CHEMOMETRIC **BRAIN**

Near infrared spectroscopy,
a tool for better quality control and faster decisions

Scientific Lead

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www.chemometricbrain.io

Better quality control, faster decisions

Chemometric Brain

One global platform for easy spectroscopy use

Any NIRS Hardware

Any Food Product

- ✓ **Easy-to-use** interface
- ✓ **No trained personnel** needed
- ✓ **Any NIRS** hardware

- ✓ **Custom and ready** to use models
- ✓ Support from a **team of experts**
- ✓ **Any food** product

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The discovery of near infrared radiation

William Herschel, Astronomer

The discovery of near-infrared radiation was made by William Herschel (1800) when **he studied the colour responsible for the heat of sunlight** in the visible range of the electromagnetic spectrum. **Equipped with a thermometer and a prism** with which to separate the colours of sunlight, **he was able to see an increase in temperature when the thermometer was placed beyond the red region of the visible spectrum**. He called this invisible infrared radiation (Herschel, 1800).

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Short history of near infrared spectroscopy

Development of the **earliest NIRS equipment**

First studies with complex samples of agri-food origin and development of new **instruments with improved optics**

Technology boom driven by technological breakthroughs and **expansion of the IT sector**

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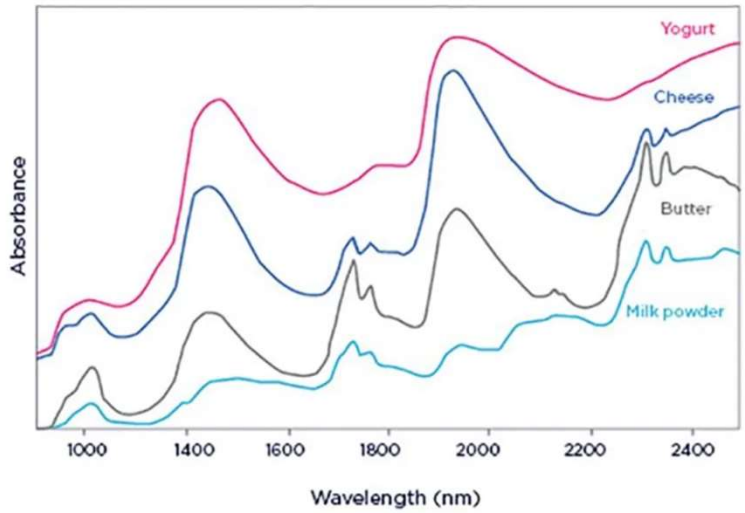
What is near infrared spectroscopy?

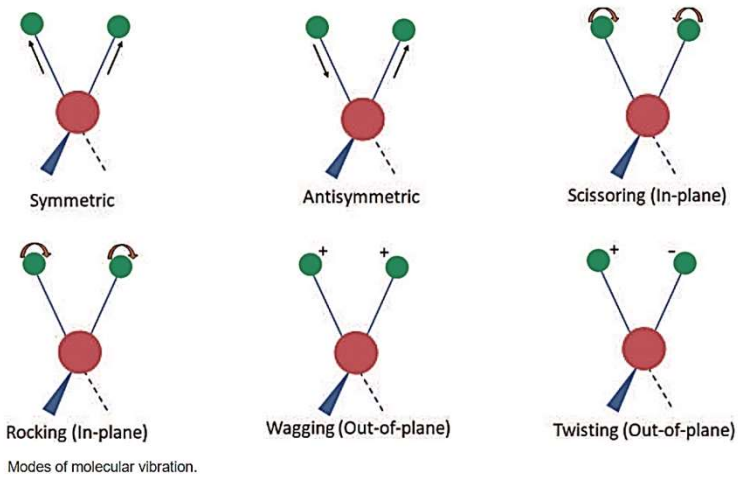
- Spectroscopy studies the **interaction between matter and light**.
- Near Infrared Spectroscopy (NIRS) works from **800nm to 2500nm**.



- Applying NIRS to any food product, **produces a unique spectra or fingerprint**, rich in chemical data.
- The representation of **the absorbance values obtained at the different wavelengths of the NIR range gives rise to a curve called NIR spectrum**, which is the result of the different overtones, combination bands and electronic absorptions of radiation of the functional groups present in the sample.

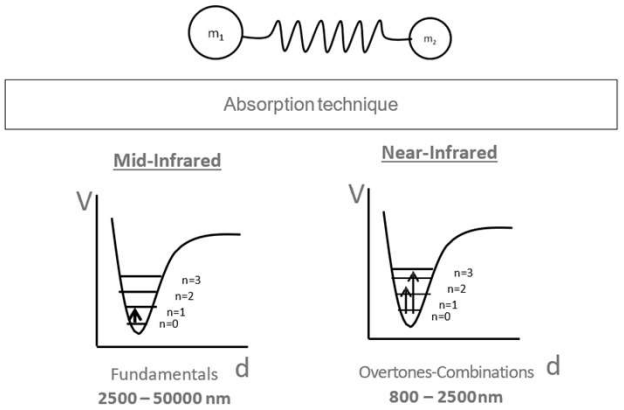
The technical basis of near infrared spectroscopy – Molecular vibrations

- **Covalent bonds** SHARE electrons between atoms in a molecule
- Bonds have length, strength & direction unique to each pair of atoms
- **Bonds act like springs** joining atoms
- Bonds vibrate at unique frequencies due to atomic masses & 'stiffness'
- **If vibration changes the dipole moment,** then **bond can absorb INFRARED photons**
- A **photon of EXACTLY the right frequency is absorbed & excites the bond to a higher vibrational state**
- Frequency = qualitative analysis: IDENTITY
- Amplitude = quantitative analysis: AMOUNT



Molecular vibrations between two atoms with respect to one atom.

