

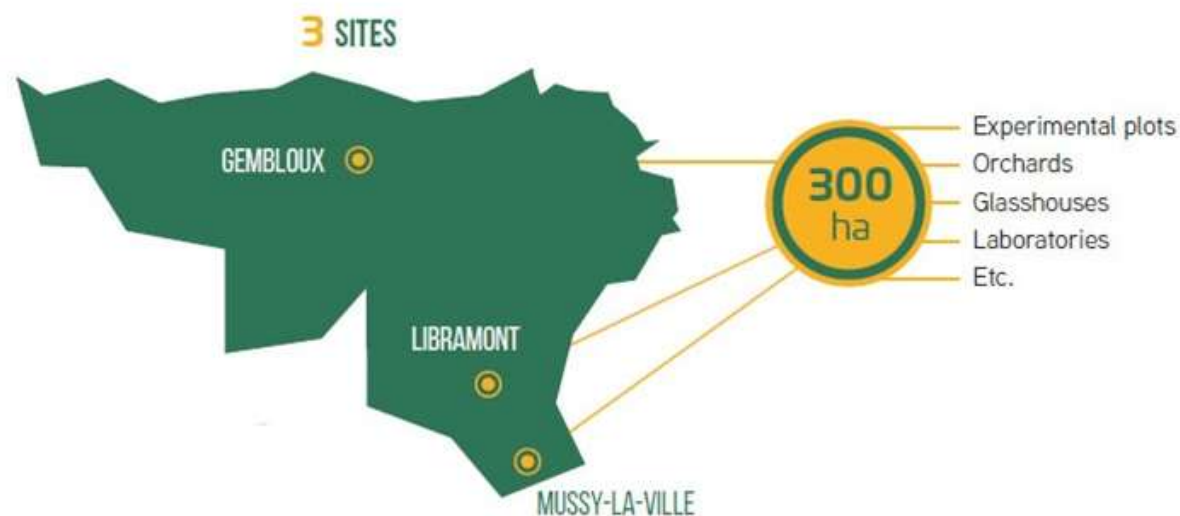


Applications of Vibrational Spectroscopy and Chemometrics in the Agro-Food Sector: Perspective from the Walloon Agricultural Research Center (CRA-W)

Antoine DERYCK, Juan Antonio FERNANDEZ PIERNA, François STEVENS,
Vincent BAETEN

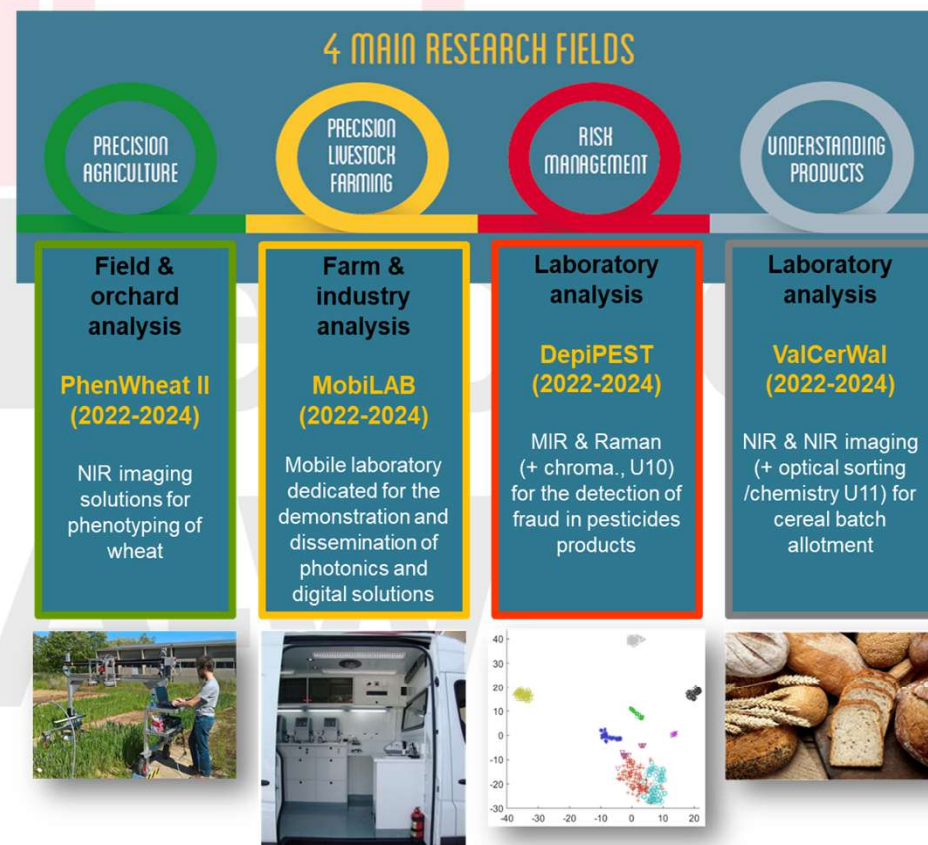
Monells – 22 May 2026





The CRA-W brings together scientific research, service and support functions in support of Walloon farmers, stockbreeders, horticulturists, forestry producers and operators in the agri-food sector

Our 130 research projects primarily aim to reduce synthetic inputs, produce more sustainably from an economic, environmental, and societal perspective, and strengthen the profitability of agricultural production, particularly by improving processing methods



General director

Sophie LEONARD a.i.

Coordination and strategy

Deputy Director general

Jean-Pierre GOFFART

Central Services Department

**Human Resources, Budget and
Finance Office**

Nathalie ROBRECHT

Logistics

Isabelle PIERRARD

Life Sciences Department

Marc LATEUR a.i.

Biological engineering

Frédéric DEBODE

**Biodiversity and plant and forest
improvement**

Marc LATEUR

Crops and forest health

François HENRIET a.i.

**Productions in agriculture
Department**

Viviane PLANCHON a.i.

Crop production

Feriel BEN ABDALLAH a.i.

Animal production

José WAVREILLE

**Agriculture, territory and
technologies integration**

Viviane PLANCHON

**Sustainability, systems and
prospectives Department**

Didier STILMANT

**Soil, water and integrated
production**

Bruno HUYGHEBAERT

Agricultural systems

Didier STILMANT a.i.

Agriculture and sustainability

Eric FROIDMONT

**Knowledge and valorization of
agricultural products Department**

Gilbert BERBEN

**Protection, control products and
residues**

Olivier PIGEON

**Valorization of agricultural
products, biomass and wood**

Jérôme DELCARTE a.i.

**Quality and authentication of
agricultural products**

Vincent BAETEN

Quality and authentication of agricultural products Unit

Implementing and validating various operations with a view to being a dynamic, innovative and sustainable research player committed to the quality and authentication of agricultural and agri-food products. The unit also seeks to boost the Walloon agri-food sectors by improving the quality, traceability and typicality of their products, focusing in particular on products from the short distribution and organic sectors.



Objectives

Developing and applying knowledge, analytical methods and innovative tools to ensure product quality and authentication.



Developing **knowledge** in the field of agri-food product quality and authentication



Ensuring a **technological and analytical watch** in the field of molecular biology, chemometrics, bioinformatics, imaging, database management, microbiology, microscopy and vibrational spectroscopy.



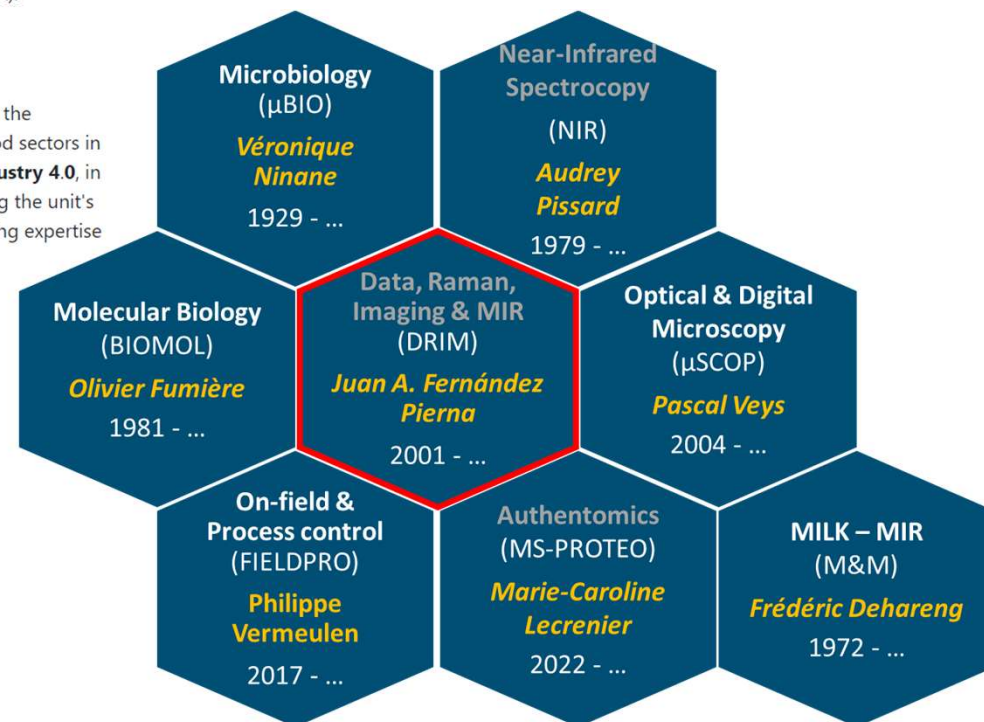
Developing **innovative, rapid and sustainable analytical methods**.



Participating in the **European Research Area (ERA)**.



Lending support to the agricultural and food sectors in the **roll-out of Industry 4.0**, in particular by sharing the unit's sensor and modelling expertise



Head of Unit: Dr Vincent Baeten

Scientific Director Unit QAP

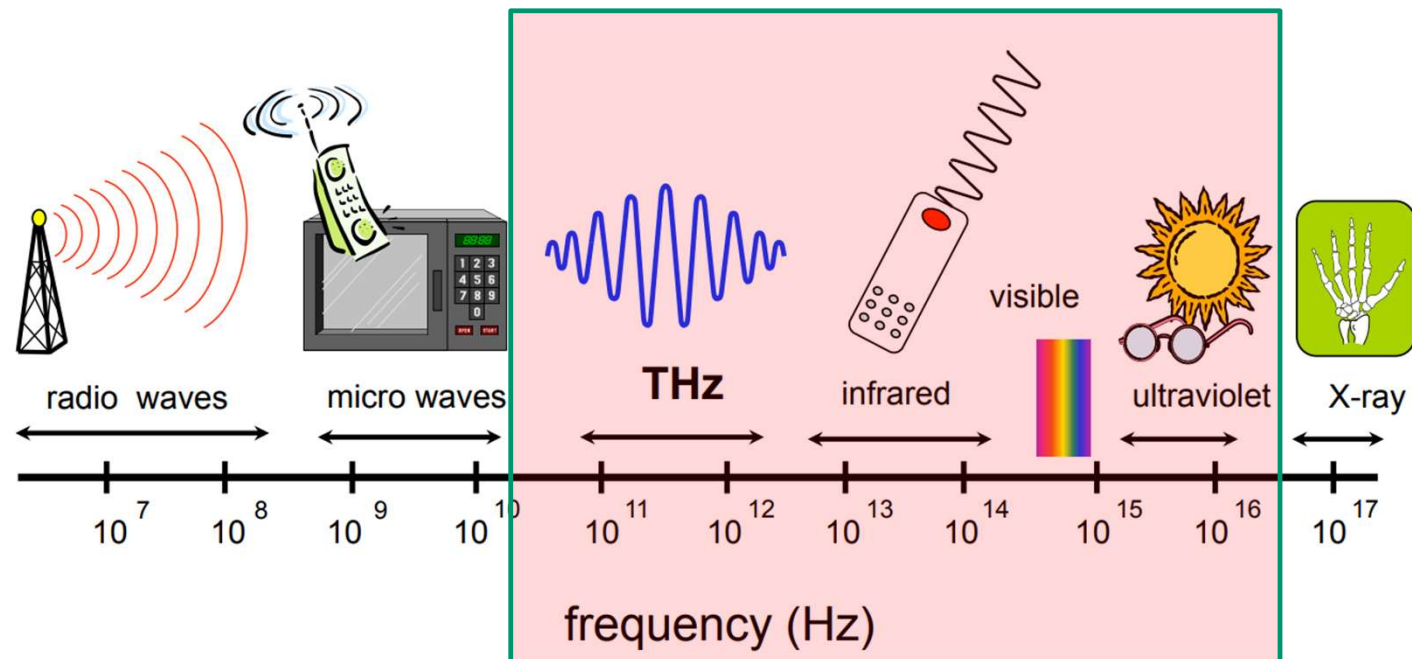


v.baeten@cra.wallonie.be

Vibrational Spectroscopy

Waves at our service...

electromagnetic spectrum of light



Source : R. Gente, N. Born, A. Rehn, M. Koch
CROP.SENSE.net Symposium, Bonn, 29.9.1014.

