# Classification of chocolates based on their frontal fluorescent « fingerprint »

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# Introduction

## Sensory evaluation


*Different cacao varieties and origins*

**208 dark chocolates**

*Same process of fabrication*

**Obtain a classification of chocolates based on their fluorescent « fingerprint » ?**

Pole 2

Pole 3

Pole 1

Pole 4

**Sensory poles**

**«Fingerprint by FFS »**

**?**

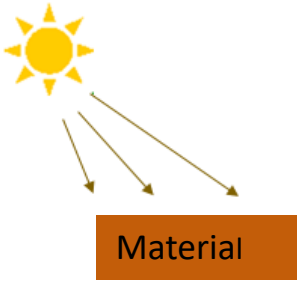
# Material and Methods
## - Front Face Fluorescence Spectroscopy (FFFS)

Fast, sensitive and non destructive analytical technique to obtain « fingerprints » 3-D of raw or processed products.

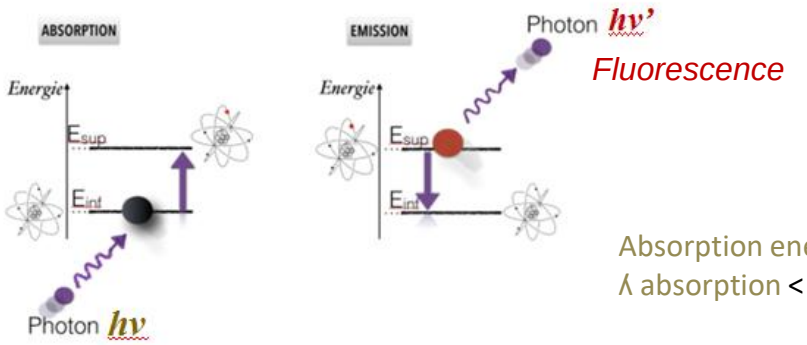
**Applications :** Following the quality control of a product or a process (ex: mechanisms of oxydation), the traceability (ex: varieties, geographical origins), …

**Benefits :** Developping fast analytical methods coupled with chemometry in order to replace long and expensive chemical analytical methods.

# Material and Methods
## - What is the fluorescence ?




Interaction light - material




Absorption energy > Emission energy
λ absorption < λ emission

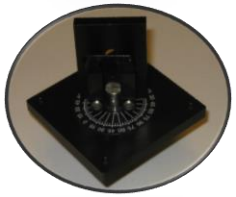
•**Fluorescence** is an emission of light induced by a return to the ground state from a substance that has absorbed an electromagnetic radiation.

•Generally, fluorescent molecules (**fluorophores**) are substances composed of **conjugated aromatic rings** or molecules plane and cyclic with one or several **π links**.

- Polyphenols : catechin, procyanidin, gallic acid, quercetin
- Vitamins (A, B2, B6, E (tocopherols), B9)
- Aromatic amino acids (Phenylalanine, Tryptophan, Tyrosine…)

# Material et Methods
## - Samples preparation and parameters of analysis

Incubator
45°C

Incidence angle 55°C

EX1: Excitation 1 (Mono1)
Start: 250.00nm
End: 650.00nm
Increment: 5.00nm
Side Entrance Slit: 2.00 nmBandpass
Side Exit Slit: 2.00 nmBandpass
First Intermediate Slit: 2.00 nmBandpass
Grating: Density 1200 (Blaze: 330)

EM1: Emission 1 (Mono2)
Start: 290.00nm
End: 800.00nm
Increment: 2.00nm
Side Entrance Slit: 3.00 nmBandpass
Side Exit Slit: 3.00 nmBandpass
First Intermediate Slit: 3.00 nmBandpass
Grating: Density 1200 (Blaze: 500)

One spectral acquisition by sample (t = 53 min)

# Results
## - Data analysis

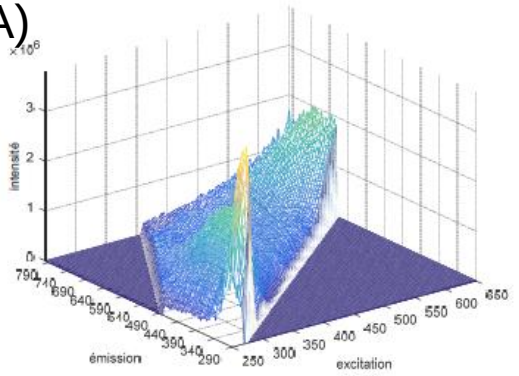
- Obtain spectral data set composed with 20 736 results by sample, or 4 313 088 data to analyze !