The technical basis of near infrared spectroscopy

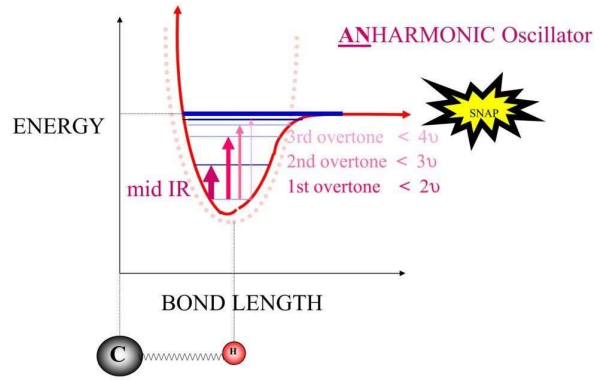


NIR absorption **bands are due to the anharmonicity of the vibrating atoms**. The bands reflect:

- **Overtone transitions** that correspond to quantum numbers greater than one and that appear as multiples of the fundamental vibrational frequency. Overtone transitions appear between 780 and 2000 nm. First and higher overtones are much less likely than the fundamental vibrational frequency. That's the reason why the bands are weaker.

- **Combination modes** that appear in polyatomic molecules, where multiple vibrational modes interact. They are the sum of multiples of each interacting frequency. Their absorption bands emerge between 1900 and 2500 nm.

- **The non-equidistant energy states of a vibration**. That means that allowed transitions become smaller in energy.



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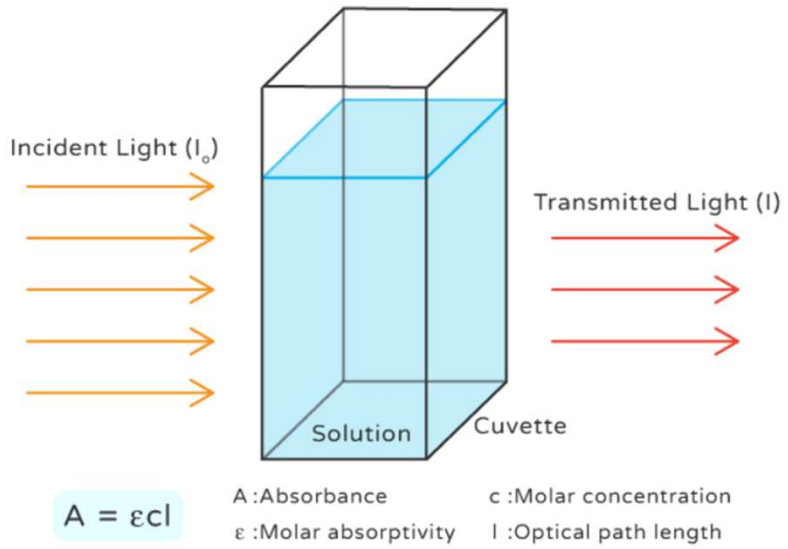
The technical basis of near infrared spectroscopy – Beer-Lambert Law

- **Beer-Lambert Law** is the basis of all forms of quantitative spectroscopy
- $A = \log\left(\frac{1}{T}\right) = \varepsilon\ c\ L$ where:
    - A : Absorbance
    - T: Transmittance
    - L: Optical path (cm)
    - ε: extinction coefficient (M-1 cm-1)
    - C: Concentration (M)



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Near infrared spectroscopy instrument operation

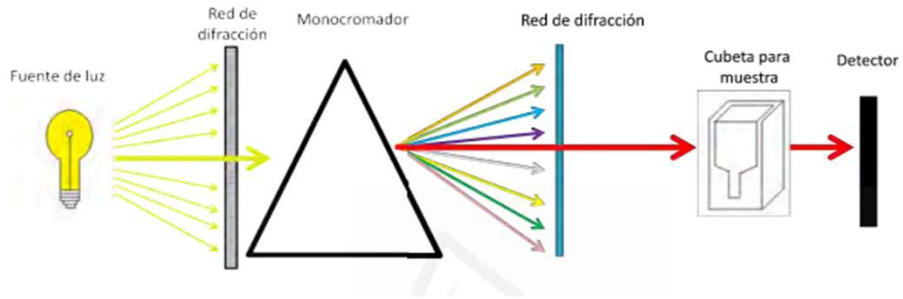
Light source: the most widely used in NIR spectroscopy is the tungsten halogen lamp (good performance, robustness, cost)

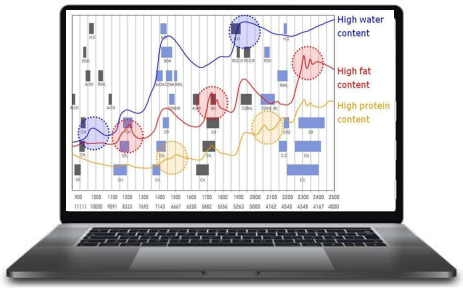
Monochromator: the light beam strikes the diffraction grating, and it is split into discrete wavelengths.