Vibrational Spectroscopy At the CRA-W

Vibrational Spectroscopy

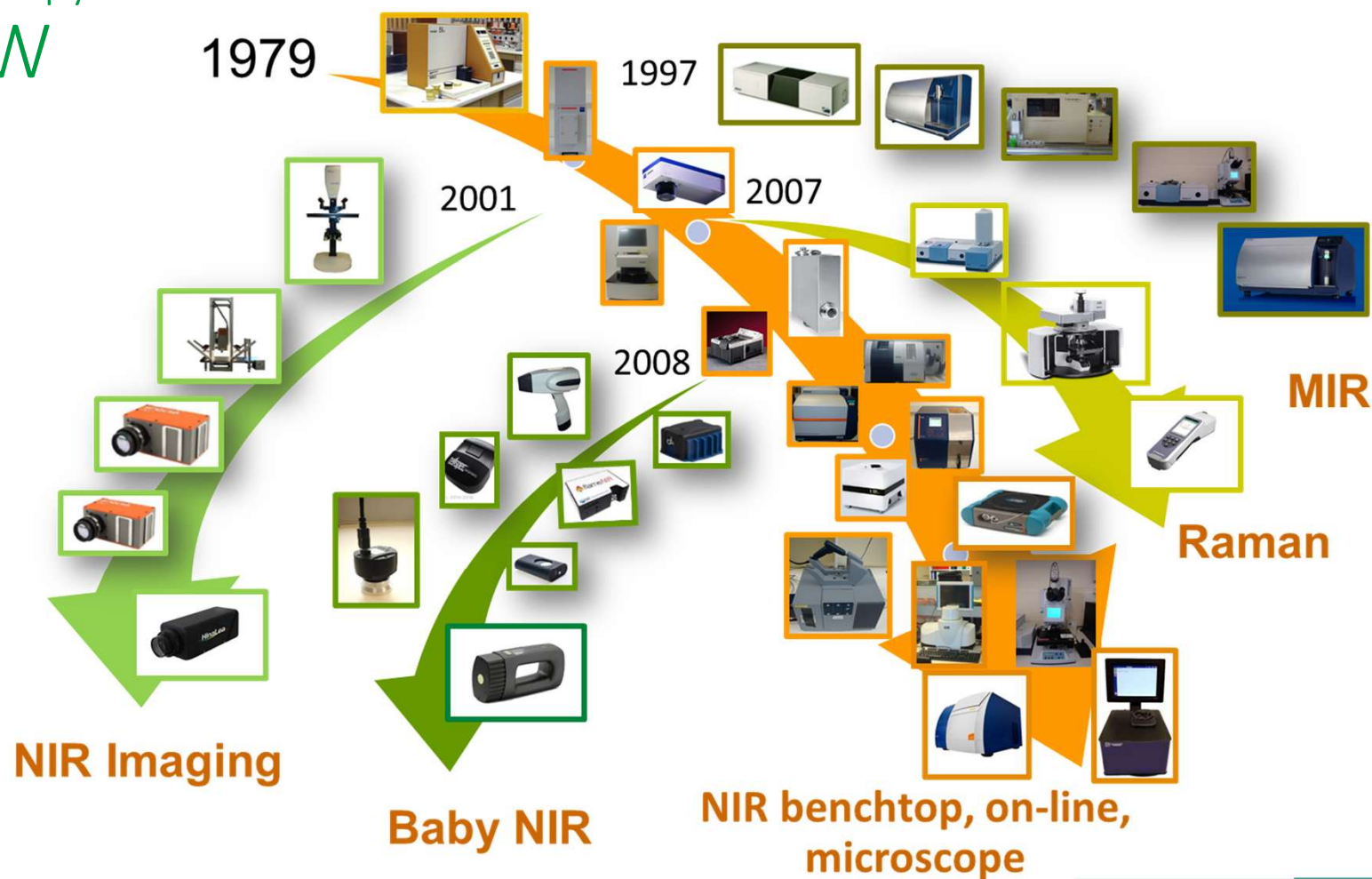
- No or limited sample prep (drying, grinding, ...)
- No additional reagents necessary
- Fast measurement even on moving sample (conveyor belt, ..)
- Non-invasive (do not alter the sample)
- Simultaneous determination of different constituents

Fast

Easy

Cost-efficient

Eco-friendly



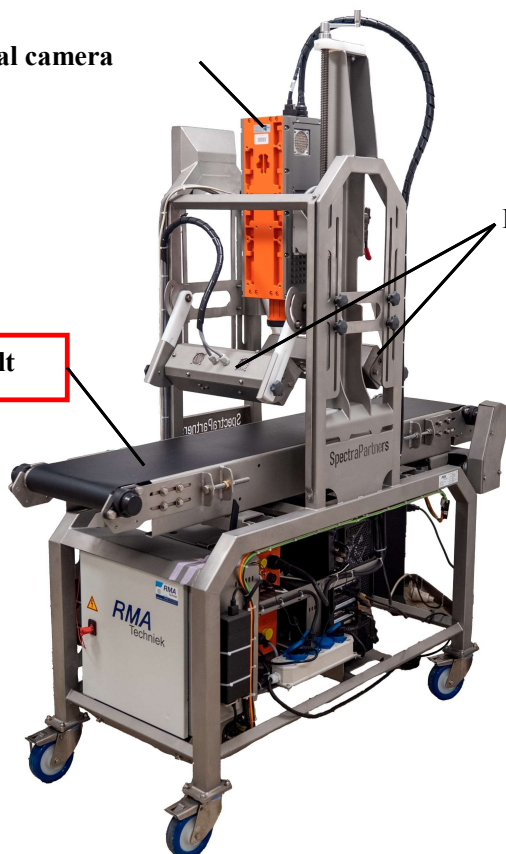
Vibrational Spectroscopy At the CRA-W

From the lab...

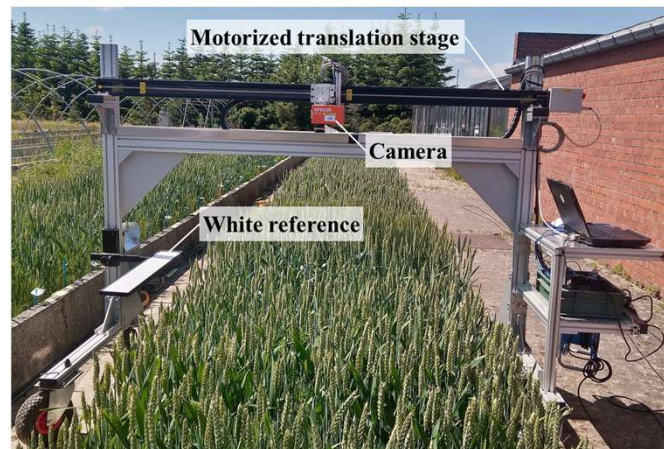
Hyperspectral camera

Conveyor belt

Halogen lamps



... To the field

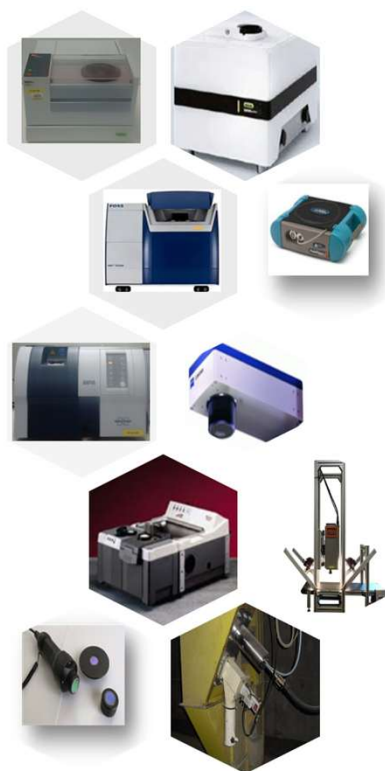


Source: Y. Curnel, CRA-W



recherche
CRA-W

Vibrational Spectroscopy At the CRA-W



- Different instrument generations
- Different brands
- Different sample presentation accessories
- Different technologies
- Bench top *versus* on-line
- Bench top *versus* hand-held

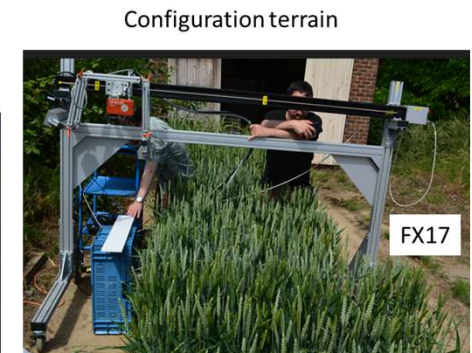
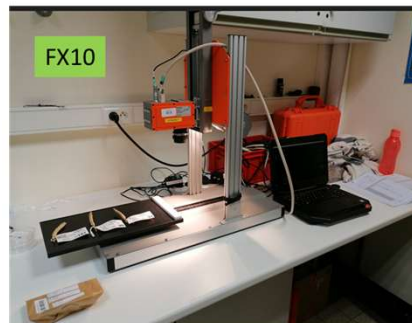
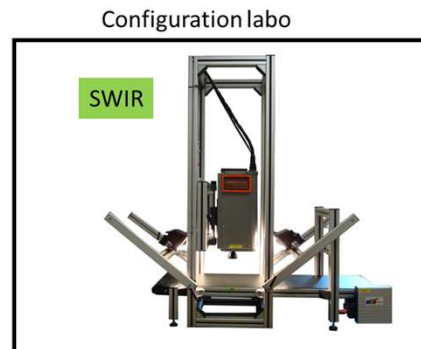
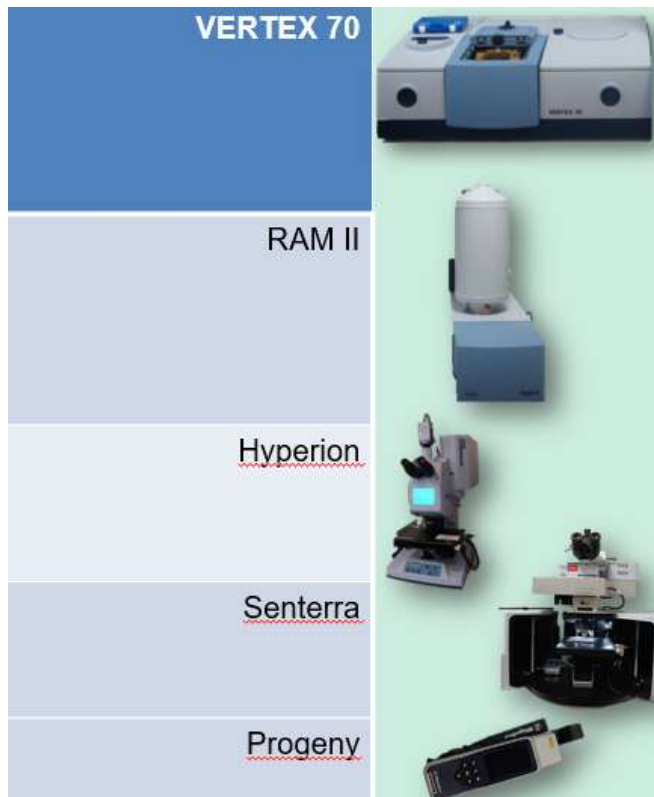
Challenges !



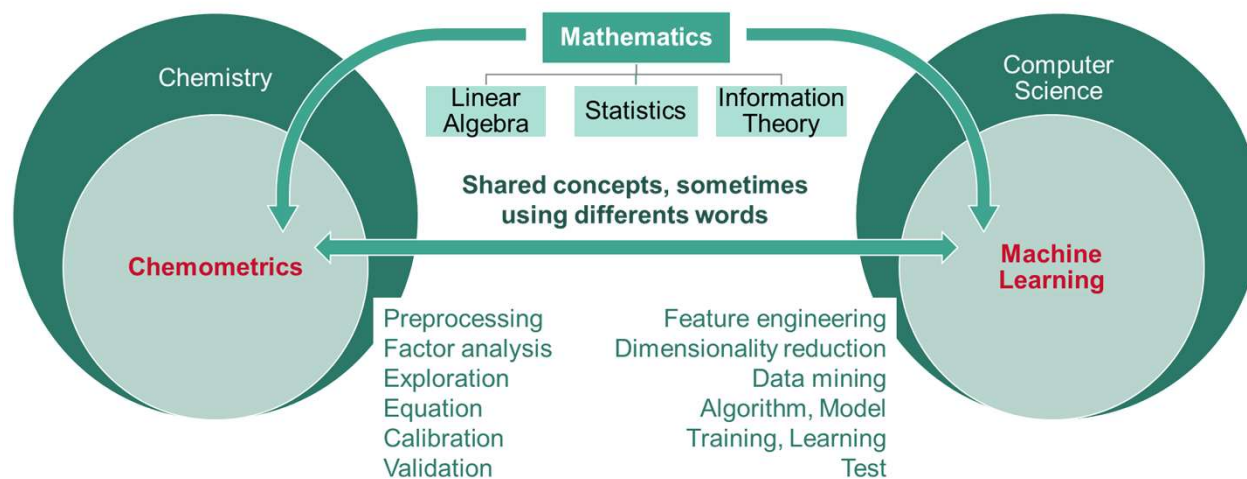
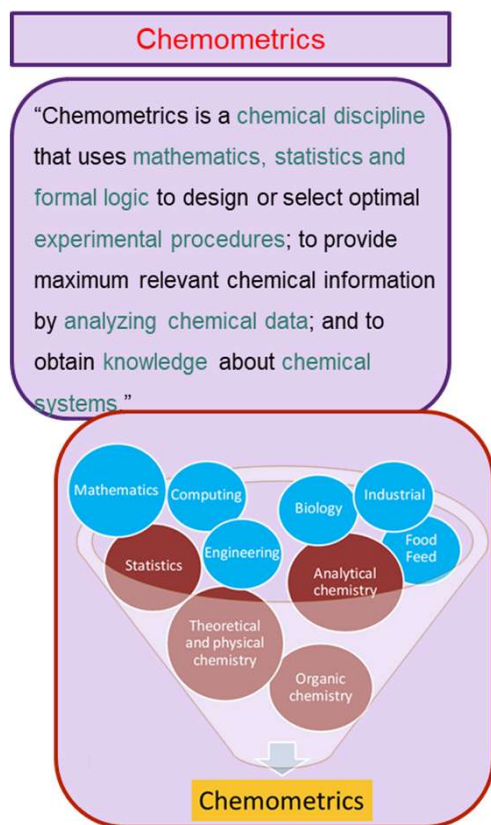
Quentin Arnould / Delphine Delhotte / Antoine Deryck /
Juan Antonio Fernández
Maxime Joissains / Nicaise Kayoka / François Stevens

