spectrum)		Test (selected bands)	
		R^2	RMSECV	R^2	RMSEP	R^2	RMSEP
N	10	0.56	0.21	0.52	0.23	0.52	0.23
P	5	0.70	0.04	0.61	0.04	0.61	0.04
K	5	0.68	0.35	0.62	0.37	0.62	0.37
Ca	5	0.68	0.81	0.69	0.78	0.69	0.78

LV = latent variable; CV = cross-validation; RMSE: root mean square error in cross-validation (CV) and test (P).

A168. Prediction of Mulberry Fruit Quality at different maturity stages using Visible-Near infrared (VIS-NIR) Hyperspectral Imaging

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Mulberry (*Morus nigra* L.) a popular perishable fruit which is consumed fresh or in processed products, is rich in nutrients and bioactive compounds. This study explores the potential of visible near-infrared (VIS-NIR) hyperspectral imaging for predicting the quality of mulberry fruit at different maturity stages. The Hyperspectral images of freshly picked mulberries were taken from 9 different maturity stages ranging from green to dark purple with a line-scan hyperspectral scanner (Version 1.4, DV srl, Padova, Italy) which consisted of visible near-infrared (Vis-NIR) sensor. The wavelength ranges from 400 to 1000 nm with 1,000 × 2000 pixels/mm of spatial resolution and 5 nm spectral resolution. For excitation a cooled halogen lamp with a stabilized power source was used. A total of 77 samples of mulberry across 9 maturity stages were used for the development of the model of internal quality variables (i.e., total soluble solids (TSS), pH, total acidity (TA), total antioxidant activity (AOX) and firmness). The spectra extracted from images were pre-processed using different methods (i.e., smoothing, mean centering, auto scale, Log (1/T), 1st Derivative, and 2nd derivative) to remove outliers and noise to develop models using Partial Least Square Regression (PLSR). The PLSR models showed promising efficiency in predicting the quality variables with R^2 predictions of 0.88, 0.83, 0.75, and 0.6 for TSS, pH, TA, firmness, and AOX, respectively. The results of this study validated the potential application of VIS-NIR hyperspectral imaging for non-destructive assessment of mulberry quality and its application for optimizing post-harvest handling assuring better quality for fresh mulberry consumption.

Keywords: Hyperspectral Imaging, VIS-NIR, non-destructive, PLS-R, mulberry quality

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