Lens: for focusing the light

Sample holder

Detector: converts the radiant energy into an electrical signal and a signal processor. This signal, amplified and converted into a digital signal by means of an analogue-to-digital converter, and is finally transmitted to a computer for storage or processing.



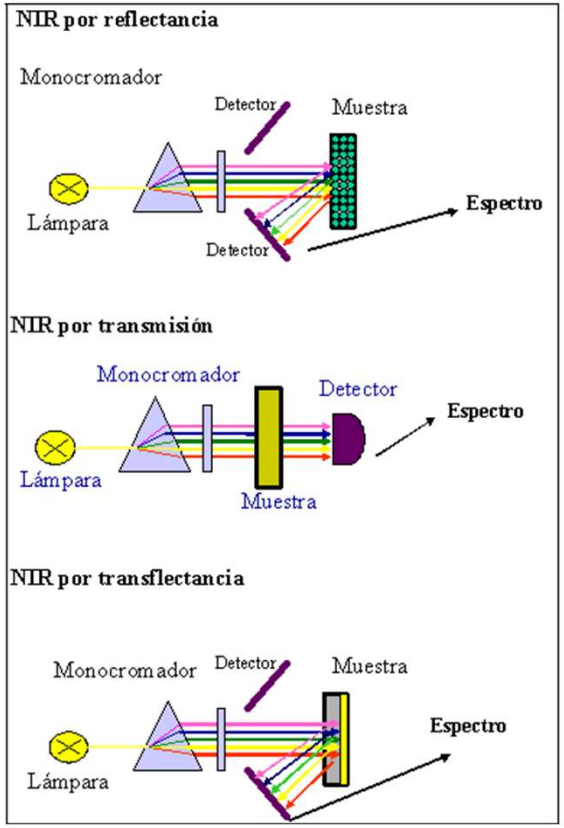


Measurement Modes

Reflectance: The sample to be analyzed is bombarded with NIR rays of different wavelengths. For each wavelength, some of the rays will be absorbed by specific chemical bonds At the same time, other **rays will be scattered and reflected by** other **chemical bonds.**

Transmission: The sample to be analyzed is bombarded with NIR rays of different wavelengths. For each wavelength, some of the rays will be absorbed by specific chemical bonds and some of the **rays will pass through the sample.**

Transflectance: Follows the **same approach as reflectance**, i.e., in these conditions again what is quantified is the **reflected energy that has not been absorbed by the sample**. The only difference is that at the end of the cuvette there is a **specular surface that causes the reflection of the radiation** and makes this radiation pass through the sample again.



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Characteristics, advantages and limitations of the technique

Characteristics

- Spectrum is a fingerprint.
- The spectrum does not have characteristic bands that you can correlate with functional groups.
- Spectra from similar materials are very similar.
- You obtain a value of absorbance at each wavelength (a lot of information).

You need to be ableto transform the information in knowledge.

Advantages

- Non-destructive analysis.
- No sample preparation and no chemical or consumables.
- Multi-Parameter Analysis
- Rapid and real time analysis data
- Deeper sample penetration compared to other spectroscopy.
- Can be portable.

Difficulties

- The spectra are not easily interpretable
- Need a lot of mathematical treatments
- Need of libraries to get results
- Overlapping bands (combination), not easy to interpret.
- Differences in spectra are often very subtle.
- Usually not for trace level analysis.

Chemometrics – extracting chemical information from data

According to the definition of the Chemometrics Society, it is “the chemical discipline that uses mathematical and statistical methods to **design or select optimal procedures and experiments, and to provide maximum chemical information by analyzing chemical data”.**

With **2** variables we can draw a **bi-dimensional** scatter plot; with **3**, we can draw a **tri-dimensional** scatter plot.

But, ***what to do when dealing with several (up to thousands) variables?***

The problem is that **most of the time the variables are not independent** of one another.
Doing univariate analysis does not take into account the **correlations between variables.**

So, multivariate analysis:

- **helps to identify variables that contribute most to the overall variability in the data.**
- **helps to isolate those variables that are related (i.e. that co-vary with each other).**