- Data set cleaning and selection of informative data range

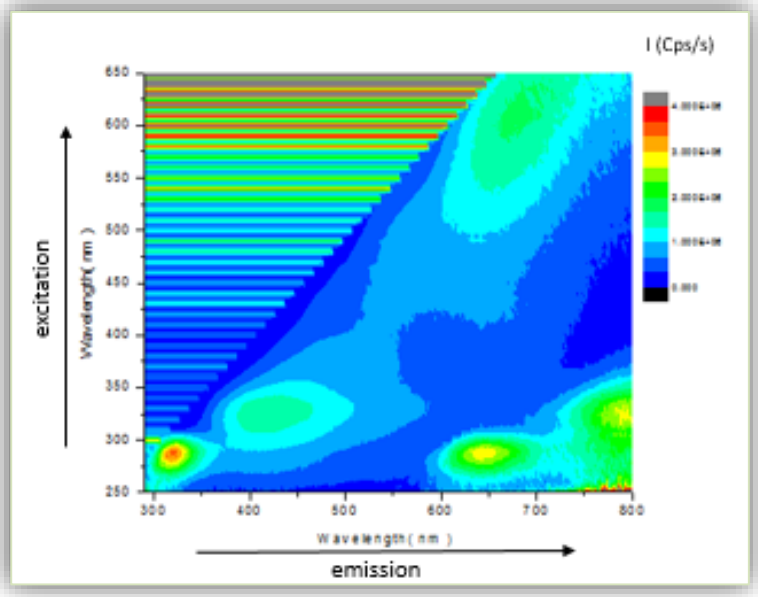
- Data analysis with chemometry:

    * Multivariate exploratory analysis (PCA, LDA)
    * Multiway data analysis (PARAFAC)

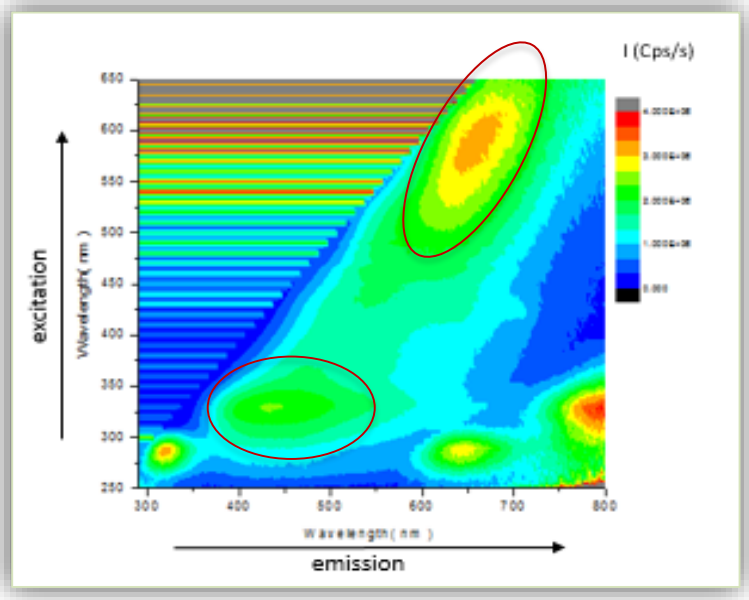
- Data pretraitement by area normalization