DRIM team

Techniques – Raman, Imaging & MIR

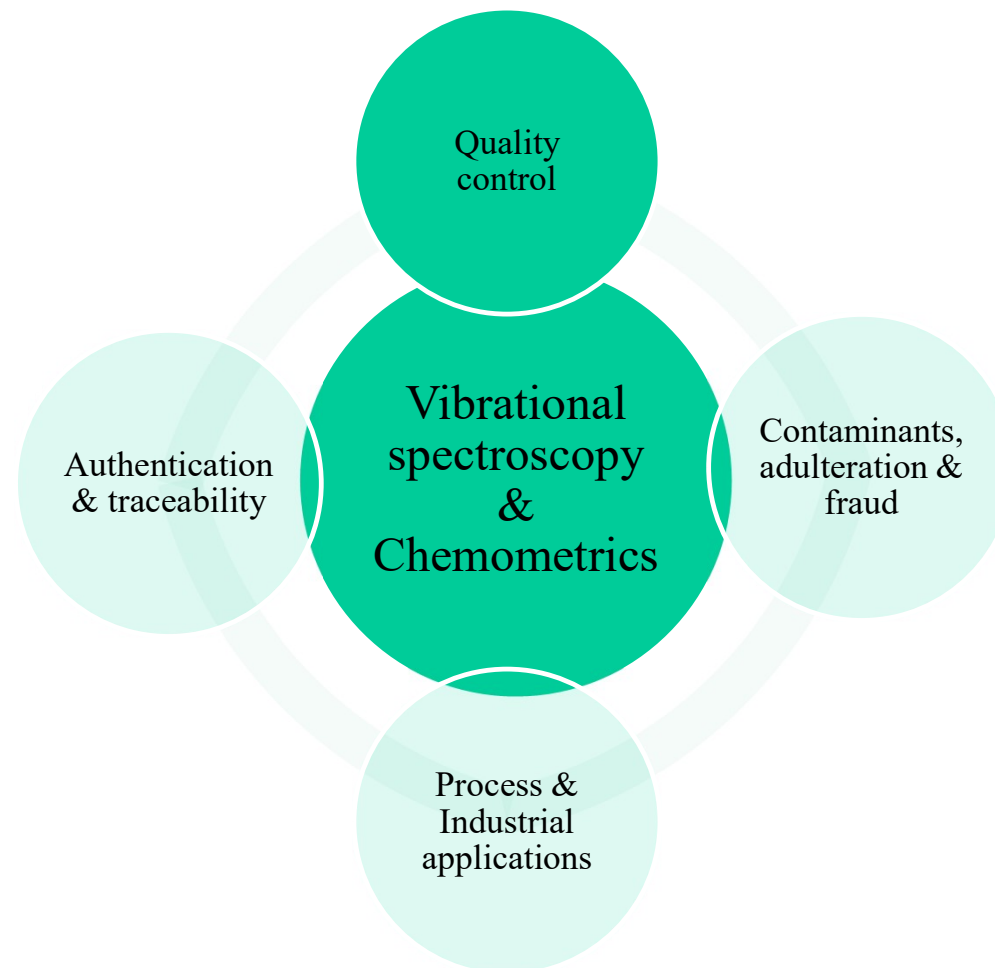


Data Sciences – Chemometrics, Machine Learning

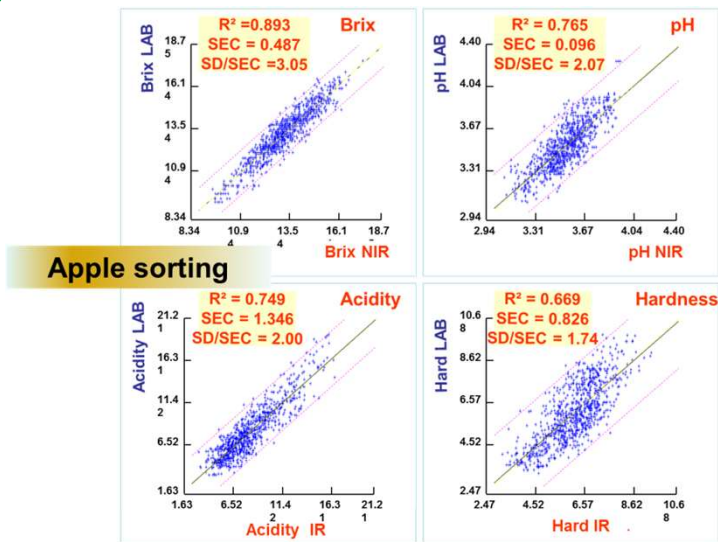


Source: Massart, D.L., et al. (1997) *Data Handling in Science and Technology 20A: Handbook of Chemometrics and Qualimetrics Part A*, p1

Why Chemometric approaches / machine learning /
multivariate analysis / ... ?



Quality control Fruits

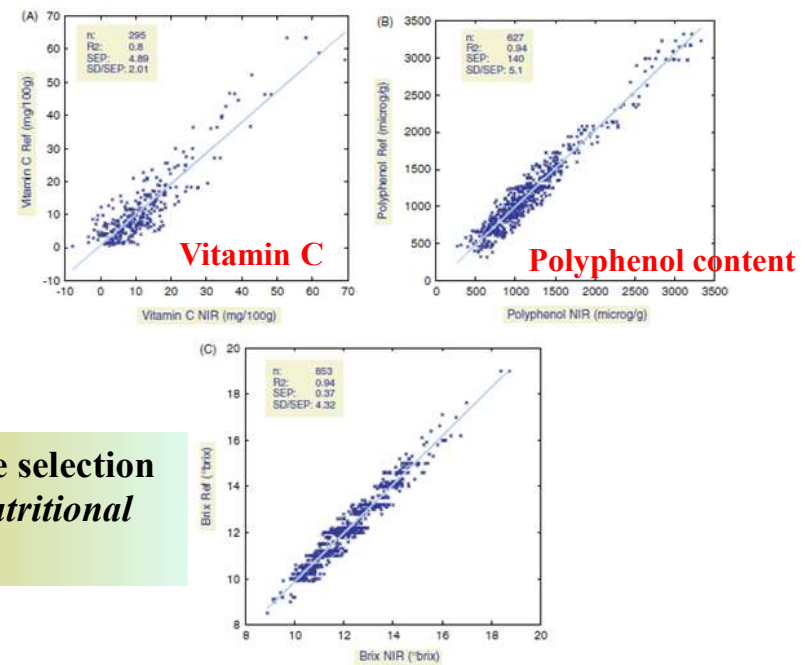


**Measurement of key parameters for the selection
of our fruits of tomorrow based on *Nutritional
criteria***

► J Sci Food Agric. 2013 Jan;93(2):238-44. doi: 10.1002/jsfa.5779. Epub 2012 Jul 2.

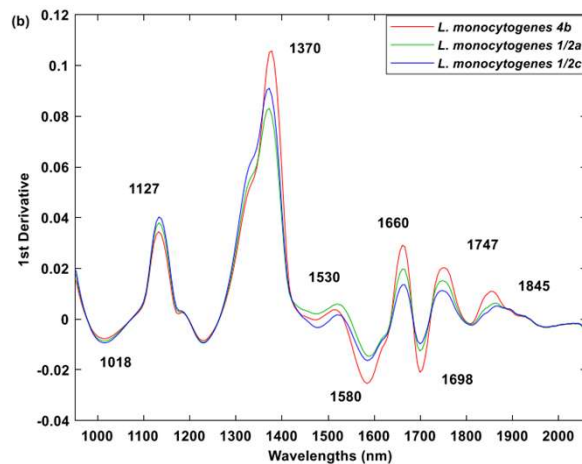
Non-destructive measurement of vitamin C, total polyphenol and sugar content in apples using near-infrared spectroscopy

Audrey Pissard ¹, Juan A Fernández Pierna, Vincent Baeten, Georges Sinnaeve, Georges Lognay, Anne Mouteau, Pascal Dupont, Alain Rondia, Marc Lateur



Quality control Meat products

Differentiation of *Listeria monocytogenes* on beef



Stellenbosch
UNIVERSITY
IYUNIVESITHI
UNIVERSITEIT



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Molecular and Biomolecular Spectroscopy
journal homepage: www.journals.elsevier.com/spectrochimica-acta-part-a-molecular-and-biomolecular-spectroscopy



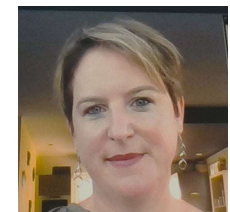
Differentiation of *Listeria monocytogenes* serotypes using near infrared hyperspectral imaging

Rumbidzai T. Matenda^a, Diane Rip^a, Juan A. Fernández Pierna^b, Vincent Baeten^b, Paul J. Williams^{a,*}

^a Department of Food Science, Stellenbosch University, Private Bag X1, Matieland, Stellenbosch 7602, South Africa
^b Quality and authentication of products Unit, Knowledge and valorization of agricultural products Department, Walloon Agricultural Research Centre (CRA-W), Chaussée de Namur, 24, 5030 Gembloux, Belgium



NAME-SA: Chemometric analysis of multi-instrument spectroscopic data for rapid meat quality assessment



fnrs
LA LIBERTÉ DE CHERCHER

LIÈGE université
Gembloux
Agro-Bio Tech

Stellenbosch
UNIVERSITY
IYUNIVESITHI
UNIVERSITEIT

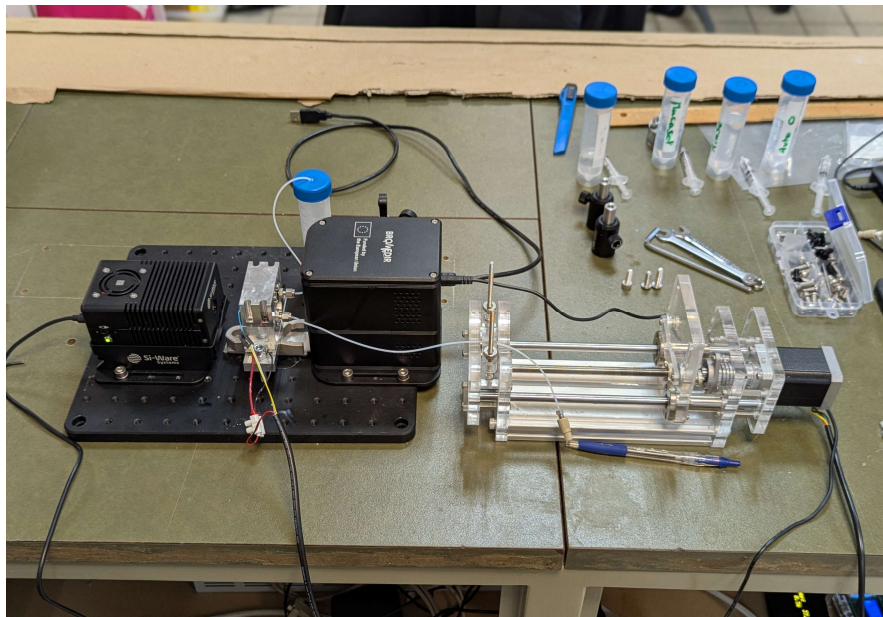
UCLouvain

AGRO
LOUVAIN

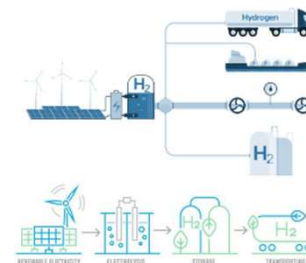
Wallonie
recherche
CRA-W

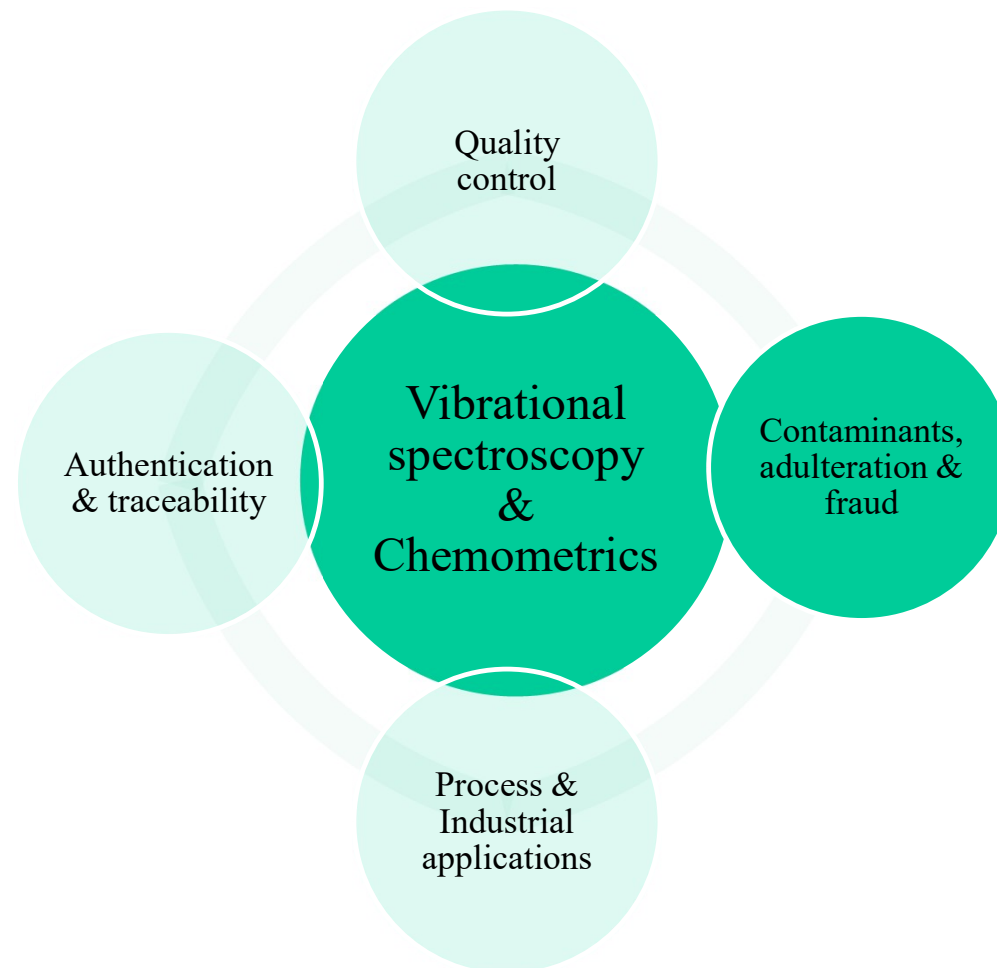
Quality control BROMEDIR

Goal: Achieve new generation of miniaturized MEMS-FTIR spectrometer for detection of larger pool of chemicals & biochemicals.