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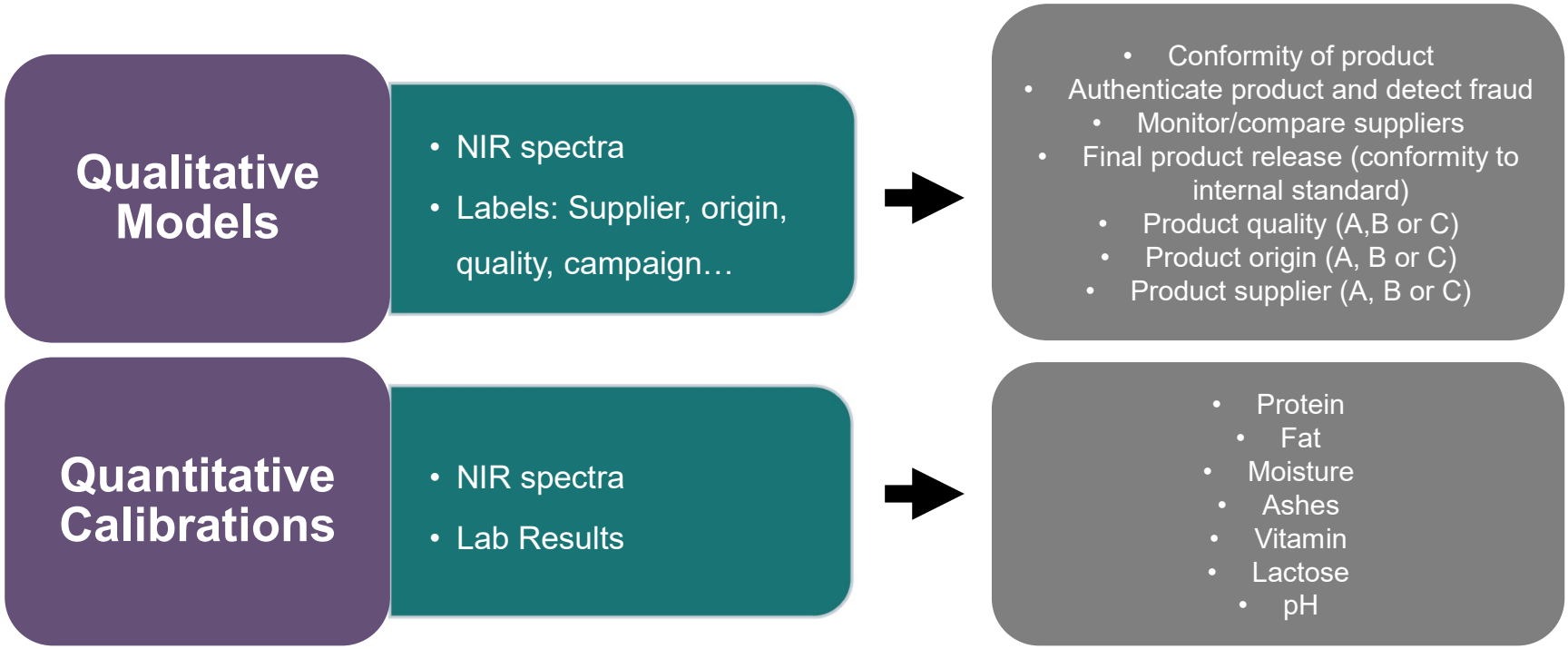
Two types of applications of NIRS technology in food operations



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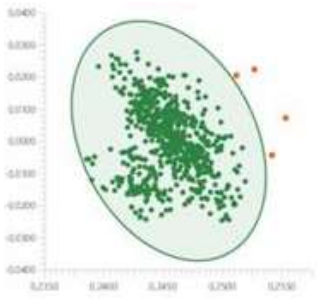
How are qualitative models built and applied to a process?

*1. Capture NIRS spectra for your **good samples** for your raw materials or final products*

*2. **Good samples** are included in a qualitative model, against which you can compare new samples*



*3. Instant **conformity validation** results upon comparing new samples*

Sample-ID	Validation	Risk Level
Casein 19032780	✗	MEDIUM
Casein 19032781	✗	HIGH
Casein 19032782	✓	VALIDATED

Good samples are samples of a product that conform to your primary and secondary properties of interest (protein, moisture, density, colour, or any other), have been tested in succesful production runs, and haven't been adulterated.

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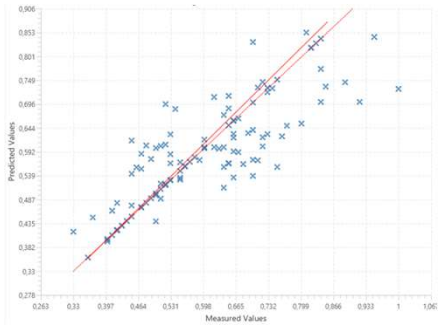
How are quantitative models built and applied to a process?

*1. Capture **NIRS spectra of samples** of your raw materials or final products.*

*2. The same samples are analysed to obtain a **reference value** and the model is developed.*



*3. **Instant results** when measuring new samples.*

Lote	Fecha	NIR
135_T	16/07/2024 13:48:50	0,662774
134_T	16/07/2024 13:48:19	0,477038
133_T	16/07/2024 13:47:50	0,66618
132_T	16/07/2024 13:47:21	0,79264
131_T	16/07/2024 13:46:50	0,372992

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Instant detection of adulterated products

Challenge:

Qualitative analysis for detection of fraud in wheat flour

Analysis:

Through **PCA**, the **fingerprints of the adulterated batches were compared to previously validated batches.**

Results:

NIR valid as a tool for food fraud detection

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New supplier homologation

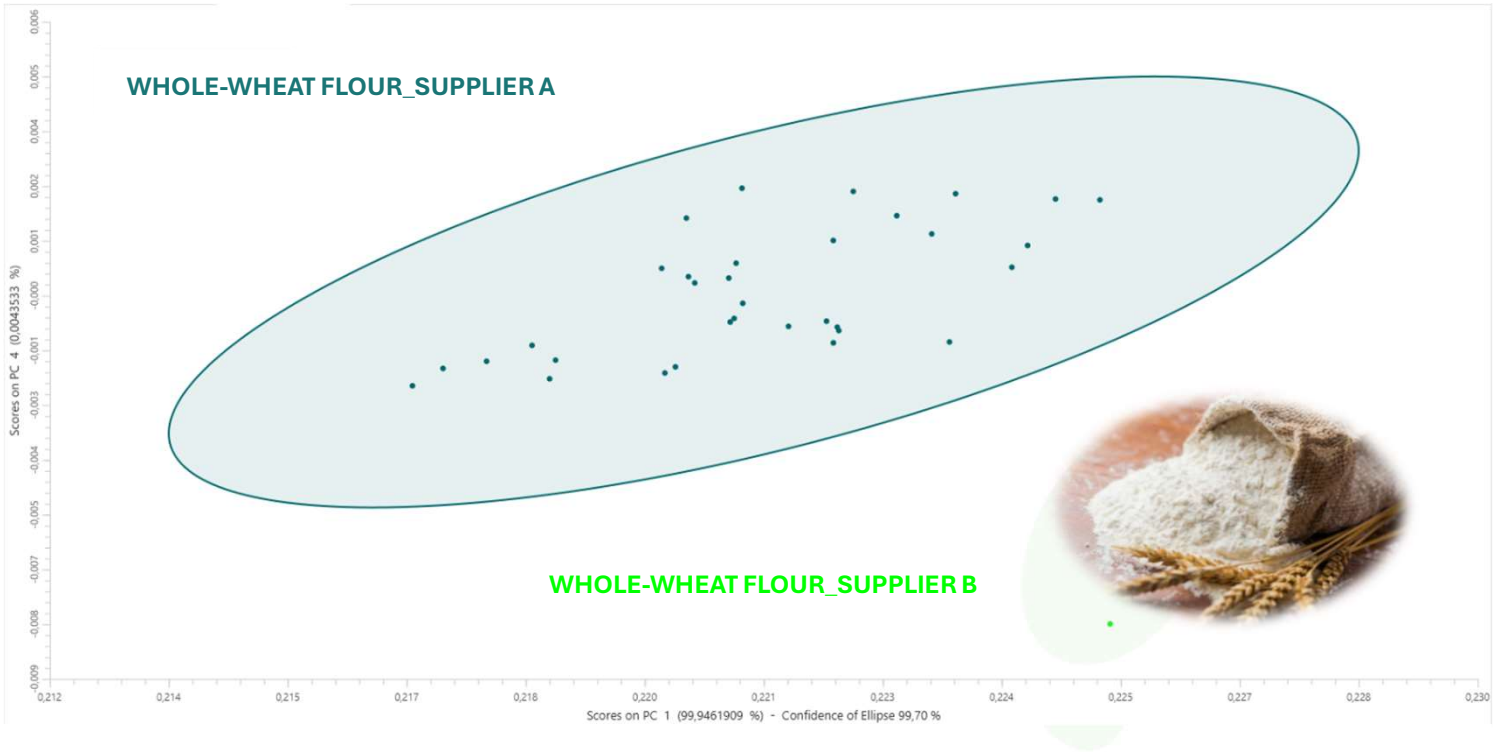
Challenge:

Use of **NIR technology to homologate** different **suppliers** of the same raw material

Approach:

Using Chemometric Brain, **samples of whole-wheat flour from different suppliers** with the **same specifications** were **analyzed by their digital spectral fingerprint**.

Through **PCA**, the fingerprints of the new batches were compared to previously validated batches.