# Results
## - Spectra 3-D




Pole 2 ou Pole 3 ou Pole 4



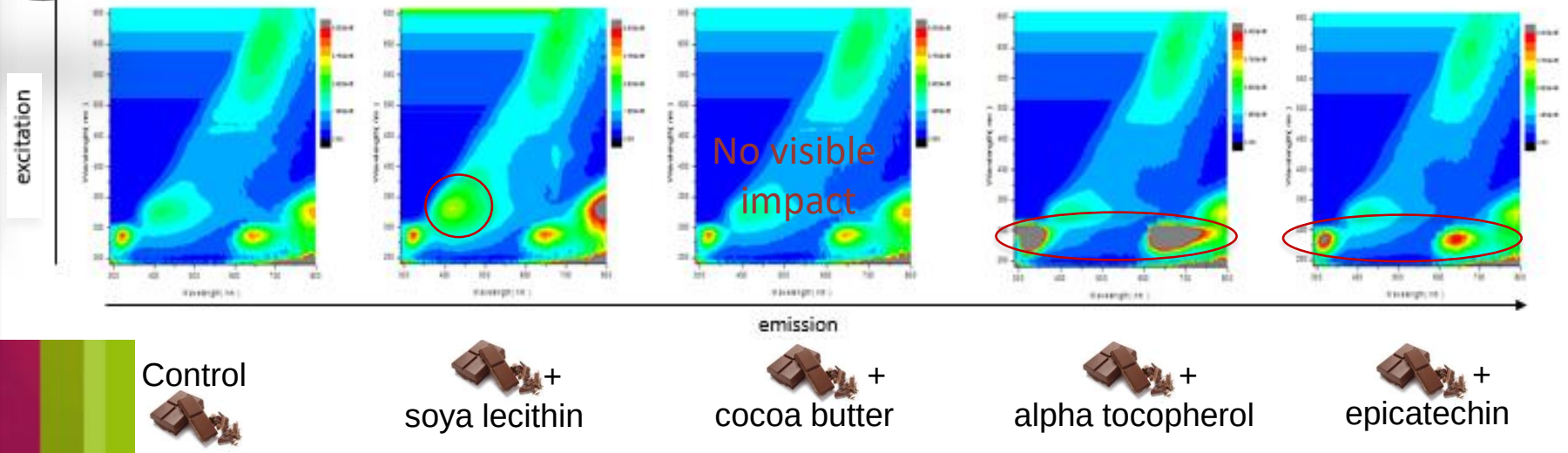

Pole 1

- Identical spectral pattern for the samples from the different sensory poles discrimination on intensity variations

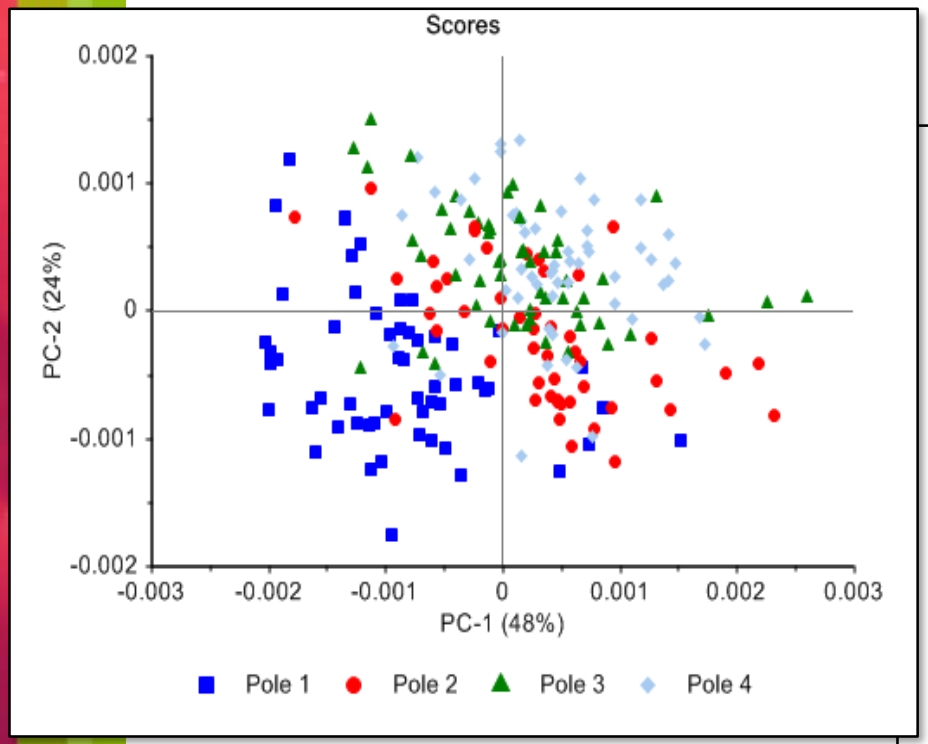
- Two typical zones for the samples from the pole 1