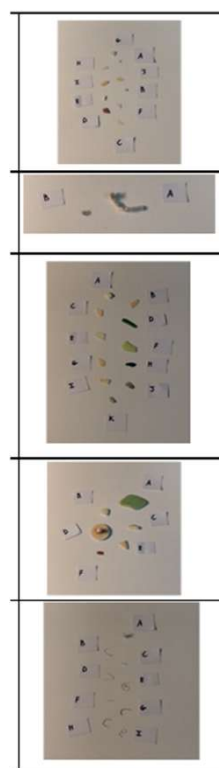
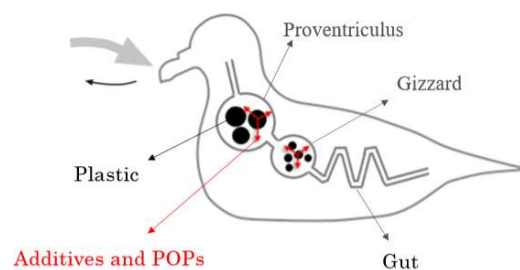
Sustainable farming
Fuel Quality
Hydrogen quality





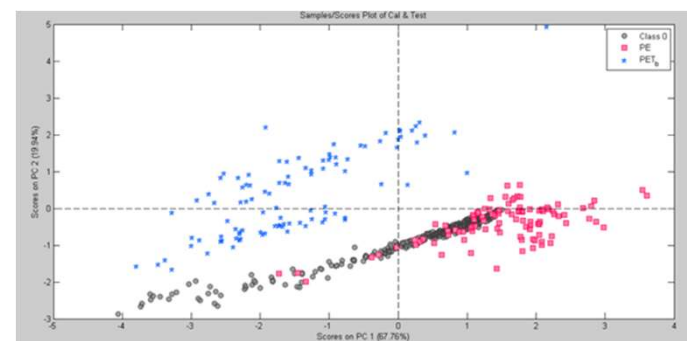
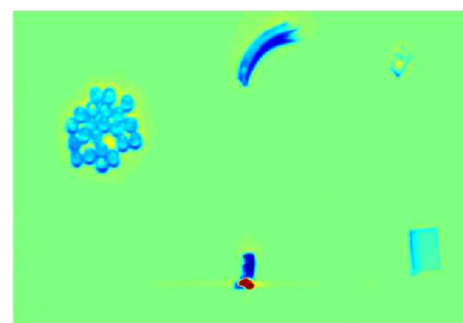
Contaminants, adulteration & fraud

Plastics and POPs



ANALYSIS OF PLASTICS EXPOSED TO SEABIRD STOMACH CONDITIONS, USING MID-INFRARED SPECTROSCOPY

Plastics are usually accompanied by additives and persistent organic pollutants (POPs).



UCLouvain

AGRO LOUVAIN

Faculté des bioingénieurs

Analysis of plastics exposed to seabird stomach conditions, using Raman, mid- and near-infrared spectroscopy

Auteur : Arthur Dubois
Promoteurs : Prof. Dr. Ir. Cathy Delbecq, Dr. Ir. Vincent Baeten
Lecteurs : Prof. Dr. Kristina Dierckx, Prof. Dr. Jean-François Rees
Encadrants : Liesbeth Van Hazel, Dr. Juan Antonio Fernández Pierra
Année académique 2023-2024
Mémoire de fin d'études présenté en vue de l'obtention du diplôme de Bioingénieur - Chimie et bio-industries

UCLouvain

AGRO LOUVAIN

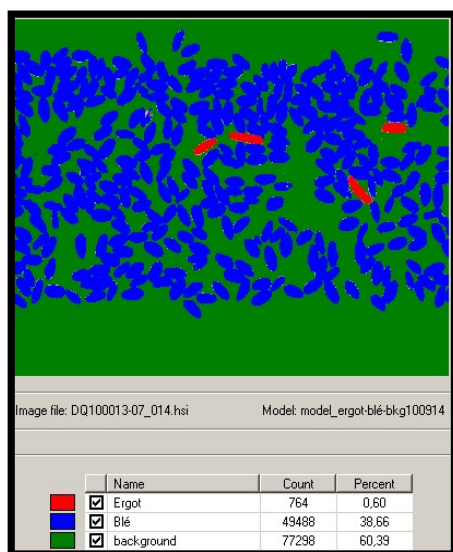
Faculté des bioingénieurs

Identification of plastics from seabird stomachs using infrared spectroscopy, and their potential link with endocrine disruption

Auteur : Albert Moenne
Promoteurs : Prof. Dr. Ir. Cathy Delbecq, Dr. Ir. Vincent Baeten
Lecteurs : Prof. Dr. Ir. Christine Dupont, Prof. Dr. Jean-François Rees
Encadrants : Dr. Liesbeth Van Hazel, Dr. Juan Antonio Fernández Pierra
Année académique 2023-2024
Mémoire de fin d'études présenté en vue de l'obtention du diplôme de Bioingénieur - Sciences agronomiques

Contaminants, adulteration & fraud

Ergot



On-line ergot detection

➤ **Fast → 30-40 kg / hour**
(Ref method = several days)

➤ **LOD <<< 500 ppm**

Contaminants, adulteration & fraud

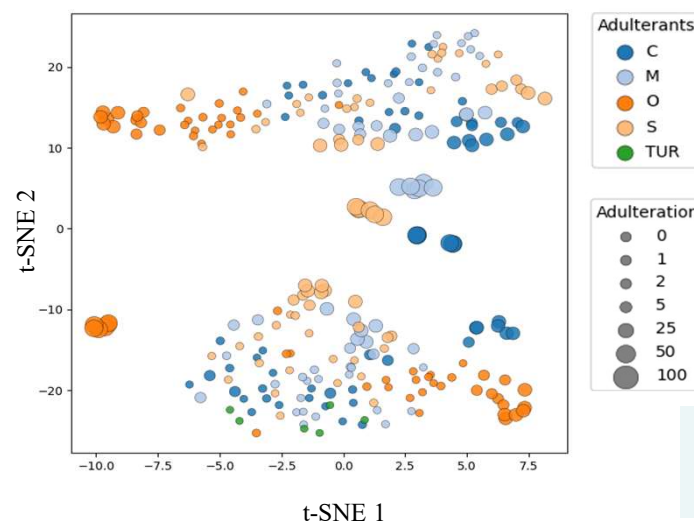
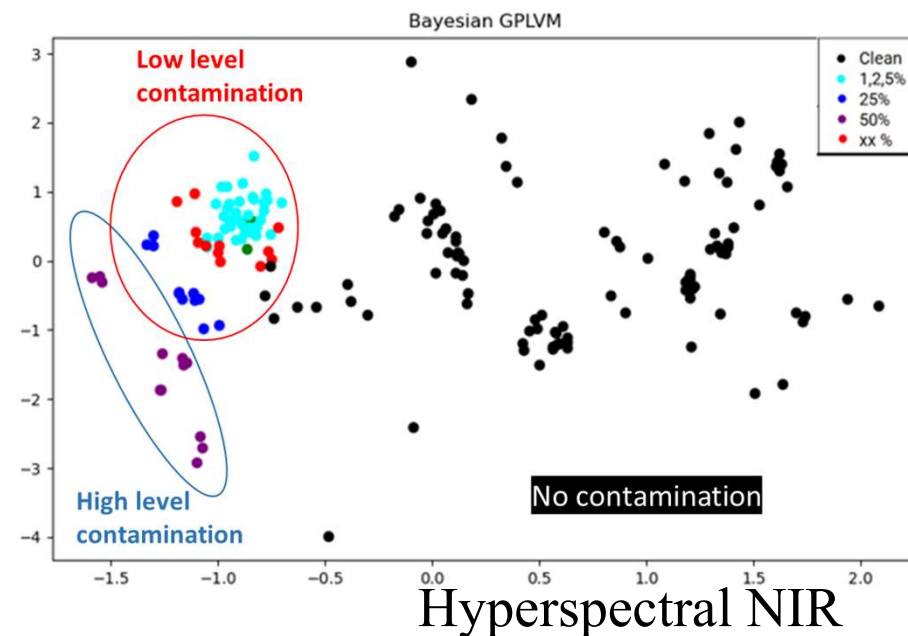
Spices - oregano adulteration



- **2 origins: Turkey and Italy**
- **4 adulterants: cistus, olive leaves, myrtle & sumac**
- **Mixed at: 1, 2, 5, 25 & 50% level**



Nicaise Kayoka



Contaminants, adulteration & fraud Spices - pepper

Poivres moulus : on vous vend de la m...

On n'est pas des pigeons !

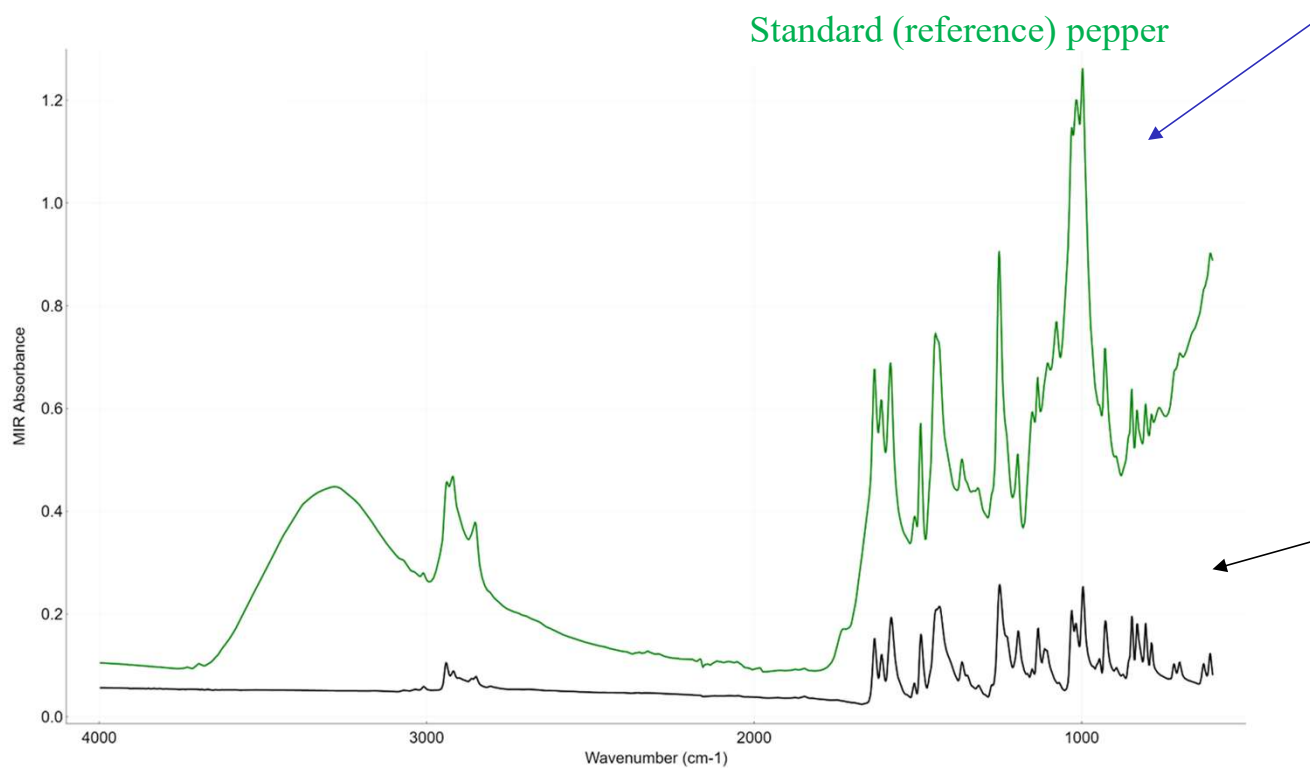
6 min | Publié le 17/11/23 | Disponible jusqu'au 16/11/2024