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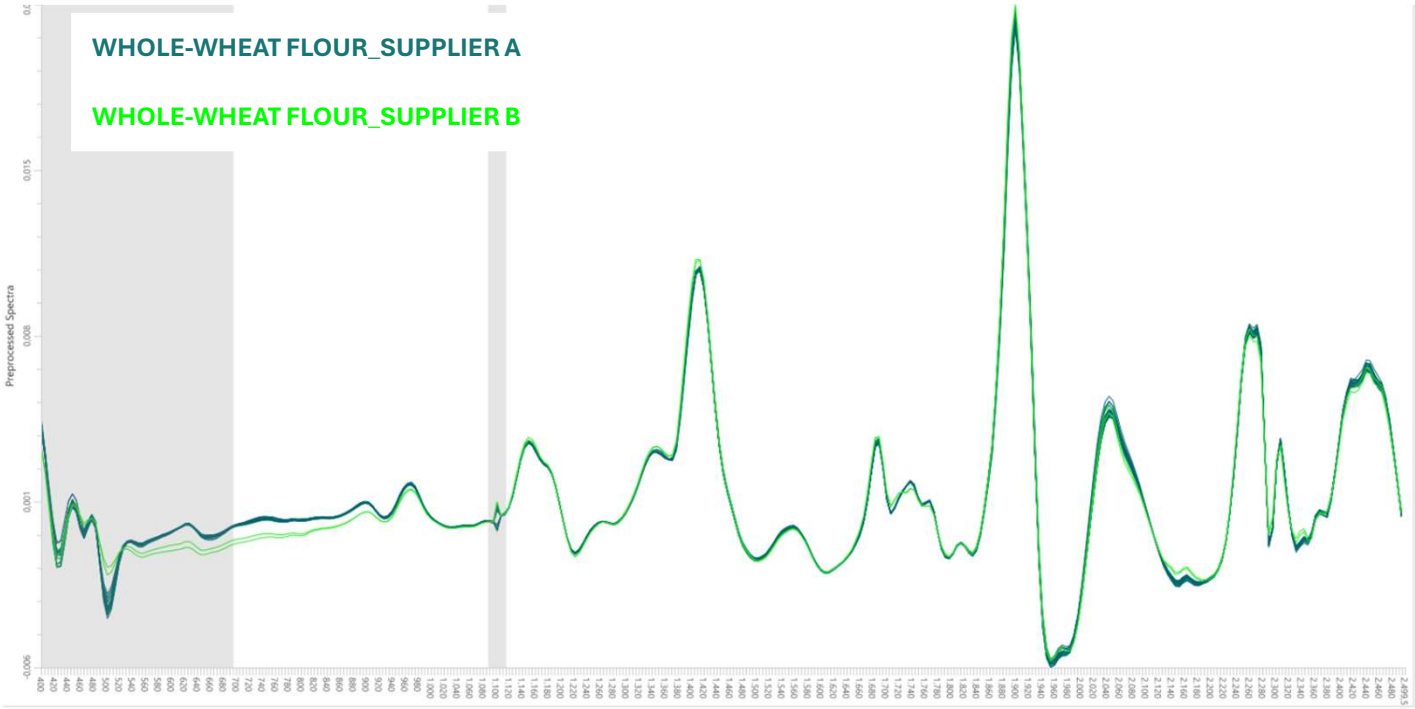
New supplier homologation

Results:

PCA revealed the **spectral fingerprint differences**, confirming the two **suppliers are not homologous** from NIR point of view.



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Various chemical properties quantified in seconds

Challenge:

Quantiative analysis of flour yields rapid determination of quality paramaters.

Analysis:

Creation of a **standard line**, applying **PCA and Regression Medthods**.

Results:

NIR as a tool for determination of nutritionals parameters. The **conventional analysis** method would take **longer time and** have a **high cost of analysis** (including sample destruction).

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Identifying manufacturing errors with advanced analysis

Challenge:

Mishap in the manufacturing process of 2 products due to **a mix-up in raw materials.**

Similar packaging, different ingredients!

Analysis:

Leveraged NIR spectrum and cutting-edge software to create a **qualitative model encompassing all batches**.

Applied Principal Component Analysis (**PCA**) for a deep dive.

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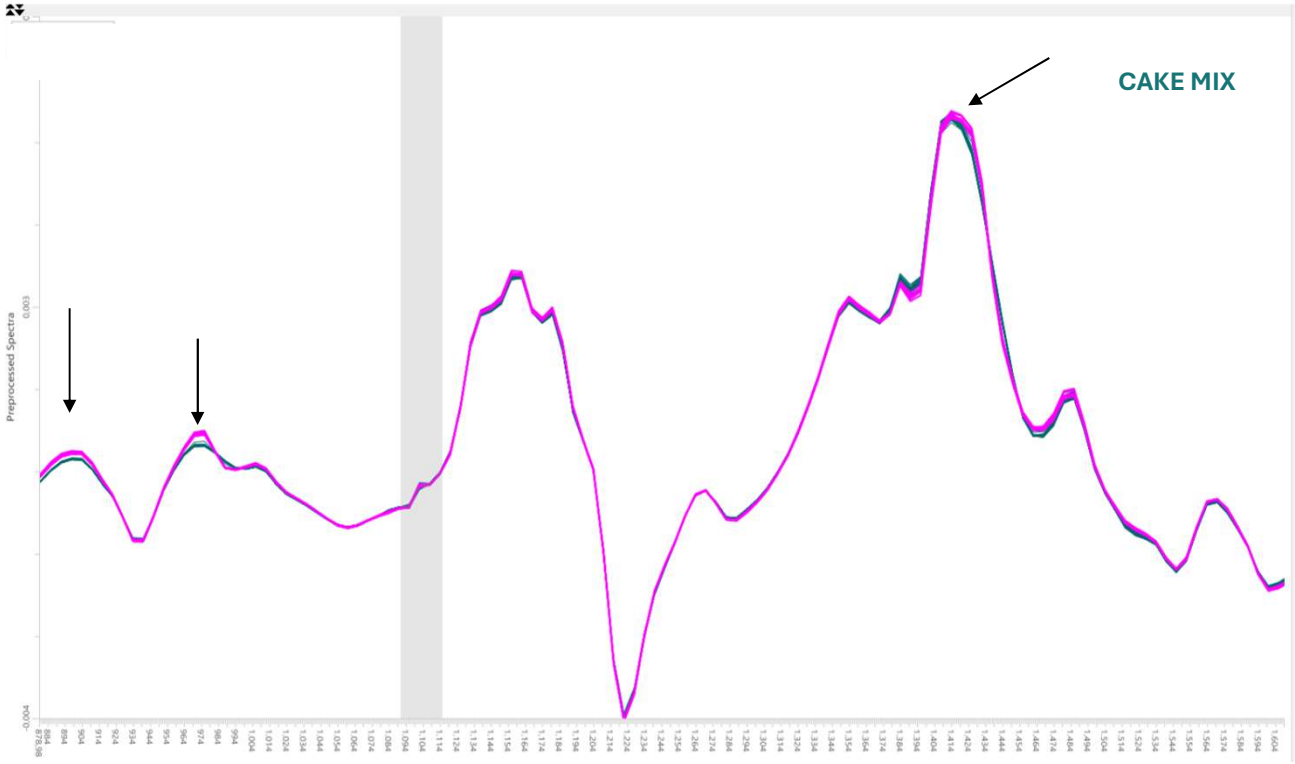
Identifying manufacturing errors with advanced analysis