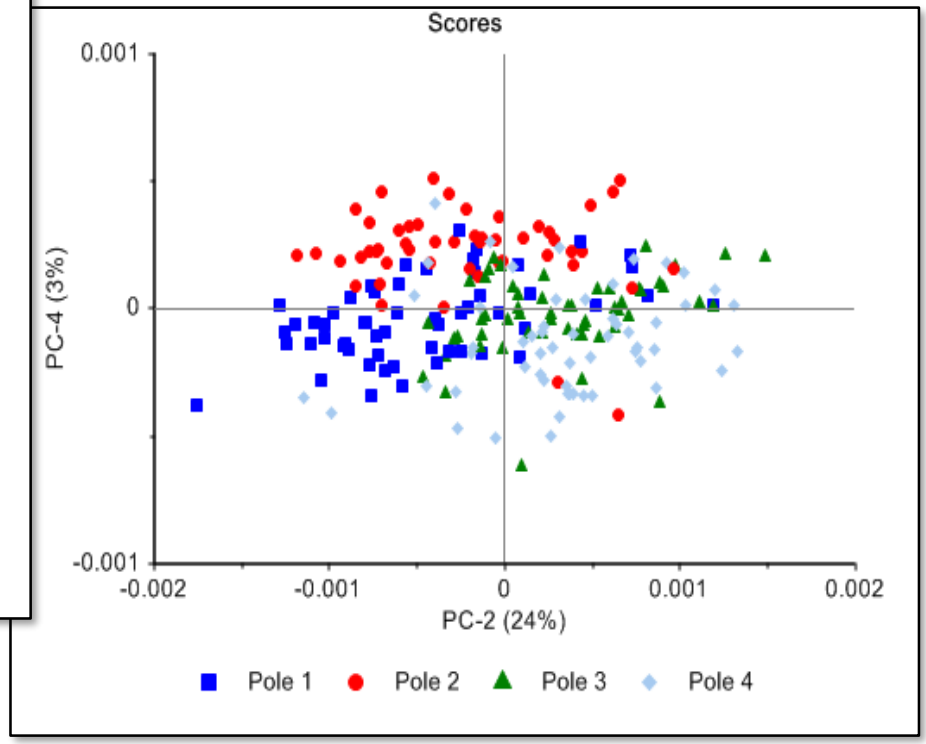
# Results
## - Characterization of fluorophores

Addition of different biochemical compounds in chocolate control



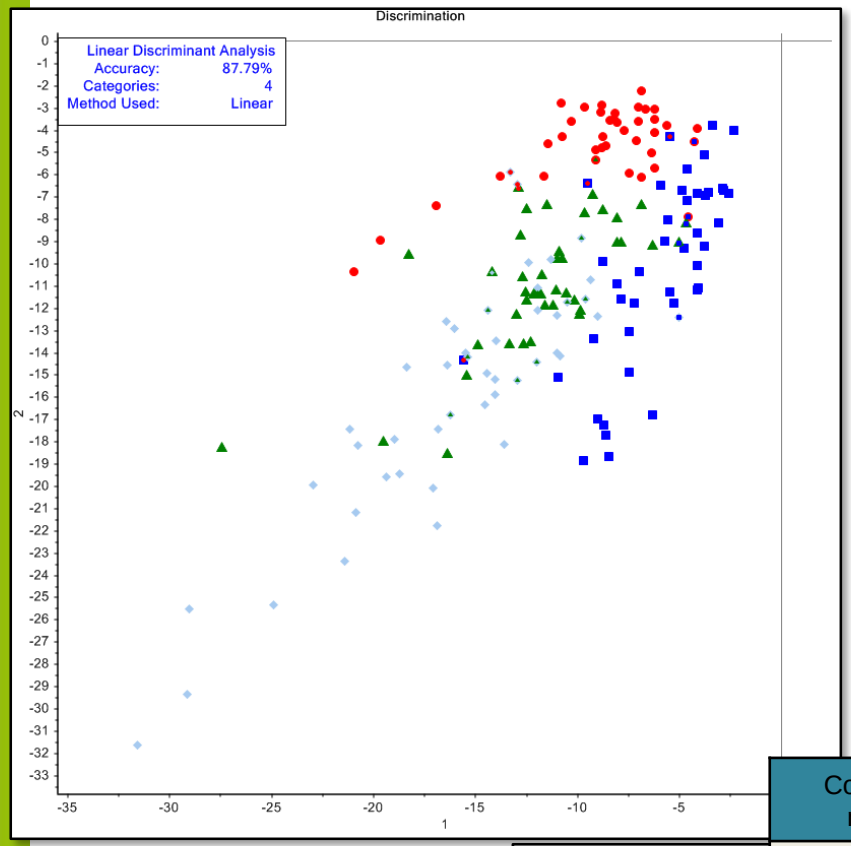
# Results
## - Principal Component Analysis (PCA)