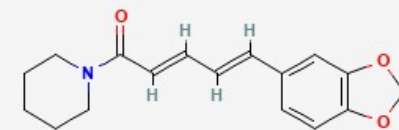
Pepper powder fraud / adulteration

Contaminants, adulteration & fraud

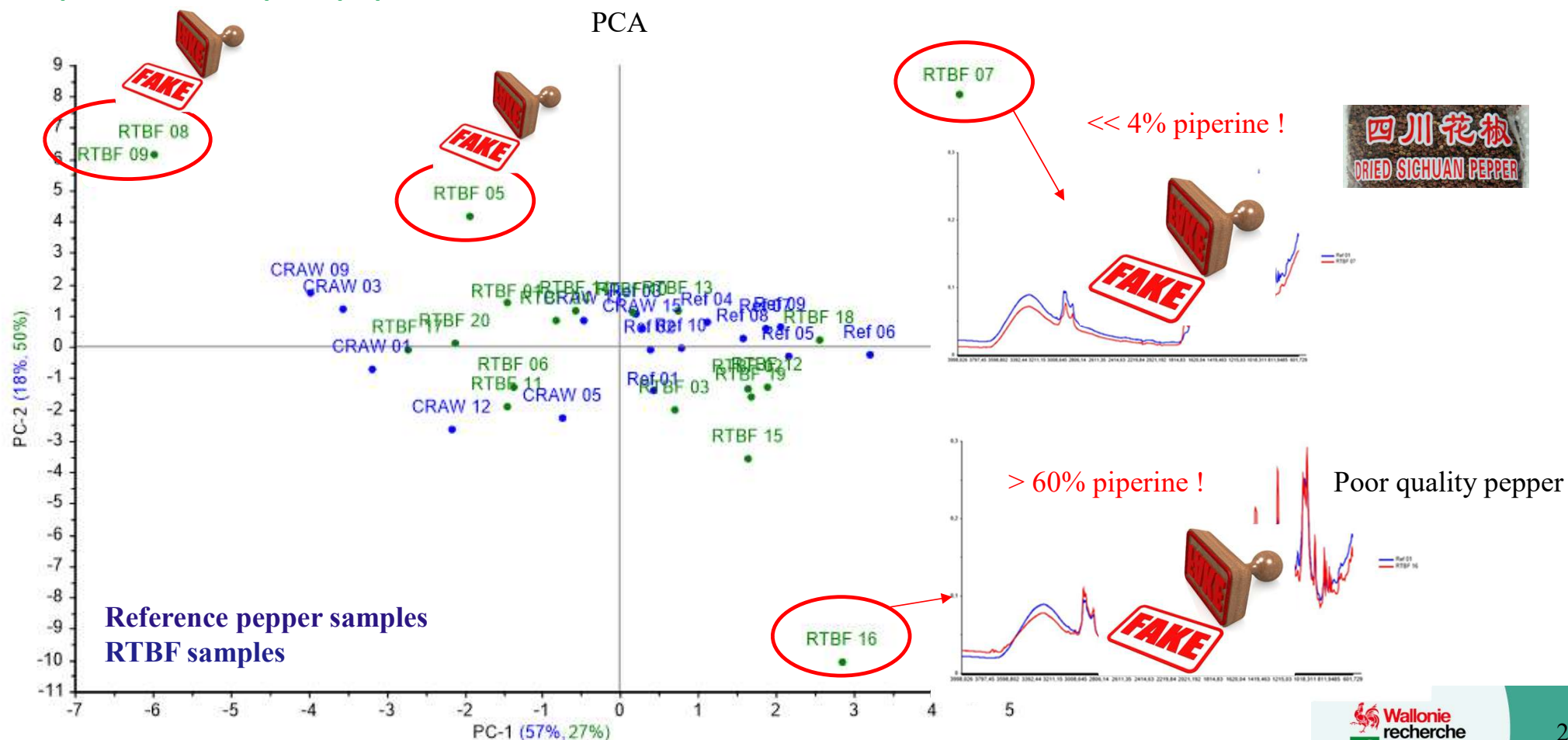
Spices - pepper



Piperine C₁₇H₁₉NO₃



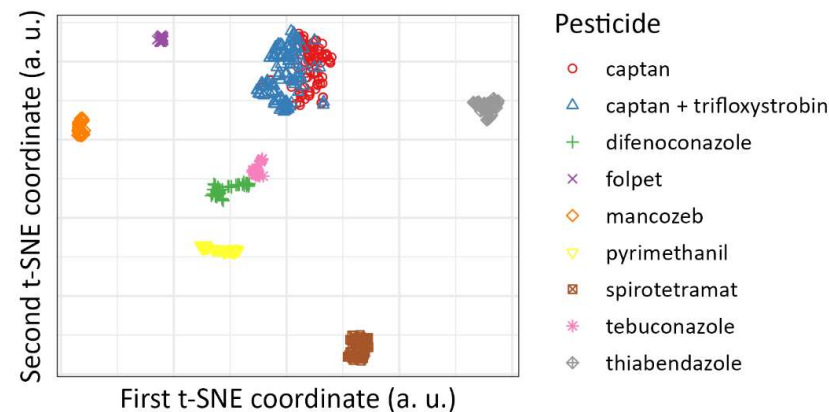
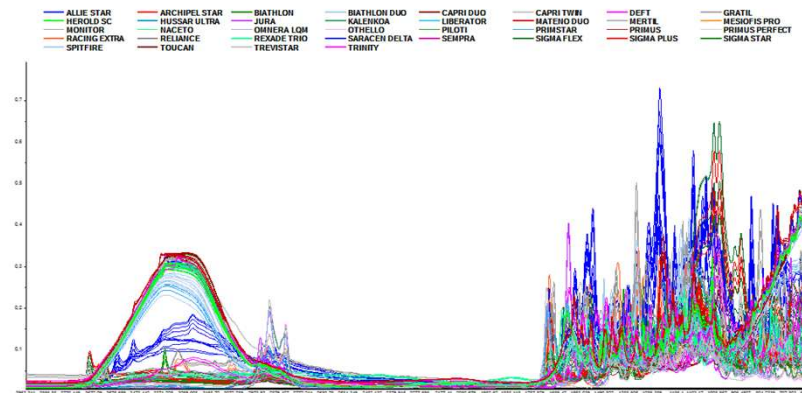
Contaminants, adulteration & fraud Spices - pepper



Some of our current projects

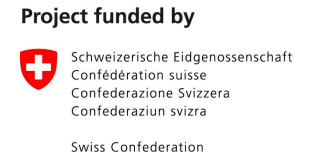
DEPIPEST

Goal: Innovative screening methodology by vibrational spectroscopy (MIR) and confirmation by chromatographic methods (GC, LC, MS) of counterfeit pesticide formulations

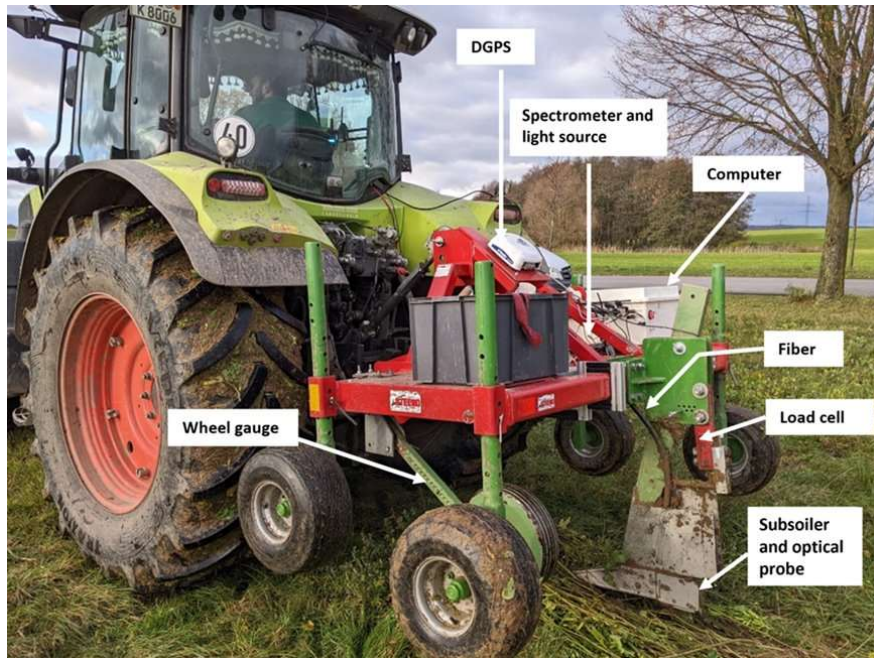


Some of our current projects

WHEATWATCHER

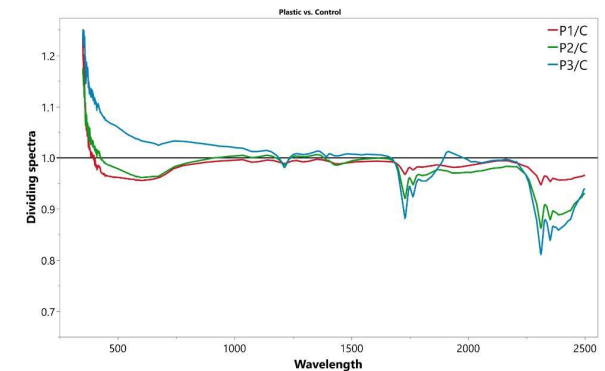


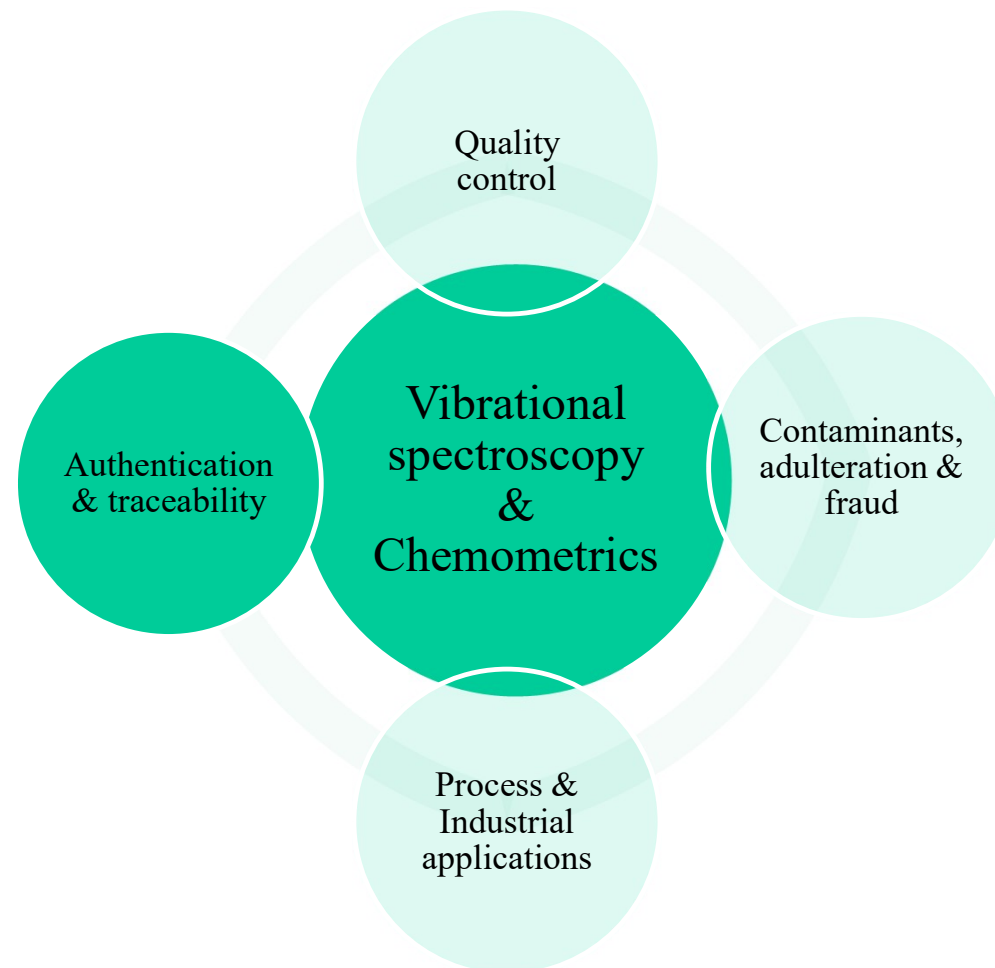
Goal: To implement an integrated digital system for monitoring soil and wheat health to improve sustainable agriculture.



Soil contaminants:

- Hydrocarbons
- Heavy metals
- Salinity
- NPK
- (Microplastics)