Results:

PCA revealed the spectral fingerprint differences, pinpointing **batches affected by the erroneous ingredient addition**.



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Identification of different protein bread blends

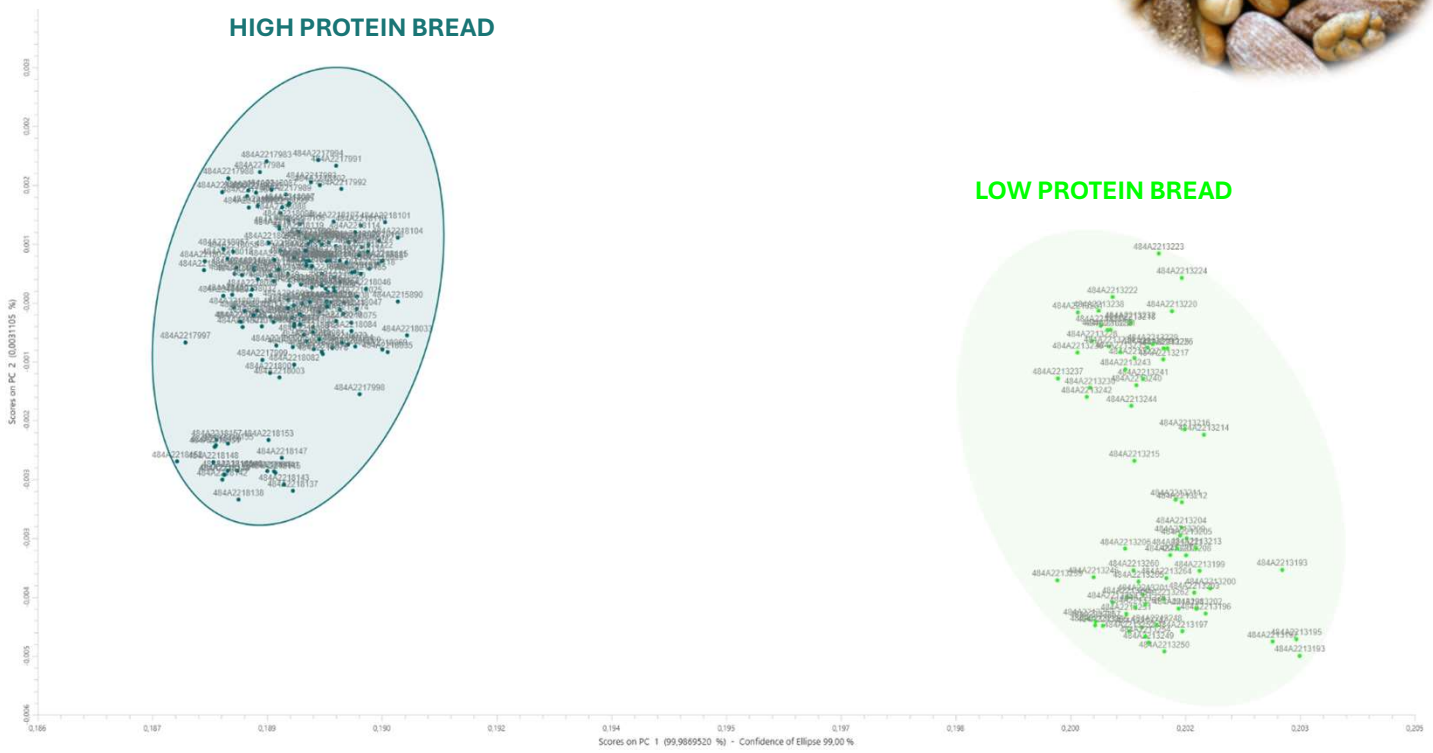
Challenge:

A company needed to **validate the protein content** in its ingredient mix without relying on complex chemical analyses.

Approach:

Using Chemometric Brain, **samples from multiple batches of high- and low-protein bread powder were analyzed** by their digital spectral fingerprint.

Through **PCA**, the fingerprints of the new batches were compared to previously validated batches.