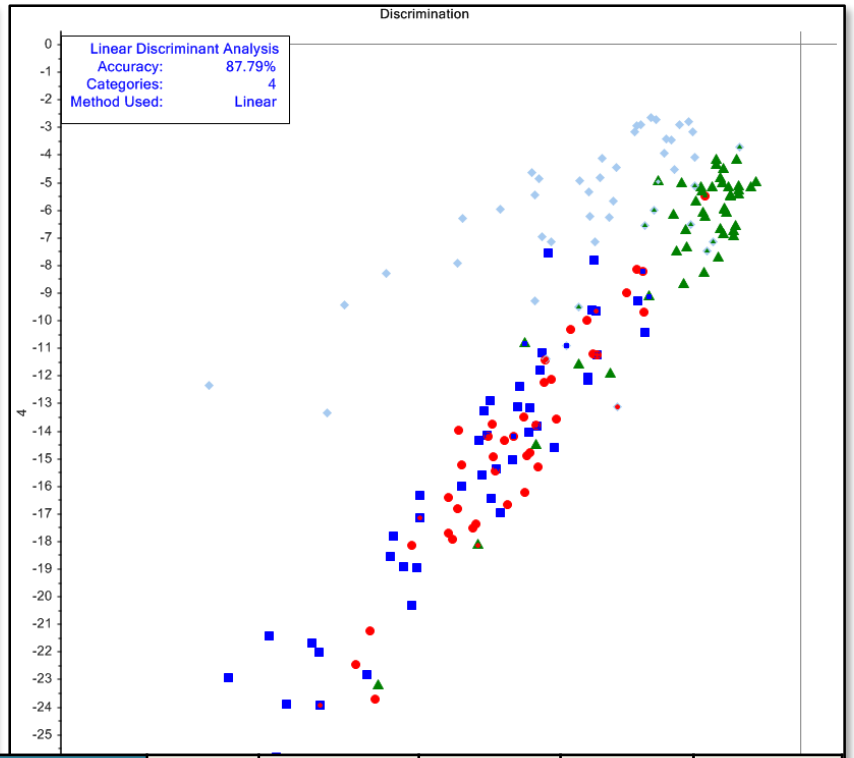



No discrimination of sensory poles

# Results
## - Linear Discriminant Analysis (LDA)



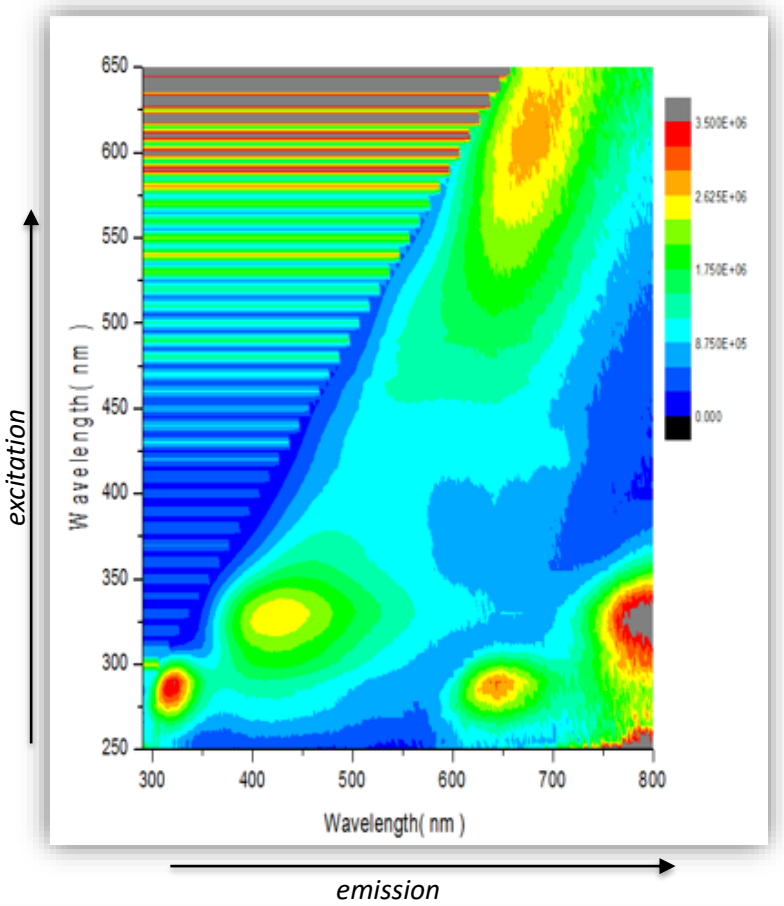



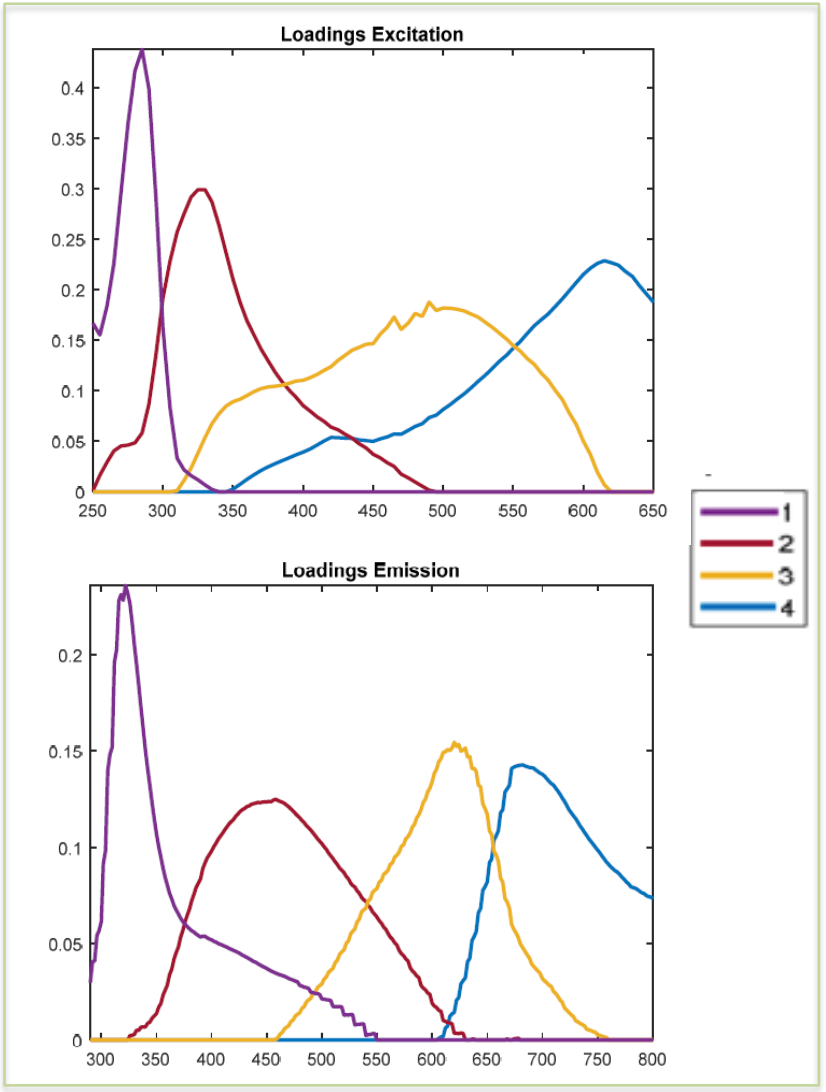

| Confusion matrix | Pole | Pole 1 (10) | Pole 2 (10) | Pole 3 (10) | Pole 4 (10) |
|---|---|---|---|---|---|
| **Prediction** | * | * | * | * | * |
| Pole 1 | * | | | | 0 |
| Pole 2 | * | | | | 1 |
| Pole 3 | * | | | **8** | 2 |
| Pole 4 | * | 0 | 2 | 1 | **7** |

30 % error

# Results

- Correlation between fluorescent spectra and loadings of PARAFAC model




Factor 1 ⟶ Polyphenols , tocopherols

Factor 2 ⟶ Fatty acids, TG, proteins

Factor 3 et 4 ⟶ ?

# Conclusion

The analysis of fluorescent « fingerprints » allows to obtain a reliable classification of chocolates in 70%.
This distribution is strongly related to the polyphenol content.

A precision of the sensory model improve the model of classification.

**Prospects :** The coupled data analysis from various methods of “rapid” chemical analysis would improve the model of classification (Multi-block data analysis).

*Thanks for your attention*