Authentication & Traceability Flax disease



Control plant

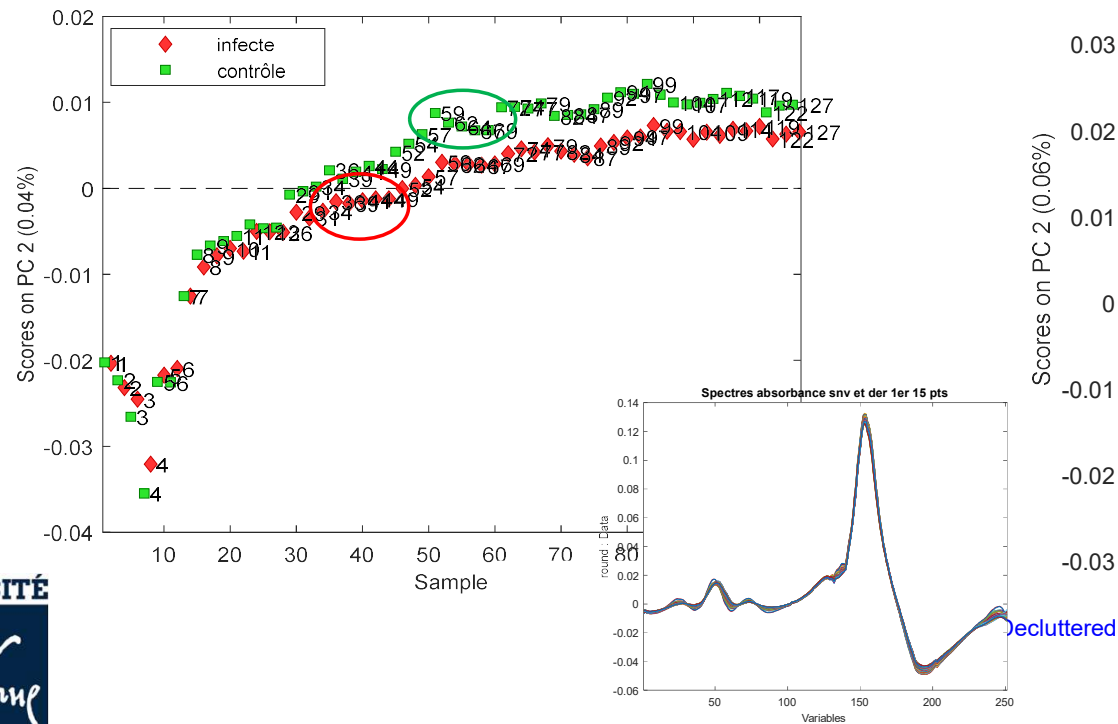
Inoculated plant



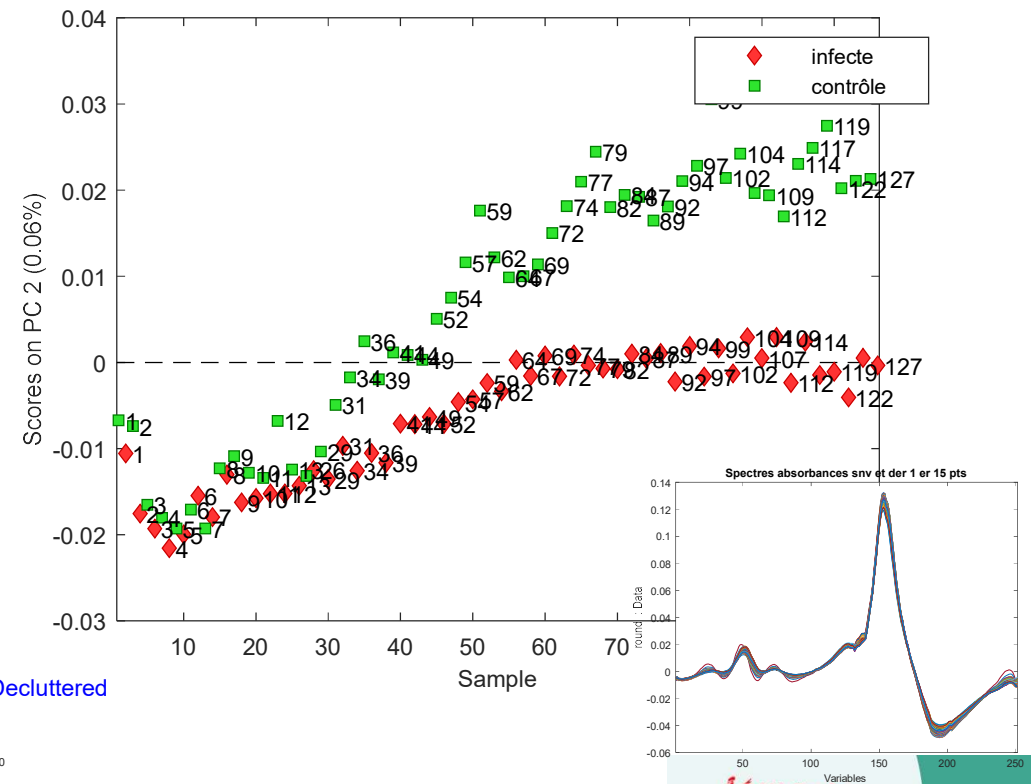
Authentication & Traceability

Flax disease

Variety more resistant

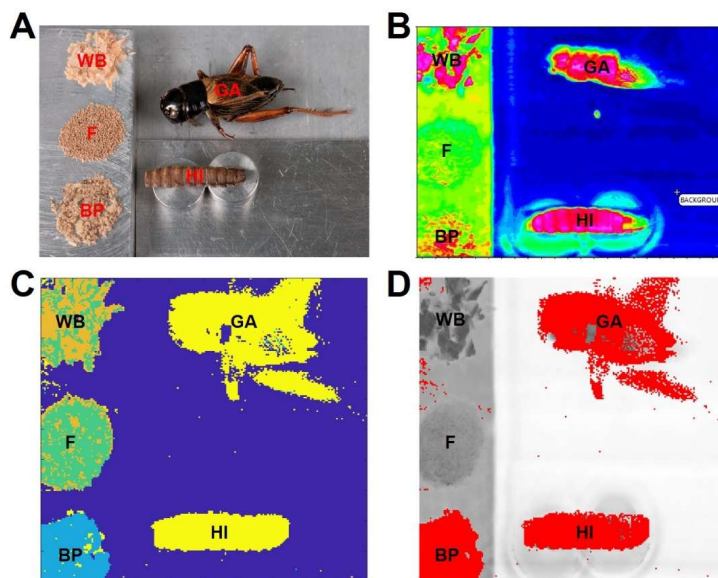
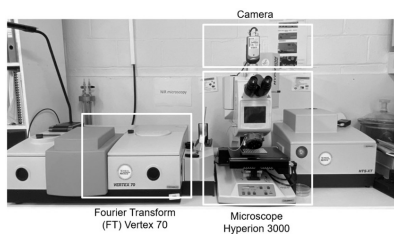
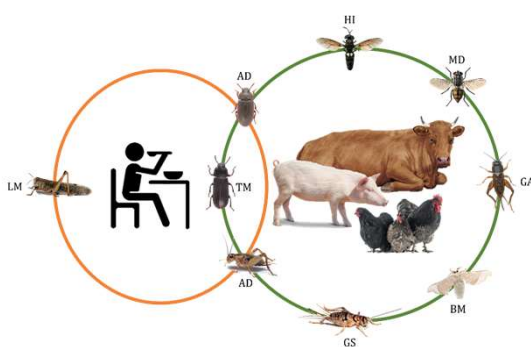


Variety less resistant



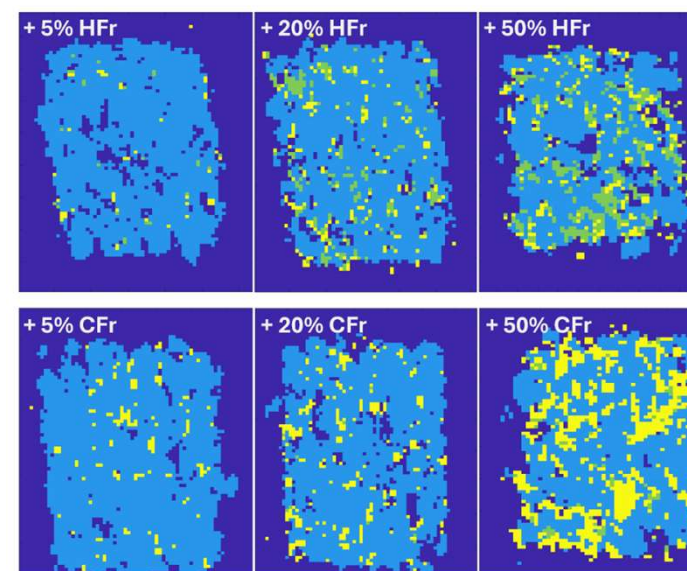
Authentication & Traceability

Detection & characterisation of insect meal intended for feedingstuffs



Photograph (A), spectral image (B), PLS-DA image processing (C) and absorbance equation image processing (D) of different samples analysed by NIRM.

WB: Wheat bran; F: Frass; BP: Bovine PAP; GA: *Gryllus assimilis*; HI: *Hermetia illucens* larvae.



PLS-DA image processing of the six samples of *T. molitor* larvae meal adulterated with 5% of HFr or CFr (**left**), 20% of HFr or CFr (**middle**) and 50% of HFr or CFr (**right**). **Dark blue**: background; **Light blue**: *T. molitor* larvae meal; **Green**: HFr; **Yellow**: CFr.

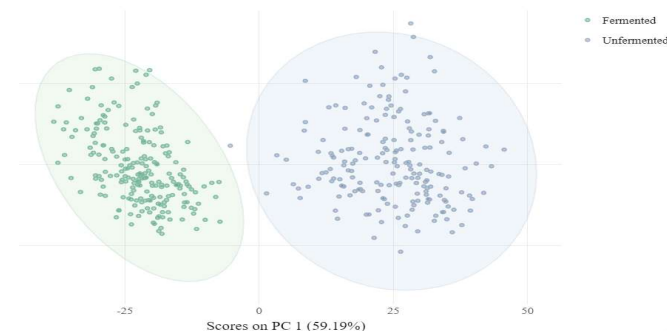
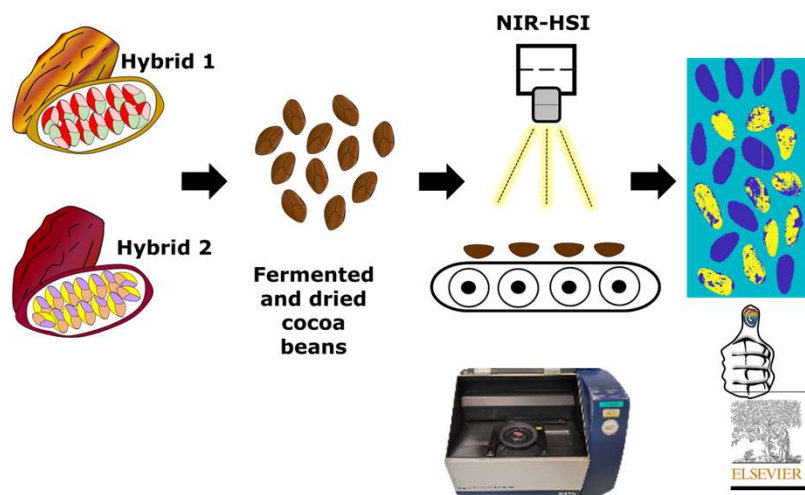
Abigaël ANSELMO

UMONS
University of Mons



Authentication & Traceability Cocoa beans

Discrimination of fermented vs unfermented cocoa beans & discrimination of 19 hybrid genotypes



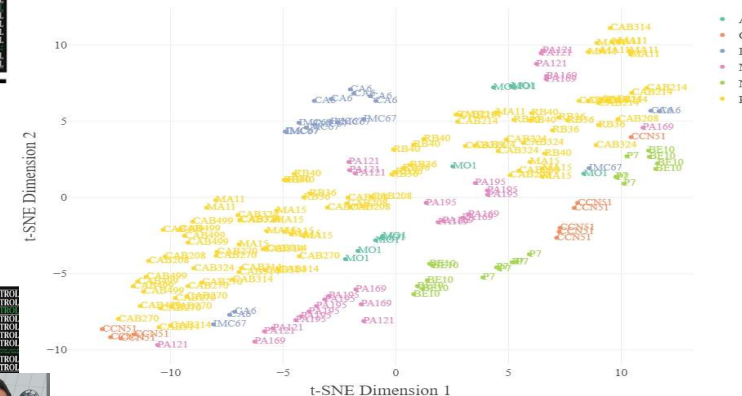
Advances in the individual authentication of cocoa beans: Vis/NIR spectroscopy as a tool to distinguish fermented from unfermented beans and classify genotypes in the eastern Amazonia

Anne Pinto^a, Antoine Deryck^b, Giulia Victória Lima^b, Ana Caroline de Oliveira^b, Fabio Gomes Moura^a, Douglas Fernandes Barbin^c, Juan Antonio Fernández Pierna^b, Vincent Baeten^b, Hervé Rogez^{b,c}



Authentication of cocoa (*Theobroma cacao*) bean hybrids by NIR-hyperspectral imaging and chemometrics

J.P. Cruz-Tirado^a, Juan Antonio Fernández Pierna^b, Hervé Rogez^c, Douglas Fernandes Barbin^b, Vincent Baeten^b



Authentication & Traceability Cereals



Discrimination between durum and common wheat kernels using near infrared hyperspectral imaging

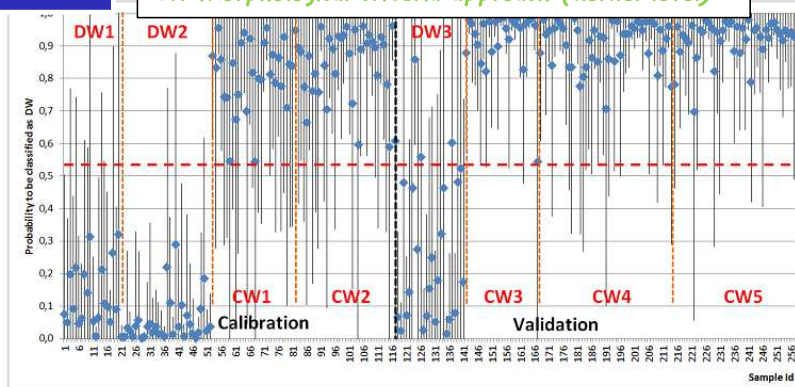
Philippe Vermeulen^{a,*}, Michele Suman^b, Juan Antonio Fernández Pierna^a, Vincent Baeten^a

^a Food and Feed Quality Unit (U15), Valorisation of Agricultural Products Department (D4), Walloon Agricultural Research Centre (CRA-W), Henseval Building, Chaussée de Namur 24, 5030, Gembloux, Belgium

^b Research Development & Quality, Barilla G. & R. Prati S.p.A, Via Mantova 166, 43100, Parma, Italy

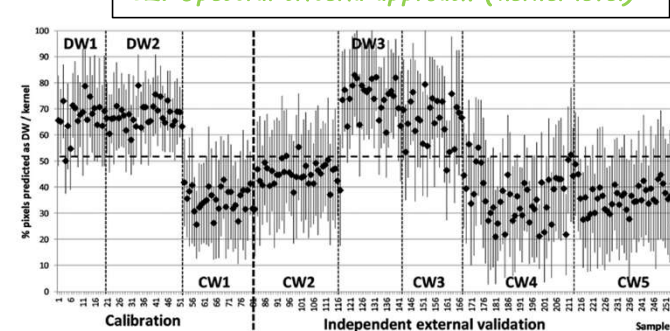
To benefit from HSI advantages for high throughput analysis : to certify batches

C1: Morphological criteria approach (kernel level)



Probability to be classified as DW (*: mean by kernel $\pm$ 2SD) after applying PLSDA model performed on 8 morphological criteria (area, perimeter, circularity, maxFeret, minFeret, aspect ratio, roundness and solidity), on the 257 images of 16 kernels.

C2: Spectral criteria approach (kernel level)



Percentage of pixels predicted as DW (*: mean by kernel $\pm$ 2SD) after applying PLSDA model performed on NIR data, on the 257 images of 16 kernels.