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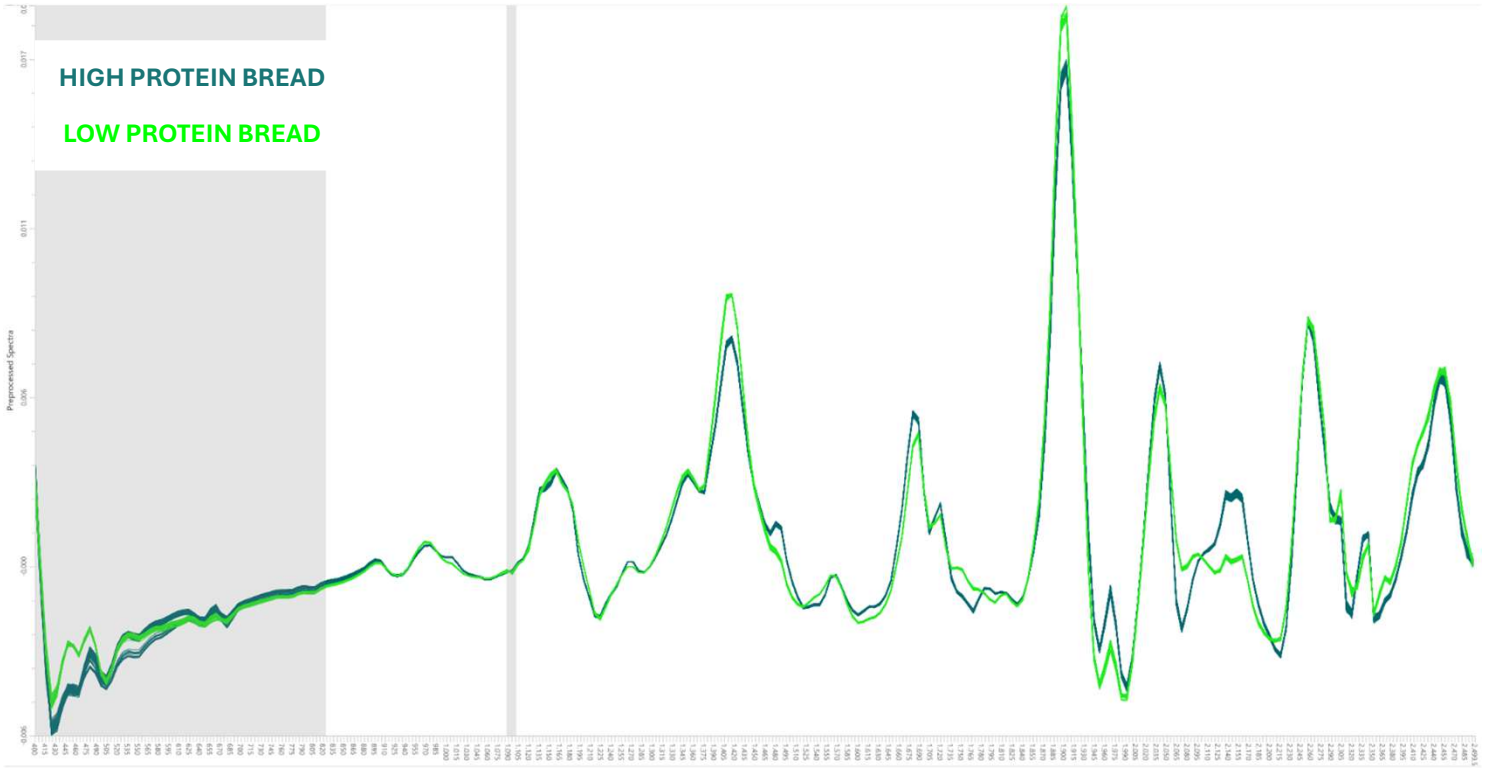
Identification of different protein bread blends

Results:

Some **batches fell outside the confidence zone of the "High Protein Bread" model**, indicating that they **did not meet the required protein level**. The spectra revealed two distinct fingerprints.



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Rapid evaluation of optimal blending time

Challenge:

Without a way to evaluate homogeneity rapidly, industrial validation will require other **lengthy tests on the final blend**.

Approach:

Qualitative analysis of three **batches** of a powder product **blended** for **4, 6, and 8 minutes.**

Results:

Full homogeneity of the mix is achieved in **6 minutes** blending time.

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End-to-end control in powder blending

Raw Material Quality Control

- ✓ Food fraud detection
- ✓ Supplier consistency
- ✓ Changes in formulation/ extraction

Blending Time Optimization

- ✓ Optimal blending time

Final Product Quality Control

- ✓ Correct formulation control
- ✓ Optimal homogeneity

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Better control of your supply chain and production, just a step away

FOOD FRAUD

APPROVE RAW MATERIALS

PREVENT PRODUCTION DEVIATIONS

CLASSIFY PRODUCT TO INTERNAL QUALITY LEVELS

PREVENT RAW MATERIAL DEVIATIONS

MONITOR SUPPLIERS

ENSURE PRODUCT HOMOGENEITY

DETERMINE PHYSICAL-CHEMICAL PROPERTIES

Get all these insights on our **software**, **without the need to be an expert,** with **ready-to-use or custom solutions**

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