Authentication & Traceability Cereals

Data fusion – 2 approaches combination

Spectral and
spatial
information
combination

		on 4,105 grains				on 257 samples			
		DW (1,231 grains)		CW (2,874 grains)		DW (77 samples)		CW (180 samples)	
		Nb	%	Nb	%	Nb	%	Nb	%
1 criterion		1 right criteria		0 right criteria					
Morphological criteria	C1 (16 grains)	1,084	88.1	2,712	94.4	73	94.8	180	100
NIR spectral profile	C2 (16 grains)	1,156	93.9	2,618	91.1	77	100	174	96.7
2 criteria		1 or 2 right criteria		0 right criteria		mean 2 criteria		mean 2 criteria	
C1+C2 (16 grains)		1,216	98.8	2,471	86.0	77	100	180	100

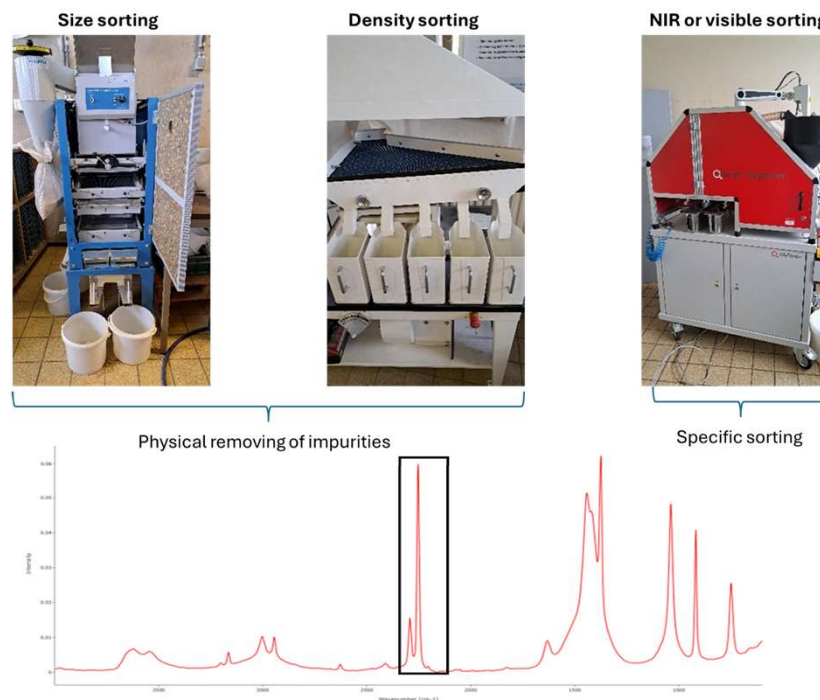


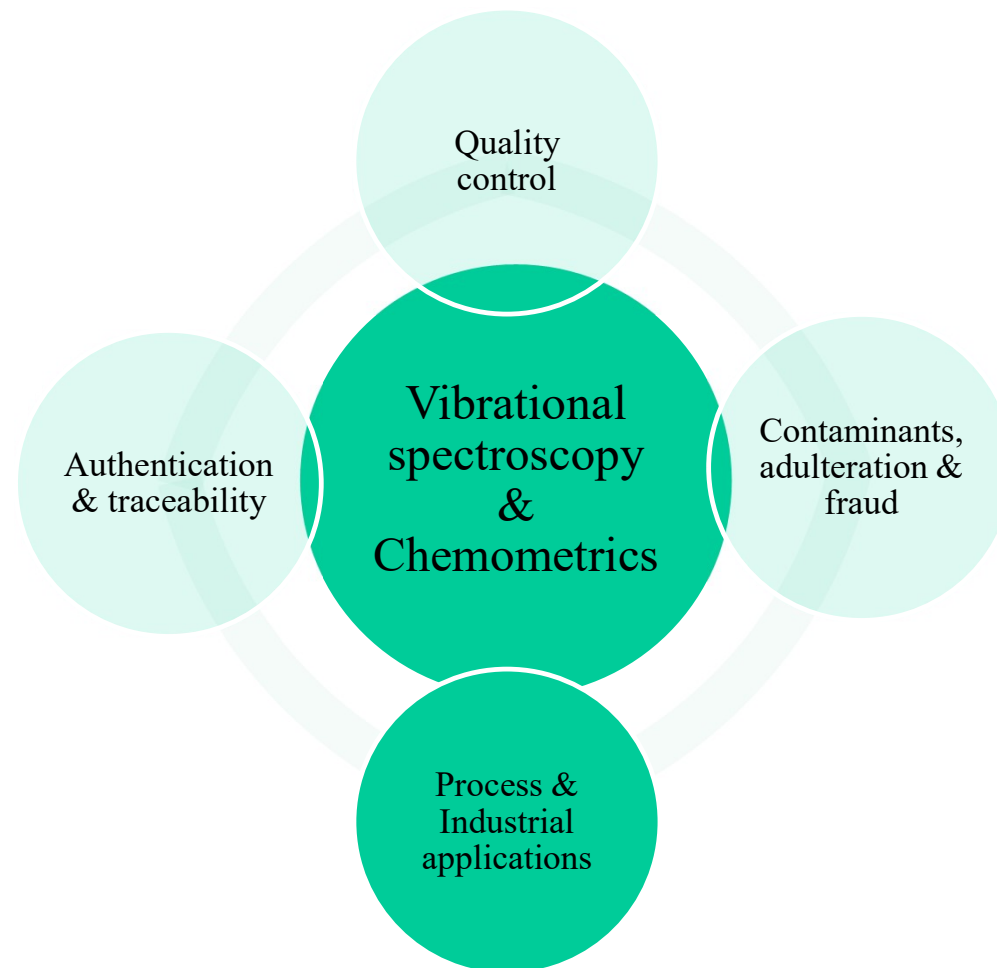
Qsorter

Some of our current projects

BELGOLEO

Goal: To develop an oilseed flax sector in Belgium: creation of a range of high value-added products that are nutritionally, ecologically, and economically viable.



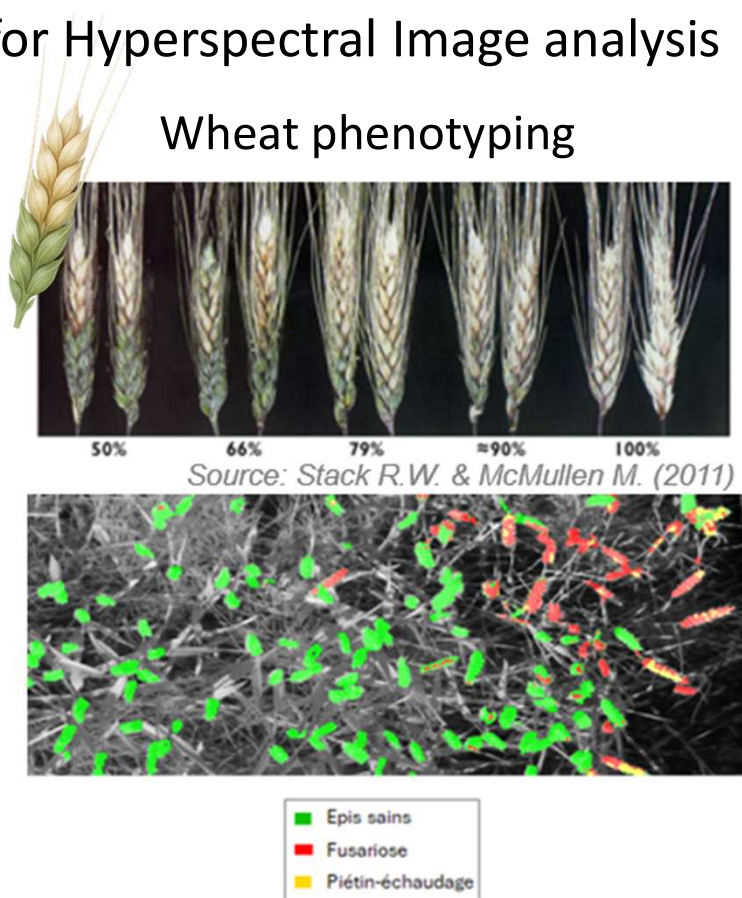


Vibrational Spectroscopy & Chemometrics

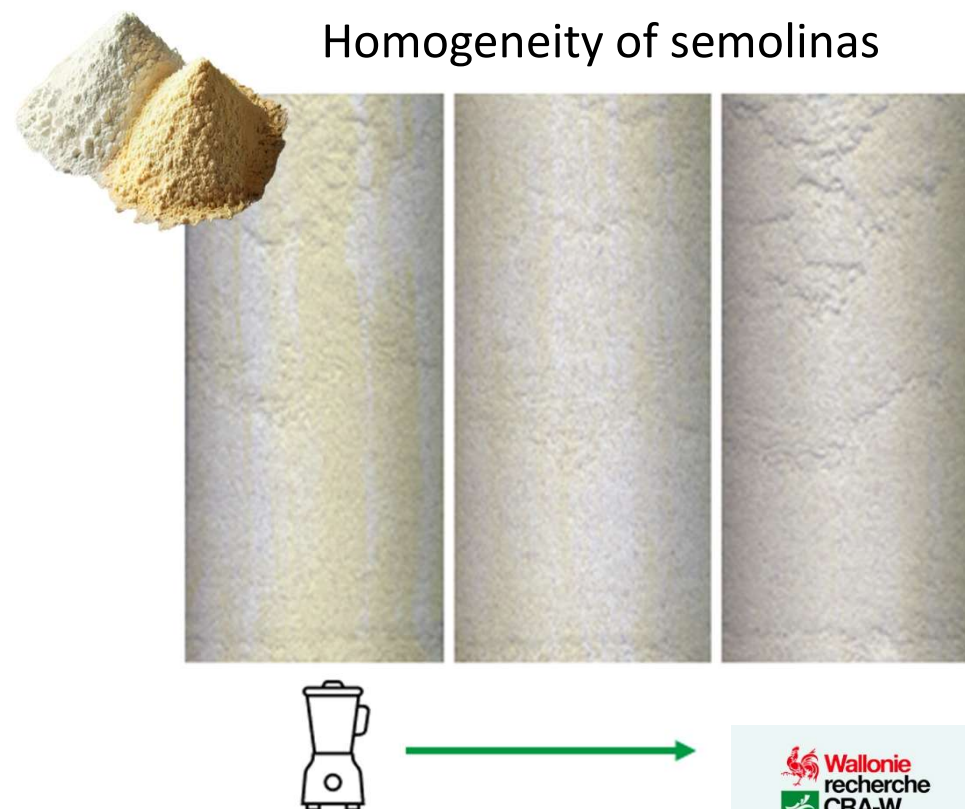
Qualispectra

Goal: To improve food safety by developing advanced Machine Learning algorithms for Hyperspectral Image analysis

Wheat phenotyping



Homogeneity of semolinas



Vibrational Spectroscopy & Chemometrics

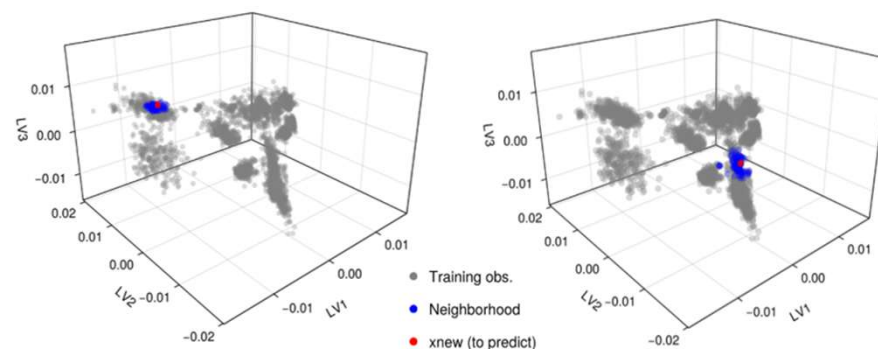
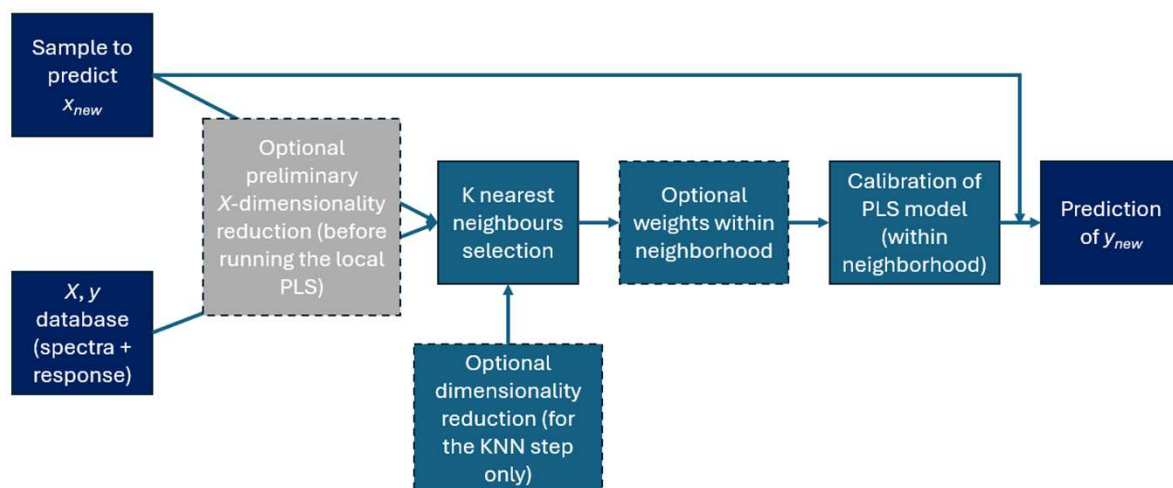
Other Areas of Work

- Instrument transfert (handheld, imaging...)
- Extension to other technologies
- Use of simplified methods (Local techniques, homogeneity algorithm)
- Deep learning / AI

Perspectives: Use of simplified chemometric methods

Local approaches

Goal: Investigating the potential of local methods for NIR data



A step-by-step tutorial to local partial least squares analyses for near-infrared spectroscopic data analysis

Antoine Deryck^{a,*}, Juan Antonio Fernández Pierna^a, Vincent Baeten^a, Matthieu Lesnoff^{b,c,d}



Exploiting the spatial information of hyperspectral images using AI (PhD)



Quality and authentication of agricultural products Unit

Vibrational Spectroscopy

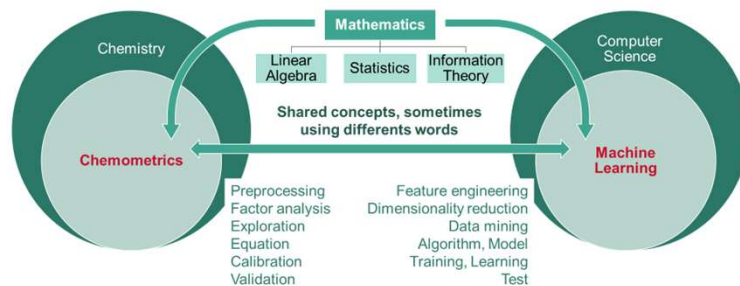
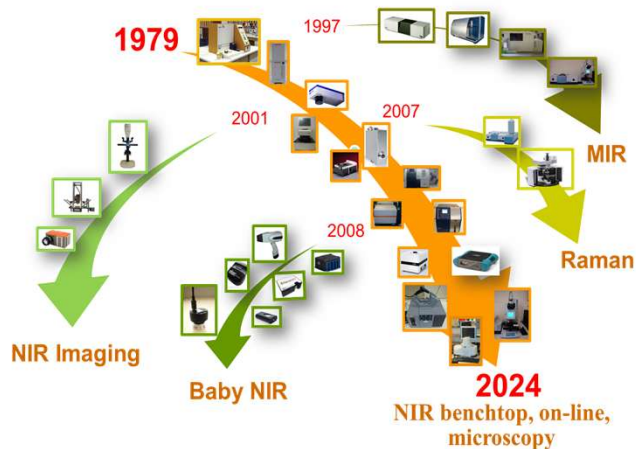
- No or limited sample prep (drying, grinding, ...)
- No additional reagents necessary
- Fast measurement even on moving sample (conveyor belt, ...)
- Non-invasive (do not alter the sample)
- Simultaneous determination of different constituents

Fast

Easy

Cost-efficient

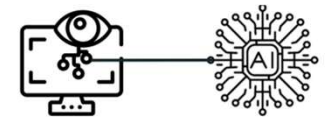
Eco-friendly



KU LEUVEN



Mission



- Exploit state-of-the-art **computer vision** algorithms and **artificial intelligence** techniques to solutions for **industry-specific application problems**
- Extend the **academic state-of-the-art** inspired by industrial constraints
- **Increase robustness** of experimental algorithms to industry standards under real-life constraints
- Optimize algorithms to **real-time** performance
- Implement advanced algorithms on **embedded systems**: μ C, FPGA, DSP, embedded GPU, server, cloud



Perspectives: Use of simplified chemometric methods

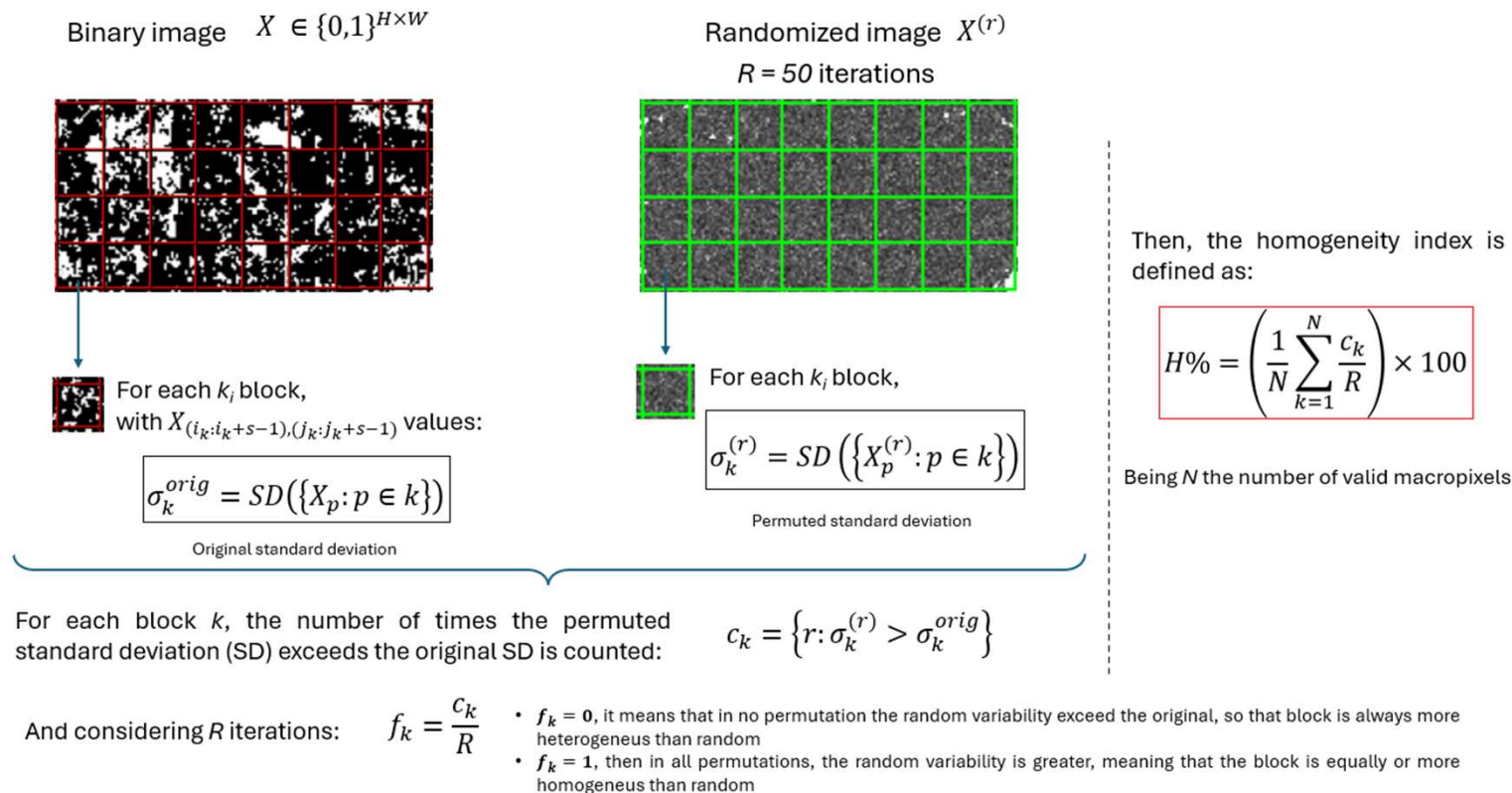
Qualispectra - Homogeneity



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Goal: Development of an algorithm that takes into account spatial distribution of components



Perspectives: Use of simplified chemometric methods

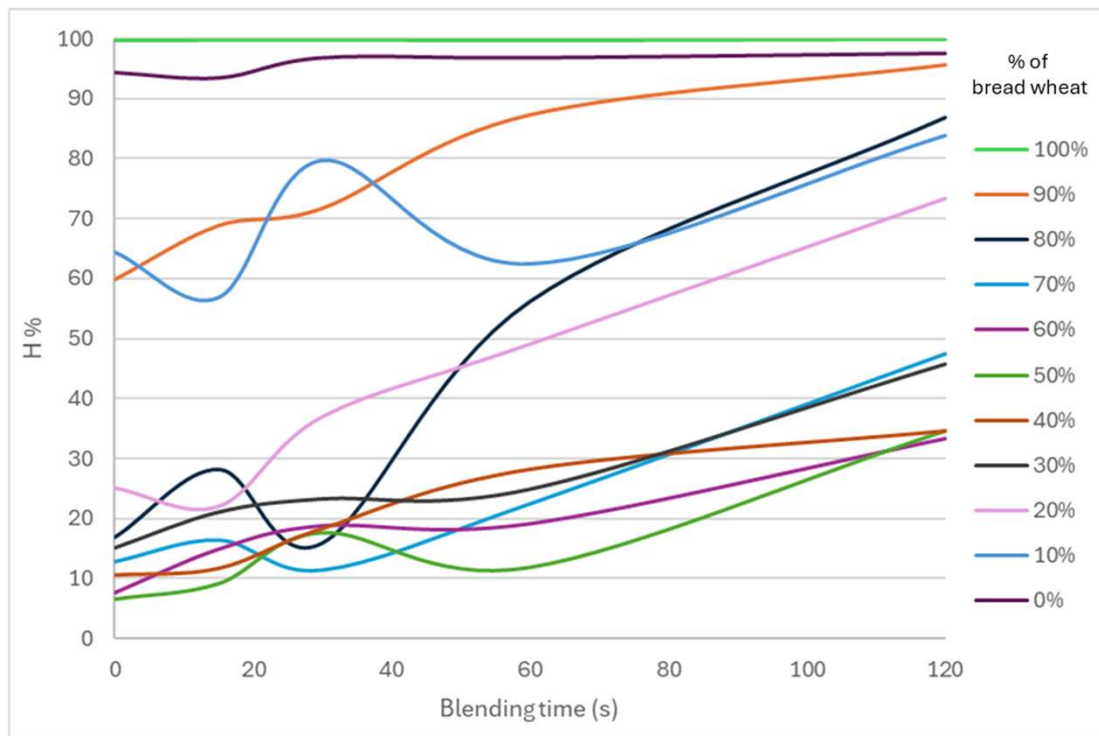
Qualispectra - Homogeneity



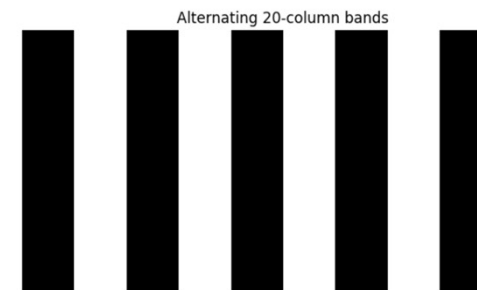
Universidad
de Jaén

cetic
Your Connection to ICT Research

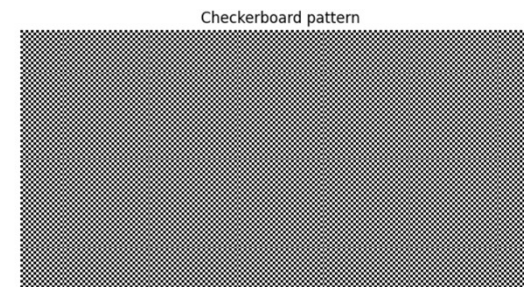
Mixtures of semolina of durum and bread wheat



Artificial Images



~ 0%
Homogeneity

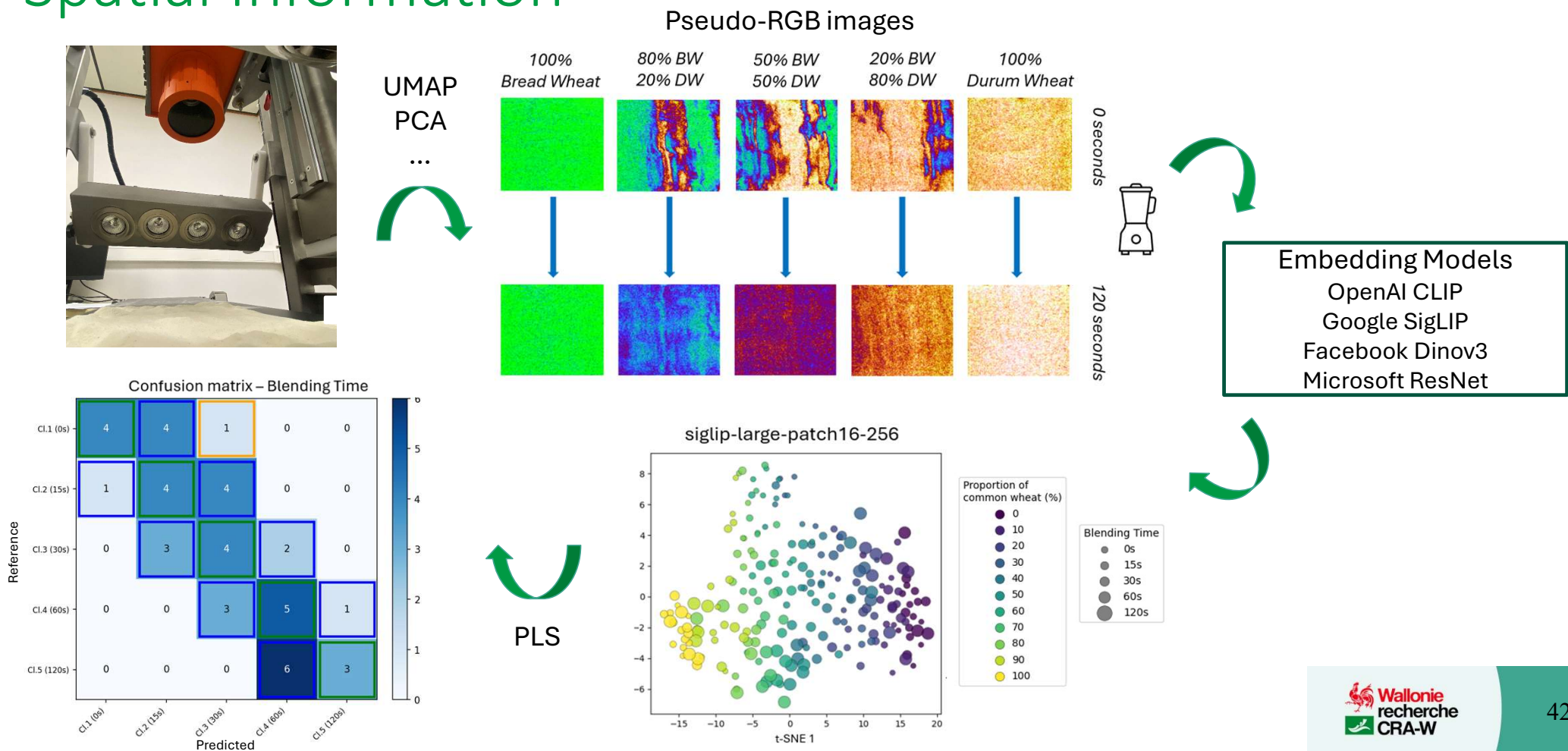


~ 100%
Homogeneity

Successfully applied it to HSI of compost

Perspectives: Use of AI methods

Using Pre-Trained Embeddings Models to Capture Spatial Information



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Data sciences **R**aman **I**maging **M**id-IR
laboratory



Quentin Arnould / Delphine Delhotte / Antoine
Deryck / Juan Antonio Fernández
Maxime Joissains / Nicaise Kayoka / François
Stevens



Gràcies!

